



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:13 AM UTC

PDB ID : 4GO3 / pdb_00004go3
Title : Crystal structure of PnpE from Pseudomonas sp. WBC-3
Authors : Su, J.; Zhang, C.; Liu, S.; Zhu, D.; Gu, L.
Deposited on : 2012-08-18
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

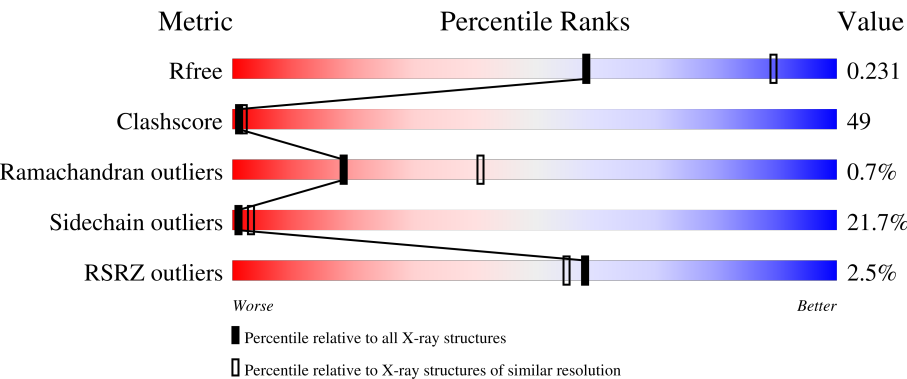
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	495	% 39%47%12%..
1	B	495	2% 41%43%13%..
1	C	495	% 41%42%15%..
1	D	495	% 41%45%12%..
1	E	495	2% 40%46%12%..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	495	3% 35% 48% 15% .
1	G	495	4% 32% 48% 16% ..
1	H	495	4% 41% 43% 14% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 29686 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 Putative gamma-hydroxymuconic semialdehyde dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3685	2333	652	684	16			
1	B	487	Total	C	N	O	S	0	1	0
			3692	2338	654	684	16			
1	C	487	Total	C	N	O	S	0	1	0
			3691	2337	652	686	16			
1	D	487	Total	C	N	O	S	0	0	0
			3685	2333	652	684	16			
1	E	485	Total	C	N	O	S	0	0	0
			3665	2321	646	682	16			
1	F	487	Total	C	N	O	S	0	0	0
			3685	2333	652	684	16			
1	G	487	Total	C	N	O	S	0	0	0
			3685	2333	652	684	16			
1	H	487	Total	C	N	O	S	0	0	0
			3685	2333	652	684	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	426	ASN	SER	engineered mutation	UNP C1I208
A	484	HIS	TYR	engineered mutation	UNP C1I208
A	488	LEU	-	expression tag	UNP C1I208
A	489	GLY	-	expression tag	UNP C1I208
A	490	HIS	-	expression tag	UNP C1I208
A	491	HIS	-	expression tag	UNP C1I208
A	492	HIS	-	expression tag	UNP C1I208
A	493	HIS	-	expression tag	UNP C1I208
A	494	HIS	-	expression tag	UNP C1I208
A	495	HIS	-	expression tag	UNP C1I208
B	426	ASN	SER	engineered mutation	UNP C1I208
B	484	HIS	TYR	engineered mutation	UNP C1I208
B	488	LEU	-	expression tag	UNP C1I208

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	489	GLY	-	expression tag	UNP C1I208
B	490	HIS	-	expression tag	UNP C1I208
B	491	HIS	-	expression tag	UNP C1I208
B	492	HIS	-	expression tag	UNP C1I208
B	493	HIS	-	expression tag	UNP C1I208
B	494	HIS	-	expression tag	UNP C1I208
B	495	HIS	-	expression tag	UNP C1I208
C	426	ASN	SER	engineered mutation	UNP C1I208
C	484	HIS	TYR	engineered mutation	UNP C1I208
C	488	LEU	-	expression tag	UNP C1I208
C	489	GLY	-	expression tag	UNP C1I208
C	490	HIS	-	expression tag	UNP C1I208
C	491	HIS	-	expression tag	UNP C1I208
C	492	HIS	-	expression tag	UNP C1I208
C	493	HIS	-	expression tag	UNP C1I208
C	494	HIS	-	expression tag	UNP C1I208
C	495	HIS	-	expression tag	UNP C1I208
D	426	ASN	SER	engineered mutation	UNP C1I208
D	484	HIS	TYR	engineered mutation	UNP C1I208
D	488	LEU	-	expression tag	UNP C1I208
D	489	GLY	-	expression tag	UNP C1I208
D	490	HIS	-	expression tag	UNP C1I208
D	491	HIS	-	expression tag	UNP C1I208
D	492	HIS	-	expression tag	UNP C1I208
D	493	HIS	-	expression tag	UNP C1I208
D	494	HIS	-	expression tag	UNP C1I208
D	495	HIS	-	expression tag	UNP C1I208
E	426	ASN	SER	engineered mutation	UNP C1I208
E	484	HIS	TYR	engineered mutation	UNP C1I208
E	488	LEU	-	expression tag	UNP C1I208
E	489	GLY	-	expression tag	UNP C1I208
E	490	HIS	-	expression tag	UNP C1I208
E	491	HIS	-	expression tag	UNP C1I208
E	492	HIS	-	expression tag	UNP C1I208
E	493	HIS	-	expression tag	UNP C1I208
E	494	HIS	-	expression tag	UNP C1I208
E	495	HIS	-	expression tag	UNP C1I208
F	426	ASN	SER	engineered mutation	UNP C1I208
F	484	HIS	TYR	engineered mutation	UNP C1I208
F	488	LEU	-	expression tag	UNP C1I208
F	489	GLY	-	expression tag	UNP C1I208
F	490	HIS	-	expression tag	UNP C1I208

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	491	HIS	-	expression tag	UNP C1I208
F	492	HIS	-	expression tag	UNP C1I208
F	493	HIS	-	expression tag	UNP C1I208
F	494	HIS	-	expression tag	UNP C1I208
F	495	HIS	-	expression tag	UNP C1I208
G	426	ASN	SER	engineered mutation	UNP C1I208
G	484	HIS	TYR	engineered mutation	UNP C1I208
G	488	LEU	-	expression tag	UNP C1I208
G	489	GLY	-	expression tag	UNP C1I208
G	490	HIS	-	expression tag	UNP C1I208
G	491	HIS	-	expression tag	UNP C1I208
G	492	HIS	-	expression tag	UNP C1I208
G	493	HIS	-	expression tag	UNP C1I208
G	494	HIS	-	expression tag	UNP C1I208
G	495	HIS	-	expression tag	UNP C1I208
H	426	ASN	SER	engineered mutation	UNP C1I208
H	484	HIS	TYR	engineered mutation	UNP C1I208
H	488	LEU	-	expression tag	UNP C1I208
H	489	GLY	-	expression tag	UNP C1I208
H	490	HIS	-	expression tag	UNP C1I208
H	491	HIS	-	expression tag	UNP C1I208
H	492	HIS	-	expression tag	UNP C1I208
H	493	HIS	-	expression tag	UNP C1I208
H	494	HIS	-	expression tag	UNP C1I208
H	495	HIS	-	expression tag	UNP C1I208

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	29	Total O 29 29	0	0
2	B	29	Total O 29 29	0	0
2	C	31	Total O 31 31	0	0
2	D	24	Total O 24 24	0	0
2	E	30	Total O 30 30	0	0
2	F	34	Total O 34 34	0	0
2	G	23	Total O 23 23	0	0

Continued on next page...

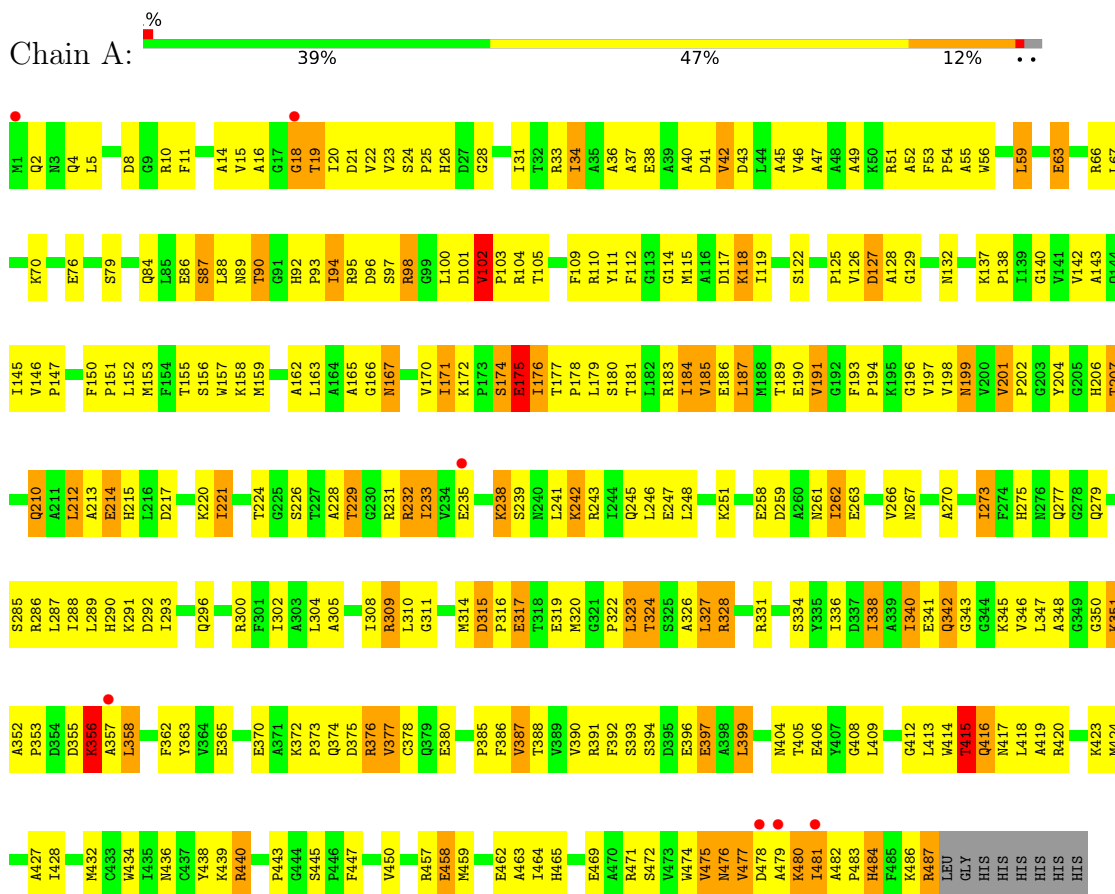
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	H	13	Total	O	0	0
			13	13		

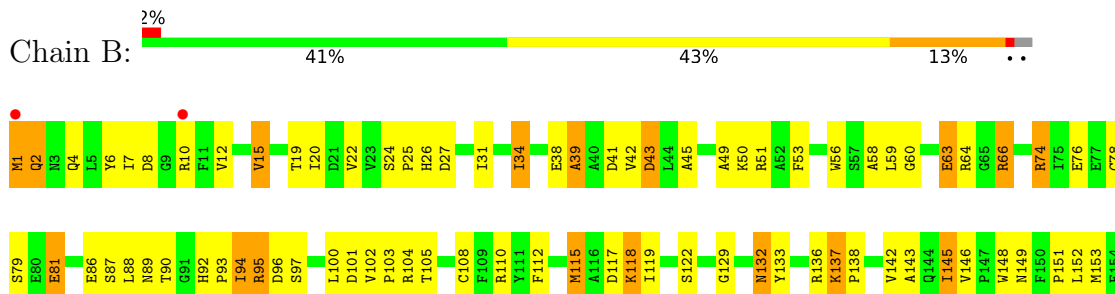
3 Residue-property plots

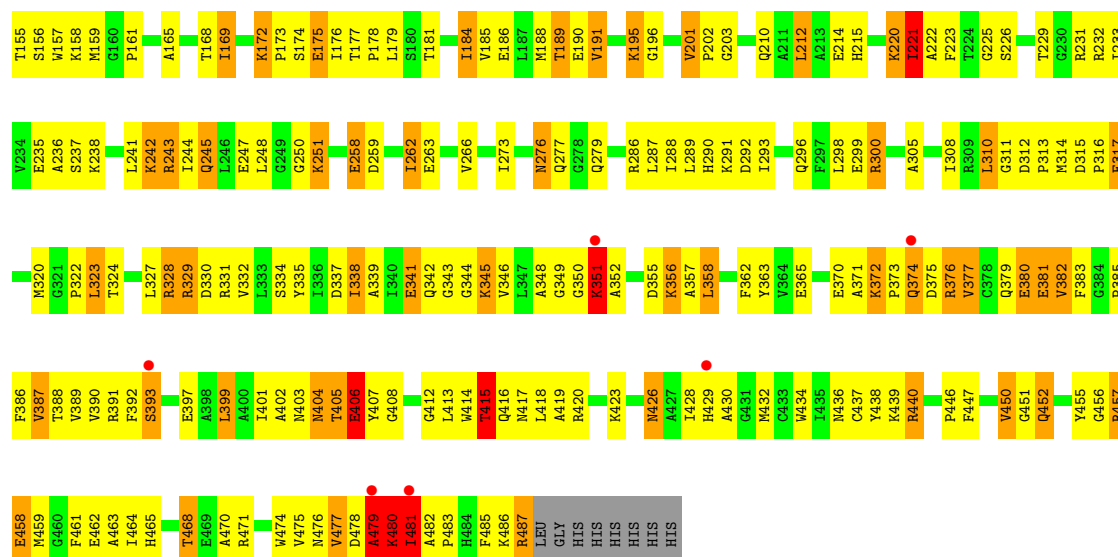
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

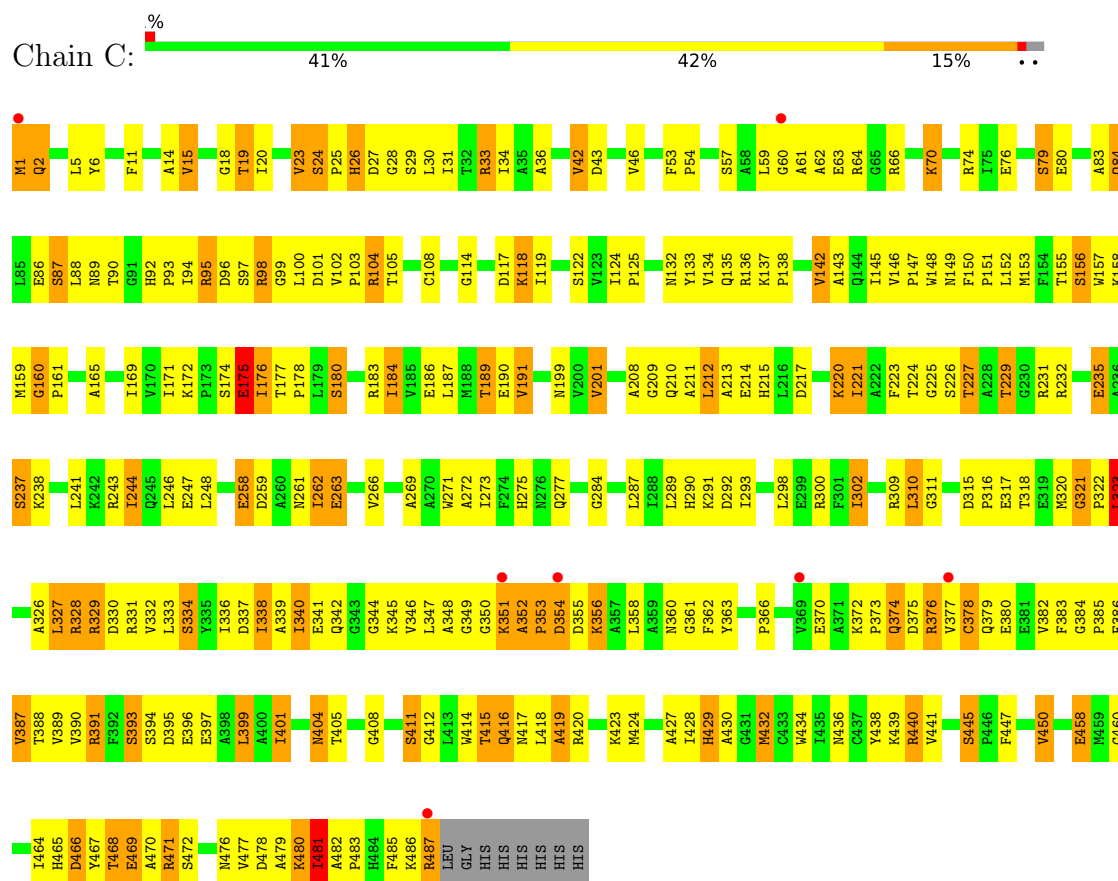


• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

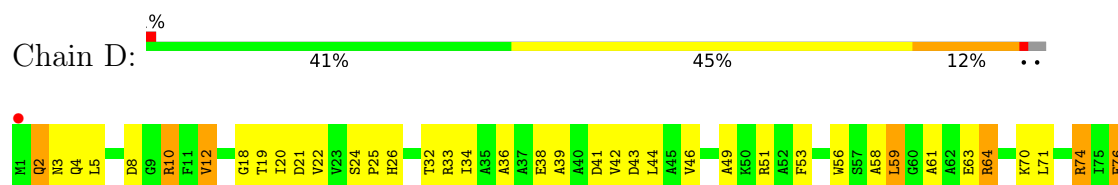


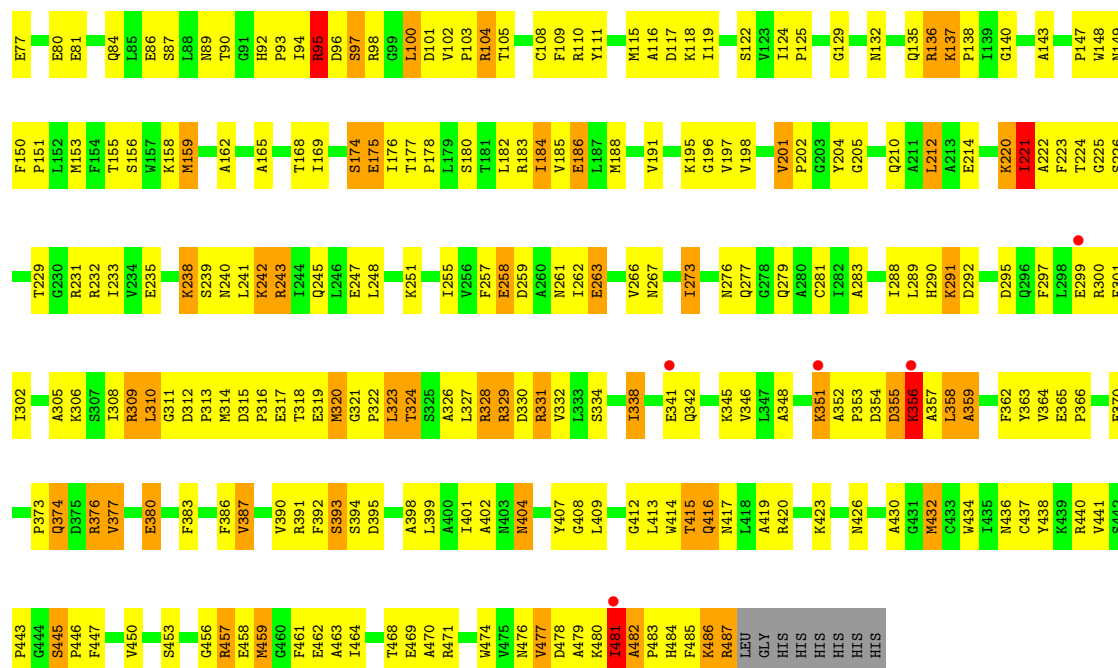


• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

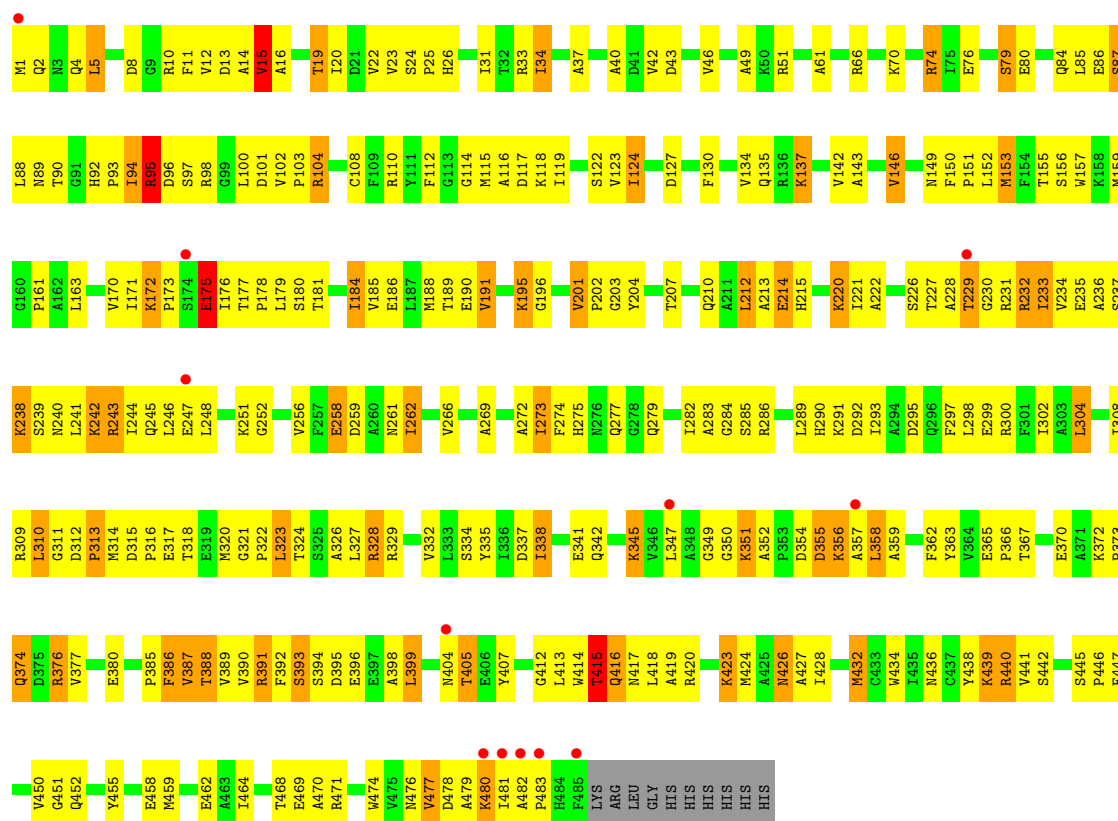


• Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase

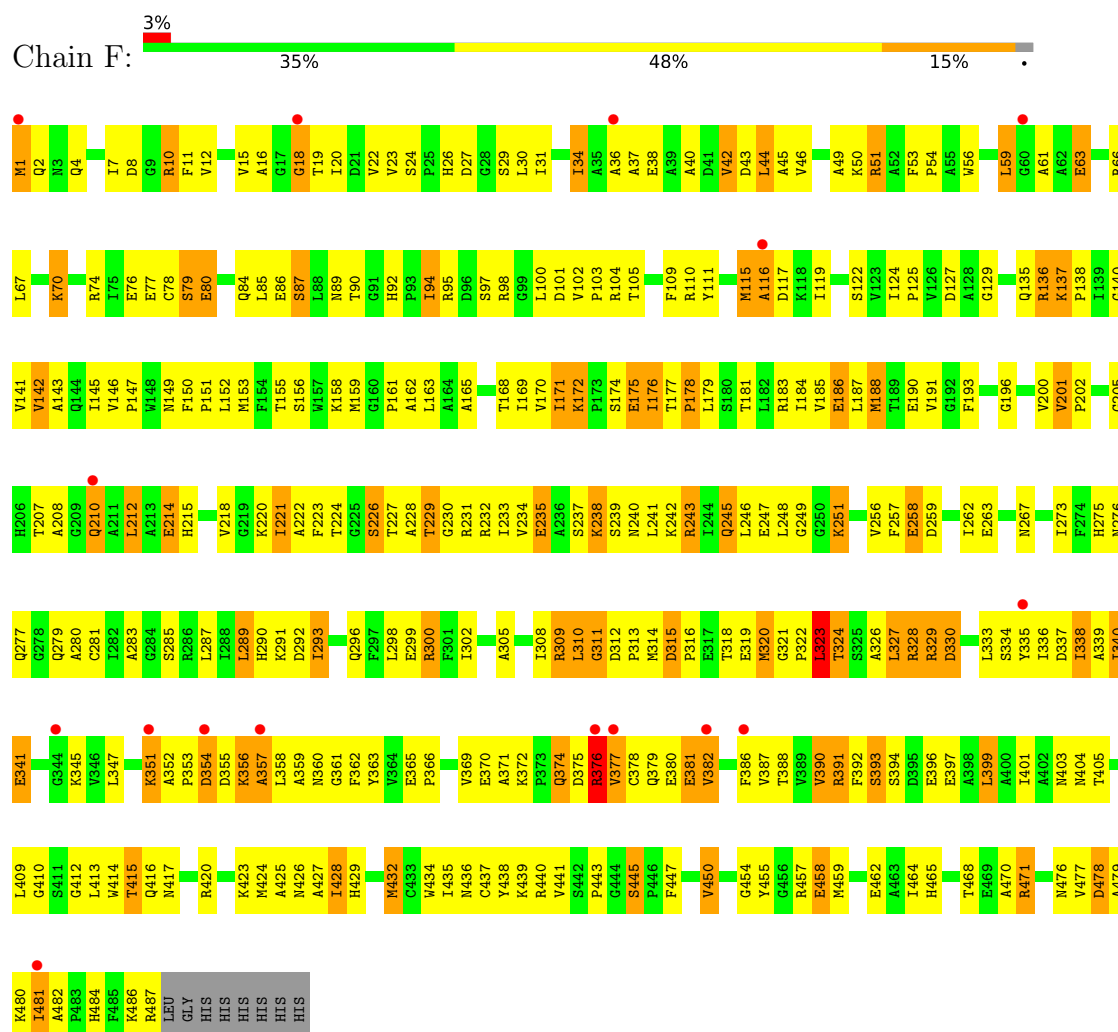




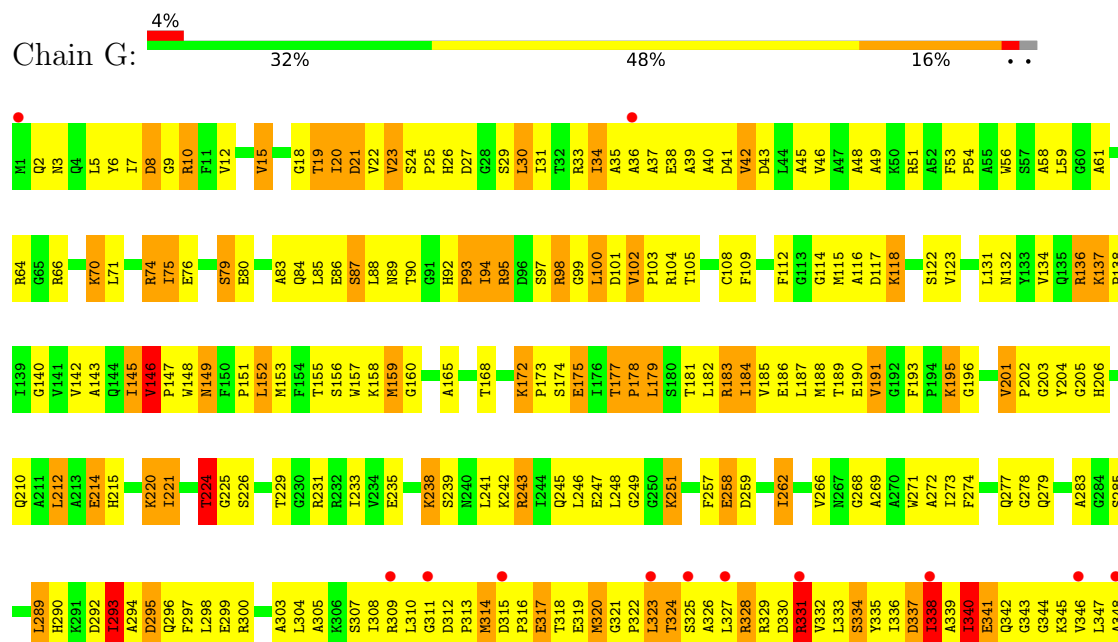
● Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase



● Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase



- Molecule 1: Putative gamma-hydroxymuconic semialdehyde dehydrogenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.53Å 144.25Å 138.29Å 90.00° 93.59° 90.00°	Depositor
Resolution (Å)	41.68 – 2.70 41.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.5 (41.68-2.70) 96.4 (41.68-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.12 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.223 , 0.237 0.218 , 0.231	Depositor DCC
R_{free} test set	4296 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å ²)	38.6	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29686	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.50% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.26	2/3761 (0.1%)	1.01	16/5101 (0.3%)
1	B	1.25	5/3772 (0.1%)	1.05	15/5116 (0.3%)
1	C	1.32	2/3770 (0.1%)	1.05	15/5113 (0.3%)
1	D	1.30	7/3761 (0.2%)	1.06	21/5101 (0.4%)
1	E	1.29	3/3741 (0.1%)	1.02	9/5076 (0.2%)
1	F	1.21	1/3761 (0.0%)	1.12	19/5101 (0.4%)
1	G	1.21	1/3761 (0.0%)	1.27	49/5101 (1.0%)
1	H	1.19	3/3761 (0.1%)	1.05	20/5101 (0.4%)
All	All	1.25	24/30088 (0.1%)	1.08	164/40810 (0.4%)

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	B	0	2
1	G	0	1
All	All	0	3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	222	ALA	CA-CB	-6.87	1.44	1.53
1	B	222	ALA	CA-CB	-6.85	1.44	1.53
1	H	222	ALA	CA-CB	-6.79	1.44	1.53
1	A	125	PRO	C-O	-6.47	1.18	1.24
1	C	352	ALA	CA-C	-6.18	1.46	1.53
1	D	100	LEU	C-O	-6.01	1.16	1.24
1	D	58	ALA	CA-CB	-5.78	1.43	1.53
1	B	58	ALA	CA-CB	-5.75	1.43	1.53
1	G	58	ALA	CA-CB	-5.74	1.43	1.53
1	D	221	ILE	C-O	-5.69	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	221	ILE	C-O	-5.64	1.18	1.24
1	H	221	ILE	C-O	-5.64	1.18	1.24
1	C	310	LEU	C-O	-5.42	1.17	1.24
1	D	310	LEU	C-O	-5.41	1.17	1.24
1	E	310	LEU	C-O	-5.40	1.17	1.24
1	B	132	ASN	C-O	-5.36	1.17	1.24
1	F	352	ALA	CA-C	-5.34	1.46	1.53
1	B	310	LEU	C-O	-5.30	1.17	1.24
1	H	470	ALA	CA-CB	-5.30	1.45	1.53
1	E	470	ALA	CA-CB	-5.28	1.45	1.53
1	D	346	VAL	C-O	-5.14	1.19	1.24
1	A	346	VAL	C-O	-5.13	1.19	1.24
1	D	419	ALA	N-CA	-5.10	1.40	1.46
1	E	163	LEU	C-O	-5.08	1.18	1.24

All (164) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	315	ASP	N-CA-C	-18.96	86.18	110.07
1	G	315	ASP	CB-CA-C	18.01	134.27	108.87
1	B	480	LYS	CA-C-N	15.22	144.19	120.13
1	B	480	LYS	C-N-CA	15.22	144.19	120.13
1	G	477	VAL	CB-CA-C	15.15	136.14	111.29
1	F	462	GLU	N-CA-C	13.93	127.82	111.11
1	F	115	MET	CB-CA-C	-12.57	88.44	109.55
1	D	358	LEU	N-CA-C	-12.21	100.70	114.62
1	D	482	ALA	CB-CA-C	11.69	134.40	110.31
1	A	340	ILE	N-CA-C	11.03	121.52	110.82
1	A	340	ILE	CB-CA-C	-10.66	98.08	112.04
1	F	462	GLU	CB-CA-C	-10.61	93.84	110.81
1	F	327	LEU	N-CA-C	9.67	121.51	110.97
1	B	479	ALA	CB-CA-C	9.66	129.65	110.42
1	F	315	ASP	N-CA-C	-9.58	95.93	109.24
1	F	116	ALA	N-CA-C	9.45	122.76	111.33
1	D	481	ILE	CB-CA-C	-9.16	99.49	111.13
1	A	233	ILE	N-CA-C	-8.85	102.20	111.58
1	F	357	ALA	N-CA-C	-8.51	102.89	113.18
1	D	355	ASP	CB-CA-C	8.39	125.11	110.85
1	G	315	ASP	CA-C-N	8.38	129.43	120.12
1	G	315	ASP	C-N-CA	8.38	129.43	120.12
1	B	382	VAL	N-CA-C	-8.05	99.19	109.58
1	G	83	ALA	CB-CA-C	-8.03	98.28	110.88

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	480	LYS	CB-CA-C	8.02	121.40	109.29
1	G	354	ASP	N-CA-C	-7.91	103.52	113.01
1	G	95	ARG	N-CA-C	-7.66	102.58	112.23
1	F	376	ARG	N-CA-C	7.57	120.25	111.02
1	C	382	VAL	N-CA-C	-7.50	98.99	108.89
1	G	83	ALA	N-CA-C	7.46	119.05	111.07
1	F	116	ALA	CB-CA-C	-7.46	98.00	110.68
1	F	315	ASP	CB-CA-C	7.37	119.99	109.38
1	E	15	VAL	CB-CA-C	-7.20	99.48	111.29
1	C	477	VAL	N-CA-C	7.14	124.19	109.34
1	A	484	HIS	N-CA-C	-7.11	103.57	111.82
1	D	482	ALA	CA-C-N	7.09	127.52	119.93
1	D	482	ALA	C-N-CA	7.09	127.52	119.93
1	D	358	LEU	CB-CA-C	7.04	118.64	109.28
1	H	160	GLY	O-C-N	6.97	123.58	121.07
1	G	23	VAL	N-CA-C	6.87	119.75	109.17
1	G	224	THR	N-CA-C	-6.86	96.18	110.80
1	G	168	THR	N-CA-C	-6.78	100.49	110.52
1	G	369	VAL	N-CA-C	6.64	117.83	107.28
1	E	415	THR	CB-CA-C	-6.62	98.20	111.17
1	A	415	THR	CB-CA-C	-6.61	98.22	111.17
1	H	415	THR	CB-CA-C	-6.59	98.25	111.17
1	B	415	THR	CB-CA-C	-6.59	98.26	111.17
1	G	357	ALA	CB-CA-C	6.53	123.42	110.42
1	C	64	ARG	N-CA-C	-6.49	104.39	112.90
1	G	317	GLU	N-CA-C	-6.46	105.53	113.41
1	G	295	ASP	CB-CA-C	-6.46	100.20	110.86
1	F	18	GLY	N-CA-C	6.44	118.89	111.36
1	F	356	LYS	N-CA-C	-6.39	104.71	114.16
1	G	384	GLY	CA-C-N	6.38	127.82	119.84
1	G	384	GLY	C-N-CA	6.38	127.82	119.84
1	C	95	ARG	N-CA-C	-6.37	105.36	113.01
1	B	479	ALA	CA-C-N	-6.32	109.84	121.41
1	B	479	ALA	C-N-CA	-6.32	109.84	121.41
1	G	397	GLU	N-CA-C	-6.31	103.93	111.69
1	D	356	LYS	CB-CA-C	-6.29	97.91	110.42
1	H	352	ALA	N-CA-C	-6.26	101.00	110.39
1	G	453	SER	N-CA-C	-6.19	105.31	112.92
1	C	160	GLY	CA-C-N	6.18	125.40	118.97
1	C	160	GLY	C-N-CA	6.18	125.40	118.97
1	D	482	ALA	N-CA-C	-6.14	99.93	109.87
1	D	64	ARG	N-CA-C	-6.05	104.76	111.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	95	ARG	N-CA-C	-5.99	105.23	112.54
1	H	311	GLY	N-CA-C	5.94	118.59	110.69
1	B	311	GLY	N-CA-C	5.90	118.54	110.69
1	F	311	GLY	N-CA-C	5.89	118.53	110.69
1	D	351	LYS	N-CA-C	5.88	115.61	107.73
1	B	406	GLU	N-CA-C	-5.82	105.94	113.16
1	D	357	ALA	N-CA-C	-5.79	104.62	112.26
1	G	477	VAL	CA-C-N	5.76	130.62	121.18
1	G	477	VAL	C-N-CA	5.76	130.62	121.18
1	H	371	ALA	N-CA-C	5.75	115.61	108.19
1	C	311	GLY	N-CA-C	5.71	118.57	110.74
1	A	18	GLY	N-CA-C	5.70	118.03	111.36
1	D	311	GLY	N-CA-C	5.70	118.55	110.74
1	E	311	GLY	N-CA-C	5.70	118.54	110.74
1	H	336	ILE	CB-CA-C	-5.67	104.48	112.14
1	A	311	GLY	N-CA-C	5.66	118.50	110.74
1	G	486	LYS	N-CA-C	-5.66	98.73	110.80
1	F	137	LYS	N-CA-C	-5.66	101.75	110.58
1	A	323	LEU	N-CA-C	-5.66	103.06	110.53
1	B	39	ALA	CB-CA-C	-5.65	99.17	110.42
1	F	323	LEU	N-CA-C	-5.65	103.07	110.53
1	H	326	ALA	CB-CA-C	-5.65	98.08	109.55
1	E	323	LEU	N-CA-C	-5.64	103.09	110.53
1	B	323	LEU	N-CA-C	-5.62	103.07	110.43
1	E	175	GLU	N-CA-C	-5.61	106.28	113.01
1	H	484	HIS	N-CA-C	-5.60	105.18	111.28
1	H	115	MET	N-CA-C	-5.60	105.57	112.90
1	G	415	THR	CB-CA-C	-5.59	100.21	111.17
1	C	231	ARG	N-CA-C	-5.58	105.34	111.82
1	G	18	GLY	N-CA-C	-5.58	105.12	112.82
1	E	5	LEU	N-CA-C	-5.57	103.14	110.43
1	G	100	LEU	N-CA-C	5.56	122.63	110.80
1	H	88	LEU	N-CA-C	-5.53	106.70	113.50
1	H	339	ALA	N-CA-C	-5.50	106.41	113.23
1	G	359	ALA	N-CA-C	-5.50	106.41	113.01
1	G	477	VAL	N-CA-C	-5.50	97.90	109.34
1	A	175	GLU	N-CA-C	-5.50	106.27	112.87
1	F	376	ARG	CB-CA-C	-5.50	102.18	110.92
1	G	23	VAL	CB-CA-C	-5.50	103.69	111.38
1	G	93	PRO	N-CA-C	-5.49	101.16	112.47
1	C	481	ILE	N-CA-C	5.49	114.27	106.53
1	H	252	GLY	N-CA-C	5.48	119.53	110.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	269	ALA	N-CA-C	-5.48	105.22	111.14
1	A	358	LEU	N-CA-C	-5.47	104.15	111.87
1	C	26	HIS	CB-CA-C	5.46	119.46	110.88
1	C	323	LEU	N-CA-C	-5.46	103.69	110.41
1	G	146	VAL	N-CA-C	5.46	113.67	109.19
1	G	152	LEU	N-CA-C	5.46	116.91	111.07
1	A	317	GLU	N-CA-C	-5.46	105.98	113.30
1	G	340	ILE	CB-CA-C	-5.46	104.71	111.70
1	H	338	ILE	N-CA-C	-5.44	105.61	113.07
1	D	419	ALA	N-CA-C	5.43	116.88	111.07
1	A	476	ASN	CA-C-N	-5.42	117.66	122.97
1	A	476	ASN	C-N-CA	-5.42	117.66	122.97
1	G	317	GLU	CB-CA-C	5.42	118.72	109.24
1	G	484	HIS	N-CA-C	-5.41	105.47	111.36
1	G	418	LEU	N-CA-C	5.40	117.59	111.11
1	G	324	THR	N-CA-C	5.40	117.92	111.71
1	H	234	VAL	N-CA-C	-5.38	104.77	112.35
1	F	115	MET	N-CA-C	5.37	120.70	113.72
1	D	186	GLU	N-CA-C	-5.33	105.03	112.45
1	G	137	LYS	N-CA-C	5.32	116.69	110.31
1	G	416	GLN	N-CA-C	-5.32	105.63	113.61
1	G	233	ILE	N-CA-C	-5.31	104.32	111.44
1	C	321	GLY	CA-C-N	-5.30	115.12	120.85
1	C	321	GLY	C-N-CA	-5.30	115.12	120.85
1	C	355	ASP	CB-CA-C	-5.30	101.16	109.70
1	G	295	ASP	N-CA-C	5.30	118.08	111.24
1	G	131	LEU	N-CA-C	-5.30	99.80	108.76
1	B	169	ILE	N-CA-C	5.27	116.25	108.45
1	D	359	ALA	CB-CA-C	5.27	119.49	110.74
1	H	175	GLU	N-CA-C	-5.26	106.13	112.54
1	G	102	VAL	N-CA-C	5.25	120.23	108.88
1	G	386	PHE	N-CA-C	-5.21	99.78	108.32
1	F	354	ASP	CB-CA-C	-5.21	104.00	111.91
1	B	481	ILE	CB-CA-C	-5.20	104.53	111.13
1	G	100	LEU	CB-CA-C	-5.20	100.07	110.42
1	E	95	ARG	N-CA-C	-5.19	105.80	111.82
1	B	60	GLY	N-CA-C	-5.18	100.90	113.18
1	H	382	VAL	N-CA-C	-5.17	102.84	109.30
1	H	129	GLY	N-CA-C	-5.16	108.33	114.48
1	D	484	HIS	N-CA-C	-5.16	105.31	111.03
1	G	123	VAL	N-CA-C	-5.15	100.22	107.75
1	E	252	GLY	N-CA-C	5.14	118.22	111.03

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	395	ASP	N-CA-C	-5.14	106.52	112.89
1	C	415	THR	CB-CA-C	-5.13	101.27	113.02
1	D	346	VAL	N-CA-C	5.13	115.61	108.84
1	A	346	VAL	N-CA-C	5.11	115.59	108.84
1	H	263	GLU	CA-C-N	5.11	127.12	120.28
1	H	263	GLU	C-N-CA	5.11	127.12	120.28
1	G	331	ARG	N-CA-C	-5.09	107.24	113.50
1	G	395	ASP	N-CA-C	-5.05	105.90	111.71
1	A	102	VAL	CB-CA-C	-5.05	108.90	113.70
1	H	64	ARG	N-CA-C	-5.05	105.86	111.36
1	D	358	LEU	CA-C-N	5.05	128.39	120.82
1	D	358	LEU	C-N-CA	5.05	128.39	120.82
1	F	354	ASP	N-CA-C	-5.02	102.92	110.70
1	A	315	ASP	CA-C-O	5.01	123.03	119.32

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	479	ALA	Peptide
1	B	480	LYS	Peptide
1	G	477	VAL	Peptide

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	3685	0	3676	359	4
1	B	3692	0	3683	432	18
1	C	3691	0	3680	345	2
1	D	3685	0	3678	309	2
1	E	3665	0	3651	379	2
1	F	3685	0	3677	430	10
1	G	3685	0	3678	476	0
1	H	3685	0	3675	347	15
2	A	29	0	0	18	1
2	B	29	0	0	32	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	31	0	0	34	0
2	D	24	0	0	15	0
2	E	30	0	0	30	0
2	F	34	0	0	21	0
2	G	23	0	0	28	0
2	H	13	0	0	11	0
All	All	29686	0	29398	2911	27

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 49.

