Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 04:36 AM BST

PDB ID	:	1SID
Title	:	MURINE POLYOMAVIRUS COMPLEXED WITH 3'SIALYL LACTOSE
Authors	:	Stehle, T.; Harrison, S.C.
Deposited on	:	1995-12-12
Resolution	:	3.65 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 following versions of software and data (see references ⓘ) were used in the production of this report:

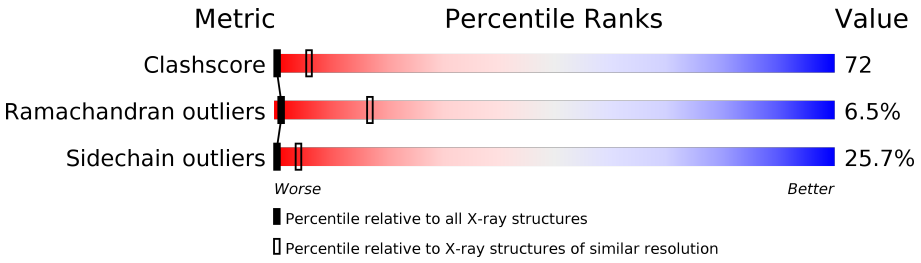
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)

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 on 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	383	23% 50% 20% • •
1	B	383	25% 46% 22% • •
1	C	383	22% 48% 21% • 7%
1	D	383	20% 44% 22% • 11%
1	E	383	20% 52% 21% • •
1	F	383	20% 46% 23% • 8%
2	G	3	67% 33%
2	H	3	33% 67%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	I	3	33% 67%
2	J	3	33% 67%
2	K	3	33% 67%
2	L	3	33% 67%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17003 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.

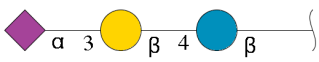
- Molecule 1 is a protein called POLYOMAVIRUS COAT PROTEIN VP1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total	C	N	O	S	0	0	0
			2849	1804	479	550	16			
1	B	367	Total	C	N	O	S	0	0	0
			2857	1808	481	552	16			
1	C	357	Total	C	N	O	S	0	0	0
			2784	1761	468	539	16			
1	D	340	Total	C	N	O	S	0	0	0
			2645	1674	445	511	15			
1	E	367	Total	C	N	O	S	0	0	0
			2857	1808	481	552	16			
1	F	354	Total	C	N	O	S	0	0	0
			2753	1740	461	536	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	SER	conflict	UNP P49302
B	6	ALA	SER	conflict	UNP P49302
C	6	ALA	SER	conflict	UNP P49302
D	6	ALA	SER	conflict	UNP P49302
E	6	ALA	SER	conflict	UNP P49302
F	6	ALA	SER	conflict	UNP P49302

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto pyranose-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	G	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	H	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	I	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	J	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	K	3	Total	C	N	O	0	0	0
			43	23	1	19			
2	L	3	Total	C	N	O	0	0	0
			43	23	1	19			

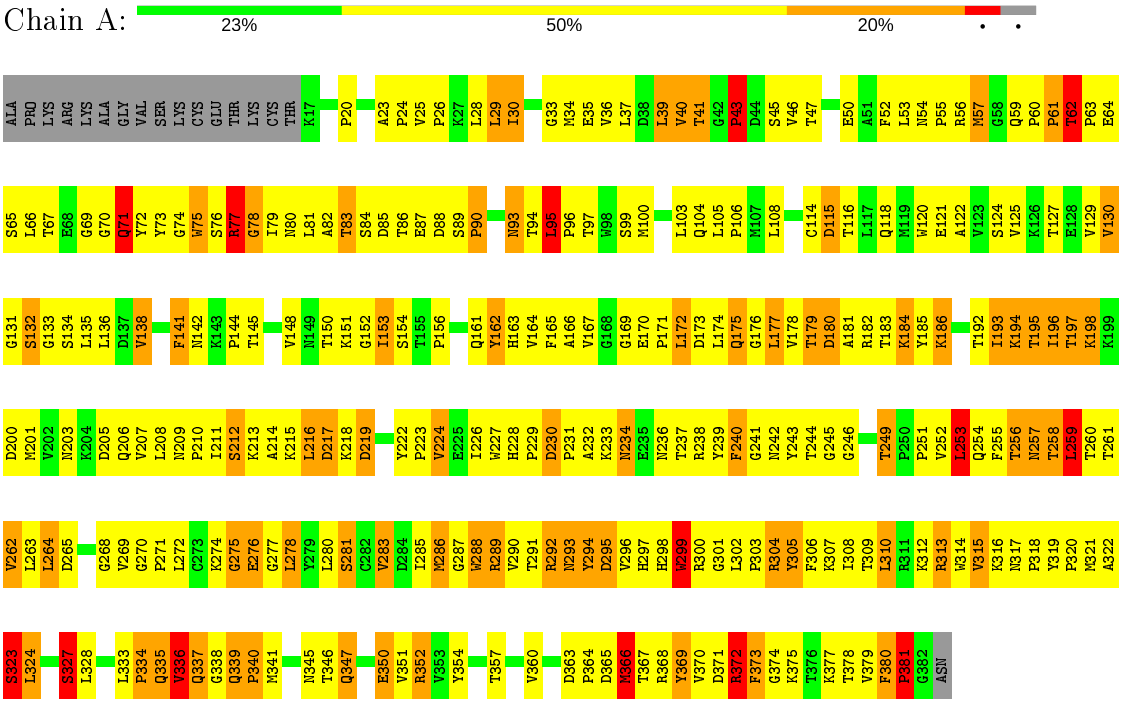
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

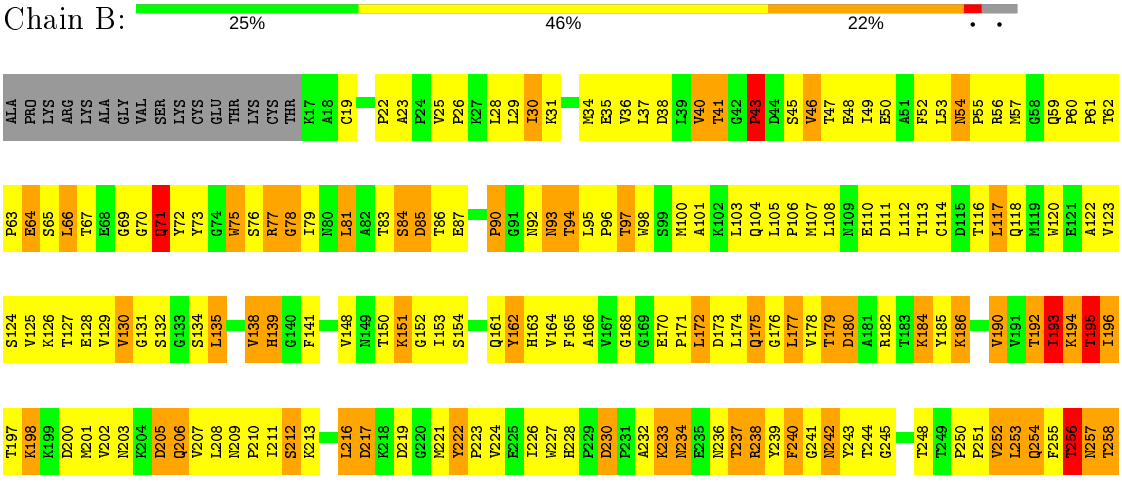
- Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

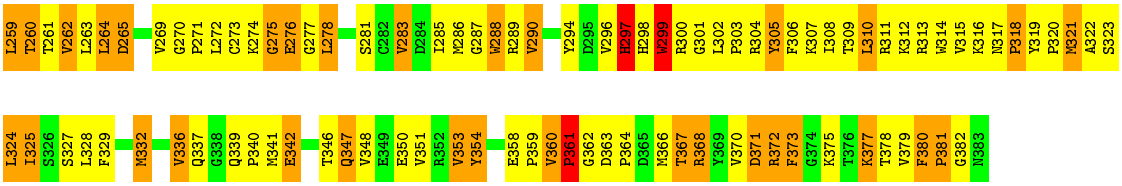
Chain A:



- Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

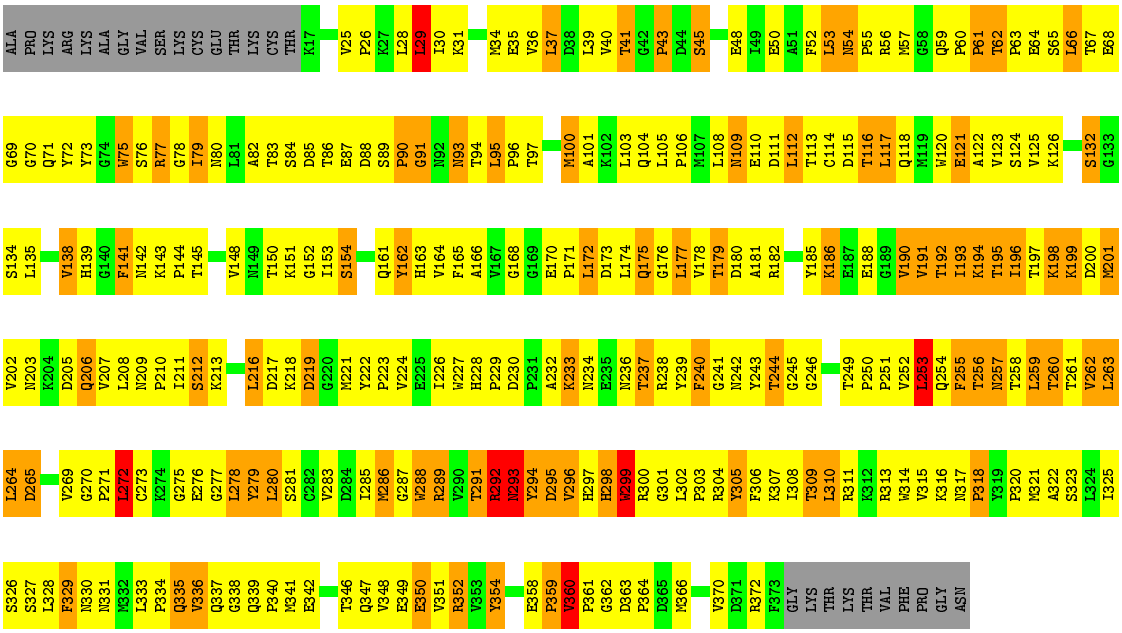
Chain B:





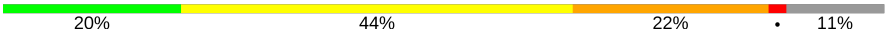
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

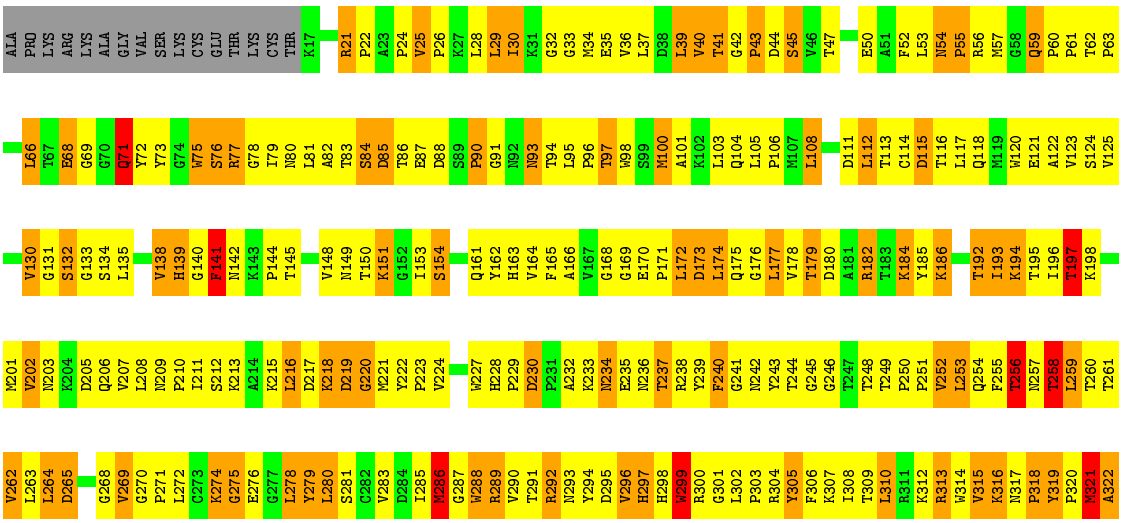
Chain C:

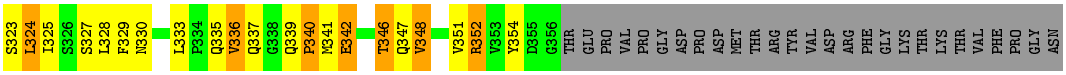


• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

Chain D:

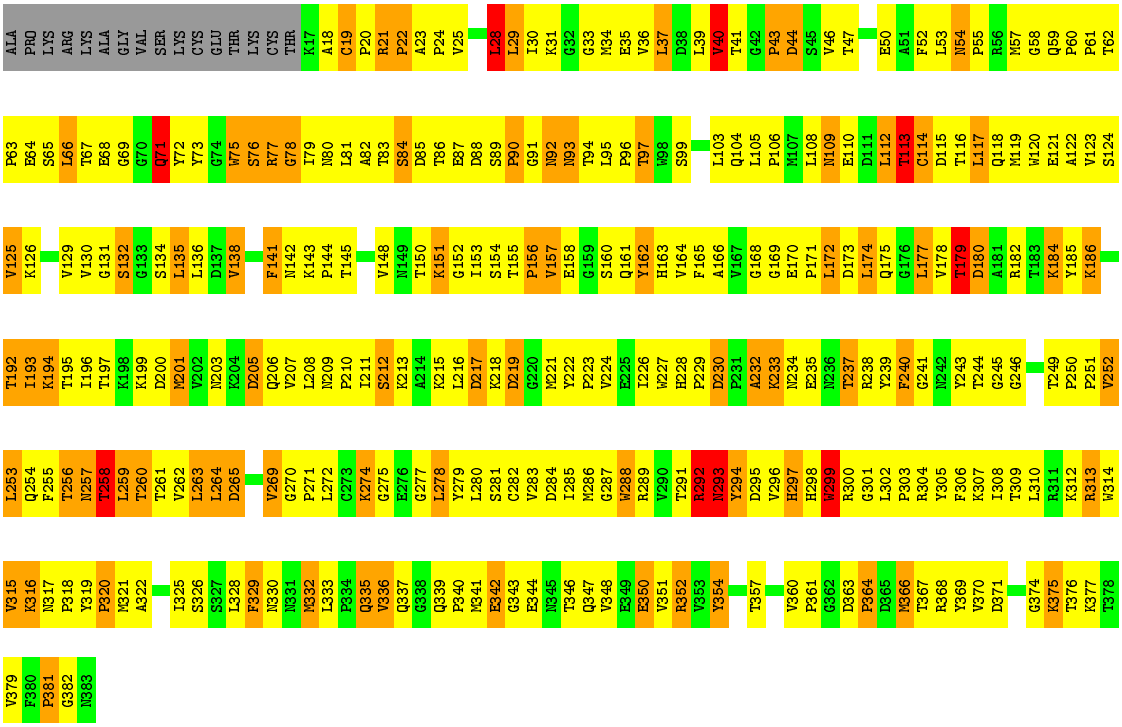






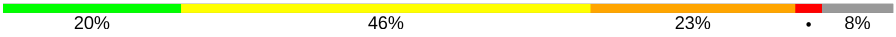
• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

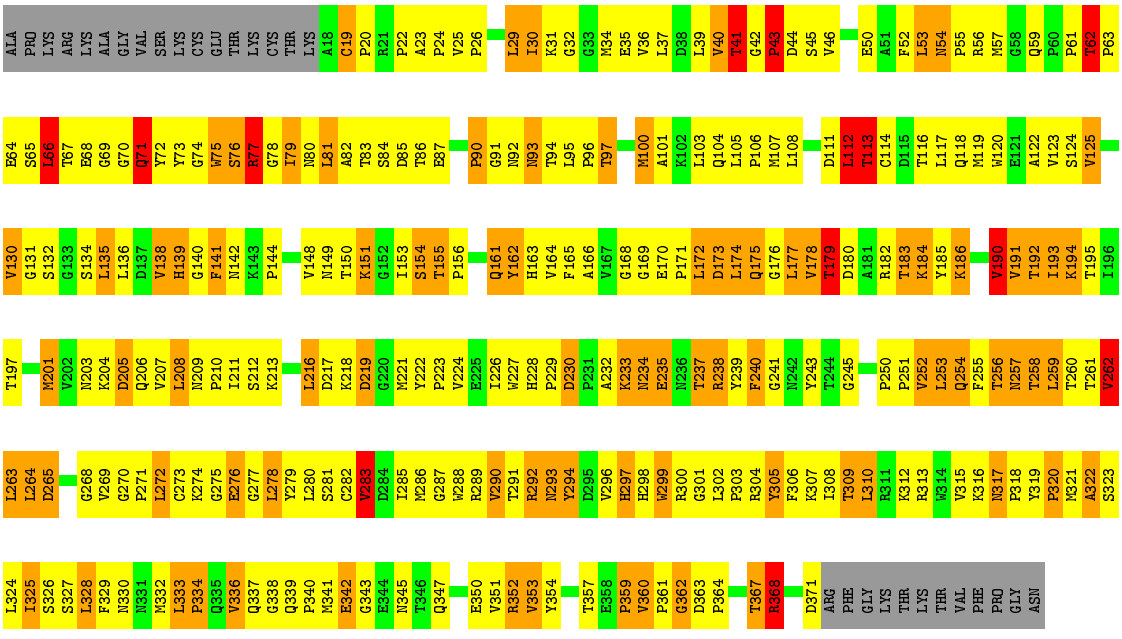
Chain E:



• Molecule 1: POLYOMAVIRUS COAT PROTEIN VP1

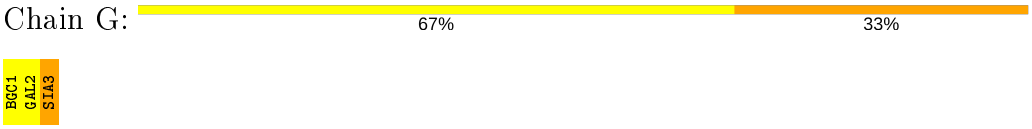
Chain F:





• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain G:



• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain H:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain I:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain J:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain K:

• Molecule 2: N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain L:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α, β, γ	570.00Å 570.00Å 570.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.65	Depositor
% Data completeness (in resolution range)	73.0 (12.00-3.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.236 , 0.253	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17003	wwPDB-VP
Average B, all atoms (Å^2)	77.0	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: SIA, BGC, GAL

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	0.96	2/2920 (0.1%)	1.26	22/3981 (0.6%)
1	B	0.95	0/2927	1.25	19/3989 (0.5%)
1	C	0.97	0/2852	1.26	21/3888 (0.5%)
1	D	1.01	2/2708 (0.1%)	1.27	23/3690 (0.6%)
1	E	1.00	1/2928 (0.0%)	1.34	23/3992 (0.6%)
1	F	0.96	2/2820 (0.1%)	1.25	21/3847 (0.5%)
All	All	0.98	7/17155 (0.0%)	1.27	129/23387 (0.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	3
1	C	0	4
1	D	0	5
1	E	0	2
1	F	0	3
All	All	0	22

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	336	VAL	C-N	13.07	1.64	1.34
1	D	342	GLU	CD-OE2	6.37	1.32	1.25
1	A	336	VAL	C-N	-5.83	1.20	1.34
1	D	299	TRP	CB-CG	5.46	1.60	1.50
1	F	234	ASN	CB-CG	5.37	1.63	1.51
1	A	262	VAL	CA-CB	-5.31	1.43	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	262	VAL	CA-CB	-5.04	1.44	1.54

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	336	VAL	O-C-N	21.97	157.85	122.70
1	A	336	VAL	O-C-N	-17.79	94.24	122.70
1	E	336	VAL	CA-C-N	-16.45	81.00	117.20
1	C	29	LEU	CA-CB-CG	-11.50	88.85	115.30
1	F	264	LEU	CA-CB-CG	-11.09	89.80	115.30
1	B	275	GLY	N-CA-C	-10.19	87.64	113.10
1	C	264	LEU	CA-CB-CG	-9.45	93.56	115.30
1	D	299	TRP	CA-CB-CG	8.86	130.53	113.70
1	E	177	LEU	CA-CB-CG	-8.77	95.12	115.30
1	F	275	GLY	N-CA-C	-8.69	91.37	113.10
1	F	29	LEU	CA-CB-CG	-8.62	95.46	115.30
1	C	275	GLY	N-CA-C	-8.60	91.60	113.10
1	E	29	LEU	CA-CB-CG	-8.48	95.78	115.30
1	A	275	GLY	N-CA-C	-8.35	92.24	113.10
1	E	299	TRP	CA-CB-CG	8.34	129.54	113.70
1	F	177	LEU	CA-CB-CG	-8.23	96.38	115.30
1	A	29	LEU	CA-CB-CG	-8.18	96.49	115.30
1	B	177	LEU	CA-CB-CG	-8.08	96.73	115.30
1	E	71	GLN	CA-C-N	-8.03	99.54	117.20
1	A	177	LEU	CA-CB-CG	-7.92	97.09	115.30
1	A	71	GLN	CA-C-N	-7.68	100.31	117.20
1	F	256	THR	N-CA-C	7.54	131.35	111.00
1	D	29	LEU	CA-CB-CG	-7.52	98.00	115.30
1	B	264	LEU	CA-CB-CG	-7.44	98.18	115.30
1	B	362	GLY	N-CA-C	-7.43	94.52	113.10
1	A	336	VAL	CA-C-N	-7.42	100.88	117.20
1	D	259	LEU	N-CA-C	7.35	130.84	111.00
1	C	95	LEU	CA-CB-CG	-7.31	98.48	115.30
1	B	71	GLN	CA-C-N	-7.30	101.14	117.20
1	D	256	THR	N-CA-C	7.24	130.55	111.00
1	C	299	TRP	CA-CB-CG	7.21	127.39	113.70
1	B	299	TRP	CA-CB-CG	7.17	127.33	113.70
1	D	71	GLN	CA-C-N	-7.10	101.59	117.20
1	E	259	LEU	N-CA-C	6.98	129.86	111.00
1	E	112	LEU	CA-CB-CG	-6.92	99.38	115.30
1	D	264	LEU	CA-CB-CG	-6.86	99.51	115.30
1	E	264	LEU	CA-CB-CG	-6.83	99.58	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	256	THR	CA-C-N	-6.80	102.23	117.20
1	A	256	THR	CA-C-N	-6.73	102.39	117.20
1	F	71	GLN	CA-C-N	-6.73	102.40	117.20
1	E	259	LEU	CA-CB-CG	-6.65	100.00	115.30
1	F	263	LEU	CA-CB-CG	-6.62	100.06	115.30
1	A	299	TRP	CA-CB-CG	6.62	126.28	113.70
1	C	259	LEU	CA-CB-CG	6.62	130.52	115.30
1	C	360	VAL	CB-CA-C	-6.58	98.89	111.40
1	F	257	ASN	N-CA-CB	-6.56	98.79	110.60
1	A	264	LEU	CA-CB-CG	-6.49	100.37	115.30
1	A	259	LEU	N-CA-C	6.39	128.25	111.00
1	F	292	ARG	N-CA-C	-6.38	93.77	111.00
1	B	259	LEU	N-CA-C	6.29	127.98	111.00
1	A	256	THR	N-CA-C	6.29	127.97	111.00
1	B	377	LYS	N-CA-C	-6.27	94.06	111.00
1	D	275	GLY	N-CA-C	-6.25	97.49	113.10
1	E	78	GLY	N-CA-C	-6.22	97.55	113.10
1	E	256	THR	N-CA-C	6.20	127.75	111.00
1	E	275	GLY	N-CA-C	-6.14	97.75	113.10
1	C	253	LEU	CA-CB-CG	-6.12	101.22	115.30
1	D	256	THR	CA-C-N	-6.09	103.80	117.20
1	C	95	LEU	N-CA-C	6.07	127.39	111.00
1	F	258	THR	N-CA-C	6.07	127.38	111.00
1	B	256	THR	N-CA-C	5.97	127.11	111.00
1	F	272	LEU	CA-CB-CG	-5.97	101.58	115.30
1	B	299	TRP	N-CA-C	5.83	126.74	111.00
1	E	258	THR	N-CA-C	5.81	126.69	111.00
1	E	263	LEU	CA-CB-CG	-5.80	101.96	115.30
1	C	263	LEU	CA-CB-CG	-5.79	101.98	115.30
1	E	274	LYS	N-CA-C	-5.77	95.43	111.00
1	E	28	LEU	CA-CB-CG	-5.77	102.04	115.30
1	C	350	GLU	N-CA-C	5.74	126.49	111.00
1	D	197	THR	N-CA-C	-5.73	95.54	111.00
1	B	254	GLN	N-CA-C	5.71	126.43	111.00
1	C	292	ARG	N-CA-C	-5.71	95.59	111.00
1	E	40	VAL	CB-CA-C	-5.71	100.55	111.40
1	B	380	PHE	N-CA-C	-5.67	95.70	111.00
1	C	91	GLY	N-CA-C	-5.67	98.93	113.10
1	C	256	THR	N-CA-C	5.67	126.30	111.00
1	B	40	VAL	CB-CA-C	-5.66	100.64	111.40
1	D	258	THR	N-CA-C	5.61	126.14	111.00
1	F	238	ARG	N-CA-C	-5.60	95.89	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	TRP	N-CA-C	5.59	126.11	111.00
1	D	40	VAL	N-CA-C	5.57	126.05	111.00
1	F	254	GLN	N-CA-C	5.57	126.05	111.00
1	A	289	ARG	N-CA-C	-5.57	95.95	111.00
1	D	259	LEU	CA-CB-CG	-5.57	102.49	115.30
1	E	232	ALA	N-CA-C	-5.57	95.96	111.00
1	B	78	GLY	N-CA-C	-5.56	99.19	113.10
1	A	257	ASN	N-CA-CB	-5.54	100.64	110.60
1	D	177	LEU	CB-CG-CD2	-5.53	101.59	111.00
1	C	177	LEU	N-CA-C	-5.51	96.11	111.00
1	D	40	VAL	CA-C-N	-5.49	105.13	117.20
1	C	289	ARG	N-CA-C	-5.47	96.24	111.00
1	A	253	LEU	CA-CB-CG	-5.45	102.76	115.30
1	D	296	VAL	N-CA-C	-5.45	96.29	111.00
1	E	76	SER	N-CA-C	-5.43	96.33	111.00
1	F	177	LEU	CB-CA-C	-5.42	99.89	110.20
1	F	283	VAL	CB-CA-C	-5.42	101.10	111.40
1	F	256	THR	C-N-CA	5.42	135.25	121.70
1	D	324	LEU	CA-CB-CG	5.36	127.63	115.30
1	D	274	LYS	N-CA-C	-5.35	96.55	111.00
1	F	289	ARG	N-CA-C	-5.35	96.55	111.00
1	D	280	LEU	CA-CB-CG	-5.35	102.99	115.30
1	F	299	TRP	N-CA-C	5.35	125.44	111.00
1	D	42	GLY	N-CA-C	-5.34	99.76	113.10
1	A	62	THR	N-CA-C	5.33	125.40	111.00
1	A	381	PRO	CA-N-CD	-5.29	104.10	111.50
1	C	299	TRP	N-CA-C	5.28	125.27	111.00
1	A	71	GLN	CB-CA-C	5.22	120.83	110.40
1	B	353	VAL	CB-CA-C	-5.21	101.50	111.40
1	B	289	ARG	N-CA-C	-5.20	96.95	111.00
1	B	94	THR	N-CA-C	-5.20	96.97	111.00
1	B	19	CYS	N-CA-C	-5.19	96.99	111.00
1	E	292	ARG	N-CA-C	-5.19	97.00	111.00
1	D	177	LEU	CB-CA-C	-5.17	100.37	110.20
1	F	114	CYS	N-CA-C	-5.16	97.08	111.00
1	D	141	PHE	N-CA-C	5.12	124.81	111.00
1	F	53	LEU	CA-CB-CG	5.10	127.02	115.30
1	E	336	VAL	C-N-CA	-5.08	109.00	121.70
1	A	78	GLY	N-CA-C	-5.08	100.40	113.10
1	D	286	MET	CG-SD-CE	5.07	108.30	100.20
1	C	177	LEU	CB-CA-C	-5.05	100.60	110.20
1	C	360	VAL	CG1-CB-CG2	5.05	118.98	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	289	ARG	N-CA-C	-5.04	97.38	111.00
1	A	258	THR	N-CA-C	5.04	124.59	111.00
1	C	280	LEU	CA-CB-CG	-5.02	103.75	115.30
1	A	95	LEU	CA-CB-CG	-5.01	103.77	115.30
1	C	272	LEU	CA-CB-CG	-5.01	103.78	115.30
1	A	153	ILE	CB-CA-C	-5.01	101.59	111.60
1	E	277	GLY	N-CA-C	5.01	125.62	113.10
1	B	238	ARG	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	TYR	Sidechain
1	A	305	TYR	Sidechain
1	A	336	VAL	Mainchain,Peptide
1	A	71	GLN	Mainchain
1	B	162	TYR	Sidechain
1	B	305	TYR	Sidechain
1	B	71	GLN	Mainchain
1	C	162	TYR	Sidechain
1	C	279	TYR	Sidechain
1	C	298	HIS	Mainchain
1	C	305	TYR	Sidechain
1	D	162	TYR	Sidechain
1	D	305	TYR	Sidechain
1	D	319	TYR	Mainchain
1	D	354	TYR	Sidechain
1	D	71	GLN	Mainchain
1	E	162	TYR	Sidechain
1	E	71	GLN	Mainchain
1	F	162	TYR	Sidechain
1	F	305	TYR	Sidechain
1	F	71	GLN	Mainchain

5.2 Too-close contacts (i)

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	2849	0	2814	457	2
1	B	2857	0	2820	454	0
1	C	2784	0	2743	441	0
1	D	2645	0	2616	404	0
1	E	2857	0	2821	472	0
1	F	2753	0	2710	420	0
2	G	43	0	37	1	0
2	H	43	0	37	5	0
2	I	43	0	37	3	0
2	J	43	0	37	1	0
2	K	43	0	37	3	0
2	L	43	0	37	5	0
All	All	17003	0	16746	2434	2

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 72.

