



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:57 AM UTC

PDB ID : 4WHB / pdb_00004whb
Title : Crystal structure of phenylurea hydrolase B
Authors : Sugrue, E.; Carr, P.D.; Khurana, J.L.; Jackson, C.J.
Deposited on : 2014-09-21
Resolution : 2.96 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

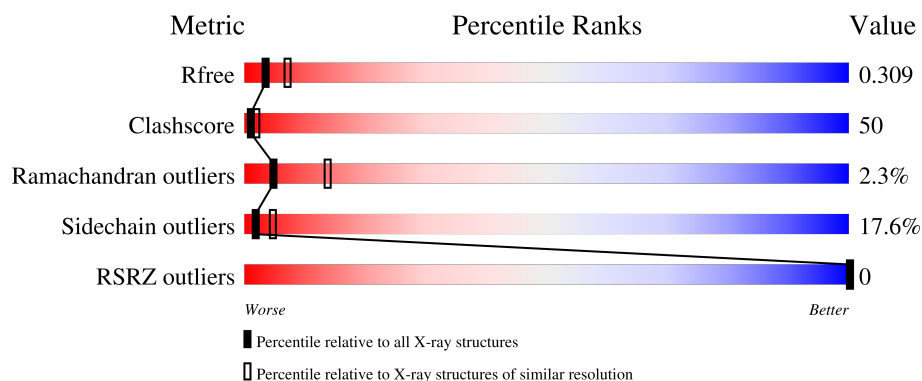
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

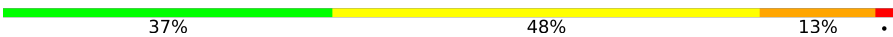
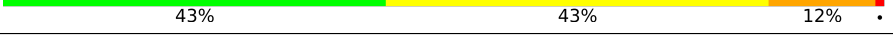
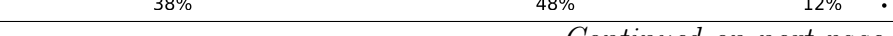
The reported resolution of this entry is 2.96 Å.

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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	461	
1	B	461	
1	C	461	
1	D	461	
1	E	461	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	461	 33% 52% 12% •
1	G	461	 39% 48% 11% •
1	H	461	 32% 50% 15% •

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 55405 atoms, of which 27459 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 Phenylurea hydrolase B.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	E	459	Total	C	H	N	O	S	0	0	0
			6918	2190	3430	618	670	10			
1	A	459	Total	C	H	N	O	S	0	0	0
			6915	2190	3427	618	670	10			
1	B	459	Total	C	H	N	O	S	0	2	0
			6944	2196	3445	622	671	10			
1	C	459	Total	C	H	N	O	S	0	2	0
			6941	2196	3442	622	671	10			
1	D	459	Total	C	H	N	O	S	0	0	0
			6917	2190	3429	618	670	10			
1	F	459	Total	C	H	N	O	S	0	0	0
			6916	2190	3428	618	670	10			
1	G	459	Total	C	H	N	O	S	0	0	0
			6917	2190	3429	618	670	10			
1	H	459	Total	C	H	N	O	S	0	0	0
			6917	2190	3429	618	670	10			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	4	Total	O	0	0
			4	4		
3	A	3	Total	O	0	0
			3	3		
3	B	3	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

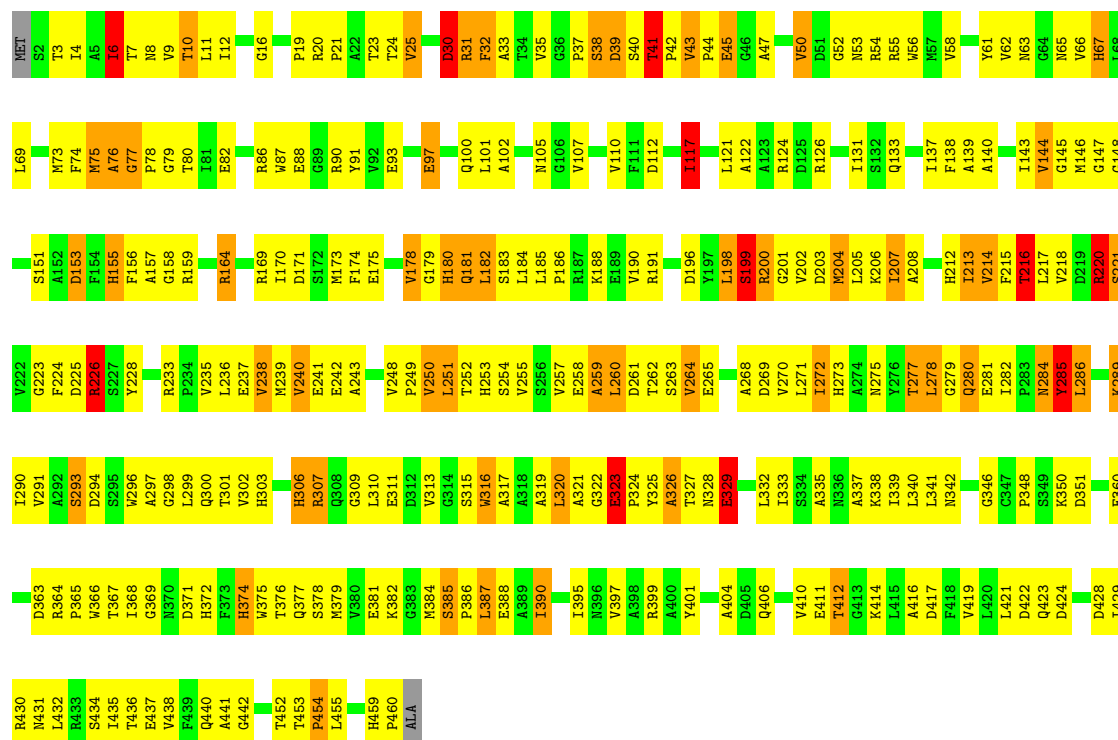
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	O 2	0	0
3	F	3	Total 3	O 3	0	0
3	G	1	Total 1	O 1	0	0
3	H	3	Total 3	O 3	0	0

3 Residue-property plots

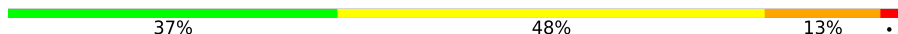
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

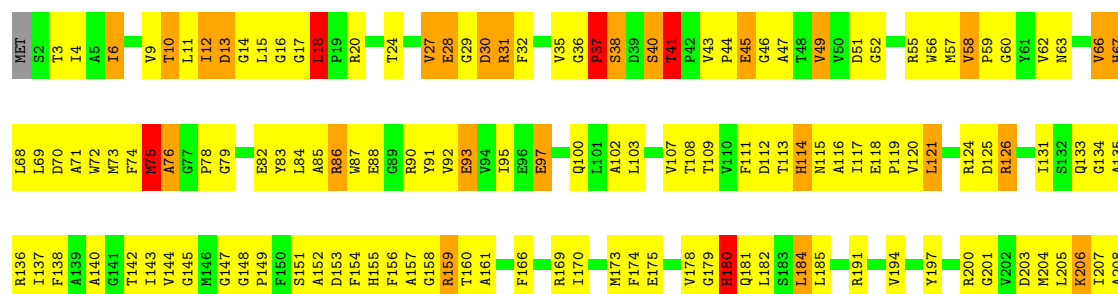
• Molecule 1: Phenylurea hydrolase B

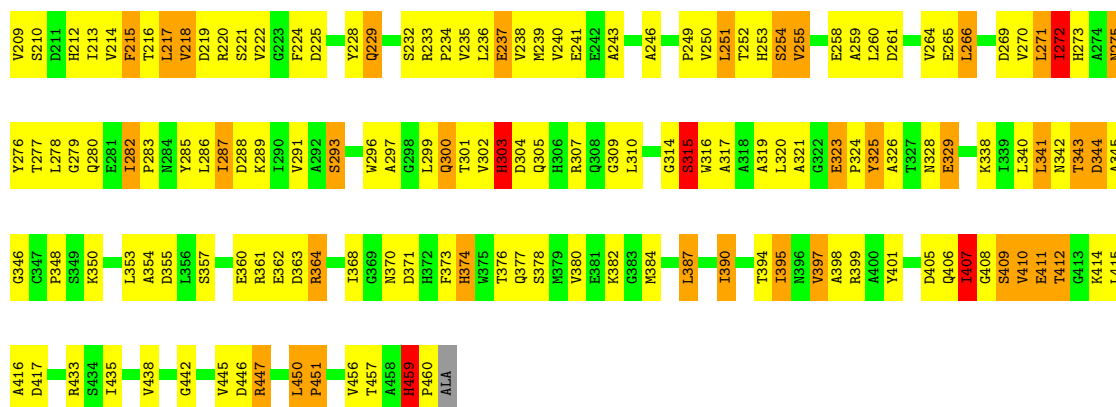
Chain E: 



• Molecule 1: Phenylurea hydrolase B

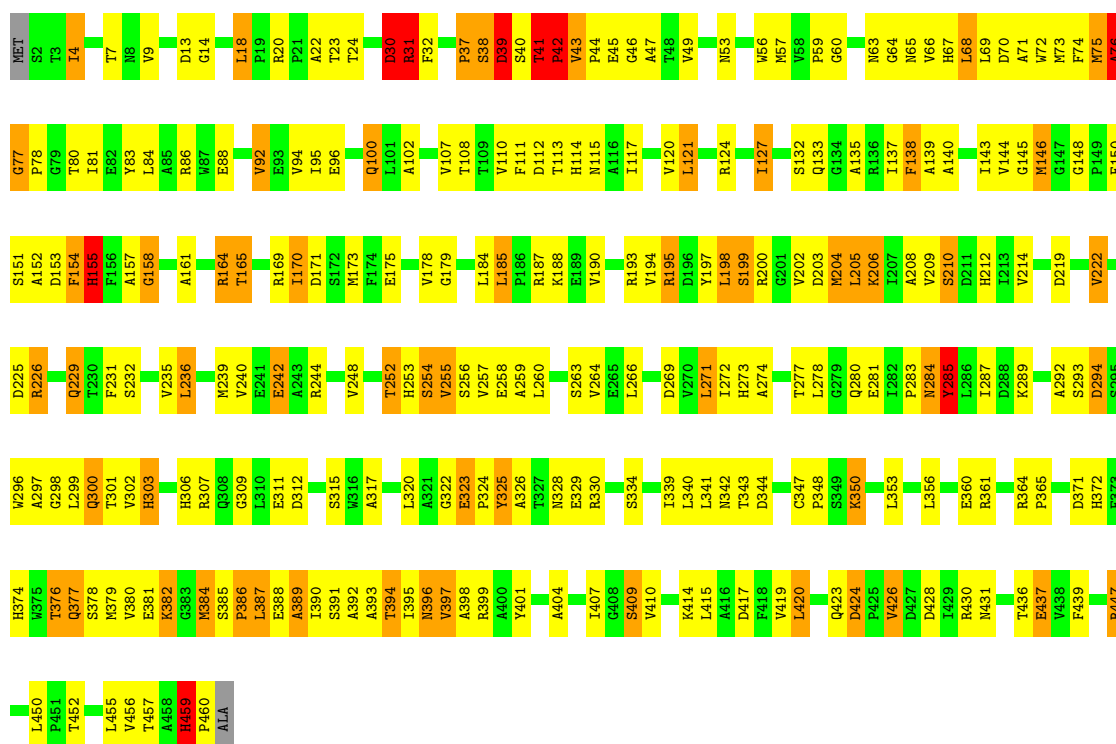
Chain A: 





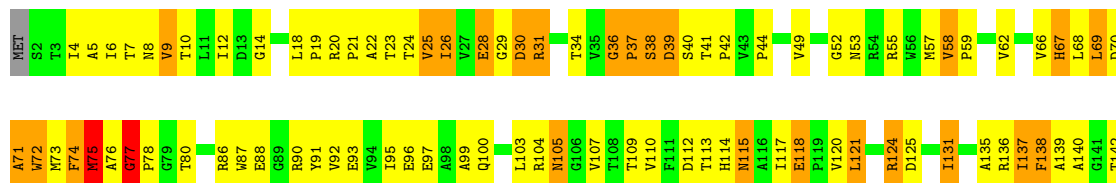
• Molecule 1: Phenylurea hydrolase B

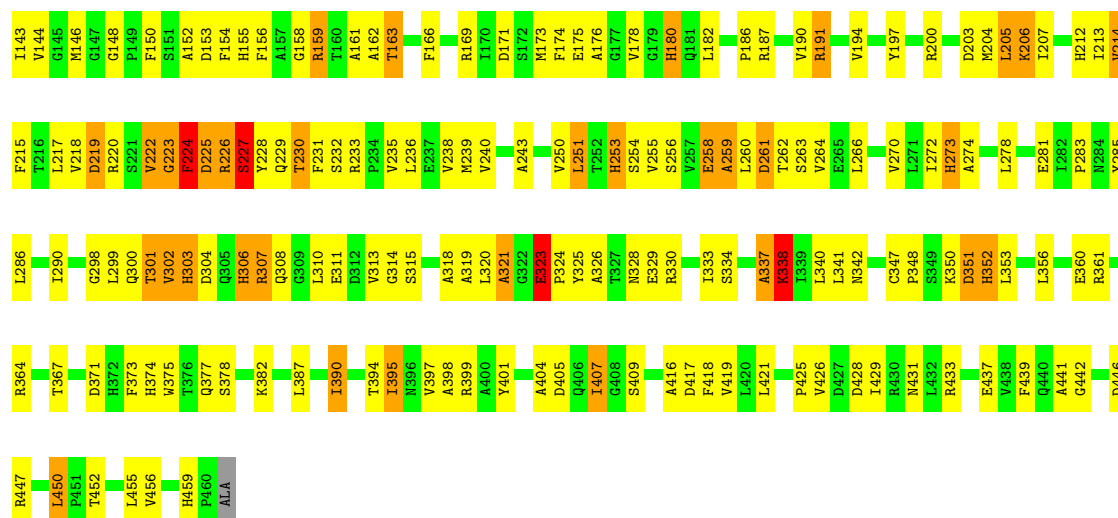
Chain B: 43% 41% 13% .



• Molecule 1: Phenylurea hydrolase B

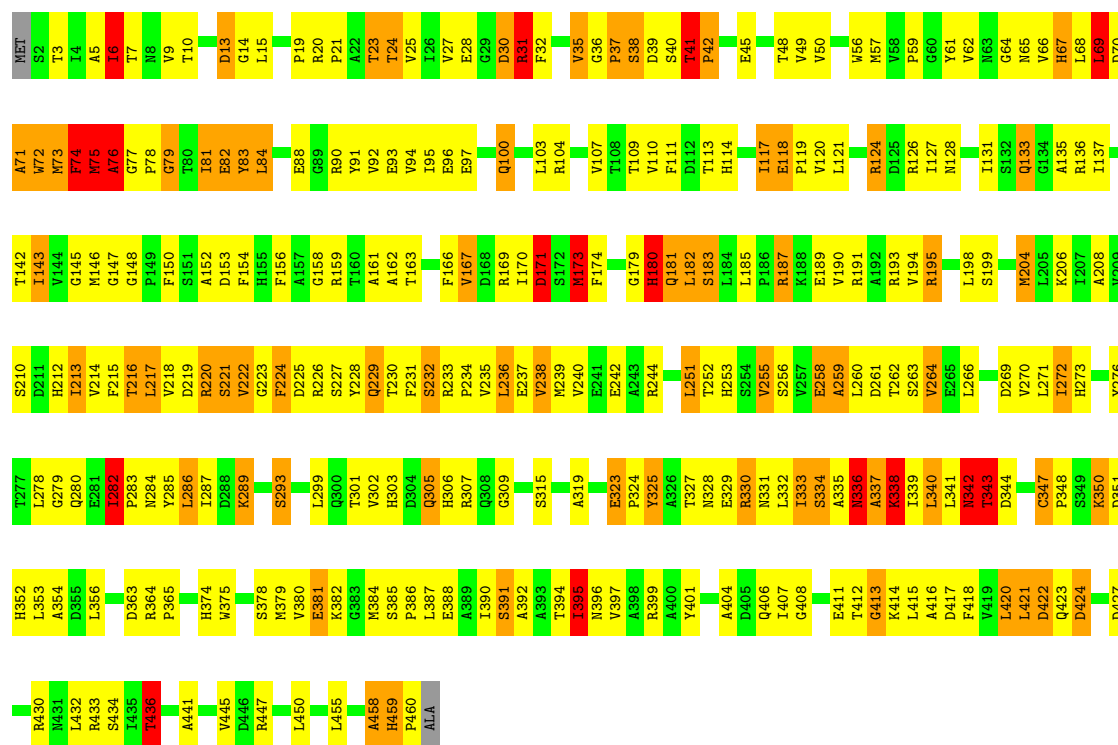
Chain C: 43% 43% 12% .





• Molecule 1: Phenylurea hydrolase B

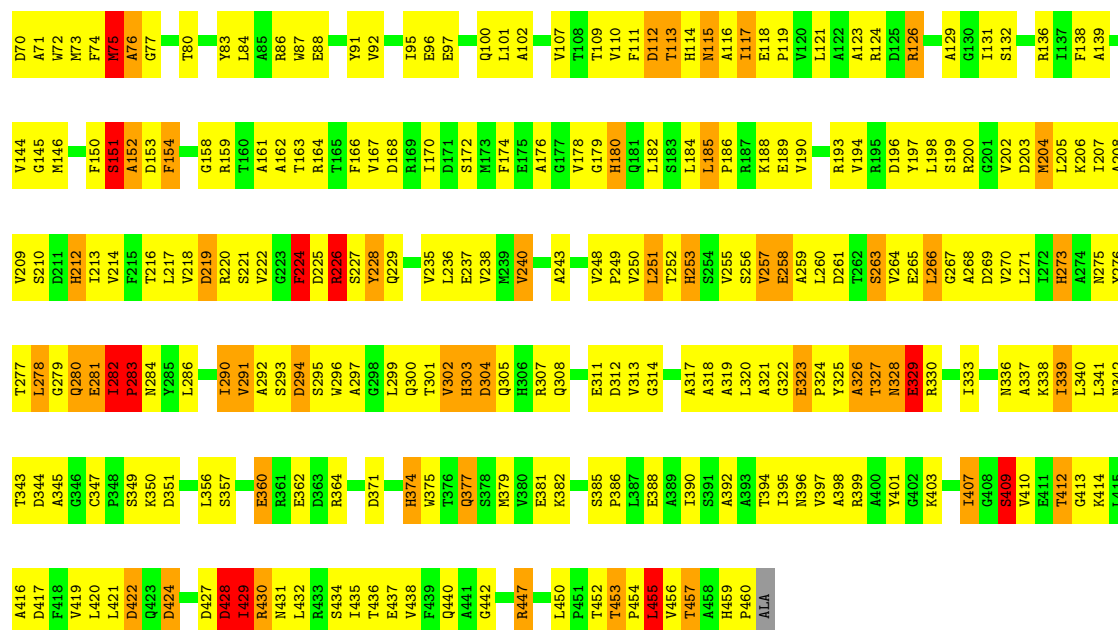
Chain D: 38% 43% 15%



• Molecule 1: Phenylurea hydrolase B

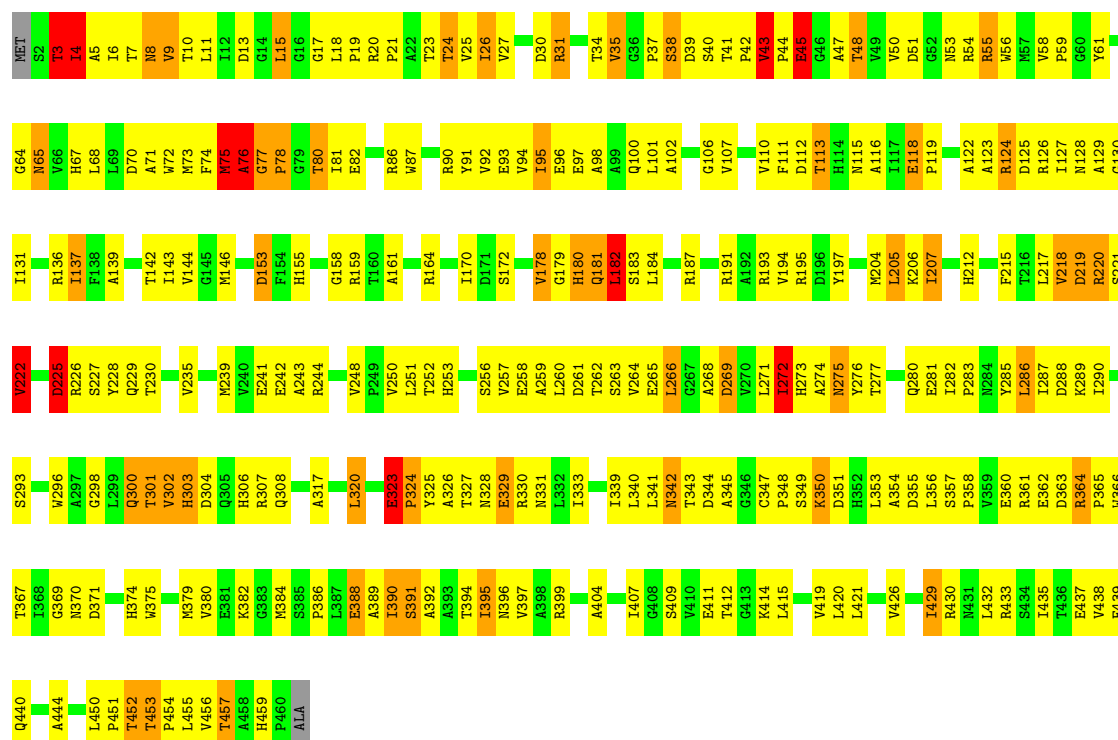
Chain F: 33% 52% 12%





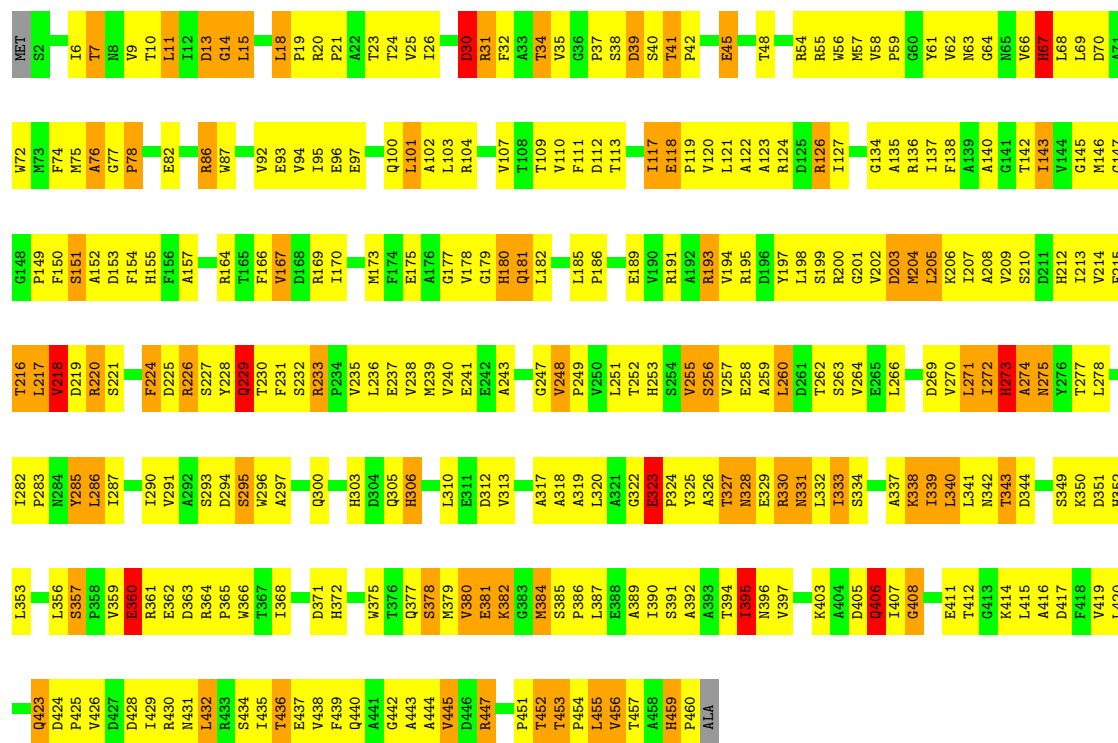
• Molecule 1: Phenylurea hydrolase B

Chain G: 39% 48% 11% .



• Molecule 1: Phenylurea hydrolase B

Chain H: 32% 50% 15% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.37Å 100.53Å 238.55Å 90.00° 98.37° 90.00°	Depositor
Resolution (Å)	39.59 – 2.96 39.59 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.9 (39.59-2.96) 89.7 (39.59-2.96)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.95Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.252 , 0.309 0.263 , 0.309	Depositor DCC
R_{free} test set	3768 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	1.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.39$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	0.085 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55405	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.7450e-03.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.98	12/3560 (0.3%)	1.22	36/4857 (0.7%)
1	B	1.15	10/3576 (0.3%)	1.26	34/4878 (0.7%)
1	C	0.96	13/3576 (0.4%)	1.19	42/4878 (0.9%)
1	D	1.08	11/3560 (0.3%)	1.24	32/4857 (0.7%)
1	E	1.03	6/3560 (0.2%)	1.19	30/4857 (0.6%)
1	F	0.96	12/3560 (0.3%)	1.21	34/4857 (0.7%)
1	G	0.99	10/3560 (0.3%)	1.19	25/4857 (0.5%)
1	H	0.95	10/3560 (0.3%)	1.21	32/4857 (0.7%)
All	All	1.01	84/28512 (0.3%)	1.21	265/38898 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	6
1	C	0	5
1	D	0	7
1	E	0	4
1	F	0	3
1	G	0	7
1	H	0	1
All	All	0	39

All (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	76	ALA	CA-C	-9.17	1.40	1.52
1	E	43	VAL	C-N	7.45	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	181	GLN	CD-OE1	7.32	1.37	1.23
1	G	323	GLU	C-N	6.97	1.39	1.33
1	G	300	GLN	CD-OE1	6.85	1.36	1.23
1	H	272	ILE	CA-C	-6.82	1.45	1.53
1	C	229	GLN	CD-OE1	6.61	1.36	1.23
1	D	229	GLN	CD-OE1	6.39	1.35	1.23
1	H	272	ILE	N-CA	-6.20	1.39	1.46
1	D	342	ASN	C-O	-6.16	1.17	1.24
1	G	75	MET	CA-C	-6.13	1.45	1.52
1	B	284	ASN	CA-C	-6.11	1.45	1.53
1	F	377	GLN	CD-OE1	6.07	1.35	1.23
1	A	229	GLN	CD-OE1	6.04	1.35	1.23
1	D	305	GLN	CD-OE1	5.95	1.34	1.23
1	E	41	THR	CA-C	5.91	1.60	1.52
1	B	398	ALA	C-O	-5.76	1.16	1.24
1	B	303	HIS	CA-C	-5.76	1.45	1.53
1	G	65	ASN	CG-OD1	5.74	1.34	1.23
1	D	336	ASN	CG-OD1	5.71	1.34	1.23
1	A	275	ASN	CA-C	-5.65	1.45	1.52
1	F	374	HIS	ND1-CE1	5.64	1.38	1.32
1	A	76	ALA	N-CA	-5.60	1.39	1.46
1	H	423	GLN	CD-OE1	5.59	1.34	1.23
1	F	455	LEU	N-CA	-5.58	1.40	1.46
1	C	105	ASN	CG-ND2	-5.57	1.21	1.33
1	E	300	GLN	CD-OE1	5.56	1.34	1.23
1	B	76	ALA	N-CA	-5.56	1.38	1.45
1	D	305	GLN	CD-NE2	-5.56	1.21	1.33
1	D	180	HIS	C-O	-5.56	1.17	1.24
1	A	76	ALA	CA-C	-5.55	1.45	1.52
1	B	18	LEU	C-N	5.52	1.40	1.33
1	H	26	ILE	C-O	-5.50	1.18	1.24
1	C	261	ASP	C-O	-5.50	1.17	1.24
1	C	67	HIS	CD2-NE2	-5.48	1.31	1.37
1	C	303	HIS	ND1-CE1	5.48	1.38	1.32
1	D	344	ASP	C-O	-5.48	1.17	1.24
1	H	67	HIS	ND1-CE1	5.47	1.38	1.32
1	D	180	HIS	CA-C	-5.45	1.46	1.52
1	D	67	HIS	CD2-NE2	-5.43	1.31	1.37
1	F	65	ASN	CG-OD1	5.41	1.33	1.23
1	F	431	ASN	CG-OD1	5.41	1.33	1.23
1	G	76	ALA	CA-C	-5.39	1.46	1.52
1	H	273	HIS	ND1-CE1	5.39	1.38	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	GLY	C-O	5.38	1.28	1.23
1	A	459	HIS	ND1-CE1	5.34	1.37	1.32
1	F	212	HIS	CD2-NE2	-5.33	1.31	1.37
1	A	114	HIS	ND1-CE1	5.32	1.37	1.32
1	F	253	HIS	CA-C	-5.32	1.46	1.52
1	F	67	HIS	CD2-NE2	-5.27	1.32	1.37
1	A	342	ASN	CG-ND2	-5.26	1.22	1.33
1	C	180	HIS	ND1-CE1	5.25	1.37	1.32
1	E	67	HIS	ND1-CE1	5.25	1.37	1.32
1	B	114	HIS	CD2-NE2	-5.24	1.32	1.37
1	H	300	GLN	CD-OE1	5.24	1.33	1.23
1	C	227	SER	CA-CB	-5.22	1.47	1.53
1	G	331	ASN	CG-OD1	5.21	1.33	1.23
1	G	78	PRO	N-CD	5.19	1.55	1.47
1	A	303	HIS	ND1-CE1	5.17	1.37	1.32
1	G	8	ASN	CG-OD1	5.16	1.33	1.23
1	B	459	HIS	ND1-CE1	5.15	1.37	1.32
1	A	374	HIS	CD2-NE2	-5.14	1.32	1.37
1	C	459	HIS	ND1-CE1	5.14	1.37	1.32
1	C	459	HIS	CD2-NE2	-5.14	1.32	1.37
1	B	42	PRO	N-CD	5.13	1.55	1.47
1	E	155	HIS	CD2-NE2	-5.13	1.32	1.37
1	F	377	GLN	CD-NE2	-5.12	1.22	1.33
1	F	180	HIS	ND1-CE1	5.11	1.37	1.32
1	A	374	HIS	ND1-CE1	5.10	1.37	1.32
1	D	436	THR	CA-C	-5.10	1.48	1.52
1	G	182	LEU	C-O	-5.10	1.17	1.24
1	C	229	GLN	CD-NE2	-5.08	1.22	1.33
1	H	360	GLU	C-O	-5.07	1.17	1.24
1	H	273	HIS	CD2-NE2	-5.06	1.32	1.37
1	D	343	THR	C-O	-5.06	1.18	1.23
1	F	280	GLN	CD-NE2	-5.06	1.22	1.33
1	C	273	HIS	CD2-NE2	-5.05	1.32	1.37
1	G	303	HIS	ND1-CE1	5.05	1.37	1.32
1	A	303	HIS	CD2-NE2	-5.04	1.32	1.37
1	H	229	GLN	CD-OE1	5.04	1.33	1.23
1	C	261	ASP	CA-C	-5.03	1.46	1.52
1	B	459	HIS	CD2-NE2	-5.02	1.32	1.37
1	F	342	ASN	CG-ND2	-5.01	1.22	1.33
1	C	225	ASP	CA-C	5.01	1.59	1.52