All (2911) 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:H:263:GLU:CG	1:H:300:ARG:NH2	1.68	1.51
1:G:10:ARG:NH1	1:G:12:VAL:CG1	1.73	1.50
1:B:479:ALA:HB1	1:B:480:LYS:CB	1.44	1.47
1:B:479:ALA:HB1	1:B:480:LYS:CG	1.43	1.46
1:B:238:LYS:CE	1:F:235:GLU:HG2	1.50	1.41
1:A:159:MET:CE	1:A:198:VAL:HG11	1.47	1.41
1:B:238:LYS:NZ	1:F:235:GLU:HG2	1.31	1.37
1:H:49:ALA:HB1	1:H:168:THR:CG2	1.55	1.37
1:B:238:LYS:NZ	1:F:235:GLU:CG	1.87	1.36
1:A:159:MET:CE	1:A:198:VAL:CG1	2.01	1.36
1:E:74:ARG:NH2	1:E:190:GLU:OE1	1.56	1.35
1:D:115:MET:HE1	1:D:461:PHE:CE1	1.59	1.34
1:C:432:MET:HE1	1:C:447:PHE:CD1	1.60	1.34
1:A:159:MET:HE1	1:A:198:VAL:CG1	1.55	1.34
1:H:329:ARG:CD	1:H:330:ASP:OD1	1.75	1.34
1:A:97:SER:O	1:A:102:VAL:CG2	1.77	1.33
1:A:376:ARG:HD3	1:A:380:GLU:OE2	1.21	1.31
1:A:235:GLU:HB3	1:C:238:LYS:CE	1.60	1.31
1:B:115:MET:HE1	1:B:461:PHE:CE1	1.64	1.31
1:C:440:ARG:HA	2:C:530:HOH:O	1.33	1.27
1:G:338:ILE:HD12	1:G:338:ILE:C	1.54	1.27
1:A:94:ILE:O	1:A:98:ARG:HG3	1.33	1.26
1:H:263:GLU:HG3	1:H:300:ARG:NH2	1.31	1.25
1:E:376:ARG:HD2	1:E:380:GLU:OE2	1.32	1.25
1:E:159:MET:HE2	1:E:171:ILE:CD1	1.66	1.25
1:E:291:LYS:HE2	1:E:393:SER:OG	1.09	1.25
1:B:238:LYS:HZ3	1:F:235:GLU:CG	1.42	1.24