All (2434) 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:328:LEU:CD2	1:A:333:LEU:HD21	1.37	1.52
1:A:328:LEU:HD21	1:A:333:LEU:CD2	1.40	1.50
1:A:175:GLN:HB2	1:A:230:ASP:HB2	1.26	1.11
1:F:175:GLN:HB2	1:F:230:ASP:HB2	1.33	1.10
1:B:336:VAL:HA	1:B:337:GLN:N	1.68	1.09
1:A:144:PRO:HD3	1:A:292:ARG:HG2	1.35	1.08
1:D:175:GLN:HG3	1:D:213:LYS:HG2	1.37	1.05
1:A:125:VAL:HG12	1:A:263:LEU:HD21	1.34	1.04
1:B:175:GLN:HB2	1:B:230:ASP:HB2	1.39	1.03
1:E:177:LEU:HD13	1:E:207:VAL:O	1.59	1.03
1:A:71:GLN:HG3	1:B:203:ASN:HB3	1.38	1.03
1:D:66:LEU:HB3	1:D:71:GLN:HB2	1.39	1.01
1:A:37:LEU:HD23	1:A:106:PRO:HD3	1.43	1.00
1:E:233:LYS:HD3	1:E:234:ASN:HD22	1.25	0.98
1:E:112:LEU:HB3	1:E:116:THR:HG23	1.45	0.98
1:A:203:ASN:HB3	1:E:71:GLN:HG3	1.42	0.98
1:F:122:ALA:HB3	1:F:271:PRO:HD2	1.44	0.98
1:D:71:GLN:HG3	1:E:203:ASN:HB3	1.47	0.96
1:C:346:THR:HG22	1:C:348:VAL:HB	1.49	0.95
1:D:138:VAL:HB	1:D:153:ILE:HG23	1.48	0.95
1:C:168:GLY:HA3	1:C:237:THR:HG23	1.46	0.95
1:F:138:VAL:HB	1:F:153:ILE:HG23	1.48	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:CG	1:A:333:LEU:HD21	1.97	0.94
1:A:177:LEU:HD21	1:A:209:ASN:H	1.29	0.94
1:A:192:THR:HG22	1:A:193:ILE:HD12	1.46	0.94
1:D:346:THR:HG22	1:D:348:VAL:HB	1.49	0.94
1:A:372:ARG:HH11	1:A:372:ARG:HB2	1.31	0.94
1:D:178:VAL:HG11	1:D:201:MET:HE1	1.50	0.93
1:A:336:VAL:CG2	1:A:337:GLN:HA	1.98	0.93
1:A:205:ASP:HA	1:A:209:ASN:HB2	1.48	0.93
1:C:208:LEU:O	1:C:210:PRO:HD3	1.68	0.92
1:D:257:ASN:ND2	1:E:238:ARG:HA	1.85	0.92
1:A:350:GLU:HG3	1:A:351:VAL:N	1.84	0.92
1:E:175:GLN:HG3	1:E:213:LYS:HG2	1.52	0.91
1:C:71:GLN:HG3	1:D:203:ASN:HB3	1.49	0.91
1:D:176:GLY:C	1:D:177:LEU:HD12	1.90	0.91
1:A:336:VAL:HG23	1:A:337:GLN:HA	1.50	0.90
1:D:257:ASN:HB2	1:E:239:TYR:CE1	2.06	0.90
1:E:83:THR:HB	1:E:87:GLU:HB3	1.51	0.90
1:B:52:PHE:CE2	1:C:208:LEU:HD23	2.07	0.89
1:F:108:LEU:HB3	1:F:118:GLN:HE21	1.34	0.89
1:F:30:ILE:HD13	1:F:36:VAL:HG13	1.55	0.89
1:A:141:PHE:CE1	1:A:292:ARG:HG3	2.08	0.88
1:A:257:ASN:ND2	1:B:238:ARG:HA	1.87	0.88
1:F:262:VAL:HG12	1:F:264:LEU:H	1.38	0.88
1:D:336:VAL:CA	1:D:337:GLN:OE1	2.22	0.88
1:B:262:VAL:HG12	1:B:264:LEU:H	1.37	0.88
1:A:380:PHE:CG	1:A:381:PRO:HD2	2.09	0.88
1:B:205:ASP:HA	1:B:209:ASN:HB2	1.52	0.88
1:D:336:VAL:HA	1:D:337:GLN:OE1	1.73	0.88
1:E:335:GLN:HA	1:E:335:GLN:OE1	1.74	0.88
1:C:172:LEU:HD22	1:C:173:ASP:N	1.89	0.88
1:A:297:HIS:HE1	1:E:145:THR:HG21	1.38	0.88
1:A:336:VAL:HG23	1:A:337:GLN:CA	2.04	0.87
1:D:168:GLY:HA3	1:D:237:THR:HG23	1.55	0.87
1:B:346:THR:HG21	1:B:348:VAL:HG12	1.57	0.87
1:B:336:VAL:O	1:B:337:GLN:HA	1.75	0.86
1:E:253:LEU:HD23	1:E:254:GLN:H	1.40	0.86
1:C:142:ASN:C	1:C:292:ARG:HB2	1.96	0.86
1:A:177:LEU:HD13	1:A:207:VAL:O	1.73	0.86
1:C:350:GLU:CB	1:F:233:LYS:HB3	2.06	0.86
1:E:168:GLY:HA3	1:E:237:THR:HG23	1.58	0.86
1:D:265:ASP:H	1:D:270:GLY:H	1.21	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:GLY:HA3	1:B:237:THR:HG23	1.56	0.85
1:F:177:LEU:HD21	1:F:208:LEU:HA	1.58	0.85
1:A:125:VAL:CG1	1:A:263:LEU:HD21	2.07	0.85
1:D:286:MET:HA	1:D:286:MET:HE3	1.58	0.85
1:C:138:VAL:HB	1:C:153:ILE:HG23	1.57	0.84
1:D:104:GLN:HE22	1:D:276:GLU:HB2	1.42	0.84
1:B:71:GLN:HG3	1:C:203:ASN:HB3	1.58	0.84
1:B:131:GLY:HA3	1:C:177:LEU:HD12	1.57	0.84
1:D:286:MET:CE	1:D:286:MET:HA	2.08	0.84
1:E:141:PHE:CE1	1:E:292:ARG:HG3	2.12	0.84
1:B:346:THR:CG2	1:B:348:VAL:HG12	2.08	0.84
1:C:62:THR:OG1	1:C:63:PRO:HD3	1.78	0.84
1:A:192:THR:HG22	1:A:193:ILE:CD1	2.07	0.83
1:B:379:VAL:HG12	1:B:380:PHE:O	1.76	0.83
1:F:83:THR:HB	1:F:87:GLU:HB3	1.58	0.83
1:A:175:GLN:CB	1:A:230:ASP:HB2	2.09	0.83
1:A:262:VAL:HG12	1:A:264:LEU:H	1.41	0.83
1:A:76:SER:O	1:A:298:HIS:HB2	1.78	0.83
1:B:37:LEU:HD23	1:B:106:PRO:HD3	1.59	0.83
1:B:138:VAL:HB	1:B:153:ILE:HG23	1.61	0.83
1:D:257:ASN:HB2	1:E:239:TYR:CD1	2.13	0.83
1:B:77:ARG:HB2	1:B:93:ASN:HB2	1.61	0.82
1:F:168:GLY:HA3	1:F:237:THR:HG23	1.62	0.82
1:B:83:THR:HB	1:B:87:GLU:HB3	1.59	0.82
1:B:222:TYR:HB3	1:B:227:TRP:CD1	2.15	0.82
1:D:178:VAL:HG22	1:D:179:THR:H	1.42	0.82
1:A:340:PRO:HG2	1:A:347:GLN:HE22	1.44	0.82
1:D:114:CYS:HB2	1:D:116:THR:HG22	1.62	0.82
1:B:233:LYS:HG2	1:B:234:ASN:N	1.95	0.81
1:E:177:LEU:HD21	1:E:209:ASN:H	1.42	0.81
1:A:138:VAL:HB	1:A:153:ILE:HG23	1.61	0.81
1:A:63:PRO:O	1:A:71:GLN:NE2	2.14	0.81
1:D:336:VAL:C	1:D:337:GLN:OE1	2.18	0.81
1:B:257:ASN:HD22	1:B:257:ASN:H	1.28	0.81
1:C:50:GLU:CD	1:D:233:LYS:HA	2.01	0.81
1:C:350:GLU:HG3	1:F:233:LYS:HG2	1.62	0.80
1:C:205:ASP:HA	1:C:209:ASN:HB2	1.62	0.80
1:D:76:SER:O	1:D:298:HIS:HB2	1.80	0.80
1:F:203:ASN:O	1:F:206:GLN:HB3	1.81	0.80
1:B:22:PRO:HG2	1:F:359:PRO:HB3	1.64	0.80
1:C:176:GLY:O	1:C:177:LEU:HD23	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:163:HIS:HA	1:F:283:VAL:O	1.81	0.80
1:F:142:ASN:C	1:F:292:ARG:HB2	2.02	0.80
1:C:50:GLU:OE1	1:D:233:LYS:HA	1.82	0.79
1:A:41:THR:O	1:A:45:SER:HB3	1.82	0.79
1:D:104:GLN:NE2	1:D:276:GLU:HB2	1.97	0.79
1:E:313:ARG:HH11	1:E:313:ARG:HG2	1.47	0.79
1:F:168:GLY:CA	1:F:237:THR:HG23	2.11	0.79
1:E:122:ALA:HA	1:E:310:LEU:HB3	1.65	0.79
1:B:258:THR:HB	1:B:259:LEU:HD22	1.63	0.79
1:B:308:ILE:N	1:B:308:ILE:HD12	1.97	0.79
1:D:174:LEU:N	1:D:174:LEU:HD12	1.98	0.79
1:D:83:THR:HB	1:D:87:GLU:HB3	1.64	0.79
1:E:272:LEU:N	1:E:272:LEU:HD12	1.98	0.79
1:C:161:GLN:HE22	1:C:251:PRO:HA	1.47	0.79
1:B:217:ASP:O	1:F:336:VAL:HG13	1.82	0.79
1:B:163:HIS:HA	1:B:283:VAL:O	1.83	0.78
1:F:308:ILE:HD12	1:F:308:ILE:N	1.98	0.78
1:F:208:LEU:O	1:F:210:PRO:HD3	1.84	0.78
1:C:352:ARG:NE	1:F:233:LYS:HE3	1.97	0.78
1:D:144:PRO:HD3	1:D:292:ARG:HG2	1.64	0.78
1:E:118:GLN:HB2	1:E:314:TRP:CZ3	2.18	0.78
1:A:208:LEU:O	1:A:210:PRO:HD3	1.83	0.78
1:B:177:LEU:HD21	1:B:208:LEU:HA	1.63	0.78
1:B:350:GLU:HG3	1:B:351:VAL:N	1.99	0.78
1:C:175:GLN:HB2	1:C:230:ASP:HB2	1.64	0.78
1:B:251:PRO:HD2	1:C:245:GLY:HA3	1.65	0.78
1:A:239:TYR:CD1	1:E:257:ASN:HB2	2.19	0.78
1:A:69:GLY:C	1:A:71:GLN:H	1.84	0.78
1:B:161:GLN:HE22	1:B:251:PRO:HA	1.48	0.78
1:C:109:ASN:HB3	1:C:117:LEU:HD21	1.66	0.78
1:C:52:PHE:CE1	1:D:208:LEU:HD23	2.19	0.78
1:E:62:THR:OG1	1:E:63:PRO:HD3	1.83	0.78
1:A:97:THR:HG22	1:A:223:PRO:HA	1.66	0.78
1:A:141:PHE:CD2	1:B:84:SER:HA	2.19	0.78
1:A:207:VAL:HG23	1:A:208:LEU:H	1.48	0.77
1:B:263:LEU:O	1:B:270:GLY:HA2	1.84	0.77
1:D:71:GLN:HG3	1:E:203:ASN:CB	2.14	0.77
1:A:222:TYR:HB3	1:A:227:TRP:CD1	2.19	0.77
1:B:341:MET:HE3	1:B:346:THR:HG22	1.66	0.77
1:D:258:THR:HB	1:D:259:LEU:HD22	1.66	0.77
1:D:111:ASP:HB3	1:D:116:THR:HG23	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:341:MET:CE	1:F:347:GLN:HB2	2.14	0.77
1:A:194:LYS:HA	1:A:197:THR:O	1.85	0.77
1:B:97:THR:HA	1:B:223:PRO:HA	1.67	0.77
1:C:233:LYS:CE	1:F:350:GLU:HG2	2.13	0.77
1:A:124:SER:HA	1:A:263:LEU:HG	1.67	0.77
1:E:178:VAL:HG22	1:E:179:THR:N	1.99	0.77
1:D:153:ILE:HG12	1:E:297:HIS:ND1	2.00	0.77
1:F:177:LEU:HD13	1:F:207:VAL:O	1.85	0.76
1:A:288:TRP:HZ3	1:A:299:TRP:CE2	2.03	0.76
1:C:112:LEU:H	1:C:112:LEU:HD22	1.49	0.76
1:D:66:LEU:HD23	1:D:66:LEU:H	1.51	0.76
1:E:122:ALA:O	1:E:271:PRO:HD2	1.85	0.76
1:F:288:TRP:HE3	1:F:299:TRP:HB3	1.49	0.76
1:D:251:PRO:HD2	1:E:245:GLY:HA3	1.68	0.76
1:A:257:ASN:HB2	1:B:239:TYR:CE2	2.20	0.76
1:D:178:VAL:HG22	1:D:179:THR:N	2.00	0.76
1:D:90:PRO:HB2	1:D:186:LYS:HE3	1.66	0.76
1:C:197:THR:O	1:C:197:THR:HG23	1.85	0.76
1:D:346:THR:CG2	1:D:348:VAL:HB	2.15	0.76
1:D:78:GLY:HA2	1:D:298:HIS:HB3	1.65	0.76
1:F:321:MET:O	1:F:324:LEU:HG	1.86	0.76
1:A:177:LEU:CD2	1:A:209:ASN:H	1.98	0.76
1:B:288:TRP:HZ3	1:B:299:TRP:CE2	2.04	0.76
1:C:176:GLY:C	1:C:177:LEU:HD23	2.07	0.76
1:E:76:SER:O	1:E:298:HIS:HB2	1.86	0.76
1:B:304:ARG:HD3	1:B:306:PHE:CZ	2.21	0.75
1:F:341:MET:HE1	1:F:347:GLN:HB2	1.68	0.75
1:A:370:VAL:HG13	1:A:374:GLY:O	1.86	0.75
1:C:175:GLN:HE21	1:C:176:GLY:N	1.84	0.75
1:D:122:ALA:HB3	1:D:271:PRO:HD2	1.67	0.75
1:C:28:LEU:HD23	1:C:29:LEU:N	2.02	0.75
1:D:269:VAL:HG12	1:D:270:GLY:O	1.87	0.75
1:C:308:ILE:HD12	1:C:308:ILE:H	1.51	0.75
1:B:125:VAL:HG12	1:B:263:LEU:HD21	1.67	0.75
1:C:313:ARG:HG2	1:C:314:TRP:N	2.02	0.75
1:D:72:TYR:O	1:D:75:TRP:HB2	1.86	0.75
1:D:133:GLY:N	1:E:228:HIS:HE1	1.83	0.75
1:C:175:GLN:HE21	1:C:176:GLY:H	1.35	0.74
1:D:30:ILE:HD13	1:D:36:VAL:HG13	1.67	0.74
1:B:339:GLN:HG2	1:B:340:PRO:HD2	1.69	0.74
1:C:346:THR:CG2	1:C:348:VAL:HB	2.16	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:172:LEU:HD22	1:F:173:ASP:N	2.02	0.74
1:F:142:ASN:O	1:F:292:ARG:HB2	1.85	0.74
1:A:52:PHE:CE2	1:B:208:LEU:HD22	2.22	0.74
1:B:22:PRO:HB2	1:F:360:VAL:HG23	1.70	0.74
1:B:103:LEU:HD22	1:F:341:MET:HG3	1.69	0.74
1:B:135:LEU:HD12	1:B:135:LEU:N	2.03	0.74
1:C:75:TRP:NE1	1:C:300:ARG:HB2	2.03	0.74
1:A:79:ILE:HD11	1:A:298:HIS:HA	1.69	0.74
1:D:258:THR:C	1:D:259:LEU:HD22	2.08	0.74
1:F:320:PRO:O	1:F:323:SER:HB3	1.88	0.74
1:A:135:LEU:N	1:A:135:LEU:HD12	2.02	0.73
1:C:172:LEU:HD22	1:C:173:ASP:H	1.51	0.73
1:D:177:LEU:N	1:D:177:LEU:HD12	2.02	0.73
1:E:75:TRP:NE1	1:E:300:ARG:HB2	2.03	0.73
1:B:219:ASP:HB2	1:F:338:GLY:HA2	1.69	0.73
1:F:91:GLY:N	1:F:186:LYS:HZ1	1.86	0.73
1:C:39:LEU:HD12	1:C:40:VAL:H	1.52	0.73
1:E:66:LEU:HD23	1:E:66:LEU:H	1.51	0.73
1:A:39:LEU:HD12	1:A:40:VAL:N	2.03	0.73
1:C:77:ARG:HB2	1:C:93:ASN:HB2	1.69	0.73
1:E:109:ASN:OD1	1:E:117:LEU:HA	1.87	0.73
1:E:175:GLN:HB2	1:E:230:ASP:HB2	1.69	0.73
1:B:272:LEU:HD12	1:B:272:LEU:N	2.03	0.73
1:B:30:ILE:HD13	1:B:36:VAL:HG13	1.69	0.73
1:E:350:GLU:HG3	1:E:351:VAL:N	2.02	0.73
1:C:175:GLN:HG2	1:C:213:LYS:HG2	1.70	0.73
1:C:71:GLN:HA	1:C:71:GLN:NE2	1.94	0.73
1:D:54:ASN:HD22	1:D:55:PRO:HD2	1.53	0.73
1:E:123:VAL:HG13	1:E:264:LEU:HD13	1.70	0.73
1:E:305:TYR:HE1	1:E:307:LYS:HB2	1.53	0.73
1:A:69:GLY:HA3	1:A:71:GLN:HE22	1.53	0.73
1:F:238:ARG:NH2	1:F:265:ASP:HB3	2.04	0.73
1:F:75:TRP:NE1	1:F:300:ARG:HB2	2.04	0.73
1:D:240:PHE:CD1	1:D:240:PHE:N	2.56	0.73
1:E:233:LYS:HD2	1:E:234:ASN:N	2.03	0.73
1:E:163:HIS:HA	1:E:283:VAL:O	1.89	0.73
1:C:203:ASN:O	1:C:206:GLN:HB3	1.87	0.72
1:C:286:MET:HE3	1:C:286:MET:HA	1.70	0.72
1:C:76:SER:O	1:C:298:HIS:HB2	1.89	0.72
1:B:125:VAL:CG1	1:B:263:LEU:HD21	2.18	0.72
1:F:296:VAL:HG11	2:L:3:SIA:H32	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:THR:HB	1:E:194:LYS:HD3	1.70	0.72
1:A:62:THR:OG1	1:A:63:PRO:HD3	1.89	0.72
1:B:170:GLU:HB2	1:B:171:PRO:HD2	1.69	0.72
1:E:121:GLU:HG2	1:E:271:PRO:O	1.88	0.72
1:A:203:ASN:CB	1:E:71:GLN:HG3	2.16	0.72
1:B:131:GLY:CA	1:C:177:LEU:HD12	2.20	0.72
1:F:150:THR:O	1:F:150:THR:HG22	1.87	0.72
1:A:122:ALA:HB3	1:A:271:PRO:HD2	1.71	0.72
1:F:30:ILE:HG12	1:F:31:LYS:N	2.02	0.72
1:A:153:ILE:HD11	1:B:297:HIS:HB3	1.72	0.72
1:A:50:GLU:HG2	1:B:233:LYS:HA	1.71	0.72
1:D:112:LEU:H	1:D:112:LEU:HD12	1.54	0.72
1:F:144:PRO:HD3	1:F:292:ARG:CG	2.20	0.72
1:C:340:PRO:HG2	1:C:347:GLN:HG3	1.72	0.72
1:D:28:LEU:HG	1:D:29:LEU:N	2.03	0.72
1:D:71:GLN:HE21	1:D:73:TYR:HB2	1.53	0.72
1:F:350:GLU:HG3	1:F:351:VAL:N	2.04	0.72
1:C:313:ARG:HG2	1:C:314:TRP:H	1.52	0.72
1:D:25:VAL:HG23	1:D:26:PRO:HD2	1.71	0.72
1:D:262:VAL:HG12	1:D:264:LEU:H	1.55	0.72
1:D:263:LEU:O	1:D:270:GLY:HA2	1.90	0.71
1:F:218:LYS:HB2	1:F:222:TYR:CE1	2.25	0.71
1:D:257:ASN:HD21	1:E:238:ARG:HA	1.53	0.71
1:F:178:VAL:HG22	1:F:179:THR:H	1.54	0.71
1:B:105:LEU:HB2	1:B:276:GLU:O	1.91	0.71
1:D:174:LEU:H	1:D:174:LEU:HD12	1.53	0.71
1:D:180:ASP:OD2	1:D:182:ARG:HD3	1.90	0.71
1:F:350:GLU:HG3	1:F:351:VAL:H	1.55	0.71
1:A:52:PHE:CZ	1:B:208:LEU:HD22	2.26	0.71
1:C:108:LEU:HD11	1:C:120:TRP:CE2	2.26	0.71
1:D:287:GLY:O	1:D:299:TRP:HB2	1.91	0.71
1:B:360:VAL:HG12	1:B:361:PRO:O	1.90	0.71
1:E:368:ARG:CZ	1:E:377:LYS:HE3	2.21	0.71
1:F:106:PRO:HD2	1:F:120:TRP:HE1	1.55	0.71
1:A:194:LYS:HD3	1:A:194:LYS:H	1.56	0.70
1:A:71:GLN:HA	1:A:71:GLN:OE1	1.85	0.70
1:C:269:VAL:HG12	1:C:270:GLY:O	1.91	0.70
1:F:180:ASP:HB3	1:F:182:ARG:CG	2.21	0.70
1:B:328:LEU:O	1:B:332:MET:SD	2.49	0.70
1:C:100:MET:HG2	1:C:216:LEU:HD13	1.72	0.70
1:D:318:PRO:HG2	1:D:319:TYR:CD2	2.26	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:PRO:HB3	1:D:95:LEU:HD11	1.71	0.70
1:A:161:GLN:HE22	1:A:251:PRO:HA	1.57	0.70
1:B:373:PHE:N	1:B:373:PHE:CD1	2.59	0.70
1:C:232:ALA:HB3	1:C:234:ASN:O	1.91	0.70
1:C:352:ARG:HE	1:F:233:LYS:HE3	1.56	0.70
1:F:65:SER:HB3	1:F:68:GLU:HG2	1.73	0.70
1:B:79:ILE:HD11	1:B:298:HIS:HA	1.74	0.70
1:D:176:GLY:O	1:D:177:LEU:HD12	1.91	0.70
1:B:296:VAL:HG11	2:H:3:SIA:H32	1.72	0.70
1:C:50:GLU:OE2	1:D:233:LYS:HA	1.92	0.70
1:E:112:LEU:O	1:E:116:THR:HG22	1.92	0.70
1:E:135:LEU:HD13	1:E:135:LEU:N	2.06	0.70
1:E:138:VAL:HB	1:E:153:ILE:HD12	1.72	0.70
1:E:209:ASN:OD1	1:E:211:ILE:HD13	1.92	0.70
1:E:208:LEU:O	1:E:210:PRO:HD3	1.92	0.70
1:E:259:LEU:HD22	1:E:259:LEU:N	2.07	0.70
1:F:192:THR:H	1:F:195:THR:HB	1.57	0.70
1:B:193:ILE:HD12	1:B:193:ILE:N	2.06	0.70
1:D:57:MET:HB2	1:D:96:PRO:HB3	1.74	0.70
1:E:186:LYS:HE2	1:E:186:LYS:N	2.05	0.70
1:E:71:GLN:NE2	1:E:73:TYR:HB2	2.07	0.70
1:A:30:ILE:HG12	1:A:36:VAL:HG13	1.74	0.70
1:A:39:LEU:HD12	1:A:40:VAL:H	1.56	0.70
1:C:95:LEU:HD23	1:C:96:PRO:HD2	1.74	0.70
1:F:66:LEU:HD23	1:F:66:LEU:H	1.56	0.70
1:B:122:ALA:HA	1:B:310:LEU:HB3	1.73	0.70
1:B:341:MET:C	1:B:346:THR:HG23	2.13	0.70
1:D:175:GLN:HB2	1:D:230:ASP:HB2	1.73	0.70
1:F:194:LYS:HD3	1:F:194:LYS:H	1.56	0.70
1:F:259:LEU:HD13	1:F:259:LEU:N	2.07	0.70
1:A:178:VAL:HG22	1:A:179:THR:N	2.07	0.69
1:C:233:LYS:NZ	1:F:350:GLU:HG2	2.07	0.69
1:F:108:LEU:HD11	1:F:120:TRP:CE2	2.27	0.69
1:F:106:PRO:HD2	1:F:120:TRP:NE1	2.07	0.69
1:A:211:ILE:HD12	1:A:211:ILE:N	2.07	0.69
1:B:192:THR:HB	1:B:193:ILE:HD12	1.74	0.69
1:C:273:CYS:HB3	1:C:277:GLY:O	1.92	0.69
1:E:265:ASP:H	1:E:270:GLY:H	1.39	0.69
1:B:71:GLN:HG3	1:C:203:ASN:CB	2.23	0.69
1:D:103:LEU:HB2	1:D:278:LEU:HB3	1.74	0.69
1:D:285:ILE:N	1:D:285:ILE:HD12	2.07	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ASN:OD1	1:C:211:ILE:HD13	1.91	0.69
1:C:233:LYS:HB3	1:F:350:GLU:HB3	1.74	0.69
1:F:150:THR:HG21	1:F:292:ARG:HH21	1.58	0.69
1:F:233:LYS:HD3	1:F:234:ASN:N	2.07	0.69
1:A:233:LYS:HG3	1:A:234:ASN:HD22	1.58	0.69
1:B:178:VAL:HG22	1:B:179:THR:N	2.08	0.69
1:F:111:ASP:HB3	1:F:116:THR:HG22	1.74	0.69
1:A:308:ILE:HD12	1:A:308:ILE:N	2.07	0.69
1:C:126:LYS:HG3	1:C:260:THR:HG23	1.75	0.69
1:D:224:VAL:HG21	1:D:283:VAL:HG11	1.74	0.69
1:E:175:GLN:CB	1:E:230:ASP:HB2	2.23	0.69
1:E:293:ASN:OD1	1:E:294:TYR:HB2	1.91	0.69
1:F:97:THR:HA	1:F:223:PRO:HA	1.75	0.69
1:A:239:TYR:CE1	1:E:257:ASN:HB2	2.28	0.69
1:C:163:HIS:HA	1:C:283:VAL:O	1.92	0.69
1:F:104:GLN:HE21	1:F:105:LEU:N	1.90	0.69
1:A:205:ASP:CA	1:A:209:ASN:HB2	2.23	0.68
1:B:257:ASN:HB3	1:C:239:TYR:CE2	2.28	0.68
1:D:317:ASN:HD22	1:D:318:PRO:HD2	1.56	0.68
1:E:170:GLU:HB2	1:E:171:PRO:HD2	1.73	0.68
1:E:246:GLY:HA3	1:E:249:THR:OG1	1.93	0.68
1:A:203:ASN:O	1:A:206:GLN:HB3	1.94	0.68
1:A:275:GLY:O	1:A:277:GLY:N	2.26	0.68
1:B:161:GLN:NE2	1:B:251:PRO:HA	2.07	0.68
1:D:141:PHE:CE1	1:D:292:ARG:HG3	2.28	0.68
1:B:256:THR:HG23	1:B:258:THR:H	1.58	0.68
1:F:177:LEU:CD2	1:F:208:LEU:HA	2.23	0.68
1:F:278:LEU:HD22	1:F:280:LEU:HD21	1.76	0.68
1:A:177:LEU:HD21	1:A:209:ASN:N	2.06	0.68
1:A:336:VAL:CB	1:A:337:GLN:HA	2.23	0.68
1:C:233:LYS:HG3	1:C:234:ASN:H	1.58	0.68
1:E:265:ASP:OD1	1:E:269:VAL:HB	1.94	0.68
1:A:228:HIS:HB3	1:A:229:PRO:HD2	1.75	0.68
1:C:287:GLY:O	1:C:299:TRP:HB2	1.94	0.68
1:E:203:ASN:O	1:E:206:GLN:HB3	1.93	0.68
1:E:305:TYR:CE1	1:E:307:LYS:HB2	2.28	0.68
1:A:50:GLU:HA	1:A:306:PHE:O	1.93	0.68
1:A:56:ARG:NH1	1:A:56:ARG:HB2	2.09	0.68
1:F:240:PHE:N	1:F:240:PHE:CD1	2.58	0.68
1:F:265:ASP:OD1	1:F:269:VAL:HB	1.94	0.68
1:A:304:ARG:HD3	1:A:306:PHE:CZ	2.29	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ASN:HD21	1:D:239:TYR:H	1.42	0.68
1:C:308:ILE:HD12	1:C:308:ILE:N	2.07	0.68
1:C:69:GLY:C	1:C:71:GLN:H	1.97	0.68
1:C:52:PHE:CD1	1:D:208:LEU:HD23	2.29	0.68
1:E:179:THR:O	1:E:206:GLN:HG3	1.94	0.68
1:E:75:TRP:CZ2	1:E:300:ARG:HD2	2.29	0.68
1:C:318:PRO:HB3	1:F:363:ASP:H	1.58	0.68
1:C:28:LEU:HD23	1:C:30:ILE:N	2.09	0.68
1:F:41:THR:HB	1:F:45:SER:OG	1.93	0.68
1:F:72:TYR:O	1:F:75:TRP:HB2	1.94	0.68
1:A:105:LEU:HB3	1:A:120:TRP:NE1	2.09	0.68
1:C:257:ASN:HD22	1:C:257:ASN:H	1.41	0.68
1:F:317:ASN:HD22	1:F:318:PRO:HD2	1.58	0.68
1:B:318:PRO:HG2	1:B:319:TYR:H	1.58	0.67
1:E:110:GLU:HA	1:E:110:GLU:OE1	1.94	0.67
1:F:105:LEU:HB2	1:F:276:GLU:O	1.93	0.67
1:C:293:ASN:OD1	1:C:294:TYR:HB2	1.94	0.67
1:E:112:LEU:HB3	1:E:116:THR:CG2	2.23	0.67
1:F:209:ASN:OD1	1:F:211:ILE:HD13	1.94	0.67
1:A:72:TYR:O	1:A:75:TRP:HB2	1.95	0.67
1:B:52:PHE:CD2	1:C:208:LEU:HD23	2.30	0.67
1:C:153:ILE:HD11	1:D:297:HIS:HB3	1.76	0.67
1:C:335:GLN:HA	1:C:335:GLN:OE1	1.91	0.67
1:A:69:GLY:HA3	1:A:71:GLN:NE2	2.10	0.67
1:C:105:LEU:HB3	1:C:120:TRP:CD1	2.29	0.67
1:D:211:ILE:HD12	1:D:211:ILE:N	2.09	0.67
1:E:317:ASN:HD22	1:E:318:PRO:HD2	1.58	0.67
1:C:193:ILE:CD1	1:C:201:MET:SD	2.83	0.67
1:C:168:GLY:CA	1:C:237:THR:HG23	2.22	0.67
1:D:233:LYS:HG3	1:D:234:ASN:N	2.10	0.67
1:C:350:GLU:HB3	1:F:233:LYS:HB3	1.75	0.67
1:F:269:VAL:HG12	1:F:270:GLY:O	1.94	0.67
1:E:46:VAL:HG12	1:E:47:THR:N	2.09	0.67
1:A:150:THR:HG21	1:A:292:ARG:HH21	1.59	0.67
1:A:192:THR:HG23	1:A:226:ILE:CD1	2.24	0.67
1:E:308:ILE:HD12	1:E:308:ILE:N	2.10	0.67
1:A:97:THR:HG22	1:A:223:PRO:CA	2.24	0.67
1:E:178:VAL:HG22	1:E:179:THR:H	1.58	0.67
1:F:125:VAL:HB	1:F:263:LEU:HD11	1.77	0.67
1:B:69:GLY:C	1:B:71:GLN:H	1.97	0.66
1:D:172:LEU:HD22	1:D:173:ASP:N	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:LEU:HD12	1:E:105:LEU:N	2.10	0.66
1:E:57:MET:CB	1:E:96:PRO:HA	2.25	0.66
1:F:336:VAL:HA	1:F:337:GLN:N	2.11	0.66
1:A:186:LYS:H	1:A:186:LYS:HD2	1.61	0.66
1:A:324:LEU:HA	1:A:327:SER:HB2	1.77	0.66
1:C:79:ILE:HB	1:C:297:HIS:O	1.94	0.66
1:E:255:PHE:O	1:E:256:THR:HB	1.94	0.66
1:B:313:ARG:HG2	1:B:314:TRP:N	2.10	0.66
1:C:135:LEU:N	1:C:135:LEU:HD22	2.10	0.66
1:C:123:VAL:HG13	1:C:264:LEU:HD13	1.77	0.66
1:F:288:TRP:HZ3	1:F:299:TRP:CD2	2.14	0.66
1:B:164:VAL:HG22	1:B:241:GLY:HA3	1.77	0.66
1:C:100:MET:C	1:C:100:MET:SD	2.73	0.66
1:D:207:VAL:HG23	1:D:208:LEU:N	2.10	0.66
1:E:308:ILE:CG2	1:E:310:LEU:HD23	2.25	0.66
1:D:208:LEU:O	1:D:210:PRO:HD3	1.95	0.66
1:D:145:THR:HG21	1:E:297:HIS:HE1	1.60	0.66
1:A:163:HIS:HA	1:A:283:VAL:O	1.96	0.66
1:E:194:LYS:H	1:E:194:LYS:HD3	1.59	0.66
1:F:55:PRO:HD3	1:F:303:PRO:CA	2.26	0.66
1:E:288:TRP:HZ3	1:E:299:TRP:CE2	2.13	0.66
1:F:108:LEU:HB3	1:F:118:GLN:NE2	2.09	0.66
1:F:288:TRP:CZ3	1:F:299:TRP:CD2	2.84	0.66
1:A:90:PRO:HG2	1:A:185:TYR:HA	1.78	0.66
1:B:124:SER:HA	1:B:261:THR:O	1.95	0.65
1:C:193:ILE:N	1:C:193:ILE:HD12	2.12	0.65
1:C:166:ALA:HA	1:C:238:ARG:O	1.97	0.65
1:D:114:CYS:HB2	1:D:116:THR:CG2	2.26	0.65
1:E:97:THR:HG22	1:E:222:TYR:O	1.95	0.65
1:F:192:THR:H	1:F:195:THR:CB	2.09	0.65
1:F:69:GLY:C	1:F:71:GLN:H	1.98	0.65
1:A:175:GLN:HB2	1:A:230:ASP:CB	2.16	0.65
1:B:125:VAL:HA	1:B:307:LYS:O	1.97	0.65
1:B:76:SER:O	1:B:298:HIS:HB2	1.96	0.65
1:D:164:VAL:HG22	1:D:241:GLY:HA3	1.78	0.65
1:C:352:ARG:NH2	1:F:233:LYS:O	2.29	0.65
1:A:150:THR:HG21	1:A:292:ARG:NH2	2.12	0.65
1:A:297:HIS:CE1	1:E:145:THR:HG21	2.27	0.65
1:E:125:VAL:HG13	1:E:125:VAL:O	1.96	0.65
1:F:144:PRO:HD3	1:F:292:ARG:HG2	1.76	0.65
1:A:336:VAL:HG23	1:A:337:GLN:N	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HD12	1:F:353:VAL:O	1.97	0.65
1:A:83:THR:HB	1:A:87:GLU:HG2	1.79	0.65
1:B:84:SER:O	1:B:86:THR:N	2.30	0.65
1:D:308:ILE:N	1:D:308:ILE:HD12	2.11	0.65
1:E:142:ASN:C	1:E:292:ARG:HB2	2.16	0.65
1:B:108:LEU:HD11	1:B:120:TRP:CE2	2.32	0.65
1:C:105:LEU:HB3	1:C:120:TRP:NE1	2.12	0.65
1:C:144:PRO:HD3	1:C:292:ARG:CG	2.27	0.65
1:D:79:ILE:HD11	1:D:299:TRP:CZ3	2.31	0.65
1:E:97:THR:HG22	1:E:222:TYR:C	2.17	0.65
1:F:286:MET:HA	1:F:286:MET:HE3	1.79	0.65
1:C:79:ILE:HD13	1:C:94:THR:HG23	1.79	0.65
1:D:97:THR:HG22	1:D:222:TYR:C	2.16	0.65
1:D:30:ILE:CD1	1:D:36:VAL:HG13	2.26	0.65
1:A:84:SER:HA	1:E:141:PHE:CD2	2.31	0.65
1:E:150:THR:O	1:E:150:THR:HG22	1.95	0.65
1:E:233:LYS:HD3	1:E:234:ASN:ND2	2.06	0.65
1:F:243:TYR:CZ	1:F:245:GLY:CA	2.80	0.65
1:B:71:GLN:CG	1:C:203:ASN:HB3	2.26	0.65
1:C:77:ARG:CB	1:C:93:ASN:HB2	2.27	0.65
1:D:233:LYS:HG3	1:D:234:ASN:H	1.61	0.65
1:F:265:ASP:H	1:F:270:GLY:H	1.43	0.65
1:A:257:ASN:HD22	1:B:239:TYR:H	1.45	0.65
1:A:306:PHE:HB3	1:A:308:ILE:CD1	2.27	0.65
1:A:350:GLU:CG	1:A:351:VAL:N	2.58	0.65
1:B:208:LEU:O	1:B:210:PRO:HD3	1.97	0.65
1:D:317:ASN:ND2	1:D:318:PRO:HD2	2.12	0.65
1:F:238:ARG:HH21	1:F:265:ASP:HB3	1.60	0.65
1:F:255:PHE:O	1:F:256:THR:HB	1.97	0.65
1:B:238:ARG:HH21	1:B:265:ASP:HB3	1.62	0.65
1:D:111:ASP:HB3	1:D:116:THR:CG2	2.26	0.65
1:D:193:ILE:N	1:D:193:ILE:HD12	2.11	0.65
1:D:265:ASP:OD1	1:D:269:VAL:HB	1.96	0.65
1:E:368:ARG:HA	1:E:376:THR:O	1.97	0.65
1:A:83:THR:HG22	1:A:87:GLU:HB3	1.79	0.64
1:D:193:ILE:H	1:D:193:ILE:HD12	1.62	0.64
1:E:222:TYR:HB3	1:E:227:TRP:CD1	2.32	0.64
1:F:103:LEU:HB2	1:F:278:LEU:HB3	1.79	0.64
1:A:105:LEU:HB3	1:A:106:PRO:HD2	1.79	0.64
1:B:275:GLY:O	1:B:277:GLY:N	2.29	0.64
1:B:324:LEU:O	1:B:328:LEU:HD23	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LYS:HD3	1:C:198:LYS:H	1.61	0.64
1:F:111:ASP:HB3	1:F:116:THR:CG2	2.27	0.64
1:F:319:TYR:HD1	1:F:320:PRO:HD2	1.61	0.64
1:A:246:GLY:HA3	1:A:249:THR:OG1	1.97	0.64
1:F:285:ILE:N	1:F:285:ILE:HD12	2.12	0.64
1:B:71:GLN:HE21	1:B:73:TYR:HB2	1.61	0.64
1:D:35:GLU:HG2	1:D:36:VAL:N	2.13	0.64
1:D:71:GLN:HA	1:D:71:GLN:NE2	2.06	0.64
1:A:328:LEU:HD11	1:A:333:LEU:CD2	2.26	0.64
1:A:336:VAL:CB	1:A:337:GLN:CA	2.75	0.64
1:C:193:ILE:O	1:C:196:ILE:HG23	1.98	0.64
1:D:106:PRO:HD2	1:D:120:TRP:HE1	1.61	0.64
1:E:54:ASN:HD22	1:E:55:PRO:HD2	1.62	0.64
1:A:233:LYS:HG3	1:A:234:ASN:N	2.12	0.64
1:B:177:LEU:HD22	1:B:207:VAL:C	2.18	0.64
1:C:193:ILE:HD11	1:C:201:MET:SD	2.38	0.64
1:C:97:THR:HG22	1:C:223:PRO:CA	2.27	0.64
1:E:233:LYS:HD2	1:E:234:ASN:H	1.62	0.64
1:E:90:PRO:HB2	1:E:186:LYS:HE3	1.79	0.64
1:F:90:PRO:HB2	1:F:95:LEU:HD11	1.79	0.64
1:B:262:VAL:HG12	1:B:264:LEU:HB2	1.79	0.64
1:C:286:MET:CE	1:C:286:MET:HA	2.28	0.64
1:C:84:SER:O	1:C:86:THR:N	2.30	0.64
1:D:55:PRO:HD3	1:D:303:PRO:HA	1.80	0.64
1:D:76:SER:HG	1:D:299:TRP:HE3	1.46	0.64
1:E:103:LEU:HB2	1:E:278:LEU:HB3	1.80	0.64
1:A:69:GLY:O	1:A:71:GLN:N	2.30	0.64
1:C:192:THR:HB	1:C:194:LYS:HD3	1.79	0.64
1:A:192:THR:HG21	1:A:194:LYS:HE2	1.79	0.64
1:B:259:LEU:N	1:B:259:LEU:HD22	2.13	0.64
1:B:324:LEU:H	1:B:324:LEU:HD22	1.62	0.64
1:C:103:LEU:HB2	1:C:278:LEU:HB3	1.78	0.64
1:C:193:ILE:HG12	1:C:201:MET:CE	2.28	0.64
1:D:233:LYS:CG	1:D:234:ASN:H	2.10	0.64
1:F:161:GLN:HE22	1:F:251:PRO:HA	1.63	0.64
1:A:105:LEU:HD12	1:A:105:LEU:N	2.13	0.63
1:A:380:PHE:CD1	1:A:381:PRO:HD2	2.33	0.63
1:B:177:LEU:HD13	1:B:207:VAL:O	1.98	0.63
1:C:211:ILE:N	1:C:211:ILE:HD12	2.12	0.63
1:D:258:THR:HB	1:D:259:LEU:CD2	2.29	0.63
1:D:335:GLN:NE2	1:D:335:GLN:HA	2.13	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:TYR:CZ	1:E:245:GLY:HA2	2.33	0.63
1:E:84:SER:O	1:E:86:THR:N	2.31	0.63
1:E:83:THR:CB	1:E:87:GLU:HB3	2.27	0.63
1:A:308:ILE:HG22	1:A:310:LEU:HD12	1.79	0.63
1:D:186:LYS:H	1:D:186:LYS:HD2	1.62	0.63
1:F:269:VAL:HA	1:F:313:ARG:NH2	2.13	0.63
1:A:179:THR:O	1:A:206:GLN:HG3	1.97	0.63
1:A:207:VAL:HG23	1:A:208:LEU:N	2.14	0.63
1:B:161:GLN:HE22	1:B:251:PRO:CA	2.11	0.63
1:B:257:ASN:HD21	1:C:239:TYR:H	1.44	0.63
1:D:170:GLU:HB2	1:D:171:PRO:HD2	1.80	0.63
1:E:115:ASP:HB3	1:E:317:ASN:H	1.62	0.63
1:F:182:ARG:HG3	1:F:183:THR:H	1.63	0.63
1:A:306:PHE:HB3	1:A:308:ILE:HD11	1.79	0.63
1:B:185:TYR:CD2	1:B:192:THR:HG21	2.32	0.63
1:B:100:MET:SD	1:B:101:ALA:N	2.71	0.63
1:D:55:PRO:HD3	1:D:303:PRO:CA	2.29	0.63
1:F:264:LEU:HD23	1:F:268:GLY:HA2	1.81	0.63
1:B:178:VAL:HG11	1:B:201:MET:HE1	1.79	0.63
1:D:239:TYR:C	1:D:240:PHE:CD1	2.72	0.63
1:B:186:LYS:HE2	1:B:186:LYS:N	2.13	0.63
1:E:169:GLY:HA3	1:E:272:LEU:O	1.99	0.63
1:F:108:LEU:HD11	1:F:120:TRP:CZ2	2.34	0.63
1:A:172:LEU:HD22	1:A:173:ASP:N	2.13	0.63
1:C:121:GLU:HG2	1:C:271:PRO:O	1.98	0.63
1:C:186:LYS:N	1:C:186:LYS:HE2	2.13	0.63
1:C:97:THR:HG22	1:C:223:PRO:HA	1.81	0.63
1:C:265:ASP:OD1	1:C:269:VAL:HB	1.99	0.63
1:A:257:ASN:HD21	1:B:238:ARG:HA	1.60	0.63
1:C:100:MET:SD	1:C:101:ALA:N	2.72	0.63
1:F:263:LEU:O	1:F:270:GLY:HA2	1.98	0.63
1:B:103:LEU:HD13	1:F:341:MET:HB3	1.81	0.63
1:B:269:VAL:HG12	1:B:270:GLY:O	1.98	0.62
1:C:240:PHE:CD1	1:C:240:PHE:N	2.66	0.62
1:D:313:ARG:HG2	1:D:314:TRP:H	1.63	0.62
1:A:304:ARG:HG2	1:A:306:PHE:CE1	2.33	0.62
1:D:268:GLY:O	1:D:313:ARG:NH2	2.32	0.62
1:A:288:TRP:CE3	1:A:299:TRP:HB3	2.34	0.62
1:A:336:VAL:CG2	1:A:337:GLN:CA	2.70	0.62
1:C:115:ASP:CG	1:C:116:THR:H	2.03	0.62
1:C:341:MET:SD	1:C:348:VAL:HG23	2.40	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:153:ILE:HD11	1:C:297:HIS:HB2	1.82	0.62
1:D:78:GLY:CA	1:D:298:HIS:HB3	2.29	0.62
1:D:313:ARG:HG2	1:D:314:TRP:N	2.14	0.62
1:E:130:VAL:O	1:E:302:LEU:HD22	1.99	0.62
1:E:66:LEU:HB3	1:E:71:GLN:HB2	1.81	0.62
1:F:269:VAL:HA	1:F:313:ARG:HH21	1.65	0.62
1:F:81:LEU:HD23	1:F:82:ALA:O	2.00	0.62
1:A:131:GLY:O	1:A:134:SER:HB3	1.99	0.62
1:A:97:THR:HA	1:A:223:PRO:HA	1.79	0.62
1:A:288:TRP:HB3	1:A:297:HIS:O	1.99	0.62
1:D:76:SER:OG	1:D:299:TRP:CE3	2.52	0.62
1:F:81:LEU:HG	1:F:82:ALA:H	1.64	0.62
1:B:52:PHE:CZ	1:F:347:GLN:HB3	2.35	0.62
1:D:57:MET:O	1:D:57:MET:HG3	2.00	0.62
1:E:142:ASN:O	1:E:292:ARG:HB2	2.00	0.62
1:F:233:LYS:HD3	1:F:234:ASN:H	1.63	0.62
1:A:175:GLN:HG2	1:A:212:SER:O	2.00	0.62
1:B:185:TYR:HA	1:B:186:LYS:HE2	1.82	0.62
1:E:240:PHE:N	1:E:240:PHE:CD1	2.64	0.62
1:A:164:VAL:HA	1:A:241:GLY:HA3	1.81	0.62
1:A:371:ASP:O	1:A:373:PHE:N	2.33	0.62
1:D:272:LEU:HD12	1:D:272:LEU:N	2.15	0.62
1:E:162:TYR:CE1	1:E:283:VAL:HG21	2.35	0.62
1:E:304:ARG:HD3	1:E:306:PHE:CZ	2.34	0.62
1:A:203:ASN:HD22	1:E:71:GLN:HE21	1.46	0.62
1:E:77:ARG:O	1:E:298:HIS:CG	2.52	0.62
1:F:317:ASN:HD22	1:F:318:PRO:CD	2.13	0.62
1:F:90:PRO:CB	1:F:95:LEU:HD11	2.30	0.62
1:B:185:TYR:HB2	1:B:194:LYS:HE3	1.82	0.62
1:D:179:THR:O	1:D:206:GLN:HG3	2.00	0.62
1:A:175:GLN:HG3	1:A:213:LYS:CE	2.30	0.62
1:F:125:VAL:O	1:F:125:VAL:HG13	2.00	0.62
1:F:232:ALA:HB3	1:F:234:ASN:O	1.99	0.62
1:A:130:VAL:HG23	1:A:303:PRO:HG2	1.82	0.61
1:B:117:LEU:HD12	1:B:117:LEU:H	1.63	0.61
1:D:217:ASP:OD1	1:D:218:LYS:HD3	1.99	0.61
1:A:216:LEU:HD23	1:A:222:TYR:CD1	2.35	0.61
1:A:77:ARG:O	1:A:298:HIS:CG	2.53	0.61
1:E:366:MET:HG2	1:E:367:THR:N	2.15	0.61
1:B:56:ARG:HE	1:F:339:GLN:NE2	1.97	0.61
1:A:328:LEU:HD11	1:A:333:LEU:HD23	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ASP:OD2	1:C:182:ARG:HD3	2.00	0.61
1:E:193:ILE:HG12	1:E:201:MET:CE	2.30	0.61
1:E:285:ILE:N	1:E:285:ILE:HD12	2.14	0.61
1:E:308:ILE:HG22	1:E:310:LEU:HD23	1.80	0.61
1:A:233:LYS:HA	1:E:50:GLU:HG2	1.82	0.61
1:F:19:CYS:HB3	1:F:20:PRO:CD	2.31	0.61
1:A:121:GLU:O	1:A:310:LEU:HB2	1.99	0.61
1:B:165:PHE:CZ	1:B:240:PHE:CE1	2.88	0.61
1:B:262:VAL:CG1	1:B:264:LEU:HB2	2.30	0.61
1:B:35:GLU:O	1:B:38:ASP:HB2	2.00	0.61
1:D:43:PRO:O	1:D:312:LYS:HB2	2.00	0.61
1:D:76:SER:OG	1:D:299:TRP:HE3	1.84	0.61
1:A:135:LEU:HD12	1:A:135:LEU:H	1.66	0.61
1:A:193:ILE:O	1:A:196:ILE:HG23	2.01	0.61
1:D:66:LEU:HD12	1:E:182:ARG:HB3	1.83	0.61
1:B:101:ALA:HB2	1:F:339:GLN:HB2	1.81	0.61
1:B:203:ASN:O	1:B:206:GLN:HB3	2.00	0.61
1:C:251:PRO:HD2	1:D:245:GLY:HA3	1.83	0.61
1:E:136:LEU:O	1:E:138:VAL:HG22	2.01	0.61
1:E:318:PRO:HG2	1:E:319:TYR:CD2	2.36	0.61
1:B:177:LEU:CD2	1:B:208:LEU:HA	2.31	0.61
1:B:186:LYS:HE2	1:B:186:LYS:H	1.66	0.61
1:C:256:THR:HB	1:D:240:PHE:HA	1.82	0.61
1:C:304:ARG:HD3	1:C:306:PHE:CZ	2.36	0.61
1:D:54:ASN:HD21	1:E:208:LEU:CB	2.14	0.61
1:E:218:LYS:N	1:E:218:LYS:HD2	2.16	0.61
1:A:336:VAL:HB	1:A:337:GLN:CA	2.31	0.61
1:C:300:ARG:HH11	1:C:300:ARG:HG3	1.65	0.61
1:C:118:GLN:HB3	1:C:314:TRP:CE3	2.36	0.61
1:A:288:TRP:HE3	1:A:299:TRP:HB3	1.65	0.61
1:D:253:LEU:HD23	1:D:254:GLN:N	2.16	0.61
1:B:103:LEU:CD2	1:F:341:MET:HG3	2.30	0.61
1:A:233:LYS:HG3	1:A:234:ASN:ND2	2.15	0.61
1:B:22:PRO:HG2	1:F:359:PRO:CB	2.31	0.61
1:C:170:GLU:HB2	1:C:171:PRO:HD2	1.83	0.61
1:C:341:MET:CE	1:C:347:GLN:HB2	2.30	0.61
1:D:178:VAL:CG2	1:D:179:THR:H	2.14	0.61
1:D:306:PHE:HB3	1:D:308:ILE:HD11	1.83	0.61
1:A:84:SER:HB3	1:A:86:THR:HG22	1.83	0.60
1:D:232:ALA:HB3	1:D:235:GLU:OE1	2.01	0.60
1:E:170:GLU:CD	1:E:274:LYS:HD2	2.22	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:324:LEU:HD12	1:F:325:ILE:N	2.16	0.60
1:A:141:PHE:HD2	1:B:84:SER:HA	1.63	0.60
1:D:203:ASN:O	1:D:206:GLN:HB3	2.01	0.60
1:F:104:GLN:NE2	1:F:105:LEU:N	2.49	0.60
1:B:25:VAL:HG21	1:F:360:VAL:HG13	1.81	0.60
1:A:240:PHE:CD1	1:A:240:PHE:N	2.65	0.60
1:B:46:VAL:HG12	1:B:47:THR:H	1.66	0.60
1:D:84:SER:O	1:D:86:THR:N	2.34	0.60
1:E:55:PRO:HD3	1:E:303:PRO:HB3	1.82	0.60
1:E:333:LEU:HD22	1:E:333:LEU:H	1.66	0.60
1:F:211:ILE:N	1:F:211:ILE:HD12	2.16	0.60
1:F:94:THR:O	1:F:95:LEU:HD23	2.01	0.60
1:A:251:PRO:HG2	1:B:243:TYR:HE2	1.66	0.60
1:A:35:GLU:HG2	1:A:36:VAL:N	2.15	0.60
1:B:30:ILE:HG12	1:B:31:LYS:N	2.17	0.60
1:B:346:THR:HG21	1:B:348:VAL:CG1	2.31	0.60
1:C:207:VAL:HG23	1:C:208:LEU:N	2.15	0.60
1:C:79:ILE:HD11	1:C:299:TRP:CZ3	2.37	0.60
1:D:91:GLY:N	1:D:186:LYS:HZ1	1.99	0.60
1:D:168:GLY:CA	1:D:237:THR:HG23	2.28	0.60
1:E:79:ILE:HD11	1:E:299:TRP:CZ3	2.36	0.60
1:F:291:THR:OG1	1:F:296:VAL:HB	2.01	0.60
1:C:111:ASP:CG	1:C:114:CYS:HB3	2.21	0.60
1:C:192:THR:O	1:C:196:ILE:HG22	2.02	0.60
1:D:192:THR:O	1:D:196:ILE:HG22	2.00	0.60
1:D:265:ASP:CG	1:D:269:VAL:HB	2.21	0.60
1:E:207:VAL:HG23	1:E:208:LEU:N	2.16	0.60
1:A:257:ASN:HB2	1:B:239:TYR:CZ	2.36	0.60
1:B:269:VAL:HA	1:B:313:ARG:NH2	2.16	0.60
1:C:105:LEU:N	1:C:105:LEU:HD12	2.16	0.60
1:D:133:GLY:CA	1:E:228:HIS:HE1	2.13	0.60
1:F:19:CYS:HB3	1:F:20:PRO:HD2	1.82	0.60
1:F:317:ASN:ND2	1:F:319:TYR:H	1.99	0.60
1:E:313:ARG:CG	1:E:313:ARG:HH11	2.14	0.60
1:F:233:LYS:HD3	1:F:234:ASN:HB2	1.83	0.60
1:F:125:VAL:HG11	1:F:263:LEU:HD21	1.82	0.60
1:E:370:VAL:HG22	1:E:375:LYS:CB	2.32	0.60
1:F:205:ASP:HA	1:F:209:ASN:HB2	1.84	0.60
1:B:240:PHE:N	1:B:240:PHE:CD1	2.68	0.60
1:B:341:MET:CE	1:B:348:VAL:HB	2.31	0.60
1:C:111:ASP:OD2	1:C:114:CYS:HB3	2.02	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:SER:HA	1:C:135:LEU:HD23	1.83	0.60
1:C:152:GLY:HA2	1:D:295:ASP:HB3	1.83	0.60
1:C:194:LYS:H	1:C:194:LYS:HD3	1.65	0.60
1:C:194:LYS:HG2	1:C:195:THR:H	1.66	0.60
1:D:193:ILE:CD1	1:D:194:LYS:HD3	2.32	0.60
1:C:118:GLN:HB3	1:C:314:TRP:CZ3	2.37	0.60
1:C:265:ASP:H	1:C:270:GLY:H	1.50	0.60
1:F:285:ILE:H	1:F:285:ILE:HD12	1.65	0.60
1:A:251:PRO:HG2	1:B:245:GLY:HA3	1.84	0.59
1:B:257:ASN:ND2	1:C:239:TYR:H	2.00	0.59
1:C:265:ASP:HB3	1:C:270:GLY:H	1.66	0.59
1:A:153:ILE:HG12	1:B:297:HIS:ND1	2.17	0.59
1:A:336:VAL:HB	1:A:338:GLY:H	1.67	0.59
1:B:207:VAL:HG23	1:B:208:LEU:H	1.67	0.59
1:B:251:PRO:HD2	1:C:245:GLY:CA	2.32	0.59
1:D:348:VAL:HG12	1:D:348:VAL:O	2.02	0.59
1:A:328:LEU:CD1	1:A:333:LEU:HD21	2.32	0.59
1:A:336:VAL:HB	1:A:337:GLN:HA	1.84	0.59
1:C:197:THR:O	1:C:199:LYS:N	2.35	0.59
1:C:142:ASN:O	1:C:292:ARG:HB2	2.01	0.59
1:C:346:THR:HG22	1:C:348:VAL:CB	2.27	0.59
1:C:57:MET:HB3	1:C:96:PRO:HB3	1.84	0.59
1:D:193:ILE:HD12	1:D:194:LYS:HD3	1.83	0.59
1:D:30:ILE:HD12	1:D:39:LEU:HD23	1.84	0.59
1:F:288:TRP:CZ3	1:F:299:TRP:CE3	2.89	0.59
1:F:288:TRP:HE3	1:F:299:TRP:CB	2.15	0.59
1:F:55:PRO:HD3	1:F:303:PRO:HA	1.83	0.59
1:A:25:VAL:HG13	1:A:26:PRO:HD2	1.84	0.59
1:A:142:ASN:O	1:A:292:ARG:HB2	2.01	0.59
1:A:69:GLY:C	1:A:71:GLN:N	2.55	0.59
1:B:59:GLN:HE21	1:B:71:GLN:HE22	1.47	0.59
1:C:125:VAL:HA	1:C:307:LYS:O	2.02	0.59
1:E:193:ILE:O	1:E:196:ILE:HG23	2.01	0.59
1:E:278:LEU:HD22	1:E:279:TYR:N	2.17	0.59
1:E:306:PHE:HB3	1:E:308:ILE:CD1	2.32	0.59
1:F:263:LEU:HB3	1:F:271:PRO:HD3	1.85	0.59
1:F:50:GLU:HA	1:F:306:PHE:O	2.00	0.59
1:B:135:LEU:CD1	1:B:135:LEU:N	2.64	0.59
1:E:35:GLU:HG2	1:E:36:VAL:N	2.16	0.59
1:E:88:ASP:O	1:E:184:LYS:HB2	2.03	0.59
1:D:47:THR:O	1:D:310:LEU:HD12	2.03	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:HD21	1:E:209:ASN:N	2.15	0.59
1:F:192:THR:HB	1:F:194:LYS:HD3	1.84	0.59
1:A:82:ALA:HB1	1:A:88:ASP:HA	1.85	0.59
1:C:285:ILE:N	1:C:285:ILE:HD12	2.17	0.59
1:D:62:THR:OG1	1:D:63:PRO:HD3	2.03	0.59
1:A:295:ASP:HB3	1:E:152:GLY:HA2	1.84	0.59
1:F:300:ARG:HG3	1:F:301:GLY:N	2.18	0.59
1:B:238:ARG:NH2	1:B:265:ASP:HB3	2.18	0.59
1:E:306:PHE:HB3	1:E:308:ILE:HD11	1.84	0.59
1:B:108:LEU:HB3	1:B:118:GLN:HE21	1.67	0.59
1:B:339:GLN:NE2	1:B:347:GLN:NE2	2.51	0.59
1:C:117:LEU:HD13	1:C:118:GLN:N	2.17	0.59
1:F:197:THR:HG23	1:F:197:THR:O	2.02	0.59
1:A:369:TYR:N	1:A:369:TYR:CD1	2.71	0.59
1:B:75:TRP:NE1	1:B:300:ARG:HB2	2.18	0.59
1:E:238:ARG:NH2	1:E:265:ASP:HB3	2.17	0.59
1:E:367:THR:CG2	1:E:368:ARG:N	2.66	0.59
1:E:57:MET:HB2	1:E:96:PRO:HB3	1.85	0.59
1:F:186:LYS:CD	1:F:186:LYS:H	2.16	0.59
1:A:296:VAL:HG11	2:G:3:SIA:H32	1.83	0.59
1:A:233:LYS:HG3	1:A:234:ASN:H	1.68	0.58
1:A:300:ARG:HG3	1:A:301:GLY:N	2.17	0.58
1:A:122:ALA:HA	1:A:310:LEU:HB3	1.85	0.58
1:A:43:PRO:HA	1:A:312:LYS:HD2	1.85	0.58
1:B:222:TYR:H	1:B:222:TYR:HD1	1.50	0.58
1:C:145:THR:HG21	1:D:297:HIS:HE1	1.68	0.58
1:C:285:ILE:H	1:C:285:ILE:HD12	1.68	0.58
1:C:57:MET:HA	1:C:96:PRO:HA	1.83	0.58
1:D:125:VAL:HB	1:D:263:LEU:HD11	1.85	0.58
1:E:228:HIS:HB3	1:E:229:PRO:HD2	1.84	0.58
1:E:66:LEU:CD2	1:E:66:LEU:H	2.12	0.58
1:F:80:ASN:HB3	1:F:90:PRO:O	2.02	0.58
1:A:211:ILE:O	1:A:213:LYS:N	2.36	0.58
1:B:43:PRO:HA	1:B:312:LYS:HD2	1.85	0.58
1:C:69:GLY:O	1:C:71:GLN:N	2.36	0.58
1:D:52:PHE:CE1	1:E:208:LEU:HD22	2.38	0.58
1:E:150:THR:HG21	1:E:292:ARG:HH21	1.67	0.58
1:E:368:ARG:NH2	1:E:377:LYS:HE3	2.18	0.58
1:F:62:THR:OG1	1:F:63:PRO:HD3	2.04	0.58
1:A:80:ASN:HB3	1:A:90:PRO:O	2.03	0.58
1:F:90:PRO:HD2	1:F:186:LYS:HE3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ASN:HD21	1:A:289:ARG:HG3	1.68	0.58
1:A:79:ILE:HG21	1:E:153:ILE:CD1	2.34	0.58
1:E:28:LEU:HG	1:E:29:LEU:N	2.19	0.58
1:F:201:MET:HA	1:F:201:MET:CE	2.33	0.58
1:B:165:PHE:CZ	1:B:240:PHE:HE1	2.21	0.58
1:B:306:PHE:HB3	1:B:308:ILE:HD11	1.84	0.58
1:B:34:MET:O	1:B:37:LEU:HB2	2.04	0.58
1:C:207:VAL:HG23	1:C:208:LEU:H	1.69	0.58
1:D:106:PRO:HD2	1:D:120:TRP:NE1	2.17	0.58
1:D:50:GLU:OE2	1:E:233:LYS:HA	2.03	0.58
1:E:166:ALA:HA	1:E:238:ARG:O	2.03	0.58
1:A:313:ARG:NH1	1:E:23:ALA:HB1	2.19	0.58
1:E:60:PRO:HB2	1:E:61:PRO:HD2	1.84	0.58
1:F:208:LEU:HD23	1:F:208:LEU:O	2.04	0.58
1:A:106:PRO:HD2	1:A:120:TRP:HE1	1.69	0.58
1:A:175:GLN:HA	1:A:213:LYS:HA	1.85	0.58
1:B:205:ASP:CA	1:B:209:ASN:HB2	2.30	0.58
1:B:358:GLU:HG3	1:B:359:PRO:O	2.03	0.58
1:C:178:VAL:HG22	1:C:179:THR:N	2.18	0.58
1:D:108:LEU:HB3	1:D:118:GLN:HE21	1.68	0.58
1:F:252:VAL:O	1:F:253:LEU:HD12	2.04	0.58
1:A:135:LEU:CD1	1:A:135:LEU:H	2.17	0.58
1:A:135:LEU:N	1:A:135:LEU:CD1	2.66	0.58
1:B:25:VAL:HG12	1:B:26:PRO:HD2	1.86	0.58
1:D:339:GLN:HG2	1:D:340:PRO:HD2	1.85	0.58
1:F:122:ALA:HA	1:F:310:LEU:HB3	1.85	0.58
1:F:69:GLY:O	1:F:71:GLN:N	2.37	0.58
1:A:129:VAL:HB	1:A:253:LEU:HD21	1.84	0.58
1:A:150:THR:HG22	1:A:150:THR:O	2.02	0.58
1:B:177:LEU:CD2	1:B:205:ASP:O	2.51	0.58
1:B:310:LEU:H	1:B:310:LEU:HD12	1.69	0.58
1:C:233:LYS:HG3	1:C:234:ASN:N	2.19	0.58
1:E:315:VAL:HG12	1:E:316:LYS:H	1.67	0.58
1:E:296:VAL:HG11	2:K:3:SIA:H32	1.86	0.58
1:E:92:ASN:OD1	1:E:186:LYS:HD2	2.04	0.58
1:E:208:LEU:HD23	1:E:210:PRO:HG3	1.86	0.58
1:E:150:THR:HG21	1:E:292:ARG:NH2	2.19	0.58
1:A:205:ASP:HA	1:A:209:ASN:CB	2.29	0.58
1:B:162:TYR:CE1	1:B:224:VAL:HG11	2.39	0.58
1:C:202:VAL:HG12	1:C:203:ASN:OD1	2.04	0.58
1:C:50:GLU:HG2	1:C:307:LYS:HG3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:125:VAL:HA	1:E:307:LYS:O	2.04	0.58
1:E:35:GLU:HG2	1:E:36:VAL:H	1.69	0.58
1:E:90:PRO:HB3	1:E:95:LEU:HD11	1.86	0.58
1:F:100:MET:SD	1:F:101:ALA:N	2.77	0.58