All (265) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	215	PHE	N-CA-C	11.63	127.53	112.41
1	A	275	ASN	N-CA-C	-11.11	99.56	113.55
1	G	77	GLY	N-CA-C	11.03	125.24	112.00
1	A	272	ILE	N-CA-C	-10.01	95.64	109.46
1	F	46	GLY	N-CA-C	-9.30	101.91	115.30
1	D	41	THR	CA-C-N	9.19	130.64	119.98
1	D	41	THR	C-N-CA	9.19	130.64	119.98
1	G	184	LEU	N-CA-C	9.14	121.33	111.36
1	A	76	ALA	N-CA-C	-9.12	91.37	110.80
1	C	39	ASP	N-CA-C	-8.35	100.85	112.45
1	E	220	ARG	N-CA-C	-8.34	99.53	110.53
1	A	41	THR	N-CA-C	8.27	128.09	109.81
1	F	282	ILE	C-N-CD	8.21	138.67	120.60
1	E	33	ALA	N-CA-C	8.18	119.97	111.14
1	D	6	ILE	N-CA-C	8.14	119.42	107.37
1	G	361	ARG	N-CA-C	8.14	120.23	111.36
1	E	79	GLY	N-CA-C	-7.97	103.53	115.00
1	B	86	ARG	N-CA-C	-7.94	99.30	110.50
1	B	39	ASP	N-CA-C	-7.76	102.35	112.68
1	F	39	ASP	N-CA-C	-7.74	102.78	111.14
1	D	325	TYR	N-CA-C	7.73	119.79	111.36
1	E	69	LEU	N-CA-C	-7.60	103.07	112.88
1	B	344	ASP	N-CA-C	-7.60	98.77	110.10
1	G	75	MET	N-CA-C	-7.56	96.94	108.96
1	C	222	VAL	N-CA-C	7.44	119.28	112.29
1	C	159	ARG	N-CA-C	-7.37	103.27	111.82
1	D	216	THR	N-CA-C	-7.37	104.29	113.28
1	G	181	GLN	N-CA-C	-7.33	101.40	110.41
1	F	283	PRO	CA-N-CD	-7.30	101.29	111.50
1	B	43	VAL	N-CA-C	7.29	116.09	108.95
1	D	171	ASP	N-CA-C	-7.26	100.75	110.55
1	H	273	HIS	N-CA-C	7.25	121.08	111.28
1	E	43	VAL	N-CA-C	7.25	115.76	109.02
1	B	70	ASP	N-CA-C	7.08	119.35	109.15
1	B	154	PHE	N-CA-C	-7.06	98.99	108.74
1	F	152	ALA	N-CA-C	-7.04	98.81	109.79
1	B	155	HIS	CB-CA-C	7.01	120.78	110.26
1	A	18	LEU	CA-C-N	7.01	128.60	119.84
1	A	18	LEU	C-N-CA	7.01	128.60	119.84
1	H	273	HIS	CB-CG-CD2	-6.98	122.12	131.20
1	C	180	HIS	CB-CG-CD2	-6.94	122.18	131.20
1	H	117	ILE	N-CA-C	6.87	116.98	110.53
1	C	337	ALA	N-CA-C	6.86	118.76	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	282	ILE	CA-C-N	-6.85	112.93	119.85
1	D	282	ILE	C-N-CA	-6.85	112.93	119.85
1	E	155	HIS	CB-CG-CD2	-6.83	122.32	131.20
1	D	42	PRO	N-CA-C	6.83	122.01	110.95
1	D	69	LEU	N-CA-C	-6.83	98.11	109.24
1	B	76	ALA	CA-C-N	6.76	133.86	121.70
1	B	76	ALA	C-N-CA	6.76	133.86	121.70
1	C	230	THR	N-CA-C	6.75	118.43	111.14
1	H	272	ILE	CA-C-O	6.75	129.19	120.69
1	A	159	ARG	N-CA-C	-6.73	104.02	111.36
1	C	77	GLY	CA-C-N	-6.71	113.39	120.03
1	C	77	GLY	C-N-CA	-6.71	113.39	120.03
1	E	67	HIS	CB-CG-CD2	-6.70	122.49	131.20
1	B	294	ASP	N-CA-C	6.70	120.63	111.39
1	E	374	HIS	N-CA-C	-6.69	103.98	111.28
1	A	282	ILE	CA-C-N	-6.66	113.93	120.52
1	A	282	ILE	C-N-CA	-6.66	113.93	120.52
1	F	258	GLU	N-CA-C	-6.66	101.17	110.35
1	B	18	LEU	CA-C-N	-6.65	113.11	119.76
1	B	18	LEU	C-N-CA	-6.65	113.11	119.76
1	H	248	VAL	CA-C-N	-6.65	113.13	119.85
1	H	248	VAL	C-N-CA	-6.65	113.13	119.85
1	B	459	HIS	CB-CG-CD2	-6.64	122.56	131.20
1	E	38	SER	CB-CA-C	-6.63	108.91	116.54
1	A	67	HIS	CB-CG-CD2	-6.63	122.58	131.20
1	A	180	HIS	N-CA-C	-6.63	96.68	110.80
1	E	43	VAL	CB-CA-C	-6.63	104.51	111.00
1	A	303	HIS	CB-CG-CD2	-6.62	122.59	131.20
1	F	212	HIS	CB-CG-CD2	-6.61	122.61	131.20
1	A	459	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	B	127	ILE	N-CA-C	6.55	117.18	110.82
1	F	374	HIS	CB-CG-CD2	-6.54	122.70	131.20
1	G	323	GLU	CA-C-N	-6.54	113.42	121.00
1	G	323	GLU	C-N-CA	-6.54	113.42	121.00
1	E	86	ARG	N-CA-C	6.53	118.19	111.14
1	B	42	PRO	CA-N-CD	-6.51	102.39	111.50
1	C	321	ALA	N-CA-C	6.51	118.45	111.36
1	D	395	ILE	CB-CA-C	-6.49	103.54	112.24
1	C	67	HIS	CB-CG-CD2	-6.49	122.77	131.20
1	G	4	ILE	N-CA-C	6.49	118.78	109.51
1	A	114	HIS	CB-CG-CD2	-6.48	122.78	131.20
1	C	459	HIS	CB-CG-CD2	-6.45	122.81	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	455	LEU	N-CA-C	-6.45	107.27	114.62
1	H	323	GLU	CA-C-N	-6.42	112.38	119.19
1	H	323	GLU	C-N-CA	-6.42	112.38	119.19
1	H	219	ASP	N-CA-C	6.42	119.54	110.23
1	D	255	VAL	N-CA-C	6.42	118.27	112.17
1	G	77	GLY	CA-C-N	-6.39	114.14	120.98
1	G	77	GLY	C-N-CA	-6.39	114.14	120.98
1	H	273	HIS	CB-CG-ND1	6.39	132.28	122.70
1	C	303	HIS	CB-CG-CD2	-6.38	122.91	131.20
1	B	138	PHE	N-CA-C	-6.35	98.85	109.07
1	H	14	GLY	N-CA-C	-6.33	106.98	115.21
1	C	20	ARG	CA-C-N	-6.32	114.22	120.98
1	C	20	ARG	C-N-CA	-6.32	114.22	120.98
1	F	385	SER	CA-C-N	6.30	126.78	119.47
1	F	385	SER	C-N-CA	6.30	126.78	119.47
1	D	67	HIS	CB-CG-CD2	-6.30	123.01	131.20
1	B	114	HIS	CB-CG-CD2	-6.29	123.03	131.20
1	F	273	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	F	67	HIS	CB-CG-CD2	-6.25	123.08	131.20
1	H	67	HIS	CB-CG-CD2	-6.24	123.09	131.20
1	C	306	HIS	CB-CG-CD2	-6.23	123.10	131.20
1	A	58	VAL	CA-C-N	-6.23	113.86	120.03
1	A	58	VAL	C-N-CA	-6.23	113.86	120.03
1	F	180	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	C	180	HIS	CB-CG-ND1	6.21	132.01	122.70
1	A	374	HIS	CB-CG-CD2	-6.19	123.16	131.20
1	H	35	VAL	N-CA-C	6.19	116.77	107.80
1	F	424	ASP	N-CA-C	6.15	118.39	109.04
1	D	13	ASP	N-CA-C	-6.15	104.68	111.82
1	F	428	ASP	N-CA-C	6.14	123.89	110.80
1	G	95	ILE	CB-CA-C	-6.13	103.76	112.22
1	B	459	HIS	CB-CG-ND1	6.13	131.89	122.70
1	B	41	THR	N-CA-C	6.12	123.34	109.81
1	E	323	GLU	CA-C-N	-6.06	112.76	119.19
1	E	323	GLU	C-N-CA	-6.06	112.76	119.19
1	D	173	MET	N-CA-C	-6.06	104.01	111.40
1	D	15	LEU	N-CA-C	-6.06	105.47	112.92
1	B	347	CYS	CA-C-N	6.04	126.01	120.03
1	B	347	CYS	C-N-CA	6.04	126.01	120.03
1	C	18	LEU	CA-C-N	-6.02	113.74	119.76
1	C	18	LEU	C-N-CA	-6.02	113.74	119.76
1	F	75	MET	CA-C-N	6.02	131.21	122.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	75	MET	C-N-CA	6.02	131.21	122.36
1	G	303	HIS	CB-CG-CD2	-6.00	123.40	131.20
1	F	224	PHE	N-CA-C	6.00	119.30	108.69
1	F	43	VAL	CA-C-N	5.99	125.54	119.19
1	F	43	VAL	C-N-CA	5.99	125.54	119.19
1	E	43	VAL	CA-C-N	-5.97	113.66	120.89
1	E	43	VAL	C-N-CA	-5.97	113.66	120.89
1	E	155	HIS	CB-CG-ND1	5.96	131.64	122.70
1	E	326	ALA	N-CA-C	5.92	118.97	111.69
1	H	406	GLN	N-CA-C	5.91	120.34	112.30
1	B	325	TYR	N-CA-C	5.90	117.51	111.14
1	E	77	GLY	CA-C-N	-5.89	112.48	119.84
1	E	77	GLY	C-N-CA	-5.89	112.48	119.84
1	A	279	GLY	N-CA-C	5.85	119.84	113.58
1	B	303	HIS	N-CA-C	-5.84	103.23	110.41
1	G	95	ILE	N-CA-C	5.84	116.61	110.72
1	A	86	ARG	N-CA-C	-5.83	102.83	110.53
1	D	75	MET	N-CA-C	-5.82	98.40	110.80
1	C	36	GLY	CA-C-N	5.80	127.09	119.84
1	C	36	GLY	C-N-CA	5.80	127.09	119.84
1	G	27	VAL	N-CA-C	5.79	115.99	108.35
1	E	67	HIS	CB-CG-ND1	5.78	131.38	122.70
1	A	315	SER	N-CA-C	5.78	119.11	112.57
1	D	307	ARG	N-CA-C	-5.78	104.67	110.97
1	G	364	ARG	CA-C-N	5.76	125.61	119.28
1	G	364	ARG	C-N-CA	5.76	125.61	119.28
1	B	205	LEU	N-CA-C	5.73	117.74	108.34
1	A	40	SER	N-CA-C	5.73	121.30	113.97
1	G	183	SER	N-CA-C	-5.72	105.05	111.28
1	A	374	HIS	CB-CG-ND1	5.72	131.28	122.70
1	C	450	LEU	C-N-CD	5.71	133.15	120.60
1	H	34	THR	N-CA-C	5.70	118.14	111.02
1	H	274	ALA	N-CA-C	5.69	118.26	111.71
1	F	212	HIS	CB-CG-ND1	5.69	131.24	122.70
1	C	306	HIS	CB-CG-ND1	5.69	131.23	122.70
1	D	330	ARG	N-CA-C	-5.68	105.09	111.28
1	B	77	GLY	CA-C-N	-5.67	113.86	119.93
1	B	77	GLY	C-N-CA	-5.67	113.86	119.93
1	A	114	HIS	CB-CG-ND1	5.66	131.19	122.70
1	A	450	LEU	C-N-CD	5.66	133.05	120.60
1	B	155	HIS	CB-CG-CD2	-5.66	123.85	131.20
1	C	273	HIS	CB-CG-CD2	-5.65	123.86	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	75	MET	N-CA-C	-5.64	101.93	110.28
1	A	459	HIS	CB-CG-ND1	5.64	131.16	122.70
1	A	407	ILE	N-CA-C	5.61	121.02	109.34
1	H	200	ARG	N-CA-C	-5.61	105.27	111.71
1	C	77	GLY	N-CA-C	5.60	123.76	112.34
1	B	317	ALA	N-CA-C	-5.59	106.22	113.16
1	G	159	ARG	N-CA-C	-5.59	104.81	111.69
1	C	459	HIS	CB-CG-ND1	5.58	131.06	122.70
1	E	41	THR	N-CA-C	5.57	122.13	109.81
1	C	67	HIS	CB-CG-ND1	5.57	131.06	122.70
1	F	326	ALA	N-CA-C	5.57	117.16	111.14
1	C	225	ASP	N-CA-C	5.57	121.31	113.02
1	F	374	HIS	CB-CG-ND1	5.56	131.04	122.70
1	B	158	GLY	N-CA-C	-5.55	108.47	115.08
1	F	180	HIS	CB-CG-ND1	5.55	131.03	122.70
1	D	74	PHE	N-CA-C	-5.54	103.17	110.43
1	C	258	GLU	N-CA-C	-5.54	103.32	110.19
1	G	225	ASP	N-CA-C	5.54	122.59	110.80
1	A	67	HIS	CB-CG-ND1	5.53	131.00	122.70
1	D	337	ALA	N-CA-C	5.52	117.29	111.28
1	F	339	ILE	N-CA-C	5.50	116.41	108.48
1	B	30	ASP	N-CA-C	-5.50	99.09	110.80
1	F	40	SER	N-CA-C	-5.48	100.40	108.79
1	F	3	THR	N-CA-C	5.48	117.64	109.59
1	H	76	ALA	N-CA-C	-5.47	105.21	111.07
1	D	344	ASP	CA-C-O	-5.47	114.41	120.70
1	F	67	HIS	CB-CG-ND1	5.47	130.91	122.70
1	D	78	PRO	N-CA-C	5.47	119.90	111.21
1	H	272	ILE	N-CA-C	-5.46	100.80	108.12
1	E	240	VAL	N-CA-C	5.46	116.24	110.72
1	F	357	SER	N-CA-C	5.46	117.92	110.01
1	B	285	TYR	CA-C-N	5.45	127.59	120.28
1	B	285	TYR	C-N-CA	5.45	127.59	120.28
1	D	217	LEU	N-CA-C	-5.45	106.48	113.02
1	H	395	ILE	CB-CA-C	-5.45	104.89	112.02
1	F	282	ILE	N-CA-C	5.44	120.63	108.88
1	H	67	HIS	CB-CG-ND1	5.44	130.86	122.70
1	C	303	HIS	CB-CG-ND1	5.43	130.84	122.70
1	A	17	GLY	N-CA-C	-5.42	106.37	112.33
1	H	216	THR	N-CA-C	-5.42	106.64	113.20
1	A	254	SER	CA-C-O	5.39	126.48	120.77
1	D	67	HIS	CB-CG-ND1	5.38	130.77	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	93	GLU	N-CA-C	5.38	117.23	111.36
1	A	303	HIS	CB-CG-ND1	5.37	130.76	122.70
1	C	224	PHE	N-CA-C	5.37	122.24	110.80
1	G	303	HIS	CB-CG-ND1	5.36	130.74	122.70
1	H	334	SER	N-CA-C	-5.36	105.52	111.36
1	H	143	ILE	N-CA-C	-5.35	102.69	109.80
1	C	148	GLY	CA-C-N	5.34	125.67	119.47
1	C	148	GLY	C-N-CA	5.34	125.67	119.47
1	H	384	MET	N-CA-C	5.34	117.60	108.90
1	C	71	ALA	CA-C-N	5.33	127.73	120.54
1	C	71	ALA	C-N-CA	5.33	127.73	120.54
1	F	273	HIS	CB-CG-ND1	5.32	130.69	122.70
1	H	86	ARG	N-CA-C	-5.32	103.12	110.35
1	D	315	SER	N-CA-C	-5.31	103.13	110.35
1	A	215	PHE	CA-C-N	5.30	131.24	121.70
1	A	215	PHE	C-N-CA	5.30	131.24	121.70
1	H	260	LEU	N-CA-C	-5.29	104.94	111.40
1	E	216	THR	N-CA-C	-5.29	106.83	113.28
1	D	347	CYS	CA-C-N	5.28	125.57	119.92
1	D	347	CYS	C-N-CA	5.28	125.57	119.92
1	C	261	ASP	N-CA-C	-5.27	105.43	111.07
1	F	409	SER	N-CA-C	5.26	115.08	108.45
1	C	74	PHE	N-CA-C	-5.26	105.55	111.28
1	E	117	ILE	N-CA-C	5.26	115.40	110.30
1	C	301	THR	N-CA-C	5.25	116.78	108.96
1	C	115	ASN	N-CA-C	5.24	115.27	107.88
1	B	41	THR	C-N-CD	5.23	132.11	120.60
1	E	335	ALA	N-CA-C	-5.22	106.76	113.02
1	E	190	VAL	N-CA-C	-5.21	105.63	110.53
1	G	43	VAL	N-CA-C	-5.20	99.49	107.71
1	E	255	VAL	CB-CA-C	-5.20	105.21	110.93
1	E	284	ASN	N-CA-C	-5.20	102.91	110.24
1	C	176	ALA	CB-CA-C	-5.19	110.17	117.23
1	H	7	THR	N-CA-C	5.19	117.53	108.76
1	A	78	PRO	CB-CA-C	-5.14	107.55	111.87
1	D	424	ASP	CA-C-N	-5.14	113.63	119.28
1	D	424	ASP	C-N-CA	-5.14	113.63	119.28
1	A	148	GLY	CA-C-N	5.13	124.92	119.28
1	A	148	GLY	C-N-CA	5.13	124.92	119.28
1	F	76	ALA	N-CA-C	-5.11	104.25	111.56
1	G	272	ILE	N-CA-C	-5.11	104.48	110.05
1	B	114	HIS	CB-CG-ND1	5.11	130.36	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	79	GLY	N-CA-C	-5.10	107.76	114.95
1	E	329	GLU	N-CA-C	-5.09	105.73	111.28
1	H	357	SER	CA-C-N	5.07	124.79	119.82
1	H	357	SER	C-N-CA	5.07	124.79	119.82
1	G	222	VAL	N-CA-C	-5.07	100.18	107.37
1	C	69	LEU	N-CA-C	-5.05	106.95	113.02
1	C	273	HIS	CB-CG-ND1	5.05	130.28	122.70
1	H	459	HIS	N-CA-C	5.05	118.49	108.59
1	E	32	PHE	CB-CA-C	-5.04	102.28	109.84
1	H	408	GLY	N-CA-C	5.02	120.66	114.69
1	D	408	GLY	N-CA-C	5.01	120.66	114.69
1	G	257	VAL	N-CA-C	-5.01	105.61	110.42

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	217	LEU	Peptide
1	A	293	SER	Peptide
1	A	344	ASP	Peptide
1	A	37	PRO	Peptide
1	A	38	SER	Peptide
1	A	75	MET	Peptide
1	B	30	ASP	Peptide
1	B	38	SER	Peptide
1	B	386	PRO	Peptide
1	B	407	ILE	Peptide
1	B	409	SER	Peptide
1	B	76	ALA	Peptide
1	C	138	PHE	Peptide
1	C	227	SER	Peptide
1	C	315	SER	Peptide
1	C	38	SER	Peptide
1	C	77	GLY	Peptide
1	D	180	HIS	Peptide
1	D	38	SER	Peptide
1	D	41	THR	Peptide
1	D	42	PRO	Peptide
1	D	458	ALA	Peptide
1	D	69	LEU	Peptide
1	D	76	ALA	Peptide
1	E	30	ASP	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	E	39	ASP	Peptide
1	E	41	THR	Peptide
1	E	6	ILE	Peptide
1	F	284	ASN	Peptide
1	F	38	SER	Peptide
1	F	75	MET	Peptide
1	G	218	VAL	Peptide
1	G	222	VAL	Peptide
1	G	3	THR	Peptide
1	G	30	ASP	Peptide
1	G	39	ASP	Peptide
1	G	75	MET	Peptide
1	G	76	ALA	Peptide
1	H	218	VAL	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3488	3427	3427	399	1
1	B	3499	3445	3437	312	0
1	C	3499	3442	3437	273	1
1	D	3488	3429	3429	389	5
1	E	3488	3430	3429	324	0
1	F	3488	3428	3428	400	1
1	G	3488	3429	3429	263	5
1	H	3488	3429	3429	443	1
2	A	1	0	0	0	0
3	A	3	0	0	2	0
3	B	3	0	0	0	0
3	D	2	0	0	2	0
3	E	4	0	0	0	0
3	F	3	0	0	1	0
3	G	1	0	0	1	0
3	H	3	0	0	1	0
All	All	27946	27459	27445	2782	7

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 50.

All (2782) 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:6:ILE:HB	1:H:25:VAL:CG1	1.25	1.64
1:B:391:SER:CB	1:B:394:THR:HB	1.15	1.63
1:A:251:LEU:HD12	1:A:270:VAL:CB	1.46	1.45
1:E:224:PHE:CD1	1:E:278:LEU:HD11	1.51	1.43
1:F:322:GLY:HA2	1:F:326:ALA:CB	1.48	1.42
1:H:6:ILE:CB	1:H:25:VAL:CG1	1.99	1.39
1:C:227:SER:OG	1:C:228:TYR:HA	1.25	1.36
1:A:251:LEU:CD1	1:A:270:VAL:HB	1.55	1.36
1:F:72:TRP:O	1:F:76:ALA:CB	1.75	1.32
1:F:97:GLU:OE1	1:F:456:VAL:CG1	1.76	1.32
1:A:287:ILE:O	1:A:291:VAL:HG23	1.29	1.29
1:F:453:THR:O	1:F:455:LEU:CD2	1.81	1.27
1:B:391:SER:CB	1:B:394:THR:CB	2.11	1.26
1:D:70:ASP:O	1:D:72:TRP:N	1.69	1.26
1:B:389:ALA:O	1:B:392:ALA:CB	1.82	1.26
1:C:6:ILE:HG22	1:C:25:VAL:O	1.10	1.23
1:F:72:TRP:O	1:F:76:ALA:HB2	1.10	1.23
1:B:391:SER:HB3	1:B:394:THR:CB	1.68	1.22
1:C:6:ILE:HG21	1:C:25:VAL:CG2	1.67	1.22
1:D:7:THR:HA	1:D:24:THR:CG2	1.68	1.21
1:A:251:LEU:HD12	1:A:270:VAL:CG1	1.69	1.21
1:H:423:GLN:NE2	3:H:501:HOH:O	1.62	1.18
1:H:206:LYS:HE3	1:H:272:ILE:HG21	1.24	1.18
1:E:429:ILE:O	1:E:432:LEU:HD12	1.44	1.18
1:A:251:LEU:CD1	1:A:270:VAL:CB	2.13	1.18
1:F:322:GLY:O	1:F:323:GLU:HB2	1.40	1.18
1:F:453:THR:O	1:F:455:LEU:HD23	1.40	1.18
1:H:145:GLY:CA	1:H:179:GLY:HA2	1.73	1.17
1:H:204:MET:HA	1:H:248:VAL:CG1	1.72	1.17
1:B:389:ALA:O	1:B:392:ALA:HB1	1.39	1.17
1:C:323:GLU:CB	1:C:324:PRO:HD2	1.76	1.15
1:F:217:LEU:CD1	1:F:226:ARG:HH22	1.59	1.15
1:H:253:HIS:CD2	1:H:273:HIS:CE1	2.33	1.15
1:H:253:HIS:CD2	1:H:273:HIS:NE2	2.13	1.15
1:C:6:ILE:O	1:C:24:THR:HG23	1.43	1.15
1:G:68:LEU:HB3	1:G:95:ILE:HG23	1.27	1.15
1:B:301:THR:HG21	1:B:379:MET:CE	1.76	1.15
1:F:323:GLU:HB3	1:F:324:PRO:HD3	1.28	1.15

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:THR:HB	1:F:28:GLU:OE2	1.47	1.14
1:B:299:LEU:HD23	1:B:329:GLU:HB3	1.26	1.14
1:B:301:THR:HG21	1:B:379:MET:HE3	1.30	1.13
1:H:204:MET:HA	1:H:248:VAL:HG12	1.23	1.13
1:D:219:ASP:HB3	1:D:222:VAL:HG11	1.31	1.13
1:H:6:ILE:CB	1:H:25:VAL:HG13	1.70	1.13
1:A:75:MET:CE	1:A:212:HIS:HE1	1.63	1.12
1:A:459:HIS:HB2	1:A:460:PRO:HA	1.26	1.12
1:A:75:MET:CE	1:A:212:HIS:CE1	2.30	1.12
1:H:206:LYS:CE	1:H:272:ILE:HG21	1.78	1.12
1:H:6:ILE:CB	1:H:25:VAL:HG12	1.70	1.11
1:H:145:GLY:HA2	1:H:179:GLY:HA2	1.22	1.11
1:H:255:VAL:O	1:H:278:LEU:HD12	1.51	1.11
1:F:275:ASN:O	1:F:325:TYR:HD1	1.31	1.10
1:H:255:VAL:HB	1:H:278:LEU:HD11	1.12	1.10
1:D:32:PHE:HE2	1:D:412:THR:N	1.47	1.10
1:F:264:VAL:CG1	1:F:293:SER:HB2	1.79	1.09
1:F:322:GLY:CA	1:F:326:ALA:HB2	1.81	1.09
1:E:153:ASP:HB3	1:E:212:HIS:HB3	1.29	1.09
1:H:6:ILE:HD12	1:H:25:VAL:HG11	1.25	1.09
1:E:235:VAL:O	1:E:239:MET:HG3	1.52	1.09
1:D:70:ASP:CG	1:D:72:TRP:O	1.96	1.08
1:A:251:LEU:CD1	1:A:270:VAL:CG1	2.28	1.08
1:C:304:ASP:HA	1:C:307:ARG:HG2	1.09	1.08
1:F:97:GLU:CD	1:F:456:VAL:HG12	1.78	1.08
1:D:332:LEU:O	1:D:337:ALA:HB2	1.52	1.08
1:D:333:ILE:HD13	1:D:334:SER:N	1.68	1.08
1:E:224:PHE:CE1	1:E:278:LEU:HD11	1.88	1.07
1:C:224:PHE:HE1	1:C:325:TYR:OH	1.32	1.07
1:F:323:GLU:HB3	1:F:324:PRO:CD	1.80	1.07
1:H:278:LEU:HA	1:H:325:TYR:OH	1.50	1.07
1:H:356:LEU:HB2	1:H:360:GLU:HG3	1.35	1.07
1:C:6:ILE:CG2	1:C:25:VAL:O	2.03	1.07
1:F:325:TYR:O	1:F:329:GLU:OE2	1.73	1.07
1:D:84:LEU:HD23	1:D:91:TYR:OH	1.55	1.06
1:H:6:ILE:HB	1:H:25:VAL:HG12	1.10	1.06
1:G:97:GLU:O	1:G:101:LEU:HD12	1.55	1.06
1:A:13:ASP:O	1:A:410:VAL:HG23	1.52	1.06
1:G:124:ARG:NH1	1:G:125:ASP:OD1	1.88	1.06
1:A:235:VAL:O	1:A:238:VAL:HG12	1.54	1.06
1:E:224:PHE:CD1	1:E:278:LEU:CD1	2.39	1.05