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:229:THR:HG23	1:H:232:ARG:NH2	1.51	1.24
1:H:87:SER:OG	1:H:92:HIS:O	1.55	1.23
1:H:329:ARG:HD2	1:H:330:ASP:OD1	1.18	1.23
1:D:273:ILE:HD12	1:D:273:ILE:O	1.37	1.22
1:A:97:SER:O	1:A:102:VAL:HG23	1.06	1.22
1:F:273:ILE:HG12	1:F:387:VAL:CG2	1.69	1.22
1:F:326:ALA:O	1:F:330:ASP:OD1	1.57	1.22
1:B:238:LYS:NZ	1:F:235:GLU:CD	1.98	1.21
1:F:181:THR:O	1:F:184:ILE:HG22	1.37	1.21
1:G:10:ARG:NH1	1:G:12:VAL:HG11	0.90	1.21
1:A:183:ARG:NH1	1:A:186:GLU:OE1	1.73	1.21
1:H:263:GLU:HG2	1:H:300:ARG:NH2	1.39	1.21
1:D:210:GLN:O	1:D:214:GLU:HG2	1.39	1.20
1:D:259:ASP:OD1	1:D:415:THR:CG2	1.88	1.20
1:E:231:ARG:NH2	1:H:239:SER:O	1.75	1.19
1:F:338:ILE:HD11	1:F:376:ARG:NE	1.57	1.19
1:B:479:ALA:CB	1:B:480:LYS:HB3	1.70	1.19
1:A:217:ASP:OD2	1:B:374:GLN:NE2	1.77	1.18
1:G:293:ILE:HD12	1:G:293:ILE:C	1.61	1.17
1:B:238:LYS:CE	1:F:235:GLU:CG	2.21	1.17
1:G:347:LEU:HD11	1:G:370:GLU:HG3	1.25	1.16
1:E:273:ILE:O	1:E:273:ILE:HD12	1.46	1.16
1:F:377:VAL:CG1	1:F:388:THR:HG21	1.76	1.16
1:D:323:LEU:HD23	1:D:323:LEU:N	1.53	1.15
1:G:350:GLY:O	1:G:351:LYS:HG2	1.46	1.15
1:B:132:ASN:ND2	1:F:445:SER:OG	1.79	1.15
1:A:210:GLN:O	1:A:214:GLU:HG2	1.44	1.15
1:H:99:GLY:C	1:H:100:LEU:HD23	1.72	1.15
1:G:357:ALA:C	1:G:358:LEU:HD12	1.72	1.14
1:G:481:ILE:N	1:G:481:ILE:HD12	1.58	1.14
1:D:259:ASP:OD1	1:D:415:THR:HG22	0.98	1.14
1:G:251:LYS:HB2	1:G:407:TYR:CD1	1.81	1.14
1:E:291:LYS:CE	1:E:393:SER:OG	1.95	1.14
1:E:159:MET:HE2	1:E:171:ILE:HD13	1.29	1.13
1:E:15:VAL:HG12	1:E:16:ALA:N	1.47	1.13
1:B:405:THR:CG2	1:B:407:TYR:H	1.59	1.13
1:C:408:GLY:O	1:C:430:ALA:HA	1.49	1.13
1:G:310:LEU:HD12	1:G:320:MET:HG2	1.19	1.12
1:H:49:ALA:HB1	1:H:168:THR:HG22	1.21	1.12
1:H:328:ARG:HH11	1:H:328:ARG:CG	1.59	1.12
1:A:86:GLU:O	1:A:90:THR:OG1	1.66	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ILE:HD12	1:A:233:ILE:HG23	1.28	1.12
1:B:351:LYS:HG3	1:B:352:ALA:H	1.09	1.12
1:B:426:ASN:O	1:F:137:LYS:NZ	1.82	1.12
1:B:405:THR:HG22	1:B:407:TYR:N	1.63	1.12
1:C:2:GLN:HA	1:C:2:GLN:HE21	1.06	1.12
1:A:376:ARG:CD	1:A:380:GLU:OE2	1.97	1.12
1:A:21:ASP:OD1	1:A:33:ARG:HD3	1.50	1.11
1:E:235:GLU:O	1:E:238:LYS:HD3	1.49	1.11
1:F:183:ARG:NH1	1:F:186:GLU:OE1	1.82	1.11
1:A:132:ASN:ND2	1:C:445:SER:OG	1.84	1.11
1:F:38:GLU:HA	1:F:207:THR:HG22	1.30	1.11
1:H:328:ARG:NH1	1:H:328:ARG:HG2	1.47	1.11
1:E:110:ARG:NH2	2:E:517:HOH:O	1.84	1.11
1:D:415:THR:HG21	1:D:420:ARG:HH11	1.12	1.10
1:C:2:GLN:HA	1:C:2:GLN:NE2	1.57	1.10
1:C:262:ILE:O	1:C:266:VAL:HG23	1.50	1.10
1:F:61:ALA:HB1	1:F:116:ALA:O	1.52	1.10
1:F:273:ILE:CG1	1:F:387:VAL:HG22	1.80	1.10
1:F:471:ARG:NH2	2:F:531:HOH:O	1.82	1.10
1:G:3:ASN:ND2	1:G:33:ARG:O	1.83	1.10
1:F:338:ILE:CD1	1:F:376:ARG:HE	1.65	1.10
1:H:338:ILE:O	1:H:338:ILE:HD13	1.50	1.10
1:H:329:ARG:HG3	1:H:329:ARG:HH11	0.99	1.09
1:G:363:TYR:N	2:G:519:HOH:O	1.84	1.09
1:B:238:LYS:HZ2	1:F:235:GLU:CD	1.57	1.09
1:D:10:ARG:HG2	1:D:10:ARG:HH11	1.03	1.09
1:D:137:LYS:NZ	1:G:426:ASN:ND2	1.99	1.09
1:G:87:SER:HB2	1:G:94:ILE:CD1	1.82	1.09
1:B:479:ALA:CB	1:B:480:LYS:CB	2.30	1.08
1:F:38:GLU:HA	1:F:207:THR:CG2	1.81	1.08
1:H:464:ILE:O	1:H:468:THR:HG23	1.52	1.08
1:G:183:ARG:HD2	1:G:183:ARG:O	1.52	1.08
1:B:479:ALA:CB	1:B:480:LYS:CG	2.30	1.08
1:B:479:ALA:HB1	1:B:480:LYS:HB3	1.13	1.08
1:G:338:ILE:HD12	1:G:338:ILE:O	1.53	1.08
1:F:234:VAL:O	1:F:237:SER:OG	1.67	1.08
1:A:484:HIS:O	1:C:95:ARG:NH2	1.87	1.07
1:H:8:ASP:OD2	1:H:51:ARG:NH2	1.86	1.07
1:E:239:SER:O	1:H:231:ARG:NH2	1.87	1.07
1:G:327:LEU:CD2	1:G:331:ARG:HD2	1.84	1.07
1:D:351:LYS:CG	1:D:352:ALA:H	1.68	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:LYS:HB2	1:G:407:TYR:HD1	0.91	1.07
1:A:55:ALA:C	2:A:525:HOH:O	1.95	1.06
1:B:320:MET:HE1	1:B:385:PRO:CB	1.84	1.06
1:B:100:LEU:O	1:B:104:ARG:HG3	1.55	1.06
1:F:210:GLN:O	1:F:214:GLU:HG3	1.56	1.06
1:G:335:TYR:O	1:G:339:ALA:HB2	1.55	1.06
1:F:210:GLN:O	1:F:214:GLU:CG	2.03	1.05
1:F:443:PRO:CA	1:F:459:MET:HE3	1.86	1.05
1:H:351:LYS:HG3	1:H:352:ALA:H	1.20	1.05
1:G:10:ARG:HH11	1:G:12:VAL:CG1	1.47	1.05
1:E:104:ARG:NE	1:E:153:MET:CE	2.20	1.05
1:A:235:GLU:CB	1:C:238:LYS:HE3	1.86	1.05
1:B:329:ARG:HH11	1:B:329:ARG:HG3	1.15	1.04
1:A:235:GLU:HB3	1:C:238:LYS:HE3	1.07	1.04
1:A:481:ILE:HG13	1:A:482:ALA:N	1.67	1.04
1:G:376:ARG:HH11	1:G:376:ARG:CG	1.70	1.04
1:C:302:ILE:CD1	1:C:347:LEU:HB3	1.87	1.04
1:G:201:VAL:O	1:G:201:VAL:HG13	1.57	1.04
1:G:376:ARG:HH11	1:G:376:ARG:HG3	0.90	1.04
1:A:43:ASP:OD1	1:B:374:GLN:HG2	1.54	1.04
1:G:94:ILE:HD13	1:G:314:MET:HE2	1.33	1.04
1:A:462:GLU:OE1	1:C:136:ARG:NH2	1.89	1.04
1:A:42:VAL:O	1:A:46:VAL:HG23	1.56	1.03
1:H:481:ILE:HD12	1:H:482:ALA:H	1.23	1.03
1:A:221:ILE:CD1	1:A:233:ILE:CG2	2.36	1.03
1:G:362:PHE:C	2:G:519:HOH:O	2.01	1.03
1:A:159:MET:CE	1:A:198:VAL:HG13	1.85	1.03
1:B:136:ARG:NH2	2:B:514:HOH:O	1.89	1.03
1:F:443:PRO:HA	1:F:459:MET:CE	1.88	1.02
1:F:481:ILE:HD12	1:F:482:ALA:H	1.22	1.02
1:G:25:PRO:HD2	2:G:512:HOH:O	1.59	1.02
1:C:302:ILE:HD11	1:C:347:LEU:HB3	1.39	1.02
1:G:293:ILE:C	1:G:293:ILE:CD1	2.30	1.02
1:A:158:LYS:HD3	1:A:458:GLU:OE2	1.60	1.02
1:A:258:GLU:HB3	1:A:290:HIS:CD2	1.93	1.02
1:D:309:ARG:HG2	1:D:309:ARG:NH1	1.59	1.02
1:F:94:ILE:O	1:F:98:ARG:HG3	1.58	1.02
1:H:159:MET:HE2	1:H:171:ILE:HD13	1.42	1.02
1:B:401:ILE:O	1:B:404:ASN:HB3	1.60	1.02
1:H:281:CYS:SG	2:H:503:HOH:O	2.17	1.02
1:A:232:ARG:HA	1:A:235:GLU:CG	1.89	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:ASN:ND2	1:G:445:SER:OG	1.92	1.01
1:D:351:LYS:HG3	1:D:352:ALA:H	1.21	1.01
1:E:15:VAL:CG1	1:E:16:ALA:N	2.16	1.01
1:F:338:ILE:HD11	1:F:376:ARG:HE	0.86	1.01
1:G:90:THR:O	1:G:324:THR:HG22	1.59	1.01
1:G:376:ARG:HG3	1:G:376:ARG:NH1	1.64	1.01
1:F:377:VAL:HG12	1:F:388:THR:HG21	1.39	1.01
1:A:232:ARG:CA	1:A:235:GLU:HG2	1.90	1.01
1:G:481:ILE:H	1:G:481:ILE:CD1	1.69	1.01
1:D:115:MET:HE1	1:D:461:PHE:CD1	1.95	1.01
1:D:137:LYS:HZ1	1:G:426:ASN:ND2	1.54	1.01
1:G:151:PRO:CG	1:G:177:THR:OG1	2.08	1.01
1:G:10:ARG:HH12	1:G:12:VAL:CG1	1.53	1.00
1:H:259:ASP:OD1	1:H:415:THR:HG22	1.58	1.00
1:H:49:ALA:CB	1:H:168:THR:CG2	2.39	1.00
1:C:432:MET:CE	1:C:447:PHE:CD1	2.44	1.00
1:G:322:PRO:HG3	1:G:363:TYR:CZ	1.96	1.00
1:B:152:LEU:CD1	1:B:184:ILE:CD1	2.39	1.00
1:C:302:ILE:HD11	1:C:347:LEU:CB	1.91	1.00
1:F:86:GLU:O	1:F:90:THR:OG1	1.80	1.00
1:B:439:LYS:NZ	2:B:501:HOH:O	1.93	0.99
1:B:479:ALA:HB1	1:B:480:LYS:HG2	1.41	0.99
1:H:273:ILE:HD13	1:H:285:SER:HA	1.41	0.99
1:B:2:GLN:HE21	1:B:2:GLN:HA	1.24	0.99
1:F:339:ALA:HB2	1:F:377:VAL:HG21	1.39	0.99
1:B:238:LYS:HE2	1:F:235:GLU:HG2	1.39	0.99
1:D:309:ARG:HH11	1:D:309:ARG:CG	1.74	0.99
1:G:373:PRO:HG2	1:G:374:GLN:OE1	1.60	0.99
1:A:221:ILE:HD12	1:A:233:ILE:CG2	1.92	0.98
1:F:210:GLN:NE2	2:F:527:HOH:O	1.97	0.98
1:A:232:ARG:HA	1:A:235:GLU:HG2	0.99	0.98
1:A:251:LYS:NZ	2:A:524:HOH:O	1.95	0.98
1:G:309:ARG:NH1	1:G:317:GLU:HB3	1.77	0.98
1:A:159:MET:HE3	1:A:198:VAL:HG13	1.44	0.98
1:C:26:HIS:O	1:C:361:GLY:HA3	1.62	0.98
1:G:358:LEU:HD12	1:G:358:LEU:N	1.78	0.98
1:D:309:ARG:HG2	1:D:309:ARG:HH11	0.82	0.98
1:F:415:THR:HG21	1:F:420:ARG:HD2	1.43	0.98
1:A:94:ILE:O	1:A:98:ARG:CG	2.11	0.98
1:E:42:VAL:HG13	1:E:212:LEU:HD13	1.44	0.98
1:D:8:ASP:OD2	1:D:51:ARG:NH2	1.95	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:115:MET:O	1:F:115:MET:HG3	1.64	0.97
1:G:257:PHE:HZ	1:G:424:MET:HE2	1.29	0.97
1:B:405:THR:HG22	1:B:407:TYR:H	0.81	0.97
1:D:328:ARG:HH11	1:D:383:PHE:HB3	1.28	0.97
1:A:100:LEU:O	1:A:104:ARG:HG3	1.65	0.97
1:G:94:ILE:HD13	1:G:314:MET:CE	1.94	0.97
1:G:481:ILE:HD12	1:G:481:ILE:H	0.81	0.97
1:H:102:VAL:HG22	1:H:152:LEU:HD21	1.45	0.97
1:B:74:ARG:NH2	2:B:525:HOH:O	1.97	0.97
1:C:6:TYR:OH	1:C:189:THR:HG21	1.63	0.97
1:G:373:PRO:HD2	1:G:374:GLN:OE1	1.63	0.97
1:B:238:LYS:CD	1:F:235:GLU:HG3	1.93	0.97
1:B:238:LYS:HD3	1:F:235:GLU:HG3	1.47	0.97
1:E:226:SER:OG	1:E:229:THR:HG22	1.64	0.97
1:D:188:MET:HE1	1:D:198:VAL:HG21	1.45	0.97
1:F:26:HIS:O	1:F:361:GLY:HA3	1.65	0.97
1:C:375:ASP:OD2	2:C:507:HOH:O	1.83	0.97
1:G:408:GLY:O	1:G:430:ALA:HA	1.65	0.97
1:G:322:PRO:HB3	2:G:519:HOH:O	1.65	0.96
1:A:47:ALA:HB2	1:B:374:GLN:HB2	1.44	0.96
1:C:153:MET:O	1:C:156:SER:OG	1.84	0.96
1:C:23:VAL:HG12	1:C:29:SER:O	1.64	0.96
1:H:328:ARG:HH11	1:H:328:ARG:HG2	0.81	0.96
1:E:159:MET:HE2	1:E:171:ILE:HD12	1.44	0.96
1:D:309:ARG:HD3	1:D:319:GLU:OE1	1.62	0.96
1:D:329:ARG:NH2	1:D:330:ASP:OD1	1.99	0.96
1:H:240:ASN:OD1	2:H:506:HOH:O	1.84	0.96
1:B:95:ARG:NH2	1:F:484:HIS:O	1.99	0.96
1:D:259:ASP:CG	1:D:415:THR:HG22	1.89	0.96
1:E:478:ASP:N	2:E:514:HOH:O	1.97	0.96
1:A:132:ASN:ND2	1:C:445:SER:HG	1.59	0.96
1:C:190:GLU:OE2	2:C:516:HOH:O	1.84	0.96
1:E:476:ASN:O	2:E:508:HOH:O	1.82	0.96
1:F:443:PRO:HA	1:F:459:MET:HE3	0.96	0.96
1:F:481:ILE:HD12	1:F:482:ALA:N	1.80	0.96
1:B:381:GLU:OE1	2:B:527:HOH:O	1.81	0.95
1:D:95:ARG:NH2	1:G:484:HIS:O	1.99	0.95
1:E:479:ALA:O	1:E:480:LYS:HD3	1.66	0.95
1:F:201:VAL:O	1:F:201:VAL:HG12	1.65	0.95
1:G:273:ILE:HD13	1:G:285:SER:HA	1.47	0.95
1:D:93:PRO:O	1:D:96:ASP:HB2	1.64	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:SER:HA	1:E:101:ASP:HB2	1.46	0.95
1:F:26:HIS:O	1:F:361:GLY:CA	2.13	0.95
1:G:322:PRO:HG3	1:G:363:TYR:CE1	2.00	0.95
1:G:278:GLY:HA3	1:G:384:GLY:O	1.65	0.95
1:B:320:MET:HE1	1:B:385:PRO:HB3	1.47	0.95
1:E:477:VAL:C	2:E:514:HOH:O	2.07	0.95
1:F:432:MET:HE1	1:F:447:PHE:CD1	2.01	0.95
1:G:37:ALA:CB	1:G:201:VAL:HG22	1.97	0.95
1:B:137:LYS:HG3	1:B:471:ARG:HG3	1.49	0.95
1:B:22:VAL:CG2	1:B:34:ILE:CG2	2.44	0.95
1:B:132:ASN:ND2	1:F:445:SER:HG	1.61	0.94
1:D:426:ASN:OD1	1:G:137:LYS:NZ	1.99	0.94
1:B:152:LEU:HD11	1:B:184:ILE:HD11	1.48	0.94
1:C:2:GLN:NE2	2:C:521:HOH:O	1.99	0.94
1:F:335:TYR:OH	1:F:380:GLU:OE1	1.84	0.94
1:C:480:LYS:O	1:C:480:LYS:HD3	1.67	0.94
1:C:415:THR:HG22	1:C:416:GLN:H	1.28	0.94
1:A:471:ARG:NH1	1:C:428:ILE:O	2.00	0.94
1:B:479:ALA:CB	1:B:480:LYS:HG2	1.93	0.94
1:A:226:SER:OG	1:A:229:THR:HG22	1.65	0.94
1:G:241:LEU:O	2:G:504:HOH:O	1.85	0.94
1:A:22:VAL:CG2	1:A:34:ILE:CG2	2.46	0.93
1:E:258:GLU:OE1	2:E:516:HOH:O	1.84	0.93
1:G:87:SER:CB	1:G:94:ILE:CD1	2.46	0.93
1:G:358:LEU:N	1:G:358:LEU:CD1	2.30	0.93
1:B:334:SER:O	1:B:338:ILE:HG22	1.68	0.93
1:G:338:ILE:C	1:G:338:ILE:CD1	2.30	0.93
1:D:10:ARG:HH11	1:D:10:ARG:CG	1.82	0.93
1:G:415:THR:HG21	1:G:420:ARG:HD2	1.46	0.93
1:F:117:ASP:OD2	2:F:524:HOH:O	1.85	0.93
1:D:257:PHE:HB2	1:D:415:THR:HG23	1.51	0.93
1:F:273:ILE:HG21	1:F:387:VAL:HG21	1.50	0.93
1:D:323:LEU:N	1:D:323:LEU:CD2	2.30	0.93
1:C:24:SER:OG	2:C:512:HOH:O	1.85	0.93
1:A:232:ARG:CB	1:A:235:GLU:OE2	2.16	0.93
1:E:351:LYS:HE2	1:E:352:ALA:O	1.69	0.93
1:G:363:TYR:CA	2:G:519:HOH:O	2.10	0.93
1:E:351:LYS:O	1:E:365:GLU:HG3	1.69	0.93
1:B:22:VAL:HG21	1:B:34:ILE:HG21	1.50	0.92
1:F:429:HIS:O	2:F:516:HOH:O	1.87	0.92
1:D:351:LYS:CG	1:D:352:ALA:N	2.30	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:326:ALA:HB2	1:F:362:PHE:CZ	2.05	0.92
1:F:94:ILE:O	1:F:94:ILE:HG13	1.68	0.92
1:F:377:VAL:CG1	1:F:388:THR:CG2	2.48	0.92
1:F:326:ALA:HB2	1:F:362:PHE:CE1	2.05	0.92
1:F:404:ASN:O	1:F:405:THR:HG22	1.69	0.92
1:F:458:GLU:OE1	2:F:511:HOH:O	1.88	0.92
1:B:226:SER:OG	1:B:229:THR:HG22	1.70	0.92
1:E:259:ASP:OD1	1:E:415:THR:HG22	1.70	0.92
1:H:355:ASP:C	1:H:357:ALA:H	1.77	0.92
1:H:127:ASP:OD1	2:H:509:HOH:O	1.86	0.91
1:H:229:THR:HG23	1:H:232:ARG:HH22	1.25	0.91
1:A:481:ILE:HG13	1:A:482:ALA:H	1.27	0.91
1:A:221:ILE:CD1	1:A:233:ILE:HG21	1.97	0.91
1:H:229:THR:CG2	1:H:232:ARG:NH2	2.33	0.91
1:C:2:GLN:HE21	1:C:2:GLN:CA	1.81	0.91
1:E:479:ALA:O	1:E:480:LYS:HE2	1.71	0.91
1:D:226:SER:OG	1:D:229:THR:HG22	1.71	0.91
1:E:201:VAL:O	1:E:201:VAL:HG12	1.68	0.91
1:G:226:SER:OG	1:G:229:THR:HG22	1.71	0.91
1:H:329:ARG:HG3	1:H:329:ARG:NH1	1.69	0.91
1:D:462:GLU:OE1	1:G:136:ARG:NH2	2.04	0.91
1:B:273:ILE:HG12	1:B:387:VAL:HG22	1.53	0.91
1:B:329:ARG:HG3	1:B:329:ARG:NH1	1.77	0.91
1:B:101:ASP:OD1	2:B:511:HOH:O	1.87	0.90
1:F:23:VAL:HG12	1:F:24:SER:O	1.71	0.90
1:G:457:ARG:HG2	1:G:457:ARG:HH11	1.36	0.90
1:E:386:PHE:O	1:E:386:PHE:HD1	1.54	0.90
1:C:23:VAL:CG1	1:C:29:SER:O	2.19	0.90
1:D:323:LEU:HD23	1:D:323:LEU:H	1.30	0.90
1:G:289:LEU:HD11	1:G:389:VAL:HG13	1.54	0.90
1:B:22:VAL:HG21	1:B:34:ILE:CG2	2.02	0.90
1:D:356:LYS:HA	1:D:359:ALA:HB2	1.54	0.90
1:G:293:ILE:HD12	1:G:294:ALA:N	1.85	0.90
1:A:55:ALA:O	2:A:525:HOH:O	1.83	0.90
1:E:152:LEU:CD1	1:E:184:ILE:CD1	2.49	0.90
1:B:136:ARG:NE	2:B:514:HOH:O	1.96	0.90
1:A:235:GLU:HB3	1:C:238:LYS:HE2	1.52	0.90
1:C:26:HIS:O	1:C:361:GLY:CA	2.19	0.90
1:E:404:ASN:O	1:E:405:THR:HG22	1.72	0.90
1:G:97:SER:HA	1:G:101:ASP:HB2	1.51	0.90
1:C:482:ALA:O	2:C:529:HOH:O	1.88	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:351:LYS:O	1:F:365:GLU:HG3	1.71	0.90
1:C:439:LYS:O	2:C:530:HOH:O	1.90	0.89
1:B:41:ASP:OD2	2:B:522:HOH:O	1.89	0.89
1:E:104:ARG:NE	1:E:153:MET:HE3	1.84	0.89
1:B:63:GLU:OE1	1:B:66:ARG:NH1	2.05	0.89
1:C:259:ASP:OD1	1:C:415:THR:HG23	1.72	0.89
1:C:315:ASP:OD1	1:C:316:PRO:HD2	1.72	0.89
1:E:15:VAL:HG12	1:E:16:ALA:H	1.30	0.89
1:G:373:PRO:CD	1:G:374:GLN:OE1	2.19	0.89
1:C:220:LYS:HE3	1:C:466:ASP:O	1.73	0.89
1:D:2:GLN:NE2	2:D:506:HOH:O	2.04	0.89
1:G:327:LEU:HD21	1:G:331:ARG:HD2	1.54	0.89
1:G:373:PRO:CG	1:G:374:GLN:OE1	2.20	0.89
1:A:159:MET:HE3	1:A:198:VAL:CG1	1.99	0.89
1:F:329:ARG:NH1	2:F:510:HOH:O	1.99	0.89
1:G:210:GLN:HG2	2:G:517:HOH:O	1.71	0.89
1:B:101:ASP:O	1:B:105:THR:OG1	1.91	0.89
1:E:377:VAL:HG21	1:E:386:PHE:CZ	2.08	0.88
1:G:22:VAL:HG23	1:G:34:ILE:HG23	1.55	0.88
1:C:440:ARG:CA	2:C:530:HOH:O	2.02	0.88
1:B:357:ALA:HB2	1:G:12:VAL:HG12	1.53	0.88
1:C:467:TYR:OH	2:C:508:HOH:O	1.90	0.88
1:H:329:ARG:HH11	1:H:329:ARG:CG	1.86	0.88
1:B:238:LYS:HB2	1:F:231:ARG:HG2	1.55	0.88
1:E:210:GLN:O	1:E:214:GLU:HG2	1.73	0.88
1:A:213:ALA:O	1:A:242:LYS:HE2	1.74	0.88
1:H:148:TRP:CD1	1:H:176:ILE:HD12	2.09	0.88
1:E:42:VAL:CG1	1:E:212:LEU:HD13	2.02	0.88
1:G:363:TYR:CG	2:G:519:HOH:O	2.25	0.88
1:H:99:GLY:O	1:H:100:LEU:HD23	1.72	0.88
1:A:259:ASP:OD1	1:A:415:THR:HG22	1.74	0.88
1:F:415:THR:HG21	1:F:420:ARG:CD	2.04	0.88
1:B:479:ALA:HB1	1:B:480:LYS:CD	2.03	0.88
1:B:479:ALA:HA	1:B:480:LYS:HB3	1.55	0.88
1:F:338:ILE:CD1	1:F:376:ARG:NE	2.29	0.88
1:G:148:TRP:HB3	1:G:177:THR:CG2	2.03	0.88
1:B:351:LYS:HG3	1:B:352:ALA:N	1.87	0.87
1:E:159:MET:CE	1:E:171:ILE:HD13	2.04	0.87
1:H:273:ILE:HG12	1:H:387:VAL:HG22	1.54	0.87
1:B:76:GLU:CD	1:B:110:ARG:NH1	2.33	0.87
1:B:415:THR:HG21	1:B:420:ARG:HD2	1.57	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:108:CYS:HB3	1:H:156:SER:HB2	1.54	0.87
1:D:10:ARG:HG2	1:D:10:ARG:NH1	1.86	0.87
1:B:329:ARG:HD2	1:B:330:ASP:N	1.89	0.87
1:A:22:VAL:HG23	1:A:34:ILE:CG2	2.04	0.87
1:A:377:VAL:HG13	1:A:388:THR:HG21	1.54	0.87
1:D:20:ILE:HG21	1:D:175:GLU:HB3	1.55	0.86
1:B:351:LYS:CG	1:B:352:ALA:H	1.88	0.86
1:D:351:LYS:O	1:D:365:GLU:HG3	1.75	0.86
1:A:8:ASP:OD2	1:A:51:ARG:NH2	2.06	0.86
1:E:320:MET:HE1	1:E:366:PRO:HG3	1.55	0.86
1:D:457:ARG:HG2	1:D:457:ARG:HH11	1.39	0.86
1:C:142:VAL:HG22	1:C:220:LYS:HB3	1.56	0.86
1:D:36:ALA:O	2:D:524:HOH:O	1.91	0.86
1:C:2:GLN:NE2	1:C:2:GLN:CA	2.36	0.86
1:C:23:VAL:N	2:C:520:HOH:O	1.96	0.86
1:G:335:TYR:O	1:G:339:ALA:CB	2.24	0.86
1:C:24:SER:CB	2:C:512:HOH:O	2.22	0.86
1:A:56:TRP:HA	2:A:525:HOH:O	1.74	0.85
1:A:310:LEU:CD2	1:A:353:PRO:HG2	2.06	0.85
1:E:104:ARG:CZ	1:E:153:MET:HE1	2.05	0.85
1:E:370:GLU:OE2	2:E:518:HOH:O	1.94	0.85
1:E:377:VAL:CG2	1:E:386:PHE:CZ	2.58	0.85
1:B:417:ASN:HD22	1:B:420:ARG:HB2	1.41	0.85
1:B:479:ALA:CB	1:B:480:LYS:CE	2.54	0.85
1:E:87:SER:OG	1:E:92:HIS:O	1.94	0.85
1:B:238:LYS:HZ3	1:F:235:GLU:CD	1.70	0.85
1:G:138:PRO:HG3	1:G:165:ALA:O	1.75	0.85
1:A:415:THR:HG21	1:A:420:ARG:HD2	1.57	0.85
1:E:292:ASP:OD2	2:E:529:HOH:O	1.93	0.85
1:H:86:GLU:OE1	1:H:151:PRO:HD2	1.77	0.85
1:G:249:GLY:O	1:G:453:SER:OG	1.94	0.85
1:A:232:ARG:HB3	1:A:235:GLU:OE2	1.76	0.85
1:B:416:GLN:NE2	2:B:503:HOH:O	1.98	0.85
1:E:415:THR:HG21	1:E:420:ARG:HD2	1.57	0.85
1:C:87:SER:OG	1:C:92:HIS:O	1.94	0.85
1:E:318:THR:O	2:E:512:HOH:O	1.94	0.85
1:E:396:GLU:OE1	2:E:520:HOH:O	1.94	0.85
1:F:51:ARG:O	2:F:528:HOH:O	1.94	0.85
1:A:47:ALA:HB2	1:B:374:GLN:CB	2.05	0.84
1:D:10:ARG:NE	2:D:504:HOH:O	2.11	0.84
1:H:49:ALA:HB1	1:H:168:THR:HG21	1.58	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:GLU:O	1:D:90:THR:OG1	1.94	0.84
1:A:221:ILE:HD13	1:A:233:ILE:HG21	1.57	0.84
1:A:404:ASN:O	1:A:405:THR:CG2	2.25	0.84
1:C:379:GLN:NE2	1:C:404:ASN:OD1	2.10	0.84
1:G:310:LEU:CD2	1:G:353:PRO:HG3	2.06	0.84
1:G:327:LEU:CD2	1:G:331:ARG:CD	2.55	0.84
1:B:334:SER:O	1:B:338:ILE:CG2	2.24	0.84
1:G:87:SER:OG	1:G:92:HIS:O	1.96	0.84
1:B:81:GLU:OE1	2:B:518:HOH:O	1.93	0.84
1:E:152:LEU:HD11	1:E:184:ILE:HD11	1.58	0.84
1:H:355:ASP:OD1	1:H:357:ALA:HB3	1.77	0.84
1:D:80:GLU:OE1	1:D:98:ARG:NH2	2.11	0.84
1:F:124:ILE:O	2:F:514:HOH:O	1.95	0.84
1:D:458:GLU:O	1:D:459:MET:HB2	1.76	0.84
1:H:377:VAL:HG21	1:H:386:PHE:CZ	2.13	0.84
1:A:41:ASP:OD1	2:A:511:HOH:O	1.93	0.84
1:B:238:LYS:CD	1:F:235:GLU:CG	2.52	0.84
1:C:326:ALA:HB2	1:C:362:PHE:CE1	2.12	0.84
1:D:481:ILE:HG22	1:D:482:ALA:N	1.93	0.84
1:E:320:MET:CE	1:E:366:PRO:HG3	2.08	0.84
1:G:100:LEU:O	1:G:104:ARG:HG3	1.78	0.84
1:H:26:HIS:ND1	1:H:363:TYR:OH	1.95	0.84
1:H:237:SER:O	2:H:506:HOH:O	1.96	0.84
1:H:408:GLY:O	1:H:430:ALA:HA	1.76	0.83
1:H:415:THR:HG21	1:H:420:ARG:HD2	1.57	0.83
1:A:4:GLN:OE1	2:A:518:HOH:O	1.96	0.83
1:A:273:ILE:HG13	1:A:273:ILE:O	1.76	0.83
1:C:318:THR:CG2	1:C:320:MET:O	2.26	0.83
1:G:22:VAL:HG21	1:G:34:ILE:CG2	2.09	0.83
1:A:404:ASN:O	1:A:405:THR:HG22	1.77	0.83
1:B:244:ILE:N	2:B:524:HOH:O	1.87	0.83
1:B:287:LEU:HD22	1:B:289:LEU:HD21	1.60	0.83
1:D:8:ASP:OD1	1:D:195:LYS:HG3	1.77	0.83
1:E:22:VAL:CG2	1:E:34:ILE:CG2	2.57	0.83
1:E:227:THR:HG23	1:H:241:LEU:HD11	1.61	0.83
1:A:129:GLY:HA3	1:A:479:ALA:HB3	1.60	0.83
1:C:397:GLU:O	1:C:401:ILE:HG13	1.77	0.83
1:D:235:GLU:O	1:D:238:LYS:HG2	1.79	0.83
1:E:386:PHE:O	1:E:386:PHE:CD1	2.30	0.83
1:B:479:ALA:CA	1:B:480:LYS:HB3	2.08	0.83
1:E:248:LEU:HD12	1:H:241:LEU:HD13	1.59	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:351:LYS:HG3	1:H:352:ALA:N	1.90	0.83
1:A:213:ALA:O	1:A:242:LYS:CE	2.27	0.82
1:B:479:ALA:HB2	1:B:480:LYS:NZ	1.93	0.82
1:C:290:HIS:HD2	1:C:292:ASP:H	1.22	0.82
1:G:87:SER:CB	1:G:94:ILE:HD12	2.09	0.82
1:G:151:PRO:HG2	1:G:177:THR:OG1	1.79	0.82
1:B:100:LEU:O	1:B:104:ARG:CG	2.28	0.82
1:G:22:VAL:CG2	1:G:34:ILE:CG2	2.57	0.82
1:H:481:ILE:HD12	1:H:482:ALA:N	1.92	0.82
1:C:417:ASN:ND2	1:C:420:ARG:H	1.76	0.82
1:F:257:PHE:HB2	1:F:415:THR:HG23	1.58	0.82
1:B:22:VAL:CG2	1:B:34:ILE:HG21	2.08	0.82
1:D:415:THR:HG21	1:D:420:ARG:NH1	1.93	0.82
1:F:371:ALA:O	2:F:517:HOH:O	1.98	0.82
1:B:137:LYS:NZ	1:F:426:ASN:OD1	2.12	0.82
1:H:102:VAL:HG22	1:H:152:LEU:CD2	2.10	0.82
1:A:20:ILE:HG13	1:A:36:ALA:HB2	1.61	0.82
1:F:259:ASP:O	1:F:416:GLN:HG3	1.79	0.82
1:G:289:LEU:CD1	1:G:389:VAL:HG13	2.07	0.82
1:C:229:THR:OG1	1:C:232:ARG:NH2	2.13	0.82
1:G:340:ILE:HG22	1:G:341:GLU:N	1.95	0.82
1:B:376:ARG:NH1	1:B:380:GLU:OE1	2.13	0.81
1:F:336:ILE:O	1:F:340:ILE:HG12	1.80	0.81
1:H:158:LYS:HD3	1:H:458:GLU:OE2	1.80	0.81
1:C:57:SER:O	2:C:523:HOH:O	1.98	0.81
1:D:302:ILE:O	1:D:306:LYS:HG3	1.80	0.81
1:F:258:GLU:HG3	1:F:290:HIS:CG	2.16	0.81
1:H:138:PRO:HG3	1:H:165:ALA:O	1.79	0.81
1:D:204:TYR:C	2:D:517:HOH:O	2.23	0.81
1:A:43:ASP:OD1	1:B:374:GLN:CG	2.28	0.81
1:A:47:ALA:CB	1:B:374:GLN:HB2	2.10	0.81
1:D:334:SER:O	1:D:338:ILE:HG23	1.81	0.81
1:E:153:MET:HB2	2:E:510:HOH:O	1.79	0.81
1:D:184:ILE:O	1:D:188:MET:HG3	1.80	0.81
1:F:355:ASP:OD1	2:F:518:HOH:O	1.99	0.81
1:G:445:SER:O	2:G:507:HOH:O	1.98	0.81
1:A:221:ILE:CD1	1:A:233:ILE:HG23	1.99	0.81
1:B:259:ASP:OD1	1:B:415:THR:HG22	1.81	0.81
1:B:320:MET:HE1	1:B:385:PRO:CG	2.11	0.81
1:F:101:ASP:OD1	2:F:503:HOH:O	1.98	0.81
1:F:417:ASN:HD22	1:F:420:ARG:H	1.27	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:148:TRP:CB	1:G:177:THR:CG2	2.59	0.81
1:D:328:ARG:O	1:D:332:VAL:HG23	1.81	0.81
1:G:476:ASN:OD1	1:G:479:ALA:HB3	1.81	0.81
1:B:136:ARG:CZ	2:B:514:HOH:O	2.19	0.80
1:F:291:LYS:HE2	1:F:393:SER:HB3	1.63	0.80
1:C:175:GLU:OE2	2:C:522:HOH:O	1.98	0.80
1:C:480:LYS:O	1:C:480:LYS:CD	2.29	0.80
1:C:93:PRO:O	1:C:96:ASP:HB2	1.81	0.80
1:D:2:GLN:HE21	1:D:2:GLN:HA	1.44	0.80
1:C:210:GLN:O	1:C:214:GLU:HG2	1.81	0.80
1:E:376:ARG:CD	1:E:380:GLU:OE2	2.22	0.80
1:G:201:VAL:O	1:G:201:VAL:CG1	2.30	0.80
1:A:273:ILE:HG21	1:A:387:VAL:CG2	2.11	0.80
1:B:20:ILE:HD13	1:B:175:GLU:HB3	1.61	0.80
1:F:152:LEU:O	1:F:155:THR:OG1	1.99	0.80
1:E:153:MET:CB	2:E:510:HOH:O	2.27	0.80
1:B:2:GLN:HE21	1:B:2:GLN:CA	1.92	0.80
1:D:328:ARG:HA	1:D:328:ARG:HE	1.47	0.80
1:B:335:TYR:HA	1:B:338:ILE:HG23	1.62	0.80
1:F:221:ILE:O	1:F:221:ILE:CG2	2.30	0.80
1:G:475:VAL:HG12	1:G:477:VAL:HG12	1.63	0.80
1:D:273:ILE:HG21	1:D:387:VAL:HG22	1.64	0.80
1:F:53:PHE:CE1	1:F:140:GLY:HA2	2.17	0.80
1:G:259:ASP:O	1:G:416:GLN:NE2	2.16	0.80
1:E:314:MET:HA	1:E:314:MET:HE2	1.64	0.79
1:F:27:ASP:OD1	1:F:29:SER:CB	2.30	0.79
1:A:52:ALA:O	2:A:529:HOH:O	2.00	0.79
1:A:152:LEU:CD1	1:A:184:ILE:CD1	2.59	0.79
1:A:210:GLN:O	1:A:214:GLU:CG	2.30	0.79
1:A:338:ILE:HD13	1:A:376:ARG:HH21	1.48	0.79
1:B:152:LEU:HD12	1:B:184:ILE:CD1	2.12	0.79
1:B:337:ASP:O	1:B:341:GLU:HG2	1.82	0.79
1:E:226:SER:OG	1:E:229:THR:CG2	2.30	0.79
1:H:327:LEU:O	1:H:331:ARG:HG3	1.83	0.79
1:E:201:VAL:O	1:E:201:VAL:CG1	2.29	0.79
1:G:338:ILE:O	1:G:338:ILE:CD1	2.30	0.79
1:H:338:ILE:O	1:H:338:ILE:CD1	2.30	0.79
1:B:115:MET:CE	1:B:461:PHE:CE1	2.59	0.79
1:E:22:VAL:HG21	1:E:34:ILE:HG21	1.63	0.79
1:F:94:ILE:HG12	1:F:98:ARG:NH1	1.97	0.79
1:D:338:ILE:HD11	1:D:376:ARG:HB3	1.65	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:377:VAL:HG11	1:F:388:THR:HG21	1.63	0.79
1:H:49:ALA:C	1:H:168:THR:HG21	2.08	0.79
1:A:355:ASP:O	1:A:357:ALA:N	2.16	0.79
1:B:6:TYR:OH	1:B:189:THR:HG21	1.82	0.79
1:C:432:MET:HE1	1:C:447:PHE:HD1	1.47	0.79
1:D:2:GLN:NE2	1:D:2:GLN:HA	1.97	0.79
1:F:377:VAL:HG11	1:F:388:THR:CG2	2.13	0.79
1:A:33:ARG:NH2	1:F:8:ASP:OD2	2.16	0.79
1:B:74:ARG:NH1	1:B:78:CYS:SG	2.56	0.79
1:D:291:LYS:HE2	1:D:393:SER:HB2	1.65	0.79
1:E:235:GLU:O	1:E:238:LYS:CD	2.30	0.79
1:F:404:ASN:O	1:F:405:THR:CG2	2.30	0.79
1:F:459:MET:N	2:F:506:HOH:O	2.15	0.79
1:H:99:GLY:O	1:H:100:LEU:CD2	2.30	0.79
1:H:333:LEU:HD22	1:H:351:LYS:HE2	1.63	0.79
1:A:56:TRP:CA	2:A:525:HOH:O	2.29	0.78
1:H:25:PRO:HA	1:H:362:PHE:CE2	2.18	0.78
1:D:185:VAL:HG23	1:D:188:MET:HE2	1.63	0.78
1:F:429:HIS:HB3	2:F:516:HOH:O	1.83	0.78
1:G:53:PHE:CE1	1:G:140:GLY:HA2	2.17	0.78
1:D:188:MET:HE1	1:D:198:VAL:CG2	2.13	0.78
1:D:204:TYR:O	2:D:517:HOH:O	2.02	0.78
1:E:479:ALA:O	1:E:480:LYS:CD	2.30	0.78
1:F:227:THR:CG2	1:F:231:ARG:NH1	2.45	0.78
1:G:350:GLY:O	1:G:351:LYS:CG	2.30	0.78
1:H:20:ILE:HD13	1:H:175:GLU:HB3	1.63	0.78
1:B:76:GLU:OE2	1:B:110:ARG:NH1	2.15	0.78
1:B:344:GLY:C	1:B:345:LYS:HD3	2.09	0.78
1:F:38:GLU:HG2	1:F:207:THR:HG21	1.65	0.78
1:F:259:ASP:OD1	1:F:415:THR:HG22	1.82	0.78
1:B:428:ILE:O	1:F:471:ARG:NH1	2.16	0.78
1:C:190:GLU:CD	2:C:516:HOH:O	2.23	0.78
1:D:351:LYS:HG2	1:D:352:ALA:N	1.97	0.78
1:F:410:GLY:O	2:F:519:HOH:O	2.02	0.78
1:A:152:LEU:HD11	1:A:184:ILE:HD11	1.66	0.78
1:B:81:GLU:CB	2:B:518:HOH:O	2.31	0.78
1:E:479:ALA:O	1:E:480:LYS:CE	2.30	0.78
1:F:201:VAL:O	1:F:201:VAL:CG1	2.29	0.78
1:F:356:LYS:HA	1:F:359:ALA:HB2	1.66	0.78
1:A:232:ARG:HB2	1:A:235:GLU:OE2	1.82	0.78
1:F:273:ILE:HG12	1:F:387:VAL:HG22	0.85	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:338:ILE:HD12	1:G:339:ALA:N	1.98	0.78
2:A:515:HOH:O	1:B:374:GLN:HG3	1.81	0.78
1:B:312:ASP:OD1	1:B:313:PRO:HD2	1.83	0.78
1:F:210:GLN:O	1:F:214:GLU:HG2	1.82	0.78
1:G:76:GLU:O	1:G:79:SER:HB3	1.83	0.78
1:G:372:LYS:HB3	1:G:373:PRO:HD2	1.65	0.78
1:A:34:ILE:HD11	1:A:202:PRO:HB2	1.66	0.78
1:C:119:ILE:HD11	1:C:464:ILE:HD12	1.66	0.78
1:D:115:MET:CE	1:D:461:PHE:CE1	2.55	0.78
1:F:477:VAL:HG23	1:F:478:ASP:HB2	1.64	0.78
1:B:2:GLN:HA	1:B:2:GLN:NE2	1.97	0.78
1:F:273:ILE:CG1	1:F:387:VAL:CG2	2.52	0.78
1:C:275:HIS:NE2	2:C:524:HOH:O	2.00	0.77
1:E:248:LEU:HD11	1:H:241:LEU:HD22	1.65	0.77
1:F:335:TYR:CE2	1:F:376:ARG:CZ	2.66	0.77
1:G:221:ILE:CG2	1:G:221:ILE:O	2.31	0.77
1:B:172:LYS:NZ	1:B:203:GLY:O	2.17	0.77
1:B:238:LYS:HZ3	1:F:235:GLU:HG2	0.94	0.77
1:G:74:ARG:HG3	1:G:187:LEU:HD22	1.65	0.77
1:G:95:ARG:NH1	1:G:319:GLU:HG2	1.99	0.77
1:E:377:VAL:HG21	1:E:386:PHE:HZ	1.48	0.77
1:G:369:VAL:O	1:G:369:VAL:HG12	1.83	0.77
1:H:175:GLU:CD	1:H:175:GLU:H	1.91	0.77
1:B:94:ILE:O	1:B:94:ILE:HG13	1.83	0.77
1:F:227:THR:HA	1:F:248:LEU:HD13	1.67	0.77
1:D:257:PHE:CB	1:D:415:THR:HG23	2.15	0.77
1:F:22:VAL:HG21	1:F:34:ILE:CG2	2.15	0.77
1:G:310:LEU:HD12	1:G:320:MET:CG	2.09	0.77
1:A:102:VAL:HB	1:A:103:PRO:HD3	1.66	0.77
1:A:241:LEU:HD13	1:C:248:LEU:CD1	2.14	0.77
1:B:451:GLY:O	2:B:502:HOH:O	2.01	0.77
1:E:22:VAL:CG2	1:E:34:ILE:HG21	2.14	0.77
1:H:355:ASP:C	1:H:357:ALA:N	2.39	0.77
1:C:480:LYS:O	1:C:480:LYS:CG	2.30	0.77
1:F:2:GLN:HA	1:F:2:GLN:NE2	1.97	0.77
1:C:70:LYS:HD2	1:C:191:VAL:HG22	1.67	0.77
1:H:302:ILE:O	1:H:306:LYS:HG3	1.85	0.77
1:C:302:ILE:HD13	1:C:347:LEU:HB3	1.67	0.76
1:F:235:GLU:O	1:F:238:LYS:HD3	1.84	0.76
1:B:152:LEU:CD1	1:B:184:ILE:HD11	2.05	0.76
1:H:333:LEU:CD2	1:H:351:LYS:HE2	2.14	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:GLU:HG2	1:F:238:LYS:CE	2.16	0.76
1:B:328:ARG:NH1	1:B:331:ARG:HE	1.82	0.76
1:E:386:PHE:CD1	1:E:386:PHE:C	2.63	0.76
1:F:37:ALA:CB	1:F:201:VAL:HG13	2.15	0.76
1:G:326:ALA:N	1:G:362:PHE:CE2	2.53	0.76
1:H:124:ILE:HB	1:H:132:ASN:ND2	2.01	0.76
1:A:292:ASP:O	1:A:296:GLN:NE2	2.19	0.76
1:B:345:LYS:CD	1:B:345:LYS:N	2.49	0.76
1:H:90:THR:HG21	1:H:92:HIS:CE1	2.21	0.76
1:E:102:VAL:HB	1:E:103:PRO:HD3	1.67	0.76
1:E:104:ARG:CZ	1:E:153:MET:CE	2.61	0.76
1:A:235:GLU:CB	1:C:238:LYS:CE	2.50	0.76
1:A:37:ALA:O	2:A:519:HOH:O	2.03	0.76
1:C:408:GLY:O	1:C:430:ALA:CA	2.32	0.76
1:A:355:ASP:C	1:A:357:ALA:H	1.92	0.76
1:D:355:ASP:O	1:D:356:LYS:HB2	1.85	0.75
1:E:258:GLU:HG3	1:E:290:HIS:CD2	2.21	0.75
1:F:61:ALA:HB1	1:F:116:ALA:C	2.12	0.75
1:F:221:ILE:O	1:F:221:ILE:HG23	1.85	0.75
1:G:15:VAL:HG11	1:G:40:ALA:HB3	1.68	0.75
1:G:21:ASP:HB3	1:G:30:LEU:CD1	2.15	0.75
1:A:184:ILE:O	1:A:187:LEU:HB2	1.87	0.75
1:B:87:SER:OG	1:B:97:SER:OG	2.05	0.75
1:G:51:ARG:O	2:G:520:HOH:O	2.04	0.75
1:G:148:TRP:CD1	1:G:148:TRP:H	2.01	0.75
1:H:49:ALA:CA	1:H:168:THR:HG21	2.16	0.75
1:C:215:HIS:HD2	1:C:217:ASP:H	1.32	0.75
1:D:481:ILE:HG22	1:D:482:ALA:H	1.49	0.75
1:A:22:VAL:CG2	1:A:34:ILE:HG21	2.15	0.75
1:A:22:VAL:HG21	1:A:34:ILE:CG2	2.15	0.75
1:D:486:LYS:O	1:D:487:ARG:C	2.30	0.75
1:E:22:VAL:HG23	1:E:34:ILE:CG2	2.15	0.75
1:E:354:ASP:C	1:E:355:ASP:OD2	2.30	0.75
1:G:22:VAL:CG2	1:G:34:ILE:HG23	2.16	0.75
1:G:394:SER:HB2	1:G:396:GLU:OE2	1.87	0.75
1:A:228:ALA:O	1:A:232:ARG:NE	2.19	0.75
1:E:262:ILE:O	1:E:266:VAL:HG23	1.86	0.75
1:F:281:CYS:HB3	1:F:409:LEU:CD2	2.17	0.75
1:G:326:ALA:HB2	1:G:362:PHE:CZ	2.22	0.75
1:A:334:SER:O	1:A:338:ILE:HG23	1.85	0.75
1:D:10:ARG:CD	2:D:504:HOH:O	2.35	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:GLU:OE1	1:G:84:GLN:NE2	2.19	0.75
1:H:215:HIS:HD2	1:H:217:ASP:H	1.34	0.75
1:H:328:ARG:NE	1:H:383:PHE:HB3	2.01	0.75
1:A:34:ILE:CD1	1:A:202:PRO:HB2	2.17	0.75
1:E:329:ARG:NH1	2:E:505:HOH:O	2.16	0.75
1:F:22:VAL:HG21	1:F:34:ILE:HG21	1.68	0.75
1:F:313:PRO:HB2	1:F:314:MET:HE2	1.68	0.75
1:G:53:PHE:HB3	1:G:54:PRO:HD3	1.67	0.75
1:A:143:ALA:HB1	1:A:212:LEU:HG	1.69	0.75
1:C:404:ASN:O	1:C:405:THR:HG23	1.87	0.75
1:D:404:ASN:O	1:D:404:ASN:CG	2.29	0.75
1:G:396:GLU:CD	1:G:396:GLU:H	1.95	0.75
1:B:258:GLU:HG2	1:B:290:HIS:CD2	2.21	0.74
1:C:321:GLY:O	2:C:511:HOH:O	2.05	0.74
1:C:370:GLU:OE2	1:C:391:ARG:HD2	1.87	0.74
1:D:376:ARG:NH1	1:D:380:GLU:OE2	2.14	0.74
1:E:277:GLN:NE2	1:E:321:GLY:H	1.85	0.74
1:E:451:GLY:O	2:E:501:HOH:O	2.05	0.74
1:F:415:THR:CG2	1:F:420:ARG:HH11	1.99	0.74
1:C:63[A]:GLU:OE1	1:C:66:ARG:NE	2.19	0.74
1:H:163:LEU:CD2	1:H:169:ILE:HD12	2.17	0.74
1:A:138:PRO:HG3	1:A:165:ALA:O	1.87	0.74
1:B:115:MET:HE1	1:B:461:PHE:CD1	2.22	0.74
1:A:273:ILE:HG21	1:A:387:VAL:HG22	1.69	0.74
1:B:133:TYR:OH	2:B:521:HOH:O	2.05	0.74
1:B:344:GLY:C	1:B:345:LYS:CD	2.60	0.74
1:F:404:ASN:C	1:F:405:THR:CG2	2.60	0.74
1:G:293:ILE:CD1	1:G:293:ILE:O	2.35	0.74
1:B:337:ASP:OD2	2:B:517:HOH:O	2.05	0.74
1:D:376:ARG:CD	1:D:380:GLU:OE2	2.36	0.74
1:E:210:GLN:O	1:E:214:GLU:CG	2.36	0.74
1:G:231:ARG:O	1:G:235:GLU:HG3	1.88	0.74
1:A:457:ARG:NH1	1:C:470:ALA:O	2.21	0.74
1:B:22:VAL:HG23	1:B:34:ILE:CG2	2.16	0.74
1:D:457:ARG:NE	2:D:513:HOH:O	1.92	0.74
1:F:27:ASP:OD1	1:F:29:SER:HB3	1.86	0.74
1:F:115:MET:O	1:F:119:ILE:HG13	1.88	0.74
1:B:328:ARG:HH12	1:B:331:ARG:HE	1.36	0.74
1:E:104:ARG:HE	1:E:153:MET:HE3	1.51	0.74
1:G:357:ALA:CA	1:G:358:LEU:HD12	2.17	0.74
1:H:1:MET:HE1	1:H:31:ILE:CG2	2.18	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:329:ARG:HD3	1:H:330:ASP:OD1	1.85	0.74
1:C:334:SER:O	1:C:338:ILE:HG23	1.87	0.73
1:A:220:LYS:HZ1	1:A:245:GLN:HB2	1.51	0.73
1:B:457:ARG:NH2	1:F:470:ALA:O	2.20	0.73
1:C:404:ASN:O	1:C:404:ASN:CG	2.29	0.73
1:G:148:TRP:O	1:G:151:PRO:HD3	1.87	0.73
1:G:327:LEU:HD23	1:G:327:LEU:O	1.88	0.73
1:B:379:GLN:OE1	2:B:506:HOH:O	2.05	0.73
1:A:475:VAL:HG12	1:A:477:VAL:HG12	1.70	0.73
1:B:479:ALA:HB3	1:B:480:LYS:HE2	1.68	0.73
1:D:137:LYS:NZ	1:G:426:ASN:HD21	1.86	0.73
1:E:291:LYS:HE2	1:E:393:SER:HG	1.52	0.73
1:B:342:GLN:OE1	1:B:376:ARG:HB2	1.88	0.73
1:G:458:GLU:C	1:G:459:MET:HG2	2.14	0.73
1:D:273:ILE:O	1:D:273:ILE:CD1	2.30	0.73
1:D:458:GLU:O	1:D:459:MET:CB	2.36	0.73
1:F:246:LEU:O	1:F:454:GLY:HA3	1.87	0.73
1:C:210:GLN:O	1:C:214:GLU:CG	2.36	0.73
1:C:327:LEU:CD2	1:C:331:ARG:NH1	2.52	0.73
1:G:148:TRP:HB3	1:G:177:THR:HG22	1.69	0.73
1:C:153:MET:HE3	1:C:157:TRP:CZ2	2.23	0.73
1:E:22:VAL:HG21	1:E:34:ILE:CG2	2.19	0.73
1:G:87:SER:OG	1:G:94:ILE:HD12	1.89	0.73
1:A:56:TRP:N	2:A:525:HOH:O	2.14	0.72
1:G:148:TRP:CB	1:G:177:THR:HG21	2.19	0.72
1:G:151:PRO:HG3	1:G:177:THR:OG1	1.88	0.72
1:H:333:LEU:HD22	1:H:351:LYS:CE	2.19	0.72
1:C:351:LYS:HG3	1:C:352:ALA:H	1.53	0.72
1:D:273:ILE:HD12	1:D:273:ILE:C	2.10	0.72
1:E:266:VAL:HG22	1:E:297:PHE:CE1	2.25	0.72
1:F:338:ILE:CD1	1:F:376:ARG:CD	2.67	0.72
1:G:37:ALA:HB1	1:G:201:VAL:HG22	1.70	0.72
1:H:152:LEU:HD11	1:H:184:ILE:HD11	1.71	0.72
1:B:320:MET:CE	1:B:385:PRO:HB3	2.19	0.72
1:B:481:ILE:HB	2:B:515:HOH:O	1.88	0.72
1:C:158:LYS:HD3	1:C:458:GLU:OE2	1.88	0.72
1:G:305:ALA:HA	1:G:308:ILE:HD12	1.69	0.72
1:B:90:THR:HG22	1:B:177:THR:HG21	1.69	0.72
1:B:231:ARG:O	1:B:235:GLU:HG3	1.89	0.72
1:G:457:ARG:HG2	1:G:457:ARG:NH1	2.04	0.72
1:H:377:VAL:CG2	1:H:386:PHE:CE1	2.72	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:ARG:HA	1:A:328:ARG:HH11	1.54	0.72
1:A:424:MET:O	1:A:428:ILE:HG13	1.89	0.72
1:E:213:ALA:HA	1:E:221:ILE:HD12	1.71	0.72
1:B:22:VAL:HG23	1:B:34:ILE:HG23	1.71	0.72
1:G:22:VAL:HG21	1:G:34:ILE:HG21	1.69	0.72
1:A:377:VAL:O	2:A:524:HOH:O	2.07	0.72
1:E:104:ARG:HD2	1:E:153:MET:HE2	1.70	0.72
1:E:266:VAL:HG22	1:E:297:PHE:CD1	2.25	0.72
1:H:56:TRP:CH2	1:H:64:ARG:HG2	2.25	0.72
1:C:327:LEU:HD22	1:C:331:ARG:NH1	2.04	0.72
1:C:353:PRO:HG2	1:C:358:LEU:HD23	1.69	0.72
1:D:148:TRP:CZ3	1:D:324:THR:OG1	2.42	0.72
1:D:188:MET:HE1	1:D:198:VAL:HG11	1.71	0.72
1:F:22:VAL:CG2	1:F:34:ILE:CG2	2.68	0.72
1:F:61:ALA:CB	1:F:116:ALA:O	2.36	0.72
1:G:172:LYS:HG2	1:G:172:LYS:O	1.89	0.72
1:A:21:ASP:OD1	1:A:33:ARG:CD	2.34	0.72
1:C:337:ASP:O	1:C:341:GLU:HG3	1.90	0.72
1:C:340:ILE:HG22	1:C:341:GLU:N	2.05	0.72
1:E:97:SER:O	1:E:102:VAL:HG23	1.90	0.72
1:E:117:ASP:OD2	2:E:502:HOH:O	2.06	0.72
1:F:335:TYR:CD2	1:F:376:ARG:NH2	2.58	0.72
1:E:152:LEU:CD1	1:E:184:ILE:HD11	2.15	0.71
1:E:273:ILE:HG13	1:E:387:VAL:HG22	1.71	0.71
1:G:257:PHE:CZ	1:G:424:MET:HE2	2.20	0.71
1:A:152:LEU:CD1	1:A:184:ILE:HD11	2.18	0.71
1:B:56:TRP:CH2	1:B:64:ARG:HG2	2.25	0.71
1:C:108:CYS:HB3	1:C:156:SER:HB2	1.73	0.71
1:D:210:GLN:O	1:D:214:GLU:CG	2.29	0.71
1:F:394:SER:OG	1:F:397:GLU:HB2	1.90	0.71
1:C:373:PRO:HG3	1:C:390:VAL:HG11	1.70	0.71
1:E:231:ARG:HH21	1:H:239:SER:C	1.93	0.71
1:F:23:VAL:C	1:F:31:ILE:HD11	2.16	0.71
1:H:393:SER:OG	1:H:397:GLU:OE1	2.06	0.71
1:F:2:GLN:HA	1:F:2:GLN:HE21	1.55	0.71
1:H:163:LEU:HD21	1:H:169:ILE:HD12	1.72	0.71
1:B:377:VAL:HG13	1:B:388:THR:HG21	1.73	0.71
1:D:143:ALA:HB1	1:D:212:LEU:HG	1.70	0.71
1:G:273:ILE:HG13	1:G:273:ILE:O	1.91	0.71
1:C:417:ASN:HD22	1:C:420:ARG:H	1.38	0.71
1:H:210:GLN:O	1:H:214:GLU:HG3	1.90	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:GLN:HG3	1:E:320:MET:CG	2.20	0.71
1:G:5:LEU:HD21	1:G:35:ALA:O	1.91	0.71
1:A:2:GLN:HA	1:A:2:GLN:HE21	1.56	0.71
1:B:88:LEU:HA	1:B:314:MET:HE3	1.71	0.71
1:F:290:HIS:CD2	1:F:292:ASP:H	2.09	0.71
1:F:375:ASP:O	1:F:378:CYS:HB2	1.89	0.71
1:B:243:ARG:HB3	2:B:524:HOH:O	1.90	0.71
1:E:242:LYS:O	2:E:507:HOH:O	2.08	0.71
1:G:153:MET:HE3	1:G:157:TRP:CZ2	2.25	0.71
1:C:190:GLU:OE1	2:C:516:HOH:O	2.08	0.71
1:C:290:HIS:CD2	1:C:292:ASP:H	2.07	0.71
1:E:20:ILE:HD13	1:E:175:GLU:HB3	1.73	0.71
1:E:221:ILE:HG23	1:E:221:ILE:O	1.91	0.71
1:G:447:PHE:C	1:G:447:PHE:CD2	2.68	0.71
1:D:310:LEU:HD23	1:D:353:PRO:HG2	1.73	0.70
1:E:290:HIS:HE1	1:E:393:SER:O	1.74	0.70
1:F:227:THR:HG22	1:F:231:ARG:NH1	2.06	0.70
1:H:90:THR:CG2	1:H:92:HIS:CE1	2.74	0.70
1:E:175:GLU:CD	1:E:175:GLU:H	1.96	0.70
1:A:377:VAL:HG21	1:A:386:PHE:CZ	2.27	0.70
1:A:477:VAL:CG2	1:A:478:ASP:N	2.54	0.70
1:E:462:GLU:CD	1:H:136:ARG:HH12	1.99	0.70
1:A:26:HIS:ND1	1:A:363:TYR:OH	2.16	0.70
1:E:404:ASN:O	1:E:405:THR:CG2	2.38	0.70
1:F:415:THR:HG21	1:F:420:ARG:HH11	1.53	0.70
1:B:320:MET:CE	1:B:385:PRO:CG	2.70	0.70
1:B:417:ASN:HD22	1:B:420:ARG:CB	2.04	0.70
1:F:259:ASP:OD1	1:F:420:ARG:NH1	2.24	0.70
1:H:355:ASP:O	1:H:357:ALA:N	2.24	0.70
1:D:21:ASP:OD1	1:D:33:ARG:HD3	1.92	0.70
1:G:334:SER:O	1:G:338:ILE:HG23	1.91	0.70
1:B:345:LYS:HE2	1:C:404:ASN:HA	1.73	0.70
1:C:263:GLU:HG3	1:C:300:ARG:NH2	2.06	0.70
1:D:2:GLN:HE21	1:D:2:GLN:CA	2.00	0.70
1:F:287:LEU:HD22	1:F:289:LEU:HD21	1.72	0.70
1:H:277:GLN:HG3	1:H:320:MET:HG3	1.73	0.70
1:D:328:ARG:HE	1:D:328:ARG:CA	1.94	0.70
1:F:281:CYS:HB3	1:F:409:LEU:HD23	1.73	0.70
1:G:24:SER:OG	2:G:512:HOH:O	2.10	0.70
1:G:155:THR:O	1:G:159:MET:HG3	1.92	0.70
1:G:344:GLY:O	2:G:505:HOH:O	2.10	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:HIS:HD2	1:A:101:ASP:OD2	1.75	0.69
1:B:329:ARG:HD2	1:B:329:ARG:C	2.17	0.69
1:C:310:LEU:HD12	1:C:320:MET:HB3	1.72	0.69
1:D:115:MET:CE	1:D:461:PHE:CD1	2.75	0.69
1:E:20:ILE:HG21	1:E:175:GLU:HB3	1.74	0.69
1:E:31:ILE:CD1	1:E:88:LEU:HG	2.22	0.69
1:G:23:VAL:CG1	1:G:24:SER:N	2.54	0.69
1:H:213:ALA:O	1:H:242:LYS:HE2	1.91	0.69
1:A:22:VAL:HG23	1:A:34:ILE:HG23	1.71	0.69
1:D:477:VAL:HG22	1:D:478:ASP:N	2.07	0.69
1:F:74:ARG:NH1	1:F:78:CYS:SG	2.65	0.69
1:F:275:HIS:ND1	1:F:439:LYS:NZ	2.39	0.69
1:A:241:LEU:HD13	1:C:248:LEU:HD11	1.74	0.69
1:B:335:TYR:CA	1:B:338:ILE:HG23	2.21	0.69
1:C:415:THR:HG22	1:C:416:GLN:N	2.05	0.69
1:F:38:GLU:CA	1:F:207:THR:CG2	2.65	0.69
1:G:409:LEU:O	1:G:432:MET:HE3	1.93	0.69
1:H:99:GLY:C	1:H:100:LEU:CD2	2.59	0.69
1:H:251:LYS:HB2	1:H:407:TYR:CD1	2.28	0.69
1:A:310:LEU:CD2	1:A:353:PRO:CG	2.70	0.69
1:B:76:GLU:CD	1:B:110:ARG:HH11	2.00	0.69
1:C:259:ASP:OD1	1:C:415:THR:CG2	2.39	0.69
1:D:309:ARG:CD	1:D:319:GLU:OE1	2.39	0.69
1:H:30:LEU:HD21	1:H:33:ARG:HE	1.58	0.69
1:B:250:GLY:O	1:B:381:GLU:HG3	1.93	0.69
1:E:93:PRO:O	1:E:96:ASP:HB2	1.92	0.69
1:E:337:ASP:OD1	2:E:523:HOH:O	2.09	0.69
1:A:377:VAL:CG1	1:A:388:THR:HG21	2.23	0.69
1:B:328:ARG:O	1:B:332:VAL:HG23	1.92	0.69
1:B:328:ARG:NH2	1:B:383:PHE:H	1.91	0.69
1:B:329:ARG:HH11	1:B:329:ARG:CG	1.94	0.69
1:C:291:LYS:HE3	1:C:393:SER:OG	1.92	0.69
1:D:328:ARG:HH11	1:D:383:PHE:CB	2.03	0.69
1:E:251:LYS:HB2	1:E:407:TYR:CD1	2.26	0.69
1:E:377:VAL:HG22	1:E:386:PHE:CZ	2.27	0.69
1:E:423:LYS:HD3	2:E:526:HOH:O	1.92	0.69
1:F:129:GLY:O	1:F:477:VAL:HG22	1.93	0.69
1:E:22:VAL:HG23	1:E:34:ILE:HG23	1.75	0.69
1:G:304:LEU:HA	2:G:513:HOH:O	1.91	0.69
1:H:152:LEU:CD1	1:H:184:ILE:HD11	2.22	0.69
1:H:329:ARG:HD2	1:H:330:ASP:N	2.07	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:351:LYS:CG	1:H:352:ALA:H	2.02	0.69
1:A:355:ASP:C	1:A:357:ALA:N	2.46	0.69
1:E:370:GLU:OE1	1:E:391:ARG:NH1	2.25	0.69
1:G:87:SER:CB	1:G:94:ILE:HD13	2.23	0.69
1:A:417:ASN:ND2	1:A:420:ARG:H	1.90	0.68
1:D:4:GLN:OE1	2:D:506:HOH:O	2.11	0.68
1:D:196:GLY:N	2:D:523:HOH:O	2.00	0.68
1:E:273:ILE:HG21	1:E:387:VAL:HG21	1.74	0.68
1:B:310:LEU:HD12	1:B:320:MET:HG2	1.76	0.68
1:G:19:THR:CG2	1:G:20:ILE:N	2.56	0.68
1:E:273:ILE:CG1	1:E:387:VAL:HG22	2.22	0.68
1:F:94:ILE:HD11	1:F:98:ARG:CZ	2.24	0.68
1:G:259:ASP:OD1	1:G:415:THR:HG22	1.93	0.68
1:G:404:ASN:CG	1:G:404:ASN:O	2.36	0.68
1:H:415:THR:CG2	1:H:420:ARG:HH11	2.05	0.68
1:A:377:VAL:HG13	1:A:388:THR:CG2	2.23	0.68
1:F:43:ASP:O	2:F:522:HOH:O	2.11	0.68
1:H:56:TRP:CZ2	1:H:64:ARG:HG2	2.28	0.68
1:A:38:GLU:O	1:A:42:VAL:HG13	1.92	0.68
1:C:487:ARG:HB3	2:C:505:HOH:O	1.93	0.68
1:E:152:LEU:HD12	1:E:184:ILE:CD1	2.23	0.68
1:A:417:ASN:HD22	1:A:420:ARG:H	1.41	0.68
1:B:479:ALA:CB	1:B:480:LYS:NZ	2.55	0.68
1:E:273:ILE:HG21	1:E:387:VAL:CG2	2.24	0.68
1:F:404:ASN:C	1:F:405:THR:HG23	2.17	0.68
1:G:6:TYR:OH	1:G:189:THR:CG2	2.42	0.68
1:G:485:PHE:O	1:G:487:ARG:N	2.27	0.68
1:C:397:GLU:O	1:C:401:ILE:CG1	2.42	0.68
1:E:417:ASN:ND2	1:E:420:ARG:H	1.90	0.68
1:G:363:TYR:HA	2:G:519:HOH:O	1.87	0.68
1:H:417:ASN:ND2	1:H:420:ARG:H	1.91	0.68
1:B:481:ILE:HG23	1:B:482:ALA:N	2.08	0.68
1:H:136:ARG:HG3	1:H:468:THR:OG1	1.94	0.68
1:D:273:ILE:HG21	1:D:387:VAL:CG2	2.24	0.68
1:F:177:THR:N	1:F:178:PRO:HD3	2.08	0.68
1:G:92:HIS:O	1:G:93:PRO:C	2.35	0.68
1:B:415:THR:HB	1:B:417:ASN:H	1.59	0.67
1:H:124:ILE:HB	1:H:132:ASN:HD22	1.59	0.67
1:A:310:LEU:HD21	1:A:363:TYR:HB3	1.76	0.67
1:B:185:VAL:O	1:B:189:THR:HG22	1.94	0.67
1:B:235:GLU:HG2	1:F:238:LYS:HE3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:GLU:O	1:C:79:SER:HB3	1.93	0.67
1:D:87:SER:OG	1:D:97:SER:OG	2.11	0.67
1:F:23:VAL:C	1:F:31:ILE:CD1	2.67	0.67
1:H:329:ARG:NH1	1:H:329:ARG:CG	2.51	0.67
1:B:243:ARG:CB	2:B:524:HOH:O	2.41	0.67
1:E:345:LYS:HD3	1:E:347:LEU:HD23	1.77	0.67
1:F:63:GLU:OE1	1:F:66:ARG:HD2	1.94	0.67
1:H:6:TYR:OH	1:H:189:THR:HG21	1.94	0.67
1:H:152:LEU:O	1:H:155:THR:OG1	2.12	0.67
1:B:317:GLU:OE1	1:G:193:PHE:O	2.13	0.67
1:D:259:ASP:O	1:D:416:GLN:CG	2.42	0.67
1:G:357:ALA:HB3	1:G:358:LEU:CD1	2.24	0.67
1:A:22:VAL:HG21	1:A:34:ILE:HG21	1.73	0.67
1:E:417:ASN:HD22	1:E:420:ARG:H	1.41	0.67
1:F:338:ILE:HD11	1:F:376:ARG:CD	2.22	0.67
1:C:18:GLY:HA3	2:C:515:HOH:O	1.94	0.67
1:C:25:PRO:HA	1:C:362:PHE:CE2	2.30	0.67
1:E:2:GLN:HA	1:E:2:GLN:HE21	1.59	0.67
1:F:97:SER:HA	1:F:101:ASP:HB2	1.77	0.67
1:A:20:ILE:HD12	1:A:175:GLU:HB3	1.76	0.67
1:A:129:GLY:HA3	1:A:479:ALA:CB	2.24	0.67
1:B:486:LYS:O	1:B:487:ARG:C	2.38	0.67
1:A:277:GLN:HE21	1:A:320:MET:HG3	1.59	0.67
1:C:441:VAL:N	2:C:530:HOH:O	2.28	0.67
1:F:335:TYR:CE2	1:F:376:ARG:NH2	2.62	0.67
1:G:277:GLN:HG2	1:G:321:GLY:O	1.95	0.67
1:H:124:ILE:HD13	1:H:124:ILE:N	2.08	0.67
1:F:323:LEU:N	1:F:323:LEU:HD23	2.08	0.67
1:G:220:LYS:HG3	1:G:221:ILE:N	2.10	0.67
1:B:241:LEU:HD13	1:F:248:LEU:HD12	1.77	0.66
1:C:438:TYR:HD2	1:C:439:LYS:HG3	1.59	0.66
1:D:76:GLU:OE1	1:D:110:ARG:NH1	2.28	0.66
1:E:358:LEU:N	1:E:358:LEU:CD1	2.58	0.66
1:H:371:ALA:HB1	1:H:375:ASP:OD2	1.96	0.66
1:B:148:TRP:CH2	1:B:328:ARG:HG3	2.30	0.66
1:D:137:LYS:NZ	1:G:426:ASN:HD22	1.89	0.66
1:D:309:ARG:HD3	1:D:309:ARG:H	1.58	0.66
1:D:415:THR:CG2	1:D:420:ARG:HH11	2.01	0.66
1:F:458:GLU:O	1:F:459:MET:HB2	1.95	0.66
1:C:417:ASN:HD22	1:C:420:ARG:CB	2.08	0.66
1:C:476:ASN:OD1	1:C:479:ALA:HB3	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:462:GLU:OE2	1:H:136:ARG:NH1	2.29	0.66
1:G:424:MET:O	1:G:428:ILE:HG13	1.96	0.66
1:E:377:VAL:CG2	1:E:386:PHE:HZ	2.04	0.66
1:E:426:ASN:HD22	1:H:137:LYS:HE2	1.60	0.66
1:H:287:LEU:HD22	1:H:289:LEU:HD21	1.77	0.66
1:B:251:LYS:NZ	1:B:377:VAL:O	2.28	0.66
1:B:323:LEU:CD1	1:B:332:VAL:HG21	2.24	0.66
1:B:345:LYS:HB2	1:B:370:GLU:HB3	1.77	0.66
1:B:405:THR:HG21	1:B:407:TYR:HB2	1.78	0.66
1:F:143:ALA:HB1	1:F:212:LEU:HG	1.76	0.66
1:A:114:GLY:O	1:A:118:LYS:NZ	2.22	0.66
1:C:25:PRO:HA	1:C:362:PHE:CD2	2.30	0.66
1:C:354:ASP:C	1:C:354:ASP:OD2	2.37	0.66
1:E:295:ASP:O	1:E:299:GLU:HB2	1.96	0.66
1:F:1:MET:CG	1:F:1:MET:O	2.44	0.66
1:D:312:ASP:OD1	1:D:313:PRO:HD2	1.96	0.66
1:D:485:PHE:HE2	1:G:308:ILE:HD11	1.59	0.66
1:F:2:GLN:HE21	1:F:2:GLN:CA	2.06	0.66
1:G:340:ILE:O	1:G:342:GLN:N	2.29	0.66
1:H:92:HIS:HD2	1:H:101:ASP:OD2	1.78	0.66
1:B:210:GLN:NE2	1:B:214:GLU:OE2	2.29	0.66
1:C:340:ILE:CG2	1:C:341:GLU:N	2.59	0.66
1:D:61:ALA:HB1	1:D:116:ALA:C	2.20	0.66
1:E:258:GLU:CG	1:E:290:HIS:CD2	2.79	0.66
1:G:358:LEU:HB3	1:G:363:TYR:CE2	2.31	0.66
1:C:94:ILE:HG12	1:C:98:ARG:HD2	1.78	0.65
1:G:175:GLU:HG3	1:G:203:GLY:O	1.96	0.65
1:G:458:GLU:O	1:G:459:MET:CB	2.43	0.65
1:B:137:LYS:CG	1:B:471:ARG:HG3	2.24	0.65
1:B:468:THR:OG1	2:B:514:HOH:O	2.14	0.65
1:E:273:ILE:HD12	1:E:273:ILE:C	2.17	0.65
1:E:442:SER:OG	2:H:509:HOH:O	2.14	0.65
1:F:210:GLN:OE1	1:F:210:GLN:N	2.30	0.65
1:G:158:LYS:HE2	1:G:458:GLU:OE2	1.95	0.65
1:A:15:VAL:HG13	1:A:16:ALA:N	2.12	0.65
1:D:158:LYS:HD3	1:D:458:GLU:OE2	1.95	0.65
1:D:457:ARG:HG2	1:D:457:ARG:NH1	2.07	0.65
1:E:221:ILE:O	1:E:221:ILE:CG2	2.44	0.65
1:E:261:ASN:C	1:E:261:ASN:OD1	2.39	0.65
1:E:262:ILE:HD11	1:E:293:ILE:HB	1.78	0.65
1:B:89:ASN:O	1:B:89:ASN:ND2	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:GLU:OE1	2:B:525:HOH:O	2.14	0.65
1:G:87:SER:HB3	1:G:314:MET:HE3	1.79	0.65
1:A:100:LEU:O	1:A:104:ARG:CG	2.42	0.65
1:A:157:TRP:O	2:A:501:HOH:O	2.13	0.65
1:A:226:SER:OG	1:A:229:THR:CG2	2.41	0.65
1:C:36:ALA:O	2:C:515:HOH:O	2.15	0.65
1:F:432:MET:CE	1:F:447:PHE:CD1	2.77	0.65
1:A:159:MET:HE1	1:A:198:VAL:HG11	0.72	0.65
1:B:288:ILE:HG22	1:B:392:PHE:CD2	2.31	0.65
1:B:429[A]:HIS:CE1	1:B:450:VAL:HG11	2.32	0.65
1:D:4:GLN:HB3	1:D:12:VAL:O	1.97	0.65
1:D:188:MET:CE	1:D:198:VAL:HG11	2.26	0.65
1:G:325:SER:C	1:G:362:PHE:CD2	2.74	0.65
1:H:26:HIS:HD1	1:H:363:TYR:HH	0.67	0.65
1:B:474:TRP:HB2	1:F:434:TRP:HA	1.79	0.65
1:D:188:MET:HE1	1:D:198:VAL:CB	2.25	0.65
1:E:172:LYS:NZ	1:E:173:PRO:O	2.30	0.65
1:F:290:HIS:HD2	1:F:292:ASP:H	1.45	0.65
1:A:228:ALA:O	1:A:232:ARG:CZ	2.45	0.65
1:B:263:GLU:HG3	1:B:300:ARG:NH2	2.12	0.65
1:C:80:GLU:OE1	1:C:84:GLN:NE2	2.30	0.65
1:C:201:VAL:O	1:C:201:VAL:CG1	2.45	0.65
1:D:183:ARG:NH1	1:D:186:GLU:OE1	2.30	0.65
1:E:42:VAL:HG13	1:E:212:LEU:CD1	2.24	0.65
1:E:94:ILE:HA	1:E:97:SER:OG	1.96	0.65
1:G:310:LEU:CD1	1:G:320:MET:HG2	2.12	0.65
1:A:87:SER:OG	1:A:92:HIS:O	2.10	0.65
1:A:201:VAL:O	1:A:201:VAL:CG1	2.45	0.65
1:F:18:GLY:HA3	2:F:504:HOH:O	1.96	0.65
1:F:221:ILE:HB	1:F:242:LYS:HD3	1.77	0.65
1:H:25:PRO:HB2	1:H:322:PRO:HG2	1.78	0.65
1:B:88:LEU:CA	1:B:314:MET:HE3	2.26	0.65
1:G:87:SER:HB2	1:G:94:ILE:HD12	1.68	0.65
1:B:88:LEU:N	1:B:314:MET:HE1	2.12	0.64
1:B:201:VAL:O	1:B:201:VAL:CG1	2.45	0.64
1:C:20:ILE:HD13	1:C:175:GLU:HB3	1.79	0.64
1:D:201:VAL:O	1:D:201:VAL:CG1	2.45	0.64
1:D:404:ASN:O	1:D:404:ASN:ND2	2.30	0.64
1:H:251:LYS:HD3	1:H:380:GLU:O	1.97	0.64
1:B:137:LYS:CE	1:F:426:ASN:OD1	2.45	0.64
1:B:328:ARG:NH1	1:B:331:ARG:NE	2.45	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:479:ALA:CB	1:B:480:LYS:HE2	2.25	0.64
1:C:302:ILE:HD11	1:C:347:LEU:HB2	1.78	0.64
1:E:355:ASP:OD2	1:E:355:ASP:N	2.30	0.64
1:F:89:ASN:O	1:F:89:ASN:ND2	2.29	0.64
1:G:273:ILE:HD13	1:G:285:SER:CA	2.24	0.64
1:A:273:ILE:HD13	1:A:285:SER:HA	1.79	0.64
1:A:342:GLN:O	1:A:342:GLN:NE2	2.30	0.64
1:B:26:HIS:ND1	1:B:363:TYR:OH	2.17	0.64
1:E:104:ARG:CD	1:E:153:MET:HE2	2.26	0.64
1:A:112:PHE:HA	1:A:115:MET:HB3	1.77	0.64
1:B:405:THR:CG2	1:B:406:GLU:N	2.60	0.64
1:C:117:ASP:OD1	1:C:118:LYS:NZ	2.30	0.64
1:D:238:LYS:HD3	1:G:235:GLU:HG2	1.78	0.64
1:E:345:LYS:HD3	1:E:347:LEU:CD2	2.27	0.64
1:E:396:GLU:OE1	1:E:396:GLU:N	2.30	0.64
1:F:74:ARG:HG3	1:F:187:LEU:HD22	1.80	0.64
1:F:339:ALA:HB2	1:F:377:VAL:CG2	2.24	0.64
1:H:89:ASN:ND2	1:H:89:ASN:O	2.30	0.64
1:H:183:ARG:NH1	1:H:186:GLU:OE1	2.30	0.64
1:A:342:GLN:NE2	1:A:375:ASP:OD1	2.31	0.64
1:B:238:LYS:HD3	1:F:231:ARG:O	1.97	0.64
1:E:86:GLU:O	1:E:90:THR:OG1	2.13	0.64
1:E:358:LEU:N	1:E:358:LEU:HD12	2.13	0.64
1:G:356:LYS:O	1:G:358:LEU:N	2.30	0.64
1:C:152:LEU:CD1	1:C:184:ILE:CD1	2.75	0.64
1:D:277:GLN:NE2	1:D:321:GLY:H	1.94	0.64
1:F:330:ASP:OD1	1:F:330:ASP:N	2.30	0.64
1:H:261:ASN:C	1:H:261:ASN:OD1	2.39	0.64
1:A:220:LYS:NZ	1:A:245:GLN:HB2	2.13	0.64
1:B:479:ALA:CB	1:B:480:LYS:CD	2.71	0.64
1:E:117:ASP:OD1	1:E:117:ASP:N	2.30	0.64
1:E:479:ALA:C	1:E:480:LYS:HE2	2.22	0.64
1:F:311:GLY:O	1:F:313:PRO:HD3	1.98	0.64
1:H:302:ILE:O	1:H:306:LYS:CG	2.46	0.64
1:B:235:GLU:HG2	1:F:238:LYS:CD	2.27	0.64
1:D:39:ALA:O	1:D:43:ASP:OD1	2.15	0.64
1:E:159:MET:CE	1:E:171:ILE:CD1	2.59	0.64
1:E:417:ASN:HD22	1:E:420:ARG:HB2	1.63	0.64
1:E:477:VAL:HG23	1:E:478:ASP:HB2	1.78	0.64
1:G:94:ILE:O	1:G:98:ARG:HG3	1.98	0.64
1:A:417:ASN:HD22	1:A:420:ARG:HB2	1.63	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:ASP:OD1	1:C:316:PRO:CD	2.45	0.64
1:E:220:LYS:HG3	1:E:221:ILE:N	2.12	0.64
1:A:89:ASN:O	1:A:89:ASN:ND2	2.30	0.64
1:A:338:ILE:HD13	1:A:376:ARG:NH2	2.13	0.64
1:E:251:LYS:HG3	1:E:286:ARG:HD3	1.79	0.64
1:E:87:SER:HB3	1:E:314:MET:HE3	1.79	0.63
1:F:43:ASP:OD1	1:F:215:HIS:NE2	2.32	0.63
1:F:486:LYS:O	1:F:487:ARG:C	2.39	0.63
1:G:94:ILE:O	1:G:98:ARG:CG	2.46	0.63
1:H:39:ALA:O	1:H:42:VAL:HG22	1.97	0.63
1:A:76:GLU:OE2	1:A:110:ARG:NH1	2.31	0.63
1:C:287:LEU:HD22	1:C:289:LEU:HD21	1.80	0.63
1:G:310:LEU:CD2	1:G:353:PRO:CG	2.75	0.63
1:G:464:ILE:O	1:G:468:THR:OG1	2.14	0.63
1:D:71:LEU:O	1:D:71:LEU:HD12	1.98	0.63
1:C:175:GLU:OE1	1:C:175:GLU:N	2.30	0.63
1:F:159:MET:HE2	1:F:171:ILE:CD1	2.28	0.63
1:G:8:ASP:OD1	1:G:48:ALA:HB1	1.99	0.63
1:H:377:VAL:HG21	1:H:386:PHE:HZ	1.58	0.63
1:C:25:PRO:HB2	1:C:322:PRO:HG2	1.79	0.63
1:C:338:ILE:HD11	1:C:376:ARG:HB2	1.80	0.63
1:F:458:GLU:O	1:F:459:MET:CB	2.46	0.63
1:A:231:ARG:O	1:C:238:LYS:HE2	1.97	0.63
1:A:238:LYS:O	1:A:239:SER:C	2.42	0.63
1:C:23:VAL:HG13	1:C:29:SER:O	1.98	0.63
1:D:374:GLN:N	1:D:374:GLN:OE1	2.30	0.63
1:E:74:ARG:NH2	1:E:190:GLU:CD	2.50	0.63
1:F:220:LYS:HE2	1:F:245:GLN:HG3	1.79	0.63
1:F:320:MET:CE	1:F:366:PRO:HG3	2.29	0.63
1:G:86:GLU:O	1:G:90:THR:OG1	2.09	0.63
1:G:92:HIS:C	1:G:93:PRO:O	2.40	0.63
1:B:148:TRP:HH2	1:B:328:ARG:HG3	1.62	0.63
1:E:104:ARG:CD	1:E:153:MET:CE	2.77	0.63
1:E:334:SER:O	1:E:338:ILE:HG23	1.99	0.63
1:F:18:GLY:O	1:F:36:ALA:N	2.25	0.63
1:F:94:ILE:HG22	1:F:313:PRO:O	1.99	0.63
1:F:227:THR:HG22	1:F:231:ARG:HH11	1.63	0.63
1:G:327:LEU:HD22	1:G:331:ARG:CD	2.28	0.63
1:H:1:MET:HE1	1:H:31:ILE:HG22	1.81	0.63
1:H:90:THR:CG2	1:H:92:HIS:ND1	2.62	0.63
1:B:245:GLN:HB3	2:B:519:HOH:O	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:GLY:N	1:D:453:SER:OG	2.31	0.63
1:F:396:GLU:OE1	1:F:396:GLU:N	2.30	0.63
1:G:408:GLY:O	1:G:430:ALA:CA	2.45	0.63
1:H:273:ILE:O	1:H:273:ILE:HG13	1.99	0.63
1:H:304:LEU:HD12	1:H:304:LEU:O	1.97	0.63
1:A:127:ASP:OD2	1:A:127:ASP:N	2.30	0.63
1:D:61:ALA:HB1	1:D:116:ALA:O	1.99	0.63
1:D:374:GLN:CD	1:D:374:GLN:H	2.05	0.63
1:E:231:ARG:NE	1:H:238:LYS:O	2.30	0.63
1:E:259:ASP:OD1	1:E:415:THR:CG2	2.46	0.63
1:H:90:THR:O	1:H:324:THR:HG22	1.99	0.63
1:H:377:VAL:CG2	1:H:386:PHE:CZ	2.82	0.63
1:B:56:TRP:CZ2	1:B:64:ARG:HG2	2.33	0.62
1:B:479:ALA:HB3	1:B:480:LYS:HG2	1.80	0.62
1:D:376:ARG:HD2	1:D:380:GLU:OE2	1.99	0.62
2:E:525:HOH:O	1:H:426:ASN:HB2	1.99	0.62
1:F:162:ALA:HB3	1:F:169:ILE:HD11	1.81	0.62
1:G:6:TYR:OH	1:G:189:THR:HG21	1.99	0.62
1:G:87:SER:HB3	1:G:314:MET:CE	2.29	0.62
1:G:476:ASN:OD1	1:G:479:ALA:CB	2.46	0.62
1:C:213:ALA:HA	1:C:221:ILE:HG13	1.81	0.62
1:D:376:ARG:HD3	1:D:380:GLU:OE2	1.99	0.62
1:D:481:ILE:CG2	1:D:482:ALA:N	2.62	0.62
1:H:329:ARG:NE	1:H:330:ASP:OD1	2.33	0.62
1:B:479:ALA:HB2	1:B:480:LYS:HZ2	1.60	0.62
1:D:485:PHE:CE2	1:G:308:ILE:HD11	2.34	0.62
1:F:34:ILE:O	1:F:34:ILE:HG13	1.91	0.62
1:G:108:CYS:HB3	1:G:156:SER:HB2	1.81	0.62
1:A:15:VAL:HG11	1:A:40:ALA:CB	2.29	0.62
1:A:480:LYS:N	2:A:528:HOH:O	2.30	0.62
1:B:401:ILE:O	1:B:404:ASN:CB	2.41	0.62
1:F:409:LEU:O	1:F:432:MET:HG2	1.99	0.62
1:G:173:PRO:HG3	1:G:181:THR:HG21	1.81	0.62
1:G:356:LYS:O	1:G:357:ALA:C	2.40	0.62
1:G:356:LYS:C	1:G:358:LEU:N	2.57	0.62
1:A:409:LEU:O	1:A:432:MET:HE3	1.99	0.62
1:C:480:LYS:O	1:C:480:LYS:HG2	1.94	0.62
1:D:185:VAL:HA	1:D:188:MET:HG3	1.80	0.62
1:E:153:MET:O	1:E:156:SER:OG	2.18	0.62
1:A:406:GLU:OE1	1:A:406:GLU:HA	1.97	0.62
1:C:42:VAL:O	1:C:46:VAL:HG23	1.99	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:PHE:CZ	1:D:140:GLY:HA2	2.34	0.62
1:F:227:THR:HG21	1:F:231:ARG:HH12	1.64	0.62
1:H:335:TYR:CG	1:H:382:VAL:HG22	2.33	0.62
1:D:100:LEU:O	1:D:104:ARG:HG3	2.00	0.62
1:G:20:ILE:HD11	1:G:204:TYR:CE2	2.35	0.62
1:B:248:LEU:HD11	1:F:241:LEU:HD22	1.80	0.62
1:B:477:VAL:HG22	1:B:478:ASP:N	2.14	0.62
1:E:342:GLN:HE22	1:E:376:ARG:H	1.46	0.62
1:H:155:THR:O	1:H:159:MET:HB2	1.99	0.62
1:H:159:MET:HE2	1:H:171:ILE:CD1	2.26	0.62
1:A:309:ARG:HD3	1:A:309:ARG:C	2.24	0.62
1:B:88:LEU:N	1:B:314:MET:CE	2.63	0.62
1:B:323:LEU:HD11	1:B:332:VAL:HG21	1.82	0.62
1:C:237:SER:CB	1:C:244:ILE:HD11	2.30	0.62
1:C:356:LYS:HG2	1:C:356:LYS:O	1.97	0.62
1:F:424:MET:O	1:F:428:ILE:HG13	2.00	0.62
1:G:31:ILE:CD1	1:G:88:LEU:HG	2.30	0.62
1:G:85:LEU:O	1:G:85:LEU:HD12	2.00	0.62
1:G:238:LYS:O	1:G:239:SER:C	2.42	0.62
1:A:273:ILE:HG21	1:A:387:VAL:HG21	1.79	0.62
1:B:235:GLU:HG2	1:F:238:LYS:HD2	1.82	0.62
1:C:119:ILE:CD1	1:C:464:ILE:HD12	2.30	0.62
1:D:414:TRP:CE3	1:D:436:ASN:HA	2.35	0.62
1:G:293:ILE:HD12	1:G:293:ILE:O	1.94	0.62
1:G:309:ARG:NH1	1:G:317:GLU:CB	2.60	0.62
1:B:273:ILE:HG21	1:B:387:VAL:CG2	2.30	0.61
1:B:481:ILE:CB	2:B:515:HOH:O	2.46	0.61
1:D:239:SER:O	1:G:231:ARG:NH2	2.30	0.61
1:F:8:ASP:OD2	1:F:51:ARG:NH2	2.33	0.61
1:F:27:ASP:OD1	1:F:29:SER:N	2.29	0.61
1:H:406:GLU:OE1	1:H:406:GLU:HA	1.97	0.61
1:A:310:LEU:HD21	1:A:353:PRO:HG2	1.83	0.61
1:E:282:ILE:HG21	1:E:432:MET:HE3	1.81	0.61
1:F:326:ALA:CB	1:F:362:PHE:CE1	2.83	0.61
1:G:104:ARG:HH21	1:G:153:MET:HE1	1.63	0.61
1:A:262:ILE:O	1:A:266:VAL:HG23	2.00	0.61
1:C:486:LYS:O	1:C:487:ARG:C	2.42	0.61
1:E:157:TRP:CZ2	1:E:441:VAL:HG11	2.35	0.61
1:F:89:ASN:HD22	1:F:89:ASN:C	2.04	0.61
1:B:358:LEU:N	1:B:358:LEU:CD1	2.62	0.61
1:B:450:VAL:CG1	1:B:451:GLY:N	2.63	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:SER:HB2	1:G:94:ILE:HD11	1.80	0.61
1:H:49:ALA:O	1:H:168:THR:HG21	2.01	0.61
1:A:59:LEU:HG	1:A:63:GLU:HB3	1.81	0.61
1:B:298:LEU:HD11	1:B:389:VAL:HG11	1.82	0.61
1:D:462:GLU:OE2	1:G:465:HIS:NE2	2.16	0.61
1:H:417:ASN:HD22	1:H:420:ARG:CB	2.14	0.61
1:B:15:VAL:HG12	1:B:41:ASP:CG	2.25	0.61
1:B:158:LYS:HD3	1:B:458:GLU:OE2	2.00	0.61
1:B:481:ILE:N	2:B:515:HOH:O	2.33	0.61
1:E:185:VAL:HA	1:E:188:MET:HE3	1.81	0.61
1:G:340:ILE:C	1:G:342:GLN:N	2.56	0.61
1:B:81:GLU:HB2	2:B:518:HOH:O	1.95	0.61
1:F:100:LEU:O	1:F:104:ARG:HG3	2.01	0.61
1:F:417:ASN:ND2	1:F:420:ARG:H	1.98	0.61
1:G:136:ARG:HH21	1:G:470:ALA:HB2	1.65	0.61
1:H:142:VAL:HG11	1:H:467:TYR:HE2	1.66	0.61
1:B:152:LEU:CD1	1:B:184:ILE:HD12	2.27	0.61
1:E:277:GLN:HG3	1:E:320:MET:HG3	1.81	0.61
1:F:22:VAL:CG2	1:F:34:ILE:HG21	2.30	0.61
1:F:230:GLY:O	1:F:234:VAL:HG23	2.01	0.61
1:G:148:TRP:CA	1:G:177:THR:HG21	2.30	0.61
1:G:447:PHE:C	1:G:447:PHE:HD2	2.09	0.61
1:B:185:VAL:O	1:B:189:THR:CG2	2.49	0.61
1:E:292:ASP:CG	2:E:529:HOH:O	2.42	0.61
1:F:381:GLU:CG	1:F:381:GLU:O	2.48	0.61
1:H:49:ALA:CB	1:H:168:THR:HG21	2.18	0.61
1:B:152:LEU:HD12	1:B:184:ILE:HD13	1.82	0.61
1:G:310:LEU:HD23	1:G:353:PRO:CG	2.31	0.61
1:G:340:ILE:C	1:G:342:GLN:H	2.09	0.61
1:H:61:ALA:HB1	1:H:116:ALA:O	1.98	0.61
1:H:259:ASP:OD1	1:H:415:THR:CG2	2.42	0.61
1:A:477:VAL:HG22	1:A:478:ASP:N	2.15	0.60
1:B:137:LYS:HE2	1:F:426:ASN:OD1	2.00	0.60
1:F:310:LEU:HD21	1:F:363:TYR:HB3	1.81	0.60
1:A:25:PRO:HB2	1:A:322:PRO:HG2	1.82	0.60
1:A:213:ALA:O	1:A:242:LYS:HE3	2.01	0.60
1:A:481:ILE:CG1	1:A:482:ALA:H	2.09	0.60
1:C:18:GLY:CA	2:C:515:HOH:O	2.48	0.60
1:C:287:LEU:HD12	1:C:387:VAL:HG21	1.81	0.60
1:D:370:GLU:OE2	1:D:391:ARG:NH1	2.34	0.60
1:D:481:ILE:CG2	1:D:482:ALA:H	2.13	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:290:HIS:CE1	1:E:393:SER:O	2.53	0.60
1:A:228:ALA:O	1:A:232:ARG:NH2	2.34	0.60
1:C:63[A]:GLU:OE1	1:C:66:ARG:CZ	2.48	0.60
1:E:137:LYS:NZ	1:H:426:ASN:OD1	2.34	0.60
1:E:248:LEU:CD1	1:H:241:LEU:HD22	2.30	0.60
1:G:21:ASP:HB3	1:G:30:LEU:HD12	1.79	0.60
1:H:337:ASP:HA	1:H:340:ILE:HD12	1.83	0.60
1:H:417:ASN:HD22	1:H:420:ARG:H	1.46	0.60
1:A:309:ARG:N	1:A:319:GLU:OE1	2.22	0.60
1:F:351:LYS:O	1:F:365:GLU:CG	2.48	0.60
1:G:221:ILE:O	1:G:221:ILE:HG23	2.00	0.60
1:C:332:VAL:O	1:C:332:VAL:HG12	2.01	0.60
1:D:53:PHE:CE1	1:D:140:GLY:HA2	2.36	0.60
1:D:137:LYS:HZ3	1:G:426:ASN:ND2	1.94	0.60
1:D:485:PHE:CE2	1:G:308:ILE:CD1	2.84	0.60
1:B:34:ILE:HG13	1:B:34:ILE:O	1.92	0.60
1:E:89:ASN:OD1	1:E:177:THR:HA	2.02	0.60
1:G:143:ALA:HB1	1:G:212:LEU:HG	1.83	0.60
1:H:328:ARG:HE	1:H:383:PHE:HB3	1.63	0.60
1:A:15:VAL:HG11	1:A:40:ALA:HB3	1.83	0.60
1:D:188:MET:HE1	1:D:198:VAL:CG1	2.31	0.60
1:G:380:GLU:HG2	2:G:523:HOH:O	2.00	0.60
1:C:60:GLY:O	1:C:61:ALA:C	2.45	0.60
1:D:262:ILE:HG23	1:D:297:PHE:HD1	1.67	0.60
1:E:31:ILE:HD13	1:E:88:LEU:HG	1.83	0.60
1:E:43:ASP:OD1	1:E:215:HIS:NE2	2.35	0.60
1:D:231:ARG:HG2	1:G:238:LYS:HB2	1.84	0.60
1:D:310:LEU:HD23	1:D:353:PRO:CG	2.32	0.60
1:E:392:PHE:CD1	1:E:394:SER:O	2.54	0.60
1:A:93:PRO:O	1:A:96:ASP:HB2	2.01	0.60
1:C:2:GLN:HG3	1:C:11:PHE:CZ	2.37	0.60
1:C:23:VAL:HG11	1:C:28:GLY:O	2.02	0.60
1:E:227:THR:HA	1:E:248:LEU:HB3	1.83	0.60
1:G:26:HIS:CB	2:G:512:HOH:O	2.50	0.60
1:G:221:ILE:O	1:G:221:ILE:HG22	2.02	0.60
1:G:323:LEU:N	1:G:323:LEU:HD23	2.16	0.60
1:G:329:ARG:NH1	1:G:330:ASP:OD1	2.30	0.60
1:H:90:THR:HG22	1:H:92:HIS:ND1	2.16	0.60
1:D:201:VAL:O	1:D:201:VAL:HG12	2.01	0.59
1:E:184:ILE:O	1:E:188:MET:HG3	2.02	0.59
1:F:310:LEU:CD2	1:F:353:PRO:HG3	2.32	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:ALA:O	1:F:358:LEU:HD12	2.02	0.59
1:G:335:TYR:O	1:G:339:ALA:N	2.34	0.59
1:F:38:GLU:HA	1:F:207:THR:HG21	1.83	0.59
1:C:372:LYS:C	1:C:374:GLN:H	2.09	0.59
1:D:263:GLU:O	1:D:267:ASN:ND2	2.34	0.59
1:D:477:VAL:CG2	1:D:478:ASP:N	2.66	0.59
1:F:298:LEU:O	1:F:302:ILE:HD12	2.02	0.59
1:B:320:MET:CE	1:B:385:PRO:CB	2.71	0.59
1:C:138:PRO:HG3	1:C:165:ALA:O	2.02	0.59
1:E:283:ALA:O	2:E:527:HOH:O	2.15	0.59
1:A:355:ASP:O	1:A:356:LYS:C	2.45	0.59
1:B:38:GLU:O	1:B:41:ASP:N	2.32	0.59
1:D:20:ILE:HD13	1:D:175:GLU:HB3	1.85	0.59
1:E:143:ALA:HB1	1:E:212:LEU:HG	1.84	0.59
1:G:458:GLU:O	1:G:459:MET:HB2	2.01	0.59
1:B:201:VAL:O	1:B:201:VAL:HG12	2.01	0.59
1:C:329:ARG:NH2	1:C:330:ASP:OD1	2.30	0.59
1:E:123:VAL:C	1:E:124:ILE:HD13	2.28	0.59
1:E:337:ASP:CG	2:E:523:HOH:O	2.46	0.59
1:E:399:LEU:HD11	1:E:427:ALA:HB1	1.84	0.59
1:F:386:PHE:C	1:F:387:VAL:CG2	2.76	0.59
1:G:347:LEU:HD11	1:G:370:GLU:CG	2.18	0.59
1:H:21:ASP:HB3	1:H:30:LEU:CD1	2.32	0.59
1:A:102:VAL:CB	1:A:103:PRO:HD3	2.31	0.59
1:B:243:ARG:CA	2:B:524:HOH:O	2.50	0.59
1:D:309:ARG:HD3	1:D:309:ARG:N	2.17	0.59
1:E:76:GLU:O	1:E:79:SER:HB3	2.02	0.59
1:E:195:LYS:O	1:E:195:LYS:HG2	2.00	0.59
1:G:99:GLY:O	1:G:103:PRO:HG2	2.02	0.59
1:B:102:VAL:HB	1:B:103:PRO:HD3	1.85	0.59
1:E:417:ASN:HD22	1:E:420:ARG:CB	2.16	0.59
1:G:94:ILE:CD1	1:G:314:MET:CE	2.76	0.59
1:H:269:ALA:O	1:H:273:ILE:HG22	2.03	0.59
1:A:251:LYS:CE	2:A:524:HOH:O	2.45	0.59
1:C:370:GLU:CD	1:C:391:ARG:HH11	2.11	0.59
1:E:74:ARG:CZ	1:E:190:GLU:OE1	2.44	0.59
1:G:151:PRO:CG	1:G:177:THR:HG1	2.15	0.59
1:B:344:GLY:C	1:B:345:LYS:HD2	2.27	0.59
1:E:404:ASN:C	1:E:405:THR:CG2	2.76	0.59
1:F:40:ALA:O	1:F:44:LEU:HD12	2.03	0.59
1:F:386:PHE:C	1:F:387:VAL:HG23	2.28	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:304:LEU:HD12	1:H:304:LEU:C	2.28	0.59
1:C:137:LYS:HG3	1:C:471:ARG:HG3	1.83	0.58
1:F:320:MET:HE1	1:F:366:PRO:HG3	1.84	0.58
1:G:380:GLU:CG	2:G:523:HOH:O	2.51	0.58
1:H:30:LEU:HD21	1:H:33:ARG:NE	2.17	0.58
1:A:174:SER:C	1:A:176:ILE:H	2.11	0.58
1:A:201:VAL:O	1:A:201:VAL:HG12	2.01	0.58
1:D:417:ASN:HD22	1:D:420:ARG:H	1.48	0.58
1:E:31:ILE:HD11	1:E:88:LEU:HG	1.86	0.58
1:E:42:VAL:O	1:E:46:VAL:HG23	2.03	0.58
1:E:153:MET:HG3	2:E:510:HOH:O	2.03	0.58
1:E:258:GLU:CD	2:E:516:HOH:O	2.40	0.58
1:F:94:ILE:O	1:F:94:ILE:CG1	2.48	0.58
1:F:437:CYS:SG	1:F:440:ARG:HG3	2.43	0.58
1:H:76:GLU:O	1:H:79:SER:HB3	2.02	0.58
1:H:288:ILE:HG22	1:H:392:PHE:CD2	2.39	0.58
1:E:277:GLN:HG3	1:E:320:MET:HG2	1.83	0.58
1:G:6:TYR:CD2	1:G:185:VAL:HG21	2.39	0.58
1:G:56:TRP:CH2	1:G:64:ARG:HG2	2.39	0.58
1:H:183:ARG:O	1:H:183:ARG:HD2	2.03	0.58
1:A:162:ALA:O	1:A:167:ASN:ND2	2.30	0.58
1:C:186:GLU:O	1:C:190:GLU:HG3	2.03	0.58
1:D:137:LYS:HG3	1:D:471:ARG:HG3	1.83	0.58
1:G:23:VAL:HG13	1:G:24:SER:N	2.17	0.58
1:A:23:VAL:HG12	1:A:24:SER:N	2.17	0.58
1:A:305:ALA:HA	1:A:308:ILE:HD12	1.85	0.58
1:B:273:ILE:CG1	1:B:387:VAL:HG22	2.32	0.58
1:F:149:ASN:ND2	1:F:150:PHE:CD1	2.71	0.58
1:G:31:ILE:HD13	1:G:88:LEU:HG	1.85	0.58
1:G:459:MET:N	1:G:463:ALA:HB2	2.18	0.58
1:H:8:ASP:OD1	2:H:507:HOH:O	2.17	0.58
1:C:201:VAL:O	1:C:201:VAL:HG12	2.01	0.58
1:C:339:ALA:O	1:C:344:GLY:HA3	2.03	0.58
1:C:415:THR:CG2	1:C:416:GLN:H	2.09	0.58
1:D:5:LEU:HB2	1:D:12:VAL:HG12	1.84	0.58
1:E:447:PHE:C	1:E:447:PHE:CD2	2.82	0.58
1:C:151:PRO:HG2	1:C:177:THR:HB	1.86	0.58
1:D:175:GLU:H	1:D:175:GLU:CD	2.10	0.58
1:D:277:GLN:HE21	1:D:320:MET:HG2	1.69	0.58
1:D:326:ALA:HB2	1:D:362:PHE:CE1	2.39	0.58
1:E:155:THR:HG22	1:E:181:THR:HG23	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:GLU:HG2	1:E:204:TYR:CD1	2.39	0.58
1:G:97:SER:CA	1:G:101:ASP:HB2	2.32	0.58
1:G:293:ILE:O	1:G:293:ILE:HD13	2.04	0.58
1:A:417:ASN:HD22	1:A:420:ARG:CB	2.16	0.58
1:C:19:THR:HG23	1:C:20:ILE:N	2.17	0.58
1:C:20:ILE:HG21	1:C:175:GLU:HB3	1.86	0.58
1:C:143:ALA:HB1	1:C:212:LEU:HG	1.84	0.58
1:E:392:PHE:CE1	1:E:394:SER:O	2.57	0.58
1:G:148:TRP:CD1	1:G:148:TRP:N	2.72	0.58
1:G:323:LEU:O	1:G:362:PHE:HB2	2.04	0.58
1:G:357:ALA:HB3	1:G:358:LEU:HD11	1.86	0.58
1:E:87:SER:HB3	1:E:314:MET:CE	2.33	0.58
1:H:74:ARG:NE	1:H:77:GLU:OE1	2.37	0.58
1:A:477:VAL:HG23	1:A:478:ASP:HB2	1.85	0.57
1:B:258:GLU:HG2	1:B:290:HIS:NE2	2.19	0.57
1:B:320:MET:CE	1:B:385:PRO:HG3	2.34	0.57
1:F:145:ILE:HB	1:F:223:PHE:HD1	1.68	0.57
1:G:303:ALA:C	2:G:513:HOH:O	2.46	0.57
1:B:159:MET:HG2	1:B:169:ILE:HD13	1.86	0.57
1:B:186:GLU:HA	1:B:189:THR:HG23	1.86	0.57
1:C:259:ASP:OD2	1:C:415:THR:HG22	2.04	0.57
1:D:445:SER:HB2	1:G:132:ASN:ND2	2.19	0.57
1:E:61:ALA:HB1	1:E:116:ALA:C	2.28	0.57
1:E:308:ILE:HG21	1:E:320:MET:HE3	1.84	0.57
1:E:452:GLN:HG2	1:H:240:ASN:O	2.03	0.57
1:F:70:LYS:HB3	1:F:191:VAL:CG1	2.33	0.57
1:F:163:LEU:HG	1:F:169:ILE:HD12	1.86	0.57
1:F:338:ILE:HD13	1:F:376:ARG:HD3	1.85	0.57
1:G:136:ARG:HG3	1:G:468:THR:HB	1.86	0.57
1:H:153:MET:O	1:H:156:SER:OG	2.22	0.57
1:B:25:PRO:HB2	1:B:322:PRO:HG2	1.85	0.57
1:B:312:ASP:OD1	1:B:313:PRO:CD	2.51	0.57
1:C:432:MET:HE1	1:C:447:PHE:CG	2.31	0.57
1:H:376:ARG:C	1:H:378:CYS:H	2.11	0.57
1:B:90:THR:HG22	1:B:177:THR:CG2	2.34	0.57
1:C:174:SER:C	1:C:176:ILE:N	2.60	0.57
1:C:384:GLY:O	1:C:386:PHE:N	2.36	0.57
1:E:124:ILE:HD13	1:E:124:ILE:N	2.19	0.57
1:E:175:GLU:HG3	1:E:203:GLY:O	2.05	0.57
1:F:257:PHE:CB	1:F:415:THR:HG23	2.30	0.57
1:H:432:MET:HE1	1:H:447:PHE:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ALA:O	1:A:483:PRO:C	2.47	0.57
1:B:288:ILE:HG22	1:B:392:PHE:HD2	1.69	0.57
1:E:275:HIS:ND1	1:E:439:LYS:NZ	2.52	0.57
1:F:87:SER:HB3	1:F:314:MET:HE1	1.86	0.57
1:G:335:TYR:CE2	2:G:523:HOH:O	2.57	0.57
1:H:322:PRO:HB3	1:H:363:TYR:CD2	2.40	0.57
1:A:217:ASP:CG	1:B:374:GLN:HE22	2.11	0.57
1:A:241:LEU:CD1	1:C:248:LEU:CD1	2.81	0.57
1:C:226:SER:O	1:C:227:THR:C	2.47	0.57
1:G:70:LYS:NZ	1:G:191:VAL:O	2.38	0.57
1:G:351:LYS:O	1:G:365:GLU:HB2	2.05	0.57
1:E:277:GLN:OE1	2:E:509:HOH:O	2.18	0.57
1:H:230:GLY:O	1:H:234:VAL:HG23	2.04	0.57
1:B:117:ASP:OD1	1:B:118:LYS:NZ	2.36	0.57
1:C:269:ALA:O	1:C:273:ILE:HG22	2.03	0.57
1:G:10:ARG:NH1	1:G:12:VAL:HG13	2.07	0.57
1:H:377:VAL:HG22	1:H:386:PHE:CE1	2.39	0.57
1:B:243:ARG:HD2	1:F:455:TYR:HB3	1.87	0.57
1:B:417:ASN:ND2	1:B:420:ARG:H	2.03	0.57
1:C:318:THR:HG22	1:C:320:MET:O	2.04	0.57
1:D:117:ASP:OD1	1:D:117:ASP:N	2.30	0.57
1:E:101:ASP:O	2:E:510:HOH:O	2.18	0.57
1:G:151:PRO:CB	1:G:177:THR:OG1	2.53	0.57
1:G:396:GLU:CD	1:G:396:GLU:N	2.62	0.57
1:H:152:LEU:CD1	1:H:184:ILE:CD1	2.82	0.57
1:A:117:ASP:OD1	1:A:117:ASP:N	2.33	0.57
1:A:376:ARG:C	1:A:378:CYS:H	2.12	0.57
1:A:376:ARG:HD2	1:A:380:GLU:OE2	2.02	0.57
1:C:346:VAL:CG1	1:C:348:ALA:O	2.53	0.57
1:D:105:THR:OG1	1:D:153:MET:HA	2.04	0.57
1:G:326:ALA:HB2	1:G:362:PHE:CE1	2.40	0.57
1:A:23:VAL:CG1	1:A:24:SER:N	2.68	0.56
1:B:262:ILE:O	1:B:266:VAL:HG23	2.05	0.56
1:C:386:PHE:C	1:C:386:PHE:CD1	2.82	0.56
1:E:34:ILE:O	1:E:34:ILE:HG13	1.91	0.56
1:E:426:ASN:ND2	1:H:137:LYS:HE2	2.20	0.56
1:B:220:LYS:HE3	1:B:245:GLN:HB2	1.86	0.56
1:B:351:LYS:CG	1:B:352:ALA:N	2.53	0.56
1:E:356:LYS:HG3	1:E:356:LYS:O	2.04	0.56
1:F:386:PHE:O	1:F:387:VAL:HG22	2.05	0.56
1:A:404:ASN:O	1:A:405:THR:HG23	2.02	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:VAL:HG13	1:B:388:THR:CG2	2.35	0.56
1:B:483:PRO:HB3	1:F:267:ASN:OD1	2.06	0.56
1:D:188:MET:CE	1:D:198:VAL:HG21	2.27	0.56
1:E:177:THR:N	1:E:178:PRO:HD3	2.20	0.56
1:G:157:TRP:CE2	1:G:459:MET:CE	2.88	0.56
1:H:100:LEU:HD23	1:H:100:LEU:N	2.09	0.56
1:H:358:LEU:HB3	1:H:363:TYR:CD2	2.40	0.56
1:H:358:LEU:HD13	1:H:358:LEU:N	2.21	0.56
1:A:84:GLN:HG2	1:A:314:MET:HE1	1.88	0.56
1:B:277:GLN:HG3	1:B:320:MET:HG3	1.87	0.56
1:B:335:TYR:HA	1:B:338:ILE:CG2	2.32	0.56
1:B:404:ASN:CG	1:B:404:ASN:O	2.48	0.56
1:C:24:SER:CA	2:C:512:HOH:O	2.50	0.56
1:G:415:THR:HG21	1:G:420:ARG:CD	2.27	0.56
1:H:153:MET:HE3	1:H:157:TRP:CZ2	2.40	0.56
1:H:417:ASN:HD22	1:H:420:ARG:HB2	1.71	0.56
1:A:152:LEU:HD12	1:A:184:ILE:HD13	1.87	0.56
1:D:10:ARG:CG	1:D:10:ARG:NH1	2.49	0.56
1:D:162:ALA:HB3	1:D:169:ILE:HD11	1.88	0.56
1:G:26:HIS:N	2:G:512:HOH:O	1.89	0.56
1:G:235:GLU:O	1:G:238:LYS:HG2	2.05	0.56
1:B:290:HIS:CD2	1:B:292:ASP:H	2.24	0.56
1:C:434:TRP:CD1	1:C:440:ARG:HB2	2.40	0.56
1:G:149:ASN:N	1:G:149:ASN:OD1	2.33	0.56
1:H:404:ASN:CG	1:H:404:ASN:O	2.48	0.56
1:A:404:ASN:C	1:A:405:THR:CG2	2.78	0.56
1:C:246:LEU:HB3	1:C:248:LEU:HD21	1.87	0.56
1:F:94:ILE:HD11	1:F:98:ARG:NH2	2.21	0.56
1:H:142:VAL:HG22	1:H:220:LYS:HB3	1.88	0.56
1:H:377:VAL:HG22	1:H:386:PHE:HE1	1.69	0.56
1:B:350:GLY:O	1:B:351:LYS:HB2	2.04	0.56
1:E:155:THR:CG2	1:E:181:THR:HG23	2.35	0.56
1:F:357:ALA:C	1:F:358:LEU:HD12	2.30	0.56
1:F:441:VAL:HG13	2:F:515:HOH:O	2.04	0.56
1:H:186:GLU:O	1:H:190:GLU:HG3	2.05	0.56
1:A:320:MET:HE3	1:A:385:PRO:HG3	1.88	0.56
1:A:394:SER:OG	1:A:397:GLU:HB2	2.06	0.56
1:C:302:ILE:CD1	1:C:347:LEU:CB	2.63	0.56
1:D:310:LEU:HD12	1:D:320:MET:HB3	1.88	0.56
1:E:5:LEU:HD11	1:E:37:ALA:HB2	1.88	0.56
1:E:273:ILE:O	1:E:273:ILE:CD1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:LEU:HD13	1:E:297:PHE:HD2	1.71	0.56
1:A:290:HIS:CD2	1:A:292:ASP:HB2	2.41	0.56
1:C:27:ASP:C	1:C:27:ASP:OD1	2.46	0.56