1:F:150:THR:HG21	1:F:292:ARG:NH2	2.19	0.58
1:A:30:ILE:CG1	1:A:36:VAL:HG13	2.33	0.57
1:B:69:GLY:O	1:B:71:GLN:N	2.37	0.57
1:C:191:VAL:HG21	1:C:222:TYR:CD2	2.39	0.57
1:D:233:LYS:CG	1:D:234:ASN:N	2.66	0.57
1:D:341:MET:HE2	1:D:347:GLN:HB2	1.86	0.57
1:A:257:ASN:HD22	1:B:238:ARG:HA	1.65	0.57
1:A:34:MET:O	1:A:37:LEU:HD13	2.04	0.57
1:B:261:THR:HG22	1:B:262:VAL:N	2.19	0.57
1:B:342:GLU:N	1:B:346:THR:HG23	2.19	0.57
1:D:177:LEU:CD1	1:D:177:LEU:N	2.68	0.57
1:D:32:GLY:CA	1:D:36:VAL:HG21	2.34	0.57
1:E:61:PRO:HG2	1:E:62:THR:H	1.68	0.57
1:F:287:GLY:O	1:F:299:TRP:HB2	2.03	0.57
1:A:293:ASN:OD1	1:A:294:TYR:N	2.38	0.57
1:B:48:GLU:O	1:F:351:VAL:HA	2.03	0.57
1:C:222:TYR:HB3	1:C:227:TRP:CD1	2.40	0.57
1:C:341:MET:C	1:C:346:THR:HG23	2.25	0.57
1:D:100:MET:C	1:D:100:MET:SD	2.83	0.57
1:E:317:ASN:ND2	1:E:318:PRO:HD2	2.17	0.57
1:E:58:GLY:HA3	1:E:76:SER:HA	1.84	0.57
1:A:175:GLN:HG3	1:A:213:LYS:CD	2.34	0.57
1:B:105:LEU:N	1:B:105:LEU:HD12	2.18	0.57
1:A:251:PRO:HG2	1:B:243:TYR:CE2	2.39	0.57
1:C:263:LEU:O	1:C:270:GLY:HA2	2.04	0.57
1:A:166:ALA:HB2	1:A:239:TYR:CB	2.34	0.57
1:B:111:ASP:OD2	1:B:114:CYS:SG	2.62	0.57
1:B:209:ASN:OD1	1:B:211:ILE:HD13	2.04	0.57
1:B:222:TYR:N	1:B:222:TYR:CD1	2.72	0.57
1:B:371:ASP:O	1:B:373:PHE:N	2.37	0.57
1:D:150:THR:HG21	1:D:292:ARG:HH21	1.68	0.57
1:E:256:THR:OG1	1:E:257:ASN:N	2.37	0.57
1:F:204:LYS:NZ	1:F:204:LYS:HB3	2.18	0.57
1:F:57:MET:SD	1:F:301:GLY:HA3	2.44	0.57
1:B:164:VAL:HA	1:B:241:GLY:HA3	1.87	0.57
1:B:300:ARG:HG3	1:B:301:GLY:N	2.18	0.57
1:B:72:TYR:O	1:B:75:TRP:HB2	2.03	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:100:MET:SD	1:D:101:ALA:N	2.78	0.57
1:E:298:HIS:CD2	1:E:298:HIS:H	2.22	0.57
1:F:339:GLN:HG2	1:F:340:PRO:HD2	1.85	0.57
1:B:76:SER:OG	1:B:299:TRP:CE3	2.58	0.57
1:D:131:GLY:O	1:D:134:SER:HB3	2.05	0.57
1:A:293:ASN:OD1	1:A:294:TYR:HB2	2.05	0.57
1:A:350:GLU:HG3	1:A:351:VAL:H	1.69	0.57
1:A:378:THR:HG22	1:A:379:VAL:O	2.05	0.57
1:B:46:VAL:HG12	1:B:47:THR:N	2.19	0.57
1:E:288:TRP:CZ3	1:E:299:TRP:CE2	2.92	0.57
1:A:174:LEU:HA	1:A:230:ASP:H	1.70	0.57
1:A:263:LEU:O	1:A:270:GLY:HA2	2.04	0.57
1:C:190:VAL:HG23	1:C:221:MET:O	2.04	0.57
1:C:25:VAL:CG1	1:C:26:PRO:HD2	2.35	0.57
1:E:177:LEU:CD1	1:E:207:VAL:O	2.42	0.57
1:C:177:LEU:HD23	1:C:177:LEU:N	2.20	0.57
1:C:76:SER:OG	1:C:299:TRP:CE3	2.52	0.57
1:C:55:PRO:HD3	1:C:303:PRO:HA	1.86	0.57
1:C:363:ASP:HB3	1:C:366:MET:CE	2.35	0.57
1:E:354:TYR:N	1:E:354:TYR:CD1	2.73	0.57
1:A:243:TYR:CZ	1:A:245:GLY:HA2	2.39	0.56
1:B:166:ALA:HA	1:B:238:ARG:O	2.06	0.56
1:D:219:ASP:O	1:D:221:MET:HB2	2.05	0.56
1:E:39:LEU:HD12	1:E:39:LEU:O	2.05	0.56
1:A:232:ALA:HB3	1:A:234:ASN:O	2.05	0.56
1:A:261:THR:HG22	1:A:262:VAL:N	2.19	0.56
1:A:265:ASP:H	1:A:270:GLY:H	1.51	0.56
1:A:319:TYR:N	1:A:320:PRO:HD2	2.20	0.56
1:B:194:LYS:HG3	1:B:195:THR:H	1.71	0.56
1:C:193:ILE:O	1:C:197:THR:HG22	2.05	0.56
1:C:198:LYS:HD3	1:C:198:LYS:N	2.17	0.56
1:C:210:PRO:HA	1:C:213:LYS:HE2	1.87	0.56
1:C:246:GLY:HA3	1:C:249:THR:OG1	2.06	0.56
1:C:318:PRO:O	1:C:320:PRO:HD3	2.05	0.56
1:E:113:THR:C	1:E:115:ASP:H	2.08	0.56
1:E:34:MET:O	1:E:37:LEU:HD22	2.06	0.56
1:F:130:VAL:HG23	1:F:303:PRO:HG2	1.86	0.56
1:A:323:SER:O	1:A:327:SER:HB2	2.05	0.56
1:B:122:ALA:HB3	1:B:271:PRO:HD2	1.87	0.56
1:C:186:LYS:HE2	1:C:186:LYS:H	1.69	0.56
1:C:55:PRO:HD3	1:C:303:PRO:CA	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:77:ARG:CB	1:E:93:ASN:HB2	2.36	0.56
1:A:169:GLY:HA3	1:A:272:LEU:O	2.05	0.56
1:B:265:ASP:H	1:B:270:GLY:H	1.53	0.56
1:B:323:SER:O	1:B:327:SER:N	2.38	0.56
1:D:105:LEU:HD12	1:D:105:LEU:N	2.21	0.56
1:E:88:ASP:H	1:E:184:LYS:HD3	1.70	0.56
1:F:57:MET:HA	1:F:96:PRO:HA	1.87	0.56
1:A:20:PRO:HG2	1:B:116:THR:HG21	1.87	0.56
1:B:166:ALA:HB2	1:B:239:TYR:HB3	1.88	0.56
1:B:288:TRP:CZ3	1:B:299:TRP:CE2	2.91	0.56
1:B:50:GLU:HA	1:B:306:PHE:O	2.06	0.56
1:B:153:ILE:HG12	1:C:297:HIS:CE1	2.40	0.56
1:C:350:GLU:CD	1:C:351:VAL:H	2.09	0.56
1:D:219:ASP:O	1:D:221:MET:N	2.39	0.56
1:E:243:TYR:OH	1:E:245:GLY:HA2	2.05	0.56
1:F:186:LYS:H	1:F:186:LYS:HD2	1.71	0.56
1:F:192:THR:HG22	1:F:193:ILE:CD1	2.35	0.56
1:F:96:PRO:HG3	1:F:299:TRP:CZ2	2.40	0.56
1:A:192:THR:HG23	1:A:226:ILE:HD13	1.87	0.56
1:B:286:MET:HE3	1:B:286:MET:HA	1.87	0.56
1:D:98:TRP:HH2	1:D:164:VAL:CG1	2.18	0.56
1:E:194:LYS:HA	1:E:197:THR:O	2.06	0.56
1:C:97:THR:HA	1:C:223:PRO:HA	1.88	0.56
1:E:90:PRO:HD2	1:E:186:LYS:CE	2.35	0.56
1:D:133:GLY:H	1:E:228:HIS:HE1	1.52	0.56
1:E:291:THR:OG1	1:E:296:VAL:HB	2.06	0.56
1:E:46:VAL:HG12	1:E:47:THR:H	1.69	0.56
1:B:150:THR:HG22	1:B:150:THR:O	2.04	0.56
1:F:300:ARG:CG	1:F:301:GLY:N	2.68	0.56
1:B:175:GLN:HE21	1:B:176:GLY:N	2.04	0.56
1:B:66:LEU:HD23	1:B:66:LEU:N	2.20	0.56
1:B:256:THR:HA	1:C:239:TYR:CE1	2.41	0.56
1:C:360:VAL:HG12	1:C:361:PRO:HD2	1.87	0.56
1:F:233:LYS:HD3	1:F:234:ASN:CB	2.36	0.56
1:C:34:MET:O	1:C:37:LEU:HB2	2.06	0.56
1:F:308:ILE:HD12	1:F:308:ILE:H	1.67	0.56
1:C:144:PRO:HD3	1:C:292:ARG:HG3	1.87	0.56
1:D:164:VAL:CG2	1:D:241:GLY:HA3	2.35	0.56
1:E:90:PRO:HD2	1:E:186:LYS:HZ1	1.70	0.56
1:F:194:LYS:H	1:F:194:LYS:CD	2.19	0.56
1:A:336:VAL:HB	1:A:338:GLY:N	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:THR:CG2	1:A:87:GLU:HB3	2.36	0.55
1:B:258:THR:HB	1:B:259:LEU:CD2	2.36	0.55
1:C:192:THR:OG1	1:C:194:LYS:HE3	2.06	0.55
1:C:346:THR:C	1:C:348:VAL:H	2.08	0.55
1:F:19:CYS:CB	1:F:20:PRO:HD2	2.36	0.55
1:F:259:LEU:N	1:F:259:LEU:CD1	2.70	0.55
1:F:262:VAL:CG1	1:F:264:LEU:HB2	2.36	0.55
1:A:328:LEU:HD21	1:A:333:LEU:HD21	0.62	0.55
1:A:339:GLN:HG2	1:A:347:GLN:NE2	2.21	0.55
1:A:370:VAL:HG22	1:A:375:LYS:HE2	1.89	0.55
1:A:372:ARG:HB3	1:A:373:PHE:CE1	2.40	0.55
1:A:61:PRO:HG2	1:A:62:THR:H	1.71	0.55
1:B:257:ASN:ND2	1:C:239:TYR:O	2.39	0.55
1:C:90:PRO:HD2	1:C:186:LYS:CE	2.36	0.55
1:E:82:ALA:HB1	1:E:88:ASP:HA	1.88	0.55
1:B:370:VAL:HA	1:B:375:LYS:HA	1.89	0.55
1:B:69:GLY:C	1:B:71:GLN:N	2.60	0.55
1:C:322:ALA:HA	1:C:325:ILE:HG22	1.88	0.55
1:E:138:VAL:HG12	1:E:153:ILE:CG2	2.36	0.55
1:F:185:TYR:HB2	1:F:194:LYS:CE	2.36	0.55
1:F:164:VAL:HG22	1:F:241:GLY:HA3	1.86	0.55
1:F:62:THR:O	1:F:64:GLU:N	2.39	0.55
1:A:116:THR:HA	1:A:315:VAL:O	2.06	0.55
1:A:239:TYR:C	1:A:240:PHE:CG	2.80	0.55
1:A:161:GLN:NE2	1:A:251:PRO:HA	2.20	0.55
1:B:78:GLY:O	1:B:79:ILE:HD13	2.07	0.55
1:C:28:LEU:CD2	1:C:30:ILE:N	2.69	0.55
1:D:306:PHE:HB3	1:D:308:ILE:CD1	2.37	0.55
1:E:60:PRO:CB	1:E:61:PRO:HD2	2.35	0.55
1:A:254:GLN:HA	1:A:254:GLN:OE1	2.06	0.55
1:B:273:CYS:HB3	1:B:277:GLY:O	2.05	0.55
1:B:328:LEU:C	1:B:332:MET:SD	2.84	0.55
1:B:54:ASN:HD22	1:B:55:PRO:HD2	1.71	0.55
1:C:288:TRP:HB2	1:C:297:HIS:HB3	1.88	0.55
1:D:340:PRO:HG2	1:D:347:GLN:HG3	1.88	0.55
1:F:66:LEU:HD23	1:F:66:LEU:N	2.22	0.55
1:A:121:GLU:HG3	1:A:272:LEU:CD2	2.37	0.55
1:B:100:MET:C	1:B:100:MET:SD	2.85	0.55
1:B:176:GLY:O	1:B:177:LEU:HD23	2.07	0.55
1:D:253:LEU:HD23	1:D:254:GLN:H	1.71	0.55
1:E:125:VAL:CG1	1:E:263:LEU:HD21	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:GLN:NE2	1:E:251:PRO:HA	2.21	0.55
1:F:125:VAL:CG1	1:F:263:LEU:HD21	2.36	0.55
1:F:161:GLN:HE22	1:F:251:PRO:CA	2.19	0.55
1:C:152:GLY:HA2	1:D:295:ASP:CB	2.36	0.55
1:C:186:LYS:H	1:C:186:LYS:CD	2.20	0.55
1:C:197:THR:O	1:C:197:THR:CG2	2.54	0.55
1:D:149:ASN:O	1:D:151:LYS:HE2	2.06	0.55
1:D:304:ARG:HG2	1:D:306:PHE:CE1	2.41	0.55
1:E:121:GLU:HG3	1:E:313:ARG:HD2	1.89	0.55
1:A:193:ILE:HG12	1:A:201:MET:CE	2.37	0.55
1:A:317:ASN:ND2	1:A:320:PRO:HD3	2.21	0.55
1:C:30:ILE:HG23	1:C:36:VAL:HG13	1.87	0.55
1:D:192:THR:H	1:D:195:THR:CB	2.19	0.55
1:A:242:ASN:HB2	1:E:253:LEU:O	2.06	0.55
1:E:79:ILE:HD13	1:E:94:THR:HG23	1.89	0.55
1:F:233:LYS:HE2	1:F:234:ASN:ND2	2.21	0.55
1:B:168:GLY:CA	1:B:237:THR:HG23	2.34	0.55
1:B:258:THR:C	1:B:259:LEU:HD22	2.26	0.55
1:B:276:GLU:HG2	1:C:370:VAL:CG2	2.37	0.55
1:C:310:LEU:N	1:C:310:LEU:HD12	2.22	0.55
1:C:83:THR:HB	1:C:87:GLU:HB3	1.87	0.55
1:D:265:ASP:H	1:D:270:GLY:N	1.99	0.55
1:D:50:GLU:HG2	1:D:305:TYR:OH	2.06	0.55
1:E:150:THR:CG2	1:E:292:ARG:HH21	2.19	0.55
1:F:243:TYR:CZ	1:F:245:GLY:HA3	2.42	0.55
1:F:341:MET:HE3	1:F:347:GLN:HB2	1.87	0.55
1:C:161:GLN:NE2	1:C:251:PRO:HA	2.18	0.55
1:D:208:LEU:O	1:D:208:LEU:HG	2.06	0.55
1:D:28:LEU:HD11	1:D:30:ILE:O	2.06	0.55
1:D:342:GLU:N	1:D:346:THR:HG23	2.22	0.55
1:E:117:LEU:HD13	1:E:118:GLN:H	1.72	0.55
1:F:91:GLY:N	1:F:186:LYS:NZ	2.55	0.55
1:A:145:THR:HG21	1:B:297:HIS:CE1	2.42	0.54
1:C:53:LEU:HD22	1:C:306:PHE:CE1	2.43	0.54
1:E:341:MET:C	1:E:346:THR:HG23	2.28	0.54
1:F:175:GLN:HG3	1:F:213:LYS:NZ	2.22	0.54
1:D:133:GLY:H	1:E:228:HIS:CE1	2.24	0.54
1:D:59:GLN:NE2	1:D:69:GLY:O	2.39	0.54
1:B:175:GLN:CB	1:B:230:ASP:HB2	2.26	0.54
1:C:239:TYR:C	1:C:240:PHE:CD1	2.81	0.54
1:D:211:ILE:CD1	1:D:211:ILE:N	2.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:PRO:HD3	1:F:292:ARG:HG3	1.88	0.54
1:F:302:LEU:HB3	1:F:303:PRO:HD2	1.89	0.54
1:A:125:VAL:O	1:A:125:VAL:HG13	2.07	0.54
1:A:243:TYR:CZ	1:A:245:GLY:CA	2.91	0.54
1:B:177:LEU:HD22	1:B:205:ASP:O	2.08	0.54
1:B:50:GLU:HG2	1:C:233:LYS:HA	1.88	0.54
1:C:350:GLU:HG3	1:F:233:LYS:CG	2.33	0.54
1:A:121:GLU:HG3	1:A:272:LEU:HD23	1.89	0.54
1:A:142:ASN:C	1:A:292:ARG:HB2	2.28	0.54
1:D:161:GLN:HE22	1:D:251:PRO:HA	1.72	0.54
1:E:178:VAL:CG2	1:E:179:THR:N	2.68	0.54
1:F:105:LEU:HB3	1:F:120:TRP:CD1	2.43	0.54
1:A:286:MET:HA	1:A:286:MET:HE3	1.88	0.54
1:B:192:THR:HG22	1:B:226:ILE:CD1	2.38	0.54
1:B:252:VAL:HG13	1:C:244:THR:HA	1.89	0.54
1:C:153:ILE:HG12	1:D:297:HIS:ND1	2.22	0.54
1:E:57:MET:HB2	1:E:96:PRO:HA	1.90	0.54
1:E:59:GLN:HG3	1:E:60:PRO:N	2.22	0.54
1:F:256:THR:OG1	1:F:257:ASN:N	2.41	0.54
1:B:110:GLU:CD	1:F:322:ALA:H	2.11	0.54
1:A:78:GLY:O	1:A:79:ILE:HD13	2.08	0.54
1:B:62:THR:OG1	1:B:63:PRO:HD3	2.08	0.54
1:C:126:LYS:HG2	1:C:260:THR:HA	1.90	0.54
1:C:54:ASN:HD22	1:C:55:PRO:HD2	1.73	0.54
1:D:115:ASP:OD2	1:D:317:ASN:HB3	2.08	0.54
1:A:108:LEU:HD11	1:A:120:TRP:CE2	2.43	0.54
1:A:174:LEU:HD11	1:A:214:ALA:HB3	1.90	0.54
1:A:287:GLY:O	1:A:299:TRP:HB2	2.08	0.54
1:B:162:TYR:HE1	1:B:283:VAL:HG21	1.73	0.54
1:C:82:ALA:HB1	1:C:88:ASP:HA	1.89	0.54
1:C:31:LYS:HE3	1:D:233:LYS:NZ	2.22	0.54
1:E:287:GLY:O	1:E:299:TRP:HB2	2.07	0.54
1:F:211:ILE:O	1:F:213:LYS:N	2.40	0.54
1:F:280:LEU:HD23	1:F:280:LEU:N	2.23	0.54
1:B:346:THR:HG22	1:B:348:VAL:H	1.73	0.54
1:C:82:ALA:HB2	1:C:88:ASP:OD1	2.07	0.54
1:D:310:LEU:H	1:D:310:LEU:HD12	1.72	0.54
1:E:82:ALA:HB1	1:E:87:GLU:O	2.08	0.54
1:F:185:TYR:HB2	1:F:194:LYS:HE2	1.90	0.54
1:A:181:ALA:H	1:A:206:GLN:HE21	1.55	0.54
1:A:133:GLY:HA3	1:B:228:HIS:HE1	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:ILE:HD11	1:D:297:HIS:CB	2.37	0.54
1:C:192:THR:HB	1:C:193:ILE:HD12	1.90	0.54
1:B:178:VAL:CG2	1:B:179:THR:N	2.70	0.53
1:B:207:VAL:HG23	1:B:208:LEU:N	2.23	0.53
1:C:256:THR:HA	1:D:239:TYR:CE1	2.42	0.53
1:D:257:ASN:HD22	1:E:239:TYR:H	1.55	0.53
1:D:142:ASN:O	1:D:292:ARG:HB2	2.08	0.53
1:F:264:LEU:N	1:F:264:LEU:HD12	2.22	0.53
1:B:250:PRO:HB3	1:C:245:GLY:O	2.09	0.53
1:B:257:ASN:HB3	1:C:239:TYR:CZ	2.43	0.53
1:C:253:LEU:O	1:D:242:ASN:HB2	2.08	0.53
1:D:56:ARG:NH2	1:D:219:ASP:OD1	2.41	0.53
1:E:132:SER:O	1:E:135:LEU:HD22	2.08	0.53
1:F:339:GLN:CB	1:F:340:PRO:HD2	2.38	0.53
1:A:90:PRO:HD2	1:A:186:LYS:HE3	1.91	0.53
1:D:285:ILE:N	1:D:285:ILE:CD1	2.72	0.53
1:D:71:GLN:CG	1:E:203:ASN:HB3	2.30	0.53
1:A:192:THR:O	1:A:196:ILE:HG22	2.08	0.53
1:C:120:TRP:HA	1:C:120:TRP:CE3	2.44	0.53
1:C:174:LEU:HD23	1:C:227:TRP:HB3	1.89	0.53
1:E:138:VAL:HG12	1:E:153:ILE:HG21	1.90	0.53
1:E:208:LEU:O	1:E:208:LEU:HD23	2.09	0.53
1:E:285:ILE:HD12	1:E:285:ILE:H	1.72	0.53
1:A:203:ASN:HD22	1:E:71:GLN:NE2	2.05	0.53
1:F:262:VAL:HG12	1:F:264:LEU:HB2	1.91	0.53
1:A:308:ILE:N	1:A:308:ILE:CD1	2.72	0.53
1:A:82:ALA:HB1	1:A:87:GLU:O	2.08	0.53
1:A:84:SER:O	1:A:87:GLU:N	2.41	0.53
1:D:336:VAL:C	1:D:337:GLN:O	2.46	0.53
1:E:166:ALA:HB2	1:E:239:TYR:HB3	1.91	0.53
1:B:48:GLU:HB2	1:F:352:ARG:HG3	1.89	0.53
1:B:117:LEU:HA	1:B:314:TRP:HZ3	1.73	0.53
1:C:161:GLN:HA	1:C:285:ILE:HG22	1.90	0.53
1:D:33:GLY:O	1:D:36:VAL:HB	2.07	0.53
1:D:341:MET:CE	1:D:347:GLN:HB2	2.37	0.53
1:F:57:MET:HB2	1:F:96:PRO:HB3	1.91	0.53
2:L:2:GAL:H3	2:L:3:SIA:O1B	2.08	0.53
1:A:178:VAL:HG22	1:A:179:THR:H	1.74	0.53
1:A:124:SER:CA	1:A:263:LEU:HG	2.35	0.53
1:A:317:ASN:OD1	1:A:319:TYR:HD2	1.92	0.53
1:C:97:THR:HG22	1:C:223:PRO:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:341:MET:HA	1:C:346:THR:HG23	1.90	0.53
1:C:341:MET:HE2	1:C:347:GLN:HB2	1.90	0.53
1:C:65:SER:C	1:C:67:THR:H	2.11	0.53
1:E:164:VAL:HG22	1:E:241:GLY:HA3	1.90	0.53
1:F:150:THR:CG2	1:F:292:ARG:HH21	2.21	0.53
1:B:90:PRO:HD2	1:B:186:LYS:NZ	2.24	0.53
1:E:329:PHE:O	1:E:332:MET:N	2.42	0.53
1:A:169:GLY:O	1:A:274:LYS:HG2	2.09	0.53
1:A:323:SER:HB2	1:A:324:LEU:HG	1.91	0.53
1:A:370:VAL:HG12	1:A:371:ASP:O	2.08	0.53
1:A:372:ARG:HB3	1:A:373:PHE:CD1	2.44	0.53
1:B:300:ARG:CG	1:B:301:GLY:N	2.72	0.53
1:C:233:LYS:HB3	1:F:350:GLU:CB	2.39	0.53
1:C:363:ASP:HB3	1:C:366:MET:HE2	1.91	0.53
1:D:97:THR:HG22	1:D:222:TYR:O	2.09	0.53
1:F:135:LEU:HD13	1:F:135:LEU:N	2.24	0.53
1:F:276:GLU:OE1	1:F:276:GLU:HA	2.09	0.53
1:B:275:GLY:C	1:B:277:GLY:H	2.12	0.53
1:B:285:ILE:HD12	1:B:285:ILE:H	1.74	0.53
1:B:300:ARG:HG3	1:B:301:GLY:H	1.74	0.53
1:B:336:VAL:O	1:B:337:GLN:CA	2.53	0.53
1:C:72:TYR:O	1:C:75:TRP:HB2	2.09	0.53
1:C:89:SER:OG	1:C:186:LYS:NZ	2.42	0.53
1:D:61:PRO:HG2	1:D:62:THR:H	1.73	0.53
1:E:193:ILE:O	1:E:197:THR:HG22	2.09	0.53
1:F:265:ASP:CG	1:F:269:VAL:HB	2.28	0.53
1:A:238:ARG:NH2	1:A:265:ASP:HB3	2.23	0.52
1:B:371:ASP:C	1:B:373:PHE:H	2.12	0.52
1:E:192:THR:O	1:E:196:ILE:HG22	2.08	0.52
1:E:168:GLY:CA	1:E:237:THR:HG23	2.35	0.52
1:E:342:GLU:HG2	1:E:343:GLY:N	2.24	0.52
1:E:66:LEU:HD23	1:E:66:LEU:N	2.20	0.52
1:E:69:GLY:C	1:E:71:GLN:H	2.12	0.52
1:F:317:ASN:ND2	1:F:318:PRO:HD2	2.25	0.52
1:F:332:MET:O	1:F:334:PRO:HD3	2.09	0.52
1:F:34:MET:O	1:F:37:LEU:HB2	2.09	0.52
1:A:94:THR:O	1:A:94:THR:HG22	2.09	0.52
1:C:78:GLY:HA3	2:I:2:GAL:C4	2.39	0.52
1:E:177:LEU:HD21	1:E:208:LEU:HA	1.90	0.52
1:C:233:LYS:HE2	1:F:352:ARG:CZ	2.39	0.52
1:A:86:THR:HG23	1:A:87:GLU:N	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ALA:O	1:F:359:PRO:HA	2.09	0.52
1:B:165:PHE:CE1	1:B:240:PHE:HE1	2.27	0.52
1:B:323:SER:O	1:B:327:SER:HB3	2.08	0.52
1:D:98:TRP:HH2	1:D:164:VAL:HG11	1.73	0.52
1:A:234:ASN:HD22	1:A:234:ASN:N	2.08	0.52
1:B:285:ILE:HD12	1:B:285:ILE:N	2.23	0.52
1:D:117:LEU:HD23	1:D:118:GLN:N	2.25	0.52
1:F:150:THR:O	1:F:150:THR:CG2	2.57	0.52
1:F:168:GLY:HA2	1:F:237:THR:HA	1.92	0.52
1:D:139:HIS:HD2	1:E:88:ASP:OD2	1.92	0.52
1:F:288:TRP:HA	1:F:299:TRP:CB	2.39	0.52
1:F:300:ARG:HG3	1:F:301:GLY:H	1.74	0.52
1:A:288:TRP:HZ3	1:A:299:TRP:CD2	2.26	0.52
1:B:172:LEU:HD22	1:B:173:ASP:O	2.10	0.52
1:F:164:VAL:HA	1:F:241:GLY:HA3	1.91	0.52
1:F:76:SER:O	1:F:298:HIS:HB2	2.10	0.52
1:A:88:ASP:H	1:A:184:LYS:HD3	1.73	0.52
1:A:56:ARG:HB2	1:A:56:ARG:HH11	1.75	0.52
1:C:186:LYS:CE	1:C:186:LYS:H	2.23	0.52
1:C:272:LEU:HD12	1:C:272:LEU:N	2.25	0.52
1:D:54:ASN:HD21	1:E:208:LEU:HB2	1.74	0.52
1:F:169:GLY:O	1:F:274:LYS:HG2	2.10	0.52
1:F:321:MET:C	1:F:323:SER:H	2.13	0.52
1:F:86:THR:HG23	1:F:87:GLU:N	2.24	0.52
1:A:177:LEU:HD22	1:A:205:ASP:O	2.10	0.52
1:C:48:GLU:HG2	1:C:309:THR:HG23	1.92	0.52
1:C:75:TRP:CD1	1:C:300:ARG:HB2	2.45	0.52
1:D:90:PRO:HD2	1:D:184:LYS:O	2.09	0.52
1:E:193:ILE:N	1:E:193:ILE:HD12	2.25	0.52
1:E:80:ASN:HB3	1:E:90:PRO:O	2.10	0.52
1:F:74:GLY:O	1:F:300:ARG:NH1	2.42	0.52
1:A:297:HIS:ND1	1:E:153:ILE:HG12	2.24	0.52
1:A:81:LEU:HG	1:A:82:ALA:H	1.74	0.52
1:B:232:ALA:HB3	1:B:234:ASN:O	2.10	0.52
1:B:60:PRO:HB2	1:B:61:PRO:HD2	1.92	0.52
1:C:37:LEU:HG	1:C:106:PRO:HD3	1.92	0.52
1:D:236:ASN:OD1	1:D:271:PRO:HA	2.10	0.52
1:D:256:THR:HG23	1:D:258:THR:N	2.25	0.52
1:E:162:TYR:HE1	1:E:283:VAL:HG21	1.74	0.52
1:E:286:MET:SD	1:E:302:LEU:HD12	2.50	0.52
1:F:332:MET:HG3	1:F:333:LEU:HD22	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:VAL:CG2	1:A:179:THR:N	2.73	0.52
1:A:288:TRP:CZ3	1:A:299:TRP:CE2	2.92	0.52
1:C:194:LYS:HG2	1:C:195:THR:N	2.25	0.52
1:C:75:TRP:CZ2	1:C:300:ARG:HD2	2.45	0.52
1:D:175:GLN:OE1	1:D:208:LEU:HD11	2.10	0.52
1:D:209:ASN:OD1	1:D:211:ILE:HD13	2.09	0.52
1:E:105:LEU:HD12	1:E:105:LEU:H	1.74	0.52
1:A:208:LEU:HD13	1:E:52:PHE:CD1	2.45	0.52
1:E:83:THR:O	1:E:84:SER:HB2	2.09	0.52
1:A:243:TYR:HE2	1:E:251:PRO:HB2	1.75	0.51
1:A:262:VAL:HG12	1:A:264:LEU:N	2.20	0.51
1:B:104:GLN:HE21	1:B:105:LEU:N	2.08	0.51
1:B:194:LYS:O	1:B:196:ILE:N	2.43	0.51
1:B:341:MET:CA	1:B:346:THR:HG23	2.40	0.51
1:C:142:ASN:N	1:C:154:SER:OG	2.42	0.51
1:C:291:THR:OG1	1:C:296:VAL:HG23	2.11	0.51
1:D:123:VAL:O	1:D:263:LEU:N	2.42	0.51
1:C:233:LYS:HE3	1:F:350:GLU:HG2	1.91	0.51
1:B:48:GLU:HB2	1:F:352:ARG:CG	2.40	0.51
1:F:84:SER:HB3	1:F:86:THR:HG22	1.92	0.51
1:A:167:VAL:C	1:A:237:THR:HG23	2.31	0.51
1:C:78:GLY:HA3	2:I:2:GAL:H4	1.92	0.51
1:D:327:SER:OG	1:D:328:LEU:N	2.43	0.51
1:D:71:GLN:NE2	1:D:73:TYR:H	2.06	0.51
1:E:233:LYS:CD	1:E:234:ASN:N	2.72	0.51
1:E:33:GLY:O	1:E:36:VAL:HG23	2.10	0.51
1:F:166:ALA:HB2	1:F:239:TYR:CB	2.41	0.51
1:F:193:ILE:HD12	1:F:194:LYS:HD3	1.91	0.51
1:A:259:LEU:HD13	1:A:260:THR:H	1.74	0.51
1:B:308:ILE:N	1:B:308:ILE:CD1	2.67	0.51
1:C:198:LYS:CD	1:C:198:LYS:H	2.20	0.51
1:C:75:TRP:CE2	1:C:300:ARG:HD2	2.45	0.51
1:C:336:VAL:HA	1:C:337:GLN:N	2.25	0.51
1:D:108:LEU:HG	1:D:312:LYS:HE2	1.91	0.51
1:E:258:THR:HB	1:E:259:LEU:HD22	1.92	0.51
1:F:65:SER:HB3	1:F:68:GLU:CG	2.40	0.51
1:F:71:GLN:HE21	1:F:73:TYR:HB2	1.75	0.51
1:A:341:MET:CE	1:A:347:GLN:HB2	2.39	0.51
1:B:243:TYR:CZ	1:B:245:GLY:HA2	2.45	0.51
1:B:56:ARG:NH1	1:B:56:ARG:HB2	2.26	0.51
1:B:90:PRO:HG2	1:B:185:TYR:CE1	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:LYS:N	1:C:292:ARG:HB2	2.26	0.51
1:D:233:LYS:C	1:D:234:ASN:HD22	2.14	0.51
1:F:90:PRO:HD2	1:F:186:LYS:CE	2.41	0.51
1:A:28:LEU:HG	1:A:29:LEU:N	2.23	0.51
1:B:77:ARG:O	1:B:298:HIS:CG	2.64	0.51
1:C:234:ASN:OD1	1:F:352:ARG:NH2	2.43	0.51
1:D:207:VAL:HG23	1:D:208:LEU:H	1.74	0.51
1:D:124:SER:HA	1:D:262:VAL:HA	1.92	0.51
1:D:163:HIS:HA	1:D:283:VAL:O	2.11	0.51
1:E:109:ASN:OD1	1:E:118:GLN:N	2.43	0.51
1:E:185:TYR:HB2	1:E:194:LYS:HE2	1.91	0.51
1:E:77:ARG:O	1:E:298:HIS:ND1	2.44	0.51
1:F:96:PRO:HG3	1:F:299:TRP:HZ2	1.75	0.51
1:A:192:THR:CG2	1:A:194:LYS:HE2	2.40	0.51
1:A:193:ILE:HD13	1:A:201:MET:HG2	1.92	0.51
1:B:165:PHE:CD1	1:B:165:PHE:C	2.83	0.51
1:C:28:LEU:HD21	1:C:30:ILE:C	2.30	0.51
1:D:337:GLN:HA	1:D:337:GLN:OE1	2.10	0.51
1:E:286:MET:HE3	1:E:286:MET:HA	1.92	0.51
1:E:318:PRO:HG2	1:E:319:TYR:H	1.76	0.51
1:E:77:ARG:HB3	1:E:93:ASN:HB2	1.92	0.51
1:F:239:TYR:C	1:F:240:PHE:CD1	2.84	0.51
1:F:55:PRO:HB3	1:F:302:LEU:O	2.11	0.51
1:A:229:PRO:O	1:A:229:PRO:HG2	2.10	0.51
1:B:153:ILE:HD11	1:C:297:HIS:CG	2.46	0.51
1:B:354:TYR:N	1:B:354:TYR:CD1	2.78	0.51
1:D:308:ILE:HG22	1:D:310:LEU:HG	1.93	0.51
1:F:232:ALA:HB3	1:F:235:GLU:OE1	2.10	0.51
1:F:273:CYS:HB3	1:F:277:GLY:O	2.11	0.51
1:A:192:THR:HB	1:A:194:LYS:CE	2.41	0.51
1:B:177:LEU:CD1	1:B:207:VAL:O	2.58	0.51
1:C:106:PRO:HD2	1:C:120:TRP:HE1	1.75	0.51
1:C:211:ILE:N	1:C:211:ILE:CD1	2.74	0.51
1:C:54:ASN:HD21	1:D:208:LEU:CB	2.24	0.51
1:D:142:ASN:HD21	1:D:289:ARG:HG3	1.76	0.51
1:E:117:LEU:O	1:E:315:VAL:HG23	2.11	0.51
1:E:192:THR:HG21	1:E:194:LYS:HE2	1.92	0.51
1:E:193:ILE:HG12	1:E:201:MET:HE1	1.90	0.51
1:F:100:MET:C	1:F:100:MET:SD	2.89	0.51
1:F:180:ASP:HB3	1:F:182:ARG:HG2	1.93	0.51
1:A:145:THR:OG1	1:A:153:ILE:N	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:LEU:HD23	1:E:254:GLN:N	2.18	0.51
1:E:72:TYR:O	1:E:75:TRP:HB2	2.10	0.51
1:B:287:GLY:O	1:B:299:TRP:HB2	2.11	0.51
1:C:265:ASP:H	1:C:270:GLY:N	2.08	0.51
1:D:105:LEU:HD23	1:D:120:TRP:CD2	2.45	0.51
1:D:175:GLN:HG2	1:D:212:SER:O	2.11	0.51
1:E:192:THR:H	1:E:195:THR:HB	1.74	0.51
1:F:166:ALA:HB1	1:F:238:ARG:O	2.11	0.51
1:F:192:THR:HG22	1:F:193:ILE:HD12	1.91	0.51
1:F:209:ASN:ND2	1:F:211:ILE:HB	2.25	0.51
1:A:166:ALA:HB2	1:A:239:TYR:HB3	1.92	0.50
1:A:275:GLY:C	1:A:277:GLY:H	2.11	0.50
1:A:285:ILE:N	1:A:285:ILE:HD12	2.25	0.50
1:A:74:GLY:O	1:A:300:ARG:NH1	2.44	0.50
1:B:177:LEU:HD21	1:B:208:LEU:CA	2.39	0.50
1:B:211:ILE:N	1:B:211:ILE:HD12	2.25	0.50
1:B:239:TYR:C	1:B:240:PHE:CG	2.84	0.50
1:C:191:VAL:HG23	1:C:222:TYR:HA	1.93	0.50
1:D:300:ARG:CG	1:D:301:GLY:N	2.74	0.50
1:F:222:TYR:HB3	1:F:227:TRP:CD1	2.45	0.50
1:F:308:ILE:HG22	1:F:310:LEU:HG	1.92	0.50
1:B:243:TYR:OH	1:B:245:GLY:HA2	2.11	0.50
1:A:145:THR:HG21	1:B:297:HIS:HE1	1.75	0.50
1:B:317:ASN:OD1	1:B:318:PRO:HD2	2.11	0.50
1:B:341:MET:HA	1:B:341:MET:CE	2.41	0.50
1:C:339:GLN:CB	1:C:340:PRO:HD2	2.40	0.50
1:F:104:GLN:NE2	1:F:105:LEU:O	2.45	0.50
1:F:25:VAL:CG1	1:F:26:PRO:HD2	2.41	0.50
1:F:317:ASN:HD21	1:F:319:TYR:HB2	1.75	0.50
1:A:142:ASN:ND2	1:A:289:ARG:HG3	2.25	0.50
1:B:162:TYR:CE1	1:B:283:VAL:HG21	2.46	0.50
1:B:305:TYR:CG	1:B:306:PHE:N	2.80	0.50
1:C:265:ASP:CG	1:C:269:VAL:HB	2.31	0.50
1:D:144:PRO:HA	1:D:153:ILE:O	2.11	0.50
1:D:80:ASN:HB3	1:D:90:PRO:O	2.11	0.50
1:E:177:LEU:CD2	1:E:209:ASN:H	2.18	0.50
1:A:233:LYS:HA	1:E:50:GLU:CG	2.41	0.50
1:F:170:GLU:HB2	1:F:171:PRO:HD2	1.92	0.50
1:A:265:ASP:OD1	1:A:269:VAL:N	2.44	0.50
1:B:243:TYR:CZ	1:B:245:GLY:CA	2.94	0.50
1:B:92:ASN:OD1	1:B:186:LYS:HD2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PRO:HA	1:C:153:ILE:O	2.12	0.50
1:D:259:LEU:N	1:D:259:LEU:HD22	2.26	0.50
1:D:32:GLY:HA3	1:D:36:VAL:CG2	2.42	0.50
1:A:125:VAL:HA	1:A:307:LYS:O	2.11	0.50
1:B:86:THR:HG23	1:B:87:GLU:N	2.26	0.50
1:C:228:HIS:HB3	1:C:229:PRO:HD2	1.91	0.50
1:C:333:LEU:HD12	1:C:334:PRO:O	2.12	0.50
1:D:97:THR:HA	1:D:223:PRO:HA	1.94	0.50
1:D:66:LEU:HD23	1:D:66:LEU:N	2.24	0.50
1:D:69:GLY:C	1:D:71:GLN:H	2.15	0.50
1:B:52:PHE:CE2	1:F:347:GLN:HB3	2.47	0.50
1:A:166:ALA:HB1	1:A:238:ARG:O	2.11	0.50
1:A:170:GLU:HB2	1:A:171:PRO:HD2	1.94	0.50
1:B:288:TRP:CZ3	1:B:299:TRP:CD1	3.00	0.50
1:B:69:GLY:HA3	1:B:71:GLN:OE1	2.11	0.50
1:B:152:GLY:HA2	1:C:295:ASP:HB3	1.94	0.50
1:C:300:ARG:CG	1:C:301:GLY:N	2.75	0.50
1:D:192:THR:HG21	1:D:194:LYS:CE	2.41	0.50
1:E:112:LEU:O	1:E:116:THR:CG2	2.60	0.50
1:E:203:ASN:O	1:E:206:GLN:CB	2.60	0.50
1:E:62:THR:O	1:E:64:GLU:N	2.42	0.50
1:B:305:TYR:CE2	1:B:307:LYS:HB2	2.46	0.50
1:B:367:THR:HG22	1:B:368:ARG:H	1.77	0.50
1:E:265:ASP:H	1:E:270:GLY:N	2.09	0.50
1:A:184:LYS:O	1:A:186:LYS:HE2	2.12	0.50
1:A:180:ASP:HA	1:A:206:GLN:HE21	1.76	0.50
1:A:288:TRP:CZ3	1:A:299:TRP:CD2	2.99	0.50
1:B:197:THR:O	1:B:197:THR:HG23	2.10	0.50
1:C:192:THR:N	1:C:195:THR:OG1	2.42	0.50
1:B:50:GLU:CD	1:C:233:LYS:HA	2.31	0.50
1:D:138:VAL:HB	1:D:153:ILE:HD12	1.94	0.50
1:D:91:GLY:N	1:D:186:LYS:NZ	2.60	0.50
1:D:279:TYR:N	1:D:279:TYR:CD1	2.79	0.50
1:E:177:LEU:CD2	1:E:208:LEU:HA	2.42	0.50
1:E:243:TYR:CZ	1:E:245:GLY:CA	2.94	0.50
1:E:93:ASN:OD1	1:E:93:ASN:N	2.44	0.50
1:A:166:ALA:HB1	1:A:237:THR:HG22	1.93	0.50
1:C:25:VAL:HG13	1:C:26:PRO:HD2	1.92	0.50
1:C:278:LEU:HD23	1:C:279:TYR:N	2.26	0.50
1:D:202:VAL:HG12	1:D:203:ASN:OD1	2.12	0.50
1:D:236:ASN:ND2	1:D:272:LEU:O	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:161:GLN:HE22	1:E:251:PRO:HA	1.77	0.50
1:E:288:TRP:HB3	1:E:299:TRP:HB3	1.94	0.50
1:E:300:ARG:CG	1:E:301:GLY:N	2.74	0.50
1:A:339:GLN:HG3	1:A:340:PRO:HD2	1.94	0.49
1:B:131:GLY:O	1:B:134:SER:HB3	2.11	0.49
1:B:57:MET:SD	1:B:301:GLY:HA3	2.52	0.49
1:C:109:ASN:HB3	1:C:117:LEU:CD2	2.40	0.49
1:B:134:SER:OG	1:C:179:THR:HG23	2.11	0.49
1:C:311:ARG:NH2	1:C:313:ARG:NH2	2.59	0.49
1:D:319:TYR:HB2	1:D:324:LEU:HD23	1.93	0.49
1:E:193:ILE:CD1	1:E:201:MET:SD	3.00	0.49
1:E:162:TYR:CE1	1:E:224:VAL:HG11	2.47	0.49
1:B:117:LEU:HD12	1:B:117:LEU:N	2.26	0.49
1:B:60:PRO:CB	1:B:61:PRO:HD2	2.41	0.49
1:C:288:TRP:HA	1:C:299:TRP:HB3	1.94	0.49
1:C:311:ARG:HH21	1:C:313:ARG:NH2	2.09	0.49
1:C:62:THR:CB	1:C:63:PRO:HD3	2.42	0.49
1:D:55:PRO:CD	1:D:303:PRO:HB3	2.43	0.49
1:D:75:TRP:NE1	1:D:300:ARG:HB2	2.26	0.49
1:E:211:ILE:N	1:E:211:ILE:HD12	2.27	0.49
1:E:308:ILE:CD1	1:E:308:ILE:N	2.75	0.49
1:E:329:PHE:O	1:E:332:MET:HB2	2.12	0.49
1:F:19:CYS:CB	1:F:20:PRO:CD	2.90	0.49
1:C:350:GLU:HB2	1:F:233:LYS:HB3	1.90	0.49
1:A:177:LEU:CD2	1:A:205:ASP:O	2.59	0.49
1:A:57:MET:CB	1:A:96:PRO:HA	2.41	0.49
1:B:83:THR:O	1:B:84:SER:HB2	2.12	0.49
1:C:69:GLY:C	1:C:71:GLN:N	2.64	0.49
1:D:255:PHE:HB2	1:E:241:GLY:O	2.11	0.49
1:D:322:ALA:O	1:D:325:ILE:HB	2.11	0.49
1:E:37:LEU:HB3	1:E:106:PRO:HG2	1.93	0.49
1:E:367:THR:HG22	1:E:368:ARG:N	2.27	0.49
1:F:201:MET:HA	1:F:201:MET:HE2	1.93	0.49
1:F:175:GLN:HG3	1:F:213:LYS:CE	2.43	0.49
1:F:97:THR:HG22	1:F:222:TYR:C	2.33	0.49
2:I:2:GAL:H3	2:I:3:SIA:O1B	2.09	0.49
1:A:84:SER:HA	1:E:141:PHE:HD2	1.72	0.49
1:B:208:LEU:O	1:B:208:LEU:HD23	2.12	0.49
1:B:94:THR:O	1:B:95:LEU:HG	2.12	0.49
1:C:164:VAL:HG22	1:C:241:GLY:HA3	1.94	0.49
1:D:144:PRO:HD3	1:D:292:ARG:CG	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:TRP:N	1:D:222:TYR:O	2.43	0.49
1:D:304:ARG:HD3	1:D:306:PHE:CZ	2.46	0.49
1:E:69:GLY:O	1:E:71:GLN:N	2.44	0.49
1:C:316:LYS:HE3	1:F:359:PRO:HD2	1.94	0.49
1:F:42:GLY:O	1:F:312:LYS:NZ	2.30	0.49
1:C:349:GLU:O	1:C:350:GLU:HG2	2.12	0.49
1:D:175:GLN:HG2	1:D:176:GLY:N	2.27	0.49
1:D:69:GLY:O	1:D:71:GLN:N	2.46	0.49
1:E:122:ALA:O	1:E:271:PRO:CD	2.58	0.49
1:E:126:LYS:HG2	1:E:260:THR:HG23	1.95	0.49
1:F:285:ILE:CD1	1:F:285:ILE:H	2.25	0.49
1:C:269:VAL:HA	1:C:313:ARG:NH2	2.27	0.49
1:D:219:ASP:O	1:D:220:GLY:C	2.50	0.49
1:D:269:VAL:CG1	1:D:272:LEU:HD11	2.42	0.49
1:E:166:ALA:HB2	1:E:239:TYR:CB	2.43	0.49
1:A:177:LEU:CD1	1:A:207:VAL:O	2.53	0.49
1:A:211:ILE:HD12	1:A:211:ILE:H	1.76	0.49
1:A:253:LEU:HG	1:A:254:GLN:H	1.77	0.49
1:A:278:LEU:HD11	1:A:308:ILE:HG21	1.95	0.49
1:A:133:GLY:CA	1:B:228:HIS:HE1	2.26	0.49
1:A:50:GLU:CD	1:B:233:LYS:HB2	2.32	0.49
1:C:174:LEU:N	1:C:174:LEU:HD12	2.27	0.49
1:C:243:TYR:CZ	1:C:245:GLY:CA	2.96	0.49
1:D:175:GLN:HG2	1:D:176:GLY:H	1.77	0.49
1:D:185:TYR:HB2	1:D:194:LYS:HE3	1.93	0.49
1:E:288:TRP:CE3	1:E:299:TRP:CG	3.00	0.49
1:E:91:GLY:O	1:E:93:ASN:N	2.44	0.49
1:F:75:TRP:HE1	1:F:300:ARG:HB2	1.74	0.49
1:F:84:SER:O	1:F:87:GLU:N	2.45	0.49
1:A:264:LEU:HD23	1:A:268:GLY:HA2	1.94	0.49
1:A:118:GLN:HB2	1:A:314:TRP:CZ3	2.47	0.49
1:B:104:GLN:HE22	1:B:276:GLU:HB2	1.78	0.49
1:B:125:VAL:O	1:B:125:VAL:HG13	2.13	0.49
1:B:46:VAL:O	1:F:353:VAL:HA	2.12	0.49
1:E:114:CYS:C	1:E:116:THR:N	2.65	0.49
1:C:233:LYS:NZ	1:F:352:ARG:NE	2.61	0.49
1:F:367:THR:HG22	1:F:368:ARG:H	1.78	0.49
1:C:150:THR:O	1:C:150:THR:HG22	2.12	0.49
1:C:61:PRO:HG2	1:C:62:THR:H	1.78	0.49
1:D:203:ASN:N	1:D:203:ASN:OD1	2.44	0.49
1:D:43:PRO:HD2	1:D:44:ASP:H	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:161:GLN:NE2	1:F:251:PRO:HA	2.25	0.49
1:F:329:PHE:O	1:F:333:LEU:HB2	2.13	0.49
1:A:181:ALA:H	1:A:206:GLN:NE2	2.11	0.49
1:A:184:LYS:N	1:A:184:LYS:HD2	2.28	0.49
1:A:175:GLN:HG3	1:A:213:LYS:HD3	1.94	0.49
1:A:222:TYR:N	1:A:222:TYR:CD1	2.81	0.49
1:A:290:VAL:HG22	1:A:297:HIS:CD2	2.48	0.49
1:A:50:GLU:HG2	1:A:305:TYR:OH	2.12	0.49
1:D:172:LEU:HD22	1:D:173:ASP:O	2.12	0.49
1:D:21:ARG:HE	1:D:21:ARG:H	1.60	0.49
1:D:264:LEU:HA	1:D:264:LEU:HD12	1.42	0.49
1:D:34:MET:O	1:D:37:LEU:HB2	2.13	0.49
1:D:83:THR:CB	1:D:87:GLU:HB3	2.41	0.49
1:B:45:SER:HA	1:F:354:TYR:O	2.13	0.49
1:A:106:PRO:HD2	1:A:120:TRP:NE1	2.27	0.48
1:B:172:LEU:HD22	1:B:173:ASP:N	2.28	0.48
1:B:288:TRP:HB3	1:B:297:HIS:O	2.12	0.48
1:C:105:LEU:HB3	1:C:106:PRO:HD2	1.94	0.48
1:D:221:MET:O	1:D:223:PRO:HD3	2.13	0.48
1:F:192:THR:HG21	1:F:194:LYS:HE2	1.95	0.48
1:F:177:LEU:CD1	1:F:207:VAL:O	2.56	0.48
1:F:207:VAL:HG23	1:F:208:LEU:N	2.28	0.48
1:F:317:ASN:HD22	1:F:319:TYR:H	1.60	0.48
1:B:164:VAL:HB	1:B:283:VAL:CG2	2.42	0.48
1:B:185:TYR:CB	1:B:192:THR:HG21	2.43	0.48
1:C:41:THR:HB	1:C:45:SER:HB2	1.95	0.48
1:D:91:GLY:H	1:D:186:LYS:NZ	2.11	0.48
1:E:119:MET:HG2	1:E:315:VAL:HG21	1.95	0.48
1:A:161:GLN:HE22	1:A:251:PRO:CA	2.23	0.48
1:B:166:ALA:HB2	1:B:239:TYR:CB	2.44	0.48
1:B:180:ASP:HB3	1:B:182:ARG:HG2	1.94	0.48
1:B:162:TYR:HB3	1:B:285:ILE:HD13	1.95	0.48
1:B:50:GLU:CG	1:C:233:LYS:HA	2.43	0.48
1:D:123:VAL:HG12	1:D:124:SER:N	2.26	0.48
1:D:97:THR:HG22	1:D:223:PRO:N	2.28	0.48
1:E:125:VAL:HG12	1:E:263:LEU:HD21	1.95	0.48
1:F:111:ASP:C	1:F:113:THR:N	2.66	0.48
1:C:352:ARG:NE	1:F:234:ASN:OD1	2.47	0.48
1:A:56:ARG:NH1	1:A:219:ASP:OD1	2.46	0.48
1:A:278:LEU:HD22	1:A:280:LEU:CD2	2.43	0.48
1:A:335:GLN:HE21	1:A:336:VAL:HG22	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:TRP:HA	1:B:299:TRP:HB3	1.95	0.48
1:B:323:SER:O	1:B:327:SER:CB	2.62	0.48
1:C:162:TYR:HB3	1:C:285:ILE:HD13	1.96	0.48
1:D:24:PRO:C	1:D:25:VAL:HG12	2.32	0.48
1:A:108:LEU:HD11	1:A:120:TRP:CZ2	2.48	0.48
1:A:33:GLY:O	1:A:36:VAL:HG23	2.14	0.48
1:B:105:LEU:HB3	1:B:120:TRP:CD1	2.48	0.48
1:B:111:ASP:C	1:B:113:THR:N	2.66	0.48
1:B:50:GLU:HG2	1:B:305:TYR:OH	2.13	0.48
1:C:35:GLU:HG2	1:C:36:VAL:N	2.27	0.48
1:B:139:HIS:HD2	1:C:88:ASP:OD1	1.96	0.48
1:E:157:VAL:O	1:E:158:GLU:HG3	2.14	0.48
1:F:193:ILE:O	1:F:197:THR:HG22	2.12	0.48
1:F:65:SER:C	1:F:67:THR:H	2.16	0.48
1:A:228:HIS:CE1	1:E:131:GLY:HA2	2.49	0.48
1:A:57:MET:HE1	1:A:299:TRP:O	2.12	0.48
1:A:318:PRO:O	1:A:321:MET:HG2	2.13	0.48
1:C:39:LEU:HD12	1:C:40:VAL:N	2.25	0.48
1:C:71:GLN:HE21	1:C:73:TYR:HB2	1.79	0.48
1:E:112:LEU:O	1:E:114:CYS:N	2.47	0.48
1:F:304:ARG:HG2	1:F:305:TYR:N	2.28	0.48
1:F:39:LEU:HD12	1:F:40:VAL:H	1.78	0.48
1:B:239:TYR:C	1:B:239:TYR:CD1	2.87	0.48
1:C:125:VAL:HB	1:C:263:LEU:HD11	1.95	0.48
1:C:211:ILE:O	1:C:213:LYS:N	2.44	0.48
1:C:175:GLN:CB	1:C:230:ASP:HB2	2.41	0.48
1:C:291:THR:HB	1:C:293:ASN:HB3	1.94	0.48
1:D:207:VAL:CG2	1:D:208:LEU:N	2.77	0.48
1:A:294:TYR:CD1	1:E:151:LYS:HG2	2.48	0.48
1:E:145:THR:HB	1:E:152:GLY:HA3	1.94	0.48
1:E:305:TYR:C	1:E:306:PHE:CD1	2.87	0.48
1:E:59:GLN:HG3	1:E:60:PRO:CD	2.44	0.48
1:E:94:THR:O	1:E:95:LEU:HD23	2.14	0.48
1:F:164:VAL:HG12	1:F:165:PHE:N	2.27	0.48
1:F:104:GLN:HE22	1:F:276:GLU:HB2	1.78	0.48
1:F:55:PRO:HD3	1:F:303:PRO:HB3	1.96	0.48
1:F:75:TRP:CD1	1:F:300:ARG:HB2	2.48	0.48
1:A:233:LYS:HA	1:E:50:GLU:CD	2.34	0.48
1:C:185:TYR:HB2	1:C:194:LYS:HE2	1.96	0.48
1:C:236:ASN:OD1	1:C:272:LEU:HD12	2.14	0.48
1:C:142:ASN:HD21	1:C:289:ARG:CG	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:PHE:C	1:C:331:ASN:H	2.17	0.48
1:E:216:LEU:HD23	1:E:216:LEU:HA	1.51	0.48
1:F:69:GLY:C	1:F:71:GLN:N	2.65	0.48
1:A:340:PRO:HG2	1:A:347:GLN:NE2	2.22	0.48
1:B:288:TRP:CZ3	1:B:299:TRP:NE1	2.82	0.48
1:C:209:ASN:ND2	1:C:211:ILE:HB	2.29	0.48
1:E:209:ASN:HA	1:E:210:PRO:HD3	1.65	0.48
1:E:23:ALA:HA	1:E:24:PRO:HD3	1.63	0.48
1:E:325:ILE:O	1:E:328:LEU:HB3	2.14	0.48
1:E:370:VAL:HA	1:E:375:LYS:HA	1.96	0.48
1:F:149:ASN:O	1:F:151:LYS:HE2	2.14	0.48
1:A:233:LYS:HE2	1:A:234:ASN:HD21	1.79	0.48
1:B:185:TYR:HB2	1:B:194:LYS:CE	2.43	0.48
1:C:59:GLN:OE1	1:C:60:PRO:HD2	2.13	0.48
1:C:97:THR:CG2	1:C:223:PRO:HA	2.44	0.48
1:D:185:TYR:HB2	1:D:194:LYS:CE	2.43	0.48
1:D:264:LEU:CD2	1:D:268:GLY:HA2	2.44	0.48
1:E:279:TYR:C	1:E:280:LEU:HD23	2.34	0.48
1:E:340:PRO:O	1:E:346:THR:HA	2.13	0.48
1:A:280:LEU:HD23	1:A:280:LEU:N	2.30	0.47
1:B:366:MET:CE	1:B:377:LYS:HG2	2.44	0.47
1:C:132:SER:O	1:C:135:LEU:HD23	2.14	0.47
1:C:341:MET:CA	1:C:346:THR:HG23	2.43	0.47
1:B:139:HIS:HB3	1:C:80:ASN:O	2.13	0.47
1:D:138:VAL:CB	1:D:153:ILE:HG23	2.34	0.47
1:D:130:VAL:O	1:D:303:PRO:HD2	2.14	0.47
1:D:321:MET:O	1:D:322:ALA:C	2.52	0.47
1:D:69:GLY:HA3	1:D:71:GLN:OE1	2.13	0.47
1:E:145:THR:OG1	1:E:153:ILE:HB	2.14	0.47
1:E:304:ARG:HD3	1:E:306:PHE:CE1	2.49	0.47
1:E:69:GLY:C	1:E:71:GLN:N	2.67	0.47
1:E:90:PRO:HD2	1:E:186:LYS:NZ	2.29	0.47
1:F:91:GLY:O	1:F:93:ASN:N	2.47	0.47
1:A:100:MET:HB3	1:A:216:LEU:HD13	1.96	0.47
1:A:288:TRP:CZ3	1:A:299:TRP:CD1	3.02	0.47
1:A:296:VAL:HG12	1:A:298:HIS:HD2	1.79	0.47
1:A:328:LEU:HD21	1:A:333:LEU:HD22	1.71	0.47
1:B:161:GLN:OE1	1:B:251:PRO:HA	2.15	0.47
1:A:257:ASN:HB2	1:B:239:TYR:CD2	2.48	0.47
1:D:55:PRO:HD3	1:D:303:PRO:HB3	1.96	0.47
1:D:72:TYR:O	1:D:73:TYR:C	2.51	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:177:LEU:HA	1:E:177:LEU:HD23	1.67	0.47
1:E:192:THR:H	1:E:195:THR:CB	2.26	0.47
1:E:197:THR:HG23	1:E:197:THR:O	2.12	0.47
1:F:112:LEU:HD12	1:F:113:THR:H	1.80	0.47
1:F:120:TRP:HA	1:F:120:TRP:CE3	2.49	0.47
1:F:243:TYR:CZ	1:F:245:GLY:HA2	2.48	0.47
1:F:362:GLY:O	1:F:364:PRO:HD3	2.13	0.47
1:A:142:ASN:HD21	1:A:289:ARG:CG	2.26	0.47
1:A:82:ALA:CB	1:A:88:ASP:HA	2.44	0.47
1:E:280:LEU:N	1:E:280:LEU:HD23	2.29	0.47
1:F:243:TYR:OH	1:F:245:GLY:HA3	2.14	0.47
1:F:254:GLN:HA	1:F:254:GLN:OE1	2.14	0.47
1:A:103:LEU:HB2	1:A:278:LEU:HB3	1.95	0.47
1:A:233:LYS:CG	1:A:234:ASN:HD22	2.27	0.47
1:B:197:THR:O	1:B:197:THR:CG2	2.63	0.47
1:B:322:ALA:O	1:B:323:SER:C	2.52	0.47
1:C:175:GLN:OE1	1:C:208:LEU:HD11	2.15	0.47
1:C:181:ALA:H	1:C:206:GLN:NE2	2.12	0.47
1:E:375:LYS:HG2	1:E:375:LYS:O	2.13	0.47
1:F:224:VAL:HG21	1:F:283:VAL:HG11	1.95	0.47
1:F:77:ARG:HB2	1:F:93:ASN:HB2	1.95	0.47
1:A:175:GLN:HG3	1:A:213:LYS:HE2	1.96	0.47
1:A:305:TYR:CG	1:A:306:PHE:N	2.82	0.47
1:B:178:VAL:HG11	1:B:201:MET:CE	2.45	0.47
1:C:135:LEU:N	1:C:135:LEU:CD2	2.78	0.47
1:C:66:LEU:HD23	1:C:66:LEU:N	2.29	0.47
1:D:174:LEU:HD22	1:D:227:TRP:HB3	1.96	0.47
1:C:300:ARG:NH2	1:D:206:GLN:O	2.43	0.47
1:D:83:THR:O	1:D:84:SER:HB2	2.14	0.47
1:E:29:LEU:HA	1:E:29:LEU:HD23	1.39	0.47
1:E:37:LEU:HD13	1:E:37:LEU:H	1.80	0.47
1:E:91:GLY:O	1:E:94:THR:N	2.43	0.47
1:C:233:LYS:HD2	1:F:350:GLU:OE1	2.14	0.47
1:A:370:VAL:CG2	1:A:375:LYS:HE2	2.45	0.47
1:B:175:GLN:NE2	1:B:176:GLY:O	2.47	0.47
1:B:253:LEU:HD23	1:B:254:GLN:H	1.80	0.47
1:B:378:THR:HG22	1:B:379:VAL:N	2.29	0.47
1:C:216:LEU:HA	1:C:216:LEU:HD23	1.51	0.47
1:C:261:THR:HG22	1:C:262:VAL:N	2.30	0.47
1:D:142:ASN:ND2	1:D:289:ARG:HG3	2.29	0.47
1:E:57:MET:CA	1:E:96:PRO:HA	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:177:LEU:HD21	1:F:208:LEU:CA	2.39	0.47
1:A:181:ALA:O	1:A:201:MET:HB2	2.14	0.47
1:A:65:SER:C	1:A:67:THR:H	2.18	0.47
1:B:108:LEU:HD11	1:B:120:TRP:NE1	2.30	0.47
1:B:363:ASP:O	1:B:366:MET:HB3	2.14	0.47
1:B:40:VAL:HG12	1:B:41:THR:N	2.30	0.47
1:C:205:ASP:OD1	1:C:209:ASN:ND2	2.48	0.47
1:D:192:THR:HB	1:D:194:LYS:HD3	1.96	0.47
1:E:97:THR:HG23	1:E:223:PRO:HA	1.96	0.47
1:F:322:ALA:HB1	1:F:325:ILE:HB	1.96	0.47
2:H:2:GAL:H3	2:H:3:SIA:O1B	2.13	0.47
1:B:341:MET:HA	1:B:341:MET:HE3	1.96	0.47
1:B:94:THR:O	1:B:94:THR:HG22	2.15	0.47
1:C:209:ASN:O	1:C:212:SER:N	2.48	0.47
1:D:21:ARG:H	1:D:21:ARG:NE	2.13	0.47
1:D:32:GLY:HA3	1:D:36:VAL:HG21	1.96	0.47
1:D:50:GLU:HA	1:D:306:PHE:O	2.15	0.47
1:E:308:ILE:HG21	1:E:310:LEU:HD23	1.95	0.47
1:E:314:TRP:HA	1:E:314:TRP:CE3	2.48	0.47
1:F:105:LEU:HB3	1:F:120:TRP:NE1	2.29	0.47
1:F:180:ASP:HB3	1:F:182:ARG:HG3	1.95	0.47
1:B:75:TRP:CZ2	1:B:300:ARG:HD2	2.49	0.47
1:B:346:THR:CB	1:B:348:VAL:HG12	2.44	0.47
1:B:371:ASP:C	1:B:373:PHE:N	2.67	0.47
1:C:255:PHE:O	1:C:256:THR:HB	2.15	0.47
1:C:122:ALA:O	1:C:271:PRO:HD2	2.15	0.47
1:D:255:PHE:O	1:E:240:PHE:HA	2.15	0.47
1:D:125:VAL:HA	1:D:307:LYS:O	2.14	0.47
1:E:222:TYR:CD1	1:E:222:TYR:N	2.83	0.47
1:E:346:THR:HG22	1:E:348:VAL:HG23	1.96	0.47
1:F:136:LEU:O	1:F:138:VAL:HG22	2.15	0.47
1:C:233:LYS:CD	1:F:350:GLU:HG2	2.43	0.47
1:B:93:ASN:ND2	2:H:2:GAL:H62	2.29	0.47
1:A:192:THR:HB	1:A:194:LYS:HD3	1.97	0.47
1:A:251:PRO:CG	1:B:245:GLY:HA3	2.44	0.47
1:A:367:THR:HB	1:A:378:THR:OG1	2.15	0.47
1:B:177:LEU:HD23	1:B:205:ASP:O	2.15	0.47
1:C:28:LEU:HD23	1:C:29:LEU:C	2.34	0.47
1:C:362:GLY:O	1:C:364:PRO:HD3	2.15	0.47
1:C:66:LEU:HA	1:C:71:GLN:HB2	1.97	0.47