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HG21	1:A:239:MET:CE	1.86	1.05
1:F:97:GLU:OE1	1:F:456:VAL:HG11	1.52	1.05
1:H:77:GLY:O	1:H:155:HIS:CD2	2.09	1.05
1:H:405:ASP:OD1	1:H:406:GLN:NE2	1.89	1.05
1:C:260:LEU:O	1:C:264:VAL:HG23	1.56	1.05
1:F:279:GLY:HA2	1:F:324:PRO:HG2	1.33	1.05
1:D:7:THR:CA	1:D:24:THR:HG23	1.86	1.04
1:F:427:ASP:O	1:F:428:ASP:HB2	1.57	1.04
1:C:258:GLU:O	1:C:259:ALA:HB3	1.58	1.03
1:D:32:PHE:CE2	1:D:412:THR:N	2.24	1.03
1:D:70:ASP:OD2	1:D:73:MET:CB	2.07	1.02
1:A:210:SER:OG	1:A:254:SER:HA	1.56	1.02
1:C:323:GLU:CB	1:C:324:PRO:CD	2.36	1.02
1:D:70:ASP:OD2	1:D:73:MET:HB2	1.59	1.02
1:F:322:GLY:CA	1:F:326:ALA:CB	2.38	1.02
1:C:6:ILE:HG21	1:C:25:VAL:HG23	1.03	1.02
1:E:323:GLU:HB3	1:E:324:PRO:HD2	1.41	1.01
1:E:236:LEU:O	1:E:240:VAL:HG23	1.60	1.01
1:D:70:ASP:O	1:D:71:ALA:C	2.02	1.01
1:H:381:GLU:O	1:H:382:LYS:NZ	1.91	1.01
1:A:194:VAL:HG21	1:A:239:MET:HE3	1.41	1.01
1:B:390:ILE:C	1:B:392:ALA:HB3	1.84	1.01
1:D:6:ILE:HA	1:D:50:VAL:CG1	1.91	1.01
1:G:262:THR:O	1:G:266:LEU:HD21	1.60	1.01
1:C:227:SER:OG	1:C:228:TYR:CA	2.08	1.00
1:D:70:ASP:O	1:D:72:TRP:O	1.78	1.00
1:H:255:VAL:HB	1:H:278:LEU:CD1	1.89	1.00
1:A:240:VAL:HG21	1:A:266:LEU:HG	1.39	1.00
1:H:145:GLY:HA2	1:H:179:GLY:CA	1.91	1.00
1:B:391:SER:HB2	1:B:394:THR:CB	1.83	1.00
1:B:391:SER:HB2	1:B:394:THR:HB	1.01	1.00
1:F:73:MET:HA	1:F:76:ALA:HB1	1.39	1.00
1:D:6:ILE:O	1:D:24:THR:HG22	1.61	1.00
1:H:76:ALA:HB3	1:H:77:GLY:HA2	1.44	1.00
1:D:381:GLU:OE2	1:D:381:GLU:N	1.95	0.99
1:B:391:SER:HB3	1:B:394:THR:HB	1.00	0.99
1:H:6:ILE:CG2	1:H:25:VAL:HG12	1.91	0.99
1:H:225:ASP:OD2	1:H:226:ARG:NH2	1.94	0.99
1:E:214:VAL:HG13	1:E:215:PHE:HD1	1.23	0.99
1:A:253:HIS:ND1	1:A:273:HIS:ND1	2.10	0.99
1:B:22:ALA:O	1:B:37:PRO:HB3	1.61	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ALA:C	1:B:392:ALA:CB	2.35	0.99
1:A:251:LEU:HD11	1:A:270:VAL:HG11	1.43	0.99
1:H:143:ILE:HG21	1:H:146:MET:HE2	1.42	0.99
1:A:251:LEU:CD1	1:A:270:VAL:HG11	1.92	0.99
1:H:145:GLY:N	1:H:179:GLY:HA2	1.77	0.99
1:F:253:HIS:CE1	1:F:273:HIS:CD2	2.51	0.99
1:G:6:ILE:HG12	1:G:9:VAL:HG22	1.41	0.99
1:A:13:ASP:HA	1:A:410:VAL:HG21	1.45	0.98
1:E:226:ARG:HD2	1:E:228:TYR:HE2	1.24	0.98
1:E:252:THR:HG22	1:E:271:LEU:HA	1.44	0.98
1:A:67:HIS:HE1	1:A:344:ASP:OD1	1.46	0.98
1:H:253:HIS:HD2	1:H:273:HIS:CE1	1.72	0.98
1:B:301:THR:CG2	1:B:379:MET:HE3	1.94	0.98
1:F:257:VAL:HG23	1:F:277:THR:CG2	1.94	0.98
1:F:113:THR:HG23	1:F:206:LYS:HD3	1.42	0.98
1:H:6:ILE:HB	1:H:25:VAL:HG13	1.00	0.98
1:F:97:GLU:OE1	1:F:456:VAL:HG12	1.55	0.98
1:C:323:GLU:HB3	1:C:324:PRO:HD2	1.41	0.97
1:A:275:ASN:OD1	1:A:276:TYR:N	1.96	0.97
1:H:145:GLY:H	1:H:179:GLY:CA	1.77	0.97
1:C:323:GLU:HB2	1:C:324:PRO:HD2	1.47	0.97
1:A:271:LEU:CD1	1:A:296:TRP:O	2.12	0.96
1:F:264:VAL:HG13	1:F:293:SER:HB2	1.45	0.96
1:H:253:HIS:CD2	1:H:273:HIS:HE2	1.74	0.96
1:C:272:ILE:HG22	1:C:273:HIS:CD2	2.01	0.96
1:F:264:VAL:CG1	1:F:293:SER:CB	2.42	0.96
1:G:68:LEU:CB	1:G:95:ILE:HG23	1.95	0.96
1:A:271:LEU:HD12	1:A:296:TRP:O	1.62	0.96
1:D:190:VAL:O	1:D:194:VAL:HG23	1.66	0.96
1:C:6:ILE:CG2	1:C:25:VAL:HG23	1.94	0.96
1:H:31:ARG:NH1	1:H:415:LEU:HD11	1.79	0.96
1:H:322:GLY:HA2	1:H:326:ALA:HB2	1.48	0.96
1:B:409:SER:HB2	1:B:410:VAL:HA	1.47	0.96
1:A:4:ILE:O	1:A:27:VAL:HG23	1.66	0.96
1:B:307:ARG:HH21	1:B:322:GLY:HA2	1.29	0.96
1:D:32:PHE:CZ	1:D:414:LYS:HB2	2.00	0.95
1:A:240:VAL:HG21	1:A:266:LEU:CG	1.94	0.95
1:F:217:LEU:HD12	1:F:226:ARG:HH22	1.28	0.95
1:D:25:VAL:HG12	1:D:35:VAL:HG12	1.48	0.95
1:H:206:LYS:HE3	1:H:272:ILE:CG2	1.96	0.95
1:A:350:LYS:O	1:A:354:ALA:N	1.99	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:THR:OG1	1:D:379:MET:CE	2.14	0.95
1:D:350:LYS:HE3	1:D:460:PRO:HB3	1.45	0.95
1:F:97:GLU:CD	1:F:456:VAL:CG1	2.38	0.95
1:G:68:LEU:HB3	1:G:95:ILE:CG2	1.97	0.95
1:A:40:SER:O	1:A:41:THR:HG22	1.65	0.94
1:C:6:ILE:CG2	1:C:25:VAL:H	1.78	0.94
1:D:421:LEU:HB3	1:D:434:SER:O	1.66	0.94
1:F:322:GLY:HA2	1:F:326:ALA:HB2	0.96	0.94
1:F:453:THR:O	1:F:455:LEU:HD21	1.66	0.94
1:H:107:VAL:HG23	1:H:372:HIS:CE1	2.02	0.94
1:H:253:HIS:NE2	1:H:273:HIS:NE2	2.13	0.94
1:C:304:ASP:HA	1:C:307:ARG:CG	1.98	0.94
1:E:233:ARG:NH2	1:E:265:GLU:OE1	2.00	0.94
1:E:253:HIS:ND1	1:E:273:HIS:CD2	2.35	0.94
1:F:322:GLY:HA2	1:F:326:ALA:HB3	1.47	0.94
1:F:217:LEU:CD1	1:F:226:ARG:NH2	2.30	0.94
1:C:144:VAL:HA	1:C:178:VAL:HG11	1.50	0.93
1:G:261:ASP:OD1	1:G:289:LYS:NZ	2.01	0.93
1:D:6:ILE:C	1:D:24:THR:HG22	1.93	0.93
1:F:61:TYR:HB2	1:F:107:VAL:HG12	1.48	0.93
1:F:113:THR:CG2	1:F:206:LYS:HD3	1.99	0.93
1:H:146:MET:CE	1:H:208:ALA:HB2	1.98	0.93
1:H:145:GLY:CA	1:H:179:GLY:CA	2.47	0.93
1:E:423:GLN:OE1	1:E:431:ASN:OD1	1.86	0.93
1:A:206:LYS:NZ	3:A:603:HOH:O	1.98	0.93
1:E:321:ALA:O	1:E:326:ALA:HB2	1.69	0.92
1:B:388:GLU:O	1:B:390:ILE:N	2.02	0.92
1:G:262:THR:O	1:G:266:LEU:CD2	2.16	0.92
1:C:6:ILE:HG23	1:C:25:VAL:H	1.34	0.92
1:F:217:LEU:HD13	1:F:226:ARG:HH22	1.35	0.92
1:H:343:THR:HG23	1:H:375:TRP:HD1	1.35	0.92
1:H:225:ASP:HB2	1:H:226:ARG:HE	1.34	0.92
1:B:391:SER:N	1:B:392:ALA:HB3	1.83	0.92
1:A:67:HIS:HA	1:A:112:ASP:OD1	1.69	0.92
1:H:439:PHE:CZ	1:H:444:ALA:HB2	2.04	0.92
1:A:251:LEU:HD12	1:A:270:VAL:HB	0.93	0.92
1:G:272:ILE:HG23	1:G:342:ASN:OD1	1.68	0.92
1:A:287:ILE:C	1:A:291:VAL:HG23	1.94	0.92
1:C:259:ALA:O	1:C:263:SER:OG	1.85	0.92
1:A:206:LYS:HE3	1:A:272:ILE:HD11	1.49	0.92
1:H:142:THR:HG22	1:H:143:ILE:O	1.70	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:ILE:HG22	1:C:25:VAL:C	1.95	0.91
1:C:227:SER:HG	1:C:228:TYR:HA	1.23	0.91
1:H:6:ILE:CD1	1:H:25:VAL:HG11	1.99	0.91
1:A:235:VAL:O	1:A:238:VAL:CG1	2.18	0.91
1:B:299:LEU:CD2	1:B:329:GLU:HB3	1.99	0.91
1:F:217:LEU:HD13	1:F:226:ARG:NH2	1.84	0.91
1:H:203:ASP:O	1:H:248:VAL:HG13	1.68	0.91
1:B:225:ASP:OD1	1:B:226:ARG:N	2.03	0.90
1:D:328:ASN:O	1:D:331:ASN:N	2.02	0.90
1:A:13:ASP:C	1:A:410:VAL:HG23	1.95	0.90
1:B:388:GLU:N	1:B:388:GLU:OE1	2.04	0.90
1:D:219:ASP:HB3	1:D:222:VAL:CG1	2.01	0.90
1:F:253:HIS:ND1	1:F:273:HIS:HD2	1.69	0.90
1:E:253:HIS:ND1	1:E:273:HIS:HD2	1.67	0.90
1:D:32:PHE:HE2	1:D:412:THR:H	0.90	0.90
1:A:236:LEU:HB3	1:A:266:LEU:HD22	1.54	0.90
1:D:279:GLY:H	1:D:325:TYR:HE1	1.19	0.90
1:D:411:GLU:O	1:D:412:THR:HB	1.71	0.89
1:F:275:ASN:O	1:F:325:TYR:CD1	2.23	0.89
1:H:68:LEU:HD13	1:H:95:ILE:CG2	2.02	0.89
1:E:181:GLN:O	1:E:184:LEU:N	2.05	0.89
1:A:209:VAL:HG21	1:A:252:THR:OG1	1.72	0.89
1:H:34:THR:HG22	1:H:41:THR:HG21	1.53	0.89
1:D:7:THR:HA	1:D:24:THR:HG23	0.90	0.89
1:G:65:ASN:OD1	1:G:113:THR:OG1	1.89	0.89
1:A:350:LYS:HA	1:A:353:LEU:HB2	1.54	0.89
1:A:459:HIS:CB	1:A:460:PRO:HA	2.01	0.89
1:H:225:ASP:HB2	1:H:226:ARG:NE	1.87	0.89
1:A:191:ARG:HD2	1:A:238:VAL:CG2	2.02	0.89
1:H:6:ILE:CG1	1:H:25:VAL:HG13	2.02	0.89
1:A:13:ASP:HA	1:A:410:VAL:CG2	2.02	0.89
1:E:220:ARG:O	1:E:221:SER:OG	1.89	0.89
1:A:235:VAL:C	1:A:238:VAL:HG12	1.97	0.89
1:F:257:VAL:HG23	1:F:277:THR:HG23	1.53	0.89
1:H:6:ILE:CG1	1:H:25:VAL:CG1	2.50	0.89
1:A:71:ALA:O	1:A:74:PHE:HB2	1.74	0.88
1:A:348:PRO:HG3	1:A:364:ARG:HH12	1.37	0.88
1:H:360:GLU:OE1	1:H:361:ARG:NE	2.07	0.88
1:B:72:TRP:O	1:B:76:ALA:HB2	1.73	0.88
1:G:360:GLU:O	1:G:364:ARG:HG3	1.72	0.88
1:D:219:ASP:CB	1:D:222:VAL:HG11	2.02	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:GLY:HA2	1:F:161:ALA:HB3	1.56	0.88
1:D:387:LEU:O	1:D:391:SER:N	2.05	0.88
1:D:148:GLY:O	1:D:154:PHE:HD2	1.56	0.88
1:F:253:HIS:ND1	1:F:273:HIS:CD2	2.42	0.88
1:H:323:GLU:HB3	1:H:324:PRO:HD3	1.54	0.88
1:H:66:VAL:C	1:H:67:HIS:HD2	1.82	0.88
1:C:113:THR:HB	1:C:206:LYS:HD2	1.56	0.88
1:G:92:VAL:O	1:G:96:GLU:HG3	1.72	0.88
1:C:78:PRO:O	1:C:352:HIS:NE2	2.06	0.88
1:D:258:GLU:O	1:D:260:LEU:N	2.07	0.88
1:B:69:LEU:HD13	1:B:95:ILE:CG1	2.04	0.87
1:D:68:LEU:CD1	1:D:95:ILE:HG23	2.04	0.87
1:B:296:TRP:HZ3	1:B:396:ASN:HB3	1.39	0.87
1:H:206:LYS:NZ	1:H:272:ILE:HG21	1.88	0.87
1:G:126:ARG:HA	1:G:131:ILE:HD12	1.57	0.87
1:D:303:HIS:HB2	1:D:306:HIS:HB2	1.57	0.87
1:F:277:THR:N	1:F:325:TYR:HE1	1.71	0.87
1:A:70:ASP:OD1	1:A:71:ALA:N	2.08	0.87
1:C:254:SER:OG	1:C:260:LEU:CD1	2.22	0.87
1:H:145:GLY:N	1:H:179:GLY:CA	2.35	0.87
1:H:353:LEU:O	1:H:360:GLU:OE2	1.91	0.87
1:H:70:ASP:O	1:H:74:PHE:CE1	2.28	0.87
1:A:240:VAL:HG21	1:A:266:LEU:CD1	2.03	0.86
1:F:114:HIS:O	1:F:115:ASN:ND2	2.08	0.86
1:H:313:VAL:HG11	1:H:357:SER:CB	2.03	0.86
1:E:378:SER:O	1:E:382:LYS:HG2	1.75	0.86
1:D:30:ASP:OD1	1:D:31:ARG:N	2.08	0.86
1:F:251:LEU:CD2	1:F:270:VAL:HB	2.04	0.86
1:H:66:VAL:O	1:H:67:HIS:HD2	1.58	0.86
1:A:250:VAL:H	1:A:269:ASP:HB2	1.40	0.86
1:B:66:VAL:HG21	1:B:110:VAL:HG21	1.55	0.86
1:A:30:ASP:OD1	1:A:31:ARG:N	2.08	0.86
1:F:454:PRO:C	1:F:455:LEU:HD23	2.01	0.86
1:G:97:GLU:OE2	1:G:457:THR:OG1	1.93	0.86
1:D:233:ARG:NH1	1:D:237:GLU:OE1	2.09	0.86
1:F:68:LEU:HD13	1:F:95:ILE:HG23	1.57	0.86
1:F:159:ARG:HD2	1:F:167:VAL:HG11	1.58	0.86
1:H:202:VAL:O	1:H:204:MET:N	2.07	0.86
1:A:253:HIS:ND1	1:A:273:HIS:CE1	2.43	0.85
1:D:279:GLY:N	1:D:325:TYR:HE1	1.74	0.85
1:G:260:LEU:O	1:G:264:VAL:HG23	1.76	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:275:ASN:O	1:G:328:ASN:ND2	2.08	0.85
1:E:282:ILE:HG13	1:E:328:ASN:HD21	1.41	0.85
1:B:252:THR:HG21	1:B:263:SER:HB3	1.59	0.85
1:F:66:VAL:HG21	1:F:110:VAL:HG11	1.58	0.85
1:F:73:MET:CA	1:F:76:ALA:HB1	2.06	0.85
1:A:75:MET:HE2	1:A:212:HIS:CE1	2.10	0.85
1:D:388:GLU:HA	1:D:391:SER:OG	1.77	0.85
1:A:75:MET:HE1	1:A:212:HIS:HE1	1.39	0.84
1:E:153:ASP:HA	1:E:212:HIS:O	1.77	0.84
1:F:75:MET:N	1:F:76:ALA:HB3	1.92	0.84
1:A:175:GLU:OE1	1:A:181:GLN:OE1	1.95	0.84
1:C:323:GLU:HB3	1:C:324:PRO:CD	2.02	0.84
1:A:215:PHE:H	1:A:216:THR:HB	1.43	0.84
1:B:112:ASP:O	1:B:140:ALA:CB	2.25	0.84
1:B:153:ASP:O	1:B:212:HIS:ND1	2.09	0.84
1:D:32:PHE:HZ	1:D:414:LYS:HB2	1.42	0.83
1:F:255:VAL:HB	1:F:278:LEU:CD2	2.08	0.83
1:H:68:LEU:HD13	1:H:95:ILE:HG23	1.60	0.83
1:H:72:TRP:CE3	1:H:75:MET:CE	2.61	0.83
1:C:30:ASP:OD1	1:C:31:ARG:N	2.10	0.83
1:B:395:ILE:O	1:B:399[B]:ARG:N	2.12	0.83
1:A:237:GLU:HA	1:A:266:LEU:HD11	1.58	0.83
1:A:446:ASP:O	1:A:450:LEU:HD13	1.78	0.83
1:F:322:GLY:O	1:F:323:GLU:CB	2.23	0.83
1:F:61:TYR:OH	1:F:432:LEU:HD22	1.78	0.83
1:A:86:ARG:NH2	1:F:88:GLU:O	2.12	0.83
1:D:31:ARG:NH2	1:D:406:GLN:OE1	2.11	0.83
1:D:38:SER:OG	3:D:501:HOH:O	1.64	0.83
1:H:66:VAL:C	1:H:67:HIS:CD2	2.57	0.83
1:H:313:VAL:HG11	1:H:357:SER:HB3	1.61	0.83
1:E:179:GLY:C	1:E:180:HIS:ND1	2.37	0.83
1:E:226:ARG:HD2	1:E:228:TYR:CE2	2.12	0.83
1:C:254:SER:OG	1:C:260:LEU:HD12	1.79	0.83
1:H:282:ILE:HG13	1:H:328:ASN:OD1	1.78	0.83
1:F:251:LEU:HD22	1:F:270:VAL:HB	1.58	0.82
1:H:72:TRP:CZ3	1:H:75:MET:HE1	2.14	0.82
1:H:323:GLU:HB3	1:H:324:PRO:CD	2.09	0.82
1:F:66:VAL:HG21	1:F:110:VAL:CG1	2.09	0.82
1:H:207:ILE:HD11	1:H:239:MET:SD	2.19	0.82
1:H:275:ASN:OD1	1:H:329:GLU:HG3	1.79	0.82
1:B:385:SER:HB3	1:B:387:LEU:O	1.79	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:GLU:N	1:F:281:GLU:OE1	2.12	0.82
1:E:261:ASP:O	1:E:265:GLU:HG3	1.80	0.82
1:A:271:LEU:CD1	1:A:297:ALA:HA	2.09	0.82
1:H:146:MET:HE1	1:H:208:ALA:HB2	1.59	0.82
1:E:372:HIS:O	1:E:376:THR:HG23	1.79	0.82
1:F:253:HIS:HE1	1:F:273:HIS:NE2	1.77	0.82
1:H:220:ARG:O	1:H:221:SER:OG	1.95	0.82
1:H:225:ASP:C	1:H:226:ARG:HG2	2.05	0.82
1:H:313:VAL:HG21	1:H:357:SER:OG	1.80	0.82
1:A:210:SER:HG	1:A:254:SER:HA	1.43	0.82
1:F:428:ASP:OD2	1:F:430:ARG:CD	2.27	0.82
1:G:4:ILE:HD12	1:G:5:ALA:N	1.95	0.82
1:G:97:GLU:O	1:G:101:LEU:CD1	2.28	0.82
1:A:12:ILE:HD12	1:A:56:TRP:HD1	1.42	0.82
1:D:6:ILE:O	1:D:24:THR:CG2	2.27	0.82
1:B:113:THR:HA	1:B:140:ALA:CB	2.10	0.81
1:H:72:TRP:CZ3	1:H:75:MET:CE	2.63	0.81
1:H:143:ILE:CG2	1:H:146:MET:HE2	2.10	0.81
1:F:253:HIS:CE1	1:F:273:HIS:NE2	2.48	0.81
1:H:23:THR:HG22	1:H:37:PRO:HG3	1.62	0.81
1:A:251:LEU:HD13	1:A:270:VAL:HB	1.63	0.81
1:B:14:GLY:O	1:B:391:SER:OG	1.98	0.81
1:F:96:GLU:OE2	1:F:126:ARG:NH1	2.14	0.81
1:B:253:HIS:CD2	1:B:273:HIS:NE2	2.49	0.81
1:D:215:PHE:O	1:D:218:VAL:HG13	1.80	0.81
1:B:244:ARG:NH2	1:B:269:ASP:OD1	2.14	0.81
1:A:12:ILE:HD12	1:A:56:TRP:CD1	2.16	0.81
1:E:153:ASP:CB	1:E:212:HIS:HB3	2.10	0.81
1:E:214:VAL:HG13	1:E:215:PHE:CD1	2.14	0.81
1:C:307:ARG:NH2	1:C:311:GLU:OE2	2.14	0.81
1:B:73:MET:O	1:B:77:GLY:HA2	1.80	0.81
1:A:67:HIS:CE1	1:A:344:ASP:OD1	2.32	0.80
1:A:445:VAL:O	1:A:447:ARG:NH1	2.12	0.80
1:B:296:TRP:CZ3	1:B:396:ASN:HB3	2.17	0.80
1:D:217:LEU:HD13	1:D:226:ARG:NH1	1.95	0.80
1:H:204:MET:CA	1:H:248:VAL:CG1	2.56	0.80
1:H:357:SER:O	1:H:360:GLU:N	2.14	0.80
1:A:233:ARG:NH1	1:A:265:GLU:OE1	2.14	0.80
1:D:191:ARG:NH1	1:D:242:GLU:OE2	2.14	0.80
1:D:70:ASP:OD2	1:D:73:MET:HB3	1.80	0.80
1:F:72:TRP:O	1:F:76:ALA:HB1	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:ARG:NH2	1:B:322:GLY:CA	2.45	0.80
1:B:307:ARG:NH2	1:B:322:GLY:HA2	1.97	0.80
1:B:385:SER:C	1:B:387:LEU:O	2.24	0.80
1:D:301:THR:HG21	1:D:378:SER:CB	2.12	0.80
1:D:220:ARG:HH11	1:D:220:ARG:HG3	1.47	0.79
1:E:364:ARG:NH1	1:E:367:THR:OG1	2.16	0.79
1:G:275:ASN:ND2	1:G:276:TYR:HD1	1.81	0.79
1:E:53:ASN:O	1:E:55:ARG:NH1	2.14	0.79
1:E:124:ARG:NH1	1:E:203:ASP:OD1	2.15	0.79
1:A:191:ARG:CZ	1:A:238:VAL:HG22	2.12	0.79
1:D:272:ILE:O	1:D:273:HIS:HB2	1.83	0.79
1:H:252:THR:O	1:H:272:ILE:HB	1.82	0.79
1:H:278:LEU:CA	1:H:325:TYR:OH	2.31	0.78
1:B:395:ILE:O	1:B:399[A]:ARG:N	2.12	0.78
1:E:257:VAL:HG22	1:E:277:THR:HG22	1.65	0.78
1:E:385:SER:O	1:E:388:GLU:N	2.16	0.78
1:A:91:TYR:HE2	1:A:173:MET:HE1	1.47	0.78
1:B:303:HIS:NE2	1:B:377:GLN:HG2	1.97	0.78
1:H:342:ASN:O	1:H:375:TRP:NE1	2.16	0.78
1:E:224:PHE:CE1	1:E:278:LEU:CD1	2.65	0.78
1:B:69:LEU:HD13	1:B:95:ILE:HG12	1.66	0.78
1:G:296:TRP:HZ3	1:G:396:ASN:HD22	1.32	0.78
1:C:258:GLU:O	1:C:259:ALA:CB	2.27	0.78
1:D:7:THR:CA	1:D:24:THR:CG2	2.54	0.78
1:D:222:VAL:HG22	1:D:223:GLY:N	1.97	0.78
1:H:204:MET:HB2	1:H:249:PRO:HG2	1.65	0.78
1:D:68:LEU:HD13	1:D:95:ILE:HG23	1.64	0.78
1:D:337:ALA:O	1:D:338:LYS:HD3	1.83	0.78
1:C:217:LEU:HD23	1:C:224:PHE:HB3	1.66	0.77
1:H:143:ILE:HG21	1:H:146:MET:CE	2.13	0.77
1:A:91:TYR:O	1:A:95:ILE:HG13	1.85	0.77
1:A:206:LYS:HE3	1:A:272:ILE:CD1	2.14	0.77
1:D:75:MET:HG2	1:D:215:PHE:CE1	2.18	0.77
1:A:215:PHE:N	1:A:216:THR:HB	2.00	0.77
1:A:409:SER:OG	1:A:414:LYS:NZ	2.17	0.77
1:B:301:THR:HG21	1:B:379:MET:HE2	1.64	0.77
1:D:387:LEU:O	1:D:390:ILE:HB	1.85	0.77
1:E:323:GLU:HB3	1:E:324:PRO:CD	2.14	0.77
1:E:423:GLN:CD	1:E:431:ASN:OD1	2.27	0.77
1:B:307:ARG:HH21	1:B:322:GLY:CA	1.97	0.77
1:B:394:THR:HG22	1:B:395:ILE:N	1.98	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:MET:HA	1:G:248:VAL:HB	1.65	0.77
1:F:428:ASP:OD2	1:F:430:ARG:HD2	1.85	0.77
1:B:301:THR:CG2	1:B:379:MET:CE	2.57	0.77
1:E:257:VAL:HG22	1:E:277:THR:CG2	2.15	0.76
1:G:91:TYR:O	1:G:95:ILE:HG13	1.85	0.76
1:B:210:SER:HB2	1:B:255:VAL:CG2	2.15	0.76
1:D:301:THR:OG1	1:D:379:MET:HE2	1.83	0.76
1:D:350:LYS:HD3	1:D:458:ALA:O	1.85	0.76
1:A:66:VAL:HA	1:A:345:ALA:HB3	1.68	0.76
1:C:62:VAL:HG13	1:C:109:THR:HB	1.66	0.76
1:G:102:ALA:HB1	1:G:107:VAL:HB	1.65	0.76
1:H:406:GLN:HB2	1:H:415:LEU:HD13	1.67	0.76
1:G:250:VAL:CG1	1:G:268:ALA:HA	2.15	0.76
1:G:266:LEU:HD22	1:G:266:LEU:H	1.51	0.76
1:H:30:ASP:H	1:H:442:GLY:HA3	1.49	0.76
1:D:279:GLY:N	1:D:325:TYR:CE1	2.53	0.76
1:F:255:VAL:O	1:F:278:LEU:HD23	1.86	0.76
1:B:389:ALA:C	1:B:392:ALA:HB2	2.11	0.76
1:D:303:HIS:HB2	1:D:306:HIS:CB	2.16	0.76
1:H:260:LEU:HD12	1:H:271:LEU:HD23	1.68	0.76
1:E:225:ASP:O	1:E:226:ARG:HB3	1.86	0.76
1:A:240:VAL:CG2	1:A:266:LEU:HG	2.16	0.76
1:A:254:SER:CB	1:A:259:ALA:HB1	2.14	0.76
1:F:281:GLU:C	1:F:283:PRO:HB3	2.10	0.76
1:G:64:GLY:HA2	1:G:111:PHE:HD2	1.51	0.76
1:F:273:HIS:ND1	1:F:276:TYR:CD2	2.53	0.75
1:H:41:THR:H	1:H:42:PRO:HA	1.50	0.75
1:E:264:VAL:CG1	1:E:293:SER:CB	2.64	0.75
1:A:409:SER:C	1:A:414:LYS:HZ1	1.94	0.75
1:B:391:SER:HB2	1:B:395:ILE:H	1.51	0.75
1:D:301:THR:HG21	1:D:378:SER:HB2	1.66	0.75
1:D:301:THR:CG2	1:D:378:SER:CB	2.64	0.75
1:D:386:PRO:O	1:D:390:ILE:HG13	1.86	0.75
1:F:429:ILE:HD11	1:F:432:LEU:HD11	1.66	0.75
1:G:323:GLU:HB2	1:G:324:PRO:CD	2.16	0.75
1:G:357:SER:OG	1:G:360:GLU:HG3	1.85	0.75
1:G:275:ASN:ND2	1:G:276:TYR:CD1	2.55	0.75
1:E:224:PHE:CG	1:E:278:LEU:CD1	2.70	0.75
1:F:65:ASN:OD1	1:F:113:THR:HB	1.86	0.75
1:F:74:PHE:O	1:F:154:PHE:HB3	1.85	0.75
1:A:125:ASP:HB2	1:A:126:ARG:HH12	1.52	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:GLY:HA2	1:A:161:ALA:HB3	1.69	0.75
1:D:32:PHE:CD2	1:D:412:THR:HA	2.22	0.75
1:E:224:PHE:CG	1:E:278:LEU:HD11	2.19	0.75
1:A:75:MET:SD	1:A:215:PHE:CD2	2.79	0.75
1:D:251:LEU:HD22	1:D:270:VAL:HB	1.67	0.75
1:A:126:ARG:HG2	1:A:126:ARG:HH11	1.51	0.74
1:B:395:ILE:HG13	1:B:396:ASN:OD1	1.87	0.74
1:D:113:THR:HB	1:D:206:LYS:HD2	1.69	0.74
1:B:399[B]:ARG:HH11	1:B:399[B]:ARG:HG3	1.53	0.74
1:E:43:VAL:HG22	1:E:45:GLU:H	1.52	0.74
1:F:136:ARG:NH2	1:F:417:ASP:OD2	2.20	0.74
1:F:225:ASP:O	1:F:226:ARG:HB2	1.84	0.74
1:H:251:LEU:HD22	1:H:270:VAL:HB	1.67	0.74
1:G:24:THR:HB	1:G:41:THR:HG21	1.69	0.74
1:H:343:THR:HG23	1:H:375:TRP:CD1	2.20	0.74
1:E:279:GLY:N	1:E:325:TYR:CE1	2.55	0.74
1:H:210:SER:OG	1:H:255:VAL:HG22	1.86	0.74
1:E:24:THR:HG21	1:E:40:SER:HB2	1.69	0.74
1:E:217:LEU:HD11	1:E:223:GLY:O	1.87	0.74
1:D:30:ASP:HB2	1:D:441:ALA:O	1.86	0.74
1:H:214:VAL:O	1:H:217:LEU:HB3	1.88	0.74
1:D:25:VAL:HG12	1:D:35:VAL:CG1	2.18	0.74
1:D:385:SER:HB3	1:D:388:GLU:HG2	1.68	0.74
1:G:3:THR:HG23	1:G:47:ALA:HA	1.67	0.74
1:G:250:VAL:HG13	1:G:268:ALA:HA	1.68	0.74
1:H:6:ILE:CD1	1:H:25:VAL:CG1	2.65	0.74
1:B:40:SER:O	1:B:41:THR:OG1	2.05	0.74
1:D:217:LEU:HD13	1:D:226:ARG:HH12	1.52	0.74
1:H:260:LEU:HD12	1:H:271:LEU:CD2	2.16	0.74
1:D:25:VAL:CG1	1:D:35:VAL:HG12	2.17	0.74
1:D:187:ARG:HB3	1:D:187:ARG:NH1	2.02	0.74
1:D:278:LEU:HA	1:D:325:TYR:CE1	2.23	0.74
1:G:129:ALA:HB3	1:G:131:ILE:HG13	1.69	0.74
1:E:157:ALA:O	1:E:159:ARG:N	2.20	0.74
1:B:391:SER:CA	1:B:394:THR:HB	2.16	0.74
1:C:6:ILE:CG2	1:C:25:VAL:N	2.51	0.74
1:D:84:LEU:HD23	1:D:91:TYR:CZ	2.23	0.73
1:D:328:ASN:O	1:D:331:ASN:HB2	1.87	0.73
1:D:436:THR:O	1:D:447:ARG:NH2	2.21	0.73
1:H:107:VAL:CG2	1:H:372:HIS:CE1	2.70	0.73
1:E:207:ILE:HD12	1:E:239:MET:SD	2.28	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ASN:CG	1:A:276:TYR:H	1.95	0.73
1:B:395:ILE:HD12	1:B:399[B]:ARG:NH1	2.02	0.73
1:D:73:MET:HE1	1:D:83:TYR:CD2	2.22	0.73
1:D:84:LEU:HD22	1:D:170:ILE:CG2	2.17	0.73
1:H:6:ILE:HD12	1:H:25:VAL:CG1	2.10	0.73
1:H:72:TRP:CE3	1:H:75:MET:HE2	2.22	0.73
1:C:12:ILE:HG12	1:C:19:PRO:HB3	1.70	0.73
1:D:7:THR:HG22	1:D:24:THR:HG21	1.69	0.73
1:A:438:VAL:HG23	1:A:447:ARG:HD3	1.69	0.73
1:B:92:VAL:O	1:B:96:GLU:HG3	1.89	0.73
1:D:350:LYS:HE3	1:D:460:PRO:CB	2.17	0.73
1:C:387:LEU:HD21	1:C:426:VAL:HG22	1.69	0.73
1:H:191:ARG:NH1	1:H:241:GLU:OE2	2.22	0.73
1:C:6:ILE:O	1:C:24:THR:CG2	2.32	0.73
1:H:136:ARG:HH12	1:H:417:ASP:HB3	1.52	0.73
1:H:255:VAL:C	1:H:278:LEU:HD12	2.12	0.73
1:A:271:LEU:HD11	1:A:296:TRP:O	1.89	0.73
1:F:66:VAL:CG2	1:F:110:VAL:CG1	2.67	0.73
1:G:6:ILE:HD11	1:G:9:VAL:CG1	2.18	0.73
1:E:277:THR:CB	1:E:280:GLN:O	2.37	0.73
1:D:70:ASP:OD1	1:D:72:TRP:O	2.04	0.73
1:F:264:VAL:HG11	1:F:293:SER:HB3	1.71	0.73
1:F:278:LEU:H	1:F:325:TYR:HE1	1.36	0.73
1:A:11:LEU:HD21	1:A:13:ASP:HB3	1.70	0.72
1:F:97:GLU:OE2	1:F:456:VAL:HG12	1.89	0.72
1:E:148:GLY:N	1:E:175:GLU:OE2	2.21	0.72
1:G:252:THR:OG1	1:G:263:SER:OG	2.05	0.72
1:A:282:ILE:HG23	1:A:328:ASN:HD21	1.52	0.72
1:C:30:ASP:CG	1:C:31:ARG:H	1.97	0.72
1:C:254:SER:OG	1:C:260:LEU:HD13	1.89	0.72
1:D:301:THR:OG1	1:D:379:MET:HE3	1.89	0.72
1:F:126:ARG:NH1	1:F:132:SER:OG	2.22	0.72
1:A:203:ASP:OD1	3:A:602:HOH:O	2.08	0.72
1:B:112:ASP:O	1:B:140:ALA:HB3	1.87	0.72
1:H:175:GLU:O	1:H:178:VAL:HG22	1.88	0.72
1:D:142:THR:OG1	1:D:174:PHE:O	2.06	0.72
1:A:38:SER:OG	1:A:41:THR:N	2.23	0.72
1:A:191:ARG:CD	1:A:238:VAL:CG2	2.68	0.72
1:F:207:ILE:HG22	1:F:251:LEU:O	1.89	0.72
1:E:284:ASN:O	1:E:285:TYR:CD2	2.42	0.72
1:A:254:SER:HB2	1:A:259:ALA:CB	2.19	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:SER:HB2	1:A:259:ALA:HB1	1.69	0.72
1:C:272:ILE:HG22	1:C:273:HIS:HD2	1.53	0.72
1:E:179:GLY:O	1:E:180:HIS:ND1	2.23	0.72
1:B:253:HIS:NE2	1:B:273:HIS:NE2	2.37	0.72
1:C:6:ILE:CG2	1:C:25:VAL:CG2	2.60	0.72
1:C:28:GLU:O	1:C:30:ASP:O	2.08	0.72
1:B:69:LEU:HD13	1:B:95:ILE:HG13	1.70	0.72
1:C:319:ALA:HB1	1:C:323:GLU:OE1	1.88	0.72
1:C:224:PHE:CE1	1:C:325:TYR:OH	2.18	0.71
1:D:333:ILE:HD13	1:D:334:SER:H	1.55	0.71
1:F:182:LEU:HA	1:F:185:LEU:HD12	1.72	0.71
1:E:66:VAL:O	1:E:67:HIS:HD2	1.73	0.71
1:A:75:MET:HE1	1:A:212:HIS:CE1	2.16	0.71
1:A:12:ILE:CD1	1:A:56:TRP:CD1	2.72	0.71
1:B:195:ARG:HG2	1:B:242:GLU:HG3	1.70	0.71
1:D:158:GLY:HA2	1:D:161:ALA:HB3	1.72	0.71
1:C:59:PRO:HB3	1:C:409:SER:HA	1.73	0.71
1:D:32:PHE:HE1	1:D:415:LEU:O	1.73	0.71
1:E:204:MET:HA	1:E:248:VAL:HB	1.73	0.71
1:F:73:MET:C	1:F:76:ALA:HB3	2.15	0.71
1:B:391:SER:HA	1:B:394:THR:N	2.05	0.71
1:D:114:HIS:ND1	1:D:143:ILE:HG13	2.05	0.71
1:E:275:ASN:HB3	1:E:299:LEU:HD12	1.71	0.71
1:A:113:THR:HB	1:A:206:LYS:HG3	1.71	0.71
1:F:67:HIS:N	1:F:345:ALA:O	2.22	0.71
1:F:113:THR:HG21	1:F:206:LYS:NZ	2.06	0.71
1:F:266:LEU:H	1:F:266:LEU:HD12	1.54	0.71
1:G:220:ARG:O	1:G:221:SER:OG	2.06	0.71
1:D:231:PHE:HB2	1:D:236:LEU:HD13	1.72	0.71
1:G:95:ILE:O	1:G:98:ALA:HB3	1.90	0.71
1:H:272:ILE:HG22	1:H:273:HIS:ND1	2.05	0.71
1:B:41:THR:H	1:B:42:PRO:HA	1.56	0.71
1:H:231:PHE:CE2	1:H:239:MET:HE1	2.25	0.71
1:H:357:SER:O	1:H:360:GLU:CB	2.39	0.71
1:A:13:ASP:CA	1:A:410:VAL:HG23	2.20	0.71
1:G:4:ILE:HD12	1:G:5:ALA:H	1.54	0.71
1:H:31:ARG:NH1	1:H:415:LEU:CD1	2.54	0.71
1:A:91:TYR:CE2	1:A:173:MET:HE1	2.26	0.70
1:B:178:VAL:HG12	1:B:179:GLY:H	1.56	0.70
1:D:195:ARG:HH11	1:D:195:ARG:HG3	1.56	0.70
1:G:6:ILE:O	1:G:24:THR:HG23	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:431:ASN:O	1:H:434:SER:OG	2.09	0.70
1:D:6:ILE:HA	1:D:50:VAL:HG11	1.71	0.70
1:F:277:THR:CG2	1:F:280:GLN:O	2.40	0.70
1:F:279:GLY:CA	1:F:324:PRO:HG2	2.19	0.70
1:F:313:VAL:HG21	1:F:360:GLU:OE2	1.91	0.70
1:C:158:GLY:HA2	1:C:161:ALA:HB3	1.72	0.70
1:D:70:ASP:O	1:D:72:TRP:C	2.33	0.70
1:F:277:THR:HG21	1:F:280:GLN:O	1.91	0.70
1:H:277:THR:HG21	1:H:282:ILE:HG12	1.74	0.70
1:H:293:SER:HB2	1:H:295:SER:OG	1.92	0.70
1:A:261:ASP:OD1	1:A:289:LYS:NZ	2.21	0.70
1:C:78:PRO:O	1:C:352:HIS:CD2	2.45	0.70
1:C:395:ILE:O	1:C:399[B]:ARG:HG2	1.92	0.70
1:F:277:THR:N	1:F:325:TYR:CE1	2.58	0.70
1:F:277:THR:HG22	1:F:280:GLN:HB2	1.74	0.70
1:G:323:GLU:HB2	1:G:324:PRO:HD3	1.73	0.70
1:H:416:ALA:HB3	1:H:442:GLY:H	1.55	0.70
1:E:277:THR:OG1	1:E:280:GLN:O	2.08	0.70
1:C:25:VAL:HG21	1:C:57:MET:HE1	1.74	0.70
1:G:390:ILE:HG22	1:G:429:ILE:HD11	1.73	0.70
1:A:275:ASN:CG	1:A:276:TYR:N	2.50	0.70
1:F:455:LEU:HD23	1:F:455:LEU:N	2.06	0.70
1:E:38:SER:OG	1:E:39:ASP:N	2.22	0.70
1:E:428:ASP:HB3	1:E:431:ASN:HD22	1.56	0.70
1:A:13:ASP:CA	1:A:410:VAL:CG2	2.69	0.70
1:C:235:VAL:O	1:C:239:MET:HG3	1.92	0.70
1:D:9:VAL:HG22	1:D:23:THR:O	1.91	0.70
1:G:343:THR:HG21	1:G:371:ASP:HB2	1.74	0.70
1:E:282:ILE:HG13	1:E:328:ASN:ND2	2.07	0.69
1:A:236:LEU:HB3	1:A:266:LEU:CD2	2.22	0.69
1:B:385:SER:O	1:B:387:LEU:O	2.09	0.69
1:D:133:GLN:OE1	1:D:450:LEU:HD21	1.92	0.69
1:H:232:SER:OG	1:H:235:VAL:HG23	1.92	0.69
1:E:324:PRO:O	1:E:325:TYR:C	2.32	0.69
1:A:303:HIS:HB2	1:A:374:HIS:CE1	2.26	0.69
1:B:340:LEU:CD1	1:B:397:VAL:HA	2.22	0.69
1:F:224:PHE:CE2	1:F:278:LEU:CD1	2.75	0.69
1:F:264:VAL:HG12	1:F:293:SER:HB2	1.72	0.69
1:G:127:ILE:O	1:G:130:GLY:N	2.20	0.69
1:H:328:ASN:HA	1:H:331:ASN:HB2	1.74	0.69
1:D:75:MET:HE2	1:D:212:HIS:CE1	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:6:ILE:HG12	1:G:9:VAL:CG2	2.20	0.69
1:G:272:ILE:CG2	1:G:342:ASN:OD1	2.38	0.69
1:H:151:SER:OG	1:H:152:ALA:N	2.24	0.69
1:A:240:VAL:HG21	1:A:266:LEU:HD11	1.74	0.69
1:A:74:PHE:CZ	1:A:84:LEU:HD11	2.27	0.69
1:G:142:THR:HG22	1:G:197:TYR:OH	1.92	0.69
1:E:238:VAL:O	1:E:242:GLU:OE1	2.11	0.69
1:A:29:GLY:O	1:A:30:ASP:HB3	1.91	0.69
1:D:6:ILE:C	1:D:24:THR:CG2	2.66	0.69
1:F:264:VAL:CG1	1:F:293:SER:HB3	2.23	0.69
1:G:251:LEU:HD23	1:G:272:ILE:HD11	1.72	0.69
1:G:307:ARG:HG3	1:G:308:GLN:HG3	1.75	0.69
1:H:185:LEU:HD13	1:H:193:ARG:NH2	2.08	0.69
1:E:75:MET:CE	1:E:316:TRP:CH2	2.76	0.69
1:A:44:PRO:HB2	1:A:45:GLU:HG3	1.75	0.69
1:A:210:SER:OG	1:A:254:SER:CA	2.36	0.69
1:B:399[B]:ARG:HG3	1:B:399[B]:ARG:NH1	2.08	0.69
1:A:288:ASP:HA	1:A:291:VAL:HB	1.74	0.69
1:B:69:LEU:CD1	1:B:95:ILE:HG13	2.23	0.69
1:B:341:LEU:HD12	1:B:393:ALA:HB2	1.75	0.69
1:G:67:HIS:HA	1:G:112:ASP:OD1	1.93	0.69
1:H:6:ILE:O	1:H:24:THR:HG23	1.93	0.69
1:H:206:LYS:HZ2	1:H:272:ILE:HG21	1.57	0.69
1:E:65:ASN:O	1:E:66:VAL:HG23	1.93	0.68
1:A:14:GLY:O	1:A:15:LEU:HD23	1.93	0.68
1:A:66:VAL:HG11	1:A:368:ILE:HD11	1.73	0.68
1:D:301:THR:CG2	1:D:378:SER:HB3	2.21	0.68
1:H:407:ILE:HG22	1:H:408:GLY:N	2.08	0.68
1:A:179:GLY:C	1:A:180:HIS:O	2.28	0.68
1:C:364:ARG:NH1	1:C:367:THR:OG1	2.26	0.68
1:E:191:ARG:NH1	1:E:238:VAL:HG22	2.08	0.68
1:E:264:VAL:CG1	1:E:293:SER:HB2	2.22	0.68
1:A:363:ASP:OD1	1:A:370:ASN:OD1	2.11	0.68
1:D:75:MET:O	1:D:76:ALA:C	2.35	0.68
1:D:333:ILE:HD13	1:D:333:ILE:C	2.16	0.68
1:F:268:ALA:O	1:F:295:SER:OG	2.11	0.68
1:G:273:HIS:NE2	3:G:501:HOH:O	2.26	0.68
1:A:207:ILE:HG22	1:A:252:THR:HA	1.74	0.68
1:B:121:LEU:HD22	1:B:124:ARG:HH21	1.57	0.68
1:D:261:ASP:HB2	1:D:286:LEU:HD11	1.75	0.68
1:H:64:GLY:HA3	1:H:340:LEU:CD2	2.23	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:323:GLU:HB2	1:C:324:PRO:CD	2.13	0.68
1:F:72:TRP:C	1:F:76:ALA:CB	2.64	0.68
1:F:129:ALA:HB1	1:H:92:VAL:HG11	1.75	0.68
1:F:322:GLY:CA	1:F:326:ALA:HB3	2.18	0.68
1:H:357:SER:O	1:H:360:GLU:HB2	1.93	0.68
1:A:3:THR:O	1:A:47:ALA:HB1	1.93	0.68
1:B:111:PHE:HD2	1:B:204:MET:CE	2.06	0.68
1:F:75:MET:H	1:F:76:ALA:HB3	1.56	0.68
1:G:179:GLY:O	1:G:182:LEU:HD12	1.93	0.68
1:B:112:ASP:O	1:B:140:ALA:HB2	1.94	0.68
1:B:390:ILE:CA	1:B:392:ALA:HB3	2.23	0.68
1:F:40:SER:OG	1:F:42:PRO:HA	1.94	0.68
1:D:59:PRO:HG2	1:D:394:THR:HG21	1.74	0.68
1:F:66:VAL:O	1:F:112:ASP:HA	1.94	0.68
1:A:282:ILE:HG23	1:A:328:ASN:ND2	2.08	0.68
1:F:278:LEU:N	1:F:325:TYR:CE1	2.56	0.68
1:G:256:SER:OG	1:G:258:GLU:O	2.01	0.68
1:D:38:SER:OG	1:D:39:ASP:N	2.27	0.67
1:H:260:LEU:CD1	1:H:271:LEU:CD2	2.72	0.67
1:D:68:LEU:HD12	1:D:95:ILE:HG23	1.75	0.67
1:D:84:LEU:HD22	1:D:170:ILE:HG21	1.74	0.67
1:F:62:VAL:HA	1:F:109:THR:O	1.94	0.67
1:A:181:GLN:O	1:A:184:LEU:HD12	1.94	0.67
1:F:73:MET:CA	1:F:76:ALA:CB	2.72	0.67
1:F:328:ASN:O	1:F:329:GLU:C	2.35	0.67
1:E:323:GLU:CB	1:E:324:PRO:HD2	2.22	0.67
1:D:208:ALA:HB1	1:D:253:HIS:HD2	1.59	0.67
1:H:229:GLN:OE1	1:H:233:ARG:NH2	2.27	0.67
1:A:350:LYS:O	1:A:353:LEU:N	2.28	0.67
1:B:66:VAL:CG2	1:B:110:VAL:HG21	2.25	0.67
1:A:406:GLN:O	1:A:407:ILE:HG23	1.93	0.67
1:C:4:ILE:HG22	1:C:5:ALA:N	2.09	0.67
1:H:406:GLN:CB	1:H:415:LEU:CD1	2.73	0.67
1:F:29:GLY:O	1:F:30:ASP:HB2	1.94	0.67
1:F:292:ALA:O	3:F:502:HOH:O	2.12	0.67
1:H:217:LEU:HD13	1:H:226:ARG:HG3	1.77	0.67
1:F:45:GLU:HG2	1:F:46:GLY:H	1.60	0.67
1:F:214:VAL:O	1:F:218:VAL:HG23	1.95	0.67
1:G:370:ASN:OD1	1:G:433:ARG:NH2	2.22	0.67
1:E:399:ARG:HA	1:E:404:ALA:HB2	1.76	0.67
1:A:75:MET:HE3	1:A:212:HIS:CE1	2.28	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:VAL:CG2	1:A:252:THR:OG1	2.42	0.67
1:B:143:ILE:HG12	1:B:206:LYS:HD2	1.77	0.67
1:G:127:ILE:HD12	1:G:136:ARG:HA	1.77	0.67
1:C:217:LEU:HD23	1:C:224:PHE:CB	2.25	0.67
1:D:189:GLU:HB3	1:D:193:ARG:NH1	2.10	0.67
1:F:428:ASP:CG	1:F:430:ARG:HD2	2.19	0.67
1:A:111:PHE:HA	1:A:138:PHE:O	1.95	0.66
1:A:178:VAL:HA	1:A:182:LEU:HD11	1.77	0.66
1:A:316:TRP:CG	1:A:317:ALA:H	2.13	0.66
1:B:96:GLU:OE1	1:B:132:SER:HB2	1.95	0.66
1:D:5:ALA:O	1:D:50:VAL:HG12	1.95	0.66
1:F:307:ARG:NH2	1:F:311:GLU:OE2	2.27	0.66
1:G:6:ILE:HG22	1:G:25:VAL:O	1.94	0.66
1:A:75:MET:HE3	1:A:212:HIS:HE1	1.58	0.66
1:B:190:VAL:HG11	1:B:239:MET:HE3	1.76	0.66
1:D:341:LEU:H	1:D:397:VAL:HG12	1.61	0.66
1:H:59:PRO:HG2	1:H:394:THR:HG21	1.78	0.66
1:A:179:GLY:O	1:A:180:HIS:ND1	2.26	0.66
1:A:191:ARG:NE	1:A:238:VAL:HG22	2.09	0.66
1:C:77:GLY:O	1:C:155:HIS:ND1	2.28	0.66
1:C:124:ARG:HB2	1:C:137:ILE:HB	1.76	0.66
1:E:279:GLY:H	1:E:325:TYR:HE1	1.40	0.66
1:A:126:ARG:HG2	1:A:126:ARG:NH1	2.09	0.66
1:A:208:ALA:HA	1:A:253:HIS:HB3	1.77	0.66
1:D:340:LEU:HD12	1:D:397:VAL:HG12	1.76	0.66
1:G:358:PRO:O	1:G:362:GLU:HG3	1.95	0.66
1:F:419:VAL:HG13	1:F:438:VAL:HG22	1.77	0.66
1:C:38:SER:OG	1:C:40:SER:O	2.12	0.66
1:D:76:ALA:HB3	1:D:77:GLY:HA2	1.76	0.66
1:G:127:ILE:HG13	1:G:128:ASN:N	2.10	0.66
1:E:226:ARG:HH11	1:E:226:ARG:CA	2.08	0.66
1:A:145:GLY:H	1:A:179:GLY:HA2	1.60	0.66
1:A:287:ILE:O	1:A:291:VAL:CG2	2.25	0.66
1:G:356:LEU:HD22	1:G:360:GLU:OE1	1.95	0.66
1:E:217:LEU:HD23	1:E:217:LEU:C	2.21	0.66
1:E:319:ALA:O	1:E:325:TYR:HD2	1.79	0.66
1:C:337:ALA:O	1:C:338:LYS:HB2	1.96	0.66
1:D:6:ILE:CA	1:D:50:VAL:HG11	2.26	0.66
1:G:286:LEU:C	1:G:288:ASP:N	2.52	0.66
1:H:259:ALA:HA	1:H:262:THR:HB	1.78	0.66
1:D:56:TRP:HZ3	1:D:422:ASP:O	1.77	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:251:LEU:HD23	1:F:270:VAL:HB	1.78	0.65
1:F:304:ASP:OD1	1:F:381:GLU:CD	2.39	0.65
1:H:407:ILE:HG22	1:H:408:GLY:H	1.60	0.65
1:A:282:ILE:CG2	1:A:328:ASN:HD21	2.09	0.65
1:G:123:ALA:O	1:G:127:ILE:HG23	1.96	0.65
1:E:196:ASP:O	1:E:199:SER:HB3	1.96	0.65
1:A:316:TRP:CD1	1:A:317:ALA:H	2.13	0.65
1:D:301:THR:CG2	1:D:378:SER:HB2	2.26	0.65
1:G:277:THR:OG1	1:G:280:GLN:O	2.11	0.65
1:A:62:VAL:HG13	1:A:109:THR:HB	1.77	0.65
1:D:328:ASN:OD1	1:D:329:GLU:N	2.29	0.65
1:F:340:LEU:HD22	1:F:397:VAL:HA	1.78	0.65
1:E:226:ARG:NH1	1:E:226:ARG:HB2	2.12	0.65
1:A:88:GLU:OE1	1:A:169:ARG:NH1	2.28	0.65
1:G:339:ILE:HD11	1:G:384:MET:HE1	1.79	0.65