1:D:328:ARG:HA	1:D:328:ARG:NE	2.17	0.56
1:H:86:GLU:HG3	1:H:86:GLU:O	2.06	0.56
1:H:379:GLN:NE2	1:H:404:ASN:OD1	2.39	0.56
1:A:404:ASN:C	1:A:405:THR:HG23	2.31	0.55
1:A:481:ILE:CG1	1:A:482:ALA:N	2.54	0.55
1:C:315:ASP:C	1:C:317:GLU:H	2.13	0.55
1:E:108:CYS:HB3	1:E:156:SER:HB2	1.88	0.55
1:G:175:GLU:CG	1:G:203:GLY:O	2.54	0.55
1:G:327:LEU:HD23	1:G:331:ARG:HD2	1.85	0.55
1:H:335:TYR:O	1:H:338:ILE:HG22	2.06	0.55
1:A:23:VAL:HG12	1:A:24:SER:O	2.07	0.55
1:A:310:LEU:HD22	1:A:353:PRO:HG3	1.87	0.55
1:C:432:MET:CE	1:C:447:PHE:CE1	2.88	0.55
1:D:377:VAL:O	1:D:377:VAL:HG13	2.06	0.55
1:F:177:THR:N	1:F:178:PRO:CD	2.70	0.55
1:G:177:THR:N	1:G:178:PRO:HD3	2.20	0.55
1:G:356:LYS:C	1:G:358:LEU:H	2.14	0.55
1:H:221:ILE:HD12	1:H:233:ILE:HG23	1.89	0.55
1:A:167:ASN:ND2	1:A:167:ASN:H	2.01	0.55
1:C:27:ASP:OD1	1:C:28:GLY:N	2.40	0.55
1:C:174:SER:C	1:C:176:ILE:H	2.14	0.55
1:F:336:ILE:O	1:F:340:ILE:CG1	2.50	0.55
1:G:290:HIS:CD2	1:G:292:ASP:H	2.24	0.55
1:A:445:SER:CB	1:C:132:ASN:HD21	2.19	0.55
1:G:20:ILE:HD12	1:G:36:ALA:HB2	1.87	0.55
1:A:152:LEU:HD12	1:A:184:ILE:CD1	2.35	0.55
1:A:342:GLN:CD	1:A:375:ASP:OD1	2.50	0.55
1:B:235:GLU:CG	1:F:238:LYS:HD2	2.36	0.55
1:D:273:ILE:CD1	1:D:273:ILE:C	2.79	0.55
1:G:394:SER:OG	1:G:397:GLU:HB2	2.05	0.55
1:G:458:GLU:O	1:G:459:MET:HG2	2.06	0.55
1:H:253:ALA:HB2	1:H:286:ARG:NH2	2.21	0.55
1:C:1:MET:HE1	1:C:31:ILE:CG2	2.37	0.55
1:E:312:ASP:O	1:E:314:MET:N	2.40	0.55
1:F:181:THR:C	1:F:184:ILE:HG22	2.24	0.55
1:F:338:ILE:HD13	1:F:376:ARG:CD	2.35	0.55
1:B:337:ASP:O	1:B:341:GLU:CG	2.52	0.55
1:F:53:PHE:HB3	1:F:54:PRO:HD3	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:ILE:CG2	1:F:387:VAL:HG21	2.32	0.55
1:G:469:GLU:OE1	1:G:471:ARG:NE	2.33	0.55
2:A:515:HOH:O	1:B:374:GLN:N	2.39	0.55
1:E:23:VAL:CG1	1:E:24:SER:N	2.70	0.55
1:G:413:LEU:HD11	1:G:435:ILE:HG12	1.88	0.55
1:H:370:GLU:OE1	1:H:391:ARG:NH1	2.40	0.55
1:A:177:THR:N	1:A:178:PRO:HD3	2.22	0.55
1:A:438:TYR:HD2	1:A:439:LYS:HG3	1.72	0.55
1:B:100:LEU:C	1:B:104:ARG:HG3	2.27	0.55
1:C:323:LEU:CD1	1:C:332:VAL:HG21	2.37	0.55
1:G:151:PRO:HB3	1:G:177:THR:HG1	1.72	0.55
1:G:376:ARG:HD2	1:G:376:ARG:N	2.22	0.55
1:H:242:LYS:HG2	2:H:506:HOH:O	2.07	0.55
1:B:479:ALA:CA	1:B:480:LYS:CB	2.72	0.55
1:D:21:ASP:OD1	1:D:33:ARG:CD	2.55	0.55
1:D:485:PHE:HE2	1:G:308:ILE:CD1	2.20	0.55
1:F:231:ARG:O	1:F:235:GLU:HG3	2.07	0.55
1:H:357:ALA:C	1:H:358:LEU:HD13	2.32	0.55
1:A:328:ARG:NH1	1:A:331:ARG:HD3	2.22	0.54
1:D:305:ALA:HA	1:D:308:ILE:HD12	1.90	0.54
1:D:314:MET:O	1:D:316:PRO:HD3	2.07	0.54
1:E:374:GLN:NE2	1:E:374:GLN:H	2.03	0.54
1:F:235:GLU:O	1:F:238:LYS:CD	2.54	0.54
1:G:37:ALA:HB2	1:G:201:VAL:HG22	1.84	0.54
1:G:289:LEU:HD12	1:G:390:VAL:O	2.07	0.54
1:H:49:ALA:CA	1:H:168:THR:CG2	2.80	0.54
1:H:86:GLU:OE2	1:H:180:SER:OG	2.18	0.54
1:D:151:PRO:O	2:D:507:HOH:O	2.18	0.54
1:F:15:VAL:CG1	1:F:16:ALA:N	2.70	0.54
1:F:15:VAL:HG13	1:F:16:ALA:N	2.20	0.54
1:G:97:SER:HA	1:G:101:ASP:CB	2.30	0.54
1:H:376:ARG:HD2	1:H:380:GLU:OE2	2.07	0.54
1:A:215:HIS:HD2	1:A:217:ASP:H	1.54	0.54
1:C:147:PRO:HD3	1:C:224:THR:HB	1.88	0.54
1:E:42:VAL:HG22	1:E:201:VAL:HG11	1.89	0.54
1:E:66:ARG:HG2	2:E:511:HOH:O	2.07	0.54
1:F:447:PHE:C	1:F:447:PHE:CD2	2.85	0.54
1:A:320:MET:HE1	1:A:385:PRO:CB	2.37	0.54
1:A:477:VAL:CG2	1:A:478:ASP:HB2	2.36	0.54
1:E:19:THR:HG21	1:E:33:ARG:HD3	1.89	0.54
1:E:95:ARG:NH2	1:H:484:HIS:O	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:185:VAL:HA	1:E:188:MET:HG3	1.87	0.54
1:G:15:VAL:HG11	1:G:40:ALA:CB	2.35	0.54
2:A:515:HOH:O	1:B:373:PRO:HD2	2.06	0.54
1:B:320:MET:HE3	1:B:385:PRO:HG3	1.89	0.54
1:D:417:ASN:ND2	1:D:420:ARG:H	2.06	0.54
1:F:258:GLU:CG	1:F:290:HIS:CE1	2.91	0.54
1:F:377:VAL:HG13	1:F:386:PHE:HE1	1.72	0.54
1:G:22:VAL:CG2	1:G:34:ILE:HG21	2.32	0.54
1:G:326:ALA:N	1:G:362:PHE:CD2	2.75	0.54
1:H:290:HIS:CD2	1:H:292:ASP:H	2.26	0.54
1:H:326:ALA:O	1:H:330:ASP:CG	2.50	0.54
1:B:305:ALA:HA	1:B:308:ILE:HD12	1.90	0.54
1:B:334:SER:O	1:B:337:ASP:HB2	2.08	0.54
1:D:25:PRO:HB2	1:D:322:PRO:HG2	1.88	0.54
1:D:168:THR:HG22	1:D:197:VAL:HA	1.90	0.54
1:E:256:VAL:HG12	1:E:293:ILE:HD13	1.89	0.54
1:G:340:ILE:O	1:G:343:GLY:N	2.36	0.54
1:A:147:PRO:HG3	1:A:224:THR:HG22	1.90	0.54
1:D:426:ASN:CG	1:G:137:LYS:HZ3	2.10	0.54
1:D:469:GLU:CD	1:G:450:VAL:HG22	2.33	0.54
1:G:220:LYS:HD3	1:G:243:ARG:HB2	1.90	0.54
1:A:415:THR:CG2	1:A:420:ARG:HH11	2.21	0.54
1:A:475:VAL:HG12	1:A:475:VAL:O	2.08	0.54
1:B:345:LYS:HD3	1:B:345:LYS:N	2.19	0.54
1:B:376:ARG:HH11	1:B:380:GLU:CD	2.15	0.54
1:C:152:LEU:CD1	1:C:184:ILE:HD11	2.38	0.54
1:C:394:SER:O	1:C:395:ASP:C	2.49	0.54
1:F:22:VAL:HG23	1:F:34:ILE:HG23	1.88	0.54
1:G:147:PRO:CG	1:G:224:THR:HG22	2.38	0.54
1:G:157:TRP:CE2	1:G:459:MET:HE1	2.43	0.54
1:G:363:TYR:CD2	2:G:519:HOH:O	2.51	0.54
1:H:42:VAL:HB	1:H:212:LEU:HD13	1.90	0.54
1:C:336:ILE:HG21	1:C:350:GLY:O	2.08	0.54
1:C:417:ASN:HD22	1:C:420:ARG:HB2	1.72	0.54
1:E:291:LYS:HE2	1:E:393:SER:CB	2.25	0.54
1:G:19:THR:HA	1:G:34:ILE:O	2.08	0.54
1:G:151:PRO:O	1:G:155:THR:HG23	2.08	0.54
1:A:434:TRP:CD1	1:A:440:ARG:HB2	2.42	0.54
1:A:475:VAL:CG1	1:A:477:VAL:HG12	2.37	0.54
1:B:112:PHE:CZ	1:B:161:PRO:HG3	2.43	0.54
1:B:358:LEU:N	1:B:358:LEU:HD13	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:ARG:NH1	1:C:186:GLU:OE1	2.41	0.54
1:C:320:MET:CE	1:C:385:PRO:HG3	2.38	0.54
1:D:258:GLU:HG2	1:D:290:HIS:CD2	2.43	0.54
1:F:142:VAL:HG22	1:F:220:LYS:HB3	1.90	0.54
1:F:159:MET:HE2	1:F:171:ILE:HD13	1.89	0.54
1:F:172:LYS:O	1:F:172:LYS:CG	2.55	0.54
1:F:412:GLY:HA3	1:F:438:TYR:CE1	2.43	0.54
1:A:93:PRO:O	1:A:96:ASP:N	2.36	0.53
1:A:215:HIS:O	1:A:242:LYS:NZ	2.40	0.53
1:B:334:SER:O	1:B:338:ILE:HG23	2.07	0.53
1:F:372:LYS:O	1:F:378:CYS:SG	2.63	0.53
1:A:18:GLY:O	1:A:36:ALA:N	2.36	0.53
1:B:316:PRO:HG2	1:G:190:GLU:HG2	1.90	0.53
1:B:402:ALA:C	1:B:404:ASN:H	2.15	0.53
1:B:415:THR:CG2	1:B:420:ARG:HH11	2.21	0.53
1:C:27:ASP:O	1:C:360:ASN:HB3	2.08	0.53
1:E:239:SER:C	1:H:231:ARG:HH21	2.08	0.53
1:E:415:THR:CG2	1:E:420:ARG:HH11	2.21	0.53
1:F:70:LYS:HB3	1:F:191:VAL:HG13	1.90	0.53
1:F:76:GLU:CD	1:F:110:ARG:HH12	2.16	0.53
1:F:172:LYS:O	1:F:172:LYS:HG2	2.08	0.53
1:F:257:PHE:HB2	1:F:415:THR:CG2	2.33	0.53
1:H:273:ILE:CD1	1:H:285:SER:HA	2.27	0.53
1:D:412:GLY:HA2	1:D:434:TRP:O	2.08	0.53
1:D:415:THR:HB	1:D:417:ASN:H	1.74	0.53
1:E:241:LEU:HD11	1:H:227:THR:HG23	1.89	0.53
1:E:338:ILE:HD11	1:E:376:ARG:HB2	1.89	0.53
1:F:258:GLU:HG3	1:F:290:HIS:CD2	2.42	0.53
1:F:330:ASP:CG	2:F:510:HOH:O	2.51	0.53
1:G:327:LEU:HD22	1:G:331:ARG:HD3	1.89	0.53
1:G:357:ALA:CB	1:G:358:LEU:HD12	2.38	0.53
1:B:81:GLU:CG	2:B:518:HOH:O	2.56	0.53
1:C:432:MET:CE	1:C:447:PHE:HD1	2.10	0.53
1:D:259:ASP:O	1:D:416:GLN:HG3	2.07	0.53
1:E:312:ASP:C	1:E:312:ASP:OD1	2.51	0.53
1:F:20:ILE:HD13	1:F:175:GLU:HB3	1.91	0.53
1:F:335:TYR:CD1	1:F:382:VAL:HG13	2.44	0.53
1:G:152:LEU:CD1	1:G:184:ILE:CD1	2.86	0.53
1:G:357:ALA:CB	1:G:358:LEU:CD1	2.86	0.53
1:H:210:GLN:O	1:H:214:GLU:CG	2.56	0.53
1:H:233:ILE:O	1:H:233:ILE:HG22	2.07	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:MET:HE2	1:A:198:VAL:CG1	2.25	0.53
1:B:235:GLU:O	1:B:238:LYS:HG2	2.09	0.53
1:B:273:ILE:HG21	1:B:387:VAL:HG21	1.89	0.53
1:B:338:ILE:HA	1:B:341:GLU:HG3	1.90	0.53
1:F:258:GLU:CD	1:F:258:GLU:H	2.16	0.53
1:H:102:VAL:CG2	1:H:152:LEU:CD2	2.84	0.53
1:H:288:ILE:HG22	1:H:392:PHE:HD2	1.73	0.53
1:A:86:GLU:OE1	1:A:151:PRO:HD2	2.09	0.53
1:E:266:VAL:CG2	1:E:297:PHE:CD1	2.91	0.53
1:F:228:ALA:O	1:F:232:ARG:HG3	2.09	0.53
1:G:182:LEU:O	1:G:185:VAL:HG12	2.08	0.53
1:H:108:CYS:CB	1:H:156:SER:HB2	2.31	0.53
1:A:259:ASP:O	1:A:416:GLN:HG2	2.09	0.53
1:A:399:LEU:HD11	1:A:427:ALA:HB1	1.91	0.53
1:D:392:PHE:CE1	1:D:398:ALA:HB2	2.44	0.53
1:E:152:LEU:HD12	1:E:184:ILE:HD13	1.90	0.53
1:E:424:MET:O	1:E:428:ILE:HG13	2.09	0.53
1:F:1:MET:O	1:F:1:MET:HG3	2.09	0.53
1:F:386:PHE:O	1:F:387:VAL:CG2	2.57	0.53
1:G:289:LEU:HD12	1:G:289:LEU:H	1.73	0.53
1:G:310:LEU:HA	1:G:320:MET:O	2.08	0.53
1:H:277:GLN:HG3	1:H:320:MET:CG	2.38	0.53
1:A:474:TRP:HB2	1:C:434:TRP:HA	1.91	0.53
1:D:290:HIS:CD2	1:D:292:ASP:H	2.27	0.53
1:D:328:ARG:CA	1:D:328:ARG:NE	2.67	0.53
1:D:338:ILE:HD11	1:D:376:ARG:CB	2.38	0.53
1:E:262:ILE:CD1	1:E:293:ILE:HB	2.39	0.53
1:F:186:GLU:O	1:F:190:GLU:HG3	2.08	0.53
1:G:179:LEU:N	1:G:179:LEU:HD23	2.24	0.53
1:G:337:ASP:C	1:G:339:ALA:N	2.65	0.53
1:G:358:LEU:N	1:G:358:LEU:HD13	2.23	0.53
1:A:221:ILE:HD13	1:A:233:ILE:CG2	2.23	0.53
1:A:412:GLY:HA2	1:A:434:TRP:O	2.09	0.53
1:B:88:LEU:CA	1:B:314:MET:CE	2.87	0.53
1:C:293:ILE:C	1:C:293:ILE:HD12	2.34	0.53
1:F:256:VAL:HG12	1:F:293:ILE:HD11	1.90	0.53
1:F:277:GLN:HG3	1:F:320:MET:HG2	1.91	0.53
1:A:320:MET:HE1	1:A:385:PRO:CG	2.39	0.53
1:B:310:LEU:CD1	1:B:320:MET:HG2	2.38	0.53
1:C:310:LEU:HD11	2:C:511:HOH:O	2.09	0.53
1:C:399:LEU:HD11	1:C:427:ALA:HB1	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:258:GLU:HG2	1:F:290:HIS:CE1	2.44	0.53
1:F:399:LEU:HD11	1:F:427:ALA:HB1	1.91	0.53
1:G:10:ARG:HH11	1:G:12:VAL:HG12	1.61	0.53
1:G:348:ALA:HB3	1:G:368:VAL:HG23	1.90	0.53
1:A:22:VAL:CG2	1:A:34:ILE:HG22	2.39	0.52
1:A:86:GLU:O	1:A:86:GLU:HG3	2.08	0.52
1:A:147:PRO:CG	1:A:224:THR:HG22	2.40	0.52
1:B:296:GLN:O	1:B:300:ARG:HG3	2.09	0.52
1:C:262:ILE:O	1:C:266:VAL:CG2	2.41	0.52
1:E:228:ALA:HB1	1:E:232:ARG:NH2	2.23	0.52
1:E:298:LEU:HD21	1:E:389:VAL:HG21	1.91	0.52
1:E:469:GLU:OE2	1:H:450:VAL:HG22	2.09	0.52
1:F:22:VAL:HG23	1:F:34:ILE:CG2	2.38	0.52
1:H:339:ALA:O	1:H:344:GLY:N	2.42	0.52
1:A:167:ASN:H	1:A:167:ASN:HD22	1.57	0.52
1:B:153:MET:HE3	1:B:157:TRP:CZ2	2.44	0.52
1:C:155:THR:O	1:C:159:MET:HB2	2.09	0.52
1:F:102:VAL:HB	1:F:103:PRO:HD3	1.90	0.52
1:F:277:GLN:NE2	1:F:321:GLY:H	2.07	0.52
1:G:485:PHE:C	1:G:487:ARG:N	2.68	0.52
1:A:2:GLN:HA	1:A:2:GLN:NE2	2.23	0.52
1:B:235:GLU:CG	1:F:238:LYS:HE3	2.38	0.52
1:E:97:SER:CA	1:E:101:ASP:HB2	2.31	0.52
1:E:289:LEU:HD13	1:E:297:PHE:CD2	2.44	0.52
1:G:274:PHE:HB3	1:G:320:MET:HE1	1.90	0.52
1:H:221:ILE:HG23	1:H:221:ILE:O	2.09	0.52
1:B:214:GLU:HG3	1:B:236:ALA:HB1	1.91	0.52
1:B:477:VAL:CG2	1:B:478:ASP:N	2.72	0.52
1:C:86:GLU:HG3	1:C:86:GLU:O	2.08	0.52
1:D:221:ILE:HG23	1:D:221:ILE:O	2.09	0.52
1:E:93:PRO:CD	1:E:277:GLN:HE22	2.23	0.52
1:E:96:ASP:O	1:E:100:LEU:HB2	2.09	0.52
1:G:20:ILE:HD11	1:G:204:TYR:CZ	2.44	0.52
1:G:434:TRP:HB3	1:G:437:CYS:SG	2.49	0.52
1:G:458:GLU:O	1:G:459:MET:CG	2.57	0.52
1:G:475:VAL:CG1	1:G:477:VAL:HG12	2.37	0.52
1:B:221:ILE:HG23	1:B:221:ILE:O	2.09	0.52
1:D:184:ILE:O	1:D:188:MET:CG	2.57	0.52
1:D:374:GLN:N	1:D:374:GLN:CD	2.68	0.52
1:F:185:VAL:HA	1:F:188:MET:HB2	1.92	0.52
1:G:15:VAL:HG12	1:G:41:ASP:CG	2.34	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:SER:CB	1:G:314:MET:CE	2.87	0.52
1:G:278:GLY:HA3	1:G:384:GLY:C	2.32	0.52
1:A:310:LEU:HD22	1:A:353:PRO:CG	2.39	0.52
1:A:376:ARG:C	1:A:378:CYS:N	2.67	0.52
1:B:92:HIS:CE1	1:B:276:ASN:HD21	2.27	0.52
1:B:470:ALA:HB3	1:F:457:ARG:HE	1.75	0.52
1:C:221:ILE:O	1:C:221:ILE:CG2	2.58	0.52
1:E:25:PRO:HB2	1:E:322:PRO:HG2	1.90	0.52
1:E:412:GLY:HA2	1:E:434:TRP:O	2.09	0.52
1:F:432:MET:HE1	1:F:447:PHE:HD1	1.68	0.52
1:C:151:PRO:CG	1:C:177:THR:HB	2.40	0.52
1:F:322:PRO:HG3	1:F:363:TYR:CZ	2.44	0.52
1:G:373:PRO:HG2	1:G:374:GLN:H	1.75	0.52
1:H:458:GLU:O	1:H:459:MET:HB2	2.09	0.52
1:A:476:ASN:ND2	1:A:480:LYS:HE3	2.24	0.52
1:B:8:ASP:OD1	1:B:195:LYS:HG3	2.09	0.52
1:C:105:THR:OG1	1:C:153:MET:HA	2.09	0.52
1:C:263:GLU:CG	1:C:300:ARG:NH2	2.73	0.52
1:C:432:MET:HE1	1:C:447:PHE:CE1	2.30	0.52
1:D:188:MET:CE	1:D:198:VAL:CB	2.87	0.52
1:D:351:LYS:HG3	1:D:352:ALA:N	2.03	0.52
1:E:86:GLU:OE1	1:E:151:PRO:HD2	2.09	0.52
1:E:478:ASP:CA	2:E:514:HOH:O	2.50	0.52
1:F:26:HIS:O	1:F:361:GLY:N	2.42	0.52
1:F:240:ASN:OD1	1:F:240:ASN:N	2.41	0.52
1:G:95:ARG:HH12	1:G:319:GLU:HG2	1.73	0.52
1:H:124:ILE:N	1:H:124:ILE:CD1	2.73	0.52
1:H:126:VAL:O	1:H:127:ASP:C	2.53	0.52
1:A:377:VAL:CG1	1:A:388:THR:CG2	2.86	0.52
1:A:462:GLU:CD	1:C:136:ARG:NH2	2.65	0.52
1:C:404:ASN:O	1:C:405:THR:CG2	2.57	0.52
1:C:415:THR:HG22	1:C:417:ASN:H	1.74	0.52
1:D:182:LEU:O	1:D:185:VAL:HG12	2.10	0.52
1:H:92:HIS:CD2	1:H:101:ASP:OD2	2.62	0.52
1:B:151:PRO:HG2	1:B:177:THR:HB	1.92	0.52
1:B:315:ASP:O	1:B:317:GLU:N	2.42	0.52
1:C:31:ILE:HD13	1:C:88:LEU:HG	1.90	0.52
1:D:445:SER:HB2	1:G:132:ASN:HD21	1.74	0.52
1:H:399:LEU:HD11	1:H:427:ALA:HB1	1.91	0.52
1:A:89:ASN:C	1:A:89:ASN:HD22	2.15	0.51
1:A:155:THR:HG22	1:A:181:THR:HG23	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ALA:CB	1:G:12:VAL:HG12	2.34	0.51
1:D:223:PHE:CZ	1:D:229:THR:HG23	2.45	0.51
1:E:61:ALA:HB1	1:E:116:ALA:O	2.09	0.51
1:F:11:PHE:C	1:F:12:VAL:HG13	2.35	0.51
1:F:80:GLU:OE2	1:F:80:GLU:HA	2.06	0.51
1:G:19:THR:HG23	1:G:20:ILE:N	2.24	0.51
1:H:90:THR:HG22	1:H:92:HIS:CE1	2.45	0.51
1:H:412:GLY:HA2	1:H:434:TRP:O	2.09	0.51
1:C:152:LEU:HD12	1:C:184:ILE:CD1	2.40	0.51
1:C:411:SER:OG	1:C:432:MET:O	2.28	0.51
1:E:86:GLU:O	1:E:86:GLU:HG3	2.08	0.51
1:G:94:ILE:O	1:G:98:ARG:HG2	2.11	0.51
1:G:173:PRO:CG	1:G:181:THR:HG21	2.39	0.51
1:B:291:LYS:HG3	1:B:392:PHE:O	2.11	0.51
1:B:376:ARG:O	1:B:380:GLU:HB2	2.11	0.51
1:C:53:PHE:HB3	1:C:54:PRO:HD3	1.92	0.51
1:D:148:TRP:CE3	1:D:324:THR:OG1	2.51	0.51
1:G:137:LYS:O	1:G:468:THR:HG22	2.10	0.51
1:G:330:ASP:O	1:G:334:SER:OG	2.28	0.51
1:H:88:LEU:HD13	1:H:314:MET:HE2	1.91	0.51
1:A:267:ASN:ND2	1:C:483:PRO:HG3	2.25	0.51
1:B:223:PHE:CZ	1:B:229:THR:HG23	2.45	0.51
1:F:296:GLN:HE21	1:F:300:ARG:NH1	2.07	0.51
1:G:262:ILE:O	1:G:266:VAL:HG23	2.11	0.51
1:H:323:LEU:HD21	1:H:385:PRO:HD3	1.92	0.51
1:D:240:ASN:O	1:D:241:LEU:HB2	2.09	0.51
1:E:170:VAL:HG11	1:E:212:LEU:HD11	1.92	0.51
1:E:322:PRO:HG3	1:E:363:TYR:CZ	2.46	0.51
1:E:338:ILE:CD1	1:E:376:ARG:HB2	2.41	0.51
1:F:229:THR:HA	1:F:232:ARG:HG3	1.93	0.51
1:A:396:GLU:OE1	1:A:396:GLU:N	2.30	0.51
1:B:344:GLY:O	1:B:345:LYS:HD2	2.11	0.51
1:C:191:VAL:HG13	1:C:191:VAL:O	2.11	0.51
1:D:32:THR:HG23	1:D:33:ARG:N	2.25	0.51
1:E:5:LEU:CD1	1:E:37:ALA:HB2	2.40	0.51
1:F:377:VAL:CG1	1:F:377:VAL:O	2.55	0.51
1:G:89:ASN:OD1	1:G:177:THR:HA	2.11	0.51
1:G:328:ARG:O	1:G:332:VAL:HG23	2.10	0.51
1:A:53:PHE:CE1	1:A:140:GLY:HA2	2.46	0.51
1:B:245:GLN:NE2	1:B:457:ARG:O	2.43	0.51
1:B:259:ASP:OD1	1:B:415:THR:CG2	2.55	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:447:PHE:C	1:C:447:PHE:CD2	2.88	0.51
1:D:26:HIS:ND1	1:D:363:TYR:OH	2.25	0.51
1:E:26:HIS:ND1	1:E:363:TYR:OH	2.25	0.51
1:E:100:LEU:O	1:E:101:ASP:C	2.52	0.51
1:F:329:ARG:HD2	2:F:510:HOH:O	2.09	0.51
1:H:119:ILE:HG12	1:H:464:ILE:HG21	1.92	0.51
1:H:352:ALA:HA	1:H:364:VAL:HA	1.92	0.51
1:A:320:MET:CE	1:A:385:PRO:CG	2.88	0.51
1:C:210:GLN:O	1:C:214:GLU:HG3	2.09	0.51
1:E:455:TYR:HB3	1:H:243:ARG:HD2	1.91	0.51
1:G:102:VAL:HB	1:G:103:PRO:HD3	1.91	0.51
1:B:251:LYS:HG3	1:B:286:ARG:HD3	1.93	0.51
1:B:315:ASP:C	1:B:317:GLU:N	2.67	0.51
1:C:100:LEU:O	1:C:104:ARG:HG3	2.11	0.51
1:C:332:VAL:O	1:C:332:VAL:CG1	2.59	0.51
1:C:376:ARG:NH1	2:C:506:HOH:O	2.40	0.51
1:D:20:ILE:HG13	1:D:36:ALA:HB2	1.92	0.51
1:E:392:PHE:CE1	1:E:398:ALA:HB2	2.45	0.51
1:F:403:ASN:O	1:F:405:THR:N	2.42	0.51
1:G:298:LEU:HD21	1:G:389:VAL:HG21	1.92	0.51
1:H:4:GLN:HG3	1:H:11:PHE:HB3	1.93	0.51
1:A:25:PRO:HA	1:A:362:PHE:CE2	2.45	0.51
1:B:4:GLN:HB3	1:B:12:VAL:O	2.11	0.51
1:B:235:GLU:CD	1:F:238:LYS:HE3	2.36	0.51
1:C:119:ILE:HG12	1:C:464:ILE:HG21	1.91	0.51
1:C:329:ARG:O	1:C:330:ASP:C	2.54	0.51
1:C:354:ASP:OD2	1:C:354:ASP:O	2.29	0.51
1:D:328:ARG:NH1	1:D:383:PHE:HB3	2.11	0.51
1:G:273:ILE:HD12	1:G:283:ALA:HB1	1.93	0.51
1:H:464:ILE:O	1:H:468:THR:CG2	2.43	0.51
1:A:259:ASP:OD1	1:A:415:THR:CG2	2.55	0.50
1:B:74:ARG:HG2	1:B:191:VAL:HG23	1.92	0.50
1:B:87:SER:OG	1:B:92:HIS:O	2.30	0.50
1:B:412:GLY:HA2	1:B:434:TRP:O	2.11	0.50
1:C:92:HIS:HD2	1:C:101:ASP:OD2	1.94	0.50
1:C:323:LEU:HD11	1:C:332:VAL:HG21	1.91	0.50
1:C:327:LEU:CD2	1:C:331:ARG:HH12	2.22	0.50
1:C:460:GLY:HA3	2:C:502:HOH:O	2.11	0.50
1:D:153:MET:CG	1:D:153:MET:O	2.57	0.50
1:D:446:PRO:HD2	1:G:134:VAL:HG21	1.93	0.50
1:D:481:ILE:HD12	1:G:440:ARG:HH12	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:PHE:CE2	1:G:308:ILE:HG12	2.45	0.50
1:E:241:LEU:HD13	1:H:248:LEU:HD12	1.93	0.50
1:A:322:PRO:HG3	1:A:363:TYR:CZ	2.46	0.50
1:B:455:TYR:HB3	1:F:243:ARG:HD2	1.93	0.50
1:C:14:ALA:HB2	1:C:36:ALA:O	2.11	0.50
1:D:25:PRO:HA	1:D:362:PHE:CE2	2.47	0.50
1:D:137:LYS:HZ1	1:G:426:ASN:HD22	1.45	0.50
1:G:210:GLN:O	1:G:214:GLU:HG2	2.12	0.50
1:G:377:VAL:HG21	1:G:386:PHE:CZ	2.47	0.50
1:G:425:ALA:HB2	1:G:435:ILE:HD11	1.93	0.50
1:C:415:THR:HG21	1:C:420:ARG:HD2	1.93	0.50
1:E:20:ILE:HG21	1:E:175:GLU:CB	2.40	0.50
1:E:304:LEU:HD12	1:E:304:LEU:C	2.36	0.50
1:F:53:PHE:CZ	1:F:140:GLY:HA2	2.45	0.50
1:F:249:GLY:HA2	1:F:281:CYS:SG	2.51	0.50
1:G:15:VAL:HG12	1:G:41:ASP:OD1	2.11	0.50
1:H:246:LEU:O	1:H:454:GLY:HA3	2.12	0.50
1:H:415:THR:HG21	1:H:420:ARG:HH11	1.76	0.50
1:C:322:PRO:HG3	1:C:363:TYR:CZ	2.46	0.50
1:F:258:GLU:HG3	1:F:290:HIS:ND1	2.26	0.50
1:F:335:TYR:HE2	1:F:376:ARG:CZ	2.23	0.50
1:G:152:LEU:CD1	1:G:184:ILE:HD11	2.41	0.50
1:G:313:PRO:HG3	1:G:322:PRO:CD	2.41	0.50
1:H:182:LEU:O	1:H:185:VAL:HG12	2.11	0.50
1:B:478:ASP:OD1	1:B:478:ASP:O	2.30	0.50
1:E:240:ASN:O	1:H:452:GLN:HG2	2.11	0.50
1:F:205:GLY:O	1:F:210:GLN:OE1	2.30	0.50
1:B:221:ILE:HD12	1:B:233:ILE:HG23	1.92	0.50
1:B:408:GLY:O	1:B:430:ALA:HA	2.12	0.50
1:B:486:LYS:O	1:B:487:ARG:O	2.30	0.50
1:C:412:GLY:HA2	1:C:434:TRP:O	2.11	0.50
1:C:414:TRP:CE3	1:C:436:ASN:HA	2.47	0.50
1:E:137:LYS:HG3	1:E:471:ARG:HG3	1.92	0.50
1:E:291:LYS:NZ	1:E:393:SER:OG	2.43	0.50
1:F:67:LEU:HB3	1:F:193:PHE:CE1	2.47	0.50
1:G:309:ARG:CZ	1:G:317:GLU:HB3	2.39	0.50
1:G:311:GLY:O	1:G:363:TYR:OH	2.24	0.50
1:A:89:ASN:ND2	1:A:89:ASN:C	2.66	0.50
1:B:238:LYS:CD	1:F:231:ARG:O	2.58	0.50
1:B:351:LYS:O	1:B:365:GLU:HG3	2.11	0.50
1:C:14:ALA:CB	2:C:515:HOH:O	2.58	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:ASN:OD1	1:C:404:ASN:O	2.29	0.50
1:D:92:HIS:HD2	1:D:101:ASP:OD2	1.94	0.50
1:D:119:ILE:HG12	1:D:464:ILE:HG21	1.93	0.50
1:E:14:ALA:O	1:E:15:VAL:C	2.54	0.50
1:E:302:ILE:HD11	1:E:347:LEU:CD1	2.42	0.50
1:E:370:GLU:CD	1:E:391:ARG:NH1	2.70	0.50
1:G:92:HIS:O	1:G:93:PRO:O	2.30	0.50
1:G:157:TRP:CD2	1:G:459:MET:HE2	2.47	0.50
1:A:174:SER:C	1:A:176:ILE:N	2.63	0.50
1:C:27:ASP:OD1	1:C:29:SER:OG	2.30	0.50
1:C:80:GLU:OE1	1:C:84:GLN:OE1	2.30	0.50
1:D:42:VAL:HG13	1:D:212:LEU:HD13	1.94	0.50
1:E:89:ASN:ND2	1:E:89:ASN:O	2.45	0.50
1:F:15:VAL:HG11	1:F:40:ALA:HB3	1.94	0.50
1:F:159:MET:HE2	1:F:171:ILE:HD12	1.93	0.50
1:F:229:THR:O	1:F:233:ILE:HG12	2.11	0.50
1:A:20:ILE:CD1	1:A:175:GLU:HB3	2.41	0.50
1:B:251:LYS:CG	1:B:286:ARG:HD3	2.42	0.50
1:B:335:TYR:C	1:B:338:ILE:HG23	2.36	0.50
1:E:351:LYS:CE	1:E:352:ALA:O	2.51	0.50
1:G:89:ASN:O	1:G:89:ASN:ND2	2.45	0.50
1:G:148:TRP:CA	1:G:177:THR:CG2	2.89	0.50
1:G:344:GLY:N	2:G:515:HOH:O	2.44	0.50
1:H:240:ASN:OD1	1:H:242:LYS:NZ	2.42	0.50
1:H:294:ALA:O	1:H:298:LEU:HG	2.12	0.50
1:B:258:GLU:CG	1:B:290:HIS:CD2	2.91	0.49
1:C:340:ILE:HG22	1:C:341:GLU:H	1.74	0.49
1:D:102:VAL:HB	1:D:103:PRO:HD3	1.94	0.49
1:F:158:LYS:O	1:F:161:PRO:HD2	2.12	0.49
1:H:108:CYS:HB3	1:H:156:SER:CB	2.34	0.49
1:B:259:ASP:CG	1:B:415:THR:HG22	2.37	0.49
1:C:152:LEU:HD11	1:C:184:ILE:HD11	1.94	0.49
1:C:302:ILE:HD11	1:C:347:LEU:CD1	2.42	0.49
1:E:248:LEU:CD1	1:H:241:LEU:HD13	2.36	0.49
1:E:315:ASP:OD2	1:E:317:GLU:HB2	2.11	0.49
1:F:27:ASP:OD1	1:F:29:SER:OG	2.30	0.49
1:F:141:VAL:HG22	1:F:168:THR:OG1	2.11	0.49
1:F:251:LYS:CD	1:F:285:SER:OG	2.60	0.49
1:H:329:ARG:CD	1:H:330:ASP:N	2.75	0.49
1:A:302:ILE:HD13	1:A:347:LEU:HB3	1.95	0.49
1:B:129:GLY:O	1:B:477:VAL:HG13	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:80:GLU:HA	1:D:80:GLU:OE2	2.11	0.49
1:D:329:ARG:HG2	1:D:364:VAL:CG2	2.43	0.49
1:E:149:ASN:HB2	1:E:279:GLN:O	2.12	0.49
1:E:291:LYS:CE	1:E:393:SER:HG	2.15	0.49
1:E:323:LEU:HD13	1:E:328:ARG:HG3	1.95	0.49
1:E:349:GLY:N	2:E:503:HOH:O	1.87	0.49
1:F:76:GLU:O	1:F:79:SER:HB3	2.13	0.49
1:F:413:LEU:C	1:F:413:LEU:HD12	2.37	0.49
1:A:273:ILE:HD11	1:A:386:PHE:O	2.12	0.49
1:A:373:PRO:HG3	1:A:390:VAL:HG11	1.94	0.49
1:A:377:VAL:HG13	1:A:377:VAL:O	2.11	0.49
1:B:2:GLN:CA	1:B:2:GLN:NE2	2.61	0.49
1:B:450:VAL:HG12	1:B:451:GLY:N	2.26	0.49
1:C:18:GLY:N	2:C:515:HOH:O	2.46	0.49
1:C:310:LEU:CD2	1:C:353:PRO:HG3	2.43	0.49
1:C:481:ILE:O	1:C:483:PRO:HD3	2.13	0.49
1:D:18:GLY:HA2	1:E:33:ARG:NH2	2.27	0.49
1:D:289:LEU:O	1:D:391:ARG:HA	2.12	0.49
1:E:373:PRO:HG3	1:E:390:VAL:HG11	1.95	0.49
1:F:42:VAL:O	1:F:46:VAL:HG23	2.12	0.49
1:F:280:ALA:HB3	1:F:283:ALA:HB2	1.94	0.49
1:F:337:ASP:HA	1:F:340:ILE:HG13	1.93	0.49
1:H:323:LEU:O	1:H:362:PHE:HD2	1.95	0.49
1:B:373:PRO:HG3	1:B:390:VAL:HG11	1.94	0.49
1:D:56:TRP:CE2	1:D:64:ARG:HD3	2.48	0.49
1:D:315:ASP:O	1:D:318:THR:HB	2.12	0.49
1:E:146:VAL:HG22	1:E:173:PRO:HA	1.95	0.49
1:F:37:ALA:HB1	1:F:201:VAL:HG13	1.91	0.49
1:F:458:GLU:CG	2:F:506:HOH:O	2.60	0.49
1:B:315:ASP:C	1:B:317:GLU:H	2.19	0.49
1:D:89:ASN:O	1:D:89:ASN:ND2	2.45	0.49
1:D:150:PHE:O	1:D:151:PRO:C	2.55	0.49
1:D:241:LEU:HD22	1:G:248:LEU:CD1	2.42	0.49
1:E:23:VAL:HG12	1:E:24:SER:N	2.27	0.49
1:E:447:PHE:HD2	1:E:447:PHE:O	1.95	0.49
1:G:100:LEU:O	1:G:104:ARG:CG	2.54	0.49
1:H:145:ILE:HG23	1:H:172:LYS:HE3	1.94	0.49
1:B:429[A]:HIS:CE1	1:B:450:VAL:CG1	2.96	0.49
1:C:1:MET:O	1:C:1:MET:HG2	2.06	0.49
1:C:59:LEU:O	1:C:59:LEU:HG	2.12	0.49
1:F:23:VAL:O	1:F:31:ILE:HD11	2.11	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:313:PRO:HG3	1:F:322:PRO:HD3	1.93	0.49
1:F:328:ARG:O	1:F:329:ARG:C	2.55	0.49
1:A:53:PHE:HB3	1:A:54:PRO:HD3	1.94	0.49
1:G:412:GLY:HA2	1:G:434:TRP:O	2.13	0.49
1:H:261:ASN:OD1	1:H:261:ASN:O	2.30	0.49
1:A:114:GLY:O	1:A:118:LYS:HG3	2.11	0.49
1:A:478:ASP:O	1:A:478:ASP:OD1	2.30	0.49
1:B:343:GLY:O	1:B:345:LYS:HD3	2.12	0.49
1:B:357:ALA:HB2	1:G:12:VAL:CG1	2.36	0.49
1:C:277:GLN:HE21	1:C:320:MET:HG3	1.76	0.49
1:D:220:LYS:HA	1:D:243:ARG:O	2.13	0.49
1:F:370:GLU:HG3	2:F:517:HOH:O	2.13	0.49
1:G:347:LEU:CD1	1:G:370:GLU:HG3	2.18	0.49
1:H:117:ASP:OD1	1:H:117:ASP:N	2.44	0.49
1:C:372:LYS:C	1:C:374:GLN:N	2.65	0.49
1:D:373:PRO:HG3	1:D:390:VAL:HG11	1.94	0.49
1:F:10:ARG:HD3	1:F:11:PHE:O	2.12	0.49
1:H:273:ILE:HD11	1:H:386:PHE:O	2.12	0.49
1:H:458:GLU:O	1:H:459:MET:CB	2.61	0.49
1:A:14:ALA:O	1:A:15:VAL:C	2.55	0.48
1:A:351:LYS:O	1:A:365:GLU:HG3	2.13	0.48
1:C:333:LEU:HD23	1:C:336:ILE:HD12	1.94	0.48
1:C:372:LYS:O	1:C:374:GLN:N	2.46	0.48
1:D:138:PRO:HG3	1:D:165:ALA:O	2.12	0.48
1:E:350:GLY:N	1:E:367:THR:HG23	2.28	0.48
1:F:163:LEU:CD1	1:F:188:MET:HE2	2.43	0.48
1:F:376:ARG:C	1:F:378:CYS:H	2.20	0.48
1:F:392:PHE:CD1	1:F:392:PHE:C	2.91	0.48
1:G:87:SER:OG	1:G:97:SER:OG	2.31	0.48
1:A:210:GLN:NE2	1:A:214:GLU:OE2	2.46	0.48
1:C:221:ILE:HG22	1:C:244:ILE:HG23	1.95	0.48
1:E:235:GLU:O	1:E:238:LYS:CE	2.60	0.48
1:H:114:GLY:O	1:H:118:LYS:HG3	2.13	0.48
1:H:155:THR:HG22	1:H:159:MET:HE3	1.94	0.48
1:B:329:ARG:C	1:B:329:ARG:CD	2.82	0.48
1:B:418:LEU:O	1:B:419:ALA:C	2.56	0.48
1:C:74:ARG:NH2	2:C:516:HOH:O	2.47	0.48
1:C:370:GLU:OE1	1:C:391:ARG:NH1	2.47	0.48
1:D:149:ASN:HB2	1:D:279:GLN:O	2.13	0.48
1:E:84:GLN:HG3	1:E:94:ILE:HD11	1.95	0.48
1:F:227:THR:HG21	1:F:231:ARG:NH1	2.22	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:112:PHE:HA	1:H:115:MET:HB3	1.95	0.48
1:H:379:GLN:NE2	1:H:404:ASN:O	2.46	0.48
1:A:137:LYS:HG3	1:A:471:ARG:HG3	1.95	0.48
1:B:223:PHE:HZ	1:B:229:THR:HG23	1.79	0.48
1:B:248:LEU:CD1	1:F:241:LEU:HD13	2.44	0.48
1:B:355:ASP:O	1:B:357:ALA:N	2.47	0.48
1:B:404:ASN:O	1:B:404:ASN:OD1	2.30	0.48
1:D:155:THR:O	1:D:159:MET:HG3	2.14	0.48
1:D:328:ARG:NH1	1:D:383:PHE:CB	2.73	0.48
1:E:350:GLY:O	1:E:351:LYS:HB3	2.13	0.48
1:E:414:TRP:CE3	1:E:436:ASN:HA	2.49	0.48
1:G:157:TRP:NE1	1:G:459:MET:HE1	2.28	0.48
1:G:195:LYS:HG2	1:G:195:LYS:O	2.14	0.48
1:H:2:GLN:HG3	1:H:11:PHE:CZ	2.49	0.48
1:H:195:LYS:O	2:H:510:HOH:O	2.19	0.48
1:A:105:THR:OG1	1:A:153:MET:HA	2.12	0.48
1:B:243:ARG:HD2	1:F:455:TYR:CB	2.43	0.48
1:D:309:ARG:NH1	1:D:309:ARG:CG	2.45	0.48
1:E:150:PHE:O	1:E:151:PRO:C	2.55	0.48
1:E:370:GLU:CD	1:E:391:ARG:HH11	2.22	0.48
1:E:434:TRP:CD1	1:E:440:ARG:HB2	2.49	0.48
1:F:27:ASP:O	1:F:360:ASN:HB3	2.13	0.48
1:F:38:GLU:CB	1:F:207:THR:CG2	2.92	0.48
1:F:150:PHE:N	1:F:151:PRO:HD3	2.28	0.48
1:G:159:MET:O	1:G:160:GLY:C	2.56	0.48
1:A:251:LYS:HG3	1:A:286:ARG:CD	2.43	0.48
1:A:445:SER:HB2	1:C:132:ASN:ND2	2.29	0.48
1:B:289:LEU:O	1:B:391:ARG:HA	2.14	0.48
1:B:405:THR:CG2	1:B:407:TYR:HD1	2.26	0.48
1:C:80:GLU:OE1	1:C:84:GLN:CD	2.57	0.48
1:C:83:ALA:HA	1:C:97:SER:HB3	1.96	0.48
1:D:376:ARG:HD3	1:E:376:ARG:HD3	1.95	0.48
1:G:399:LEU:HD11	1:G:427:ALA:HB1	1.96	0.48
1:H:342:GLN:HE22	1:H:376:ARG:H	1.60	0.48
1:B:229:THR:O	1:B:232:ARG:HB2	2.14	0.48
1:B:414:TRP:CE3	1:B:436:ASN:HA	2.49	0.48
1:C:87:SER:OG	1:C:97:SER:OG	2.31	0.48
1:C:315:ASP:OD1	1:C:317:GLU:HB2	2.13	0.48
1:D:302:ILE:HG23	1:D:348:ALA:HB2	1.96	0.48
1:D:394:SER:O	1:D:395:ASP:C	2.56	0.48
1:E:338:ILE:HD11	1:E:376:ARG:CB	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:ILE:HG23	1:F:45:ALA:HA	1.94	0.48
1:F:89:ASN:ND2	1:F:89:ASN:C	2.68	0.48
1:G:74:ARG:O	1:G:75:ILE:C	2.56	0.48
1:G:333:LEU:O	1:G:334:SER:C	2.56	0.48
1:A:150:PHE:O	1:A:151:PRO:C	2.55	0.48
1:A:418:LEU:O	1:A:419:ALA:C	2.56	0.48
1:G:293:ILE:HD13	1:G:297:PHE:HB2	1.96	0.48
1:G:310:LEU:HD13	1:G:366:PRO:HD3	1.96	0.48
1:H:195:LYS:HA	2:H:504:HOH:O	2.13	0.48
1:H:414:TRP:CE3	1:H:436:ASN:HA	2.49	0.48
1:A:414:TRP:CE3	1:A:436:ASN:HA	2.49	0.48
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.57	0.48
1:B:143:ALA:HB1	1:B:212:LEU:HG	1.96	0.48
1:C:376:ARG:C	1:C:378:CYS:H	2.21	0.48
1:D:34:ILE:HD13	1:D:178:PRO:HG3	1.95	0.48
1:E:153:MET:CG	2:E:510:HOH:O	2.54	0.48
1:F:337:ASP:O	1:F:341:GLU:HG2	2.14	0.48
1:G:215:HIS:O	1:G:242:LYS:NZ	2.47	0.48
1:H:10:ARG:HH22	1:H:195:LYS:HE3	1.79	0.48
1:H:99:GLY:O	1:H:100:LEU:HD22	2.13	0.48
1:B:174:SER:C	1:B:176:ILE:H	2.21	0.48
1:B:263:GLU:HG3	1:B:300:ARG:HH22	1.78	0.48
1:C:117:ASP:OD1	2:C:519:HOH:O	2.20	0.48
1:F:163:LEU:HD11	1:F:188:MET:HE2	1.96	0.48
1:F:412:GLY:HA2	1:F:434:TRP:O	2.14	0.48
1:F:414:TRP:CE3	1:F:436:ASN:HA	2.49	0.48
1:H:42:VAL:HG21	1:H:211:ALA:HB1	1.95	0.48
1:H:93:PRO:O	1:H:96:ASP:HB2	2.14	0.48
1:A:15:VAL:CG1	1:A:16:ALA:N	2.76	0.47
1:B:262:ILE:HD11	1:B:293:ILE:HB	1.96	0.47
1:B:452:GLN:HG2	1:F:241:LEU:HD12	1.95	0.47
1:C:289:LEU:HD12	1:C:389:VAL:CG1	2.44	0.47
1:C:338:ILE:O	1:C:342:GLN:HG3	2.14	0.47
1:F:109:PHE:CZ	1:F:156:SER:HA	2.49	0.47
1:F:185:VAL:O	1:F:188:MET:HB2	2.14	0.47
1:H:251:LYS:CB	1:H:407:TYR:CD1	2.97	0.47
1:H:330:ASP:O	1:H:334:SER:OG	2.29	0.47
1:C:411:SER:O	1:C:434:TRP:CE3	2.67	0.47
1:E:230:GLY:O	1:E:233:ILE:HB	2.13	0.47
1:G:245:GLN:HG3	1:G:456:GLY:HA3	1.96	0.47
1:A:273:ILE:HG12	1:A:387:VAL:HG22	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:LYS:HG2	1:A:352:ALA:H	1.78	0.47
1:B:273:ILE:HG21	1:B:387:VAL:HG22	1.96	0.47
1:D:223:PHE:HZ	1:D:229:THR:HG23	1.79	0.47
1:E:19:THR:HG23	1:E:33:ARG:HB3	1.96	0.47
1:E:127:ASP:HB2	1:E:130:PHE:CD1	2.50	0.47
1:E:235:GLU:O	1:E:238:LYS:HE2	2.14	0.47
1:F:94:ILE:CD1	1:F:98:ARG:CZ	2.91	0.47
1:F:309:ARG:HG3	1:F:319:GLU:HG3	1.95	0.47
1:F:377:VAL:CG1	1:F:386:PHE:HE1	2.26	0.47
1:F:381:GLU:O	1:F:381:GLU:HG2	2.13	0.47
1:G:76:GLU:O	1:G:79:SER:CB	2.59	0.47
1:H:42:VAL:O	1:H:46:VAL:HG23	2.14	0.47
1:H:377:VAL:HG22	1:H:377:VAL:O	2.14	0.47
1:A:155:THR:CG2	1:A:181:THR:HG23	2.44	0.47
1:A:248:LEU:HD11	1:C:241:LEU:HD22	1.96	0.47
1:B:465:HIS:CE1	1:F:465:HIS:CE1	3.03	0.47
1:C:223:PHE:CZ	1:C:229:THR:HG22	2.50	0.47
1:C:237:SER:O	1:C:238:LYS:C	2.55	0.47
1:C:323:LEU:HD21	1:C:385:PRO:HD3	1.96	0.47
1:D:41:ASP:HA	1:D:44:LEU:HD12	1.96	0.47
1:D:93:PRO:O	1:D:96:ASP:CB	2.51	0.47
1:D:276:ASN:O	1:D:277:GLN:HB2	2.14	0.47
1:F:159:MET:HG2	1:F:169:ILE:HD13	1.94	0.47
1:F:374:GLN:H	1:F:374:GLN:HG3	1.49	0.47
1:G:277:GLN:CG	1:G:321:GLY:O	2.60	0.47
1:H:408:GLY:O	1:H:430:ALA:CA	2.57	0.47
1:B:231:ARG:HB3	1:F:238:LYS:HB2	1.96	0.47
1:B:316:PRO:HG2	1:G:190:GLU:CG	2.44	0.47
1:B:429[A]:HIS:NE2	1:B:450:VAL:CG1	2.77	0.47
1:E:259:ASP:CG	1:E:415:THR:HG22	2.37	0.47
1:G:25:PRO:O	1:G:361:GLY:CA	2.62	0.47
1:G:95:ARG:HH11	1:G:319:GLU:HA	1.79	0.47
1:G:151:PRO:CB	1:G:177:THR:HG1	2.25	0.47
1:G:340:ILE:O	1:G:341:GLU:C	2.56	0.47
1:G:459:MET:H	1:G:463:ALA:HB2	1.79	0.47
1:A:19:THR:HG23	1:A:20:ILE:N	2.29	0.47
1:B:25:PRO:HA	1:B:362:PHE:CE2	2.48	0.47
1:B:115:MET:O	1:B:115:MET:HG3	2.12	0.47
1:E:248:LEU:CD1	1:H:241:LEU:CD2	2.92	0.47
1:F:208:ALA:O	1:F:212:LEU:HB2	2.15	0.47
1:H:418:LEU:O	1:H:419:ALA:C	2.56	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:GLU:O	1:A:42:VAL:CG1	2.60	0.47
1:A:191:VAL:O	1:A:191:VAL:HG13	2.14	0.47
1:A:439:LYS:HB3	1:A:439:LYS:HE3	1.58	0.47
1:B:92:HIS:NE2	1:B:149:ASN:O	2.47	0.47
1:B:238:LYS:HE2	1:F:235:GLU:CG	2.15	0.47
1:C:320:MET:HE1	1:C:385:PRO:HG3	1.97	0.47
1:C:374:GLN:O	1:C:375:ASP:C	2.58	0.47
1:D:109:PHE:CZ	1:D:156:SER:HA	2.50	0.47
1:D:408:GLY:O	1:D:430:ALA:HA	2.15	0.47
1:D:443:PRO:HA	1:D:459:MET:SD	2.54	0.47
1:E:40:ALA:O	1:E:43:ASP:HB2	2.15	0.47
1:E:114:GLY:O	1:E:118:LYS:NZ	2.30	0.47
1:E:157:TRP:HZ2	1:E:441:VAL:HG11	1.77	0.47
1:F:335:TYR:CD2	1:F:376:ARG:CZ	2.98	0.47
1:G:84:GLN:HA	1:G:94:ILE:HD11	1.95	0.47
1:G:104:ARG:NH2	1:G:153:MET:HE1	2.29	0.47
1:G:206:HIS:O	2:G:517:HOH:O	2.20	0.47
1:G:403:ASN:HD21	1:G:428:ILE:HA	1.79	0.47
1:H:94:ILE:C	1:H:96:ASP:H	2.23	0.47
1:H:160:GLY:N	1:H:161:PRO:HD2	2.29	0.47
1:H:289:LEU:O	1:H:391:ARG:HA	2.14	0.47
1:A:90:THR:O	1:A:324:THR:HB	2.15	0.47
1:B:455:TYR:CB	1:F:243:ARG:HD2	2.44	0.47
1:C:149:ASN:OD1	1:C:149:ASN:N	2.39	0.47
1:E:185:VAL:HG23	1:E:188:MET:HE3	1.96	0.47
1:E:328:ARG:O	1:E:332:VAL:HG23	2.14	0.47
1:F:149:ASN:ND2	1:F:150:PHE:HD1	2.11	0.47
1:F:310:LEU:HD22	1:F:353:PRO:HG3	1.97	0.47
1:G:108:CYS:HB3	1:G:156:SER:CB	2.44	0.47
1:H:327:LEU:HD23	1:H:327:LEU:HA	1.68	0.47
1:B:351:LYS:HB2	1:B:351:LYS:HE3	1.36	0.47
1:B:374:GLN:O	1:B:375:ASP:C	2.58	0.47
1:D:56:TRP:CH2	1:D:64:ARG:HG2	2.50	0.47
1:D:229:THR:HA	1:D:232:ARG:NH1	2.30	0.47
1:E:11:PHE:HE2	1:E:186:GLU:HG3	1.80	0.47
1:E:418:LEU:O	1:E:419:ALA:C	2.57	0.47
1:A:194:PRO:HD2	1:A:197:VAL:HG21	1.97	0.47
1:A:447:PHE:C	1:A:447:PHE:CD2	2.93	0.47
1:B:241:LEU:HD22	1:F:246:LEU:CD1	2.45	0.47
1:B:248:LEU:CD1	1:F:241:LEU:HD22	2.44	0.47
2:B:502:HOH:O	1:F:241:LEU:O	2.21	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:245:GLN:HG3	1:D:456:GLY:HA3	1.97	0.47
1:D:486:LYS:O	1:D:487:ARG:O	2.33	0.47
1:F:38:GLU:CG	1:F:207:THR:HG21	2.40	0.47
1:F:86:GLU:OE2	1:F:152:LEU:HB2	2.13	0.47
1:F:369:VAL:O	1:F:388:THR:HA	2.14	0.47
1:H:10:ARG:NH2	1:H:195:LYS:HE3	2.31	0.47
1:H:174:SER:OG	1:H:177:THR:OG1	2.33	0.47
1:A:263:GLU:HG3	1:A:300:ARG:NH2	2.30	0.46
1:B:235:GLU:OE2	1:F:238:LYS:HE3	2.15	0.46
1:B:446:PRO:HB3	1:B:457:ARG:HG3	1.97	0.46
1:F:79:SER:HB2	1:F:102:VAL:HG11	1.96	0.46
1:F:90:THR:O	1:F:324:THR:HB	2.15	0.46
1:F:111:TYR:CG	1:F:443:PRO:HB2	2.49	0.46
1:F:222:ALA:HA	1:F:245:GLN:HB2	1.95	0.46
1:G:314:MET:O	1:G:316:PRO:HD3	2.15	0.46
1:H:238:LYS:HE2	1:H:238:LYS:HB2	1.64	0.46
1:H:447:PHE:C	1:H:447:PHE:CD2	2.93	0.46
1:A:109:PHE:CZ	1:A:156:SER:HA	2.50	0.46
1:A:342:GLN:OE1	1:A:375:ASP:OD1	2.33	0.46
1:C:429:HIS:CE1	1:C:450:VAL:HG13	2.51	0.46
1:D:136:ARG:HA	1:D:136:ARG:HD2	1.66	0.46
1:G:148:TRP:HA	1:G:177:THR:HG21	1.97	0.46
1:G:251:LYS:HA	1:G:251:LYS:HD2	1.57	0.46
1:H:227:THR:O	1:H:231:ARG:HG3	2.15	0.46
1:A:22:VAL:HG21	1:A:34:ILE:HG22	1.94	0.46
1:A:270:ALA:HB2	1:A:304:LEU:HD23	1.98	0.46
1:A:289:LEU:O	1:A:391:ARG:HA	2.14	0.46
1:B:415:THR:HG21	1:B:420:ARG:HH11	1.80	0.46
1:C:328:ARG:O	1:C:332:VAL:HG23	2.15	0.46
1:E:214:GLU:O	1:E:215:HIS:C	2.56	0.46
1:F:11:PHE:O	1:F:12:VAL:CG1	2.64	0.46
1:F:256:VAL:HG12	1:F:293:ILE:CD1	2.44	0.46
1:G:380:GLU:CB	2:G:523:HOH:O	2.64	0.46
1:H:137:LYS:HG3	1:H:471:ARG:HG3	1.97	0.46
1:H:233:ILE:O	1:H:233:ILE:CG2	2.63	0.46
1:H:338:ILE:CD1	1:H:338:ILE:C	2.87	0.46
1:A:145:ILE:HG23	1:A:172:LYS:HE3	1.97	0.46
1:A:246:LEU:HD13	1:C:241:LEU:HD22	1.97	0.46
1:B:53:PHE:HA	1:B:168:THR:CG2	2.46	0.46
1:C:338:ILE:HD11	1:C:376:ARG:CB	2.43	0.46
1:C:351:LYS:CG	1:C:352:ALA:H	2.24	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:SER:C	1:C:396:GLU:N	2.72	0.46
1:D:262:ILE:O	1:D:263:GLU:C	2.58	0.46
1:D:320:MET:CE	1:D:366:PRO:HG3	2.46	0.46
1:E:289:LEU:O	1:E:391:ARG:HA	2.16	0.46
1:E:415:THR:HG21	1:E:420:ARG:HH11	1.81	0.46
1:F:23:VAL:CG1	1:F:24:SER:O	2.54	0.46
1:G:94:ILE:HG23	1:G:98:ARG:NE	2.30	0.46
1:G:148:TRP:HA	1:G:177:THR:CG2	2.45	0.46
1:G:289:LEU:O	1:G:391:ARG:HA	2.15	0.46
1:H:231:ARG:O	1:H:235:GLU:HG3	2.15	0.46
1:H:376:ARG:HD3	1:H:376:ARG:HA	1.79	0.46
1:A:287:LEU:HD22	1:A:289:LEU:HD21	1.97	0.46
1:A:486:LYS:O	1:A:487:ARG:HB2	2.14	0.46
1:B:89:ASN:OD1	1:B:177:THR:HA	2.15	0.46
1:F:218:VAL:O	1:F:242:LYS:HE3	2.15	0.46
1:F:356:LYS:HA	1:F:359:ALA:CB	2.42	0.46
1:F:432:MET:HE1	1:F:447:PHE:CG	2.47	0.46
1:H:136:ARG:HG3	1:H:468:THR:CB	2.45	0.46
1:C:19:THR:CG2	1:C:20:ILE:N	2.76	0.46
1:D:205:GLY:C	2:D:517:HOH:O	2.58	0.46
1:D:251:LYS:HB2	1:D:407:TYR:CD1	2.51	0.46
1:E:95:ARG:HD3	1:E:318:THR:O	2.16	0.46
1:F:23:VAL:HG12	1:F:24:SER:C	2.38	0.46
1:F:138:PRO:HG3	1:F:165:ALA:O	2.16	0.46
1:F:390:VAL:HG11	1:F:401:ILE:HD13	1.97	0.46
1:G:337:ASP:O	1:G:339:ALA:N	2.49	0.46
1:H:23:VAL:CG1	1:H:24:SER:N	2.78	0.46
1:H:100:LEU:O	1:H:101:ASP:C	2.58	0.46
1:B:15:VAL:HG12	1:B:41:ASP:OD1	2.16	0.46
1:E:258:GLU:HG3	1:E:290:HIS:CG	2.51	0.46
1:F:61:ALA:O	1:F:116:ALA:HB1	2.16	0.46
1:G:34:ILE:HD12	1:G:202:PRO:HB2	1.98	0.46
1:H:136:ARG:NE	1:H:468:THR:OG1	2.39	0.46
1:H:311:GLY:O	1:H:312:ASP:C	2.59	0.46
1:A:415:THR:HG21	1:A:420:ARG:HH11	1.80	0.46
1:B:251:LYS:HE3	2:B:526:HOH:O	2.16	0.46
1:B:447:PHE:CD2	1:B:447:PHE:C	2.93	0.46
1:B:470:ALA:HB3	1:F:457:ARG:NE	2.30	0.46
1:B:479:ALA:HB2	1:B:480:LYS:HZ3	1.80	0.46
1:D:220:LYS:HE2	1:D:243:ARG:HB2	1.98	0.46
1:D:295:ASP:OD1	1:D:391:ARG:NH2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:289:LEU:CD1	1:E:297:PHE:CD2	2.99	0.46
1:E:335:TYR:HE2	1:E:380:GLU:OE1	1.99	0.46
1:E:480:LYS:HD3	1:E:480:LYS:HA	1.60	0.46
1:G:27:ASP:OD1	1:G:29:SER:HB2	2.16	0.46
1:G:112:PHE:HA	1:G:115:MET:HB3	1.98	0.46
1:G:357:ALA:CA	1:G:358:LEU:CD1	2.91	0.46
1:A:5:LEU:O	1:A:11:PHE:HA	2.15	0.46
1:B:290:HIS:CD2	1:B:292:ASP:HB2	2.51	0.46
1:B:328:ARG:NH1	1:B:331:ARG:CD	2.79	0.46
1:B:417:ASN:HB3	1:B:420:ARG:HB3	1.96	0.46
1:C:151:PRO:HG2	1:C:177:THR:CB	2.45	0.46
1:E:152:LEU:CD1	1:E:184:ILE:HD12	2.40	0.46
1:E:310:LEU:HD12	1:E:320:MET:HB3	1.97	0.46
1:F:34:ILE:CD1	1:F:202:PRO:HB2	2.45	0.46
1:F:94:ILE:HG12	1:F:98:ARG:CZ	2.46	0.46
1:A:31:ILE:HD13	1:A:88:LEU:HG	1.98	0.46
1:A:315:ASP:C	1:A:317:GLU:H	2.23	0.46
1:D:474:TRP:CG	1:G:434:TRP:CD1	3.04	0.46
1:E:85:LEU:HD11	1:E:179:LEU:HB3	1.98	0.46
1:G:295:ASP:C	1:G:297:PHE:N	2.73	0.46
1:G:400:ALA:O	1:G:404:ASN:HB3	2.16	0.46
1:H:376:ARG:C	1:H:378:CYS:N	2.72	0.46
1:A:279:GLN:HE21	1:A:279:GLN:HB2	1.58	0.45
1:C:289:LEU:HD12	1:C:389:VAL:HG13	1.99	0.45
1:C:440:ARG:HA	1:C:440:ARG:HD2	1.42	0.45
1:D:459:MET:N	1:D:463:ALA:HB2	2.32	0.45
1:F:18:GLY:C	1:F:36:ALA:HB3	2.40	0.45
1:F:226:SER:OG	1:F:229:THR:CG2	2.64	0.45
1:F:310:LEU:CD2	1:F:353:PRO:CG	2.94	0.45
1:G:56:TRP:CZ2	1:G:64:ARG:HG2	2.52	0.45
1:G:365:GLU:O	1:G:366:PRO:C	2.57	0.45
1:G:409:LEU:O	1:G:432:MET:CE	2.63	0.45
1:H:276:ASN:O	1:H:277:GLN:HB2	2.15	0.45
1:A:336:ILE:HG21	1:A:350:GLY:O	2.16	0.45
1:A:394:SER:HB2	1:A:396:GLU:OE1	2.16	0.45
1:B:86:GLU:O	1:B:90:THR:OG1	2.29	0.45
1:B:405:THR:CG2	1:B:407:TYR:HB2	2.45	0.45
1:C:145:ILE:HD12	1:C:221:ILE:HD11	1.98	0.45
1:D:188:MET:CE	1:D:198:VAL:HB	2.46	0.45
1:D:312:ASP:OD1	1:D:313:PRO:CD	2.64	0.45
1:F:305:ALA:HA	1:F:308:ILE:HD12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:TYR:OH	1:G:189:THR:HG22	2.13	0.45
1:G:392:PHE:HB2	1:G:397:GLU:HB3	1.97	0.45
1:G:431:GLY:C	1:G:432:MET:HG3	2.40	0.45
1:H:105:THR:OG1	1:H:153:MET:HA	2.16	0.45
1:B:258:GLU:HG3	1:B:290:HIS:CG	2.50	0.45
1:C:352:ALA:C	1:C:353:PRO:O	2.59	0.45
1:D:447:PHE:C	1:D:447:PHE:CD2	2.93	0.45
1:E:153:MET:CA	2:E:510:HOH:O	2.63	0.45
1:E:234:VAL:CG2	1:E:246:LEU:HD11	2.46	0.45
1:G:94:ILE:CD1	1:G:314:MET:HE1	2.46	0.45
1:H:149:ASN:OD1	1:H:149:ASN:N	2.42	0.45
1:H:162:ALA:HB3	1:H:169:ILE:HD11	1.97	0.45
1:H:241:LEU:N	2:H:506:HOH:O	2.48	0.45
1:H:459:MET:N	1:H:463:ALA:HB2	2.31	0.45
1:A:2:GLN:HB3	1:A:11:PHE:CE1	2.51	0.45
1:E:92:HIS:HD2	1:E:101:ASP:OD2	1.99	0.45
1:E:122:SER:O	1:E:134:VAL:N	2.43	0.45
1:B:355:ASP:C	1:B:357:ALA:N	2.72	0.45
1:F:20:ILE:HG21	1:F:175:GLU:HB3	1.98	0.45
1:F:136:ARG:HA	1:F:136:ARG:HD2	1.62	0.45
1:F:239:SER:OG	1:F:240:ASN:OD1	2.35	0.45
1:F:251:LYS:HD3	1:F:285:SER:OG	2.17	0.45
1:G:6:TYR:OH	1:G:9:GLY:HA2	2.16	0.45
1:G:310:LEU:HD23	1:G:353:PRO:HG2	1.98	0.45
1:G:310:LEU:HD23	1:G:353:PRO:HG3	1.85	0.45
1:H:90:THR:HG21	1:H:92:HIS:ND1	2.31	0.45
1:H:94:ILE:C	1:H:96:ASP:N	2.73	0.45
1:A:258:GLU:CD	1:A:258:GLU:H	2.24	0.45
1:B:458:GLU:O	1:B:459:MET:HB2	2.16	0.45
1:E:185:VAL:CA	1:E:188:MET:HE3	2.46	0.45
1:F:415:THR:HG21	1:F:420:ARG:HD3	1.95	0.45
1:G:95:ARG:HD3	1:G:318:THR:O	2.17	0.45
1:A:251:LYS:HG3	1:A:286:ARG:HD3	1.98	0.45
1:A:372:LYS:HD3	1:A:372:LYS:HA	1.79	0.45
1:A:413:LEU:C	1:A:413:LEU:HD12	2.42	0.45
1:B:43:ASP:HA	1:B:215:HIS:HE2	1.81	0.45
1:B:405:THR:CG2	1:B:407:TYR:N	2.44	0.45
1:C:211:ALA:O	1:C:215:HIS:HB2	2.17	0.45
1:E:220:LYS:HA	1:E:243:ARG:O	2.16	0.45
1:F:56:TRP:O	1:F:59:LEU:HB2	2.16	0.45
1:F:70:LYS:HB3	1:F:191:VAL:HG11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:415:THR:HG22	1:F:420:ARG:HH11	1.77	0.45
1:G:19:THR:HG22	1:G:20:ILE:N	2.27	0.45
1:G:147:PRO:HG2	1:G:224:THR:HG22	1.98	0.45
1:H:339:ALA:O	1:H:344:GLY:HA3	2.17	0.45
1:A:49:ALA:HA	1:A:196:GLY:O	2.16	0.45
1:A:184:ILE:HG22	1:A:185:VAL:N	2.31	0.45
1:A:459:MET:N	1:A:463:ALA:HB2	2.32	0.45
1:B:329:ARG:NH1	1:B:329:ARG:CG	2.56	0.45
1:C:25:PRO:HD2	2:C:512:HOH:O	2.16	0.45
1:F:159:MET:O	1:F:163:LEU:HB2	2.17	0.45
1:G:109:PHE:CZ	1:G:156:SER:HA	2.51	0.45
1:H:177:THR:N	1:H:178:PRO:HD3	2.31	0.45
1:H:312:ASP:O	1:H:318:THR:OG1	2.17	0.45
1:H:335:TYR:CD2	1:H:382:VAL:HG22	2.51	0.45
1:A:92:HIS:CD2	1:A:101:ASP:OD2	2.62	0.45
1:A:370:GLU:OE1	1:A:391:ARG:NH1	2.49	0.45
1:B:377:VAL:HG21	1:B:386:PHE:CZ	2.52	0.45
1:E:112:PHE:CZ	1:E:161:PRO:HG3	2.52	0.45
1:F:76:GLU:OE1	1:F:110:ARG:NH1	2.50	0.45
1:G:31:ILE:HD11	1:G:88:LEU:HG	1.98	0.45
1:G:85:LEU:HD12	1:G:85:LEU:C	2.42	0.45
1:G:86:GLU:O	1:G:86:GLU:HG3	2.15	0.45
1:G:205:GLY:O	1:G:210:GLN:N	2.50	0.45
1:G:377:VAL:HG22	1:G:386:PHE:CE1	2.52	0.45
1:H:3:ASN:HB2	1:H:34:ILE:HG22	1.99	0.45
1:H:112:PHE:CE2	1:H:161:PRO:HD3	2.52	0.45
1:H:306:LYS:HE3	1:H:306:LYS:HB3	1.31	0.45
1:A:326:ALA:HB2	1:A:362:PHE:CE1	2.52	0.45
1:B:7:ILE:HG23	1:B:45:ALA:HA	1.99	0.45
1:B:405:THR:HG23	1:B:406:GLU:N	2.31	0.45
1:B:459:MET:N	1:B:463:ALA:HB2	2.31	0.45
1:C:386:PHE:O	1:C:386:PHE:HD1	2.00	0.45
1:C:460:GLY:CA	2:C:502:HOH:O	2.64	0.45
1:C:469:GLU:OE2	2:C:513:HOH:O	2.20	0.45
1:E:49:ALA:HA	1:E:196:GLY:O	2.17	0.45
1:E:248:LEU:HD11	1:H:241:LEU:CD2	2.42	0.45
1:E:277:GLN:HE21	1:E:321:GLY:H	1.61	0.45
1:F:18:GLY:O	1:F:36:ALA:HB3	2.17	0.45
1:F:86:GLU:OE1	1:F:90:THR:HG21	2.16	0.45
1:G:313:PRO:HG3	1:G:322:PRO:HD2	1.98	0.45
1:H:20:ILE:HD13	1:H:175:GLU:CB	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:273:ILE:HG21	1:H:387:VAL:CG2	2.47	0.45
1:A:201:VAL:N	1:A:202:PRO:HD3	2.33	0.44
1:A:424:MET:HE3	1:A:424:MET:HB3	1.75	0.44
1:C:348:ALA:O	1:C:349:GLY:C	2.61	0.44
1:C:417:ASN:HD22	1:C:420:ARG:N	2.10	0.44
1:D:49:ALA:HA	1:D:196:GLY:O	2.18	0.44
1:D:185:VAL:HG23	1:D:188:MET:CE	2.40	0.44
1:E:328:ARG:HE	1:E:328:ARG:HB2	1.54	0.44
1:F:85:LEU:HD11	1:F:179:LEU:HB2	1.98	0.44
1:F:273:ILE:HG12	1:F:386:PHE:O	2.17	0.44
1:G:2:GLN:NE2	1:G:2:GLN:HA	2.33	0.44
1:G:105:THR:OG1	1:G:153:MET:HA	2.17	0.44
1:H:258:GLU:H	1:H:258:GLU:HG3	1.15	0.44
1:H:258:GLU:HG2	1:H:290:HIS:CD2	2.52	0.44
1:A:277:GLN:CD	1:A:277:GLN:N	2.75	0.44
1:B:174:SER:C	1:B:176:ILE:N	2.74	0.44
1:B:279:GLN:HE21	1:B:279:GLN:HB2	1.58	0.44
1:C:124:ILE:HA	1:C:125:PRO:HD3	1.88	0.44
1:C:134:VAL:HA	1:C:472:SER:HA	1.99	0.44
1:C:329:ARG:O	1:C:332:VAL:N	2.50	0.44
1:D:259:ASP:O	1:D:416:GLN:HG2	2.14	0.44
1:D:356:LYS:HA	1:D:359:ALA:CB	2.35	0.44
1:F:105:THR:OG1	1:F:153:MET:HA	2.17	0.44
1:G:195:LYS:O	1:G:195:LYS:CG	2.65	0.44
1:G:338:ILE:HD12	1:G:339:ALA:CA	2.47	0.44
1:H:86:GLU:OE2	1:H:180:SER:CB	2.65	0.44
1:H:92:HIS:O	1:H:93:PRO:C	2.59	0.44
1:A:176:ILE:C	1:A:177:THR:HG23	2.43	0.44
1:B:413:LEU:C	1:B:413:LEU:HD12	2.42	0.44
1:C:418:LEU:O	1:C:419:ALA:C	2.58	0.44
1:D:119:ILE:HD11	1:D:464:ILE:HD12	1.99	0.44
1:D:147:PRO:HG3	1:D:224:THR:O	2.16	0.44
1:E:274:PHE:HB3	1:E:320:MET:HE2	1.99	0.44
1:E:337:ASP:O	1:E:341:GLU:HG3	2.16	0.44
1:F:238:LYS:O	1:F:239:SER:C	2.60	0.44
1:G:49:ALA:HA	1:G:196:GLY:O	2.18	0.44
1:G:71:LEU:HD22	1:G:188:MET:HG3	1.99	0.44
1:G:257:PHE:HZ	1:G:424:MET:CE	2.14	0.44
1:A:235:GLU:HB2	1:C:235:GLU:OE2	2.18	0.44
1:A:258:GLU:OE2	1:A:420:ARG:NH1	2.50	0.44
1:A:342:GLN:NE2	1:A:375:ASP:CG	2.76	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:ARG:HH11	1:A:380:GLU:CD	2.25	0.44
1:A:465:HIS:CE1	1:C:465:HIS:CE1	3.05	0.44
1:A:477:VAL:HG23	1:A:478:ASP:N	2.32	0.44
1:C:60:GLY:O	1:C:62:ALA:N	2.51	0.44
1:D:201:VAL:N	1:D:202:PRO:HD3	2.33	0.44
1:D:281:CYS:HB3	1:D:409:LEU:CD2	2.47	0.44
1:D:288:ILE:HG22	1:D:392:PHE:CD2	2.52	0.44
1:E:326:ALA:HB2	1:E:362:PHE:CE1	2.52	0.44
1:F:376:ARG:C	1:F:378:CYS:N	2.73	0.44
1:G:59:LEU:HD12	1:G:59:LEU:HA	1.56	0.44
1:G:71:LEU:O	1:G:75:ILE:HG13	2.17	0.44
1:G:183:ARG:HD2	1:G:183:ARG:C	2.13	0.44
1:G:328:ARG:O	1:G:328:ARG:HD3	2.17	0.44
1:G:446:PRO:HB3	1:G:457:ARG:HD2	1.99	0.44
1:H:104:ARG:NH2	1:H:153:MET:HE1	2.33	0.44
1:H:358:LEU:N	1:H:358:LEU:CD1	2.80	0.44
1:A:97:SER:O	1:A:102:VAL:HG22	1.98	0.44
1:A:259:ASP:O	1:A:416:GLN:CG	2.65	0.44
1:B:175:GLU:CD	1:B:175:GLU:H	2.25	0.44
1:B:391:ARG:HD3	2:B:513:HOH:O	2.16	0.44
1:C:429:HIS:CE1	1:C:450:VAL:CG1	3.01	0.44
1:E:151:PRO:CG	1:E:177:THR:HB	2.47	0.44
1:E:251:LYS:HB2	1:E:407:TYR:HD1	1.80	0.44
1:G:85:LEU:HD11	1:G:179:LEU:HB2	1.99	0.44
1:G:353:PRO:C	1:G:355:ASP:N	2.75	0.44
1:G:413:LEU:HD12	1:G:413:LEU:C	2.42	0.44
1:H:10:ARG:CG	1:H:10:ARG:HH11	2.30	0.44
1:A:204:TYR:HB3	1:A:206:HIS:CE1	2.53	0.44
1:A:235:GLU:CB	1:C:238:LYS:HE2	2.32	0.44
1:A:340:ILE:HG22	1:A:341:GLU:N	2.28	0.44
1:B:179:LEU:HA	1:B:179:LEU:HD23	1.56	0.44
1:C:1:MET:O	1:C:2:GLN:C	2.59	0.44
1:D:137:LYS:HB3	1:D:138:PRO:HD2	2.00	0.44
1:D:241:LEU:HD22	1:G:248:LEU:HD11	1.98	0.44
1:D:331:ARG:HE	1:D:331:ARG:HB2	1.41	0.44
1:D:377:VAL:HG13	1:D:386:PHE:HE1	1.83	0.44
1:D:480:LYS:O	1:D:480:LYS:HG2	2.17	0.44
1:E:185:VAL:O	1:E:188:MET:HB2	2.17	0.44
1:E:315:ASP:C	1:E:317:GLU:H	2.26	0.44
1:F:220:LYS:HE2	1:F:245:GLN:CG	2.47	0.44
1:H:26:HIS:HA	1:H:363:TYR:CE2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:49:ALA:HA	1:H:196:GLY:O	2.18	0.44
1:H:163:LEU:HG	1:H:169:ILE:CD1	2.47	0.44
1:B:372:LYS:O	1:B:375:ASP:HB2	2.18	0.44
1:B:403:ASN:C	1:B:405:THR:H	2.26	0.44
1:B:412:GLY:HA3	1:B:438:TYR:CE1	2.53	0.44
1:C:415:THR:CG2	1:C:417:ASN:H	2.30	0.44
1:C:485:PHE:O	1:C:486:LYS:C	2.59	0.44
1:D:56:TRP:O	1:D:59:LEU:HB2	2.18	0.44
1:D:412:GLY:HA3	1:D:438:TYR:CE1	2.53	0.44
1:E:365:GLU:O	1:E:367:THR:OG1	2.30	0.44
1:E:413:LEU:C	1:E:413:LEU:HD12	2.42	0.44
1:F:24:SER:N	1:F:31:ILE:HD11	2.32	0.44
1:F:176:ILE:C	1:F:178:PRO:HD3	2.42	0.44
1:G:440:ARG:HE	1:G:440:ARG:HB3	1.64	0.44
1:H:31:ILE:O	1:H:32:THR:HB	2.18	0.44
1:H:329:ARG:HD2	1:H:330:ASP:H	1.80	0.44
1:B:87:SER:HB3	1:B:314:MET:HE2	1.99	0.44
1:B:201:VAL:N	1:B:202:PRO:HD3	2.33	0.44
1:B:323:LEU:HD12	1:B:329:ARG:HA	1.99	0.44
1:C:14:ALA:O	1:C:15:VAL:C	2.61	0.44
1:C:333:LEU:HD22	1:C:351:LYS:HE3	1.99	0.44
1:E:237:SER:OG	1:E:244:ILE:HD11	2.18	0.44
1:E:447:PHE:CD2	1:E:447:PHE:O	2.71	0.44
1:F:94:ILE:CG1	1:F:98:ARG:CZ	2.96	0.44
1:F:333:LEU:HA	1:F:333:LEU:HD23	1.72	0.44
1:F:353:PRO:C	1:F:355:ASP:H	2.26	0.44
1:G:328:ARG:HD3	1:G:328:ARG:C	2.42	0.44
1:H:221:ILE:HD11	1:H:233:ILE:CD1	2.48	0.44
1:A:23:VAL:CG1	1:A:28:GLY:HA2	2.48	0.44
1:B:34:ILE:CD1	1:B:202:PRO:HB2	2.47	0.44
1:B:237:SER:HA	1:B:242:LYS:HD2	1.99	0.44
1:B:399:LEU:O	1:B:399:LEU:HD22	2.18	0.44
1:C:124:ILE:HB	1:C:132:ASN:HD22	1.83	0.44
1:C:272:ALA:HA	1:C:439:LYS:HD3	1.99	0.44
1:C:291:LYS:HE3	1:C:393:SER:HG	1.81	0.44
1:C:298:LEU:HD21	1:C:389:VAL:HG21	1.99	0.44
1:D:20:ILE:HG21	1:D:175:GLU:CB	2.35	0.44
1:D:178:PRO:O	1:D:182:LEU:HG	2.18	0.44
1:D:188:MET:CE	1:D:198:VAL:CG1	2.93	0.44
1:E:312:ASP:HA	1:E:313:PRO:HD3	1.91	0.44
1:F:1:MET:O	1:F:1:MET:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:PHE:CZ	1:F:276:ASN:ND2	2.85	0.44
1:F:256:VAL:CG1	1:F:293:ILE:HD11	2.48	0.44
1:G:327:LEU:CD2	1:G:327:LEU:O	2.62	0.44
1:H:273:ILE:HB	1:H:284:GLY:O	2.18	0.44
1:H:310:LEU:HA	1:H:320:MET:O	2.18	0.44
1:A:171:ILE:HG13	1:A:172:LYS:N	2.32	0.43
1:A:472:SER:O	1:C:432:MET:HA	2.18	0.43
1:B:185:VAL:HA	1:B:188:MET:HB2	2.00	0.43
1:B:248:LEU:HD12	1:F:241:LEU:HD13	2.01	0.43
1:B:335:TYR:CD1	1:B:382:VAL:HG13	2.53	0.43
1:C:100:LEU:HA	1:C:100:LEU:HD23	1.63	0.43
1:E:80:GLU:CD	1:E:98:ARG:HE	2.26	0.43
1:E:323:LEU:HD21	1:E:385:PRO:HD3	2.00	0.43
1:F:425:ALA:HB2	1:F:435:ILE:HD11	2.00	0.43
1:F:476:ASN:OD1	1:F:479:ALA:HB3	2.18	0.43
1:G:21:ASP:HB3	1:G:30:LEU:HD11	1.99	0.43
1:G:274:PHE:HB3	1:G:320:MET:CE	2.48	0.43
1:H:30:LEU:CD2	1:H:33:ARG:HE	2.27	0.43
1:H:413:LEU:C	1:H:413:LEU:HD12	2.42	0.43
1:A:261:ASN:C	1:A:261:ASN:OD1	2.61	0.43
1:A:412:GLY:HA3	1:A:438:TYR:CE1	2.53	0.43
1:B:112:PHE:HA	1:B:115:MET:HB3	2.00	0.43
1:B:119:ILE:HG12	1:B:464:ILE:HG21	2.00	0.43
1:D:255:ILE:O	1:D:414:TRP:HD1	2.01	0.43
1:D:432:MET:HA	1:G:472:SER:O	2.18	0.43
1:E:335:TYR:CE2	1:E:380:GLU:OE1	2.71	0.43
1:F:49:ALA:HA	1:F:196:GLY:O	2.18	0.43
1:G:85:LEU:HD11	1:G:179:LEU:CB	2.47	0.43
1:H:102:VAL:HB	1:H:103:PRO:HD3	2.00	0.43
1:A:231:ARG:HB2	1:A:232:ARG:HH21	1.83	0.43
1:B:339:ALA:HA	2:B:520:HOH:O	2.18	0.43
1:B:417:ASN:HD22	1:B:420:ARG:H	1.63	0.43
1:D:266:VAL:HG13	1:D:301:PHE:HD2	1.83	0.43
1:E:12:VAL:O	1:E:12:VAL:HG23	2.18	0.43
1:E:241:LEU:CD1	1:H:227:THR:HG23	2.49	0.43
1:E:248:LEU:CD1	1:H:241:LEU:CD1	2.95	0.43
1:E:256:VAL:HG12	1:E:293:ILE:CD1	2.48	0.43
1:A:119:ILE:HG12	1:A:464:ILE:HG21	2.00	0.43
1:A:242:LYS:O	2:A:516:HOH:O	2.21	0.43
1:A:273:ILE:CD1	1:A:386:PHE:O	2.66	0.43
1:C:14:ALA:CB	1:C:36:ALA:O	2.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:GLU:H	1:C:258:GLU:HG3	1.34	0.43
1:C:259:ASP:CG	1:C:415:THR:HG22	2.44	0.43
1:D:111:TYR:OH	2:D:503:HOH:O	1.96	0.43
1:D:330:ASP:O	1:E:232:ARG:NH2	2.51	0.43
1:E:412:GLY:HA3	1:E:438:TYR:CE1	2.53	0.43
1:F:46:VAL:HA	1:F:170:VAL:HG21	1.99	0.43
1:F:59:LEU:HD13	1:F:63:GLU:HB3	1.99	0.43
1:F:330:ASP:O	1:F:334:SER:OG	2.30	0.43
1:F:429:HIS:CE1	1:F:450:VAL:CG1	3.01	0.43
1:G:61:ALA:HB1	1:G:116:ALA:O	2.19	0.43
1:G:246:LEU:O	1:G:454:GLY:HA3	2.18	0.43
1:G:371:ALA:O	1:G:390:VAL:HG23	2.18	0.43
1:H:163:LEU:O	1:H:164:ALA:C	2.60	0.43
1:H:279:GLN:HE21	1:H:279:GLN:HB2	1.64	0.43
1:B:434:TRP:HB3	1:B:437:CYS:SG	2.59	0.43
1:C:98:ARG:O	1:C:103:PRO:HD3	2.18	0.43
1:C:372:LYS:C	1:C:374:GLN:HG2	2.43	0.43
1:C:374:GLN:H	1:C:374:GLN:HG2	1.15	0.43
1:C:408:GLY:C	1:C:430:ALA:HA	2.33	0.43
1:C:412:GLY:HA3	1:C:438:TYR:CE1	2.53	0.43
1:E:222:ALA:HA	1:E:245:GLN:HB3	2.00	0.43
1:E:248:LEU:HD12	1:H:241:LEU:CD1	2.39	0.43
1:E:404:ASN:C	1:E:405:THR:HG23	2.43	0.43
1:G:7:ILE:HG23	1:G:45:ALA:HA	1.99	0.43
1:G:366:PRO:HA	1:G:385:PRO:HB2	2.00	0.43
1:H:10:ARG:HH11	1:H:10:ARG:HG2	1.82	0.43
1:H:412:GLY:HA3	1:H:438:TYR:CE1	2.53	0.43
1:A:15:VAL:HG13	1:A:16:ALA:H	1.79	0.43
1:A:128:ALA:O	1:A:479:ALA:HB3	2.19	0.43
1:B:25:PRO:HB2	1:B:322:PRO:CG	2.49	0.43
1:B:49:ALA:HA	1:B:196:GLY:O	2.18	0.43
1:B:310:LEU:HA	1:B:320:MET:O	2.18	0.43
1:C:108:CYS:CB	1:C:156:SER:HB2	2.45	0.43
1:C:220:LYS:HD2	1:C:243:ARG:HB2	2.00	0.43
1:C:243:ARG:C	1:C:244:ILE:HG12	2.42	0.43
1:E:201:VAL:N	1:E:202:PRO:HD3	2.34	0.43
1:E:445:SER:HA	1:E:446:PRO:HD3	1.93	0.43
1:G:320:MET:CG	1:G:320:MET:O	2.66	0.43
1:H:211:ALA:O	1:H:215:HIS:HB2	2.19	0.43
1:A:163:LEU:O	1:A:166:GLY:N	2.49	0.43
1:B:417:ASN:ND2	1:B:420:ARG:HB2	2.21	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:LEU:O	1:C:59:LEU:CG	2.67	0.43
1:E:70:LYS:HE3	1:E:191:VAL:O	2.19	0.43
1:E:258:GLU:HG2	1:E:290:HIS:CD2	2.53	0.43
1:F:11:PHE:CZ	1:F:186:GLU:HG3	2.54	0.43
1:H:196:GLY:N	2:H:504:HOH:O	2.04	0.43
1:A:179:LEU:HA	1:A:179:LEU:HD23	1.74	0.43
1:B:92:HIS:HD2	1:B:101:ASP:OD2	2.00	0.43
1:B:221:ILE:CD1	1:B:233:ILE:HG23	2.49	0.43
1:C:86:GLU:OE1	1:C:151:PRO:HD2	2.18	0.43
1:C:99:GLY:O	1:C:100:LEU:HD23	2.18	0.43
1:C:150:PHE:N	1:C:151:PRO:HD3	2.34	0.43
1:D:312:ASP:HA	1:D:313:PRO:HD3	1.89	0.43
1:D:474:TRP:HB2	1:G:434:TRP:CD1	2.54	0.43
1:E:226:SER:HG	1:E:229:THR:HG22	1.79	0.43
1:E:315:ASP:C	1:E:317:GLU:N	2.77	0.43
1:G:377:VAL:HG22	1:G:386:PHE:HE1	1.83	0.43
1:G:377:VAL:CG2	1:G:386:PHE:CE1	3.01	0.43
1:A:155:THR:O	1:A:159:MET:HB2	2.19	0.43
1:B:108:CYS:HB3	1:B:156:SER:HB2	2.01	0.43
1:B:212:LEU:HD12	1:B:212:LEU:HA	1.77	0.43
1:C:74:ARG:HG3	1:C:187:LEU:HD22	2.01	0.43
1:C:223:PHE:CZ	1:C:229:THR:CG2	3.01	0.43
1:D:89:ASN:OD1	1:D:177:THR:HA	2.19	0.43
1:D:457:ARG:NH1	1:D:457:ARG:CG	2.75	0.43
1:E:34:ILE:CD1	1:E:202:PRO:HB2	2.49	0.43
1:E:93:PRO:HD3	1:E:277:GLN:HE22	1.83	0.43
1:E:259:ASP:O	1:E:416:GLN:CG	2.67	0.43
1:F:147:PRO:HD3	1:F:224:THR:HB	2.01	0.43
1:F:376:ARG:HG2	1:F:377:VAL:N	2.34	0.43
1:G:257:PHE:HB2	1:G:415:THR:HG23	2.01	0.43
1:G:372:LYS:O	1:G:373:PRO:C	2.61	0.43
1:G:404:ASN:O	1:G:404:ASN:OD1	2.37	0.43
1:H:100:LEU:O	1:H:104:ARG:HG3	2.19	0.43
1:H:102:VAL:N	1:H:103:PRO:CD	2.82	0.43
1:H:171:ILE:HG23	1:H:200:VAL:HG13	2.01	0.43
1:H:353:PRO:C	1:H:355:ASP:H	2.27	0.43
1:A:59:LEU:HD12	1:A:59:LEU:HA	1.56	0.43
1:A:67:LEU:HD13	1:A:193:PHE:HA	1.99	0.43
1:B:485:PHE:O	1:B:486:LYS:C	2.61	0.43
1:C:26:HIS:C	1:C:361:GLY:CA	2.87	0.43
1:D:143:ALA:O	1:D:221:ILE:HA	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:ARG:HD3	1:D:380:GLU:CD	2.43	0.43
1:E:137:LYS:HE3	1:H:426:ASN:OD1	2.18	0.43
1:E:151:PRO:HG3	1:E:177:THR:OG1	2.18	0.43
1:E:302:ILE:CD1	1:E:347:LEU:HB3	2.49	0.43
1:E:377:VAL:HG22	1:E:386:PHE:CE1	2.54	0.43
1:F:221:ILE:O	1:F:221:ILE:HG22	2.16	0.43
1:G:268:GLY:O	1:G:272:ALA:N	2.51	0.43
1:H:355:ASP:O	1:H:356:LYS:C	2.62	0.43
1:A:323:LEU:HD21	1:A:385:PRO:HD3	2.00	0.42
1:B:440:ARG:HA	1:B:440:ARG:HD2	1.50	0.42
1:D:22:VAL:CG2	1:D:34:ILE:HG23	2.49	0.42
1:D:261:ASN:C	1:D:261:ASN:OD1	2.60	0.42
1:D:401:ILE:O	1:D:402:ALA:C	2.62	0.42
1:D:441:VAL:HG13	2:D:505:HOH:O	2.20	0.42
1:F:315:ASP:OD1	1:F:316:PRO:HD2	2.19	0.42
1:F:326:ALA:HA	1:F:362:PHE:CD1	2.54	0.42
1:H:146:VAL:HA	1:H:147:PRO:HD3	1.81	0.42
1:H:486:LYS:O	1:H:487:ARG:HB2	2.19	0.42
1:A:288:ILE:HG22	1:A:392:PHE:CD2	2.54	0.42
1:B:251:LYS:HG3	1:B:286:ARG:CD	2.49	0.42
1:B:405:THR:HG23	1:B:407:TYR:HD1	1.83	0.42
1:C:160:GLY:N	1:C:161:PRO:CD	2.82	0.42
1:E:119:ILE:HG12	1:E:464:ILE:HG21	2.01	0.42
1:E:251:LYS:HA	1:E:251:LYS:HD2	1.70	0.42
1:E:372:LYS:HA	1:E:372:LYS:HD2	1.76	0.42
1:F:23:VAL:O	1:F:31:ILE:CD1	2.67	0.42
1:G:350:GLY:C	1:G:351:LYS:CG	2.92	0.42
1:B:155:THR:HB	1:B:159:MET:CE	2.48	0.42
1:B:357:ALA:HB3	1:B:358:LEU:HD13	2.01	0.42
1:D:42:VAL:HG22	1:D:201:VAL:HG11	2.01	0.42
1:D:71:LEU:HD12	1:D:71:LEU:C	2.44	0.42
1:D:437:CYS:HB2	1:D:440:ARG:HD3	2.01	0.42
1:E:102:VAL:CB	1:E:103:PRO:HD3	2.44	0.42
1:E:272:ALA:O	1:E:284:GLY:N	2.43	0.42
1:F:279:GLN:OE1	1:F:324:THR:HG23	2.19	0.42
1:F:376:ARG:CG	1:F:377:VAL:N	2.79	0.42
1:G:226:SER:HG	1:G:229:THR:HG22	1.82	0.42
1:G:337:ASP:C	1:G:339:ALA:H	2.27	0.42
1:H:42:VAL:HG21	1:H:211:ALA:CB	2.49	0.42
1:A:89:ASN:OD1	1:A:177:THR:HA	2.19	0.42
1:A:119:ILE:HD11	1:A:464:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:CG	1:B:290:HIS:CG	3.02	0.42
1:B:338:ILE:HD11	1:B:376:ARG:CB	2.49	0.42
1:D:38:GLU:O	1:D:39:ALA:C	2.61	0.42
1:D:151:PRO:HG3	1:D:177:THR:OG1	2.20	0.42
1:D:474:TRP:HB2	1:G:434:TRP:HA	2.02	0.42
1:E:119:ILE:HD11	1:E:464:ILE:HD12	2.01	0.42
1:E:477:VAL:CG2	1:E:478:ASP:N	2.82	0.42
1:G:87:SER:HB2	1:G:94:ILE:HD13	1.79	0.42
1:G:293:ILE:HD12	1:G:294:ALA:CA	2.47	0.42
1:G:412:GLY:HA3	1:G:438:TYR:CE1	2.53	0.42
1:H:343:GLY:O	1:H:344:GLY:C	2.61	0.42
1:A:302:ILE:HG23	1:A:348:ALA:HB2	2.01	0.42
1:A:309:ARG:HB2	1:A:319:GLU:OE1	2.18	0.42
1:C:89:ASN:O	1:C:89:ASN:ND2	2.53	0.42
1:C:273:ILE:HB	1:C:284:GLY:O	2.20	0.42
1:C:320:MET:HE1	1:C:385:PRO:CG	2.49	0.42
1:C:373:PRO:HB3	1:C:401:ILE:HG23	2.01	0.42
1:E:4:GLN:NE2	1:E:13:ASP:OD1	2.46	0.42
1:E:258:GLU:CD	1:E:258:GLU:H	2.26	0.42
1:E:315:ASP:OD1	1:E:316:PRO:HD2	2.19	0.42
1:E:350:GLY:CA	1:E:367:THR:HG23	2.50	0.42
1:G:432:MET:HE2	1:G:448:GLY:O	2.19	0.42
1:A:350:GLY:O	1:A:351:LYS:HB2	2.19	0.42
1:C:31:ILE:CD1	1:C:88:LEU:HG	2.50	0.42
1:C:94:ILE:O	1:C:98:ARG:HD2	2.19	0.42
1:D:56:TRP:CE3	1:D:59:LEU:HD22	2.54	0.42
1:F:23:VAL:C	1:F:31:ILE:HD12	2.41	0.42
1:F:92:HIS:HD2	1:F:101:ASP:OD2	2.02	0.42
1:G:117:ASP:OD1	1:G:118:LYS:NZ	2.39	0.42
1:G:327:LEU:HD21	1:G:331:ARG:CD	2.32	0.42
1:G:358:LEU:HB3	1:G:363:TYR:CD2	2.53	0.42
1:A:199:ASN:N	1:A:199:ASN:ND2	2.67	0.42
1:B:323:LEU:HD21	1:B:385:PRO:HD3	2.00	0.42
1:C:151:PRO:CG	1:C:177:THR:CB	2.97	0.42
1:F:37:ALA:HB3	1:F:201:VAL:HG13	1.98	0.42
1:F:234:VAL:O	1:F:235:GLU:C	2.61	0.42
1:F:312:ASP:O	1:F:318:THR:OG1	2.35	0.42
1:G:258:GLU:HG3	1:G:290:HIS:CG	2.54	0.42
1:G:305:ALA:C	1:G:307:SER:H	2.27	0.42
1:H:326:ALA:C	1:H:328:ARG:N	2.74	0.42
1:A:102:VAL:HB	1:A:103:PRO:CD	2.43	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:LEU:O	1:A:305:ALA:C	2.63	0.42
1:A:314:MET:O	1:A:316:PRO:HD3	2.19	0.42
1:B:138:PRO:HG3	1:B:165:ALA:O	2.20	0.42
1:B:290:HIS:HD2	1:B:292:ASP:HB2	1.83	0.42
1:B:457:ARG:HD2	1:B:457:ARG:HA	1.88	0.42
1:D:95:ARG:NH1	1:D:319:GLU:HA	2.35	0.42
1:D:129:GLY:HA3	1:D:479:ALA:HB2	2.01	0.42
1:D:240:ASN:OD1	1:D:240:ASN:N	2.46	0.42
1:E:482:ALA:O	1:E:483:PRO:C	2.62	0.42
1:F:289:LEU:O	1:F:391:ARG:HA	2.20	0.42
1:G:10:ARG:HH12	1:G:12:VAL:HG11	0.59	0.42
1:A:45:ALA:HB1	1:A:170:VAL:HG13	2.01	0.42
1:A:327:LEU:O	1:A:328:ARG:C	2.62	0.42
1:B:242:LYS:HE3	1:B:242:LYS:HB3	1.33	0.42
1:C:376:ARG:O	1:C:379:GLN:N	2.48	0.42
1:E:355:ASP:O	1:E:359:ALA:N	2.50	0.42
1:E:482:ALA:HA	1:E:483:PRO:HD2	1.77	0.42
1:F:22:VAL:HG11	1:F:179:LEU:HD11	2.02	0.42
1:G:186:GLU:O	1:G:189:THR:N	2.51	0.42
1:G:417:ASN:HB3	1:G:420:ARG:HB3	2.01	0.42
1:H:5:LEU:O	1:H:11:PHE:HA	2.20	0.42
1:H:197:VAL:HG12	1:H:198:VAL:HG23	2.02	0.42
1:H:221:ILE:CD1	1:H:233:ILE:HD12	2.50	0.42
1:A:100:LEU:O	1:A:101:ASP:C	2.58	0.42
1:B:89:ASN:ND2	1:B:89:ASN:C	2.77	0.42
1:B:93:PRO:O	1:B:96:ASP:HB2	2.20	0.42
1:B:329:ARG:HD2	1:B:330:ASP:CA	2.50	0.42
1:B:346:VAL:HG13	1:B:348:ALA:O	2.20	0.42
1:D:3:ASN:O	1:D:34:ILE:HA	2.20	0.42
1:F:312:ASP:HA	1:F:313:PRO:HD2	1.81	0.42
1:F:340:ILE:HG12	1:F:340:ILE:H	1.62	0.42
1:G:90:THR:O	1:G:324:THR:CG2	2.49	0.42
1:G:451:GLY:O	2:G:503:HOH:O	2.21	0.42
1:H:210:GLN:HG3	1:H:214:GLU:CD	2.44	0.42
1:A:343:GLY:O	1:A:345:LYS:HE3	2.20	0.41
1:B:458:GLU:O	1:B:459:MET:CB	2.68	0.41
1:C:146:VAL:HA	1:C:147:PRO:HD3	1.86	0.41
1:C:215:HIS:CD2	1:C:217:ASP:H	2.23	0.41
1:G:102:VAL:CB	1:G:103:PRO:HD3	2.50	0.41
1:H:111:TYR:CG	1:H:443:PRO:HB2	2.55	0.41
1:B:8:ASP:OD2	1:B:51:ARG:NH2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:TRP:CH2	1:C:383:PHE:HD2	2.38	0.41
1:D:242:LYS:HZ2	1:D:242:LYS:HG2	1.68	0.41
1:G:34:ILE:CD1	1:G:202:PRO:HB2	2.50	0.41
1:G:148:TRP:HH2	1:G:328:ARG:CG	2.33	0.41
1:B:119:ILE:HD11	1:B:464:ILE:HD12	2.01	0.41
1:B:129:GLY:HA2	1:B:478:ASP:HB3	2.02	0.41
1:B:371:ALA:C	1:B:372:LYS:HD3	2.45	0.41
1:B:452:GLN:HG3	1:F:240:ASN:O	2.20	0.41
1:C:2:GLN:HG3	1:C:11:PHE:CE2	2.55	0.41
1:C:289:LEU:CD1	1:C:389:VAL:HG13	2.50	0.41
1:E:25:PRO:HA	1:E:362:PHE:CE2	2.55	0.41
1:F:61:ALA:CB	1:F:117:ASP:HA	2.50	0.41
1:G:6:TYR:CZ	1:G:9:GLY:HA2	2.55	0.41
1:G:114:GLY:O	1:G:118:LYS:HG3	2.20	0.41
1:G:172:LYS:HE2	1:G:204:TYR:O	2.19	0.41
1:H:476:ASN:OD1	1:H:479:ALA:HB3	2.20	0.41
1:A:15:VAL:CG1	1:A:40:ALA:HB3	2.51	0.41
1:A:38:GLU:HA	1:A:207:THR:HB	2.01	0.41
1:A:151:PRO:CG	1:A:177:THR:HB	2.50	0.41
1:A:440:ARG:HA	1:A:440:ARG:HD2	1.43	0.41
1:A:458:GLU:C	1:A:459:MET:HG2	2.45	0.41
1:B:88:LEU:HA	1:B:314:MET:CE	2.46	0.41
1:B:476:ASN:CB	1:F:436:ASN:O	2.68	0.41
1:C:94:ILE:C	1:C:96:ASP:N	2.77	0.41
1:C:152:LEU:HB2	1:C:180:SER:OG	2.20	0.41
1:C:208:ALA:O	1:C:209:GLY:C	2.61	0.41
1:C:424:MET:HE3	1:C:424:MET:HB3	1.74	0.41
1:C:476:ASN:ND2	1:C:481:ILE:HD11	2.35	0.41
1:D:476:ASN:HB2	1:G:437:CYS:HB3	2.02	0.41
1:D:482:ALA:HA	1:D:483:PRO:HD2	1.64	0.41
1:E:176:ILE:C	1:E:178:PRO:HD3	2.46	0.41
1:E:213:ALA:HB2	1:E:221:ILE:CD1	2.51	0.41
1:H:14:ALA:O	1:H:15:VAL:C	2.61	0.41
1:H:221:ILE:HD11	1:H:233:ILE:HD12	2.03	0.41
1:A:310:LEU:HD23	1:A:353:PRO:HG2	1.96	0.41
1:A:392:PHE:HB2	1:A:397:GLU:HB3	2.02	0.41
1:B:221:ILE:O	1:B:221:ILE:CG2	2.68	0.41
1:B:345:LYS:HZ3	1:B:345:LYS:HG3	1.70	0.41
1:B:438:TYR:O	1:B:439:LYS:HB2	2.19	0.41
1:D:74:ARG:HD3	1:D:77:GLU:OE1	2.21	0.41
1:E:428:ILE:O	1:H:471:ARG:NH1	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:74:ARG:NH2	1:F:190:GLU:OE1	2.53	0.41
1:F:124:ILE:HG22	1:F:125:PRO:HD2	2.03	0.41
1:F:311:GLY:O	1:F:312:ASP:C	2.63	0.41
1:G:340:ILE:HD11	1:G:346:VAL:CG2	2.51	0.41
1:H:235:GLU:O	1:H:238:LYS:HG3	2.21	0.41
1:H:325:SER:OG	1:H:328:ARG:HB2	2.20	0.41
1:A:56:TRP:O	1:A:59:LEU:HB2	2.20	0.41
1:A:111:TYR:CG	1:A:443:PRO:HB2	2.56	0.41
1:B:177:THR:N	1:B:178:PRO:HD3	2.35	0.41
1:B:405:THR:HG23	1:B:406:GLU:H	1.85	0.41
1:C:259:ASP:CG	1:C:415:THR:CG2	2.94	0.41
1:D:76:GLU:CD	1:D:110:ARG:HH12	2.29	0.41
1:F:124:ILE:HA	1:F:125:PRO:HD3	1.73	0.41
1:F:315:ASP:HA	1:F:316:PRO:HD3	1.85	0.41
1:F:458:GLU:C	1:F:459:MET:HG2	2.44	0.41
1:G:53:PHE:CD1	1:G:140:GLY:HA2	2.53	0.41
1:G:89:ASN:ND2	1:G:89:ASN:C	2.78	0.41
1:G:279:GLN:HE21	1:G:279:GLN:HB2	1.52	0.41
1:G:358:LEU:C	1:G:360:ASN:H	2.29	0.41
1:H:126:VAL:C	1:H:127:ASP:O	2.62	0.41
1:H:416:GLN:H	1:H:416:GLN:HG2	1.60	0.41
1:A:377:VAL:CG2	1:A:386:PHE:CE1	3.03	0.41
1:B:145:ILE:HG12	1:B:172:LYS:HD3	2.03	0.41
1:B:152:LEU:HD11	1:B:184:ILE:CD1	2.17	0.41
1:B:277:GLN:N	1:B:277:GLN:CD	2.79	0.41
1:B:434:TRP:CD1	1:B:440:ARG:HB2	2.55	0.41
1:D:108:CYS:HB3	1:D:156:SER:HB2	2.03	0.41
1:D:377:VAL:O	1:D:377:VAL:CG1	2.59	0.41
1:F:234:VAL:O	1:F:237:SER:N	2.51	0.41
1:F:336:ILE:HG12	1:F:386:PHE:CE2	2.55	0.41
1:C:53:PHE:N	1:C:54:PRO:CD	2.84	0.41
1:C:114:GLY:O	1:C:118:LYS:HG3	2.21	0.41
1:C:376:ARG:C	1:C:378:CYS:N	2.75	0.41
1:D:22:VAL:HG21	1:D:34:ILE:CG2	2.50	0.41
1:D:341:GLU:OE2	2:D:522:HOH:O	2.20	0.41
1:D:470:ALA:HB3	1:G:457:ARG:NE	2.36	0.41
1:H:330:ASP:OD1	1:H:330:ASP:N	2.52	0.41
1:A:70:LYS:HB3	1:A:191:VAL:HG22	2.03	0.41
1:A:238:LYS:H	1:A:238:LYS:HG3	1.64	0.41
1:A:290:HIS:HD2	1:A:292:ASP:HB2	1.85	0.41
1:B:66:ARG:HH11	1:B:66:ARG:CG	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:PRO:HG3	1:B:181:THR:HG21	2.03	0.41
1:B:392:PHE:CD1	1:B:392:PHE:C	2.98	0.41
1:C:225:GLY:O	1:C:248:LEU:HA	2.21	0.41
1:C:261:ASN:OD1	1:C:261:ASN:C	2.64	0.41
1:D:18:GLY:HA3	2:D:524:HOH:O	2.20	0.41
1:D:42:VAL:O	1:D:46:VAL:HG23	2.21	0.41
1:D:174:SER:C	1:D:176:ILE:N	2.76	0.41
1:D:273:ILE:HD13	1:D:283:ALA:HB1	2.02	0.41
1:D:309:ARG:NE	1:D:319:GLU:CD	2.79	0.41
1:E:15:VAL:HG12	1:E:16:ALA:CA	2.40	0.41
1:E:137:LYS:CE	1:H:426:ASN:OD1	2.68	0.41
1:E:236:ALA:C	1:E:238:LYS:N	2.77	0.41
1:E:314:MET:O	1:E:316:PRO:HD3	2.21	0.41
1:F:61:ALA:HB1	1:F:117:ASP:HA	2.03	0.41
1:F:302:ILE:HD11	1:F:347:LEU:HD13	2.03	0.41
1:G:23:VAL:HG12	1:G:24:SER:N	2.29	0.41
1:G:25:PRO:O	1:G:361:GLY:HA2	2.21	0.41
1:G:38:GLU:O	1:G:39:ALA:C	2.64	0.41
1:G:152:LEU:HD12	1:G:184:ILE:CD1	2.50	0.41
1:G:312:ASP:HA	1:G:313:PRO:HD3	1.84	0.41
1:G:464:ILE:HD13	1:G:464:ILE:HA	1.87	0.41
1:H:69:LEU:HD23	1:H:69:LEU:HA	1.91	0.41
1:A:20:ILE:HD13	1:A:204:TYR:CE1	2.56	0.41
1:A:126:VAL:HG11	1:A:474:TRP:CH2	2.56	0.41
1:A:445:SER:CB	1:C:132:ASN:ND2	2.82	0.41
1:B:456:GLY:O	1:B:457:ARG:HD3	2.21	0.41
1:B:462:GLU:OE2	1:F:136:ARG:NH1	2.54	0.41
1:C:137:LYS:O	1:C:468:THR:HA	2.21	0.41
1:D:124:ILE:HA	1:D:125:PRO:HD3	1.95	0.41
1:D:225:GLY:O	1:D:248:LEU:HA	2.21	0.41
1:E:285:SER:O	1:E:388:THR:HG23	2.21	0.41
1:E:312:ASP:C	1:E:314:MET:N	2.78	0.41
1:E:357:ALA:HB3	1:E:358:LEU:CD1	2.51	0.41
1:E:426:ASN:O	1:E:426:ASN:CG	2.64	0.41
1:G:42:VAL:O	1:G:46:VAL:HG23	2.21	0.41
1:H:172:LYS:NZ	1:H:203:GLY:O	2.53	0.41
1:B:20:ILE:HG21	1:B:175:GLU:HB3	2.03	0.40
1:D:177:THR:N	1:D:178:PRO:HD3	2.36	0.40
1:D:338:ILE:CD1	1:D:376:ARG:CB	2.99	0.40
1:F:11:PHE:C	1:F:12:VAL:CG1	2.93	0.40
1:F:27:ASP:CG	1:F:29:SER:HB3	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:ILE:CG2	1:F:125:PRO:HD2	2.52	0.40
1:G:335:TYR:CZ	2:G:523:HOH:O	2.47	0.40
1:H:185:VAL:HG11	1:H:200:VAL:HG21	2.04	0.40
1:A:53:PHE:N	1:A:54:PRO:CD	2.84	0.40
1:B:1:MET:HE1	1:B:31:ILE:HG22	2.03	0.40
1:B:24:SER:HA	1:B:25:PRO:HD3	1.86	0.40
1:B:152:LEU:HD13	1:B:184:ILE:HD12	2.00	0.40
1:B:348:ALA:O	1:B:349:GLY:C	2.64	0.40
1:C:153:MET:HE3	1:C:157:TRP:CE2	2.57	0.40
1:E:151:PRO:HG2	1:E:177:THR:HB	2.03	0.40
1:E:238:LYS:HB2	1:H:231:ARG:HB3	2.03	0.40
1:E:474:TRP:HB2	1:H:434:TRP:HD1	1.86	0.40
1:F:191:VAL:CG1	1:F:191:VAL:O	2.66	0.40
1:G:145:ILE:C	1:G:146:VAL:CG1	2.94	0.40
1:G:158:LYS:NZ	2:G:521:HOH:O	2.49	0.40
1:G:304:LEU:N	2:G:513:HOH:O	2.54	0.40
1:H:53:PHE:CE1	1:H:140:GLY:HA2	2.56	0.40
1:H:372:LYS:O	1:H:373:PRO:C	2.63	0.40
1:A:275:HIS:ND1	1:A:439:LYS:NZ	2.70	0.40
1:B:355:ASP:O	1:B:358:LEU:N	2.50	0.40
1:C:323:LEU:N	1:C:323:LEU:HD23	2.37	0.40
1:E:24:SER:HA	1:E:25:PRO:HD3	1.88	0.40
1:E:238:LYS:O	1:H:231:ARG:NE	2.33	0.40
1:G:34:ILE:O	1:G:34:ILE:HG13	2.17	0.40
1:G:362:PHE:N	1:G:362:PHE:CD1	2.88	0.40
1:B:27:ASP:C	1:B:27:ASP:OD1	2.63	0.40
1:B:76:GLU:OE1	1:B:110:ARG:NH1	2.36	0.40
1:B:225:GLY:O	1:B:248:LEU:HA	2.21	0.40
1:C:5:LEU:O	1:C:11:PHE:HA	2.21	0.40
1:C:25:PRO:CD	2:C:512:HOH:O	2.69	0.40
1:C:310:LEU:HD23	1:C:353:PRO:HG3	2.03	0.40
1:D:89:ASN:ND2	1:D:89:ASN:C	2.78	0.40
1:D:469:GLU:OE1	1:G:450:VAL:HG22	2.22	0.40
1:E:269:ALA:O	1:E:273:ILE:HG22	2.22	0.40
1:E:312:ASP:OD1	1:E:313:PRO:HD2	2.21	0.40
1:G:84:GLN:HA	1:G:314:MET:HE1	2.03	0.40
1:G:94:ILE:HD12	1:G:94:ILE:HA	1.95	0.40
1:G:225:GLY:O	1:G:248:LEU:HA	2.21	0.40
1:G:337:ASP:O	1:G:338:ILE:C	2.63	0.40
1:G:373:PRO:CG	1:G:374:GLN:H	2.34	0.40
1:H:24:SER:HA	1:H:25:PRO:HD2	1.91	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:142:VAL:HG11	1:H:467:TYR:CE2	2.50	0.40
1:A:476:ASN:HD21	1:A:480:LYS:HE3	1.86	0.40
1:B:15:VAL:HG13	2:B:522:HOH:O	2.21	0.40
1:B:148:TRP:HB3	1:B:174:SER:OG	2.22	0.40
1:C:133:TYR:CD1	1:C:133:TYR:C	2.98	0.40
1:C:320:MET:HE3	1:C:385:PRO:HG3	2.04	0.40
1:D:94:ILE:HA	1:D:97:SER:OG	2.21	0.40
1:E:115:MET:O	1:E:119:ILE:HG13	2.21	0.40
1:E:314:MET:HA	1:E:314:MET:CE	2.45	0.40
1:F:188:MET:O	1:F:193:PHE:HB2	2.21	0.40
1:G:305:ALA:C	1:G:307:SER:N	2.79	0.40
1:G:414:TRP:CE3	1:G:436:ASN:HA	2.57	0.40
1:H:273:ILE:HG21	1:H:387:VAL:HG21	2.04	0.40
1:H:278:GLY:HA3	1:H:384:GLY:O	2.21	0.40