1:D:161:GLN:OE1	1:D:251:PRO:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:LYS:HG3	1:E:152:GLY:H	1.79	0.47
1:E:305:TYR:CD1	1:E:306:PHE:N	2.83	0.47
1:A:165:PHE:HB2	1:A:281:SER:O	2.15	0.47
1:A:239:TYR:CE1	1:E:257:ASN:CB	2.96	0.47
1:A:283:VAL:O	1:A:283:VAL:HG23	2.15	0.47
1:B:31:LYS:HD2	1:C:233:LYS:NZ	2.30	0.47
1:B:321:MET:O	1:B:325:ILE:HG12	2.15	0.47
1:B:41:THR:HB	1:B:45:SER:OG	2.14	0.47
1:C:197:THR:O	1:C:198:LYS:C	2.54	0.47
1:C:288:TRP:CB	1:C:297:HIS:HB3	2.45	0.47
1:C:67:THR:OG1	1:C:68:GLU:N	2.47	0.47
1:F:52:PHE:HA	1:F:304:ARG:O	2.15	0.47
1:F:325:ILE:HD13	1:F:328:LEU:HD23	1.97	0.47
1:B:49:ILE:HG12	1:F:351:VAL:HG22	1.97	0.47
1:A:167:VAL:HG13	1:A:280:LEU:HD22	1.96	0.46
1:A:288:TRP:HB2	1:A:297:HIS:HD2	1.80	0.46
1:A:96:PRO:HG3	1:A:299:TRP:CZ2	2.50	0.46
1:C:123:VAL:HG13	1:C:264:LEU:CD1	2.44	0.46
1:C:91:GLY:O	1:C:94:THR:HB	2.15	0.46
1:D:177:LEU:CD2	1:D:207:VAL:O	2.63	0.46
1:D:234:ASN:N	1:D:234:ASN:HD22	2.13	0.46
1:F:125:VAL:HA	1:F:307:LYS:O	2.15	0.46
1:A:196:ILE:HG21	1:A:227:TRP:CH2	2.50	0.46
1:A:265:ASP:CG	1:A:269:VAL:HB	2.35	0.46
1:B:104:GLN:NE2	1:B:105:LEU:N	2.63	0.46
1:D:94:THR:O	1:D:94:THR:HG22	2.16	0.46
1:E:194:LYS:C	1:E:196:ILE:N	2.68	0.46
1:E:50:GLU:HG3	1:E:307:LYS:HG3	1.96	0.46
1:F:107:MET:C	1:F:108:LEU:HD12	2.36	0.46
1:F:279:TYR:C	1:F:280:LEU:HD23	2.35	0.46
1:A:194:LYS:CD	1:A:194:LYS:H	2.27	0.46
1:A:233:LYS:HE2	1:A:234:ASN:ND2	2.30	0.46
1:A:253:LEU:O	1:B:242:ASN:HB2	2.16	0.46
1:A:318:PRO:C	1:A:320:PRO:HD2	2.35	0.46
1:B:152:GLY:O	1:B:153:ILE:HD13	2.14	0.46
1:B:164:VAL:CG2	1:B:241:GLY:HA3	2.45	0.46
1:B:257:ASN:ND2	1:B:257:ASN:H	2.05	0.46
1:C:341:MET:HE1	1:C:347:GLN:HB2	1.98	0.46
1:D:93:ASN:ND2	1:D:93:ASN:H	2.13	0.46
1:A:208:LEU:N	1:E:54:ASN:HD21	2.12	0.46
1:E:71:GLN:HE21	1:E:73:TYR:HB2	1.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:182:ARG:HG3	1:F:183:THR:N	2.30	0.46
1:F:228:HIS:HB3	1:F:229:PRO:HD2	1.98	0.46
1:C:350:GLU:CG	1:F:233:LYS:HB3	2.43	0.46
1:B:219:ASP:CB	1:F:338:GLY:HA2	2.42	0.46
1:F:84:SER:O	1:F:86:THR:N	2.48	0.46
1:A:237:THR:O	1:E:257:ASN:ND2	2.49	0.46
1:A:239:TYR:C	1:A:240:PHE:CD1	2.88	0.46
1:A:259:LEU:HD13	1:A:260:THR:N	2.31	0.46
1:B:262:VAL:HG12	1:B:264:LEU:N	2.17	0.46
1:C:194:LYS:O	1:C:196:ILE:N	2.48	0.46
1:D:178:VAL:CG2	1:D:179:THR:N	2.69	0.46
1:D:243:TYR:CZ	1:D:245:GLY:CA	2.99	0.46
1:D:346:THR:C	1:D:348:VAL:H	2.16	0.46
1:D:60:PRO:CB	1:D:61:PRO:HD2	2.44	0.46
1:F:209:ASN:HD21	1:F:211:ILE:HB	1.80	0.46
1:B:125:VAL:HG11	1:B:263:LEU:HD21	1.95	0.46
1:B:103:LEU:O	1:B:277:GLY:HA2	2.15	0.46
1:B:35:GLU:O	1:B:36:VAL:C	2.53	0.46
1:D:243:TYR:CZ	1:D:245:GLY:HA2	2.50	0.46
1:D:274:LYS:C	1:D:275:GLY:O	2.50	0.46
1:D:224:VAL:CG2	1:D:283:VAL:HG11	2.42	0.46
1:A:180:ASP:C	1:A:182:ARG:H	2.17	0.46
1:A:77:ARG:HB2	1:A:93:ASN:HB2	1.97	0.46
1:B:108:LEU:HB3	1:B:118:GLN:HG3	1.97	0.46
1:B:310:LEU:N	1:B:310:LEU:HD12	2.28	0.46
1:C:145:THR:OG1	1:C:153:ILE:N	2.49	0.46
1:C:175:GLN:NE2	1:C:176:GLY:N	2.60	0.46
1:B:251:PRO:HB2	1:C:243:TYR:HE2	1.81	0.46
1:D:50:GLU:OE2	1:E:233:LYS:CA	2.63	0.46
1:D:69:GLY:C	1:D:71:GLN:N	2.69	0.46
1:E:141:PHE:CD1	1:E:292:ARG:HG3	2.47	0.46
1:F:139:HIS:HB2	1:F:140:GLY:H	1.65	0.46
1:F:265:ASP:OD1	1:F:269:VAL:N	2.48	0.46
2:K:2:GAL:H3	2:K:3:SIA:O1B	2.11	0.46
1:A:271:PRO:C	1:A:272:LEU:HG	2.36	0.46
1:A:288:TRP:CE3	1:A:299:TRP:CG	3.04	0.46
1:A:56:ARG:CB	1:A:56:ARG:HH11	2.28	0.46
1:A:88:ASP:O	1:A:184:LYS:HB2	2.16	0.46
1:B:104:GLN:C	1:B:105:LEU:HD12	2.36	0.46
1:B:265:ASP:OD1	1:B:269:VAL:HB	2.15	0.46
1:C:300:ARG:NH1	1:C:300:ARG:HG3	2.29	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:341:MET:C	1:D:346:THR:HG23	2.36	0.46
1:E:197:THR:HG23	1:E:199:LYS:O	2.15	0.46
1:F:285:ILE:N	1:F:285:ILE:CD1	2.78	0.46
1:A:257:ASN:HD22	1:B:239:TYR:N	2.13	0.46
1:A:297:HIS:CG	1:E:153:ILE:HG12	2.50	0.46
1:B:152:GLY:HA2	1:C:295:ASP:O	2.15	0.46
1:B:219:ASP:C	1:B:221:MET:N	2.68	0.46
1:D:192:THR:HG21	1:D:194:LYS:HE2	1.98	0.46
1:D:291:THR:OG1	1:D:296:VAL:HB	2.16	0.46
1:D:39:LEU:HD12	1:D:40:VAL:N	2.30	0.46
1:C:141:PHE:HD2	1:D:84:SER:HA	1.81	0.46
1:E:43:PRO:O	1:E:312:LYS:HD2	2.16	0.46
1:F:25:VAL:HG13	1:F:26:PRO:HD2	1.98	0.46
1:F:54:ASN:HD22	1:F:55:PRO:HD2	1.80	0.46
1:A:333:LEU:HA	1:A:334:PRO:HD3	1.52	0.46
1:A:375:LYS:HE3	1:A:375:LYS:HB2	1.63	0.46
1:B:107:MET:C	1:B:108:LEU:HD12	2.36	0.46
1:B:111:ASP:C	1:B:113:THR:H	2.20	0.46
1:B:25:VAL:CG1	1:B:26:PRO:HD2	2.45	0.46
1:C:28:LEU:C	1:C:28:LEU:HD23	2.35	0.46
1:D:145:THR:HG21	1:E:297:HIS:CE1	2.46	0.46
1:D:239:TYR:C	1:D:240:PHE:CG	2.89	0.46
1:D:55:PRO:HD3	1:D:303:PRO:CB	2.46	0.46
1:F:191:VAL:HA	1:F:195:THR:HG21	1.98	0.46
1:F:190:VAL:HG23	1:F:223:PRO:HD3	1.97	0.46
1:A:177:LEU:HD23	1:A:177:LEU:HA	1.70	0.46
1:A:243:TYR:CE2	1:E:251:PRO:HB2	2.50	0.46
1:A:93:ASN:OD1	1:A:93:ASN:N	2.49	0.46
1:B:185:TYR:CG	1:B:192:THR:HG21	2.49	0.46
1:B:31:LYS:HD2	1:C:233:LYS:HZ2	1.81	0.46
1:B:380:PHE:HA	1:B:381:PRO:HD2	1.59	0.46
1:B:56:ARG:CZ	1:B:56:ARG:HB2	2.45	0.46
1:C:103:LEU:N	1:C:103:LEU:HD22	2.31	0.46
1:D:218:LYS:HB3	1:D:219:ASP:H	1.42	0.46
1:D:319:TYR:CB	1:D:324:LEU:HD23	2.46	0.46
1:E:259:LEU:HA	1:E:259:LEU:HD13	1.46	0.46
1:F:174:LEU:HD12	1:F:174:LEU:H	1.81	0.46
1:F:95:LEU:HA	1:F:96:PRO:HD2	1.75	0.46
1:A:196:ILE:HG21	1:A:227:TRP:HH2	1.81	0.45
1:B:90:PRO:HD2	1:B:186:LYS:HZ3	1.81	0.45
1:B:274:LYS:C	1:B:275:GLY:O	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:ARG:C	1:B:373:PHE:CD1	2.89	0.45
1:B:86:THR:HG23	1:B:87:GLU:H	1.82	0.45
1:C:105:LEU:CB	1:C:120:TRP:CD1	2.96	0.45
1:C:186:LYS:C	1:C:188:GLU:N	2.69	0.45
1:C:191:VAL:HG21	1:C:222:TYR:CG	2.50	0.45
1:D:302:LEU:HB3	1:D:303:PRO:HD2	1.98	0.45
1:D:59:GLN:HA	1:D:60:PRO:HD2	1.81	0.45
1:E:207:VAL:CG2	1:E:208:LEU:N	2.78	0.45
1:E:223:PRO:CG	1:E:226:ILE:HD12	2.45	0.45
1:F:172:LEU:HD22	1:F:172:LEU:C	2.37	0.45
1:F:176:GLY:O	1:F:177:LEU:HD23	2.16	0.45
1:F:32:GLY:CA	1:F:36:VAL:HG21	2.46	0.45
1:F:59:GLN:HE22	1:F:69:GLY:HA3	1.80	0.45
1:A:87:GLU:HA	1:A:184:LYS:NZ	2.31	0.45
1:C:315:VAL:HG23	1:C:316:LYS:O	2.16	0.45
1:D:95:LEU:HA	1:D:96:PRO:HD2	1.67	0.45
1:F:262:VAL:HG12	1:F:264:LEU:N	2.19	0.45
1:A:174:LEU:HD13	1:A:227:TRP:HB3	1.97	0.45
1:A:233:LYS:CG	1:A:234:ASN:N	2.79	0.45
1:A:60:PRO:HB2	1:A:61:PRO:HD2	1.97	0.45
1:A:85:ASP:O	1:A:182:ARG:NH1	2.50	0.45
1:B:103:LEU:HB2	1:B:278:LEU:HB3	1.98	0.45
1:B:205:ASP:HA	1:B:209:ASN:CB	2.37	0.45
1:B:233:LYS:C	1:B:234:ASN:HD22	2.20	0.45
1:B:55:PRO:HB3	1:B:302:LEU:O	2.17	0.45
1:C:223:PRO:HG3	1:C:226:ILE:HD12	1.98	0.45
1:D:252:VAL:HA	1:E:243:TYR:O	2.16	0.45
1:D:315:VAL:HG23	1:D:316:LYS:N	2.29	0.45
1:E:115:ASP:O	1:E:316:LYS:HA	2.16	0.45
1:E:134:SER:C	1:E:136:LEU:H	2.19	0.45
1:E:360:VAL:HA	1:E:361:PRO:HD2	1.60	0.45
1:F:103:LEU:HA	1:F:103:LEU:HD13	1.62	0.45
1:F:204:LYS:HB3	1:F:204:LYS:HZ3	1.80	0.45
1:F:57:MET:CB	1:F:96:PRO:HB3	2.47	0.45
1:A:114:CYS:C	1:A:116:THR:H	2.20	0.45
1:B:232:ALA:C	1:B:234:ASN:N	2.70	0.45
1:C:56:ARG:HH22	1:C:219:ASP:CG	2.19	0.45
1:E:178:VAL:CG2	1:E:179:THR:H	2.25	0.45
1:F:112:LEU:HD12	1:F:113:THR:N	2.32	0.45
1:F:79:ILE:HD13	1:F:94:THR:HG23	1.97	0.45
1:A:172:LEU:C	1:A:172:LEU:HD22	2.37	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:CG2	1:A:292:ARG:HH21	2.28	0.45
1:A:57:MET:SD	1:A:301:GLY:HA3	2.57	0.45
1:A:75:TRP:NE1	1:A:300:ARG:HB2	2.32	0.45
1:B:130:VAL:O	1:B:302:LEU:HD22	2.16	0.45
1:B:193:ILE:O	1:B:197:THR:HG22	2.17	0.45
1:C:142:ASN:HD21	1:C:289:ARG:HG3	1.81	0.45
1:C:339:GLN:HB3	1:C:340:PRO:HD2	1.98	0.45
1:D:164:VAL:HA	1:D:241:GLY:HA3	1.98	0.45
1:D:161:GLN:NE2	1:D:251:PRO:HA	2.31	0.45
1:D:251:PRO:HD2	1:E:245:GLY:CA	2.43	0.45
1:D:66:LEU:CB	1:D:71:GLN:HB2	2.29	0.45
1:E:185:TYR:HB2	1:E:194:LYS:CE	2.47	0.45
1:D:133:GLY:HA3	1:E:228:HIS:CE1	2.51	0.45
1:E:264:LEU:HD12	1:E:270:GLY:HA3	1.99	0.45
1:A:145:THR:OG1	1:A:153:ILE:HB	2.16	0.45
1:A:300:ARG:HG3	1:A:301:GLY:H	1.80	0.45
1:B:265:ASP:CG	1:B:269:VAL:HB	2.37	0.45
1:D:280:LEU:HD23	1:D:280:LEU:HA	1.63	0.45
1:E:291:THR:O	1:E:293:ASN:N	2.50	0.45
1:F:197:THR:O	1:F:197:THR:CG2	2.64	0.45
1:F:29:LEU:HD23	1:F:29:LEU:HA	1.55	0.45
1:A:370:VAL:HA	1:A:374:GLY:O	2.17	0.45
1:B:105:LEU:N	1:B:105:LEU:CD1	2.79	0.45
1:B:126:LYS:HG2	1:B:260:THR:HG23	1.98	0.45
1:B:339:GLN:CG	1:B:340:PRO:HD2	2.45	0.45
1:B:95:LEU:HA	1:B:96:PRO:HD2	1.60	0.45
1:C:288:TRP:HA	1:C:299:TRP:CB	2.46	0.45
1:C:322:ALA:O	1:C:326:SER:HB2	2.16	0.45
1:C:325:ILE:O	1:C:328:LEU:HB2	2.16	0.45
1:D:348:VAL:CG1	1:D:348:VAL:O	2.63	0.45
1:D:79:ILE:HA	1:D:79:ILE:HD13	1.69	0.45
1:E:112:LEU:HD23	1:E:112:LEU:HA	1.58	0.45
1:E:114:CYS:C	1:E:116:THR:H	2.20	0.45
1:E:118:GLN:HB2	1:E:314:TRP:CH2	2.49	0.45
1:E:136:LEU:HD23	1:E:136:LEU:HA	1.68	0.45
1:E:245:GLY:O	1:E:249:THR:HG21	2.17	0.45
1:E:291:THR:HB	1:E:293:ASN:HB3	1.98	0.45
1:E:143:LYS:NZ	1:E:295:ASP:OD2	2.46	0.45
1:F:194:LYS:HA	1:F:197:THR:O	2.16	0.45
1:F:55:PRO:HD3	1:F:303:PRO:CB	2.46	0.45
1:B:93:ASN:HD21	2:H:2:GAL:H62	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:CD1	1:A:105:LEU:N	2.79	0.45
1:A:88:ASP:O	1:A:184:LYS:HD3	2.17	0.45
1:A:264:LEU:HA	1:A:264:LEU:HD12	1.68	0.45
1:A:300:ARG:CG	1:A:301:GLY:N	2.80	0.45
1:B:290:VAL:HG13	1:B:297:HIS:HA	1.99	0.45
1:B:52:PHE:CD2	1:C:208:LEU:CD2	2.99	0.45
1:B:62:THR:O	1:B:64:GLU:N	2.48	0.45
1:C:105:LEU:HD21	1:C:310:LEU:HD22	1.99	0.45
1:C:194:LYS:O	1:C:197:THR:N	2.50	0.45
1:C:162:TYR:CE2	1:C:224:VAL:HG11	2.52	0.45
1:C:165:PHE:O	1:C:239:TYR:HA	2.17	0.45
1:D:228:HIS:HB3	1:D:229:PRO:HD2	1.99	0.45
1:D:327:SER:O	1:D:330:ASN:N	2.49	0.45
1:E:300:ARG:HG3	1:E:301:GLY:N	2.32	0.45
1:E:43:PRO:CG	1:E:44:ASP:H	2.30	0.45
1:A:263:LEU:N	1:A:263:LEU:HD23	2.32	0.45
1:A:328:LEU:CG	1:A:333:LEU:CD2	2.84	0.45
1:A:369:TYR:N	1:A:369:TYR:HD1	2.15	0.45
1:B:151:LYS:HD3	1:B:151:LYS:HA	1.59	0.45
1:B:341:MET:HA	1:B:346:THR:HG23	1.98	0.45
1:C:52:PHE:CD1	1:D:208:LEU:CD2	2.99	0.45
1:D:30:ILE:CD1	1:D:39:LEU:HD23	2.47	0.45
1:E:239:TYR:C	1:E:240:PHE:CD1	2.90	0.45
1:E:254:GLN:HA	1:E:254:GLN:OE1	2.17	0.45
1:A:224:VAL:CG1	1:A:283:VAL:HG11	2.47	0.45
1:A:372:ARG:NH1	1:A:372:ARG:HB2	2.13	0.45
1:A:365:ASP:HB3	1:A:380:PHE:HE2	1.82	0.45
1:B:172:LEU:CD2	1:B:173:ASP:N	2.80	0.45
1:C:100:MET:HB2	1:C:280:LEU:O	2.17	0.45
1:C:354:TYR:CD1	1:C:354:TYR:N	2.85	0.45
1:E:232:ALA:HB3	1:E:235:GLU:OE1	2.16	0.45
1:D:257:ASN:HD22	1:E:238:ARG:HA	1.78	0.45
1:E:117:LEU:O	1:E:314:TRP:HE3	2.00	0.45
1:E:325:ILE:O	1:E:326:SER:C	2.55	0.45
1:E:57:MET:HA	1:E:96:PRO:HA	1.98	0.45
1:F:161:GLN:OE1	1:F:251:PRO:HA	2.17	0.45
1:A:125:VAL:N	1:A:261:THR:O	2.49	0.44
1:B:302:LEU:HB3	1:B:303:PRO:HD2	1.99	0.44
1:B:78:GLY:C	1:B:79:ILE:HD13	2.38	0.44
1:C:67:THR:OG1	1:C:68:GLU:HG3	2.16	0.44
1:C:79:ILE:HA	1:C:79:ILE:HD13	1.71	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:PHE:CD1	1:D:292:ARG:CB	3.01	0.44
1:D:90:PRO:HD2	1:D:186:LYS:CE	2.46	0.44
1:E:104:GLN:HE21	1:E:105:LEU:N	2.13	0.44
1:F:193:ILE:HG12	1:F:201:MET:HE1	1.97	0.44
1:F:91:GLY:H	1:F:186:LYS:NZ	2.15	0.44
1:A:207:VAL:HB	1:E:54:ASN:ND2	2.32	0.44
1:A:352:ARG:HG3	1:A:354:TYR:HE1	1.81	0.44
1:A:366:MET:HA	1:A:380:PHE:CZ	2.53	0.44
1:A:79:ILE:HG21	1:E:153:ILE:HD11	1.98	0.44
1:B:180:ASP:C	1:B:182:ARG:H	2.20	0.44
1:B:203:ASN:N	1:B:203:ASN:OD1	2.47	0.44
1:B:358:GLU:OE2	1:B:368:ARG:NH2	2.50	0.44
1:C:139:HIS:HD2	1:D:88:ASP:OD1	2.00	0.44
1:E:174:LEU:HD11	1:E:215:LYS:O	2.17	0.44
1:F:208:LEU:C	1:F:208:LEU:HD23	2.37	0.44
1:A:138:VAL:CB	1:A:153:ILE:HG23	2.39	0.44
1:A:104:GLN:HE22	1:A:276:GLU:HB2	1.81	0.44
1:A:89:SER:HA	1:A:184:LYS:HB2	1.99	0.44
1:A:52:PHE:CD2	1:B:208:LEU:HD13	2.52	0.44
1:B:76:SER:CB	1:B:299:TRP:CE3	3.01	0.44
1:B:318:PRO:CG	1:B:319:TYR:H	2.27	0.44
1:B:341:MET:HA	1:B:346:THR:CG2	2.47	0.44
1:D:151:LYS:HD3	1:D:151:LYS:HA	1.79	0.44
1:D:216:LEU:HA	1:D:216:LEU:HD23	1.70	0.44
1:D:50:GLU:HG2	1:D:305:TYR:CZ	2.51	0.44
1:D:335:GLN:HA	1:D:335:GLN:HE21	1.83	0.44
1:E:155:THR:HA	1:E:156:PRO:HD2	1.87	0.44
1:E:118:GLN:HA	1:E:313:ARG:O	2.17	0.44
1:E:318:PRO:HG2	1:E:319:TYR:N	2.31	0.44
1:E:46:VAL:CG1	1:E:47:THR:N	2.78	0.44
1:F:342:GLU:HG2	1:F:343:GLY:N	2.33	0.44
1:A:193:ILE:N	1:A:193:ILE:HD12	2.33	0.44
1:A:192:THR:CB	1:A:194:LYS:HE2	2.47	0.44
1:B:105:LEU:HB3	1:B:120:TRP:NE1	2.32	0.44
1:B:85:ASP:OD2	1:B:182:ARG:NH1	2.50	0.44
1:C:37:LEU:HA	1:C:37:LEU:HD12	1.76	0.44
1:D:161:GLN:HE22	1:D:251:PRO:CA	2.31	0.44
1:D:305:TYR:CG	1:D:306:PHE:N	2.85	0.44
1:E:131:GLY:O	1:E:134:SER:HB3	2.17	0.44
1:E:164:VAL:HG12	1:E:165:PHE:N	2.32	0.44
1:E:217:ASP:C	1:E:218:LYS:HD2	2.38	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:21:ARG:HA	1:E:22:PRO:HD2	1.74	0.44
1:F:177:LEU:HD23	1:F:177:LEU:HA	1.64	0.44
1:A:164:VAL:HG12	1:A:165:PHE:N	2.32	0.44
1:A:196:ILE:HG13	1:A:197:THR:N	2.31	0.44
1:A:238:ARG:HA	1:E:257:ASN:HD22	1.83	0.44
1:A:288:TRP:CZ3	1:A:299:TRP:CG	3.05	0.44
1:A:336:VAL:CG2	1:A:337:GLN:N	2.70	0.44
1:A:54:ASN:ND2	1:B:207:VAL:HB	2.32	0.44
1:C:350:GLU:HG3	1:F:233:LYS:NZ	2.33	0.44
1:D:246:GLY:HA3	1:D:249:THR:OG1	2.16	0.44
1:D:259:LEU:HA	1:D:259:LEU:HD13	1.81	0.44
1:D:308:ILE:N	1:D:308:ILE:CD1	2.78	0.44
1:E:250:PRO:HA	1:E:251:PRO:HD3	1.54	0.44
1:E:370:VAL:HG22	1:E:375:LYS:HA	1.99	0.44
1:E:89:SER:OG	1:E:186:LYS:NZ	2.51	0.44
1:F:111:ASP:C	1:F:113:THR:H	2.21	0.44
1:F:94:THR:HG22	1:F:94:THR:O	2.17	0.44
1:A:194:LYS:C	1:A:196:ILE:N	2.70	0.44
1:A:339:GLN:HA	1:A:340:PRO:HD2	1.57	0.44
1:B:193:ILE:HG12	1:B:201:MET:CE	2.47	0.44
1:C:125:VAL:HG23	1:C:308:ILE:HG13	1.99	0.44
1:D:264:LEU:HG	1:D:268:GLY:HA2	1.99	0.44
1:D:321:MET:O	1:D:324:LEU:N	2.50	0.44
1:E:285:ILE:N	1:E:285:ILE:CD1	2.79	0.44
1:F:177:LEU:CD2	1:F:205:ASP:O	2.65	0.44
1:F:211:ILE:N	1:F:211:ILE:CD1	2.81	0.44
1:A:255:PHE:HE2	1:B:162:TYR:CE2	2.35	0.44
1:A:59:GLN:HG3	1:A:60:PRO:O	2.17	0.44
1:B:97:THR:HG22	1:B:222:TYR:C	2.38	0.44
1:C:209:ASN:C	1:C:211:ILE:H	2.20	0.44
1:D:60:PRO:HB2	1:D:61:PRO:HD2	1.99	0.44
1:E:201:MET:HE2	1:E:201:MET:HB3	1.87	0.44
1:E:50:GLU:HA	1:E:306:PHE:O	2.18	0.44
1:F:141:PHE:CE2	1:F:292:ARG:NH1	2.85	0.44
1:F:164:VAL:HA	1:F:240:PHE:O	2.17	0.44
1:A:104:GLN:HE21	1:A:105:LEU:N	2.16	0.44
1:A:216:LEU:HD23	1:A:216:LEU:HA	1.84	0.44
1:B:367:THR:HB	1:B:378:THR:CB	2.48	0.44
1:C:175:GLN:OE1	1:C:208:LEU:CD1	2.66	0.44
1:C:239:TYR:C	1:C:239:TYR:CD1	2.91	0.44
1:D:142:ASN:HA	1:D:290:VAL:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:GLN:HB2	1:E:230:ASP:CB	2.45	0.44
1:E:229:PRO:HG2	1:E:229:PRO:O	2.18	0.44
1:E:166:ALA:CA	1:E:238:ARG:O	2.66	0.44
1:E:313:ARG:CG	1:E:313:ARG:NH1	2.77	0.44
1:E:65:SER:C	1:E:67:THR:H	2.21	0.44
1:C:350:GLU:HG3	1:F:233:LYS:CB	2.48	0.44
1:A:161:GLN:OE1	1:A:251:PRO:HA	2.18	0.44
1:A:233:LYS:CG	1:A:234:ASN:H	2.30	0.44
1:A:243:TYR:OH	1:A:245:GLY:HA2	2.18	0.44
1:A:300:ARG:HG3	1:A:300:ARG:HH11	1.83	0.44
1:B:30:ILE:HG23	1:F:353:VAL:CG2	2.47	0.44
1:B:319:TYR:HA	1:B:320:PRO:HD3	1.66	0.44
1:C:177:LEU:HA	1:C:205:ASP:O	2.18	0.44
1:C:323:SER:O	1:C:327:SER:N	2.51	0.44
1:D:186:LYS:H	1:D:186:LYS:CD	2.26	0.44
1:D:169:GLY:HA3	1:D:272:LEU:O	2.17	0.44
1:E:174:LEU:HD12	1:E:174:LEU:H	1.82	0.44
1:E:363:ASP:HA	1:E:364:PRO:HD3	1.67	0.44
1:F:166:ALA:HB2	1:F:239:TYR:HB3	2.00	0.44
1:F:175:GLN:NE2	1:F:176:GLY:O	2.51	0.44
1:F:91:GLY:H	1:F:186:LYS:HZ1	1.65	0.44
1:F:269:VAL:CG1	1:F:272:LEU:HD11	2.48	0.44
1:A:136:LEU:HA	1:A:136:LEU:HD23	1.57	0.43
1:A:286:MET:HA	1:A:286:MET:CE	2.48	0.43
1:B:98:TRP:HH2	1:B:164:VAL:HG12	1.83	0.43
1:C:117:LEU:HD13	1:C:118:GLN:H	1.83	0.43
1:C:233:LYS:HE3	1:C:233:LYS:HB2	1.25	0.43
1:D:327:SER:O	1:D:328:LEU:C	2.56	0.43
1:E:103:LEU:HD22	1:E:103:LEU:N	2.33	0.43
1:E:105:LEU:CD1	1:E:105:LEU:N	2.78	0.43
1:E:232:ALA:C	1:E:234:ASN:H	2.21	0.43
1:F:168:GLY:N	1:F:237:THR:HG23	2.31	0.43
1:A:100:MET:C	1:A:100:MET:SD	2.97	0.43
1:A:138:VAL:O	1:A:153:ILE:HG23	2.18	0.43
1:B:129:VAL:HB	1:B:253:LEU:HD21	1.98	0.43
1:B:177:LEU:HA	1:B:177:LEU:HD23	1.75	0.43
1:B:255:PHE:HA	1:B:255:PHE:HD1	1.70	0.43
1:D:133:GLY:CA	1:E:228:HIS:CE1	2.97	0.43
1:E:219:ASP:C	1:E:221:MET:N	2.72	0.43
1:E:72:TYR:O	1:E:73:TYR:C	2.57	0.43
1:F:290:VAL:HG22	1:F:297:HIS:HD2	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TRP:CE2	1:B:300:ARG:HD2	2.53	0.43
1:B:368:ARG:HG2	1:B:375:LYS:HE3	1.99	0.43
1:C:144:PRO:HD3	1:C:292:ARG:HG2	1.98	0.43
1:C:288:TRP:HZ3	1:C:299:TRP:CE2	2.37	0.43
1:C:50:GLU:CG	1:C:307:LYS:HG3	2.49	0.43
1:C:321:MET:O	1:C:325:ILE:HG22	2.18	0.43
1:D:150:THR:HG22	1:D:150:THR:O	2.18	0.43
1:D:91:GLY:H	1:D:186:LYS:CE	2.32	0.43
1:D:76:SER:CB	1:D:299:TRP:HE3	2.31	0.43
1:E:185:TYR:HB2	1:E:194:LYS:NZ	2.33	0.43
1:E:39:LEU:O	1:E:40:VAL:C	2.56	0.43
1:E:91:GLY:H	1:E:186:LYS:HE3	1.82	0.43
1:F:111:ASP:O	1:F:113:THR:N	2.51	0.43
1:F:123:VAL:O	1:F:263:LEU:N	2.50	0.43
1:F:162:TYR:CE1	1:F:283:VAL:HG21	2.53	0.43
1:A:170:GLU:OE2	1:A:274:LYS:HD2	2.18	0.43
1:B:153:ILE:HD11	1:C:297:HIS:CB	2.48	0.43
1:B:193:ILE:HG22	1:B:212:SER:HB3	2.00	0.43
1:B:209:ASN:HA	1:B:210:PRO:HD3	1.88	0.43
1:B:216:LEU:HA	1:B:216:LEU:HD23	1.64	0.43
1:B:57:MET:HB2	1:B:96:PRO:HB3	1.99	0.43
1:D:105:LEU:HB3	1:D:120:TRP:CD1	2.54	0.43
1:D:125:VAL:N	1:D:261:THR:O	2.51	0.43
1:D:25:VAL:CG2	1:D:26:PRO:HD2	2.44	0.43
1:D:287:GLY:C	1:D:299:TRP:HB2	2.38	0.43
1:D:300:ARG:HG3	1:D:301:GLY:N	2.32	0.43
1:E:288:TRP:HE3	1:E:299:TRP:CG	2.36	0.43
1:F:216:LEU:HA	1:F:216:LEU:HD23	1.52	0.43
1:F:59:GLN:NE2	1:F:69:GLY:HA3	2.34	0.43
1:B:78:GLY:HA3	2:H:2:GAL:O3	2.18	0.43
1:B:92:ASN:HD21	1:B:190:VAL:HG12	1.83	0.43
1:B:161:GLN:CD	1:B:251:PRO:HA	2.38	0.43
1:B:288:TRP:HE3	1:B:299:TRP:HB3	1.82	0.43
1:C:41:THR:HB	1:C:45:SER:CB	2.47	0.43
1:B:139:HIS:HD2	1:C:88:ASP:OD2	2.01	0.43
1:D:29:LEU:HA	1:D:29:LEU:HD23	1.48	0.43
1:E:239:TYR:C	1:E:240:PHE:CG	2.91	0.43
1:F:224:VAL:CG2	1:F:283:VAL:HG11	2.48	0.43
1:F:239:TYR:C	1:F:240:PHE:CG	2.92	0.43
1:F:124:SER:HA	1:F:261:THR:O	2.19	0.43
1:F:328:LEU:HG	1:F:329:PHE:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:GLY:O	1:F:94:THR:N	2.49	0.43
1:A:198:LYS:H	1:A:198:LYS:HG2	1.26	0.43
1:A:265:ASP:OD1	1:A:269:VAL:HB	2.18	0.43
1:B:182:ARG:O	1:B:184:LYS:HD2	2.18	0.43
1:B:194:LYS:O	1:B:195:THR:C	2.56	0.43
1:B:232:ALA:C	1:B:234:ASN:H	2.21	0.43
1:B:304:ARG:HD3	1:B:306:PHE:CE1	2.52	0.43
1:B:358:GLU:HB2	1:B:359:PRO:HD2	2.00	0.43
1:B:83:THR:CB	1:B:87:GLU:HB3	2.39	0.43
1:C:203:ASN:OD1	1:C:203:ASN:N	2.52	0.43
1:C:69:GLY:HA3	1:C:71:GLN:OE1	2.19	0.43
1:D:194:LYS:C	1:D:196:ILE:N	2.71	0.43
1:D:165:PHE:CE1	1:D:240:PHE:CD1	3.07	0.43
1:D:82:ALA:HB1	1:D:87:GLU:O	2.18	0.43
1:E:283:VAL:O	1:E:283:VAL:HG23	2.17	0.43
1:F:78:GLY:HA3	2:L:2:GAL:C4	2.49	0.43
1:A:328:LEU:HD23	1:A:333:LEU:HD11	2.01	0.43
1:A:95:LEU:HA	1:A:96:PRO:HD2	1.71	0.43
1:B:236:ASN:O	1:B:271:PRO:HB3	2.18	0.43
1:B:30:ILE:HG23	1:B:36:VAL:HG13	2.00	0.43
1:C:115:ASP:O	1:C:116:THR:C	2.57	0.43
1:D:133:GLY:N	1:E:228:HIS:CE1	2.72	0.43
1:F:123:VAL:HB	1:F:309:THR:O	2.19	0.43
1:F:250:PRO:HA	1:F:251:PRO:HD3	1.77	0.43
1:F:288:TRP:HZ3	1:F:299:TRP:CE2	2.35	0.43
1:F:80:ASN:OD1	1:F:90:PRO:O	2.36	0.43
1:A:261:THR:CG2	1:A:262:VAL:N	2.81	0.43
1:A:278:LEU:HD22	1:A:280:LEU:HD23	1.99	0.43
1:B:250:PRO:HA	1:B:251:PRO:HD3	1.55	0.43
1:C:161:GLN:HE22	1:C:251:PRO:CA	2.25	0.43
1:C:205:ASP:O	1:C:207:VAL:N	2.51	0.43
1:C:350:GLU:CD	1:C:351:VAL:N	2.71	0.43
1:C:95:LEU:HA	1:C:96:PRO:HD2	1.86	0.43
1:E:175:GLN:HA	1:E:213:LYS:HA	1.99	0.43
1:A:231:PRO:HG2	1:E:305:TYR:CD2	2.53	0.43
1:F:105:LEU:HD23	1:F:120:TRP:CD2	2.54	0.43
1:F:184:LYS:O	1:F:186:LYS:HE2	2.19	0.43
1:F:54:ASN:HD22	1:F:303:PRO:HB3	1.83	0.43
1:F:317:ASN:HD22	1:F:318:PRO:N	2.16	0.43
1:F:322:ALA:C	1:F:324:LEU:N	2.69	0.43
1:A:340:PRO:O	1:A:346:THR:HA	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ASN:HD21	1:C:239:TYR:N	2.14	0.43
1:C:233:LYS:CG	1:C:234:ASN:N	2.82	0.43
1:C:308:ILE:HG22	1:C:309:THR:N	2.33	0.43
1:D:175:GLN:HG3	1:D:213:LYS:CG	2.28	0.43
1:D:302:LEU:HA	1:D:302:LEU:HD23	1.86	0.43
1:E:125:VAL:CG1	1:E:125:VAL:O	2.65	0.43
1:E:129:VAL:HB	1:E:253:LEU:HD21	2.00	0.43
1:E:284:ASP:OD1	1:E:304:ARG:NH1	2.51	0.43
1:F:278:LEU:HD22	1:F:280:LEU:CD2	2.46	0.43
1:F:291:THR:HB	1:F:293:ASN:HB3	2.00	0.43
1:F:361:PRO:HG2	1:F:364:PRO:HG3	2.00	0.43
2:J:2:GAL:H3	2:J:3:SIA:O1B	2.16	0.43
1:A:215:LYS:O	1:A:222:TYR:CZ	2.72	0.43
1:A:280:LEU:HD13	1:A:306:PHE:CD2	2.54	0.43
1:A:82:ALA:HB2	1:A:88:ASP:OD1	2.19	0.43
1:B:153:ILE:CD1	1:C:79:ILE:HG21	2.48	0.43
1:B:288:TRP:CE3	1:B:299:TRP:HB3	2.54	0.43
1:D:288:TRP:HA	1:D:299:TRP:CB	2.49	0.43
1:E:160:SER:HA	1:E:244:THR:O	2.17	0.43
1:E:144:PRO:HD3	1:E:292:ARG:HD3	2.01	0.43
1:E:363:ASP:O	1:E:366:MET:HB3	2.18	0.43
1:E:82:ALA:CB	1:E:88:ASP:HA	2.49	0.43
1:F:23:ALA:HA	1:F:24:PRO:HD3	1.74	0.43
1:F:305:TYR:C	1:F:306:PHE:CD1	2.92	0.43
1:F:97:THR:HG22	1:F:223:PRO:CA	2.49	0.43
1:A:176:GLY:C	1:A:177:LEU:HG	2.38	0.42
1:C:249:THR:HA	1:C:250:PRO:HD3	1.61	0.42
1:C:337:GLN:HB2	1:C:338:GLY:H	1.67	0.42
1:E:265:ASP:OD1	1:E:269:VAL:N	2.49	0.42
1:E:318:PRO:HG2	1:E:319:TYR:CG	2.54	0.42
1:F:218:LYS:HB2	1:F:222:TYR:HE1	1.78	0.42
1:F:336:VAL:CA	1:F:337:GLN:N	2.82	0.42
1:A:142:ASN:ND2	1:A:289:ARG:CG	2.82	0.42
1:B:192:THR:CB	1:B:193:ILE:HD12	2.48	0.42
1:C:111:ASP:OD1	1:C:114:CYS:HB3	2.19	0.42
1:C:171:PRO:HD3	1:C:279:TYR:CE2	2.53	0.42
1:D:77:ARG:O	1:D:298:HIS:ND1	2.52	0.42
1:E:164:VAL:HA	1:E:241:GLY:HA3	2.01	0.42
1:E:125:VAL:HG11	1:E:263:LEU:HD21	2.00	0.42
1:E:265:ASP:CG	1:E:269:VAL:HB	2.40	0.42
1:E:52:PHE:CD1	1:E:52:PHE:C	2.93	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:LYS:NZ	1:F:204:LYS:CB	2.81	0.42
1:F:351:VAL:CG1	1:F:352:ARG:N	2.82	0.42
1:A:291:THR:O	1:A:293:ASN:N	2.53	0.42
1:A:46:VAL:HG12	1:A:47:THR:N	2.35	0.42
1:B:123:VAL:O	1:B:263:LEU:N	2.52	0.42
1:B:197:THR:O	1:B:198:LYS:C	2.58	0.42
1:B:25:VAL:HG21	1:F:360:VAL:HA	2.00	0.42
1:B:308:ILE:H	1:B:308:ILE:HD12	1.80	0.42
1:B:311:ARG:HH21	1:B:313:ARG:NH2	2.17	0.42
1:B:54:ASN:HD22	1:B:55:PRO:CD	2.31	0.42
1:C:254:GLN:O	1:C:256:THR:N	2.52	0.42
1:C:316:LYS:HE3	1:F:359:PRO:HB2	2.01	0.42
1:D:132:SER:O	1:D:135:LEU:CD2	2.68	0.42
1:D:166:ALA:HB1	1:D:238:ARG:O	2.19	0.42
1:D:171:PRO:HG2	1:D:215:LYS:HD2	2.02	0.42
1:E:105:LEU:HB3	1:E:120:TRP:NE1	2.35	0.42
1:E:121:GLU:CG	1:E:313:ARG:HD2	2.49	0.42
1:E:368:ARG:HG3	1:E:376:THR:O	2.20	0.42
1:F:182:ARG:CG	1:F:183:THR:H	2.32	0.42
1:F:75:TRP:CE2	1:F:300:ARG:HD2	2.54	0.42
1:F:83:THR:CB	1:F:87:GLU:HB3	2.39	0.42
1:C:79:ILE:HG22	1:C:79:ILE:O	2.19	0.42
1:D:125:VAL:CG1	1:D:263:LEU:HD21	2.49	0.42
1:D:172:LEU:C	1:D:172:LEU:HD22	2.38	0.42
1:D:57:MET:HB2	1:D:96:PRO:CB	2.46	0.42
1:E:109:ASN:HD22	1:E:110:GLU:H	1.65	0.42
1:D:251:PRO:HB2	1:E:243:TYR:CE2	2.55	0.42
1:E:296:VAL:HG12	1:E:298:HIS:HD2	1.84	0.42
1:F:302:LEU:HD23	1:F:302:LEU:HA	1.76	0.42
1:F:112:LEU:HD23	1:F:321:MET:SD	2.59	0.42
1:C:111:ASP:C	1:C:113:THR:H	2.22	0.42
1:C:117:LEU:HD22	1:C:117:LEU:HA	1.45	0.42
1:C:57:MET:HB3	1:C:96:PRO:CB	2.48	0.42
1:D:153:ILE:HD13	1:D:153:ILE:HA	1.81	0.42
1:D:218:LYS:H	1:D:222:TYR:HE2	1.66	0.42
1:D:269:VAL:HG13	1:D:272:LEU:HD11	2.02	0.42
1:E:164:VAL:HA	1:E:240:PHE:O	2.20	0.42
1:E:339:GLN:HA	1:E:340:PRO:HD3	1.76	0.42
1:E:90:PRO:HD2	1:E:184:LYS:O	2.18	0.42
1:F:97:THR:HG22	1:F:223:PRO:N	2.35	0.42
1:F:339:GLN:CG	1:F:340:PRO:HD2	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PHE:HB2	1:B:241:GLY:O	2.19	0.42
1:B:117:LEU:HA	1:B:314:TRP:CZ3	2.52	0.42
1:B:209:ASN:C	1:B:211:ILE:H	2.22	0.42
1:B:360:VAL:HG12	1:B:361:PRO:N	2.34	0.42
1:C:100:MET:SD	1:C:101:ALA:HA	2.60	0.42
1:C:302:LEU:HB3	1:C:303:PRO:HD2	2.01	0.42
1:D:198:LYS:HA	1:D:198:LYS:HD3	1.52	0.42
1:D:285:ILE:HG22	1:D:287:GLY:N	2.34	0.42
1:E:175:GLN:HG2	1:E:212:SER:O	2.20	0.42
1:E:207:VAL:HG23	1:E:208:LEU:H	1.85	0.42
1:E:232:ALA:C	1:E:234:ASN:N	2.70	0.42
1:A:162:TYR:CE2	1:E:255:PHE:HE2	2.37	0.42
1:E:30:ILE:CG1	1:E:31:LYS:N	2.82	0.42
1:E:97:THR:HA	1:E:223:PRO:HA	2.00	0.42
1:B:118:GLN:HA	1:B:313:ARG:O	2.19	0.42
1:B:117:LEU:CD1	1:B:315:VAL:HG22	2.50	0.42
1:B:354:TYR:N	1:B:354:TYR:HD1	2.18	0.42
1:D:202:VAL:O	1:D:203:ASN:C	2.58	0.42
1:D:238:ARG:HG3	1:D:263:LEU:HA	2.01	0.42
1:D:308:ILE:H	1:D:308:ILE:HD12	1.83	0.42
1:F:131:GLY:O	1:F:134:SER:HB3	2.20	0.42
1:F:341:MET:HE1	1:F:347:GLN:CB	2.44	0.42
1:A:172:LEU:HD13	1:A:174:LEU:HD23	2.02	0.42
1:A:85:ASP:CG	1:A:182:ARG:HH12	2.22	0.42
1:A:72:TYR:O	1:A:73:TYR:C	2.57	0.42
1:B:178:VAL:HG22	1:B:179:THR:H	1.84	0.42
1:B:236:ASN:OD1	1:B:271:PRO:HA	2.20	0.42
1:C:125:VAL:O	1:C:125:VAL:HG13	2.19	0.42
1:E:151:LYS:HA	1:E:151:LYS:HD3	1.79	0.42
1:E:180:ASP:HB3	1:E:182:ARG:HG2	2.01	0.42
1:E:288:TRP:HE3	1:E:299:TRP:HB3	1.83	0.42
1:E:370:VAL:HG22	1:E:375:LYS:HB2	2.02	0.42
1:E:81:LEU:HG	1:E:82:ALA:H	1.85	0.42
1:F:155:THR:HA	1:F:156:PRO:HD2	1.81	0.42
1:C:350:GLU:HG3	1:F:233:LYS:HB3	2.01	0.42
1:F:166:ALA:HB1	1:F:237:THR:HG22	2.02	0.42
1:F:324:LEU:HA	1:F:327:SER:HB2	2.02	0.42
1:A:238:ARG:HH21	1:A:265:ASP:HB3	1.84	0.42
1:A:23:ALA:HA	1:A:24:PRO:HD3	1.84	0.42
1:A:302:LEU:HD23	1:A:302:LEU:HA	1.66	0.42
1:A:328:LEU:CD2	1:A:333:LEU:CD2	2.31	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:GLU:CB	1:B:171:PRO:HD2	2.44	0.42
1:B:265:ASP:OD1	1:B:269:VAL:N	2.53	0.42
1:B:380:PHE:C	1:B:382:GLY:N	2.73	0.42
1:C:209:ASN:O	1:C:211:ILE:N	2.53	0.42
1:C:126:LYS:CG	1:C:260:THR:HG23	2.48	0.42
1:D:139:HIS:HB2	1:D:140:GLY:H	1.67	0.42
1:D:140:GLY:O	1:D:154:SER:OG	2.35	0.42
1:E:142:ASN:ND2	1:E:289:ARG:HG3	2.35	0.42
1:E:175:GLN:HG3	1:E:213:LYS:CG	2.35	0.42
1:E:271:PRO:C	1:E:272:LEU:HD12	2.40	0.42
1:E:79:ILE:HD11	1:E:299:TRP:HZ3	1.80	0.42
1:E:300:ARG:HG3	1:E:301:GLY:H	1.85	0.42
1:F:91:GLY:H	1:F:186:LYS:CE	2.32	0.42
1:A:368:ARG:HH21	1:A:377:LYS:HG2	1.84	0.42
1:B:288:TRP:CE3	1:B:299:TRP:CG	3.08	0.42
1:C:233:LYS:HE2	1:F:352:ARG:NH1	2.35	0.42
1:D:117:LEU:HD23	1:D:118:GLN:H	1.83	0.42
1:E:333:LEU:HD22	1:E:333:LEU:N	2.34	0.42
1:F:286:MET:CE	1:F:286:MET:HA	2.48	0.42
1:A:52:PHE:HA	1:A:304:ARG:O	2.20	0.41
1:B:180:ASP:O	1:B:182:ARG:N	2.53	0.41
1:B:211:ILE:O	1:B:213:LYS:N	2.53	0.41
1:C:104:GLN:HE21	1:C:105:LEU:N	2.18	0.41
1:C:115:ASP:O	1:C:317:ASN:HB2	2.20	0.41
1:D:193:ILE:CG2	1:D:212:SER:HB3	2.50	0.41
1:D:278:LEU:CD2	1:D:278:LEU:C	2.89	0.41
1:E:138:VAL:O	1:E:153:ILE:HG23	2.20	0.41
1:E:180:ASP:OD1	1:E:182:ARG:HG2	2.20	0.41
1:A:39:LEU:O	1:A:41:THR:N	2.53	0.41
1:B:101:ALA:HB2	1:F:339:GLN:CB	2.49	0.41
1:B:192:THR:HB	1:B:194:LYS:HG2	2.01	0.41
1:C:132:SER:CA	1:C:135:LEU:HD23	2.48	0.41
1:C:193:ILE:CG2	1:C:212:SER:HB3	2.50	0.41
1:C:299:TRP:H	1:C:299:TRP:HE3	1.68	0.41
1:D:193:ILE:O	1:D:197:THR:HG22	2.20	0.41
1:D:59:GLN:OE1	1:D:77:ARG:HD2	2.19	0.41
1:E:117:LEU:HA	1:E:117:LEU:HD22	1.51	0.41
1:E:194:LYS:H	1:E:194:LYS:CD	2.28	0.41
1:E:193:ILE:HD11	1:E:201:MET:SD	2.61	0.41
1:E:59:GLN:HG3	1:E:60:PRO:HD2	2.01	0.41
1:F:218:LYS:O	1:F:219:ASP:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:219:ASP:C	1:F:221:MET:N	2.68	0.41
1:F:66:LEU:HB3	1:F:71:GLN:HB2	2.02	0.41
1:F:78:GLY:HA3	2:L:2:GAL:O4	2.20	0.41
1:A:174:LEU:HB2	1:A:228:HIS:O	2.20	0.41
1:A:166:ALA:CB	1:A:238:ARG:O	2.68	0.41
1:A:54:ASN:HD22	1:A:55:PRO:HD2	1.85	0.41
1:B:108:LEU:HB3	1:B:118:GLN:NE2	2.35	0.41
1:B:348:VAL:O	1:B:348:VAL:HG13	2.19	0.41
1:C:108:LEU:HD11	1:C:120:TRP:NE1	2.35	0.41
1:B:54:ASN:ND2	1:C:207:VAL:HB	2.35	0.41
1:C:50:GLU:OE2	1:D:233:LYS:CA	2.64	0.41
1:D:318:PRO:O	1:D:319:TYR:CD1	2.73	0.41
1:E:269:VAL:HG12	1:E:270:GLY:O	2.20	0.41
1:E:298:HIS:HD2	1:E:298:HIS:H	1.67	0.41
1:E:321:MET:O	1:E:322:ALA:C	2.59	0.41
1:E:332:MET:HA	1:E:332:MET:CE	2.50	0.41
1:E:337:GLN:OE1	1:E:337:GLN:HA	2.19	0.41
1:E:83:THR:HG22	1:E:84:SER:N	2.35	0.41
1:F:56:ARG:HH12	1:F:219:ASP:CG	2.23	0.41
1:F:62:THR:CB	1:F:63:PRO:HD3	2.50	0.41
1:F:78:GLY:HA3	2:L:2:GAL:H4	2.02	0.41
1:B:176:GLY:O	1:B:177:LEU:CD2	2.69	0.41
1:B:194:LYS:O	1:B:197:THR:N	2.54	0.41
1:B:379:VAL:O	1:B:380:PHE:C	2.59	0.41
1:C:115:ASP:CG	1:C:116:THR:N	2.72	0.41
1:C:193:ILE:H	1:C:193:ILE:HD12	1.84	0.41
1:C:271:PRO:C	1:C:272:LEU:HG	2.40	0.41
1:C:62:THR:O	1:C:64:GLU:N	2.54	0.41
1:E:113:THR:C	1:E:115:ASP:N	2.74	0.41
1:E:370:VAL:HG13	1:E:374:GLY:C	2.41	0.41
1:E:86:THR:HG23	1:E:87:GLU:N	2.35	0.41
1:F:177:LEU:HD22	1:F:205:ASP:O	2.20	0.41
1:A:105:LEU:HB3	1:A:106:PRO:CD	2.47	0.41
1:A:217:ASP:OD1	1:A:218:LYS:HD3	2.20	0.41
1:A:169:GLY:HA3	1:A:236:ASN:ND2	2.36	0.41
1:C:193:ILE:HD12	1:C:194:LYS:HD3	2.02	0.41
1:C:25:VAL:HG12	1:C:26:PRO:CD	2.50	0.41
1:C:358:GLU:HG3	1:C:359:PRO:O	2.20	0.41
1:D:262:VAL:HG12	1:D:264:LEU:HB2	2.01	0.41
1:E:257:ASN:HB3	1:E:258:THR:H	1.41	0.41
1:E:278:LEU:HD22	1:E:278:LEU:C	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:57:MET:CB	1:E:96:PRO:HB3	2.47	0.41
1:F:192:THR:HG23	1:F:226:ILE:CD1	2.51	0.41
1:F:81:LEU:CG	1:F:82:ALA:H	2.33	0.41
1:C:178:VAL:CG2	1:C:179:THR:N	2.81	0.41
1:D:186:LYS:N	1:D:186:LYS:CD	2.83	0.41
1:D:272:LEU:N	1:D:272:LEU:CD1	2.80	0.41
1:F:123:VAL:HG12	1:F:124:SER:N	2.33	0.41
1:E:78:GLY:HA3	2:K:2:GAL:O4	2.20	0.41
1:A:178:VAL:CG2	1:A:179:THR:H	2.32	0.41
1:A:350:GLU:OE2	1:A:352:ARG:HD2	2.21	0.41
1:C:222:TYR:N	1:C:222:TYR:CD1	2.89	0.41
1:C:105:LEU:HB2	1:C:276:GLU:O	2.21	0.41
1:D:125:VAL:HG12	1:D:263:LEU:HD21	2.03	0.41
1:D:68:GLU:HG2	1:D:68:GLU:H	1.64	0.41
1:E:143:LYS:HA	1:E:292:ARG:HA	2.02	0.41
1:E:97:THR:CG2	1:E:223:PRO:HA	2.51	0.41
1:E:264:LEU:HD12	1:E:264:LEU:HA	1.63	0.41
1:F:316:LYS:HE2	1:F:316:LYS:HB3	1.77	0.41
1:F:43:PRO:CD	1:F:44:ASP:H	2.33	0.41
1:B:185:TYR:CA	1:B:186:LYS:HE2	2.49	0.41
1:B:205:ASP:O	1:B:207:VAL:N	2.54	0.41
1:B:65:SER:C	1:B:67:THR:H	2.24	0.41
1:C:352:ARG:HE	1:F:234:ASN:CG	2.24	0.41
1:C:64:GLU:O	1:C:66:LEU:HD23	2.21	0.41
1:D:193:ILE:O	1:D:196:ILE:HG23	2.20	0.41
1:E:150:THR:CG2	1:E:292:ARG:NH2	2.82	0.41
1:E:288:TRP:CE3	1:E:299:TRP:HB3	2.55	0.41
1:F:315:VAL:HG23	1:F:316:LYS:N	2.35	0.41
1:A:145:THR:HB	1:A:152:GLY:HA3	2.03	0.41
1:A:367:THR:H	1:A:380:PHE:HE1	1.69	0.41
1:B:185:TYR:CD2	1:B:192:THR:CG2	3.01	0.41
1:B:61:PRO:HG2	1:B:62:THR:H	1.86	0.41
1:C:117:LEU:HD13	1:C:118:GLN:O	2.20	0.41
1:C:207:VAL:CG2	1:C:208:LEU:N	2.84	0.41
1:C:171:PRO:HD3	1:C:279:TYR:CZ	2.56	0.41
1:A:233:LYS:HE2	1:E:31:LYS:HD2	2.02	0.41
1:E:346:THR:HG22	1:E:348:VAL:CG2	2.51	0.41
1:E:62:THR:OG1	1:E:63:PRO:CD	2.61	0.41
1:F:184:LYS:N	1:F:184:LYS:HD2	2.35	0.41
1:F:97:THR:HG22	1:F:223:PRO:HA	2.03	0.41
1:A:165:PHE:CD2	1:A:166:ALA:N	2.89	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ILE:HG12	1:A:201:MET:HE3	2.03	0.41
1:A:285:ILE:H	1:A:285:ILE:HD12	1.85	0.41
1:A:328:LEU:HD21	1:A:333:LEU:CG	2.36	0.41
1:A:132:SER:HB2	1:B:243:TYR:HB2	2.02	0.41
1:B:305:TYR:C	1:B:306:PHE:CD1	2.94	0.41
1:B:320:PRO:O	1:B:324:LEU:HD22	2.21	0.41
1:B:66:LEU:CD2	1:B:66:LEU:N	2.83	0.41
1:D:120:TRP:O	1:D:272:LEU:HA	2.21	0.41
1:D:135:LEU:HD22	1:D:135:LEU:N	2.36	0.41
1:D:153:ILE:HG12	1:E:297:HIS:CG	2.53	0.41
1:D:352:ARG:HG3	1:D:352:ARG:HH11	1.86	0.41
1:D:43:PRO:CD	1:D:44:ASP:H	2.33	0.41
1:E:144:PRO:HG3	1:E:292:ARG:HG2	2.02	0.41
1:E:177:LEU:HD11	1:E:208:LEU:HA	2.03	0.41
1:E:194:LYS:O	1:E:196:ILE:N	2.54	0.41
1:E:124:SER:HA	1:E:261:THR:O	2.21	0.41
1:E:170:GLU:HB3	1:E:274:LYS:HD2	2.03	0.41
1:F:288:TRP:HA	1:F:299:TRP:HB3	2.02	0.41
1:A:79:ILE:HG23	1:A:79:ILE:HD12	1.78	0.41
1:B:257:ASN:N	1:B:257:ASN:HD22	2.03	0.41
1:C:123:VAL:O	1:C:263:LEU:N	2.50	0.41
1:C:142:ASN:O	1:C:143:LYS:C	2.59	0.41
1:C:164:VAL:HG12	1:C:165:PHE:N	2.36	0.41
1:C:177:LEU:HD22	1:C:208:LEU:HA	2.03	0.41
1:C:352:ARG:NH1	1:C:352:ARG:HG2	2.36	0.41
1:D:254:GLN:HA	1:D:254:GLN:OE1	2.20	0.41
1:D:310:LEU:N	1:D:310:LEU:HD12	2.36	0.41
1:E:18:ALA:O	1:E:19:CYS:C	2.59	0.41
1:E:208:LEU:CD2	1:E:210:PRO:HG3	2.50	0.41
1:E:238:ARG:HG3	1:E:263:LEU:HA	2.02	0.41
1:E:165:PHE:HB2	1:E:282:CYS:HB3	2.02	0.41
1:E:351:VAL:HG12	1:E:352:ARG:N	2.36	0.41
1:F:134:SER:C	1:F:136:LEU:H	2.24	0.41
1:F:142:ASN:HB2	1:F:154:SER:HB3	2.02	0.41
1:F:192:THR:N	1:F:195:THR:HB	2.32	0.41
1:F:359:PRO:O	1:F:360:VAL:C	2.59	0.41
1:F:84:SER:C	1:F:86:THR:N	2.73	0.41
1:A:176:GLY:O	1:A:177:LEU:HG	2.21	0.40
1:A:30:ILE:CD1	1:A:36:VAL:HG13	2.51	0.40
1:A:62:THR:O	1:A:64:GLU:N	2.55	0.40
1:B:194:LYS:C	1:B:196:ILE:N	2.74	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:GLN:NE2	1:B:71:GLN:HA	2.25	0.40
1:C:192:THR:H	1:C:195:THR:HG1	1.66	0.40
1:C:209:ASN:HA	1:C:210:PRO:HD3	1.71	0.40
1:C:124:SER:HA	1:C:261:THR:O	2.21	0.40
1:C:272:LEU:HD12	1:C:272:LEU:H	1.86	0.40
1:C:285:ILE:CD1	1:C:285:ILE:N	2.84	0.40
1:C:90:PRO:HD2	1:C:186:LYS:NZ	2.36	0.40
1:D:145:THR:OG1	1:D:153:ILE:N	2.52	0.40
1:D:174:LEU:N	1:D:174:LEU:CD1	2.68	0.40
1:D:288:TRP:CE3	1:D:299:TRP:HB3	2.56	0.40
1:D:320:PRO:O	1:D:321:MET:C	2.58	0.40
1:E:211:ILE:N	1:E:211:ILE:CD1	2.84	0.40
1:E:174:LEU:HD22	1:E:227:TRP:HB3	2.03	0.40
1:C:352:ARG:CZ	1:F:233:LYS:HB2	2.51	0.40
1:A:192:THR:N	1:A:195:THR:OG1	2.51	0.40
1:B:127:THR:OG1	1:B:128:GLU:N	2.54	0.40
1:B:346:THR:C	1:B:348:VAL:H	2.24	0.40
1:B:366:MET:HE3	1:B:377:LYS:HG2	2.02	0.40
1:C:132:SER:C	1:C:135:LEU:HD23	2.42	0.40
1:C:77:ARG:O	1:C:298:HIS:CG	2.74	0.40
1:D:249:THR:HA	1:D:250:PRO:HD3	1.87	0.40
1:D:255:PHE:HE2	1:E:162:TYR:CE2	2.40	0.40
1:D:117:LEU:HB3	1:D:315:VAL:HG22	2.03	0.40
1:E:186:LYS:HE2	1:E:186:LYS:H	1.82	0.40
1:E:144:PRO:HD3	1:E:292:ARG:HG2	2.04	0.40
1:F:203:ASN:N	1:F:203:ASN:OD1	2.54	0.40
1:F:280:LEU:HD13	1:F:306:PHE:CD2	2.56	0.40
1:A:25:VAL:HG13	1:A:26:PRO:CD	2.51	0.40
1:A:115:ASP:O	1:A:316:LYS:HA	2.21	0.40
1:B:122:ALA:CA	1:B:310:LEU:HB3	2.48	0.40
1:B:117:LEU:CA	1:B:314:TRP:HZ3	2.34	0.40
1:B:378:THR:CG2	1:B:379:VAL:N	2.84	0.40
1:C:135:LEU:H	1:C:135:LEU:HD22	1.85	0.40
1:C:205:ASP:CA	1:C:209:ASN:HB2	2.42	0.40
1:C:86:THR:HG23	1:C:87:GLU:N	2.37	0.40
1:D:174:LEU:HA	1:D:230:ASP:H	1.86	0.40
1:D:21:ARG:HA	1:D:22:PRO:HD3	1.96	0.40
1:D:288:TRP:CE3	1:D:299:TRP:CG	3.08	0.40
1:D:32:GLY:N	1:D:36:VAL:HG21	2.35	0.40
1:D:57:MET:O	1:D:57:MET:CG	2.69	0.40
1:E:103:LEU:CD2	1:E:103:LEU:N	2.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:205:ASP:HA	1:E:209:ASN:HB2	2.02	0.40
1:E:172:LEU:HD21	1:E:229:PRO:HA	2.03	0.40
1:E:287:GLY:C	1:E:299:TRP:HB2	2.42	0.40
1:F:151:LYS:HA	1:F:151:LYS:HD3	1.73	0.40
1:F:144:PRO:HA	1:F:153:ILE:O	2.21	0.40
1:F:321:MET:C	1:F:323:SER:N	2.74	0.40
1:F:39:LEU:HD12	1:F:40:VAL:N	2.35	0.40
1:A:180:ASP:OD2	1:A:182:ARG:HD2	2.22	0.40
1:A:76:SER:CB	1:A:299:TRP:CE3	3.04	0.40
1:A:45:SER:OG	1:A:312:LYS:HE3	2.20	0.40
1:B:233:LYS:HG2	1:B:234:ASN:HD22	1.85	0.40
1:C:100:MET:SD	1:C:101:ALA:CA	3.09	0.40
1:C:280:LEU:HD23	1:C:280:LEU:HA	1.66	0.40
1:C:288:TRP:CA	1:C:299:TRP:HB3	2.50	0.40
1:C:352:ARG:HH21	1:F:233:LYS:C	2.24	0.40
1:D:121:GLU:CG	1:D:269:VAL:O	2.70	0.40
1:D:54:ASN:HA	1:D:55:PRO:HD2	1.67	0.40
1:E:113:THR:O	1:E:115:ASP:N	2.54	0.40
1:A:243:TYR:O	1:E:252:VAL:HA	2.20	0.40
1:F:35:GLU:O	1:F:36:VAL:C	2.58	0.40
1:A:105:LEU:HB3	1:A:120:TRP:HE1	1.82	0.40
1:A:305:TYR:CE2	1:A:307:LYS:HB2	2.57	0.40
1:A:363:ASP:OD1	1:A:366:MET:N	2.54	0.40
1:C:111:ASP:O	1:C:114:CYS:O	2.39	0.40
1:C:208:LEU:O	1:C:208:LEU:HG	2.21	0.40
1:C:52:PHE:CD1	1:C:52:PHE:C	2.95	0.40
1:D:236:ASN:OD1	1:D:272:LEU:HD12	2.21	0.40
1:D:71:GLN:HE21	1:D:73:TYR:H	1.68	0.40
1:C:153:ILE:HD13	1:D:79:ILE:HG21	2.03	0.40
1:E:153:ILE:HD13	1:E:153:ILE:HA	1.89	0.40
1:E:259:LEU:CD2	1:E:259:LEU:N	2.79	0.40
1:E:162:TYR:CD1	1:E:283:VAL:HG21	2.56	0.40
1:E:37:LEU:N	1:E:37:LEU:HD13	2.36	0.40
1:F:136:LEU:HD23	1:F:136:LEU:HA	1.82	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:LYS:CD	1:A:328:LEU:O[2_555]	1.75	0.45
1:A:217:ASP:O	1:A:336:VAL:O[2_555]	2.05	0.15