1:H:322:GLY:HA2	1:H:326:ALA:CB	2.23	0.65
1:E:145:GLY:CA	1:E:179:GLY:HA2	2.26	0.65
1:B:391:SER:CA	1:B:394:THR:H	2.10	0.65
1:C:259:ALA:O	1:C:263:SER:N	2.30	0.65
1:D:412:THR:O	1:D:414:LYS:N	2.26	0.65
1:F:87:TRP:CH2	1:F:455:LEU:O	2.49	0.65
1:H:34:THR:HG22	1:H:41:THR:CG2	2.26	0.65
1:H:146:MET:HE2	1:H:208:ALA:HB2	1.77	0.65
1:H:356:LEU:HB2	1:H:360:GLU:CG	2.21	0.65
1:C:26:ILE:CD1	1:C:41:THR:OG1	2.44	0.65
1:D:32:PHE:CE2	1:D:412:THR:CA	2.80	0.65
1:F:178:VAL:HG12	1:F:179:GLY:H	1.59	0.65
1:H:378:SER:O	1:H:380:VAL:O	2.14	0.65
1:E:217:LEU:HD23	1:E:217:LEU:O	1.96	0.65
1:A:275:ASN:O	1:A:328:ASN:ND2	2.28	0.65
1:C:74:PHE:HA	1:C:80:THR:OG1	1.97	0.65
1:G:326:ALA:HA	1:G:329:GLU:OE1	1.96	0.65
1:E:207:ILE:HD11	1:E:236:LEU:HD23	1.79	0.65
1:B:144:VAL:HG22	1:B:178:VAL:HG11	1.78	0.65
1:B:395:ILE:HD12	1:B:399[B]:ARG:CZ	2.26	0.65
1:F:166:PHE:CE1	1:F:170:ILE:HD11	2.32	0.65
1:F:323:GLU:CB	1:F:324:PRO:CD	2.69	0.65
1:H:204:MET:CA	1:H:248:VAL:HG12	2.14	0.65
1:C:4:ILE:HG22	1:C:5:ALA:H	1.62	0.64
1:D:62:VAL:HG13	1:D:109:THR:HB	1.79	0.64
1:H:140:ALA:HA	1:H:204:MET:HG2	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:PHE:CD2	1:A:278:LEU:HD22	2.32	0.64
1:C:103:LEU:HD12	1:C:107:VAL:O	1.97	0.64
1:D:301:THR:HG23	1:D:382:LYS:NZ	2.13	0.64
1:G:421:LEU:HD11	1:G:432:LEU:HD23	1.79	0.64
1:H:6:ILE:CG2	1:H:9:VAL:HG21	2.28	0.64
1:D:231:PHE:HB2	1:D:236:LEU:CD1	2.27	0.64
1:A:178:VAL:HG12	1:A:179:GLY:N	2.12	0.64
1:F:308:GLN:O	1:F:312:ASP:N	2.31	0.64
1:H:96:GLU:OE2	1:H:126:ARG:NH2	2.30	0.64
1:E:257:VAL:CG2	1:E:277:THR:HG22	2.27	0.64
1:B:389:ALA:C	1:B:392:ALA:HB3	2.21	0.64
1:D:195:ARG:HD2	1:D:242:GLU:OE1	1.98	0.64
1:H:39:ASP:OD1	1:H:39:ASP:N	2.29	0.64
1:H:202:VAL:O	1:H:203:ASP:C	2.39	0.64
1:G:253:HIS:ND1	1:G:273:HIS:HD2	1.96	0.64
1:G:274:ALA:HB3	1:G:298:GLY:O	1.98	0.64
1:B:340:LEU:HD11	1:B:397:VAL:HA	1.79	0.64
1:D:65:ASN:OD1	1:D:66:VAL:N	2.30	0.64
1:F:282:ILE:HG22	1:F:286:LEU:HB3	1.80	0.64
1:G:9:VAL:O	1:G:23:THR:HG22	1.98	0.64
1:B:74:PHE:CZ	1:B:84:LEU:HD21	2.33	0.64
1:F:70:ASP:OD1	1:F:71:ALA:N	2.30	0.64
1:F:63:ASN:ND2	1:F:371:ASP:OD2	2.30	0.64
1:F:279:GLY:O	1:F:280:GLN:OE1	2.14	0.64
1:G:6:ILE:HD11	1:G:9:VAL:HG13	1.79	0.64
1:H:67:HIS:CD2	1:H:67:HIS:N	2.64	0.64
1:B:143:ILE:HD12	1:B:146:MET:HE1	1.79	0.64
1:F:257:VAL:HG23	1:F:277:THR:HG21	1.77	0.64
1:F:268:ALA:O	1:F:295:SER:CB	2.45	0.64
1:B:299:LEU:HD23	1:B:329:GLU:CB	2.16	0.63
1:D:70:ASP:O	1:D:72:TRP:CA	2.46	0.63
1:G:390:ILE:HG22	1:G:429:ILE:CD1	2.28	0.63
1:H:180:HIS:O	1:H:182:LEU:N	2.30	0.63
1:E:226:ARG:HH11	1:E:226:ARG:CB	2.10	0.63
1:A:238:VAL:O	1:A:241:GLU:HG2	1.98	0.63
1:C:178:VAL:O	1:C:182:LEU:HG	1.97	0.63
1:G:262:THR:O	1:G:266:LEU:HD22	1.98	0.63
1:G:391:SER:O	1:G:396:ASN:OD1	2.16	0.63
1:E:419:VAL:HG23	1:E:438:VAL:HG22	1.79	0.63
1:A:45:GLU:C	1:A:47:ALA:H	2.05	0.63
1:A:153:ASP:HB3	1:A:212:HIS:HB3	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:GLU:HA	1:A:266:LEU:CD1	2.28	0.63
1:C:318:ALA:O	1:C:319:ALA:C	2.41	0.63
1:D:171:ASP:OD1	1:D:171:ASP:N	2.28	0.63
1:F:73:MET:HG2	1:F:73:MET:O	1.99	0.63
1:F:290:ILE:HG23	1:F:291:VAL:N	2.14	0.63
1:F:395:ILE:HA	1:F:398:ALA:HB3	1.79	0.63
1:H:332:LEU:HD22	1:H:337:ALA:HB2	1.81	0.63
1:B:31:ARG:NH1	1:B:415:LEU:N	2.46	0.63
1:F:14:GLY:HA2	1:F:390:ILE:HD13	1.80	0.63
1:E:75:MET:CE	1:E:316:TRP:CZ3	2.81	0.63
1:E:290:ILE:HA	1:E:293:SER:OG	1.98	0.63
1:A:348:PRO:HG3	1:A:364:ARG:NH1	2.12	0.63
1:D:32:PHE:CD2	1:D:412:THR:CA	2.81	0.63
1:F:74:PHE:CD1	1:F:80:THR:HG23	2.33	0.63
1:F:311:GLU:HG2	1:F:318:ALA:HB1	1.80	0.63
1:G:94:VAL:HG13	1:G:456:VAL:HG23	1.81	0.63
1:A:251:LEU:CD1	1:A:270:VAL:CG2	2.76	0.63
1:A:251:LEU:HD11	1:A:270:VAL:CG1	2.12	0.63
1:C:26:ILE:HD12	1:C:34:THR:OG1	1.99	0.63
1:H:6:ILE:CD1	1:H:57:MET:SD	2.87	0.63
1:C:69:LEU:HB2	1:C:115:ASN:OD1	1.98	0.63
1:F:118:GLU:CG	1:F:119:PRO:HD3	2.29	0.63
1:F:258:GLU:C	1:F:260:LEU:H	2.07	0.63
1:E:175:GLU:O	1:E:178:VAL:N	2.22	0.63
1:C:251:LEU:N	1:C:251:LEU:HD12	2.14	0.63
1:D:459:HIS:ND1	1:D:459:HIS:O	2.31	0.63
1:E:277:THR:HB	1:E:280:GLN:O	1.98	0.63
1:A:250:VAL:N	1:A:269:ASP:HB2	2.14	0.63
1:B:253:HIS:CD2	1:B:273:HIS:CE1	2.87	0.63
1:C:224:PHE:HE1	1:C:325:TYR:HH	0.85	0.63
1:D:96:GLU:O	1:D:100:GLN:N	2.32	0.63
1:D:350:LYS:CD	1:D:458:ALA:O	2.46	0.63
1:F:97:GLU:OE2	1:F:456:VAL:CG1	2.46	0.63
1:C:31:ARG:O	1:C:416:ALA:HB2	1.98	0.62
1:F:279:GLY:HA2	1:F:324:PRO:CG	2.20	0.62
1:G:286:LEU:C	1:G:288:ASP:H	2.06	0.62
1:H:7:THR:HA	1:H:24:THR:HG23	1.80	0.62
1:H:87:TRP:HB3	1:H:94:VAL:HG21	1.80	0.62
1:A:191:ARG:NE	1:A:238:VAL:CG2	2.61	0.62
1:G:127:ILE:HD13	1:G:137:ILE:HG12	1.81	0.62
1:A:224:PHE:HB3	1:A:278:LEU:HD13	1.79	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:HIS:CG	1:D:71:ALA:HB3	2.35	0.62
1:F:178:VAL:HG12	1:F:179:GLY:N	2.15	0.62
1:A:250:VAL:H	1:A:269:ASP:CB	2.11	0.62
1:A:275:ASN:OD1	1:A:276:TYR:CD2	2.53	0.62
1:E:25:VAL:HB	1:E:35:VAL:HG12	1.81	0.62
1:A:75:MET:SD	1:A:215:PHE:HD2	2.22	0.62
1:B:307:ARG:NH2	1:B:322:GLY:HA3	2.13	0.62
1:D:124:ARG:O	1:D:128:ASN:ND2	2.28	0.62
1:D:195:ARG:HE	1:D:242:GLU:HB3	1.64	0.62
1:F:313:VAL:CG2	1:F:360:GLU:OE2	2.47	0.62
1:G:181:GLN:O	1:G:182:LEU:HD12	2.00	0.62
1:H:153:ASP:O	1:H:212:HIS:ND1	2.33	0.62
1:H:253:HIS:HE2	1:H:273:HIS:HE2	1.42	0.62
1:D:56:TRP:CZ3	1:D:422:ASP:O	2.53	0.62
1:D:222:VAL:CG2	1:D:223:GLY:N	2.62	0.62
1:D:273:HIS:NE2	3:D:502:HOH:O	2.30	0.62
1:F:153:ASP:OD2	1:F:180:HIS:NE2	2.32	0.62
1:A:115:ASN:OD1	1:A:116:ALA:N	2.32	0.62
1:C:113:THR:HB	1:C:206:LYS:CD	2.28	0.62
1:D:339:ILE:HG22	1:D:340:LEU:N	2.15	0.62
1:D:350:LYS:CE	1:D:460:PRO:HB3	2.26	0.62
1:G:286:LEU:O	1:G:288:ASP:N	2.33	0.62
1:H:406:GLN:HB2	1:H:415:LEU:CD1	2.29	0.62
1:F:75:MET:CE	1:F:212:HIS:HE1	2.13	0.62
1:H:164:ARG:HA	1:H:167:VAL:HB	1.80	0.62
1:C:10:THR:HA	1:C:21:PRO:HA	1.81	0.62
1:F:255:VAL:HA	1:F:276:TYR:O	2.00	0.62
1:E:226:ARG:CD	1:E:228:TYR:HE2	2.07	0.61
1:E:264:VAL:HG12	1:E:293:SER:CB	2.30	0.61
1:A:72:TRP:O	1:A:76:ALA:HA	2.00	0.61
1:D:305:GLN:O	1:D:309:GLY:N	2.32	0.61
1:F:227:SER:O	1:F:228:TYR:O	2.17	0.61
1:G:26:ILE:HD11	1:G:42:PRO:O	2.00	0.61
1:H:146:MET:HE1	1:H:208:ALA:CB	2.30	0.61
1:H:149:PRO:O	1:H:155:HIS:N	2.33	0.61
1:H:303:HIS:ND1	1:H:306:HIS:HB2	2.15	0.61
1:A:191:ARG:HD2	1:A:238:VAL:HG21	1.82	0.61
1:B:178:VAL:HG21	1:B:197:TYR:CG	2.34	0.61
1:B:341:LEU:CD1	1:B:393:ALA:HB2	2.31	0.61
1:B:380:VAL:HG13	1:B:384:MET:O	2.00	0.61
1:B:385:SER:CB	1:B:387:LEU:O	2.47	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:LEU:HD13	1:H:226:ARG:CG	2.31	0.61
1:H:240:VAL:O	1:H:241:GLU:HB3	2.00	0.61
1:H:406:GLN:HB3	1:H:415:LEU:CD1	2.30	0.61
1:A:236:LEU:O	1:A:240:VAL:HG23	1.99	0.61
1:C:66:VAL:HG21	1:C:110:VAL:HB	1.83	0.61
1:C:219:ASP:OD1	1:C:222:VAL:N	2.33	0.61
1:D:339:ILE:HD13	1:D:384:MET:HE3	1.82	0.61
1:H:6:ILE:CG2	1:H:25:VAL:CG1	2.61	0.61
1:E:226:ARG:HH11	1:E:226:ARG:HA	1.63	0.61
1:B:195:ARG:O	1:B:199:SER:OG	2.18	0.61
1:B:396:ASN:OD1	1:B:396:ASN:N	2.33	0.61
1:E:169:ARG:NH2	1:D:351:ASP:OD2	2.34	0.61
1:A:73:MET:HE1	1:A:83:TYR:HB2	1.83	0.61
1:A:235:VAL:HA	1:A:238:VAL:CG1	2.30	0.61
1:C:121:LEU:HD21	1:C:124:ARG:NH2	2.15	0.61
1:A:125:ASP:HB2	1:A:126:ARG:NH1	2.14	0.61
1:A:180:HIS:O	1:A:181:GLN:HB2	1.99	0.61
1:A:253:HIS:CE1	1:A:273:HIS:CE1	2.87	0.61
1:B:44:PRO:HD2	1:B:47:ALA:HB2	1.82	0.61
1:C:302:VAL:HA	1:C:374:HIS:HE1	1.65	0.61
1:D:136:ARG:CZ	1:D:415:LEU:HD13	2.31	0.61
1:A:235:VAL:CA	1:A:238:VAL:HG12	2.30	0.61
1:A:254:SER:HB3	1:A:259:ALA:HB1	1.81	0.61
1:C:6:ILE:HG21	1:C:25:VAL:HG22	1.75	0.61
1:D:387:LEU:HA	1:D:390:ILE:HB	1.82	0.61
1:H:201:GLY:C	1:H:202:VAL:HG22	2.25	0.61
1:H:253:HIS:CD2	1:H:273:HIS:HE1	2.15	0.61
1:H:340:LEU:HD21	1:H:397:VAL:HG13	1.81	0.61
1:E:178:VAL:HG22	1:E:182:LEU:HD11	1.83	0.61
1:E:272:ILE:HG22	1:E:273:HIS:CE1	2.36	0.61
1:E:309:GLY:O	1:E:313:VAL:HG23	2.01	0.61
1:D:6:ILE:CG1	1:D:50:VAL:HG11	2.30	0.61
1:F:324:PRO:O	1:F:328:ASN:HB3	2.00	0.61
1:G:386:PRO:O	1:G:390:ILE:HG23	2.00	0.61
1:G:389:ALA:O	1:G:392:ALA:HB3	2.01	0.61
1:B:372:HIS:O	1:B:376:THR:OG1	2.17	0.61
1:C:142:THR:OG1	1:C:174:PHE:O	2.16	0.61
1:D:301:THR:HG21	1:D:378:SER:HB3	1.80	0.61
1:G:178:VAL:HG12	1:G:179:GLY:H	1.65	0.61
1:H:240:VAL:HG12	1:H:241:GLU:N	2.16	0.61
1:E:38:SER:HG	1:E:39:ASP:H	1.49	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:CE	1:A:272:ILE:CD1	2.79	0.61
1:C:72:TRP:O	1:C:75:MET:O	2.19	0.61
1:E:329:GLU:O	1:E:333:ILE:HG13	2.00	0.60
1:D:153:ASP:O	1:D:212:HIS:ND1	2.29	0.60
1:F:73:MET:C	1:F:76:ALA:CB	2.73	0.60
1:F:453:THR:C	1:F:455:LEU:HD23	2.24	0.60
1:B:393:ALA:O	1:B:397:VAL:HG23	2.01	0.60
1:F:150:PHE:HB2	1:F:167:VAL:HG13	1.84	0.60
1:C:58:VAL:HG23	1:C:419:VAL:HB	1.82	0.60
1:C:236:LEU:HD13	1:C:266:LEU:HD11	1.84	0.60
1:C:307:ARG:HG3	1:C:308:GLN:N	2.16	0.60
1:G:68:LEU:HD11	1:G:137:ILE:HG21	1.83	0.60
1:A:100:GLN:OE1	1:A:451:PRO:CB	2.49	0.60
1:B:424:ASP:O	1:B:431:ASN:OD1	2.19	0.60
1:D:282:ILE:HB	1:D:287:ILE:CD1	2.32	0.60
1:C:214:VAL:O	1:C:217:LEU:N	2.26	0.60
1:D:97:GLU:HA	1:D:100:GLN:HE21	1.66	0.60
1:G:102:ALA:O	1:G:107:VAL:N	2.34	0.60
1:G:362:GLU:O	1:G:363:ASP:HB2	2.01	0.60
1:H:63:ASN:HA	1:H:341:LEU:HD23	1.83	0.60
1:H:356:LEU:CB	1:H:360:GLU:HG3	2.20	0.60
1:E:185:LEU:HD12	1:E:186:PRO:HD2	1.83	0.60
1:A:238:VAL:HG13	1:A:239:MET:N	2.17	0.60
1:B:389:ALA:O	1:B:392:ALA:HB3	1.94	0.60
1:B:399[B]:ARG:HA	1:B:404:ALA:HB2	1.83	0.60
1:D:180:HIS:O	1:D:181:GLN:HB3	2.01	0.60
1:F:87:TRP:CZ2	1:F:455:LEU:O	2.54	0.60
1:F:255:VAL:HB	1:F:278:LEU:HD23	1.83	0.60
1:H:178:VAL:HG11	1:H:197:TYR:CG	2.36	0.60
1:E:153:ASP:CA	1:E:212:HIS:O	2.49	0.60
1:B:197:TYR:O	1:B:200:ARG:HB2	2.01	0.60
1:F:23:THR:HA	1:F:37:PRO:HA	1.83	0.60
1:B:139:ALA:N	1:B:203:ASP:OD2	2.35	0.60
1:F:166:PHE:CZ	1:F:170:ILE:HD11	2.37	0.60
1:F:323:GLU:O	1:F:327:THR:OG1	2.18	0.60
1:G:9:VAL:O	1:G:23:THR:CG2	2.50	0.60
1:H:208:ALA:HA	1:H:253:HIS:CB	2.32	0.60
1:H:231:PHE:CZ	1:H:239:MET:HE1	2.36	0.60
1:E:264:VAL:HG12	1:E:293:SER:HB2	1.84	0.60
1:B:391:SER:N	1:B:394:THR:H	2.00	0.60
1:G:6:ILE:HD13	1:G:9:VAL:HG21	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:206:LYS:HE2	1:E:253:HIS:HB2	1.84	0.60
1:E:214:VAL:HG22	1:E:215:PHE:CD1	2.37	0.60
1:B:31:ARG:HH11	1:B:415:LEU:N	2.00	0.60
1:A:296:TRP:CE3	1:A:338:LYS:HB3	2.36	0.59
1:D:412:THR:C	1:D:414:LYS:H	2.08	0.59
1:G:56:TRP:O	1:G:420:LEU:HA	2.02	0.59
1:H:41:THR:N	1:H:42:PRO:HA	2.16	0.59
1:A:75:MET:SD	1:A:215:PHE:CE2	2.95	0.59
1:D:411:GLU:O	1:D:412:THR:CB	2.46	0.59
1:D:420:LEU:O	1:D:436:THR:OG1	2.19	0.59
1:F:277:THR:HB	1:F:280:GLN:O	2.03	0.59
1:F:317:ALA:C	1:F:319:ALA:H	2.08	0.59
1:H:68:LEU:CD1	1:H:95:ILE:HG23	2.32	0.59
1:D:244:ARG:NH2	1:D:269:ASP:OD2	2.32	0.59
1:H:361:ARG:O	1:H:362:GLU:C	2.45	0.59
1:E:75:MET:HE1	1:E:316:TRP:CZ3	2.38	0.59
1:A:3:THR:HA	1:A:28:GLU:HA	1.84	0.59
1:A:206:LYS:CE	1:A:272:ILE:HD11	2.29	0.59
1:B:96:GLU:OE1	1:B:132:SER:CB	2.50	0.59
1:B:397:VAL:O	1:B:401:TYR:HD1	1.85	0.59
1:D:136:ARG:NH2	1:D:417:ASP:OD2	2.34	0.59
1:D:252:THR:HG22	1:D:271:LEU:HA	1.84	0.59
1:C:136:ARG:NH2	1:C:417:ASP:OD2	2.34	0.59
1:F:35:VAL:HG12	1:F:36:GLY:H	1.68	0.59
1:F:235:VAL:HA	1:F:238:VAL:HB	1.83	0.59
1:G:282:ILE:HG13	1:G:328:ASN:OD1	2.02	0.59
1:H:207:ILE:CD1	1:H:239:MET:SD	2.90	0.59
1:E:75:MET:HE1	1:E:316:TRP:HZ3	1.68	0.59
1:E:429:ILE:HG13	1:E:432:LEU:CD1	2.32	0.59
1:H:100:GLN:HG2	1:H:134:GLY:HA2	1.83	0.59
1:B:254:SER:OG	1:B:271:LEU:CD2	2.51	0.59
1:B:254:SER:OG	1:B:271:LEU:HD21	2.02	0.59
1:B:303:HIS:HB2	1:B:306:HIS:H	1.67	0.59
1:C:299:LEU:O	1:C:375:TRP:NE1	2.31	0.59
1:C:399[B]:ARG:HD3	1:C:404:ALA:CB	2.33	0.59
1:D:195:ARG:HG3	1:D:195:ARG:NH1	2.17	0.59
1:F:204:MET:HA	1:F:248:VAL:HB	1.84	0.59
1:H:169:ARG:O	1:H:173:MET:HB2	2.03	0.59
1:H:317:ALA:O	1:H:318:ALA:C	2.44	0.59
1:H:428:ASP:OD2	1:H:430:ARG:NH1	2.36	0.59
1:B:102:ALA:HB1	1:B:107:VAL:HB	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LYS:O	1:B:293:SER:N	2.30	0.59
1:B:391:SER:N	1:B:392:ALA:CB	2.62	0.59
1:G:391:SER:C	1:G:396:ASN:OD1	2.46	0.59
1:D:187:ARG:HB3	1:D:187:ARG:HH11	1.66	0.59
1:D:232:SER:HB2	1:D:234:PRO:HD2	1.83	0.59
1:E:214:VAL:CG1	1:E:215:PHE:HD1	2.09	0.59
1:A:363:ASP:OD2	1:A:374:HIS:ND1	2.35	0.59
1:C:397:VAL:O	1:C:401:TYR:HD1	1.86	0.59
1:D:289:LYS:O	1:D:293:SER:HB2	2.03	0.59
1:A:74:PHE:C	1:A:76:ALA:N	2.59	0.58
1:A:409:SER:CB	1:A:414:LYS:NZ	2.65	0.58
1:D:73:MET:HE3	1:D:74:PHE:HE1	1.67	0.58
1:G:259:ALA:HA	1:G:262:THR:HB	1.84	0.58
1:H:150:PHE:HA	1:H:155:HIS:O	2.02	0.58
1:A:409:SER:CB	1:A:414:LYS:HZ3	2.15	0.58
1:B:436:THR:O	1:B:447:ARG:NH2	2.36	0.58
1:F:269:ASP:O	1:F:296:TRP:HB2	2.03	0.58
1:F:322:GLY:O	1:F:323:GLU:OE1	2.20	0.58
1:G:388:GLU:HA	1:G:391:SER:OG	2.04	0.58
1:H:6:ILE:HG22	1:H:9:VAL:HG22	1.84	0.58
1:A:179:GLY:O	1:A:180:HIS:O	2.20	0.58
1:B:391:SER:HB3	1:B:394:THR:OG1	2.03	0.58
1:F:64:GLY:HA3	1:F:341:LEU:O	2.04	0.58
1:G:326:ALA:HA	1:G:329:GLU:HB2	1.84	0.58
1:D:6:ILE:HA	1:D:50:VAL:HG13	1.84	0.58
1:D:100:GLN:HG2	1:D:450:LEU:HD22	1.86	0.58
1:F:226:ARG:CB	1:F:226:ARG:HH11	2.16	0.58
1:G:217:LEU:HB2	1:G:219:ASP:HB2	1.86	0.58
1:H:213:ILE:HG22	1:H:213:ILE:O	2.01	0.58
1:E:290:ILE:O	1:E:293:SER:OG	2.19	0.58
1:A:240:VAL:CG2	1:A:266:LEU:CG	2.77	0.58
1:B:117:ILE:HA	1:B:120:VAL:HG12	1.85	0.58
1:F:38:SER:HB2	1:F:40:SER:N	2.17	0.58
1:F:45:GLU:CG	1:F:46:GLY:H	2.16	0.58
1:E:279:GLY:N	1:E:325:TYR:HE1	1.97	0.58
1:B:66:VAL:CG2	1:B:110:VAL:CG2	2.82	0.58
1:D:301:THR:HG22	1:D:302:VAL:N	2.18	0.58
1:G:122:ALA:O	1:G:126:ARG:HG3	2.04	0.58
1:H:206:LYS:HE3	1:H:272:ILE:CB	2.34	0.58
1:E:10:THR:HA	1:E:21:PRO:HA	1.85	0.58
1:D:49:VAL:HG23	1:D:49:VAL:O	2.02	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:ARG:O	1:D:447:ARG:HD3	2.03	0.58
1:D:195:ARG:NH2	1:D:242:GLU:O	2.28	0.58
1:F:75:MET:CE	1:F:212:HIS:CE1	2.86	0.58
1:G:258:GLU:O	1:G:259:ALA:HB3	2.04	0.58
1:E:74:PHE:HA	1:E:80:THR:OG1	2.04	0.58
1:B:41:THR:N	1:B:42:PRO:HA	2.17	0.58
1:B:73:MET:HA	1:B:76:ALA:CB	2.34	0.58
1:C:240:VAL:O	1:C:243:ALA:HB3	2.03	0.58
1:D:10:THR:HA	1:D:21:PRO:HA	1.85	0.58
1:D:68:LEU:HD13	1:D:95:ILE:CG2	2.34	0.58
1:G:380:VAL:HA	1:G:384:MET:HB2	1.84	0.58
1:C:9:VAL:HG13	1:C:52:GLY:HA3	1.86	0.58
1:D:75:MET:O	1:D:76:ALA:O	2.21	0.58
1:D:214:VAL:O	1:D:217:LEU:HB3	2.04	0.58
1:F:290:ILE:CD1	1:F:337:ALA:HA	2.34	0.58
1:F:375:TRP:HH2	1:F:392:ALA:HB1	1.69	0.58
1:G:363:ASP:O	1:G:374:HIS:CE1	2.56	0.58
1:G:388:GLU:O	1:G:391:SER:OG	2.22	0.58
1:E:303:HIS:HB2	1:E:306:HIS:H	1.67	0.58
1:B:187:ARG:HB3	1:B:235:VAL:HG22	1.85	0.58
1:B:190:VAL:O	1:B:194:VAL:HG23	2.04	0.58
1:F:113:THR:HG21	1:F:206:LYS:HD3	1.85	0.58
1:F:126:ARG:NH1	1:F:132:SER:HG	2.01	0.58
1:A:11:LEU:HD11	1:A:410:VAL:HG11	1.86	0.57
1:B:258:GLU:O	1:B:259:ALA:HB3	2.03	0.57
1:D:79:GLY:HA2	1:D:82:GLU:OE1	2.04	0.57
1:E:224:PHE:CG	1:E:278:LEU:HD12	2.37	0.57
1:B:273:HIS:HB3	1:B:300:GLN:HE21	1.69	0.57
1:D:227:SER:C	1:D:228:TYR:HD1	2.12	0.57
1:G:94:VAL:HG22	1:G:455:LEU:HD22	1.84	0.57
1:H:145:GLY:H	1:H:179:GLY:HA3	1.64	0.57
1:E:9:VAL:O	1:E:23:THR:OG1	2.18	0.57
1:E:23:THR:HG22	1:E:37:PRO:HG3	1.85	0.57
1:A:66:VAL:HG11	1:A:368:ILE:CD1	2.34	0.57
1:A:97:GLU:OE2	1:A:451:PRO:HG3	2.05	0.57
1:A:250:VAL:O	1:A:270:VAL:N	2.36	0.57
1:B:60:GLY:HA2	1:B:419:VAL:HG23	1.86	0.57
1:F:429:ILE:O	1:F:429:ILE:HG13	2.04	0.57
1:G:67:HIS:N	1:G:345:ALA:O	2.31	0.57
1:H:231:PHE:HB2	1:H:236:LEU:HD21	1.84	0.57
1:E:213:ILE:CG2	1:E:216:THR:HG22	2.34	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HG23	1:A:216:THR:HG21	1.87	0.57
1:B:240:VAL:O	1:B:244:ARG:HG2	2.04	0.57
1:G:127:ILE:HD11	1:G:137:ILE:H	1.69	0.57
1:B:391:SER:CA	1:B:394:THR:N	2.68	0.57
1:D:146:MET:O	1:D:179:GLY:HA3	2.04	0.57
1:F:30:ASP:O	1:F:416:ALA:CB	2.52	0.57
1:F:111:PHE:CE1	1:F:138:PHE:HD2	2.22	0.57
1:G:13:ASP:O	1:G:409:SER:OG	2.12	0.57
1:C:351:ASP:OD2	1:H:166:PHE:HB2	2.04	0.57
1:D:117:ILE:HA	1:D:120:VAL:HG12	1.86	0.57
1:H:6:ILE:HG21	1:H:25:VAL:HG12	1.85	0.57
1:H:225:ASP:CB	1:H:226:ARG:HE	2.13	0.57
1:E:225:ASP:O	1:E:226:ARG:CB	2.53	0.57
1:E:301:THR:HG21	1:E:379:MET:SD	2.45	0.57
1:A:51:ASP:O	1:A:55:ARG:NH2	2.37	0.57
1:A:343:THR:OG1	1:A:345:ALA:HB2	2.05	0.57
1:D:32:PHE:HD2	1:D:412:THR:HA	1.67	0.57
1:H:240:VAL:O	1:H:241:GLU:CB	2.53	0.57
1:H:356:LEU:HD12	1:H:360:GLU:HG3	1.86	0.57
1:E:77:GLY:N	1:E:78:PRO:CD	2.68	0.57
1:E:78:PRO:HA	1:E:155:HIS:CE1	2.40	0.57
1:E:419:VAL:HG22	1:E:435:ILE:HG23	1.85	0.57
1:A:411:GLU:CB	1:A:414:LYS:HE2	2.35	0.57
1:B:203:ASP:HB2	1:B:204:MET:HG3	1.85	0.57
1:C:28:GLU:O	1:C:29:GLY:C	2.47	0.57
1:C:219:ASP:OD1	1:C:223:GLY:N	2.37	0.57
1:F:319:ALA:O	1:F:322:GLY:O	2.23	0.57
1:G:58:VAL:O	1:G:419:VAL:N	2.33	0.57
1:E:220:ARG:C	1:E:221:SER:HG	2.01	0.57
1:B:69:LEU:CD1	1:B:95:ILE:CG1	2.80	0.57
1:B:210:SER:HB2	1:B:255:VAL:HG23	1.86	0.57
1:D:217:LEU:HD22	1:D:226:ARG:HG2	1.87	0.57
1:F:330:ARG:HG2	1:F:382:LYS:HD2	1.87	0.57
1:G:9:VAL:N	1:G:23:THR:O	2.37	0.57
1:A:32:PHE:HD2	1:A:411:GLU:O	1.88	0.57
1:B:63:ASN:HB3	1:B:110:VAL:HG23	1.86	0.57
1:C:70:ASP:CG	1:C:71:ALA:H	2.13	0.57
1:D:220:ARG:O	1:D:221:SER:OG	2.21	0.57
1:G:6:ILE:CG1	1:G:9:VAL:HG22	2.26	0.57
1:H:61:TYR:CE1	1:H:432:LEU:HD23	2.39	0.57
1:A:406:GLN:O	1:A:415:LEU:HB2	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:HIS:CE1	1:C:114:HIS:CB	2.88	0.56
1:D:217:LEU:HD11	1:D:225:ASP:OD1	2.05	0.56
1:H:109:THR:HA	1:H:136:ARG:HB2	1.86	0.56
1:H:202:VAL:O	1:H:202:VAL:HG23	2.04	0.56
1:E:278:LEU:CA	1:E:325:TYR:HE1	2.19	0.56
1:F:205:LEU:HD13	1:F:243:ALA:HB2	1.86	0.56
1:G:218:VAL:HB	1:G:219:ASP:HA	1.87	0.56
1:H:122:ALA:O	1:H:126:ARG:HD2	2.04	0.56
1:H:255:VAL:C	1:H:278:LEU:CD1	2.79	0.56
1:H:326:ALA:HA	1:H:329:GLU:OE2	2.05	0.56
1:E:19:PRO:O	1:E:21:PRO:HD3	2.04	0.56
1:E:45:GLU:C	1:E:47:ALA:N	2.61	0.56
1:E:205:LEU:HD13	1:E:243:ALA:HB2	1.87	0.56
1:A:219:ASP:HB3	1:A:222:VAL:HB	1.87	0.56
1:B:259:ALA:O	1:B:263:SER:OG	2.14	0.56
1:C:41:THR:HB	1:C:42:PRO:C	2.29	0.56
1:C:162:ALA:HB1	1:H:82:GLU:OE1	2.04	0.56
1:G:9:VAL:O	1:G:23:THR:O	2.24	0.56
1:E:284:ASN:O	1:E:285:TYR:CB	2.51	0.56
1:B:73:MET:HA	1:B:76:ALA:HB3	1.87	0.56
1:B:257:VAL:CG2	1:B:277:THR:OG1	2.53	0.56
1:A:125:ASP:CB	1:A:126:ARG:HH12	2.17	0.56
1:D:38:SER:OG	1:D:40:SER:O	2.24	0.56
1:F:6:ILE:HD11	1:F:420:LEU:HD21	1.87	0.56
1:F:304:ASP:OD1	1:F:381:GLU:OE1	2.24	0.56
1:H:189:GLU:O	1:H:193:ARG:NH2	2.39	0.56
1:E:23:THR:HA	1:E:37:PRO:HA	1.87	0.56
1:A:209:VAL:HG23	1:A:253:HIS:H	1.71	0.56
1:A:251:LEU:HD12	1:A:270:VAL:HG12	1.81	0.56
1:C:326:ALA:O	1:C:329:GLU:N	2.39	0.56
1:F:3:THR:CB	1:F:28:GLU:OE2	2.39	0.56
1:F:65:ASN:OD1	1:F:113:THR:CB	2.53	0.56
1:H:11:LEU:HB2	1:H:57:MET:HB2	1.88	0.56
1:H:260:LEU:O	1:H:264:VAL:HG23	2.04	0.56
1:E:198:LEU:O	1:E:201:GLY:N	2.24	0.56
1:A:240:VAL:CG2	1:A:266:LEU:HD11	2.35	0.56
1:C:286:LEU:O	1:C:290:ILE:HG13	2.06	0.56
1:D:220:ARG:C	1:D:222:VAL:HG12	2.30	0.56
1:D:404:ALA:O	1:D:414:LYS:NZ	2.38	0.56
1:F:154:PHE:N	1:F:154:PHE:CD1	2.73	0.56
1:F:256:SER:HB2	1:F:258:GLU:O	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:277:THR:CB	1:F:280:GLN:O	2.54	0.56
1:F:303:HIS:NE2	1:F:377:GLN:CD	2.64	0.56
1:G:127:ILE:CD1	1:G:136:ARG:HA	2.36	0.56
1:G:453:THR:O	1:G:453:THR:OG1	2.24	0.56
1:H:146:MET:SD	1:H:212:HIS:HB2	2.45	0.56
1:E:307:ARG:HB2	1:E:321:ALA:HB1	1.87	0.56
1:C:206:LYS:HZ1	1:C:253:HIS:HB2	1.70	0.56
1:D:191:ARG:HH21	1:D:238:VAL:HG22	1.69	0.56
1:F:204:MET:CE	1:F:251:LEU:HD11	2.35	0.56
1:G:317:ALA:O	1:G:320:LEU:HG	2.06	0.56
1:G:341:LEU:HG	1:G:375:TRP:CD2	2.41	0.56
1:H:6:ILE:HG22	1:H:9:VAL:CG2	2.36	0.56
1:H:68:LEU:HB3	1:H:95:ILE:HG23	1.87	0.56
1:A:253:HIS:CE1	1:A:273:HIS:ND1	2.72	0.56
1:B:151:SER:OG	1:B:152:ALA:O	2.10	0.56
1:D:195:ARG:CD	1:D:242:GLU:OE1	2.54	0.56
1:F:41:THR:OG1	1:F:42:PRO:O	2.23	0.56
1:B:73:MET:O	1:B:76:ALA:N	2.33	0.56
1:F:263:SER:O	1:F:266:LEU:HD12	2.07	0.56
1:G:323:GLU:CB	1:G:324:PRO:CD	2.84	0.56
1:G:323:GLU:CB	1:G:324:PRO:HD3	2.34	0.56
1:G:340:LEU:HG	1:G:397:VAL:HG22	1.87	0.56
1:D:181:GLN:C	1:D:183:SER:H	2.14	0.55
1:F:185:LEU:HD23	1:F:186:PRO:HD2	1.88	0.55
1:H:255:VAL:CB	1:H:278:LEU:CD1	2.75	0.55
1:H:303:HIS:NE2	1:H:305:GLN:HB2	2.20	0.55
1:E:226:ARG:HH11	1:E:226:ARG:HB2	1.67	0.55
1:B:133:GLN:HG2	1:B:450:LEU:HD11	1.88	0.55
1:B:379:MET:O	1:B:382:LYS:HB2	2.05	0.55
1:B:409:SER:HB3	1:B:414:LYS:HE3	1.89	0.55
1:C:78:PRO:HG2	1:C:352:HIS:CE1	2.40	0.55
1:C:114:HIS:CE1	1:C:143:ILE:H	2.24	0.55
1:D:124:ARG:HB2	1:D:137:ILE:HB	1.88	0.55
1:F:38:SER:HB2	1:F:40:SER:O	2.05	0.55
1:F:60:GLY:HA2	1:F:419:VAL:HG23	1.87	0.55
1:F:203:ASP:C	1:F:204:MET:HG3	2.31	0.55
1:F:264:VAL:HG13	1:F:293:SER:CB	2.22	0.55
1:G:6:ILE:HD11	1:G:9:VAL:HG11	1.86	0.55
1:H:323:GLU:CB	1:H:324:PRO:CD	2.83	0.55
1:H:352:HIS:O	1:H:356:LEU:HG	2.06	0.55
1:E:153:ASP:HB3	1:E:212:HIS:CB	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:ASP:OD1	1:E:212:HIS:O	2.24	0.55
1:A:258:GLU:C	1:A:260:LEU:H	2.15	0.55
1:B:96:GLU:O	1:B:100:GLN:NE2	2.39	0.55
1:B:155:HIS:C	1:B:155:HIS:CD2	2.84	0.55
1:D:14:GLY:O	1:D:395:ILE:HD11	2.06	0.55
1:F:277:THR:HG22	1:F:277:THR:O	2.04	0.55
1:H:328:ASN:C	1:H:328:ASN:HD22	2.13	0.55
1:C:112:ASP:O	1:C:139:ALA:HA	2.06	0.55
1:G:100:GLN:OE1	1:G:451:PRO:HA	2.06	0.55
1:E:144:VAL:HA	1:E:178:VAL:HG13	1.89	0.55
1:E:252:THR:HG21	1:E:271:LEU:HD22	1.87	0.55
1:E:385:SER:OG	1:E:388:GLU:CD	2.49	0.55
1:E:429:ILE:CD1	1:E:432:LEU:HD11	2.37	0.55
1:E:453:THR:HG23	1:E:453:THR:O	2.06	0.55
1:A:3:THR:HA	1:A:27:VAL:O	2.07	0.55
1:A:70:ASP:CG	1:A:71:ALA:H	2.08	0.55
1:A:395:ILE:HA	1:A:398:ALA:HB3	1.89	0.55
1:C:373:PHE:HB3	1:C:433:ARG:HE	1.70	0.55
1:H:6:ILE:HG13	1:H:25:VAL:HG13	1.87	0.55
1:H:41:THR:O	1:H:41:THR:HG22	2.06	0.55
1:H:208:ALA:HA	1:H:253:HIS:HB3	1.87	0.55
1:A:325:TYR:N	1:A:325:TYR:CD1	2.74	0.55
1:A:343:THR:HG21	1:A:371:ASP:OD2	2.06	0.55
1:B:280:GLN:H	1:B:280:GLN:CD	2.13	0.55
1:C:205:LEU:O	1:C:251:LEU:HD12	2.06	0.55
1:C:390:ILE:O	1:C:394:THR:HG23	2.06	0.55
1:D:6:ILE:CB	1:D:50:VAL:HG11	2.36	0.55
1:D:222:VAL:HG22	1:D:223:GLY:H	1.70	0.55
1:D:422:ASP:N	1:D:422:ASP:OD1	2.36	0.55
1:G:253:HIS:ND1	1:G:273:HIS:CD2	2.74	0.55
1:H:10:THR:HG23	1:H:21:PRO:HA	1.89	0.55
1:H:100:GLN:OE1	1:H:452:THR:OG1	2.24	0.55
1:E:213:ILE:HG22	1:E:213:ILE:O	2.05	0.55
1:B:73:MET:O	1:B:76:ALA:HB3	2.07	0.55
1:B:81:ILE:HG12	1:B:150:PHE:HE1	1.72	0.55
1:C:21:PRO:O	1:C:22:ALA:HB3	2.05	0.55
1:C:26:ILE:HD12	1:C:41:THR:OG1	2.07	0.55
1:C:92:VAL:O	1:C:96:GLU:HG3	2.07	0.55
1:G:19:PRO:HG3	1:G:426:VAL:HG21	1.88	0.55
1:G:205:LEU:HD22	1:G:243:ALA:HB2	1.88	0.55
1:H:322:GLY:O	1:H:323:GLU:HG3	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:324:PRO:O	1:E:326:ALA:N	2.40	0.55
1:B:399[A]:ARG:HA	1:B:404:ALA:HB2	1.88	0.55
1:C:318:ALA:O	1:C:320:LEU:N	2.39	0.55
1:D:76:ALA:CB	1:D:77:GLY:CA	2.85	0.55
1:D:220:ARG:HG3	1:D:220:ARG:NH1	2.19	0.55
1:H:6:ILE:HG21	1:H:9:VAL:HG21	1.88	0.55
1:H:387:LEU:O	1:H:391:SER:OG	2.21	0.55
1:E:66:VAL:O	1:E:67:HIS:CD2	2.58	0.55
1:E:285:TYR:CD1	1:E:285:TYR:C	2.84	0.55
1:A:32:PHE:CD2	1:A:411:GLU:O	2.60	0.55
1:G:58:VAL:HG23	1:G:419:VAL:HB	1.88	0.55
1:H:435:ILE:CG2	1:H:438:VAL:HG23	2.37	0.55
1:A:303:HIS:HB2	1:A:374:HIS:HE1	1.69	0.55
1:B:330:ARG:O	1:B:334:SER:OG	2.24	0.55
1:B:386:PRO:HB2	1:B:426:VAL:HG13	1.87	0.55
1:F:111:PHE:CE1	1:F:138:PHE:CD2	2.95	0.55
1:F:198:LEU:HA	1:F:202:VAL:HG22	1.89	0.55
1:F:321:ALA:O	1:F:326:ALA:HB2	2.07	0.55
1:H:287:ILE:O	1:H:291:VAL:HG23	2.07	0.55
1:E:233:ARG:HA	1:E:236:LEU:HD12	1.87	0.54
1:A:92:VAL:HG12	1:C:131:ILE:HD11	1.89	0.54
1:D:189:GLU:HB3	1:D:193:ARG:HH11	1.71	0.54
1:F:273:HIS:O	1:F:276:TYR:HB2	2.08	0.54
1:G:324:PRO:O	1:G:328:ASN:CB	2.55	0.54
1:H:379:MET:O	1:H:384:MET:N	2.37	0.54
1:A:144:VAL:HG22	1:A:178:VAL:HG11	1.88	0.54
1:A:235:VAL:O	1:A:239:MET:HG3	2.07	0.54
1:C:222:VAL:O	1:C:222:VAL:HG22	2.06	0.54
1:F:75:MET:N	1:F:76:ALA:CB	2.68	0.54
1:F:75:MET:HB3	1:F:76:ALA:HB2	1.89	0.54
1:G:153:ASP:O	1:G:212:HIS:ND1	2.40	0.54
1:H:153:ASP:OD1	1:H:213:ILE:HG13	2.07	0.54
1:H:360:GLU:HG2	1:H:361:ARG:N	2.21	0.54
1:E:214:VAL:O	1:E:217:LEU:O	2.24	0.54
1:E:429:ILE:C	1:E:431:ASN:H	2.14	0.54
1:A:149:PRO:O	1:A:154:PHE:HB3	2.07	0.54
1:A:151:SER:OG	1:A:159:ARG:NH1	2.40	0.54
1:C:124:ARG:NH1	1:C:125:ASP:OD1	2.41	0.54
1:G:45:GLU:N	1:G:45:GLU:OE1	2.39	0.54
1:H:6:ILE:CG2	1:H:9:VAL:CG2	2.85	0.54
1:C:273:HIS:HA	1:C:300:GLN:HE21	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:76:ALA:HB3	1:D:77:GLY:CA	2.37	0.54
1:B:329:GLU:OE1	1:B:379:MET:HE1	2.07	0.54
1:C:75:MET:O	1:C:76:ALA:HB3	2.08	0.54
1:C:117:ILE:HD13	1:C:200:ARG:HD3	1.88	0.54
1:D:182:LEU:HB3	1:D:231:PHE:CE2	2.42	0.54
1:D:301:THR:HG23	1:D:382:LYS:HZ3	1.71	0.54
1:F:356:LEU:HD23	1:F:360:GLU:CD	2.33	0.54
1:G:158:GLY:HA2	1:G:161:ALA:HB3	1.89	0.54
1:E:76:ALA:N	1:E:77:GLY:HA2	2.22	0.54
1:E:145:GLY:C	1:E:179:GLY:HA2	2.33	0.54
1:E:264:VAL:HG11	1:E:293:SER:OG	2.07	0.54
1:E:284:ASN:O	1:E:285:TYR:CG	2.61	0.54
1:C:70:ASP:OD2	1:C:73:MET:HB2	2.06	0.54
1:F:209:VAL:HB	1:F:253:HIS:O	2.07	0.54
1:H:6:ILE:HD13	1:H:57:MET:SD	2.48	0.54
1:H:296:TRP:CD2	1:H:338:LYS:HB3	2.42	0.54
1:H:457:THR:HA	1:H:459:HIS:CD2	2.42	0.54
1:E:340:LEU:HD11	1:E:397:VAL:HA	1.89	0.54
1:B:231:PHE:HB2	1:B:236:LEU:HD13	1.90	0.54
1:C:74:PHE:CD1	1:C:74:PHE:N	2.73	0.54
1:D:148:GLY:C	1:D:154:PHE:HD2	2.14	0.54
1:H:435:ILE:HG21	1:H:438:VAL:HG23	1.90	0.54
1:C:117:ILE:O	1:C:121:LEU:HB2	2.08	0.54
1:F:126:ARG:HH11	1:F:132:SER:HG	1.55	0.54
1:F:268:ALA:O	1:F:295:SER:HB3	2.06	0.54
1:F:428:ASP:CG	1:F:430:ARG:CD	2.79	0.54
1:A:13:ASP:C	1:A:410:VAL:CG2	2.74	0.54
1:A:74:PHE:C	1:A:76:ALA:H	2.16	0.54
1:E:102:ALA:HB1	1:E:107:VAL:HB	1.91	0.54
1:E:307:ARG:NH2	1:E:311:GLU:OE1	2.41	0.54
1:E:339:ILE:HG21	1:E:379:MET:HE2	1.90	0.54
1:C:163:THR:HB	1:C:166:PHE:HB3	1.89	0.54
1:C:254:SER:HB2	1:C:259:ALA:HB1	1.90	0.54
1:F:4:ILE:HG22	1:F:48:THR:HB	1.90	0.54
1:F:290:ILE:HG23	1:F:291:VAL:H	1.73	0.54
1:E:87:TRP:CZ2	1:E:455:LEU:O	2.61	0.53
1:A:445:VAL:C	1:A:447:ARG:HH12	2.09	0.53
1:B:38:SER:OG	1:B:39:ASP:N	2.40	0.53
1:D:72:TRP:O	1:D:73:MET:HB3	2.07	0.53
1:D:75:MET:CE	1:D:212:HIS:CE1	2.91	0.53
1:D:97:GLU:HA	1:D:100:GLN:NE2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ALA:CB	1:D:253:HIS:HD2	2.21	0.53
1:D:224:PHE:HE1	1:D:325:TYR:HH	1.54	0.53
1:F:220:ARG:NH2	1:F:314:GLY:O	2.41	0.53
1:H:203:ASP:C	1:H:248:VAL:HG13	2.33	0.53
1:H:424:ASP:OD1	1:H:426:VAL:N	2.38	0.53
1:H:436:THR:OG1	1:H:437:GLU:N	2.40	0.53
1:H:453:THR:HG22	1:H:454:PRO:HD2	1.90	0.53
1:E:38:SER:OG	1:E:39:ASP:OD1	2.25	0.53
1:E:40:SER:OG	1:E:42:PRO:HA	2.08	0.53
1:A:194:VAL:CG2	1:A:239:MET:CE	2.75	0.53
1:D:206:LYS:HG3	1:D:251:LEU:HB2	1.90	0.53
1:G:407:ILE:HG23	1:G:415:LEU:HD12	1.90	0.53
1:H:439:PHE:CE1	1:H:444:ALA:HB2	2.42	0.53
1:B:303:HIS:CD2	1:B:377:GLN:HG2	2.43	0.53
1:C:217:LEU:CD2	1:C:224:PHE:CB	2.86	0.53
1:F:5:ALA:HA	1:F:26:ILE:HA	1.90	0.53
1:F:325:TYR:O	1:F:329:GLU:CD	2.48	0.53
1:G:10:THR:HG23	1:G:10:THR:O	2.07	0.53
1:G:15:LEU:HD11	1:G:411:GLU:OE2	2.08	0.53
1:G:15:LEU:HA	1:G:395:ILE:HD11	1.90	0.53
1:H:10:THR:O	1:H:56:TRP:HA	2.07	0.53
1:A:100:GLN:OE1	1:A:451:PRO:HB2	2.07	0.53
1:A:346:GLY:O	1:A:368:ILE:N	2.41	0.53
1:D:13:ASP:OD1	1:D:14:GLY:N	2.42	0.53
1:F:6:ILE:N	1:F:25:VAL:O	2.42	0.53
1:G:76:ALA:HB1	1:G:77:GLY:C	2.33	0.53
1:H:77:GLY:O	1:H:155:HIS:CG	2.60	0.53
1:H:86:ARG:HG2	1:H:87:TRP:CE2	2.43	0.53
1:D:38:SER:HB3	1:D:41:THR:HG22	1.89	0.53
1:D:182:LEU:HB3	1:D:231:PHE:HE2	1.74	0.53
1:F:7:THR:O	1:F:52:GLY:HA3	2.08	0.53
1:F:273:HIS:ND1	1:F:276:TYR:CE2	2.76	0.53
1:F:290:ILE:HD12	1:F:337:ALA:HA	1.91	0.53
1:E:75:MET:CE	1:E:316:TRP:HH2	2.20	0.53
1:E:76:ALA:HB3	1:E:77:GLY:HA2	1.91	0.53
1:A:374:HIS:C	1:A:374:HIS:CD2	2.87	0.53
1:B:391:SER:OG	1:B:391:SER:O	2.24	0.53
1:D:252:THR:HG21	1:D:263:SER:HB3	1.90	0.53
1:D:283:PRO:HB2	1:D:285:TYR:CD2	2.44	0.53
1:D:343:THR:O	1:D:343:THR:OG1	2.26	0.53
1:H:68:LEU:CB	1:H:95:ILE:HG23	2.39	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:PRO:HB2	1:A:38:SER:O	2.08	0.53
1:A:194:VAL:HG21	1:A:239:MET:HE1	1.86	0.53
1:B:365:PRO:HG3	1:B:374:HIS:CE1	2.44	0.53
1:H:30:ASP:O	1:H:31:ARG:CB	2.56	0.53
1:H:103:LEU:HD21	1:H:445:VAL:HG21	1.90	0.53
1:A:283:PRO:O	1:A:287:ILE:HD12	2.09	0.53
1:B:22:ALA:O	1:B:37:PRO:CB	2.47	0.53
1:B:138:PHE:HA	1:B:203:ASP:OD2	2.08	0.53
1:C:117:ILE:HG13	1:C:121:LEU:HD12	1.90	0.53
1:D:380:VAL:HG13	1:D:384:MET:O	2.09	0.53
1:F:206:LYS:HB2	1:F:251:LEU:HD12	1.90	0.53
1:G:94:VAL:HG13	1:G:456:VAL:CG2	2.39	0.53
1:E:429:ILE:HG23	1:E:430:ARG:N	2.22	0.53
1:A:287:ILE:HG22	1:A:291:VAL:HG21	1.90	0.53
1:B:76:ALA:H	1:B:77:GLY:HA2	1.73	0.53
1:D:278:LEU:HA	1:D:325:TYR:HE1	1.71	0.53
1:D:351:ASP:O	1:D:354:ALA:N	2.42	0.53
1:D:412:THR:HG22	1:D:413:GLY:N	2.23	0.53
1:G:6:ILE:CG2	1:G:25:VAL:H	2.21	0.53
1:G:124:ARG:HG3	1:G:125:ASP:N	2.23	0.53
1:H:31:ARG:HH11	1:H:415:LEU:CD1	2.20	0.53
1:H:45:GLU:HG3	1:H:45:GLU:O	2.09	0.53
1:H:64:GLY:HA2	1:H:111:PHE:HD2	1.73	0.53
1:H:96:GLU:HG2	1:H:127:ILE:HD11	1.89	0.53
1:H:253:HIS:HD2	1:H:273:HIS:HE1	1.48	0.53
1:A:14:GLY:HA3	1:A:59:PRO:HG2	1.91	0.53
1:A:299:LEU:HD22	1:A:329:GLU:HB2	1.91	0.53
1:A:373:PHE:O	1:A:377:GLN:HG2	2.08	0.53
1:B:348:PRO:HG2	1:B:353:LEU:HD21	1.90	0.53
1:C:41:THR:HB	1:C:42:PRO:O	2.09	0.53
1:G:71:ALA:O	1:G:74:PHE:HB2	2.09	0.53
1:G:324:PRO:O	1:G:328:ASN:HB3	2.09	0.53
1:E:296:TRP:CE3	1:E:338:LYS:HB3	2.44	0.52
1:B:68:LEU:HB3	1:B:95:ILE:HG23	1.91	0.52
1:D:70:ASP:C	1:D:72:TRP:N	2.60	0.52
1:F:45:GLU:HG2	1:F:46:GLY:N	2.24	0.52
1:F:70:ASP:OD1	1:F:72:TRP:N	2.42	0.52