All (27) 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:B:393:SER:CB	1:H:354:ASP:O[2_545]	0.79	1.41
1:B:356:LYS:NZ	1:F:341:GLU:CB[2_454]	0.88	1.32
1:B:356:LYS:NZ	1:F:341:GLU:CA[2_454]	0.92	1.28
1:A:478:ASP:OD2	1:H:423:LYS:CE[2_445]	1.10	1.10
1:B:393:SER:OG	1:H:354:ASP:O[2_545]	1.14	1.06
1:A:478:ASP:OD2	1:H:423:LYS:CD[2_445]	1.51	0.69
1:B:356:LYS:NZ	1:F:341:GLU:C[2_454]	1.58	0.62
1:B:356:LYS:CE	1:F:341:GLU:CB[2_454]	1.59	0.61
1:B:393:SER:OG	1:H:354:ASP:C[2_545]	1.63	0.57
1:B:292:ASP:OD1	1:H:354:ASP:OD2[2_545]	1.68	0.52
1:B:393:SER:OG	1:H:356:LYS:N[2_545]	1.70	0.50
1:B:393:SER:OG	1:H:355:ASP:CA[2_545]	1.88	0.32
1:E:300:ARG:NH1	1:F:396:GLU:OE2[2_454]	1.90	0.30
1:D:8:ASP:O	1:F:1:MET:N[1_565]	1.92	0.28
1:B:393:SER:OG	1:H:355:ASP:N[2_545]	1.94	0.26
1:B:393:SER:CB	1:H:354:ASP:C[2_545]	1.96	0.24
1:B:393:SER:OG	1:H:355:ASP:C[2_545]	1.96	0.24
1:C:486:LYS:NZ	1:E:195:LYS:CE[1_545]	1.98	0.22
1:C:33:ARG:CD	2:A:517:HOH:O[2_555]	2.01	0.19
1:A:376:ARG:NH2	1:H:17:GLY:O[2_545]	2.02	0.18
1:B:356:LYS:CE	1:F:341:GLU:CA[2_454]	2.02	0.18