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	364/383 (95%)	270 (74%)	67 (18%)	27 (7%)	1 13
1	B	363/383 (95%)	280 (77%)	62 (17%)	21 (6%)	1 19
1	C	353/383 (92%)	275 (78%)	60 (17%)	18 (5%)	2 21
1	D	336/383 (88%)	264 (79%)	58 (17%)	14 (4%)	3 25
1	E	365/383 (95%)	278 (76%)	62 (17%)	25 (7%)	1 15
1	F	350/383 (91%)	271 (77%)	45 (13%)	34 (10%)	0 8
All	All	2131/2298 (93%)	1638 (77%)	354 (17%)	139 (6%)	1 17

All (139) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	PRO
1	A	62	THR
1	A	148	VAL
1	A	183	THR
1	A	276	GLU
1	A	293	ASN
1	A	322	ALA
1	A	323	SER
1	A	327	SER
1	A	334	PRO
1	A	372	ARG
1	A	381	PRO
1	B	43	PRO
1	B	77	ARG
1	B	85	ASP
1	B	276	GLU
1	C	43	PRO
1	C	62	THR
1	C	85	ASP
1	C	90	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	198	LYS
1	D	43	PRO
1	D	85	ASP
1	D	293	ASN
1	D	322	ALA
1	E	43	PRO
1	E	77	ARG
1	E	85	ASP
1	E	90	PRO
1	E	92	ASN
1	E	113	THR
1	E	258	THR
1	E	371	ASP
1	E	381	PRO
1	F	19	CYS
1	F	40	VAL
1	F	41	THR
1	F	43	PRO
1	F	61	PRO
1	F	62	THR
1	F	92	ASN
1	F	183	THR
1	F	212	SER
1	A	61	PRO
1	A	212	SER
1	B	148	VAL
1	B	198	LYS
1	B	297	HIS
1	B	318	PRO
1	C	61	PRO
1	C	70	GLY
1	C	77	ARG
1	C	212	SER
1	C	255	PHE
1	D	45	SER
1	D	55	PRO
1	D	84	SER
1	D	148	VAL
1	D	321	MET
1	E	40	VAL
1	E	84	SER
1	E	148	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	212	SER
1	E	257	ASN
1	F	70	GLY
1	F	77	ARG
1	F	113	THR
1	F	148	VAL
1	F	276	GLU
1	F	293	ASN
1	A	90	PRO
1	A	200	ASP
1	A	337	GLN
1	A	366	MET
1	B	70	GLY
1	C	116	THR
1	C	190	VAL
1	C	342	GLU
1	D	90	PRO
1	E	20	PRO
1	F	90	PRO
1	F	112	LEU
1	F	179	THR
1	F	219	ASP
1	F	322	ALA
1	F	368	ARG
1	A	156	PRO
1	B	81	LEU
1	B	84	SER
1	B	195	THR
1	B	206	GLN
1	B	325	ILE
1	B	329	PHE
1	B	361	PRO
1	B	381	PRO
1	C	148	VAL
1	C	200	ASP
1	C	206	GLN
1	C	293	ASN
1	C	318	PRO
1	D	220	GLY
1	E	22	PRO
1	E	293	ASN
1	E	320	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	379	VAL
1	E	382	GLY
1	F	66	LEU
1	F	85	ASP
1	F	208	LEU
1	F	297	HIS
1	F	334	PRO
1	F	342	GLU
1	A	70	GLY
1	A	77	ARG
1	A	339	GLN
1	A	364	PRO
1	B	193	ILE
1	B	212	SER
1	D	41	THR
1	E	179	THR
1	F	320	PRO
1	F	362	GLY
1	A	340	PRO
1	B	90	PRO
1	E	114	CYS
1	F	294	TYR
1	A	249	THR
1	B	360	VAL
1	E	125	VAL
1	F	22	PRO
1	F	125	VAL
1	F	155	THR
1	E	156	PRO
1	F	190	VAL
1	A	40	VAL
1	E	364	PRO
1	D	340	PRO
1	A	30	ILE
1	D	269	VAL