1:F:277:THR:O	1:F:278:LEU:HB2	2.09	0.52
1:F:395:ILE:O	1:F:399:ARG:N	2.29	0.52
1:G:252:THR:HG21	1:G:271:LEU:HD22	1.91	0.52
1:G:286:LEU:O	1:G:287:ILE:C	2.51	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:TRP:CZ2	1:H:424:ASP:HB2	2.44	0.52
1:H:61:TYR:CD2	1:H:372:HIS:NE2	2.78	0.52
1:H:232:SER:HG	1:H:235:VAL:HG23	1.73	0.52
1:B:257:VAL:HG23	1:B:277:THR:OG1	2.09	0.52
1:C:86:ARG:HA	1:H:86:ARG:HB2	1.90	0.52
1:D:303:HIS:HB3	1:D:306:HIS:H	1.74	0.52
1:F:205:LEU:O	1:F:250:VAL:HA	2.08	0.52
1:E:264:VAL:HG11	1:E:293:SER:CB	2.38	0.52
1:E:278:LEU:HA	1:E:325:TYR:CE1	2.43	0.52
1:B:340:LEU:HD12	1:B:397:VAL:HA	1.91	0.52
1:F:45:GLU:C	1:F:47:ALA:N	2.64	0.52
1:F:303:HIS:NE2	1:F:377:GLN:OE1	2.43	0.52
1:G:146:MET:HE2	1:G:212:HIS:HB2	1.91	0.52
1:H:20:ARG:HB3	1:H:23:THR:HG21	1.92	0.52
1:H:30:ASP:N	1:H:442:GLY:HA3	2.20	0.52
1:E:411:GLU:HB3	1:E:414:LYS:HD2	1.90	0.52
1:A:63:ASN:HA	1:A:341:LEU:CD2	2.39	0.52
1:F:427:ASP:O	1:F:428:ASP:CB	2.41	0.52
1:G:38:SER:C	1:G:40:SER:H	2.17	0.52
1:H:194:VAL:O	1:H:198:LEU:HD13	2.10	0.52
1:H:453:THR:O	1:H:455:LEU:N	2.40	0.52
1:E:73:MET:O	1:E:76:ALA:HB3	2.08	0.52
1:E:286:LEU:O	1:E:290:ILE:HG13	2.10	0.52
1:E:323:GLU:CB	1:E:324:PRO:CD	2.83	0.52
1:A:73:MET:HE3	1:A:79:GLY:O	2.10	0.52
1:A:124:ARG:NH2	1:A:201:GLY:O	2.38	0.52
1:D:10:THR:HB	1:D:56:TRP:CD1	2.44	0.52
1:D:32:PHE:CE1	1:D:415:LEU:O	2.59	0.52
1:D:278:LEU:CA	1:D:325:TYR:HE1	2.23	0.52
1:D:341:LEU:H	1:D:397:VAL:CG1	2.23	0.52
1:F:117:ILE:HG21	1:F:200:ARG:HD2	1.91	0.52
1:G:72:TRP:O	1:G:75:MET:HE2	2.09	0.52
1:H:224:PHE:N	1:H:224:PHE:CD1	2.76	0.52
1:H:235:VAL:O	1:H:238:VAL:HG12	2.10	0.52
1:E:77:GLY:O	1:E:78:PRO:C	2.48	0.52
1:E:87:TRP:CH2	1:E:455:LEU:O	2.63	0.52
1:E:207:ILE:CD1	1:E:236:LEU:HD23	2.39	0.52
1:E:385:SER:O	1:E:387:LEU:N	2.43	0.52
1:A:69:LEU:HD11	1:A:91:TYR:HB3	1.92	0.52
1:B:206:LYS:HE3	1:B:272:ILE:HG13	1.90	0.52
1:B:315:SER:OG	1:B:360:GLU:OE2	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:VAL:HG21	1:D:57:MET:HE1	1.91	0.52
1:D:36:GLY:HA3	1:D:41:THR:CG2	2.39	0.52
1:H:182:LEU:HD13	1:H:239:MET:HE2	1.91	0.52
1:H:186:PRO:HG2	1:H:189:GLU:HG3	1.91	0.52
1:H:206:LYS:HA	1:H:251:LEU:HB2	1.90	0.52
1:B:292:ALA:O	1:B:294:ASP:OD1	2.28	0.52
1:D:350:LYS:HD2	1:D:459:HIS:HA	1.92	0.52
1:F:3:THR:HB	1:F:28:GLU:CD	2.32	0.52
1:F:270:VAL:HG22	1:F:340:LEU:HD11	1.90	0.52
1:E:148:GLY:O	1:E:151:SER:OG	2.28	0.52
1:E:252:THR:CG2	1:E:271:LEU:HA	2.29	0.52
1:C:298:GLY:HA3	1:C:342:ASN:ND2	2.24	0.52
1:C:446:ASP:O	1:C:450:LEU:HD12	2.09	0.52
1:D:103:LEU:HD21	1:D:445:VAL:HG21	1.92	0.52
1:D:181:GLN:CG	1:D:182:LEU:H	2.23	0.52
1:F:59:PRO:CG	1:F:394:THR:HG21	2.40	0.52
1:G:17:GLY:O	1:G:18:LEU:C	2.53	0.52
1:G:303:HIS:O	1:G:307:ARG:HB3	2.10	0.52
1:H:232:SER:OG	1:H:235:VAL:CG2	2.57	0.52
1:E:307:ARG:CZ	1:E:311:GLU:OE1	2.58	0.52
1:A:66:VAL:HA	1:A:345:ALA:CB	2.39	0.52
1:A:235:VAL:HA	1:A:238:VAL:HG12	1.90	0.52
1:B:135:ALA:O	1:B:137:ILE:HG13	2.09	0.52
1:D:252:THR:HG21	1:D:263:SER:CB	2.39	0.52
1:F:300:GLN:OE1	1:F:344:ASP:OD1	2.28	0.52
1:G:348:PRO:HG2	1:G:353:LEU:HG	1.92	0.52
1:H:32:PHE:N	1:H:414:LYS:O	2.31	0.52
1:E:181:GLN:O	1:E:182:LEU:C	2.52	0.52
1:A:213:ILE:HG23	1:A:216:THR:CG2	2.40	0.52
1:A:276:TYR:CE1	1:A:320:LEU:HD22	2.45	0.52
1:B:30:ASP:O	1:B:31:ARG:O	2.28	0.52
1:C:144:VAL:HG13	1:C:178:VAL:HG13	1.91	0.52
1:D:148:GLY:HA3	1:D:171:ASP:HB3	1.92	0.52
1:D:222:VAL:CG2	1:D:223:GLY:H	2.23	0.52
1:E:226:ARG:CD	1:E:228:TYR:CE2	2.89	0.51
1:A:271:LEU:HD13	1:A:297:ALA:HA	1.90	0.51
1:B:56:TRP:O	1:B:420:LEU:HA	2.09	0.51
1:B:143:ILE:HG22	1:B:208:ALA:HB2	1.92	0.51
1:C:57:MET:HE3	1:C:418:PHE:CG	2.45	0.51
1:C:255:VAL:O	1:C:278:LEU:HG	2.10	0.51
1:D:332:LEU:C	1:D:337:ALA:HB2	2.31	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:129:ALA:HB3	1:G:131:ILE:CG1	2.37	0.51
1:H:107:VAL:HG23	1:H:372:HIS:HE1	1.66	0.51
1:H:180:HIS:C	1:H:182:LEU:N	2.68	0.51
1:E:329:GLU:OE1	1:E:382:LYS:HE3	2.11	0.51
1:B:64:GLY:CA	1:B:397:VAL:HG11	2.40	0.51
1:C:97:GLU:OE1	1:C:456:VAL:HG12	2.09	0.51
1:D:36:GLY:CA	1:D:41:THR:HG21	2.41	0.51
1:D:181:GLN:HG2	1:D:182:LEU:H	1.75	0.51
1:F:70:ASP:O	1:F:74:PHE:CE2	2.63	0.51
1:F:225:ASP:O	1:F:226:ARG:CB	2.55	0.51
1:E:252:THR:HG21	1:E:263:SER:HB3	1.92	0.51
1:A:287:ILE:O	1:A:291:VAL:N	2.39	0.51
1:B:77:GLY:HA3	1:B:155:HIS:CB	2.41	0.51
1:B:127:ILE:HD12	1:B:137:ILE:HD11	1.91	0.51
1:B:301:THR:OG1	1:B:378:SER:OG	2.10	0.51
1:C:105:ASN:OD1	1:C:373:PHE:CE2	2.63	0.51
1:D:143:ILE:HG23	1:D:206:LYS:HB3	1.91	0.51
1:G:143:ILE:HG12	1:G:206:LYS:HD3	1.91	0.51
1:H:31:ARG:HH11	1:H:415:LEU:HG	1.75	0.51
1:H:263:SER:O	1:H:266:LEU:N	2.42	0.51
1:H:285:TYR:CE1	1:H:286:LEU:HD12	2.45	0.51
1:A:151:SER:HA	1:A:156:PHE:HD1	1.75	0.51
1:A:204:MET:HB3	1:A:249:PRO:HG2	1.92	0.51
1:B:113:THR:HA	1:B:140:ALA:HB2	1.91	0.51
1:C:25:VAL:HG21	1:C:57:MET:CE	2.40	0.51
1:C:153:ASP:HB3	1:C:212:HIS:HB3	1.91	0.51
1:D:37:PRO:O	1:D:39:ASP:O	2.28	0.51
1:D:83:TYR:C	1:D:83:TYR:CD1	2.88	0.51
1:D:90:ARG:NH2	1:D:93:GLU:OE2	2.44	0.51
1:D:227:SER:O	1:D:228:TYR:HD1	1.92	0.51
1:D:341:LEU:HA	1:D:375:TRP:CZ2	2.46	0.51
1:F:209:VAL:HG11	1:F:259:ALA:O	2.10	0.51
1:F:257:VAL:CG2	1:F:277:THR:HG21	2.39	0.51
1:F:341:LEU:HA	1:F:375:TRP:CZ2	2.45	0.51
1:H:72:TRP:CH2	1:H:75:MET:HE1	2.44	0.51
1:A:209:VAL:N	1:A:253:HIS:O	2.43	0.51
1:A:310:LEU:HD22	1:A:360:GLU:HG2	1.93	0.51
1:B:117:ILE:HD13	1:B:200:ARG:HD2	1.92	0.51
1:B:391:SER:HB2	1:B:394:THR:CG2	2.38	0.51
1:C:26:ILE:HD11	1:C:41:THR:OG1	2.09	0.51
1:C:70:ASP:CG	1:C:71:ALA:N	2.68	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:118:GLU:HG2	1:F:119:PRO:HD3	1.92	0.51
1:F:409:SER:OG	1:F:414:LYS:HE3	2.10	0.51
1:H:67:HIS:HA	1:H:112:ASP:OD1	2.10	0.51
1:E:419:VAL:CG2	1:E:435:ILE:HG23	2.41	0.51
1:A:11:LEU:HD23	1:A:11:LEU:C	2.36	0.51
1:A:68:LEU:HD11	1:A:137:ILE:HD12	1.92	0.51
1:F:388:GLU:OE1	1:F:388:GLU:N	2.44	0.51
1:E:140:ALA:HB2	1:E:204:MET:HG2	1.91	0.51
1:E:213:ILE:HG21	1:E:216:THR:CG2	2.40	0.51
1:D:118:GLU:HB2	1:D:119:PRO:HD3	1.93	0.51
1:F:409:SER:O	1:F:414:LYS:HD2	2.11	0.51
1:H:333:ILE:HG21	1:H:384:MET:HG3	1.93	0.51
1:E:121:LEU:HD11	1:E:202:VAL:HG12	1.92	0.51
1:E:259:ALA:O	1:E:262:THR:N	2.44	0.51
1:E:272:ILE:HG22	1:E:273:HIS:ND1	2.26	0.51
1:A:302:VAL:HB	1:A:321:ALA:HA	1.92	0.51
1:C:143:ILE:HB	1:C:146:MET:HG3	1.93	0.51
1:F:356:LEU:HD23	1:F:360:GLU:OE1	2.11	0.51
1:E:180:HIS:CG	1:E:181:GLN:H	2.28	0.51
1:E:258:GLU:O	1:E:260:LEU:N	2.44	0.51
1:E:284:ASN:OD1	1:E:285:TYR:N	2.44	0.51
1:E:298:GLY:HA3	1:E:342:ASN:ND2	2.26	0.51
1:E:301:THR:OG1	1:E:378:SER:OG	2.25	0.51
1:B:100:GLN:HG2	1:B:450:LEU:HD11	1.93	0.51
1:G:68:LEU:CB	1:G:95:ILE:CG2	2.70	0.51
1:H:77:GLY:O	1:H:155:HIS:NE2	2.43	0.51
1:H:384:MET:HE1	1:H:392:ALA:HB2	1.92	0.51
1:E:117:ILE:HG23	1:E:121:LEU:HD13	1.93	0.51
1:E:213:ILE:CG2	1:E:216:THR:HB	2.41	0.51
1:B:391:SER:H	1:B:393:ALA:N	2.08	0.51
1:C:399[B]:ARG:HH11	1:C:404:ALA:HB1	1.75	0.51
1:D:218:VAL:HG23	1:D:218:VAL:O	2.11	0.51
1:F:261:ASP:HB2	1:F:286:LEU:HD11	1.93	0.51
1:H:152:ALA:HB1	1:H:213:ILE:HG12	1.93	0.51
1:A:221:SER:OG	1:G:44:PRO:HB3	2.11	0.50
1:A:288:ASP:HA	1:A:291:VAL:CB	2.40	0.50
1:C:186:PRO:O	1:C:190:VAL:HG23	2.11	0.50
1:C:204:MET:HB2	1:C:251:LEU:HD11	1.93	0.50
1:C:226:ARG:HG2	1:C:228:TYR:CZ	2.46	0.50
1:D:301:THR:CG2	1:D:302:VAL:N	2.73	0.50
1:F:61:TYR:HH	1:F:432:LEU:HD22	1.73	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:VAL:HA	1:F:178:VAL:HG11	1.92	0.50
1:H:70:ASP:O	1:H:74:PHE:CD1	2.64	0.50
1:E:55:ARG:HG2	1:E:422:ASP:OD1	2.11	0.50
1:E:332:LEU:O	1:E:337:ALA:HB3	2.11	0.50
1:A:191:ARG:HD2	1:A:238:VAL:HG23	1.89	0.50
1:B:146:MET:SD	1:B:212:HIS:CD2	3.05	0.50
1:B:203:ASP:O	1:B:248:VAL:HB	2.12	0.50
1:C:7:THR:O	1:C:8:ASN:OD1	2.29	0.50
1:C:191:ARG:HB2	1:C:238:VAL:CG1	2.40	0.50
1:C:421:LEU:CD1	1:C:425:PRO:HG3	2.40	0.50
1:D:36:GLY:HA3	1:D:41:THR:HG23	1.92	0.50
1:D:92:VAL:HG22	1:D:119:PRO:HA	1.93	0.50
1:D:150:PHE:O	1:D:159:ARG:HG2	2.11	0.50
1:F:25:VAL:HG22	1:F:35:VAL:HG13	1.93	0.50
1:F:113:THR:HG21	1:F:206:LYS:HZ3	1.76	0.50
1:H:275:ASN:CG	1:H:329:GLU:HG3	2.36	0.50
1:D:222:VAL:HG22	1:D:223:GLY:O	2.11	0.50
1:D:392:ALA:HA	1:D:396:ASN:CG	2.37	0.50
1:D:430:ARG:O	1:D:433:ARG:HB2	2.12	0.50
1:G:452:THR:O	1:G:454:PRO:HD3	2.10	0.50
1:H:101:LEU:HD21	1:H:104:ARG:HH21	1.77	0.50
1:H:340:LEU:CD2	1:H:397:VAL:HG13	2.41	0.50
1:E:326:ALA:C	1:E:328:ASN:H	2.20	0.50
1:A:235:VAL:HA	1:A:238:VAL:HG11	1.93	0.50
1:C:6:ILE:CG2	1:C:25:VAL:CA	2.89	0.50
1:C:104:ARG:HG2	1:C:447:ARG:NH1	2.26	0.50
1:D:148:GLY:O	1:D:154:PHE:CD2	2.48	0.50
1:D:215:PHE:C	1:D:218:VAL:HG13	2.36	0.50
1:D:276:TYR:CD1	1:D:325:TYR:HB3	2.47	0.50
1:F:74:PHE:C	1:F:154:PHE:HB3	2.36	0.50
1:F:118:GLU:HG3	1:F:119:PRO:HD3	1.93	0.50
1:F:422:ASP:CG	1:F:434:SER:HB3	2.36	0.50
1:G:421:LEU:HD13	1:G:432:LEU:HA	1.92	0.50
1:H:6:ILE:HG21	1:H:25:VAL:CG1	2.41	0.50
1:H:182:LEU:HD12	1:H:231:PHE:HZ	1.75	0.50
1:H:240:VAL:HG12	1:H:241:GLU:H	1.76	0.50
1:B:7:THR:HA	1:B:24:THR:HG23	1.92	0.50
1:B:356:LEU:O	1:B:361:ARG:NH1	2.44	0.50
1:C:171:ASP:O	1:C:175:GLU:HG3	2.11	0.50
1:F:35:VAL:HG23	1:F:412:THR:HG22	1.94	0.50
1:F:153:ASP:HB3	1:F:212:HIS:HB3	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:204:MET:HE3	1:F:251:LEU:HD11	1.93	0.50
1:G:37:PRO:HA	1:G:41:THR:HG23	1.94	0.50
1:G:61:TYR:HB2	1:G:107:VAL:HA	1.93	0.50
1:G:90:ARG:HD3	1:G:455:LEU:HD21	1.94	0.50
1:H:30:ASP:O	1:H:31:ARG:HB2	2.12	0.50
1:H:360:GLU:CG	1:H:361:ARG:N	2.75	0.50
1:E:252:THR:HG21	1:E:271:LEU:CD2	2.42	0.50
1:B:273:HIS:O	1:B:273:HIS:ND1	2.44	0.50
1:C:96:GLU:O	1:C:100:GLN:HG3	2.10	0.50
1:D:412:THR:CG2	1:D:413:GLY:N	2.75	0.50
1:F:224:PHE:N	1:F:224:PHE:CD1	2.80	0.50
1:F:267:GLY:C	1:F:295:SER:OG	2.54	0.50
1:A:251:LEU:HD11	1:A:270:VAL:CB	2.30	0.50
1:A:282:ILE:HG23	1:A:328:ASN:CG	2.36	0.50
1:B:68:LEU:CB	1:B:95:ILE:HG23	2.42	0.50
1:B:198:LEU:C	1:B:200:ARG:H	2.20	0.50
1:C:394:THR:OG1	1:C:395:ILE:N	2.44	0.50
1:C:417:ASP:HA	1:C:439:PHE:O	2.12	0.50
1:D:180:HIS:O	1:D:181:GLN:CB	2.60	0.50
1:D:387:LEU:C	1:D:390:ILE:HB	2.37	0.50
1:H:456:VAL:HG13	1:H:457:THR:H	1.76	0.50
1:E:45:GLU:O	1:E:47:ALA:HB2	2.11	0.50
1:A:271:LEU:HD11	1:A:296:TRP:C	2.36	0.50
1:B:387:LEU:HA	1:B:388:GLU:C	2.36	0.50
1:D:70:ASP:OD2	1:D:72:TRP:O	2.29	0.50
1:D:328:ASN:O	1:D:331:ASN:CB	2.58	0.50
1:D:387:LEU:O	1:D:390:ILE:CB	2.58	0.50
1:F:282:ILE:HB	1:F:283:PRO:HA	1.94	0.50
1:G:269:ASP:N	1:G:269:ASP:OD1	2.43	0.50
1:H:317:ALA:O	1:H:320:LEU:N	2.44	0.50
1:E:371:ASP:OD1	1:E:372:HIS:ND1	2.42	0.50
1:B:67:HIS:HA	1:B:112:ASP:OD1	2.12	0.50
1:C:131:ILE:HD13	1:C:131:ILE:N	2.26	0.50
1:D:206:LYS:HE3	1:D:272:ILE:HG13	1.93	0.50
1:D:276:TYR:HD1	1:D:325:TYR:HB3	1.77	0.50
1:F:428:ASP:OD2	1:F:430:ARG:HD3	2.09	0.50
1:H:97:GLU:OE1	1:H:451:PRO:HB2	2.12	0.50
1:H:429:ILE:HG13	1:H:432:LEU:HD13	1.93	0.50
1:H:435:ILE:HG21	1:H:438:VAL:CG2	2.42	0.50
1:B:84:LEU:HD12	1:B:150:PHE:CZ	2.47	0.49
1:B:153:ASP:CB	1:B:212:HIS:HB3	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:VAL:C	1:B:382:LYS:N	2.70	0.49
1:C:274:ALA:HB3	1:C:298:GLY:O	2.12	0.49
1:D:6:ILE:CA	1:D:50:VAL:CG1	2.74	0.49
1:D:56:TRP:CZ2	1:D:424:ASP:HB2	2.47	0.49
1:F:63:ASN:CG	1:F:66:VAL:CG1	2.85	0.49
1:G:303:HIS:HB2	1:G:306:HIS:CB	2.42	0.49
1:G:303:HIS:HB2	1:G:306:HIS:HB2	1.94	0.49
1:G:344:ASP:O	1:G:345:ALA:HB2	2.11	0.49
1:G:367:THR:HG22	1:G:369:GLY:H	1.77	0.49
1:H:455:LEU:HD12	1:H:456:VAL:H	1.76	0.49
1:A:70:ASP:CG	1:A:71:ALA:N	2.70	0.49
1:A:217:LEU:HG	1:A:225:ASP:H	1.78	0.49
1:A:459:HIS:CB	1:A:460:PRO:CA	2.85	0.49
1:B:165:THR:O	1:B:169:ARG:HB2	2.11	0.49
1:C:219:ASP:CG	1:C:222:VAL:HG12	2.36	0.49
1:F:146:MET:SD	1:F:212:HIS:CD2	3.04	0.49
1:E:217:LEU:HD21	1:E:223:GLY:O	2.13	0.49
1:B:143:ILE:HG23	1:B:206:LYS:HB3	1.95	0.49
1:B:384:MET:CE	1:B:389:ALA:HA	2.42	0.49
1:C:14:GLY:O	1:C:395:ILE:HD11	2.12	0.49
1:D:32:PHE:CD2	1:D:412:THR:N	2.73	0.49
1:D:219:ASP:C	1:D:222:VAL:CG1	2.85	0.49
1:G:127:ILE:CG1	1:G:128:ASN:N	2.74	0.49
1:G:379:MET:HB3	1:G:384:MET:SD	2.52	0.49
1:A:409:SER:O	1:A:414:LYS:NZ	2.35	0.49
1:B:66:VAL:HG22	1:B:110:VAL:CG2	2.43	0.49
1:B:260:LEU:O	1:B:264:VAL:HG23	2.11	0.49
1:C:253:HIS:HD1	1:C:273:HIS:CE1	2.29	0.49
1:D:237:GLU:HA	1:D:240:VAL:HG22	1.95	0.49
1:D:337:ALA:O	1:D:338:LYS:HB2	2.12	0.49
1:F:10:THR:HA	1:F:21:PRO:HA	1.95	0.49
1:F:263:SER:HA	1:F:266:LEU:CD1	2.42	0.49
1:F:302:VAL:HG12	1:F:303:HIS:H	1.77	0.49
1:G:111:PHE:CE2	1:G:397:VAL:HG12	2.47	0.49
1:H:233:ARG:O	1:H:237:GLU:HG3	2.12	0.49
1:H:368:ILE:HA	1:H:371:ASP:HB2	1.94	0.49
1:E:61:TYR:OH	1:E:432:LEU:HB3	2.13	0.49
1:E:66:VAL:C	1:E:67:HIS:CD2	2.90	0.49
1:E:181:GLN:C	1:E:183:SER:N	2.68	0.49
1:E:281:GLU:O	1:E:282:ILE:C	2.54	0.49
1:A:27:VAL:HG12	1:A:31:ARG:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:182:LEU:HD13	1:H:239:MET:CE	2.41	0.49
1:H:341:LEU:HD12	1:H:375:TRP:CE3	2.48	0.49
1:E:293:SER:O	1:E:294:ASP:HB3	2.12	0.49
1:A:252:THR:HG22	1:A:270:VAL:O	2.12	0.49
1:A:315:SER:O	1:A:316:TRP:HB3	2.13	0.49
1:B:153:ASP:HA	1:B:212:HIS:O	2.12	0.49
1:B:256:SER:OG	1:B:258:GLU:O	2.28	0.49
1:C:377:GLN:HA	1:C:429:ILE:HG21	1.95	0.49
1:F:121:LEU:HD22	1:F:124:ARG:HE	1.77	0.49
1:G:6:ILE:CD1	1:G:9:VAL:HG11	2.43	0.49
1:H:23:THR:CG2	1:H:37:PRO:HG3	2.40	0.49
1:H:175:GLU:O	1:H:178:VAL:CG2	2.60	0.49
1:B:66:VAL:HG22	1:B:110:VAL:HG22	1.94	0.49
1:D:282:ILE:HB	1:D:287:ILE:HD11	1.94	0.49
1:H:277:THR:CG2	1:H:282:ILE:HG12	2.42	0.49
1:B:209:VAL:HG13	1:B:236:LEU:HD21	1.93	0.49
1:C:205:LEU:O	1:C:251:LEU:CD1	2.60	0.49
1:D:6:ILE:HG23	1:D:50:VAL:CG1	2.42	0.49
1:D:152:ALA:O	1:D:153:ASP:HB2	2.12	0.49
1:D:208:ALA:HA	1:D:253:HIS:HB3	1.95	0.49
1:F:109:THR:OG1	1:F:136:ARG:NH2	2.46	0.49
1:F:282:ILE:HD12	1:F:282:ILE:H	1.78	0.49
1:G:68:LEU:HB2	1:G:95:ILE:HG23	1.91	0.49
1:H:55:ARG:HD3	1:H:420:LEU:CD1	2.43	0.49
1:E:212:HIS:O	1:E:213:ILE:CG1	2.61	0.49
1:E:307:ARG:C	1:E:307:ARG:CD	2.86	0.49
1:A:28:GLU:HG3	1:A:28:GLU:O	2.12	0.49
1:A:140:ALA:O	1:A:197:TYR:OH	2.24	0.49
1:A:145:GLY:N	1:A:179:GLY:HA2	2.26	0.49
1:A:254:SER:CB	1:A:259:ALA:CB	2.84	0.49
1:A:346:GLY:O	1:A:368:ILE:HB	2.12	0.49
1:D:37:PRO:O	1:D:39:ASP:C	2.55	0.49
1:F:68:LEU:CD1	1:F:95:ILE:HG23	2.37	0.49
1:H:75:MET:SD	1:H:215:PHE:CE2	3.06	0.49
1:H:253:HIS:NE2	1:H:273:HIS:CE1	2.69	0.49
1:B:145:GLY:H	1:B:179:GLY:HA2	1.78	0.49
1:B:340:LEU:HG	1:B:397:VAL:HG13	1.95	0.49
1:E:286:LEU:HA	1:E:289:LYS:HB3	1.94	0.48
1:A:117:ILE:HD13	1:A:200:ARG:HE	1.78	0.48
1:A:126:ARG:HH11	1:A:126:ARG:CG	2.22	0.48
1:A:282:ILE:HG23	1:A:328:ASN:OD1	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:PRO:HG3	1:B:374:HIS:NE2	2.28	0.48
1:B:395:ILE:CD1	1:B:399[B]:ARG:NH2	2.75	0.48
1:C:428:ASP:HB3	1:C:431:ASN:ND2	2.28	0.48
1:D:303:HIS:CB	1:D:306:HIS:H	2.26	0.48
1:G:6:ILE:CD1	1:G:9:VAL:CG2	2.91	0.48
1:G:112:ASP:OD2	1:G:115:ASN:ND2	2.37	0.48
1:H:155:HIS:HE1	1:H:157:ALA:HB3	1.77	0.48
1:H:283:PRO:HD2	1:H:286:LEU:HD13	1.95	0.48
1:E:40:SER:O	1:E:41:THR:OG1	2.29	0.48
1:A:82:GLU:OE2	1:F:162:ALA:HB1	2.14	0.48
1:A:251:LEU:HA	1:A:270:VAL:HB	1.95	0.48
1:C:303:HIS:CE1	1:C:306:HIS:HB2	2.48	0.48
1:D:20:ARG:O	1:D:23:THR:CG2	2.61	0.48
1:B:254:SER:O	1:B:273:HIS:CE1	2.66	0.48
1:B:309:GLY:O	1:B:312:ASP:HB2	2.13	0.48
1:D:156:PHE:O	1:D:159:ARG:HG3	2.12	0.48
1:F:145:GLY:HA2	1:F:179:GLY:O	2.13	0.48
1:G:142:THR:OG1	1:G:143:ILE:N	2.46	0.48
1:H:350:LYS:HB3	1:H:459:HIS:CE1	2.48	0.48
1:E:341:LEU:HD13	1:E:375:TRP:CE3	2.49	0.48
1:E:429:ILE:C	1:E:431:ASN:N	2.71	0.48
1:A:149:PRO:HA	1:A:154:PHE:CD2	2.48	0.48
1:B:165:THR:HG21	1:G:354:ALA:HB3	1.95	0.48
1:B:387:LEU:CB	1:B:388:GLU:HA	2.43	0.48
1:B:399[B]:ARG:HH11	1:B:399[B]:ARG:CG	2.25	0.48
1:C:67:HIS:CE1	1:C:114:HIS:HB3	2.47	0.48
1:F:30:ASP:O	1:F:416:ALA:N	2.44	0.48
1:F:210:SER:HA	1:F:229:GLN:HA	1.95	0.48
1:F:303:HIS:CE1	1:F:377:GLN:HG2	2.48	0.48
1:G:207:ILE:HD12	1:G:239:MET:SD	2.54	0.48
1:A:288:ASP:HA	1:A:291:VAL:CG2	2.43	0.48
1:A:456:VAL:O	1:A:456:VAL:HG12	2.13	0.48
1:B:111:PHE:HD2	1:B:204:MET:HE2	1.77	0.48
1:C:4:ILE:CG2	1:C:5:ALA:H	2.25	0.48
1:C:4:ILE:CG2	1:C:5:ALA:N	2.75	0.48
1:D:259:ALA:CA	1:D:262:THR:HG22	2.44	0.48
1:G:37:PRO:HA	1:G:41:THR:CG2	2.44	0.48
1:G:325:TYR:O	1:G:329:GLU:N	2.44	0.48
1:H:75:MET:SD	1:H:215:PHE:HE2	2.36	0.48
1:H:275:ASN:OD1	1:H:329:GLU:CG	2.58	0.48
1:E:263:SER:HB3	1:E:271:LEU:HD22	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:O	1:A:238:VAL:HG13	2.11	0.48
1:C:91:TYR:HE2	1:C:173:MET:HE1	1.77	0.48
1:C:281:GLU:HB2	1:C:328:ASN:OD1	2.14	0.48
1:H:356:LEU:CD1	1:H:360:GLU:HG3	2.43	0.48
1:H:359:VAL:O	1:H:360:GLU:C	2.56	0.48
1:E:148:GLY:HA3	1:E:171:ASP:OD1	2.14	0.48
1:E:379:MET:HB3	1:E:384:MET:HG3	1.95	0.48
1:C:30:ASP:CG	1:C:31:ARG:N	2.65	0.48
1:C:146:MET:SD	1:C:212:HIS:HB2	2.54	0.48
1:C:310:LEU:O	1:C:314:GLY:N	2.31	0.48
1:C:398:ALA:O	1:C:399[B]:ARG:C	2.54	0.48
1:D:97:GLU:OE1	1:D:455:LEU:HB2	2.14	0.48
1:D:136:ARG:CZ	1:D:415:LEU:CD1	2.92	0.48
1:F:260:LEU:HA	1:F:263:SER:OG	2.13	0.48
1:H:333:ILE:CD1	1:H:379:MET:SD	3.02	0.48
1:H:386:PRO:O	1:H:389:ALA:N	2.47	0.48
1:E:7:THR:O	1:E:52:GLY:HA3	2.14	0.48
1:A:182:LEU:HD22	1:A:185:LEU:HD12	1.96	0.48
1:B:108:THR:HG21	1:B:417:ASP:HB3	1.96	0.48
1:B:236:LEU:HD23	1:B:266:LEU:HD11	1.95	0.48
1:C:117:ILE:CG1	1:C:121:LEU:HD12	2.44	0.48
1:C:367:THR:O	1:C:371:ASP:HB3	2.14	0.48
1:D:181:GLN:CG	1:D:185:LEU:HD11	2.44	0.48
1:F:168:ASP:O	1:F:172:SER:OG	2.26	0.48
1:F:428:ASP:CG	1:F:430:ARG:CG	2.87	0.48
1:G:6:ILE:CG1	1:G:9:VAL:CG2	2.90	0.48
1:H:13:ASP:OD1	1:H:13:ASP:N	2.24	0.48
1:H:87:TRP:HB3	1:H:94:VAL:CG2	2.42	0.48
1:H:251:LEU:HD13	1:H:272:ILE:HD11	1.96	0.48
1:E:306:HIS:O	1:E:310:LEU:N	2.27	0.48
1:A:182:LEU:CD2	1:A:185:LEU:HD12	2.43	0.48
1:B:187:ARG:HA	1:B:190:VAL:CG2	2.44	0.48
1:B:326:ALA:HA	1:B:329:GLU:HG3	1.96	0.48
1:C:53:ASN:O	1:C:55:ARG:HG3	2.14	0.48
1:C:62:VAL:HG21	1:C:407:ILE:HG22	1.95	0.48
1:D:103:LEU:HD12	1:D:107:VAL:O	2.14	0.48
1:D:339:ILE:CG2	1:D:340:LEU:N	2.76	0.48
1:F:27:VAL:HG11	1:F:442:GLY:HA3	1.96	0.48
1:F:112:ASP:OD2	1:F:115:ASN:ND2	2.47	0.48
1:F:113:THR:HG21	1:F:206:LYS:HZ2	1.79	0.48
1:F:257:VAL:HG21	1:F:280:GLN:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:ILE:HA	1:H:173:MET:HE2	1.95	0.48
1:H:180:HIS:C	1:H:182:LEU:H	2.22	0.48
1:H:290:ILE:HA	1:H:293:SER:OG	2.13	0.48
1:H:425:PRO:CB	1:H:432:LEU:HD12	2.44	0.48
1:E:257:VAL:HG22	1:E:277:THR:HG21	1.95	0.48
1:E:429:ILE:O	1:E:432:LEU:CD1	2.38	0.48
1:A:272:ILE:HD12	1:A:272:ILE:H	1.78	0.48
1:A:416:ALA:HB3	1:A:442:GLY:N	2.28	0.48
1:C:330:ARG:O	1:C:334:SER:N	2.43	0.48
1:D:68:LEU:CD1	1:D:95:ILE:CG2	2.84	0.48
1:D:252:THR:HG21	1:D:263:SER:OG	2.13	0.48
1:F:52:GLY:O	1:F:55:ARG:HB2	2.14	0.48
1:G:144:VAL:HG13	1:G:178:VAL:CG1	2.44	0.48
1:H:110:VAL:N	1:H:136:ARG:O	2.41	0.48
1:H:232:SER:O	1:H:233:ARG:C	2.56	0.48
1:E:12:ILE:HB	1:E:58:VAL:HG12	1.96	0.47
1:E:213:ILE:HG23	1:E:216:THR:HB	1.96	0.47
1:E:214:VAL:HG22	1:E:215:PHE:CE1	2.48	0.47
1:A:152:ALA:C	1:A:154:PHE:H	2.20	0.47
1:A:414:LYS:HB2	1:A:414:LYS:HE3	1.67	0.47
1:C:262:THR:O	1:C:262:THR:HG22	2.12	0.47
1:D:152:ALA:HB1	1:D:213:ILE:HG12	1.95	0.47
1:D:153:ASP:HA	1:D:212:HIS:HB3	1.96	0.47
1:F:63:ASN:CG	1:F:66:VAL:HG13	2.39	0.47
1:F:75:MET:H	1:F:76:ALA:CB	2.24	0.47
1:F:224:PHE:N	1:F:224:PHE:HD1	2.12	0.47
1:F:255:VAL:CA	1:F:276:TYR:O	2.62	0.47
1:H:269:ASP:O	1:H:296:TRP:HB2	2.14	0.47
1:E:212:HIS:O	1:E:213:ILE:HG13	2.14	0.47
1:A:118:GLU:HB2	1:A:119:PRO:HD3	1.95	0.47
1:A:136:ARG:NH2	1:A:417:ASP:OD2	2.35	0.47
1:B:94:VAL:HG23	1:B:455:LEU:HD23	1.95	0.47
1:B:236:LEU:HA	1:B:236:LEU:HD12	1.75	0.47
1:C:302:VAL:O	1:C:382:LYS:NZ	2.34	0.47
1:D:3:THR:HA	1:D:27:VAL:O	2.13	0.47
1:D:264:VAL:HG11	1:D:289:LYS:HG2	1.95	0.47
1:G:256:SER:C	1:G:258:GLU:O	2.57	0.47
1:G:350:LYS:HA	1:G:350:LYS:HD2	1.63	0.47
1:H:62:VAL:HG13	1:H:109:THR:HB	1.96	0.47
1:A:111:PHE:HD1	1:A:138:PHE:HB2	1.79	0.47
1:A:112:ASP:OD2	1:A:115:ASN:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ARG:CD	1:A:238:VAL:HG22	2.42	0.47
1:A:218:VAL:HG13	1:A:219:ASP:HB2	1.95	0.47
1:B:326:ALA:C	1:B:328:ASN:H	2.22	0.47
1:C:307:ARG:NH2	1:C:311:GLU:CD	2.72	0.47
1:C:341:LEU:HD13	1:C:375:TRP:CD2	2.48	0.47
1:F:454:PRO:C	1:F:455:LEU:CD2	2.83	0.47
1:G:6:ILE:CD1	1:G:9:VAL:CG1	2.91	0.47
1:H:198:LEU:O	1:H:201:GLY:HA2	2.14	0.47
1:H:447:ARG:HB3	1:H:447:ARG:HH11	1.79	0.47
1:E:198:LEU:O	1:E:200:ARG:N	2.48	0.47
1:A:153:ASP:CB	1:A:212:HIS:HB3	2.44	0.47
1:C:191:ARG:HB2	1:C:238:VAL:HG11	1.95	0.47
1:C:206:LYS:HZ1	1:C:253:HIS:CB	2.28	0.47
1:D:195:ARG:HD2	1:D:242:GLU:CD	2.40	0.47
1:D:352:HIS:O	1:D:356:LEU:HD13	2.13	0.47
1:G:144:VAL:HB	1:G:207:ILE:HA	1.95	0.47
1:G:365:PRO:HG2	1:G:366:TRP:CE3	2.49	0.47
1:H:260:LEU:HD11	1:H:271:LEU:HD22	1.96	0.47
1:A:275:ASN:O	1:A:277:THR:HG23	2.14	0.47
1:C:67:HIS:HE1	1:C:114:HIS:HB2	1.80	0.47
1:F:58:VAL:HB	1:F:59:PRO:HD2	1.97	0.47
1:F:75:MET:HE2	1:F:212:HIS:CE1	2.49	0.47
1:G:395:ILE:O	1:G:399:ARG:HG3	2.14	0.47
1:E:213:ILE:CG2	1:E:216:THR:CG2	2.92	0.47
1:E:315:SER:O	1:E:317:ALA:N	2.41	0.47
1:E:324:PRO:O	1:E:327:THR:N	2.48	0.47
1:A:207:ILE:CG2	1:A:252:THR:HA	2.44	0.47
1:A:277:THR:OG1	1:A:280:GLN:O	2.11	0.47
1:A:340:LEU:HD11	1:A:397:VAL:HA	1.97	0.47
1:A:447:ARG:CZ	1:A:447:ARG:HB2	2.44	0.47
1:B:343:THR:OG1	1:B:371:ASP:HB2	2.14	0.47
1:C:270:VAL:HG12	1:C:272:ILE:HG12	1.97	0.47
1:C:319:ALA:O	1:C:323:GLU:HG3	2.15	0.47
1:C:330:ARG:HA	1:C:333:ILE:HB	1.96	0.47
1:C:341:LEU:HD12	1:C:342:ASN:N	2.30	0.47
1:F:31:ARG:HD3	1:F:413:GLY:HA2	1.97	0.47
1:F:236:LEU:HB3	1:F:266:LEU:HD21	1.97	0.47
1:F:277:THR:CG2	1:F:280:GLN:HB2	2.43	0.47
1:G:191:ARG:NH2	1:G:241:GLU:OE1	2.37	0.47
1:G:399:ARG:HG2	1:G:404:ALA:HB2	1.96	0.47
1:H:11:LEU:HB3	1:H:23:THR:OG1	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:VAL:CG2	1:E:182:LEU:HD11	2.44	0.47
1:E:251:LEU:HD22	1:E:270:VAL:HB	1.95	0.47
1:A:38:SER:OG	1:A:40:SER:N	2.48	0.47
1:A:68:LEU:HB3	1:A:95:ILE:HG23	1.97	0.47
1:A:155:HIS:CE1	1:A:157:ALA:O	2.67	0.47
1:A:180:HIS:ND1	1:A:180:HIS:C	2.72	0.47
1:A:224:PHE:CB	1:A:278:LEU:HD13	2.45	0.47
1:B:112:ASP:OD2	1:B:115:ASN:HB2	2.15	0.47
1:B:113:THR:HA	1:B:140:ALA:HB3	1.93	0.47
1:B:158:GLY:HA2	1:B:161:ALA:HB3	1.96	0.47
1:B:178:VAL:HG12	1:B:179:GLY:N	2.27	0.47
1:B:229:GLN:CD	1:B:259:ALA:HB2	2.40	0.47
1:B:391:SER:H	1:B:394:THR:H	1.62	0.47
1:B:428:ASP:HB3	1:B:431:ASN:OD1	2.15	0.47
1:C:213:ILE:HG13	1:C:213:ILE:O	2.15	0.47
1:C:219:ASP:CG	1:C:222:VAL:CG1	2.87	0.47
1:C:318:ALA:O	1:C:321:ALA:N	2.31	0.47
1:D:236:LEU:HB3	1:D:266:LEU:HD11	1.97	0.47
1:D:303:HIS:HE1	1:D:363:ASP:OD2	1.97	0.47
1:D:339:ILE:HD13	1:D:384:MET:CE	2.44	0.47
1:F:13:ASP:OD1	1:F:13:ASP:N	2.45	0.47
1:F:45:GLU:CG	1:F:46:GLY:N	2.78	0.47
1:F:59:PRO:HG2	1:F:394:THR:HG21	1.95	0.47
1:F:227:SER:O	1:F:228:TYR:C	2.58	0.47
1:F:271:LEU:HG	1:F:296:TRP:O	2.15	0.47
1:F:429:ILE:HG13	1:F:432:LEU:CD1	2.45	0.47
1:G:6:ILE:CD1	1:G:9:VAL:HG21	2.44	0.47
1:G:31:ARG:CB	1:G:414:LYS:O	2.63	0.47
1:H:38:SER:HB3	1:H:40:SER:O	2.15	0.47
1:H:191:ARG:HB2	1:H:238:VAL:HG22	1.95	0.47
1:H:210:SER:CB	1:H:255:VAL:HG22	2.43	0.47
1:H:230:THR:HB	1:H:231:PHE:HD1	1.78	0.47
1:H:459:HIS:ND1	1:H:459:HIS:O	2.47	0.47
1:E:97:GLU:OE2	1:E:454:PRO:HA	2.15	0.47
1:E:333:ILE:HG12	1:E:339:ILE:HD11	1.97	0.47
1:E:386:PRO:O	1:E:390:ILE:HB	2.14	0.47
1:B:32:PHE:HE2	1:B:409:SER:HB2	1.80	0.47
1:B:81:ILE:HG12	1:B:150:PHE:CE1	2.50	0.47
1:C:447:ARG:HA	1:C:450:LEU:HD13	1.96	0.47
1:D:19:PRO:O	1:D:21:PRO:HD3	2.15	0.47
1:D:219:ASP:CG	1:D:222:VAL:HG11	2.39	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:208:ALA:HA	1:F:253:HIS:HB3	1.97	0.47
1:G:70:ASP:OD2	1:G:73:MET:HB3	2.15	0.47
1:G:194:VAL:O	1:G:197:TYR:HB3	2.15	0.47
1:H:14:GLY:HA3	1:H:59:PRO:HG3	1.96	0.47
1:H:145:GLY:N	1:H:179:GLY:HA3	2.23	0.47
1:H:233:ARG:NH2	1:H:262:THR:OG1	2.43	0.47
1:E:75:MET:HE3	1:E:316:TRP:CH2	2.48	0.47
1:E:214:VAL:CG1	1:E:215:PHE:CD1	2.90	0.47
1:A:236:LEU:C	1:A:266:LEU:HD21	2.40	0.47
1:F:198:LEU:HD21	1:F:205:LEU:HD12	1.97	0.47
1:F:290:ILE:HG23	1:F:291:VAL:HG22	1.97	0.47
1:F:421:LEU:HA	1:F:434:SER:O	2.15	0.47
1:H:76:ALA:HB3	1:H:78:PRO:HD3	1.97	0.47
1:H:102:ALA:HB1	1:H:107:VAL:HB	1.95	0.47
1:H:317:ALA:C	1:H:319:ALA:N	2.71	0.47
1:H:406:GLN:O	1:H:415:LEU:HD13	2.14	0.47
1:E:16:GLY:HA2	1:E:387:LEU:HG	1.97	0.47
1:E:88:GLU:OE1	1:E:169:ARG:NH1	2.45	0.47
1:E:122:ALA:O	1:E:126:ARG:HG3	2.15	0.47
1:E:333:ILE:CD1	1:E:382:LYS:HB2	2.45	0.47
1:A:180:HIS:C	1:A:182:LEU:N	2.74	0.47
1:A:320:LEU:HA	1:A:325:TYR:HD2	1.80	0.47
1:B:38:SER:HB3	1:B:40:SER:O	2.14	0.47
1:C:138:PHE:O	1:C:203:ASP:HB2	2.15	0.47
1:D:240:VAL:O	1:D:244:ARG:HG2	2.15	0.47
1:F:151:SER:HB2	1:F:152:ALA:O	2.15	0.47
1:F:429:ILE:HG13	1:F:432:LEU:HD12	1.96	0.47
1:H:207:ILE:HG22	1:H:251:LEU:O	2.15	0.47
1:E:62:VAL:O	1:E:397:VAL:HG21	2.15	0.46
1:A:9:VAL:HG22	1:A:52:GLY:HA3	1.97	0.46
1:A:32:PHE:HB2	1:A:412:THR:HA	1.97	0.46
1:A:69:LEU:HD23	1:A:69:LEU:HA	1.79	0.46
1:D:341:LEU:HB3	1:D:397:VAL:HG11	1.97	0.46
1:F:297:ALA:O	1:F:340:LEU:HG	2.15	0.46
1:H:31:ARG:HH11	1:H:415:LEU:CG	2.27	0.46
1:H:74:PHE:CD1	1:H:74:PHE:N	2.83	0.46
1:E:226:ARG:NH1	1:E:226:ARG:CB	2.76	0.46
1:A:207:ILE:O	1:A:253:HIS:N	2.48	0.46
1:B:9:VAL:HG11	1:B:57:MET:HB2	1.97	0.46
1:B:31:ARG:HH11	1:B:414:LYS:C	2.23	0.46
1:E:100:GLN:CG	1:E:133:GLN:O	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:ASP:O	1:E:212:HIS:ND1	2.49	0.46
1:E:217:LEU:HD13	1:E:225:ASP:O	2.15	0.46
1:B:4:ILE:HD12	1:B:439:PHE:HE2	1.80	0.46
1:B:394:THR:HG22	1:B:395:ILE:H	1.76	0.46
1:D:88:GLU:HA	1:D:91:TYR:CE1	2.50	0.46
1:F:74:PHE:O	1:F:154:PHE:CB	2.62	0.46
1:F:92:VAL:HG22	1:F:119:PRO:HA	1.97	0.46
1:G:330:ARG:O	1:G:333:ILE:N	2.48	0.46
1:H:209:VAL:O	1:H:230:THR:N	2.38	0.46
1:H:231:PHE:CE2	1:H:239:MET:CE	2.95	0.46
1:H:439:PHE:CE2	1:H:444:ALA:HB2	2.46	0.46
1:E:250:VAL:HG22	1:E:268:ALA:HA	1.97	0.46
1:A:102:ALA:HB1	1:A:107:VAL:HB	1.98	0.46
1:A:179:GLY:O	1:A:180:HIS:C	2.59	0.46
1:A:283:PRO:HD2	1:A:286:LEU:HB2	1.97	0.46
1:B:72:TRP:HD1	1:B:364:ARG:HH22	1.64	0.46
1:B:273:HIS:HB3	1:B:300:GLN:NE2	2.29	0.46
1:C:68:LEU:HB2	1:C:95:ILE:HG23	1.98	0.46
1:D:330:ARG:O	1:D:333:ILE:HD13	2.14	0.46
1:F:112:ASP:O	1:F:139:ALA:HA	2.15	0.46
1:F:198:LEU:HD13	1:F:248:VAL:HG21	1.98	0.46
1:F:317:ALA:O	1:F:319:ALA:N	2.47	0.46
1:G:64:GLY:HA2	1:G:111:PHE:CD2	2.39	0.46
1:G:252:THR:HG21	1:G:263:SER:OG	2.16	0.46
1:H:117:ILE:HA	1:H:120:VAL:HG12	1.97	0.46
1:E:126:ARG:O	1:E:131:ILE:HG22	2.15	0.46
1:E:377:GLN:HA	1:E:429:ILE:HG21	1.96	0.46
1:A:14:GLY:CA	1:A:59:PRO:HG2	2.45	0.46
1:A:214:VAL:O	1:A:217:LEU:HB2	2.15	0.46
1:A:243:ALA:HA	1:A:246:ALA:HB3	1.96	0.46
1:D:88:GLU:OE1	1:D:169:ARG:NH1	2.48	0.46
1:D:259:ALA:HA	1:D:262:THR:HG22	1.96	0.46
1:F:257:VAL:CG2	1:F:277:THR:CG2	2.81	0.46
1:G:363:ASP:O	1:G:374:HIS:ND1	2.48	0.46
1:H:64:GLY:HA2	1:H:111:PHE:CD2	2.50	0.46
1:E:105:ASN:OD1	1:E:369:GLY:HA2	2.16	0.46
1:B:253:HIS:NE2	1:B:273:HIS:CE1	2.83	0.46
1:C:66:VAL:O	1:C:112:ASP:HA	2.16	0.46
1:C:156:PHE:H	1:C:215:PHE:HE2	1.63	0.46
1:C:166:PHE:HB2	1:H:351:ASP:OD2	2.16	0.46
1:D:74:PHE:C	1:D:76:ALA:N	2.73	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:THR:HG23	1:D:263:SER:N	2.31	0.46
1:D:381:GLU:N	1:D:381:GLU:CD	2.73	0.46
1:G:38:SER:C	1:G:40:SER:N	2.73	0.46
1:G:226:ARG:HD2	1:G:228:TYR:CE2	2.51	0.46
1:H:177:GLY:O	1:H:193:ARG:HD2	2.15	0.46
1:H:379:MET:HB3	1:H:384:MET:HB2	1.98	0.46
1:E:30:ASP:O	1:E:31:ARG:C	2.59	0.46
1:E:259:ALA:O	1:E:263:SER:N	2.46	0.46
1:B:271:LEU:HD22	1:B:274:ALA:HB2	1.98	0.46
1:D:75:MET:HG2	1:D:215:PHE:CZ	2.51	0.46
1:F:30:ASP:O	1:F:416:ALA:HB2	2.16	0.46
1:F:258:GLU:C	1:F:260:LEU:N	2.74	0.46
1:H:258:GLU:C	1:H:260:LEU:H	2.24	0.46
1:E:290:ILE:CA	1:E:293:SER:OG	2.64	0.46
1:B:169:ARG:NH2	1:G:351:ASP:OD2	2.49	0.46
1:B:297:ALA:O	1:B:339:ILE:HA	2.16	0.46
1:B:320:LEU:HD23	1:B:325:TYR:CE2	2.51	0.46
1:C:304:ASP:OD1	1:C:304:ASP:N	2.48	0.46
1:D:3:THR:HG22	1:D:28:GLU:HA	1.98	0.46
1:D:330:ARG:O	1:D:333:ILE:CD1	2.64	0.46
1:F:66:VAL:HG22	1:F:110:VAL:CG1	2.44	0.46
1:H:322:GLY:O	1:H:323:GLU:CB	2.63	0.46
1:E:77:GLY:N	1:E:78:PRO:HD3	2.30	0.46
1:E:459:HIS:HA	1:E:460:PRO:HA	1.62	0.46
1:A:142:THR:HB	1:A:174:PHE:O	2.16	0.46
1:A:282:ILE:HD11	1:A:287:ILE:HG13	1.98	0.46
1:B:44:PRO:C	1:B:46:GLY:H	2.24	0.46
1:C:447:ARG:NH1	1:C:447:ARG:HB3	2.31	0.46
1:D:147:GLY:HA3	1:D:180:HIS:CE1	2.51	0.46
1:F:74:PHE:HA	1:F:80:THR:OG1	2.16	0.46
1:F:403:LYS:HB3	1:F:407:ILE:HD12	1.97	0.46
1:E:170:ILE:HG23	1:E:174:PHE:HE1	1.81	0.46
1:E:378:SER:O	1:E:382:LYS:CG	2.57	0.46
1:A:232:SER:HB2	1:A:234:PRO:HD2	1.97	0.46
1:C:140:ALA:HA	1:C:204:MET:HG2	1.98	0.46
1:C:326:ALA:HA	1:C:329:GLU:HB2	1.97	0.46
1:F:38:SER:HB2	1:F:40:SER:C	2.41	0.46
1:H:145:GLY:CA	1:H:179:GLY:HA3	2.44	0.46
1:H:271:LEU:HB3	1:H:274:ALA:HB2	1.98	0.46
1:H:439:PHE:CE1	1:H:444:ALA:CB	2.99	0.46
1:E:429:ILE:O	1:E:431:ASN:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:ILE:N	1:A:27:VAL:O	2.48	0.45
1:A:35:VAL:HG12	1:A:36:GLY:H	1.80	0.45
1:B:153:ASP:HA	1:B:212:HIS:HB3	1.98	0.45
1:C:219:ASP:CG	1:C:223:GLY:N	2.74	0.45
1:C:360:GLU:O	1:C:364:ARG:HB2	2.15	0.45
1:G:218:VAL:N	1:G:219:ASP:HB2	2.31	0.45
1:H:75:MET:O	1:H:76:ALA:C	2.59	0.45
1:H:243:ALA:O	1:H:247:GLY:N	2.48	0.45
1:H:296:TRP:CE3	1:H:338:LYS:HB3	2.51	0.45
1:E:213:ILE:HG22	1:E:216:THR:HG22	1.96	0.45
1:A:166:PHE:O	1:A:170:ILE:HG12	2.16	0.45
1:A:275:ASN:OD1	1:A:276:TYR:CG	2.69	0.45
1:A:438:VAL:CG2	1:A:447:ARG:HD3	2.43	0.45
1:A:447:ARG:NH1	1:A:447:ARG:N	2.64	0.45