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:356:LYS:CD	1:F:341:GLU:CB[2_454]	2.03	0.17
1:B:393:SER:O	1:H:355:ASP:CA[2_545]	2.05	0.15
1:A:478:ASP:CG	1:H:423:LYS:CE[2_445]	2.06	0.14
1:D:10:ARG:NH2	1:F:4:GLN:OE1[1_565]	2.13	0.07
1:B:356:LYS:NZ	1:F:341:GLU:N[2_454]	2.15	0.05
1:B:397:GLU:OE1	1:H:356:LYS:CG[2_545]	2.17	0.03

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	485/495 (98%)	452 (93%)	31 (6%)	2 (0%)	30	54
1	B	486/495 (98%)	452 (93%)	30 (6%)	4 (1%)	16	37
1	C	486/495 (98%)	440 (90%)	41 (8%)	5 (1%)	12	32
1	D	485/495 (98%)	453 (93%)	31 (6%)	1 (0%)	43	68
1	E	483/495 (98%)	446 (92%)	35 (7%)	2 (0%)	30	54
1	F	485/495 (98%)	443 (91%)	40 (8%)	2 (0%)	30	54
1	G	485/495 (98%)	432 (89%)	45 (9%)	8 (2%)	7	20
1	H	485/495 (98%)	453 (93%)	29 (6%)	3 (1%)	21	44
All	All	3880/3960 (98%)	3571 (92%)	282 (7%)	27 (1%)	18	41