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	321/335 (96%)	244 (76%)	77 (24%)	0 5
1	B	322/335 (96%)	237 (74%)	85 (26%)	0 3
1	C	314/335 (94%)	238 (76%)	76 (24%)	0 5
1	D	298/335 (89%)	214 (72%)	84 (28%)	0 2
1	E	322/335 (96%)	241 (75%)	81 (25%)	0 4
1	F	311/335 (93%)	228 (73%)	83 (27%)	0 3
All	All	1888/2010 (94%)	1402 (74%)	486 (26%)	0 4

All (486) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	LEU
1	A	41	THR
1	A	43	PRO
1	A	53	LEU
1	A	57	MET
1	A	66	LEU
1	A	71	GLN
1	A	75	TRP
1	A	77	ARG
1	A	83	THR
1	A	93	ASN
1	A	95	LEU
1	A	99	SER
1	A	115	ASP
1	A	127	THR
1	A	130	VAL
1	A	132	SER
1	A	138	VAL
1	A	141	PHE
1	A	151	LYS
1	A	154	SER
1	A	172	LEU
1	A	175	GLN
1	A	179	THR
1	A	180	ASP
1	A	184	LYS
1	A	186	LYS
1	A	193	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	194	LYS
1	A	195	THR
1	A	196	ILE
1	A	197	THR
1	A	198	LYS
1	A	216	LEU
1	A	217	ASP
1	A	219	ASP
1	A	224	VAL
1	A	230	ASP
1	A	234	ASN
1	A	240	PHE
1	A	244	THR
1	A	252	VAL
1	A	253	LEU
1	A	256	THR
1	A	258	THR
1	A	259	LEU
1	A	278	LEU
1	A	281	SER
1	A	283	VAL
1	A	286	MET
1	A	288	TRP
1	A	292	ARG
1	A	294	TYR
1	A	295	ASP
1	A	299	TRP
1	A	304	ARG
1	A	309	THR
1	A	310	LEU
1	A	313	ARG
1	A	315	VAL
1	A	323	SER
1	A	324	LEU
1	A	327	SER
1	A	335	GLN
1	A	336	VAL
1	A	345	ASN
1	A	347	GLN
1	A	350	GLU
1	A	352	ARG
1	A	357	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	360	VAL
1	A	366	MET
1	A	369	TYR
1	A	372	ARG
1	A	373	PHE
1	A	380	PHE
1	A	381	PRO
1	B	29	LEU
1	B	30	ILE
1	B	41	THR
1	B	43	PRO
1	B	46	VAL
1	B	53	LEU
1	B	54	ASN
1	B	64	GLU
1	B	66	LEU
1	B	71	GLN
1	B	75	TRP
1	B	81	LEU
1	B	93	ASN
1	B	97	THR
1	B	112	LEU
1	B	117	LEU
1	B	130	VAL
1	B	132	SER
1	B	135	LEU
1	B	138	VAL
1	B	139	HIS
1	B	141	PHE
1	B	151	LYS
1	B	154	SER
1	B	172	LEU
1	B	174	LEU
1	B	175	GLN
1	B	179	THR
1	B	180	ASP
1	B	184	LYS
1	B	186	LYS
1	B	190	VAL
1	B	192	THR
1	B	193	ILE
1	B	194	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	195	THR
1	B	196	ILE
1	B	200	ASP
1	B	202	VAL
1	B	205	ASP
1	B	216	LEU
1	B	217	ASP
1	B	222	TYR
1	B	230	ASP
1	B	233	LYS
1	B	234	ASN
1	B	237	THR
1	B	240	PHE
1	B	242	ASN
1	B	244	THR
1	B	248	THR
1	B	252	VAL
1	B	253	LEU
1	B	256	THR
1	B	257	ASN
1	B	258	THR
1	B	260	THR
1	B	262	VAL
1	B	265	ASP
1	B	278	LEU
1	B	281	SER
1	B	283	VAL
1	B	288	TRP
1	B	290	VAL
1	B	294	TYR
1	B	297	HIS
1	B	299	TRP
1	B	309	THR
1	B	310	LEU
1	B	316	LYS
1	B	321	MET
1	B	324	LEU
1	B	332	MET
1	B	336	VAL
1	B	342	GLU
1	B	347	GLN
1	B	353	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	354	TYR
1	B	361	PRO
1	B	364	PRO
1	B	367	THR
1	B	368	ARG
1	B	371	ASP
1	B	372	ARG
1	B	373	PHE
1	C	29	LEU
1	C	37	LEU
1	C	41	THR
1	C	43	PRO
1	C	45	SER
1	C	53	LEU
1	C	54	ASN
1	C	66	LEU
1	C	75	TRP
1	C	79	ILE
1	C	93	ASN
1	C	100	MET
1	C	109	ASN
1	C	110	GLU
1	C	112	LEU
1	C	117	LEU
1	C	121	GLU
1	C	132	SER
1	C	134	SER
1	C	138	VAL
1	C	141	PHE
1	C	151	LYS
1	C	154	SER
1	C	172	LEU
1	C	175	GLN
1	C	179	THR
1	C	186	LYS
1	C	191	VAL
1	C	192	THR
1	C	193	ILE
1	C	194	LYS
1	C	195	THR
1	C	196	ILE
1	C	199	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	201	MET
1	C	216	LEU
1	C	217	ASP
1	C	218	LYS
1	C	219	ASP
1	C	233	LYS
1	C	237	THR
1	C	240	PHE
1	C	242	ASN
1	C	244	THR
1	C	252	VAL
1	C	253	LEU
1	C	257	ASN
1	C	258	THR
1	C	259	LEU
1	C	260	THR
1	C	262	VAL
1	C	265	ASP
1	C	272	LEU
1	C	278	LEU
1	C	281	SER
1	C	286	MET
1	C	288	TRP
1	C	291	THR
1	C	292	ARG
1	C	293	ASN
1	C	294	TYR
1	C	295	ASP
1	C	296	VAL
1	C	299	TRP
1	C	305	TYR
1	C	309	THR
1	C	310	LEU
1	C	329	PHE
1	C	330	ASN
1	C	335	GLN
1	C	336	VAL
1	C	352	ARG
1	C	354	TYR
1	C	359	PRO
1	C	360	VAL
1	C	372	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	21	ARG
1	D	25	VAL
1	D	30	ILE
1	D	39	LEU
1	D	41	THR
1	D	45	SER
1	D	53	LEU
1	D	54	ASN
1	D	59	GLN
1	D	66	LEU
1	D	68	GLU
1	D	71	GLN
1	D	75	TRP
1	D	76	SER
1	D	77	ARG
1	D	81	LEU
1	D	85	ASP
1	D	93	ASN
1	D	97	THR
1	D	100	MET
1	D	108	LEU
1	D	112	LEU
1	D	113	THR
1	D	115	ASP
1	D	130	VAL
1	D	132	SER
1	D	138	VAL
1	D	139	HIS
1	D	141	PHE
1	D	151	LYS
1	D	154	SER
1	D	172	LEU
1	D	173	ASP
1	D	174	LEU
1	D	179	THR
1	D	182	ARG
1	D	184	LYS
1	D	186	LYS
1	D	192	THR
1	D	193	ILE
1	D	194	LYS
1	D	197	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	202	VAL
1	D	205	ASP
1	D	216	LEU
1	D	218	LYS
1	D	219	ASP
1	D	230	ASP
1	D	234	ASN
1	D	237	THR
1	D	240	PHE
1	D	244	THR
1	D	248	THR
1	D	252	VAL
1	D	253	LEU
1	D	256	THR
1	D	258	THR
1	D	260	THR
1	D	262	VAL
1	D	265	ASP
1	D	278	LEU
1	D	279	TYR
1	D	281	SER
1	D	286	MET
1	D	288	TRP
1	D	292	ARG
1	D	294	TYR
1	D	297	HIS
1	D	299	TRP
1	D	309	THR
1	D	310	LEU
1	D	313	ARG
1	D	315	VAL
1	D	316	LYS
1	D	318	PRO
1	D	321	MET
1	D	323	SER
1	D	329	PHE
1	D	333	LEU
1	D	336	VAL
1	D	346	THR
1	D	348	VAL
1	D	351	VAL
1	D	352	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	19	CYS
1	E	21	ARG
1	E	25	VAL
1	E	28	LEU
1	E	37	LEU
1	E	41	THR
1	E	44	ASP
1	E	53	LEU
1	E	54	ASN
1	E	66	LEU
1	E	68	GLU
1	E	75	TRP
1	E	93	ASN
1	E	97	THR
1	E	99	SER
1	E	108	LEU
1	E	109	ASN
1	E	113	THR
1	E	117	LEU
1	E	132	SER
1	E	135	LEU
1	E	138	VAL
1	E	141	PHE
1	E	151	LYS
1	E	154	SER
1	E	157	VAL
1	E	172	LEU
1	E	173	ASP
1	E	174	LEU
1	E	179	THR
1	E	180	ASP
1	E	184	LYS
1	E	186	LYS
1	E	192	THR
1	E	193	ILE
1	E	194	LYS
1	E	200	ASP
1	E	201	MET
1	E	205	ASP
1	E	217	ASP
1	E	219	ASP
1	E	230	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	233	LYS
1	E	237	THR
1	E	240	PHE
1	E	252	VAL
1	E	253	LEU
1	E	258	THR
1	E	260	THR
1	E	262	VAL
1	E	265	ASP
1	E	269	VAL
1	E	278	LEU
1	E	281	SER
1	E	288	TRP
1	E	292	ARG
1	E	293	ASN
1	E	294	TYR
1	E	297	HIS
1	E	299	TRP
1	E	309	THR
1	E	313	ARG
1	E	315	VAL
1	E	316	LYS
1	E	320	PRO
1	E	329	PHE
1	E	330	ASN
1	E	332	MET
1	E	335	GLN
1	E	336	VAL
1	E	342	GLU
1	E	344	GLU
1	E	347	GLN
1	E	350	GLU
1	E	352	ARG
1	E	354	TYR
1	E	357	THR
1	E	366	MET
1	E	369	TYR
1	E	375	LYS
1	E	381	PRO
1	F	30	ILE
1	F	41	THR
1	F	43	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	46	VAL
1	F	53	LEU
1	F	54	ASN
1	F	62	THR
1	F	66	LEU
1	F	71	GLN
1	F	75	TRP
1	F	76	SER
1	F	77	ARG
1	F	79	ILE
1	F	81	LEU
1	F	93	ASN
1	F	97	THR
1	F	100	MET
1	F	112	LEU
1	F	113	THR
1	F	117	LEU
1	F	119	MET
1	F	130	VAL
1	F	132	SER
1	F	135	LEU
1	F	138	VAL
1	F	139	HIS
1	F	141	PHE
1	F	151	LYS
1	F	154	SER
1	F	161	GLN
1	F	172	LEU
1	F	173	ASP
1	F	174	LEU
1	F	175	GLN
1	F	178	VAL
1	F	179	THR
1	F	184	LYS
1	F	186	LYS
1	F	190	VAL
1	F	191	VAL
1	F	192	THR
1	F	193	ILE
1	F	194	LYS
1	F	201	MET
1	F	205	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	216	LEU
1	F	217	ASP
1	F	230	ASP
1	F	233	LYS
1	F	235	GLU
1	F	237	THR
1	F	240	PHE
1	F	252	VAL
1	F	253	LEU
1	F	258	THR
1	F	259	LEU
1	F	260	THR
1	F	262	VAL
1	F	265	ASP
1	F	278	LEU
1	F	281	SER
1	F	282	CYS
1	F	283	VAL
1	F	290	VAL
1	F	294	TYR
1	F	309	THR
1	F	310	LEU
1	F	317	ASN
1	F	325	ILE
1	F	326	SER
1	F	328	LEU
1	F	330	ASN
1	F	333	LEU
1	F	336	VAL
1	F	345	ASN
1	F	352	ARG
1	F	353	VAL
1	F	357	THR
1	F	359	PRO
1	F	360	VAL
1	F	367	THR
1	F	368	ARG
1	F	371	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	54	ASN
1	A	71	GLN
1	A	104	GLN
1	A	118	GLN
1	A	139	HIS
1	A	142	ASN
1	A	206	GLN
1	A	228	HIS
1	A	234	ASN
1	A	257	ASN
1	A	297	HIS
1	A	335	GLN
1	A	337	GLN
1	A	345	ASN
1	A	347	GLN
1	B	54	ASN
1	B	59	GLN
1	B	93	ASN
1	B	104	GLN
1	B	118	GLN
1	B	139	HIS
1	B	175	GLN
1	B	206	GLN
1	B	228	HIS
1	B	257	ASN
1	B	297	HIS
1	B	339	GLN
1	B	347	GLN
1	C	54	ASN
1	C	104	GLN
1	C	109	ASN
1	C	139	HIS
1	C	142	ASN
1	C	161	GLN
1	C	175	GLN
1	C	206	GLN
1	C	228	HIS
1	C	257	ASN
1	C	337	GLN
1	C	347	GLN
1	D	54	ASN
1	D	80	ASN
1	D	93	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	104	GLN
1	D	118	GLN
1	D	139	HIS
1	D	142	ASN
1	D	228	HIS
1	D	234	ASN
1	D	257	ASN
1	D	297	HIS
1	D	317	ASN
1	D	331	ASN
1	D	335	GLN
1	D	339	GLN
1	D	347	GLN
1	E	54	ASN
1	E	59	GLN
1	E	71	GLN
1	E	104	GLN
1	E	139	HIS
1	E	161	GLN
1	E	228	HIS
1	E	234	ASN
1	E	257	ASN
1	E	297	HIS
1	E	298	HIS
1	E	317	ASN
1	E	339	GLN
1	E	347	GLN
1	F	54	ASN
1	F	59	GLN
1	F	104	GLN
1	F	118	GLN
1	F	297	HIS
1	F	317	ASN
1	F	331	ASN
1	F	339	GLN
1	F	347	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