1:C:206:LYS:HE2	1:C:272:ILE:HG21	1.97	0.45
1:C:219:ASP:OD1	1:C:222:VAL:HG12	2.16	0.45
1:C:281:GLU:HA	1:C:328:ASN:HD21	1.82	0.45
1:F:38:SER:HB2	1:F:40:SER:H	1.82	0.45
1:H:208:ALA:HA	1:H:253:HIS:HB2	1.97	0.45
1:H:344:ASP:O	1:H:366:TRP:HD1	1.99	0.45
1:H:447:ARG:HH11	1:H:447:ARG:CB	2.29	0.45
1:E:138:PHE:HB3	1:E:204:MET:HE1	1.98	0.45
1:E:322:GLY:O	1:E:323:GLU:HB2	2.16	0.45
1:C:115:ASN:ND2	1:C:120:VAL:HB	2.31	0.45
1:C:253:HIS:ND1	1:C:273:HIS:ND1	2.55	0.45
1:D:236:LEU:O	1:D:240:VAL:HG13	2.16	0.45
1:F:198:LEU:HD11	1:F:205:LEU:HD12	1.97	0.45
1:F:226:ARG:CB	1:F:226:ARG:NH1	2.79	0.45
1:F:356:LEU:CD2	1:F:360:GLU:CD	2.89	0.45
1:G:187:ARG:HB3	1:G:235:VAL:HG22	1.98	0.45
1:G:227:SER:OG	1:G:256:SER:HB3	2.16	0.45
1:G:281:GLU:O	1:G:283:PRO:HD3	2.16	0.45
1:H:260:LEU:CD1	1:H:271:LEU:HD23	2.39	0.45
1:E:156:PHE:HA	1:E:157:ALA:C	2.42	0.45
1:A:100:GLN:NE2	1:A:133:GLN:O	2.47	0.45
1:A:140:ALA:HB2	1:A:204:MET:HG2	1.99	0.45
1:B:171:ASP:O	1:B:175:GLU:HG3	2.16	0.45
1:B:391:SER:HB2	1:B:395:ILE:N	2.27	0.45
1:C:217:LEU:CD2	1:C:224:PHE:HB2	2.46	0.45
1:F:74:PHE:N	1:F:76:ALA:HB3	2.32	0.45
1:F:258:GLU:O	1:F:260:LEU:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:261:ASP:O	1:G:265:GLU:CG	2.64	0.45
1:H:231:PHE:HB2	1:H:236:LEU:CD2	2.47	0.45
1:H:361:ARG:O	1:H:364:ARG:N	2.49	0.45
1:E:11:LEU:HD11	1:E:410:VAL:HG21	1.98	0.45
1:A:67:HIS:O	1:A:346:GLY:HA2	2.16	0.45
1:A:207:ILE:O	1:A:207:ILE:HG23	2.15	0.45
1:A:260:LEU:O	1:A:264:VAL:N	2.45	0.45
1:C:25:VAL:HG21	1:C:57:MET:SD	2.56	0.45
1:D:69:LEU:HD12	1:D:69:LEU:HA	1.83	0.45
1:D:179:GLY:H	1:D:182:LEU:HG	1.81	0.45
1:F:269:ASP:O	1:F:296:TRP:N	2.47	0.45
1:F:276:TYR:HA	1:F:325:TYR:CD1	2.52	0.45
1:F:307:ARG:O	1:F:311:GLU:HG3	2.16	0.45
1:G:35:VAL:HG12	1:G:412:THR:HG23	1.99	0.45
1:G:124:ARG:O	1:G:127:ILE:HG12	2.16	0.45
1:H:270:VAL:HA	1:H:296:TRP:O	2.17	0.45
1:H:341:LEU:HD21	1:H:372:HIS:HB3	1.98	0.45
1:E:77:GLY:HA3	1:E:155:HIS:ND1	2.32	0.45
1:E:78:PRO:HA	1:E:155:HIS:HE1	1.78	0.45
1:A:180:HIS:C	1:A:180:HIS:HD1	2.24	0.45
1:A:180:HIS:HE1	1:A:181:GLN:OE1	1.99	0.45
1:B:144:VAL:HG13	1:B:178:VAL:HG12	1.98	0.45
1:C:88:GLU:OE2	1:C:169:ARG:NH1	2.49	0.45
1:D:341:LEU:HD13	1:D:375:TRP:CE3	2.52	0.45
1:F:237:GLU:HA	1:F:240:VAL:HB	1.99	0.45
1:G:43:VAL:HG13	1:G:47:ALA:HB3	1.98	0.45
1:G:61:TYR:HD2	1:G:106:GLY:C	2.25	0.45
1:H:220:ARG:O	1:H:221:SER:CB	2.65	0.45
1:E:91:TYR:CE2	1:E:173:MET:HE1	2.51	0.45
1:E:315:SER:C	1:E:317:ALA:H	2.24	0.45
1:A:11:LEU:HD23	1:A:11:LEU:O	2.17	0.45
1:A:380:VAL:HA	1:A:384:MET:HB3	1.99	0.45
1:B:65:ASN:O	1:B:66:VAL:HG13	2.16	0.45
1:B:77:GLY:C	1:B:155:HIS:HD1	2.25	0.45
1:D:220:ARG:NH1	1:D:220:ARG:CG	2.79	0.45
1:D:387:LEU:CA	1:D:390:ILE:HB	2.46	0.45
1:F:341:LEU:HD13	1:F:375:TRP:CE3	2.52	0.45
1:G:53:ASN:O	1:G:55:ARG:NE	2.50	0.45
1:G:129:ALA:CB	1:G:131:ILE:HG13	2.44	0.45
1:H:135:ALA:O	1:H:137:ILE:HG13	2.16	0.45
1:B:65:ASN:C	1:B:66:VAL:HG13	2.42	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LEU:HD13	1:B:193:ARG:HH12	1.82	0.45
1:B:190:VAL:HG11	1:B:239:MET:CE	2.45	0.45
1:C:70:ASP:OD2	1:C:73:MET:CB	2.65	0.45
1:C:154:PHE:O	1:C:215:PHE:HD2	2.00	0.45
1:F:61:TYR:OH	1:F:432:LEU:CD2	2.57	0.45
1:F:226:ARG:NH1	1:F:226:ARG:HB3	2.32	0.45
1:F:410:VAL:O	1:F:410:VAL:HG12	2.16	0.45
1:A:120:VAL:HG13	1:A:121:LEU:HD23	1.99	0.45
1:A:321:ALA:O	1:A:326:ALA:HB2	2.17	0.45
1:C:30:ASP:HB2	1:C:441:ALA:O	2.17	0.45
1:D:335:ALA:C	1:D:336:ASN:CG	2.85	0.45
1:G:80:THR:O	1:G:81:ILE:C	2.56	0.45
1:H:322:GLY:CA	1:H:326:ALA:HB2	2.32	0.45
1:H:361:ARG:HA	1:H:364:ARG:HB2	1.98	0.45
1:A:170:ILE:O	1:A:173:MET:HB2	2.17	0.45
1:A:319:ALA:O	1:A:323:GLU:HB2	2.17	0.45
1:A:378:SER:O	1:A:382:LYS:HE2	2.17	0.45
1:B:74:PHE:CD1	1:B:80:THR:HG23	2.52	0.45
1:B:88:GLU:O	1:G:86:ARG:NH2	2.50	0.45
1:C:153:ASP:CB	1:C:212:HIS:HB3	2.47	0.45
1:F:65:ASN:O	1:F:343:THR:O	2.35	0.45
1:F:109:THR:OG1	1:F:136:ARG:NE	2.50	0.45
1:F:339:ILE:O	1:F:396:ASN:HB3	2.16	0.45
1:G:6:ILE:HG23	1:G:25:VAL:H	1.82	0.45
1:G:263:SER:O	1:G:266:LEU:HD23	2.17	0.45
1:H:197:TYR:HE2	1:H:205:LEU:HD11	1.82	0.45
1:H:327:THR:HB	1:H:330:ARG:HH11	1.81	0.45
1:E:220:ARG:O	1:E:221:SER:CB	2.64	0.44
1:F:268:ALA:C	1:F:295:SER:HG	2.23	0.44
1:H:201:GLY:O	1:H:202:VAL:HG22	2.17	0.44
1:A:191:ARG:CD	1:A:238:VAL:HG21	2.42	0.44
1:A:254:SER:HB2	1:A:259:ALA:HB3	1.96	0.44
1:B:127:ILE:HD12	1:B:137:ILE:CD1	2.47	0.44
1:D:20:ARG:O	1:D:23:THR:HG22	2.16	0.44
1:D:261:ASP:O	1:D:264:VAL:HB	2.17	0.44
1:D:302:VAL:HA	1:D:374:HIS:HE1	1.83	0.44
1:F:204:MET:HE3	1:F:401:TYR:HE1	1.82	0.44
1:G:225:ASP:OD1	1:G:225:ASP:C	2.60	0.44
1:G:286:LEU:O	1:G:289:LYS:N	2.51	0.44
1:H:214:VAL:O	1:H:217:LEU:N	2.45	0.44
1:H:456:VAL:HG13	1:H:457:THR:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:PRO:C	1:E:20:ARG:HD3	2.42	0.44
1:E:423:GLN:CB	1:E:431:ASN:OD1	2.65	0.44
1:A:45:GLU:C	1:A:47:ALA:N	2.74	0.44
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.77	0.44
1:A:220:ARG:O	1:A:221:SER:HB3	2.18	0.44
1:A:250:VAL:N	1:A:269:ASP:OD2	2.50	0.44
1:B:65:ASN:O	1:B:66:VAL:CG1	2.65	0.44
1:B:298:GLY:HA3	1:B:342:ASN:ND2	2.32	0.44
1:C:67:HIS:ND1	1:C:114:HIS:HB3	2.32	0.44
1:C:100:GLN:OE1	1:C:452:THR:HG23	2.18	0.44
1:D:48:THR:HG22	1:D:49:VAL:N	2.33	0.44
1:D:382:LYS:N	1:D:382:LYS:CD	2.80	0.44
1:F:84:LEU:O	1:F:91:TYR:OH	2.30	0.44
1:G:217:LEU:CB	1:G:219:ASP:HB2	2.46	0.44
1:H:147:GLY:O	1:H:154:PHE:CD2	2.70	0.44
1:H:155:HIS:CE1	1:H:157:ALA:HB3	2.52	0.44
1:H:285:TYR:HE1	1:H:286:LEU:HD12	1.82	0.44
1:H:297:ALA:N	1:H:338:LYS:O	2.47	0.44
1:H:425:PRO:HB3	1:H:432:LEU:HD12	1.99	0.44
1:E:147:GLY:HA2	1:E:175:GLU:HG2	1.98	0.44
1:A:324:PRO:O	1:A:328:ASN:HB2	2.18	0.44
1:B:204:MET:HA	1:B:248:VAL:HB	1.99	0.44
1:B:378:SER:O	1:B:381:GLU:HB2	2.18	0.44
1:C:59:PRO:HG2	1:C:394:THR:HG21	2.00	0.44
1:D:153:ASP:CB	1:D:212:HIS:HB3	2.48	0.44
1:F:224:PHE:CE2	1:F:278:LEU:HD12	2.52	0.44
1:F:226:ARG:HB2	1:F:226:ARG:HH11	1.83	0.44
1:H:118:GLU:HB3	1:H:119:PRO:HD3	1.98	0.44
1:E:75:MET:HE3	1:E:316:TRP:CZ3	2.52	0.44
1:E:100:GLN:HG2	1:E:133:GLN:O	2.17	0.44
1:B:153:ASP:HB3	1:B:212:HIS:HB3	1.99	0.44
1:B:164:ARG:N	1:G:355:ASP:OD2	2.49	0.44
1:B:459:HIS:HA	1:B:460:PRO:HA	1.70	0.44
1:C:253:HIS:CD2	1:C:253:HIS:O	2.70	0.44
1:C:281:GLU:HA	1:C:328:ASN:ND2	2.33	0.44
1:D:57:MET:HE3	1:D:418:PHE:CB	2.48	0.44
1:D:61:TYR:OH	1:D:432:LEU:HD22	2.18	0.44
1:D:72:TRP:O	1:D:73:MET:CB	2.66	0.44
1:D:234:PRO:O	1:D:238:VAL:HG23	2.18	0.44
1:D:235:VAL:HG12	1:D:239:MET:HE2	1.98	0.44
1:D:301:THR:C	1:D:302:VAL:HG23	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:GLU:HB3	1:D:324:PRO:CD	2.48	0.44
1:F:224:PHE:CZ	1:F:278:LEU:CD1	3.01	0.44
1:H:255:VAL:O	1:H:278:LEU:CD1	2.43	0.44
1:E:429:ILE:HD12	1:E:432:LEU:HD11	1.98	0.44
1:A:92:VAL:CG1	1:C:131:ILE:HD11	2.48	0.44
1:A:114:HIS:CG	1:A:143:ILE:HG13	2.53	0.44
1:A:178:VAL:CG1	1:A:179:GLY:N	2.79	0.44
1:A:397:VAL:O	1:A:401:TYR:HD2	2.01	0.44
1:C:117:ILE:HG23	1:C:118:GLU:H	1.81	0.44
1:C:446:ASP:O	1:C:450:LEU:CD1	2.66	0.44
1:D:227:SER:C	1:D:228:TYR:CD1	2.95	0.44
1:F:80:THR:HG22	1:F:84:LEU:HD12	1.98	0.44
1:G:260:LEU:HD21	1:G:290:ILE:HD11	1.99	0.44
1:H:456:VAL:HG22	1:H:457:THR:HG23	2.00	0.44
1:A:103:LEU:HD13	1:A:135:ALA:HA	1.99	0.44
1:A:305:GLN:O	1:A:309:GLY:N	2.43	0.44
1:B:59:PRO:HG2	1:B:394:THR:OG1	2.18	0.44
1:B:365:PRO:O	1:B:371:ASP:HA	2.18	0.44
1:C:26:ILE:CD1	1:C:34:THR:OG1	2.64	0.44
1:C:87:TRP:CZ3	1:C:455:LEU:HG	2.52	0.44
1:C:150:PHE:O	1:C:159:ARG:HB3	2.17	0.44
1:C:217:LEU:HD21	1:C:225:ASP:H	1.81	0.44
1:C:326:ALA:C	1:C:329:GLU:H	2.25	0.44
1:D:171:ASP:C	1:D:173:MET:H	2.25	0.44
1:D:190:VAL:C	1:D:194:VAL:HG23	2.40	0.44
1:D:330:ARG:HA	1:D:333:ILE:HD12	2.00	0.44
1:F:121:LEU:HA	1:F:124:ARG:HB3	1.99	0.44
1:H:120:VAL:O	1:H:123:ALA:N	2.46	0.44
1:E:297:ALA:O	1:E:339:ILE:HA	2.17	0.44
1:E:301:THR:HG22	1:E:329:GLU:OE1	2.18	0.44
1:A:92:VAL:HG13	1:A:93:GLU:N	2.33	0.44
1:A:251:LEU:CD1	1:A:270:VAL:HG21	2.47	0.44
1:B:155:HIS:CD2	1:B:157:ALA:O	2.71	0.44
1:C:273:HIS:CD2	1:C:273:HIS:N	2.86	0.44
1:C:341:LEU:HD13	1:C:375:TRP:CE3	2.53	0.44
1:D:73:MET:HE3	1:D:74:PHE:CE1	2.52	0.44
1:D:187:ARG:HB3	1:D:187:ARG:CZ	2.48	0.44
1:F:221:SER:HA	1:F:222:VAL:HA	1.72	0.44
1:F:305:GLN:O	1:F:308:GLN:N	2.48	0.44
1:F:447:ARG:CZ	1:F:447:ARG:HB2	2.47	0.44
1:G:45:GLU:C	1:G:47:ALA:N	2.75	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:110:VAL:O	1:G:137:ILE:HA	2.17	0.44
1:H:193:ARG:HB2	1:H:193:ARG:CZ	2.47	0.44
1:H:286:LEU:O	1:H:290:ILE:HG13	2.18	0.44
1:E:236:LEU:O	1:E:240:VAL:CG2	2.50	0.44
1:E:307:ARG:C	1:E:307:ARG:HD2	2.43	0.44
1:B:32:PHE:CZ	1:B:410:VAL:HG22	2.53	0.44
1:B:391:SER:N	1:B:392:ALA:CA	2.81	0.44
1:C:97:GLU:OE2	1:C:455:LEU:N	2.30	0.44
1:C:112:ASP:O	1:C:140:ALA:N	2.50	0.44
1:C:137:ILE:HG22	1:C:139:ALA:HB2	1.98	0.44
1:C:283:PRO:HG2	1:C:285:TYR:HE1	1.83	0.44
1:C:283:PRO:HG2	1:C:285:TYR:CE1	2.53	0.44
1:F:65:ASN:O	1:F:66:VAL:CG1	2.66	0.44
1:F:150:PHE:HE2	1:F:170:ILE:HD12	1.83	0.44
1:F:186:PRO:O	1:F:190:VAL:HG23	2.17	0.44
1:F:228:TYR:O	1:F:229:GLN:HG3	2.18	0.44
1:H:440:GLN:O	1:H:443:ALA:O	2.35	0.44
1:E:32:PHE:CE2	1:E:410:VAL:HA	2.52	0.43
1:E:131:ILE:HD11	1:B:124:ARG:HH22	1.82	0.43
1:E:278:LEU:HA	1:E:325:TYR:HE1	1.82	0.43
1:A:152:ALA:C	1:A:154:PHE:N	2.76	0.43
1:B:170:ILE:O	1:B:173:MET:HB2	2.18	0.43
1:C:152:ALA:HB1	1:C:213:ILE:HG22	1.99	0.43
1:C:399[B]:ARG:NH1	1:C:404:ALA:HB1	2.32	0.43
1:D:56:TRP:CZ3	1:D:423:GLN:HA	2.53	0.43
1:D:170:ILE:O	1:D:173:MET:HB3	2.18	0.43
1:D:333:ILE:O	1:D:334:SER:C	2.60	0.43
1:F:75:MET:HE1	1:F:212:HIS:HE1	1.83	0.43
1:H:72:TRP:CD2	1:H:75:MET:HE3	2.52	0.43
1:H:342:ASN:O	1:H:375:TRP:CD1	2.69	0.43
1:H:405:ASP:CG	1:H:406:GLN:HE21	2.19	0.43
1:E:4:ILE:HD12	1:E:442:GLY:O	2.18	0.43
1:E:63:ASN:ND2	1:E:371:ASP:OD2	2.51	0.43
1:A:300:GLN:OE1	1:A:344:ASP:HB2	2.19	0.43
1:B:32:PHE:CE2	1:B:409:SER:HB2	2.53	0.43
1:B:283:PRO:O	1:B:285:TYR:N	2.51	0.43
1:C:416:ALA:HB3	1:C:442:GLY:N	2.33	0.43
1:D:67:HIS:HD2	1:D:114:HIS:O	2.01	0.43
1:G:304:ASP:HA	1:G:307:ARG:HD2	2.00	0.43
1:E:429:ILE:CG2	1:E:430:ARG:N	2.80	0.43
1:A:236:LEU:O	1:A:266:LEU:HD21	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ALA:O	1:B:75:MET:HB3	2.18	0.43
1:B:84:LEU:HD13	1:B:170:ILE:HG21	2.00	0.43
1:B:138:PHE:CA	1:B:203:ASP:OD2	2.66	0.43
1:B:165:THR:HG22	1:G:355:ASP:OD1	2.19	0.43
1:C:104:ARG:CG	1:C:447:ARG:NH1	2.81	0.43
1:C:219:ASP:OD2	1:C:223:GLY:N	2.51	0.43
1:D:278:LEU:CA	1:D:325:TYR:CE1	2.96	0.43
1:D:283:PRO:HB2	1:D:285:TYR:HD2	1.83	0.43
1:F:63:ASN:OD1	1:F:66:VAL:HG13	2.17	0.43
1:F:97:GLU:OE2	1:F:457:THR:OG1	2.31	0.43
1:F:282:ILE:N	1:F:283:PRO:HB3	2.33	0.43
1:G:8:ASN:N	1:G:24:THR:OG1	2.44	0.43
1:G:178:VAL:HG21	1:G:197:TYR:CG	2.53	0.43
1:G:395:ILE:H	1:G:395:ILE:HG13	1.47	0.43
1:H:13:ASP:HB2	1:H:15:LEU:H	1.84	0.43
1:E:181:GLN:O	1:E:183:SER:N	2.51	0.43
1:A:149:PRO:HA	1:A:154:PHE:HD2	1.82	0.43
1:A:235:VAL:O	1:A:239:MET:CG	2.65	0.43
1:A:287:ILE:HG22	1:A:291:VAL:CG2	2.48	0.43
1:A:317:ALA:O	1:A:319:ALA:N	2.44	0.43
1:A:317:ALA:C	1:A:319:ALA:H	2.26	0.43
1:C:299:LEU:HG	1:C:329:GLU:CD	2.43	0.43
1:D:75:MET:SD	1:D:215:PHE:CZ	3.12	0.43
1:D:330:ARG:O	1:D:334:SER:OG	2.29	0.43
1:F:92:VAL:HG13	1:F:123:ALA:HB2	1.99	0.43
1:F:116:ALA:HB2	1:F:174:PHE:CE1	2.53	0.43
1:F:252:THR:HG23	1:F:268:ALA:CB	2.48	0.43
1:G:118:GLU:H	1:G:118:GLU:HG3	1.42	0.43
1:H:6:ILE:O	1:H:24:THR:CG2	2.63	0.43
1:H:285:TYR:CD1	1:H:285:TYR:C	2.97	0.43
1:H:306:HIS:HD2	1:H:365:PRO:HG3	1.83	0.43
1:H:333:ILE:HD11	1:H:379:MET:SD	2.59	0.43
1:E:143:ILE:HG23	1:E:206:LYS:HG2	2.00	0.43
1:E:324:PRO:HA	1:E:327:THR:HB	2.01	0.43
1:A:72:TRP:O	1:A:76:ALA:CB	2.66	0.43
1:B:258:GLU:O	1:B:259:ALA:CB	2.67	0.43
1:D:74:PHE:N	1:D:74:PHE:CD1	2.85	0.43
1:D:259:ALA:O	1:D:262:THR:HG22	2.19	0.43
1:F:264:VAL:HG12	1:F:293:SER:CB	2.37	0.43
1:F:429:ILE:CD1	1:F:432:LEU:HD11	2.42	0.43
1:G:195:ARG:NE	1:G:242:GLU:OE1	2.26	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:260:LEU:HD23	1:H:286:LEU:HD23	2.00	0.43
1:H:339:ILE:O	1:H:396:ASN:HB3	2.19	0.43
1:E:387:LEU:O	1:E:390:ILE:HG22	2.18	0.43
1:E:411:GLU:HG2	1:E:412:THR:H	1.83	0.43
1:A:6:ILE:O	1:A:24:THR:HG23	2.18	0.43
1:A:191:ARG:NE	1:A:238:VAL:HG21	2.33	0.43
1:A:355:ASP:OD2	1:F:164:ARG:HG2	2.19	0.43
1:C:93:GLU:O	1:C:97:GLU:HB2	2.18	0.43
1:C:153:ASP:H	1:C:213:ILE:HG22	1.83	0.43
1:F:290:ILE:CG2	1:F:291:VAL:N	2.81	0.43
1:G:180:HIS:C	1:G:181:GLN:O	2.59	0.43
1:G:207:ILE:HB	1:G:239:MET:HE1	1.99	0.43
1:G:215:PHE:HA	1:G:218:VAL:HA	2.01	0.43
1:G:435:ILE:HG21	1:G:438:VAL:HG23	1.99	0.43
1:H:76:ALA:CB	1:H:77:GLY:HA2	2.21	0.43
1:H:293:SER:O	1:H:294:ASP:CG	2.61	0.43
1:A:210:SER:HA	1:A:229:GLN:HA	2.00	0.43
1:A:238:VAL:CG1	1:A:239:MET:N	2.81	0.43
1:B:72:TRP:CD1	1:B:364:ARG:HH22	2.36	0.43
1:D:64:GLY:O	1:D:401:TYR:OH	2.34	0.43
1:D:167:VAL:O	1:D:171:ASP:OD1	2.37	0.43
1:D:220:ARG:O	1:D:221:SER:CB	2.66	0.43
1:F:32:PHE:CE2	1:F:416:ALA:HA	2.54	0.43
1:F:293:SER:O	1:F:294:ASP:HB2	2.18	0.43
1:G:261:ASP:O	1:G:265:GLU:HG2	2.18	0.43
1:A:13:ASP:OD1	1:A:13:ASP:N	2.41	0.43
1:A:151:SER:HA	1:A:159:ARG:HD2	2.01	0.43
1:B:41:THR:H	1:B:42:PRO:CA	2.29	0.43
1:B:380:VAL:HA	1:B:384:MET:HB3	2.01	0.43
1:D:66:VAL:CG2	1:D:110:VAL:CG1	2.96	0.43
1:D:224:PHE:HE1	1:D:325:TYR:OH	2.02	0.43
1:D:416:ALA:O	1:D:441:ALA:N	2.52	0.43
1:F:69:LEU:HA	1:F:69:LEU:HD23	1.77	0.43
1:G:4:ILE:HB	1:G:48:THR:OG1	2.18	0.43
1:G:31:ARG:HB2	1:G:414:LYS:O	2.19	0.43
1:G:87:TRP:HB3	1:G:94:VAL:HG21	2.00	0.43
1:H:58:VAL:HG23	1:H:419:VAL:HB	2.01	0.43
1:H:391:SER:O	1:H:395:ILE:HD12	2.19	0.43
1:E:261:ASP:O	1:E:265:GLU:CG	2.56	0.43
1:A:316:TRP:CG	1:A:317:ALA:N	2.81	0.43
1:A:357:SER:OG	1:A:360:GLU:HG3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:ALA:N	1:B:77:GLY:CA	2.82	0.43
1:C:114:HIS:ND1	1:C:143:ILE:HG13	2.34	0.43
1:F:131:ILE:HD13	1:H:93:GLU:OE1	2.19	0.43
1:F:203:ASP:O	1:F:249:PRO:HD2	2.19	0.43
1:G:34:THR:HA	1:G:412:THR:HG22	2.01	0.43
1:G:124:ARG:HB2	1:G:137:ILE:HG13	2.00	0.43
1:H:149:PRO:HA	1:H:154:PHE:HB3	2.01	0.43
1:H:220:ARG:C	1:H:221:SER:HG	2.11	0.43
1:H:303:HIS:CE1	1:H:306:HIS:HB2	2.52	0.43
1:E:317:ALA:O	1:E:320:LEU:N	2.51	0.43
1:A:251:LEU:HD12	1:A:251:LEU:HA	1.89	0.43
1:A:277:THR:CG2	1:A:282:ILE:HG22	2.49	0.43
1:A:303:HIS:O	1:A:307:ARG:HB2	2.18	0.43
1:C:302:VAL:HA	1:C:374:HIS:CE1	2.50	0.43
1:D:36:GLY:HA2	1:D:41:THR:HG21	2.00	0.43
1:D:158:GLY:O	1:D:162:ALA:N	2.52	0.43
1:F:67:HIS:ND1	1:F:114:HIS:HB3	2.34	0.43
1:G:195:ARG:O	1:G:195:ARG:HD3	2.19	0.43
1:G:365:PRO:HG2	1:G:366:TRP:CZ3	2.54	0.43
1:H:97:GLU:HG3	1:H:455:LEU:HB3	2.00	0.43
1:H:382:LYS:HD3	1:H:382:LYS:HA	1.73	0.43
1:E:56:TRP:NE1	1:E:424:ASP:OD1	2.52	0.42
1:E:320:LEU:N	1:E:320:LEU:HD23	2.34	0.42
1:A:43:VAL:HG11	1:A:49:VAL:HG22	2.02	0.42
1:A:353:LEU:HD21	1:A:364:ARG:NH1	2.34	0.42
1:B:198:LEU:C	1:B:200:ARG:N	2.76	0.42
1:B:390:ILE:O	1:B:391:SER:C	2.58	0.42
1:C:416:ALA:O	1:C:441:ALA:N	2.52	0.42
1:D:103:LEU:CD2	1:D:445:VAL:HG21	2.49	0.42
1:G:15:LEU:HA	1:G:395:ILE:CD1	2.48	0.42
1:G:76:ALA:HA	1:G:77:GLY:O	2.18	0.42
1:H:103:LEU:HD22	1:H:134:GLY:O	2.19	0.42
1:H:120:VAL:HG13	1:H:121:LEU:N	2.33	0.42
1:H:201:GLY:C	1:H:202:VAL:CG2	2.91	0.42
1:E:43:VAL:O	1:E:43:VAL:HG13	2.18	0.42
1:E:365:PRO:HD2	1:E:366:TRP:CE3	2.54	0.42
1:A:180:HIS:O	1:A:182:LEU:N	2.46	0.42
1:A:323:GLU:O	1:A:324:PRO:C	2.62	0.42
1:C:231:PHE:HB2	1:C:236:LEU:HD21	2.01	0.42
1:D:103:LEU:HA	1:D:107:VAL:O	2.19	0.42
1:G:146:MET:HB2	1:G:146:MET:HE3	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:338:LYS:HD2	1:H:338:LYS:HA	1.65	0.42
1:E:75:MET:HE2	1:E:316:TRP:HH2	1.84	0.42
1:E:76:ALA:HB3	1:E:77:GLY:CA	2.49	0.42
1:E:452:THR:OG1	1:E:453:THR:N	2.52	0.42
1:C:401:TYR:CD1	1:C:401:TYR:N	2.88	0.42
1:D:9:VAL:CG2	1:D:23:THR:O	2.64	0.42
1:D:282:ILE:HG22	1:D:286:LEU:HB3	2.01	0.42
1:D:284:ASN:HA	1:D:287:ILE:HB	2.00	0.42
1:F:152:ALA:O	1:F:153:ASP:HB2	2.19	0.42
1:F:217:LEU:HD12	1:F:226:ARG:NH2	2.10	0.42
1:F:229:GLN:CD	1:F:259:ALA:HB2	2.44	0.42
1:G:94:VAL:CG1	1:G:456:VAL:CG2	2.97	0.42
1:H:111:PHE:CE2	1:H:397:VAL:HG12	2.54	0.42
1:E:204:MET:HB2	1:E:249:PRO:O	2.19	0.42
1:E:214:VAL:CG2	1:E:215:PHE:CE1	3.03	0.42
1:E:421:LEU:HB3	1:E:434:SER:OG	2.19	0.42
1:A:72:TRP:O	1:A:76:ALA:CA	2.67	0.42
1:B:185:LEU:H	1:B:185:LEU:HG	1.62	0.42
1:B:384:MET:HE2	1:B:389:ALA:HA	2.01	0.42
1:B:437:GLU:HA	1:B:447:ARG:HH21	1.84	0.42
1:C:104:ARG:HG2	1:C:447:ARG:HH12	1.84	0.42
1:C:356:LEU:O	1:C:361:ARG:NE	2.52	0.42
1:G:286:LEU:HD12	1:G:286:LEU:HA	1.90	0.42
1:H:142:THR:HG22	1:H:143:ILE:N	2.34	0.42
1:H:182:LEU:HD12	1:H:231:PHE:CZ	2.54	0.42
1:H:204:MET:HE2	1:H:204:MET:HB3	1.88	0.42
1:A:12:ILE:HG21	1:A:390:ILE:HD13	2.01	0.42
1:A:14:GLY:C	1:A:15:LEU:HD23	2.44	0.42
1:A:232:SER:OG	1:A:235:VAL:HG23	2.19	0.42
1:C:227:SER:CB	1:C:228:TYR:HA	2.36	0.42
1:D:109:THR:HG23	1:D:136:ARG:HB2	2.02	0.42
1:D:166:PHE:CE1	1:D:170:ILE:HG13	2.55	0.42
1:F:14:GLY:HA2	1:F:390:ILE:CD1	2.47	0.42
1:H:96:GLU:O	1:H:100:GLN:HG3	2.19	0.42
1:H:317:ALA:O	1:H:319:ALA:N	2.52	0.42
1:H:343:THR:OG1	1:H:371:ASP:OD1	2.36	0.42
1:H:392:ALA:HA	1:H:396:ASN:HB2	2.00	0.42
1:E:385:SER:C	1:E:387:LEU:N	2.77	0.42
1:E:416:ALA:O	1:E:441:ALA:N	2.53	0.42
1:A:350:LYS:CB	1:A:459:HIS:NE2	2.82	0.42
1:B:302:VAL:HG12	1:B:306:HIS:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:GLU:HB3	1:B:324:PRO:CD	2.49	0.42
1:D:74:PHE:O	1:D:75:MET:CB	2.68	0.42
1:D:252:THR:CG2	1:D:263:SER:OG	2.68	0.42
1:F:102:ALA:HB1	1:F:107:VAL:CG2	2.49	0.42
1:F:163:THR:O	1:F:166:PHE:N	2.52	0.42
1:F:317:ALA:C	1:F:319:ALA:N	2.77	0.42
1:H:92:VAL:O	1:H:96:GLU:HG3	2.19	0.42
1:E:3:THR:HG21	1:E:44:PRO:HG2	2.01	0.42
1:E:6:ILE:HD13	1:E:50:VAL:HB	2.01	0.42
1:A:126:ARG:HH11	1:A:126:ARG:N	2.18	0.42
1:A:180:HIS:C	1:A:182:LEU:H	2.24	0.42
1:A:250:VAL:HB	1:A:269:ASP:H	1.84	0.42
1:A:286:LEU:O	1:A:289:LYS:N	2.53	0.42
1:A:373:PHE:HB3	1:A:433:ARG:HH21	1.84	0.42
1:B:73:MET:HE1	1:B:83:TYR:CG	2.55	0.42
1:B:152:ALA:C	1:B:154:PHE:H	2.27	0.42
1:D:136:ARG:HH22	1:D:417:ASP:CG	2.27	0.42
1:D:299:LEU:O	1:D:375:TRP:NE1	2.43	0.42
1:F:374:HIS:C	1:F:374:HIS:CD2	2.98	0.42
1:F:420:LEU:HD12	1:F:437:GLU:HB2	2.02	0.42
1:G:100:GLN:OE1	1:G:450:LEU:HG	2.19	0.42
1:G:304:ASP:O	1:G:307:ARG:HG2	2.20	0.42
1:E:90:ARG:NE	1:E:93:GLU:OE1	2.42	0.42
1:A:178:VAL:HA	1:A:182:LEU:CD1	2.48	0.42
1:C:373:PHE:CD2	1:C:433:ARG:HG2	2.54	0.42
1:F:4:ILE:CG2	1:F:48:THR:HB	2.49	0.42
1:F:459:HIS:HA	1:F:460:PRO:HA	1.65	0.42
1:G:76:ALA:HB1	1:G:77:GLY:CA	2.49	0.42
1:H:30:ASP:O	1:H:31:ARG:CG	2.68	0.42
1:H:138:PHE:CE2	1:H:403:LYS:HG3	2.55	0.42
1:H:182:LEU:HB3	1:H:231:PHE:HE2	1.85	0.42
1:H:224:PHE:O	1:H:224:PHE:HD1	2.03	0.42
1:E:351:ASP:OD2	1:D:169:ARG:NH2	2.53	0.42
1:A:9:VAL:HG12	1:A:10:THR:N	2.34	0.42
1:B:350:LYS:HD3	1:B:459:HIS:HB3	2.01	0.42
1:C:447:ARG:HB3	1:C:447:ARG:HH11	1.85	0.42
1:D:364:ARG:HA	1:D:365:PRO:HD2	1.95	0.42
1:F:12:ILE:O	1:F:58:VAL:HA	2.20	0.42
1:F:123:ALA:O	1:F:126:ARG:HB2	2.20	0.42
1:G:301:THR:HG22	1:G:302:VAL:H	1.85	0.42
1:G:320:LEU:HA	1:G:325:TYR:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:152:ALA:O	1:H:153:ASP:HB2	2.20	0.42
1:H:386:PRO:O	1:H:390:ILE:HD12	2.20	0.42
1:H:459:HIS:HA	1:H:460:PRO:HA	1.85	0.42
1:E:143:ILE:HD13	1:E:206:LYS:HE2	2.02	0.42
1:E:364:ARG:HA	1:E:365:PRO:HD3	1.83	0.42
1:A:60:GLY:HA3	1:A:108:THR:OG1	2.19	0.42
1:B:391:SER:CA	1:B:392:ALA:C	2.93	0.42
1:D:148:GLY:C	1:D:154:PHE:CD2	2.95	0.42
1:F:72:TRP:CD1	1:F:364:ARG:HH12	2.37	0.42
1:F:117:ILE:HD11	1:F:197:TYR:CE1	2.55	0.42
1:F:428:ASP:O	1:F:429:ILE:HG22	2.19	0.42
1:G:59:PRO:HG2	1:G:394:THR:HG21	2.02	0.42
1:G:258:GLU:O	1:G:259:ALA:CB	2.67	0.42
1:H:197:TYR:CE2	1:H:205:LEU:HD11	2.55	0.42
1:H:230:THR:HB	1:H:231:PHE:CD1	2.55	0.42
1:H:361:ARG:O	1:H:363:ASP:N	2.53	0.42
1:H:387:LEU:HD13	1:H:426:VAL:HG21	2.02	0.42
1:H:406:GLN:CB	1:H:415:LEU:HD13	2.34	0.42
1:E:146:MET:SD	1:E:212:HIS:HB2	2.60	0.41
1:E:191:ARG:HB2	1:E:238:VAL:CG1	2.49	0.41
1:E:208:ALA:HA	1:E:253:HIS:HB3	2.02	0.41
1:E:341:LEU:HA	1:E:375:TRP:CZ2	2.55	0.41
1:A:140:ALA:HB2	1:A:204:MET:CG	2.50	0.41
1:C:21:PRO:O	1:C:22:ALA:CB	2.68	0.41
1:C:36:GLY:HA2	1:C:37:PRO:HD3	1.78	0.41
1:C:259:ALA:HA	1:C:262:THR:HB	2.02	0.41
1:D:81:ILE:HD11	1:D:158:GLY:HA3	2.01	0.41
1:D:145:GLY:HA2	1:D:231:PHE:HZ	1.85	0.41
1:D:173:MET:HE2	1:D:173:MET:HB2	1.71	0.41
1:F:296:TRP:CE3	1:F:338:LYS:HB3	2.55	0.41
1:G:111:PHE:HE2	1:G:397:VAL:CG1	2.33	0.41
1:H:340:LEU:O	1:H:375:TRP:CZ2	2.73	0.41
1:H:349:SER:C	1:H:351:ASP:N	2.76	0.41
1:E:54:ARG:HG2	1:E:54:ARG:O	2.19	0.41
1:A:35:VAL:HG12	1:A:36:GLY:N	2.35	0.41
1:B:117:ILE:HD11	1:B:202:VAL:HG13	2.01	0.41
1:C:6:ILE:HG22	1:C:25:VAL:CA	2.49	0.41
1:C:340:LEU:HD23	1:C:341:LEU:N	2.35	0.41
1:D:337:ALA:O	1:D:338:LYS:CB	2.67	0.41
1:D:378:SER:O	1:D:382:LYS:HG2	2.20	0.41
1:F:100:GLN:HB3	1:F:450:LEU:HG	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:ILE:O	1:F:213:ILE:HG22	2.19	0.41
1:G:87:TRP:CE3	1:G:455:LEU:HD23	2.54	0.41
1:G:282:ILE:CG1	1:G:328:ASN:OD1	2.68	0.41
1:H:69:LEU:HD23	1:H:69:LEU:HA	1.79	0.41
1:E:286:LEU:O	1:E:286:LEU:HD23	2.20	0.41
1:E:367:THR:O	1:E:371:ASP:HB3	2.21	0.41
1:A:87:TRP:O	1:A:90:ARG:HB2	2.20	0.41
1:A:220:ARG:HH21	1:A:314:GLY:C	2.27	0.41
1:B:389:ALA:O	1:B:392:ALA:HB2	1.95	0.41
1:C:206:LYS:NZ	1:C:253:HIS:CB	2.84	0.41
1:C:227:SER:CB	1:C:228:TYR:CA	2.97	0.41
1:C:399[B]:ARG:HH11	1:C:404:ALA:CB	2.33	0.41
1:D:103:LEU:HD13	1:D:135:ALA:HB2	2.03	0.41
1:D:104:ARG:HB2	1:D:447:ARG:HG3	2.02	0.41
1:D:109:THR:HG21	1:D:407:ILE:HD13	2.01	0.41
1:D:111:PHE:HD2	1:D:204:MET:HE1	1.85	0.41
1:D:255:VAL:HA	1:D:276:TYR:O	2.21	0.41
1:D:347:CYS:HA	1:D:348:PRO:HD2	1.83	0.41
1:D:348:PRO:CG	1:D:353:LEU:HD21	2.49	0.41
1:D:378:SER:HB3	1:D:382:LYS:NZ	2.36	0.41
1:D:387:LEU:O	1:D:390:ILE:CA	2.69	0.41
1:F:386:PRO:O	1:F:390:ILE:HG13	2.20	0.41
1:H:121:LEU:HD22	1:H:124:ARG:NH1	2.35	0.41
1:E:77:GLY:H	1:E:78:PRO:HD3	1.85	0.41
1:E:97:GLU:O	1:E:101:LEU:HD12	2.20	0.41
1:B:146:MET:HE3	1:B:154:PHE:CE2	2.56	0.41
1:B:258:GLU:C	1:B:260:LEU:H	2.28	0.41
1:B:450:LEU:HD12	1:B:450:LEU:HA	1.91	0.41
1:C:194:VAL:O	1:C:197:TYR:N	2.53	0.41
1:C:398:ALA:HB1	1:C:404:ALA:N	2.35	0.41
1:C:405:ASP:OD1	1:C:405:ASP:N	2.42	0.41
1:D:187:ARG:NH1	1:D:234:PRO:HB2	2.35	0.41
1:D:270:VAL:HG13	1:D:340:LEU:HD21	2.03	0.41
1:D:333:ILE:C	1:D:335:ALA:N	2.77	0.41
1:F:121:LEU:HD11	1:F:202:VAL:HG12	2.03	0.41
1:F:194:VAL:O	1:F:197:TYR:HB3	2.20	0.41
1:F:428:ASP:C	1:F:430:ARG:H	2.28	0.41
1:G:111:PHE:HE2	1:G:397:VAL:HG12	1.86	0.41
1:H:74:PHE:N	1:H:74:PHE:HD1	2.16	0.41
1:H:306:HIS:HE2	1:H:365:PRO:HD3	1.83	0.41
1:A:239:MET:HE2	1:A:239:MET:HB3	1.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:LYS:CA	1:A:353:LEU:HB2	2.37	0.41
1:A:394:THR:HB	1:A:408:GLY:O	2.20	0.41
1:B:205:LEU:HD12	1:B:205:LEU:HA	1.89	0.41
1:B:225:ASP:CG	1:B:226:ARG:N	2.76	0.41
1:B:299:LEU:HD13	1:B:339:ILE:HG23	2.01	0.41
1:D:36:GLY:CA	1:D:41:THR:CG2	2.98	0.41
1:F:61:TYR:CZ	1:F:432:LEU:HD22	2.54	0.41
1:F:251:LEU:HD22	1:F:270:VAL:CB	2.41	0.41
1:G:8:ASN:H	1:G:24:THR:HG1	1.65	0.41
1:H:218:VAL:O	1:H:218:VAL:CG2	2.69	0.41
1:H:255:VAL:HG23	1:H:256:SER:N	2.35	0.41
1:E:143:ILE:HG12	1:E:206:LYS:HD3	2.03	0.41
1:B:165:THR:HG23	1:G:351:ASP:HB3	2.02	0.41
1:B:229:GLN:OE1	1:B:259:ALA:HB2	2.20	0.41
1:B:395:ILE:HD13	1:B:399[B]:ARG:NH2	2.35	0.41
1:C:68:LEU:C	1:C:70:ASP:H	2.26	0.41
1:G:15:LEU:HD12	1:G:409:SER:OG	2.20	0.41
1:G:219:ASP:O	1:G:220:ARG:HB2	2.20	0.41
1:H:57:MET:HE3	1:H:57:MET:HB3	1.99	0.41
1:H:120:VAL:C	1:H:123:ALA:H	2.29	0.41
1:H:152:ALA:CB	1:H:213:ILE:HG12	2.50	0.41
1:E:372:HIS:O	1:E:375:TRP:HB3	2.20	0.41
1:A:350:LYS:HB2	1:A:459:HIS:NE2	2.36	0.41
1:C:121:LEU:HD21	1:C:124:ARG:CZ	2.50	0.41
1:D:146:MET:HE3	1:D:146:MET:HB3	1.89	0.41
1:F:194:VAL:O	1:F:198:LEU:HG	2.21	0.41
1:G:5:ALA:HB1	1:G:26:ILE:HG12	2.03	0.41
1:G:116:ALA:O	1:G:119:PRO:HD2	2.20	0.41
1:H:18:LEU:HA	1:H:18:LEU:HD22	1.62	0.41
1:H:332:LEU:HD22	1:H:337:ALA:CB	2.48	0.41
1:A:18:LEU:HD12	1:A:18:LEU:H	1.86	0.41
1:A:151:SER:C	1:A:156:PHE:HD1	2.28	0.41
1:A:175:GLU:O	1:A:178:VAL:O	2.38	0.41
1:A:255:VAL:CG1	1:A:278:LEU:HG	2.51	0.41
1:B:144:VAL:O	1:B:208:ALA:HB3	2.21	0.41
1:B:256:SER:O	1:B:258:GLU:O	2.38	0.41
1:B:395:ILE:HD12	1:B:399[B]:ARG:NH2	2.35	0.41
1:C:74:PHE:N	1:C:74:PHE:HD1	2.17	0.41
1:D:38:SER:CB	1:D:40:SER:O	2.69	0.41
1:D:74:PHE:O	1:D:75:MET:HB2	2.20	0.41
1:D:91:TYR:O	1:D:94:VAL:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:VAL:HA	1:D:238:VAL:HB	2.02	0.41
1:D:272:ILE:HG23	1:D:342:ASN:OD1	2.20	0.41
1:D:319:ALA:O	1:D:323:GLU:HG3	2.21	0.41
1:G:124:ARG:CB	1:G:137:ILE:HG13	2.51	0.41
1:G:261:ASP:OD1	1:G:289:LYS:CE	2.69	0.41
1:G:341:LEU:HG	1:G:375:TRP:CE3	2.56	0.41
1:H:111:PHE:HE2	1:H:397:VAL:CG1	2.33	0.41
1:E:348:PRO:HG2	1:E:364:ARG:HH12	1.86	0.41
1:E:378:SER:HA	1:E:381:GLU:HB3	2.03	0.41
1:A:20:ARG:HA	1:A:20:ARG:HD3	1.85	0.41
1:A:114:HIS:O	1:A:115:ASN:HB2	2.20	0.41
1:A:131:ILE:HD12	1:A:131:ILE:HA	1.94	0.41
1:A:251:LEU:HD11	1:A:270:VAL:HG21	2.02	0.41
1:B:37:PRO:O	1:B:39:ASP:C	2.64	0.41
1:B:219:ASP:O	1:B:222:VAL:O	2.38	0.41
1:B:306:HIS:NE2	1:B:365:PRO:HD3	2.36	0.41
1:B:380:VAL:C	1:B:382:LYS:H	2.27	0.41
1:C:261:ASP:OD1	1:C:286:LEU:HD13	2.21	0.41
1:C:318:ALA:C	1:C:320:LEU:N	2.76	0.41
1:D:75:MET:CG	1:D:215:PHE:CE1	2.98	0.41
1:D:262:THR:O	1:D:263:SER:C	2.64	0.41
1:D:450:LEU:HD23	1:D:450:LEU:HA	1.84	0.41
1:F:73:MET:HE2	1:F:73:MET:HB3	1.87	0.41
1:F:100:GLN:OE1	1:F:452:THR:HG22	2.20	0.41
1:F:185:LEU:HD22	1:F:189:GLU:HB2	2.03	0.41
1:F:281:GLU:O	1:F:283:PRO:HB3	2.20	0.41
1:G:10:THR:HA	1:G:21:PRO:HA	2.02	0.41
1:G:256:SER:O	1:G:258:GLU:O	2.38	0.41
1:H:18:LEU:O	1:H:19:PRO:C	2.64	0.41
1:H:66:VAL:O	1:H:67:HIS:CD2	2.50	0.41
1:E:74:PHE:N	1:E:74:PHE:CD1	2.87	0.41
1:E:164:ARG:HD3	1:E:164:ARG:HA	1.76	0.41
1:E:397:VAL:O	1:E:401:TYR:HD2	2.04	0.41
1:A:353:LEU:HD23	1:A:353:LEU:HA	1.89	0.41
1:A:382:LYS:HA	1:A:382:LYS:HD3	1.82	0.41
1:A:456:VAL:O	1:A:456:VAL:CG1	2.68	0.41
1:C:232:SER:O	1:C:236:LEU:HG	2.21	0.41
1:C:326:ALA:HB1	1:C:382:LYS:HE3	2.02	0.41
1:H:11:LEU:HD13	1:H:57:MET:HB3	2.03	0.41
1:H:252:THR:CG2	1:H:271:LEU:HA	2.50	0.41
1:H:342:ASN:H	1:H:375:TRP:NE1	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:380:VAL:O	1:H:381:GLU:CB	2.68	0.41
1:E:339:ILE:HG21	1:E:379:MET:CE	2.52	0.40
1:E:346:GLY:HA2	1:E:368:ILE:HD12	2.03	0.40
1:E:363:ASP:OD2	1:E:374:HIS:ND1	2.52	0.40
1:E:416:ALA:HB3	1:E:442:GLY:HA2	2.03	0.40
1:A:16:GLY:O	1:A:387:LEU:HD13	2.21	0.40
1:A:66:VAL:CG1	1:A:368:ILE:CD1	2.98	0.40
1:B:75:MET:O	1:B:75:MET:CG	2.69	0.40
1:B:148:GLY:O	1:B:151:SER:OG	2.39	0.40
1:B:385:SER:CA	1:B:387:LEU:O	2.69	0.40
1:D:71:ALA:O	1:D:74:PHE:N	2.55	0.40
1:D:282:ILE:HB	1:D:287:ILE:HD12	2.01	0.40
1:F:11:LEU:HB2	1:F:23:THR:HG21	2.03	0.40
1:F:83:TYR:O	1:F:87:TRP:HD1	2.04	0.40
1:F:293:SER:HG	1:F:295:SER:H	1.68	0.40
1:F:428:ASP:HB3	1:F:430:ARG:HG3	2.02	0.40
1:G:129:ALA:HB3	1:G:131:ILE:CD1	2.51	0.40
1:H:182:LEU:CD2	1:H:193:ARG:NH1	2.84	0.40
1:H:206:LYS:NZ	1:H:272:ILE:CG2	2.73	0.40
1:H:260:LEU:CD1	1:H:271:LEU:HD22	2.49	0.40
1:E:124:ARG:HG3	1:E:137:ILE:O	2.21	0.40
1:A:235:VAL:CA	1:A:238:VAL:CG1	2.94	0.40
1:A:271:LEU:HD12	1:A:297:ALA:HA	1.98	0.40
1:C:99:ALA:HB1	1:C:135:ALA:H	1.86	0.40
1:C:206:LYS:NZ	1:C:253:HIS:HB2	2.35	0.40
1:D:301:THR:C	1:D:302:VAL:CG2	2.94	0.40
1:D:353:LEU:O	1:D:356:LEU:HB2	2.20	0.40
1:F:151:SER:C	1:F:152:ALA:O	2.61	0.40
1:F:301:THR:HG21	1:F:379:MET:HE1	2.04	0.40
1:G:181:GLN:O	1:G:182:LEU:CG	2.69	0.40
1:G:350:LYS:HD2	1:G:353:LEU:HD12	2.02	0.40
1:H:112:ASP:O	1:H:140:ALA:HB3	2.21	0.40
1:E:73:MET:O	1:E:76:ALA:CB	2.70	0.40
1:E:191:ARG:HB2	1:E:238:VAL:HG13	2.03	0.40
1:E:213:ILE:HG21	1:E:216:THR:HG22	2.03	0.40
1:E:315:SER:O	1:E:316:TRP:CD1	2.74	0.40
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.72	0.40
1:B:178:VAL:CG2	1:B:197:TYR:HB2	2.52	0.40
1:B:409:SER:CB	1:B:410:VAL:HA	2.32	0.40
1:C:10:THR:HB	1:C:21:PRO:HB3	2.03	0.40
1:C:347:CYS:HA	1:C:348:PRO:HD3	1.94	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:ASN:C	1:F:66:VAL:HG13	2.46	0.40
1:F:453:THR:C	1:F:455:LEU:CD2	2.77	0.40
1:E:112:ASP:HB3	1:E:139:ALA:HA	2.03	0.40
1:E:313:VAL:HG11	1:E:360:GLU:OE1	2.22	0.40
1:A:71:ALA:O	1:A:74:PHE:CB	2.58	0.40
1:A:103:LEU:HD22	1:A:134:GLY:C	2.46	0.40
1:A:191:ARG:NH1	1:A:238:VAL:HG22	2.35	0.40
1:B:30:ASP:O	1:B:31:ARG:C	2.64	0.40
1:B:73:MET:O	1:B:76:ALA:CB	2.70	0.40
1:B:77:GLY:N	1:B:78:PRO:CD	2.84	0.40
1:B:88:GLU:OE1	1:B:169:ARG:NH1	2.53	0.40
1:F:150:PHE:HE2	1:F:170:ILE:CD1	2.34	0.40
1:F:236:LEU:HB3	1:F:266:LEU:CD2	2.50	0.40
1:E:140:ALA:HB2	1:E:204:MET:CG	2.52	0.40
1:E:284:ASN:O	1:E:285:TYR:HB3	2.18	0.40
1:A:71:ALA:O	1:A:75:MET:N	2.47	0.40
1:A:117:ILE:HG13	1:A:121:LEU:HG	2.04	0.40
1:A:205:LEU:HD12	1:A:205:LEU:HA	1.93	0.40
1:B:323:GLU:O	1:B:325:TYR:N	2.54	0.40
1:C:58:VAL:CG2	1:C:419:VAL:HB	2.51	0.40
1:D:70:ASP:CG	1:D:73:MET:HB3	2.44	0.40
1:F:69:LEU:O	1:F:70:ASP:HB3	2.20	0.40
1:F:176:ALA:C	1:F:178:VAL:H	2.29	0.40
1:F:193:ARG:HA	1:F:196:ASP:HB3	2.02	0.40
1:F:204:MET:HE2	1:F:204:MET:HB2	1.78	0.40
1:F:281:GLU:N	1:F:281:GLU:CD	2.75	0.40
1:F:420:LEU:HD23	1:F:420:LEU:HA	1.92	0.40
1:G:181:GLN:CG	1:G:182:LEU:N	2.84	0.40
1:G:244:ARG:HH22	1:G:250:VAL:HG12	1.87	0.40
1:G:439:PHE:CZ	1:G:444:ALA:HB2	2.56	0.40
1:H:30:ASP:C	1:H:31:ARG:HG2	2.47	0.40
1:H:178:VAL:HG11	1:H:197:TYR:CD1	2.56	0.40
1:H:227:SER:OG	1:H:228:TYR:N	2.55	0.40
1:H:341:LEU:HA	1:H:375:TRP:CH2	2.56	0.40
1:H:360:GLU:OE2	1:H:361:ARG:CZ	2.70	0.40