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	178	PRO
1	A	356	LYS
1	C	178	PRO
1	G	341	GLU
1	G	357	ALA
1	F	178	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	296	GLN
1	G	459	MET
1	B	39	ALA
1	B	356	LYS
1	B	404	ASN
1	C	175	GLU
1	E	313	PRO
1	E	459	MET
1	B	351	LYS
1	C	353	PRO
1	C	366	PRO
1	C	419	ALA
1	F	235	GLU
1	H	356	LYS
1	H	419	ALA
1	D	459	MET
1	A	408	GLY
1	G	366	PRO
1	G	338	ILE
1	G	293	ILE
1	H	178	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/383 (98%)	300 (80%)	76 (20%)	1	4
1	B	377/383 (98%)	298 (79%)	79 (21%)	1	3
1	C	377/383 (98%)	287 (76%)	90 (24%)	1	2
1	D	376/383 (98%)	299 (80%)	77 (20%)	1	3
1	E	374/383 (98%)	300 (80%)	74 (20%)	1	4
1	F	376/383 (98%)	286 (76%)	90 (24%)	1	2
1	G	376/383 (98%)	288 (77%)	88 (23%)	1	2
1	H	376/383 (98%)	299 (80%)	77 (20%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3008/3064 (98%)	2357 (78%)	651 (22%)	1 3