18 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	$\#\|Z\| > 2$
2	BGC	G	1	2	12,12,12	0.66	0	17,17,17	0.88	1 (5%)
2	GAL	G	2	2	11,11,12	0.34	0	15,15,17	1.27	1 (6%)
2	SIA	G	3	2	17,20,21	0.61	0	21,28,31	0.96	1 (4%)
2	BGC	H	1	2	12,12,12	0.69	0	17,17,17	0.75	1 (5%)
2	GAL	H	2	2	11,11,12	0.53	0	15,15,17	1.68	1 (6%)
2	SIA	H	3	2	17,20,21	0.60	0	21,28,31	0.87	1 (4%)
2	BGC	I	1	2	12,12,12	0.70	0	17,17,17	0.81	1 (5%)
2	GAL	I	2	2	11,11,12	0.40	0	15,15,17	1.86	1 (6%)
2	SIA	I	3	2	17,20,21	0.62	0	21,28,31	0.96	1 (4%)
2	BGC	J	1	2	12,12,12	0.68	0	17,17,17	0.84	1 (5%)
2	GAL	J	2	2	11,11,12	0.24	0	15,15,17	1.57	1 (6%)
2	SIA	J	3	2	17,20,21	0.79	0	21,28,31	1.31	2 (9%)
2	BGC	K	1	2	12,12,12	0.79	0	17,17,17	1.07	1 (5%)
2	GAL	K	2	2	11,11,12	0.25	0	15,15,17	1.60	1 (6%)
2	SIA	K	3	2	17,20,21	0.65	0	21,28,31	1.18	3 (14%)
2	BGC	L	1	2	12,12,12	0.83	0	17,17,17	0.88	1 (5%)
2	GAL	L	2	2	11,11,12	0.36	0	15,15,17	1.19	1 (6%)
2	SIA	L	3	2	17,20,21	0.81	0	21,28,31	1.26	2 (9%)