All (7) 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:D:226:ARG:HE	1:G:180:HIS:HE2[1_455]	0.67	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:226:ARG:HE	1:G:180:HIS:NE2[1_455]	1.26	0.34
1:A:261:ASP:OD2	1:C:187:ARG:HH21[1_655]	1.42	0.18
1:F:219:ASP:OD2	1:H:164:ARG:NH2[1_655]	2.12	0.08
1:D:187:ARG:NH2	1:G:258:GLU:OE2[1_455]	2.13	0.07
1:D:226:ARG:NE	1:G:180:HIS:NE2[1_455]	2.18	0.02
1:D:229:GLN:H	1:G:229:GLN:O[1_455]	1.60	0.00

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	457/461 (99%)	391 (86%)	57 (12%)	9 (2%)	6	16
1	B	459/461 (100%)	420 (92%)	32 (7%)	7 (2%)	8	23
1	C	459/461 (100%)	415 (90%)	35 (8%)	9 (2%)	6	16
1	D	457/461 (99%)	410 (90%)	33 (7%)	14 (3%)	3	8
1	E	457/461 (99%)	412 (90%)	31 (7%)	14 (3%)	3	8
1	F	457/461 (99%)	402 (88%)	45 (10%)	10 (2%)	5	15
1	G	457/461 (99%)	407 (89%)	40 (9%)	10 (2%)	5	15
1	H	457/461 (99%)	401 (88%)	46 (10%)	10 (2%)	5	15
All	All	3660/3688 (99%)	3258 (89%)	319 (9%)	83 (2%)	5	14