All (651) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	19	THR
1	A	34	ILE
1	A	42	VAL
1	A	59	LEU
1	A	63	GLU
1	A	66	ARG
1	A	79	SER
1	A	87	SER
1	A	90	THR
1	A	94	ILE
1	A	95	ARG
1	A	98	ARG
1	A	102	VAL
1	A	118	LYS
1	A	122	SER
1	A	127	ASP
1	A	142	VAL
1	A	146	VAL
1	A	167	ASN
1	A	171	ILE
1	A	174	SER
1	A	175	GLU
1	A	176	ILE
1	A	180	SER
1	A	184	ILE
1	A	185	VAL
1	A	187	LEU
1	A	189	THR
1	A	190	GLU
1	A	191	VAL
1	A	199	ASN
1	A	201	VAL
1	A	207	THR
1	A	210	GLN
1	A	212	LEU
1	A	214	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	221	ILE
1	A	229	THR
1	A	232	ARG
1	A	238	LYS
1	A	242	LYS
1	A	243	ARG
1	A	247	GLU
1	A	262	ILE
1	A	273	ILE
1	A	291	LYS
1	A	293	ILE
1	A	309	ARG
1	A	324	THR
1	A	327	LEU
1	A	328	ARG
1	A	338	ILE
1	A	342	GLN
1	A	351	LYS
1	A	356	LYS
1	A	358	LEU
1	A	374	GLN
1	A	376	ARG
1	A	377	VAL
1	A	387	VAL
1	A	393	SER
1	A	397	GLU
1	A	399	LEU
1	A	415	THR
1	A	416	GLN
1	A	423	LYS
1	A	440	ARG
1	A	450	VAL
1	A	458	GLU
1	A	469	GLU
1	A	475	VAL
1	A	477	VAL
1	A	480	LYS
1	A	481	ILE
1	A	487	ARG
1	B	1	MET
1	B	2	GLN
1	B	10	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	15	VAL
1	B	19	THR
1	B	34	ILE
1	B	42	VAL
1	B	43	ASP
1	B	50	LYS
1	B	63	GLU
1	B	66	ARG
1	B	74	ARG
1	B	79	SER
1	B	81	GLU
1	B	94	ILE
1	B	95	ARG
1	B	115	MET
1	B	118	LYS
1	B	122	SER
1	B	137	LYS
1	B	142	VAL
1	B	145	ILE
1	B	146	VAL
1	B	172	LYS
1	B	175	GLU
1	B	184	ILE
1	B	189	THR
1	B	191	VAL
1	B	195	LYS
1	B	201	VAL
1	B	212	LEU
1	B	220	LYS
1	B	221	ILE
1	B	242	LYS
1	B	243	ARG
1	B	245	GLN
1	B	247	GLU
1	B	251	LYS
1	B	258	GLU
1	B	262	ILE
1	B	276	ASN
1	B	299	GLU
1	B	300	ARG
1	B	317	GLU
1	B	324	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	327	LEU
1	B	328	ARG
1	B	329	ARG
1	B	338	ILE
1	B	341	GLU
1	B	345	LYS
1	B	351	LYS
1	B	358	LEU
1	B	372	LYS
1	B	374	GLN
1	B	376	ARG
1	B	377	VAL
1	B	380	GLU
1	B	381	GLU
1	B	387	VAL
1	B	393	SER
1	B	399	LEU
1	B	405	THR
1	B	406	GLU
1	B	415	THR
1	B	423	LYS
1	B	426	ASN
1	B	432	MET
1	B	440	ARG
1	B	450	VAL
1	B	452	GLN
1	B	457	ARG
1	B	458	GLU
1	B	468	THR
1	B	475	VAL
1	B	477	VAL
1	B	480	LYS
1	B	481	ILE
1	B	487	ARG
1	C	1	MET
1	C	2	GLN
1	C	15	VAL
1	C	19	THR
1	C	23	VAL
1	C	24	SER
1	C	30	LEU
1	C	33	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	34	ILE
1	C	42	VAL
1	C	43	ASP
1	C	70	LYS
1	C	79	SER
1	C	84	GLN
1	C	87	SER
1	C	90	THR
1	C	98	ARG
1	C	102	VAL
1	C	104	ARG
1	C	118	LYS
1	C	122	SER
1	C	135	GLN
1	C	142	VAL
1	C	156	SER
1	C	169	ILE
1	C	171	ILE
1	C	172	LYS
1	C	175	GLU
1	C	176	ILE
1	C	180	SER
1	C	184	ILE
1	C	189	THR
1	C	191	VAL
1	C	199	ASN
1	C	201	VAL
1	C	212	LEU
1	C	220	LYS
1	C	221	ILE
1	C	227	THR
1	C	229	THR
1	C	235	GLU
1	C	237	SER
1	C	244	ILE
1	C	247	GLU
1	C	258	GLU
1	C	262	ILE
1	C	263	GLU
1	C	271	TRP
1	C	302	ILE
1	C	309	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	323	LEU
1	C	327	LEU
1	C	328	ARG
1	C	329	ARG
1	C	334	SER
1	C	338	ILE
1	C	340	ILE
1	C	345	LYS
1	C	351	LYS
1	C	354	ASP
1	C	356	LYS
1	C	374	GLN
1	C	376	ARG
1	C	377	VAL
1	C	378	CYS
1	C	380	GLU
1	C	387	VAL
1	C	388	THR
1	C	391	ARG
1	C	393	SER
1	C	399	LEU
1	C	401	ILE
1	C	404	ASN
1	C	411	SER
1	C	416	GLN
1	C	423	LYS
1	C	429	HIS
1	C	432	MET
1	C	440	ARG
1	C	445	SER
1	C	450	VAL
1	C	458	GLU
1	C	466	ASP
1	C	468	THR
1	C	469	GLU
1	C	471	ARG
1	C	478	ASP
1	C	480	LYS
1	C	481	ILE
1	C	487	ARG
1	D	2	GLN
1	D	10	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	12	VAL
1	D	19	THR
1	D	24	SER
1	D	59	LEU
1	D	63	GLU
1	D	70	LYS
1	D	74	ARG
1	D	76	GLU
1	D	81	GLU
1	D	84	GLN
1	D	95	ARG
1	D	97	SER
1	D	104	ARG
1	D	118	LYS
1	D	122	SER
1	D	135	GLN
1	D	136	ARG
1	D	137	LYS
1	D	159	MET
1	D	174	SER
1	D	175	GLU
1	D	180	SER
1	D	184	ILE
1	D	191	VAL
1	D	201	VAL
1	D	212	LEU
1	D	220	LYS
1	D	221	ILE
1	D	233	ILE
1	D	238	LYS
1	D	242	LYS
1	D	243	ARG
1	D	247	GLU
1	D	258	GLU
1	D	263	GLU
1	D	273	ILE
1	D	291	LYS
1	D	299	GLU
1	D	300	ARG
1	D	309	ARG
1	D	317	GLU
1	D	320	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	323	LEU
1	D	324	THR
1	D	327	LEU
1	D	328	ARG
1	D	329	ARG
1	D	331	ARG
1	D	338	ILE
1	D	342	GLN
1	D	345	LYS
1	D	354	ASP
1	D	356	LYS
1	D	358	LEU
1	D	374	GLN
1	D	376	ARG
1	D	377	VAL
1	D	380	GLU
1	D	387	VAL
1	D	393	SER
1	D	399	LEU
1	D	404	ASN
1	D	413	LEU
1	D	415	THR
1	D	416	GLN
1	D	423	LYS
1	D	432	MET
1	D	445	SER
1	D	450	VAL
1	D	457	ARG
1	D	468	THR
1	D	477	VAL
1	D	481	ILE
1	D	486	LYS
1	D	487	ARG
1	E	1	MET
1	E	8	ASP
1	E	10	ARG
1	E	15	VAL
1	E	19	THR
1	E	34	ILE
1	E	51	ARG
1	E	74	ARG
1	E	79	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	87	SER
1	E	94	ILE
1	E	95	ARG
1	E	104	ARG
1	E	124	ILE
1	E	135	GLN
1	E	137	LYS
1	E	142	VAL
1	E	146	VAL
1	E	153	MET
1	E	172	LYS
1	E	175	GLU
1	E	180	SER
1	E	184	ILE
1	E	189	THR
1	E	191	VAL
1	E	195	LYS
1	E	201	VAL
1	E	207	THR
1	E	212	LEU
1	E	214	GLU
1	E	220	LYS
1	E	229	THR
1	E	232	ARG
1	E	233	ILE
1	E	238	LYS
1	E	242	LYS
1	E	243	ARG
1	E	247	GLU
1	E	258	GLU
1	E	262	ILE
1	E	273	ILE
1	E	304	LEU
1	E	309	ARG
1	E	324	THR
1	E	327	LEU
1	E	328	ARG
1	E	338	ILE
1	E	345	LYS
1	E	351	LYS
1	E	355	ASP
1	E	356	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	358	LEU
1	E	374	GLN
1	E	376	ARG
1	E	386	PHE
1	E	387	VAL
1	E	388	THR
1	E	391	ARG
1	E	393	SER
1	E	399	LEU
1	E	405	THR
1	E	415	THR
1	E	416	GLN
1	E	423	LYS
1	E	426	ASN
1	E	432	MET
1	E	439	LYS
1	E	440	ARG
1	E	450	VAL
1	E	458	GLU
1	E	468	THR
1	E	477	VAL
1	E	480	LYS
1	E	481	ILE
1	F	1	MET
1	F	10	ARG
1	F	19	THR
1	F	30	LEU
1	F	34	ILE
1	F	42	VAL
1	F	44	LEU
1	F	50	LYS
1	F	51	ARG
1	F	59	LEU
1	F	63	GLU
1	F	70	LYS
1	F	77	GLU
1	F	79	SER
1	F	80	GLU
1	F	84	GLN
1	F	87	SER
1	F	94	ILE
1	F	95	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	122	SER
1	F	127	ASP
1	F	135	GLN
1	F	136	ARG
1	F	142	VAL
1	F	146	VAL
1	F	171	ILE
1	F	172	LYS
1	F	174	SER
1	F	175	GLU
1	F	176	ILE
1	F	186	GLU
1	F	188	MET
1	F	200	VAL
1	F	201	VAL
1	F	210	GLN
1	F	212	LEU
1	F	214	GLU
1	F	221	ILE
1	F	226	SER
1	F	229	THR
1	F	238	LYS
1	F	243	ARG
1	F	245	GLN
1	F	247	GLU
1	F	251	LYS
1	F	258	GLU
1	F	262	ILE
1	F	263	GLU
1	F	289	LEU
1	F	293	ILE
1	F	299	GLU
1	F	300	ARG
1	F	309	ARG
1	F	310	LEU
1	F	320	MET
1	F	323	LEU
1	F	324	THR
1	F	327	LEU
1	F	328	ARG
1	F	329	ARG
1	F	330	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	338	ILE
1	F	340	ILE
1	F	341	GLU
1	F	345	LYS
1	F	351	LYS
1	F	354	ASP
1	F	374	GLN
1	F	376	ARG
1	F	377	VAL
1	F	379	GLN
1	F	381	GLU
1	F	382	VAL
1	F	390	VAL
1	F	391	ARG
1	F	393	SER
1	F	399	LEU
1	F	415	THR
1	F	423	LYS
1	F	428	ILE
1	F	432	MET
1	F	445	SER
1	F	450	VAL
1	F	458	GLU
1	F	464	ILE
1	F	468	THR
1	F	471	ARG
1	F	478	ASP
1	F	480	LYS
1	F	481	ILE
1	G	8	ASP
1	G	10	ARG
1	G	15	VAL
1	G	19	THR
1	G	20	ILE
1	G	21	ASP
1	G	30	LEU
1	G	34	ILE
1	G	42	VAL
1	G	43	ASP
1	G	66	ARG
1	G	70	LYS
1	G	74	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	75	ILE
1	G	79	SER
1	G	87	SER
1	G	94	ILE
1	G	98	ARG
1	G	118	LYS
1	G	122	SER
1	G	136	ARG
1	G	142	VAL
1	G	145	ILE
1	G	146	VAL
1	G	149	ASN
1	G	159	MET
1	G	172	LYS
1	G	174	SER
1	G	175	GLU
1	G	177	THR
1	G	179	LEU
1	G	183	ARG
1	G	184	ILE
1	G	191	VAL
1	G	195	LYS
1	G	201	VAL
1	G	212	LEU
1	G	214	GLU
1	G	220	LYS
1	G	221	ILE
1	G	224	THR
1	G	238	LYS
1	G	243	ARG
1	G	247	GLU
1	G	251	LYS
1	G	258	GLU
1	G	262	ILE
1	G	271	TRP
1	G	289	LEU
1	G	293	ILE
1	G	299	GLU
1	G	300	ARG
1	G	314	MET
1	G	320	MET
1	G	323	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	328	ARG
1	G	331	ARG
1	G	334	SER
1	G	336	ILE
1	G	337	ASP
1	G	338	ILE
1	G	340	ILE
1	G	345	LYS
1	G	358	LEU
1	G	369	VAL
1	G	376	ARG
1	G	377	VAL
1	G	380	GLU
1	G	387	VAL
1	G	388	THR
1	G	390	VAL
1	G	393	SER
1	G	399	LEU
1	G	404	ASN
1	G	415	THR
1	G	416	GLN
1	G	423	LYS
1	G	432	MET
1	G	435	ILE
1	G	447	PHE
1	G	450	VAL
1	G	453	SER
1	G	457	ARG
1	G	458	GLU
1	G	468	THR
1	G	477	VAL
1	G	481	ILE
1	G	486	LYS
1	H	1	MET
1	H	4	GLN
1	H	15	VAL
1	H	19	THR
1	H	23	VAL
1	H	34	ILE
1	H	59	LEU
1	H	66	ARG
1	H	79	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	87	SER
1	H	88	LEU
1	H	95	ARG
1	H	100	LEU
1	H	118	LYS
1	H	122	SER
1	H	124	ILE
1	H	127	ASP
1	H	146	VAL
1	H	155	THR
1	H	156	SER
1	H	168	THR
1	H	175	GLU
1	H	184	ILE
1	H	191	VAL
1	H	195	LYS
1	H	200	VAL
1	H	212	LEU
1	H	214	GLU
1	H	221	ILE
1	H	229	THR
1	H	231	ARG
1	H	233	ILE
1	H	238	LYS
1	H	242	LYS
1	H	243	ARG
1	H	244	ILE
1	H	247	GLU
1	H	258	GLU
1	H	262	ILE
1	H	263	GLU
1	H	271	TRP
1	H	273	ILE
1	H	299	GLU
1	H	304	LEU
1	H	306	LYS
1	H	309	ARG
1	H	323	LEU
1	H	324	THR
1	H	325	SER
1	H	327	LEU
1	H	328	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	329	ARG
1	H	330	ASP
1	H	336	ILE
1	H	338	ILE
1	H	345	LYS
1	H	354	ASP
1	H	356	LYS
1	H	358	LEU
1	H	362	PHE
1	H	363	TYR
1	H	380	GLU
1	H	387	VAL
1	H	393	SER
1	H	399	LEU
1	H	404	ASN
1	H	415	THR
1	H	416	GLN
1	H	423	LYS
1	H	432	MET
1	H	450	VAL
1	H	458	GLU
1	H	471	ARG
1	H	477	VAL
1	H	478	ASP
1	H	480	LYS
1	H	481	ILE

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

Mol	Chain	Res	Type
1	A	2	GLN
1	A	132	ASN
1	A	144	GLN
1	A	277	GLN
1	A	290	HIS
1	A	296	GLN
1	A	342	GLN
1	A	404	ASN
1	A	417	ASN
1	B	2	GLN
1	B	84	GLN
1	B	92	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	132	ASN
1	B	276	ASN
1	B	290	HIS
1	B	417	ASN
1	B	465	HIS
1	B	484	HIS
1	C	2	GLN
1	C	132	ASN
1	C	135	GLN
1	C	215	HIS
1	C	245	GLN
1	C	277	GLN
1	C	279	GLN
1	C	290	HIS
1	C	416	GLN
1	C	417	ASN
1	C	429	HIS
1	D	2	GLN
1	D	84	GLN
1	D	132	ASN
1	D	206	HIS
1	D	277	GLN
1	D	290	HIS
1	D	404	ASN
1	D	417	ASN
1	D	429	HIS
1	D	436	ASN
1	E	2	GLN
1	E	84	GLN
1	E	132	ASN
1	E	135	GLN
1	E	144	GLN
1	E	277	GLN
1	E	290	HIS
1	E	342	GLN
1	E	374	GLN
1	E	417	ASN
1	E	426	ASN
1	F	2	GLN
1	F	144	GLN
1	F	277	GLN
1	F	290	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	296	GLN
1	F	379	GLN
1	F	416	GLN
1	F	417	ASN
1	F	429	HIS
1	F	465	HIS
1	G	2	GLN
1	G	84	GLN
1	G	132	ASN
1	G	144	GLN
1	G	290	HIS
1	G	379	GLN
1	G	426	ASN
1	H	2	GLN
1	H	4	GLN
1	H	84	GLN
1	H	92	HIS
1	H	132	ASN
1	H	135	GLN
1	H	215	HIS
1	H	277	GLN
1	H	290	HIS
1	H	342	GLN
1	H	379	GLN
1	H	417	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/495 (98%)	-0.02	7 (1%) 73 72	14, 34, 61, 93	0
1	B	487/495 (98%)	0.13	8 (1%) 70 68	16, 36, 61, 102	1 (0%)
1	C	487/495 (98%)	0.12	7 (1%) 73 72	12, 37, 62, 145	1 (0%)
1	D	487/495 (98%)	0.13	6 (1%) 76 75	14, 35, 59, 165	0
1	E	485/495 (97%)	0.18	12 (2%) 58 55	16, 37, 61, 113	0
1	F	487/495 (98%)	0.35	16 (3%) 49 45	11, 44, 76, 131	0
1	G	487/495 (98%)	0.49	21 (4%) 40 36	18, 47, 94, 137	0
1	H	487/495 (98%)	0.43	22 (4%) 38 34	16, 45, 79, 148	0
All	All	3894/3960 (98%)	0.23	99 (2%) 58 55	11, 39, 73, 165	2 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	3.9
1	G	311	GLY	3.8
1	H	359	ALA	3.7
1	D	481	ILE	3.6
1	F	116	ALA	3.5
1	F	382	VAL	3.3
1	F	1	MET	3.3
1	C	354	ASP	3.3
1	E	357	ALA	3.2
1	H	354	ASP	3.2
1	H	358	LEU	3.2
1	H	337	ASP	3.1
1	B	1	MET	3.1
1	G	377	VAL	3.1
1	F	210	GLN	3.1
1	G	396	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	229	THR	3.1
1	E	482	ALA	3.1
1	E	247	GLU	3.0
1	G	384	GLY	3.0
1	F	481	ILE	3.0
1	H	487	ARG	2.9
1	C	1	MET	2.9
1	H	361	GLY	2.9
1	E	481	ILE	2.9
1	D	356	LYS	2.8
1	G	369	VAL	2.8
1	D	351	LYS	2.8
1	H	19	THR	2.8
1	G	351	LYS	2.8
1	B	429[A]	HIS	2.8
1	H	1	MET	2.8
1	E	1	MET	2.7
1	G	357	ALA	2.7
1	F	376	ARG	2.6
1	G	36	ALA	2.6
1	G	338	ILE	2.6
1	F	351	LYS	2.6
1	E	404	ASN	2.6
1	E	480	LYS	2.5
1	G	346	VAL	2.5
1	H	481	ILE	2.5
1	H	364	VAL	2.5
1	B	351	LYS	2.5
1	B	479	ALA	2.5
1	C	351	LYS	2.4
1	E	483	PRO	2.4
1	H	382	VAL	2.4
1	E	485	PHE	2.4
1	E	174	SER	2.4
1	F	377	VAL	2.4
1	G	348	ALA	2.4
1	A	481	ILE	2.3
1	F	60	GLY	2.3
1	H	23	VAL	2.3
1	H	429	HIS	2.3
1	F	354	ASP	2.3
1	G	315	ASP	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	344	GLY	2.3
1	H	355	ASP	2.3
1	A	479	ALA	2.3
1	A	478	ASP	2.3
1	B	10	ARG	2.3
1	H	143	ALA	2.2
1	G	309	ARG	2.2
1	A	18	GLY	2.2
1	G	323	LEU	2.2
1	F	357	ALA	2.2
1	G	359	ALA	2.2
1	B	374	GLN	2.2
1	F	36	ALA	2.2
1	F	335	TYR	2.2
1	A	1	MET	2.2
1	A	357	ALA	2.2
1	C	60	GLY	2.2
1	B	393	SER	2.2
1	G	1	MET	2.1
1	C	369	VAL	2.1
1	G	386	PHE	2.1
1	A	235	GLU	2.1
1	H	480	LYS	2.1
1	F	18	GLY	2.1
1	H	21	ASP	2.1
1	H	386	PHE	2.1
1	D	341	GLU	2.1
1	E	347	LEU	2.1
1	G	325	SER	2.1
1	C	487	ARG	2.1
1	G	327	LEU	2.1
1	H	360	ASN	2.1
1	D	299	GLU	2.0
1	G	374	GLN	2.0
1	H	340	ILE	2.0
1	C	377	VAL	2.0
1	F	386	PHE	2.0
1	G	331	ARG	2.0
1	H	357	ALA	2.0
1	H	325	SER	2.0
1	B	481	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.