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
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GAL	G	2	2	-	0/2/19/22	0/1/1/1
2	SIA	G	3	2	-	1/14/34/38	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GAL	H	2	2	-	0/2/19/22	0/1/1/1
2	SIA	H	3	2	-	0/14/34/38	0/1/1/1
2	BGC	I	1	2	-	0/2/22/22	0/1/1/1
2	GAL	I	2	2	-	0/2/19/22	0/1/1/1
2	SIA	I	3	2	-	6/14/34/38	0/1/1/1
2	BGC	J	1	2	-	1/2/22/22	0/1/1/1
2	GAL	J	2	2	-	0/2/19/22	0/1/1/1
2	SIA	J	3	2	-	2/14/34/38	0/1/1/1
2	BGC	K	1	2	-	0/2/22/22	0/1/1/1
2	GAL	K	2	2	-	1/2/19/22	0/1/1/1
2	SIA	K	3	2	-	4/14/34/38	0/1/1/1
2	BGC	L	1	2	-	1/2/22/22	0/1/1/1
2	GAL	L	2	2	-	0/2/19/22	0/1/1/1
2	SIA	L	3	2	-	6/14/34/38	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	2	GAL	C1-C2-C3	-6.31	101.90	109.67
2	H	2	GAL	C1-C2-C3	-5.76	102.59	109.67
2	J	2	GAL	C1-C2-C3	-5.74	102.62	109.67
2	K	2	GAL	C1-C2-C3	-5.55	102.84	109.67
2	G	2	GAL	C1-C2-C3	-4.49	104.15	109.67
2	J	3	SIA	C8-C7-C6	-4.42	104.64	113.03
2	L	3	SIA	C8-C7-C6	-3.74	105.95	113.03
2	L	2	GAL	C1-C2-C3	-3.65	105.17	109.67
2	K	1	BGC	C4-C3-C2	-3.37	104.94	110.82
2	I	3	SIA	C3-C4-C5	-3.19	107.60	111.46
2	K	3	SIA	C3-C4-C5	-2.95	107.90	111.46
2	L	3	SIA	C4-C3-C2	2.91	115.03	109.81
2	G	1	BGC	C4-C3-C2	-2.87	105.81	110.82
2	G	3	SIA	C8-C7-C6	-2.82	107.68	113.03
2	I	1	BGC	C4-C3-C2	-2.65	106.20	110.82
2	K	3	SIA	C8-C7-C6	-2.61	108.09	113.03
2	J	1	BGC	C4-C3-C2	-2.41	106.61	110.82
2	J	3	SIA	C3-C4-C5	-2.32	108.66	111.46
2	K	3	SIA	C4-C3-C2	2.31	113.95	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	1	BGC	C4-C3-C2	-2.16	107.06	110.82
2	H	1	BGC	C4-C3-C2	-2.11	107.14	110.82
2	H	3	SIA	C4-C3-C2	2.08	113.54	109.81

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	3	SIA	C6-C7-C8-C9
2	I	3	SIA	C6-C7-C8-O8
2	I	3	SIA	O7-C7-C8-C9
2	I	3	SIA	O7-C7-C8-O8
2	K	3	SIA	C5-C6-C7-C8
2	K	3	SIA	C5-C6-C7-O7
2	K	3	SIA	O6-C6-C7-C8
2	K	3	SIA	O6-C6-C7-O7
2	J	3	SIA	C5-C6-C7-O7
2	J	3	SIA	O6-C6-C7-O7
2	L	3	SIA	C6-C7-C8-C9
2	L	3	SIA	O7-C7-C8-C9
2	L	3	SIA	O8-C8-C9-O9
2	J	1	BGC	O5-C5-C6-O6
2	K	2	GAL	O5-C5-C6-O6
2	L	3	SIA	C6-C7-C8-O8
2	L	1	BGC	O5-C5-C6-O6
2	G	3	SIA	O6-C6-C7-O7
2	L	3	SIA	O7-C7-C8-O8
2	I	3	SIA	O8-C8-C9-O9
2	L	3	SIA	C7-C8-C9-O9
2	I	3	SIA	C7-C8-C9-O9

There are no ring outliers.

11 monomers are involved in 18 short contacts:

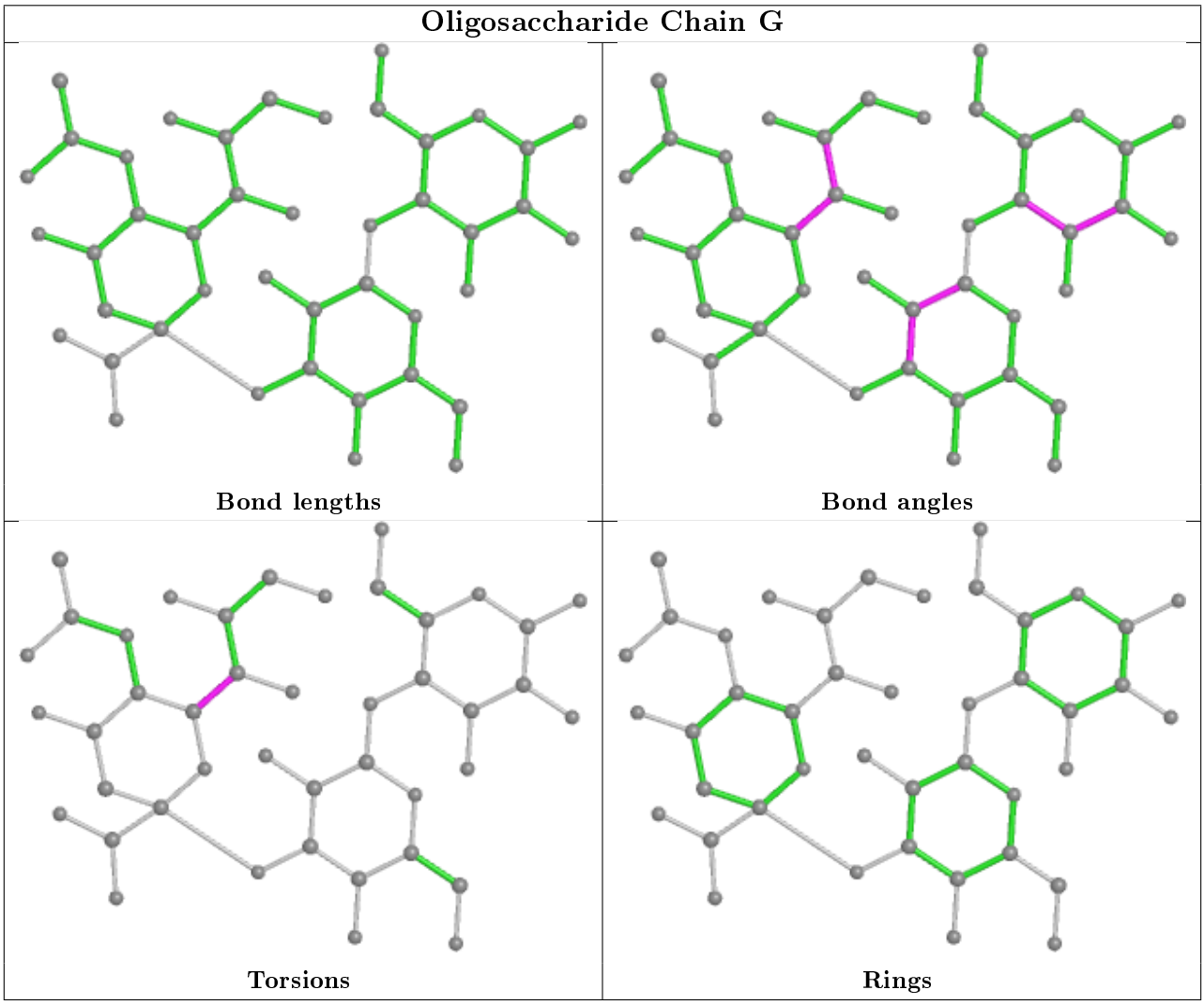
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	GAL	3	0
2	I	3	SIA	1	0
2	G	3	SIA	1	0
2	H	3	SIA	2	0
2	K	2	GAL	2	0
2	L	3	SIA	2	0

Continued on next page...

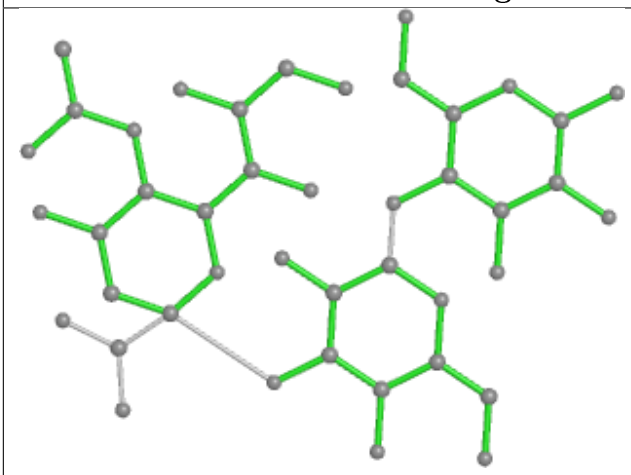
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	2	GAL	4	0
2	J	2	GAL	1	0
2	K	3	SIA	2	0
2	H	2	GAL	4	0
2	J	3	SIA	1	0

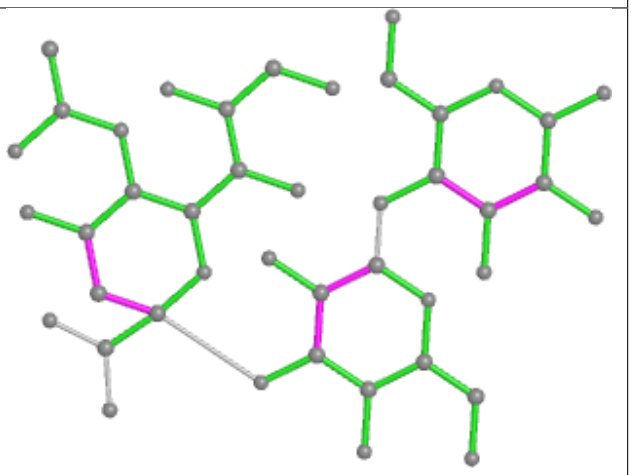
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



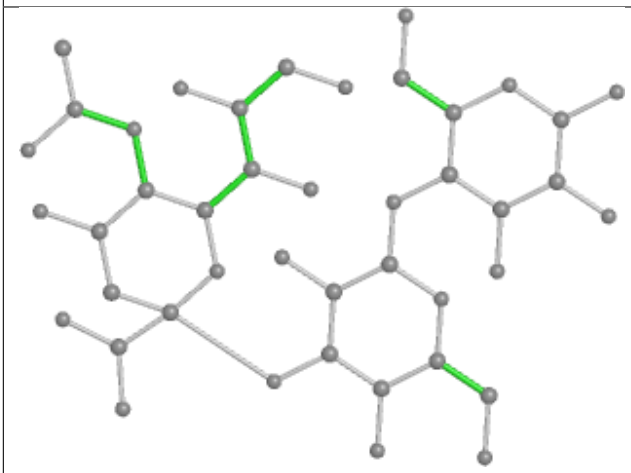
Oligosaccharide Chain H



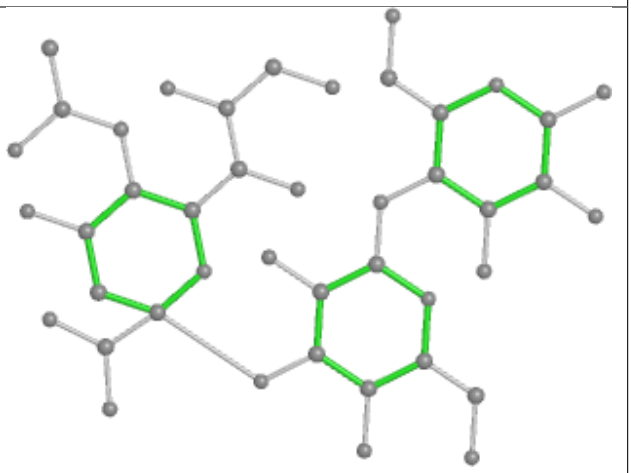
Bond lengths



Bond angles

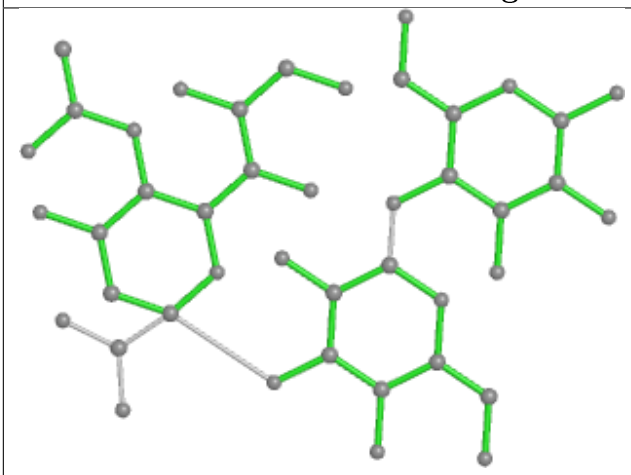


Torsions

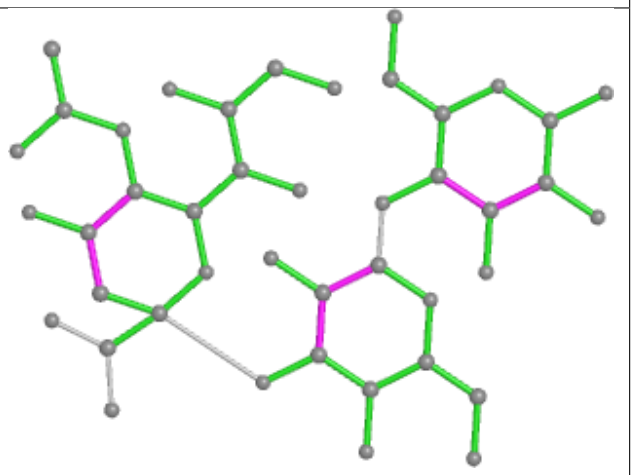


Rings

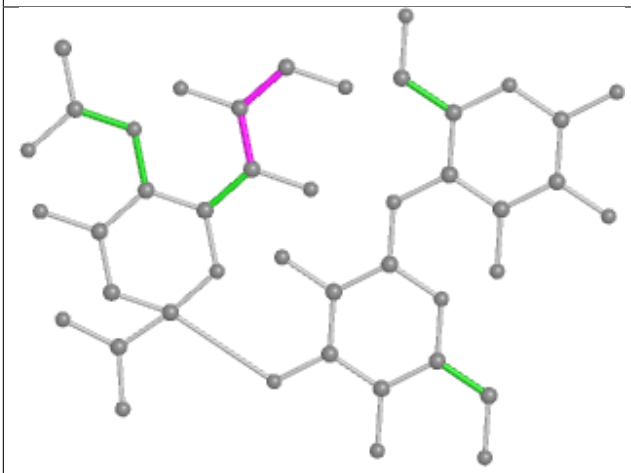
Oligosaccharide Chain I



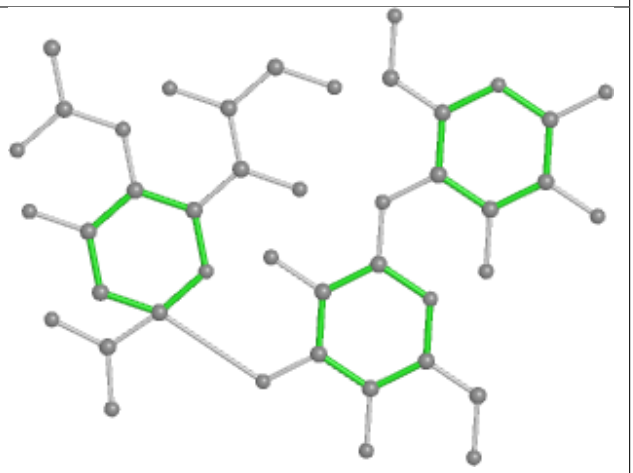
Bond lengths



Bond angles

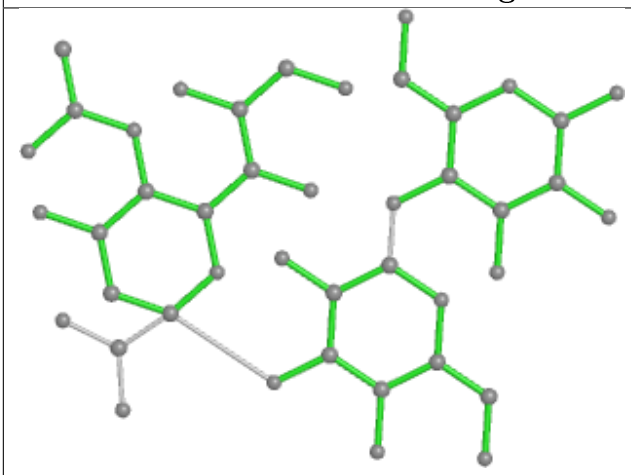


Torsions

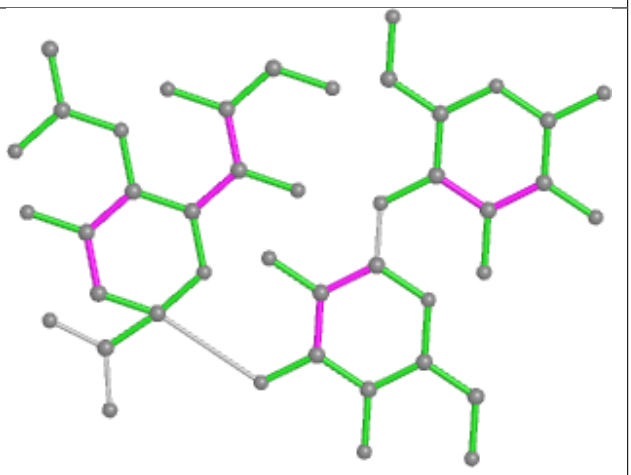


Rings

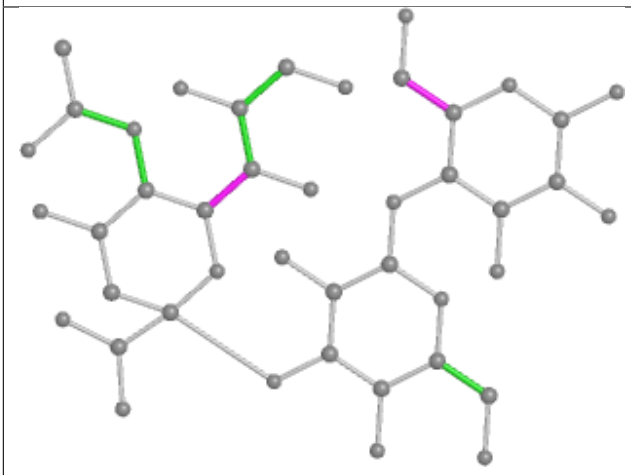
Oligosaccharide Chain J



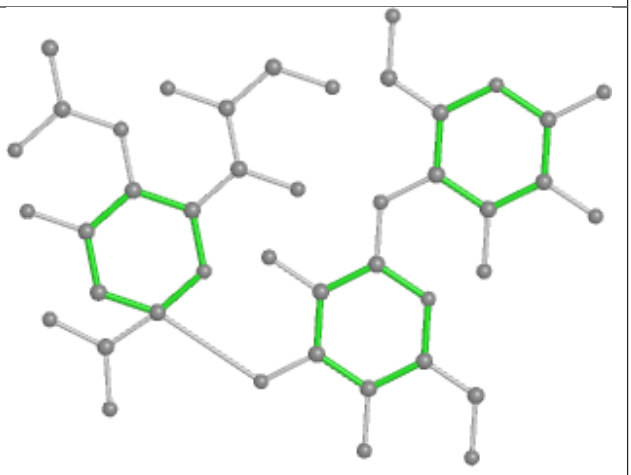
Bond lengths



Bond angles

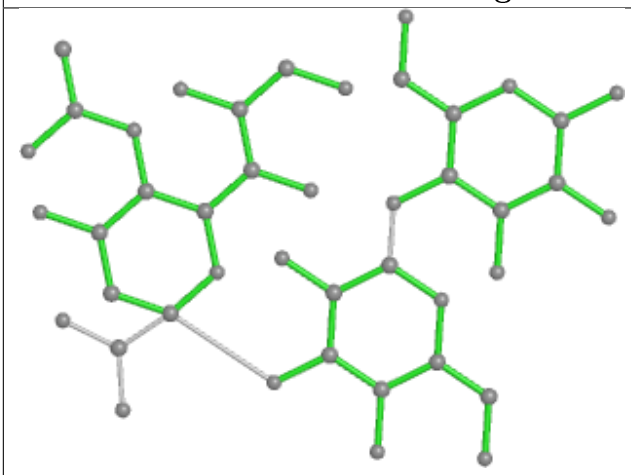


Torsions

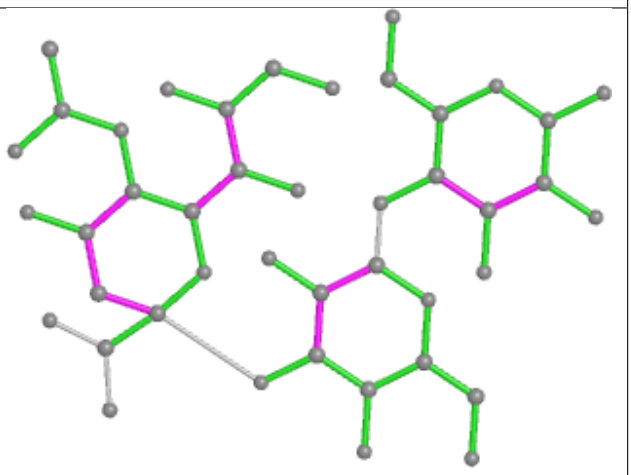


Rings

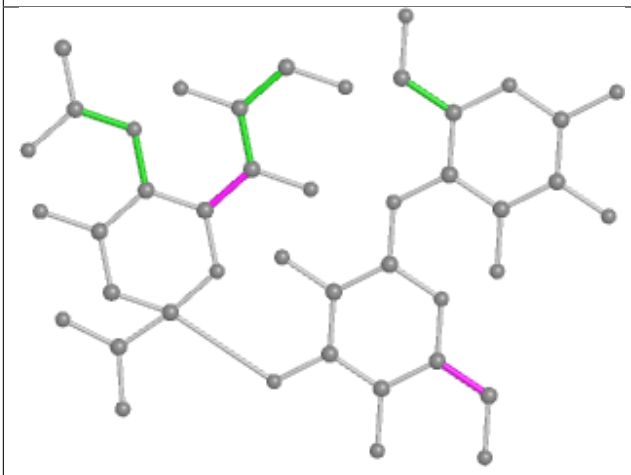
Oligosaccharide Chain K



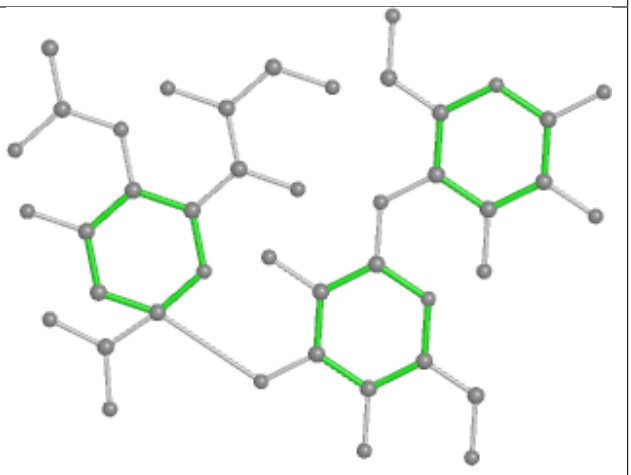
Bond lengths



Bond angles

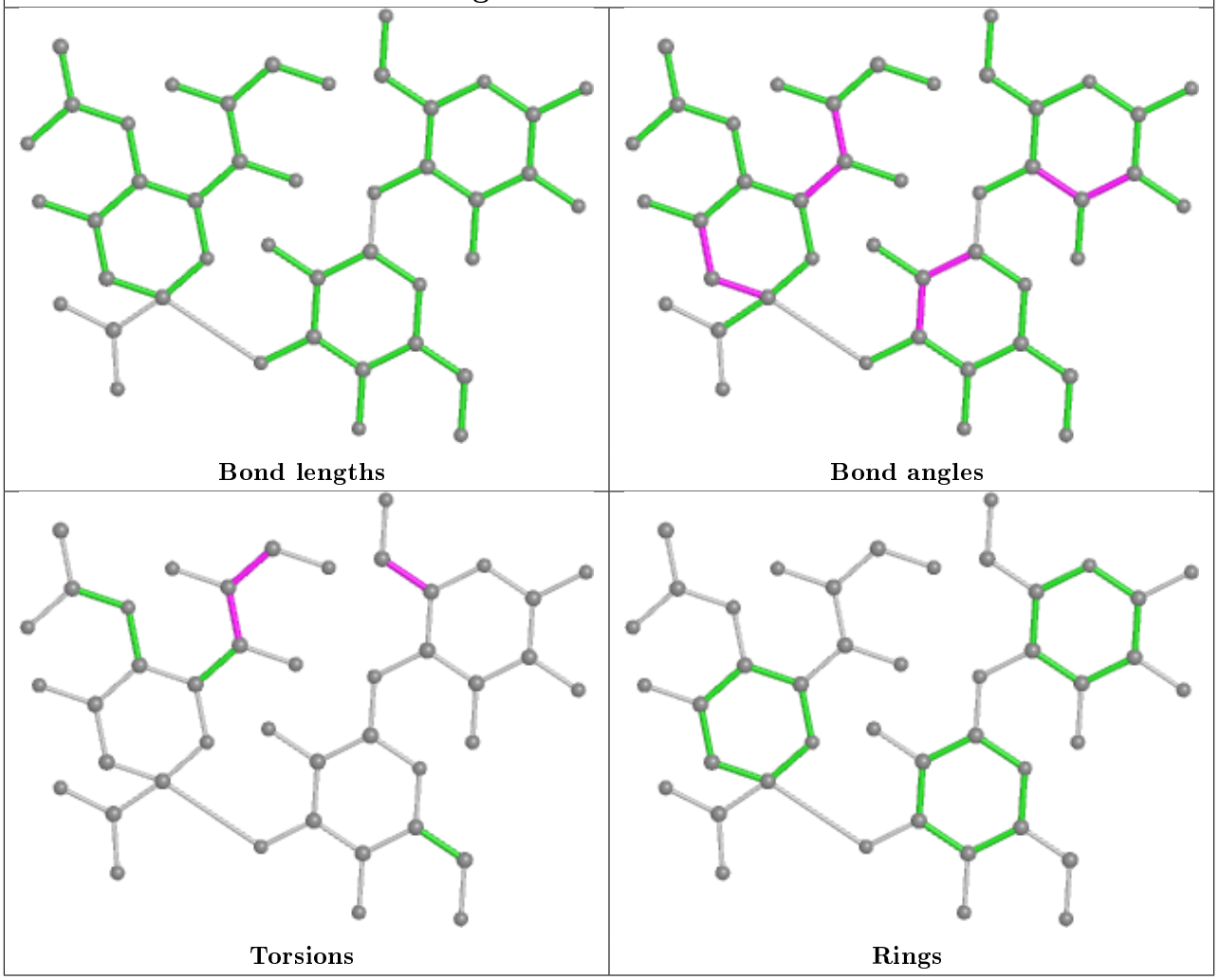


Torsions



Rings

Oligosaccharide Chain L



5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	D	1

Continued on next page...

Continued from previous page...

Mol	Chain	Number of breaks
1	C	1
1	F	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	336:VAL	C	337:GLN	N	4.77
1	B	336:VAL	C	337:GLN	N	3.16
1	F	336:VAL	C	337:GLN	N	2.96
1	C	336:VAL	C	337:GLN	N	2.91
1	E	336:VAL	C	337:GLN	N	1.64

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.