All (83) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	323	GLU
1	A	41	THR
1	A	255	VAL
1	B	31	ARG
1	B	41	THR
1	B	394	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	323	GLU
1	D	37	PRO
1	D	71	ALA
1	D	73	MET
1	D	76	ALA
1	F	30	ASP
1	F	228	TYR
1	F	283	PRO
1	F	323	GLU
1	F	429	ILE
1	G	323	GLU
1	H	203	ASP
1	H	323	GLU
1	H	360	GLU
1	E	76	ALA
1	E	158	GLY
1	E	221	SER
1	C	31	ARG
1	C	223	GLY
1	C	338	LYS
1	F	77	GLY
1	F	226	ARG
1	F	428	ASP
1	G	31	ARG
1	G	45	GLU
1	G	225	ASP
1	H	31	ARG
1	E	180	HIS
1	A	228	TYR
1	B	37	PRO
1	B	389	ALA
1	C	259	ALA
1	D	338	LYS
1	F	329	GLU
1	G	139	ALA
1	E	41	THR
1	E	182	LEU
1	E	226	ARG
1	E	259	ALA
1	E	285	TYR
1	A	37	PRO
1	A	75	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	45	GLU
1	D	181	GLN
1	D	258	GLU
1	F	151	SER
1	G	3	THR
1	G	153	ASP
1	H	30	ASP
1	H	181	GLN
1	H	456	VAL
1	A	85	ALA
1	B	42	PRO
1	B	323	GLU
1	C	219	ASP
1	C	224	PHE
1	D	31	ARG
1	D	259	ALA
1	H	41	THR
1	E	199	SER
1	E	213	ILE
1	E	316	TRP
1	A	30	ASP
1	C	44	PRO
1	G	182	LEU
1	G	452	THR
1	E	454	PRO
1	A	323	GLU
1	D	323	GLU
1	G	178	VAL
1	D	222	VAL
1	C	37	PRO
1	D	167	VAL
1	D	413	GLY
1	H	78	PRO
1	A	46	GLY
1	H	255	VAL

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	367/368 (100%)	307 (84%)	60 (16%)	2	7
1	B	368/368 (100%)	300 (82%)	68 (18%)	1	4
1	C	368/368 (100%)	319 (87%)	49 (13%)	4	12
1	D	367/368 (100%)	296 (81%)	71 (19%)	1	3
1	E	367/368 (100%)	304 (83%)	63 (17%)	2	5
1	F	367/368 (100%)	298 (81%)	69 (19%)	1	4
1	G	367/368 (100%)	298 (81%)	69 (19%)	1	4
1	H	367/368 (100%)	298 (81%)	69 (19%)	1	4
All	All	2938/2944 (100%)	2420 (82%)	518 (18%)	2	5

All (518) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	6	ILE
1	E	8	ASN
1	E	10	THR
1	E	25	VAL
1	E	30	ASP
1	E	31	ARG
1	E	41	THR
1	E	45	GLU
1	E	50	VAL
1	E	75	MET
1	E	82	GLU
1	E	97	GLU
1	E	110	VAL
1	E	117	ILE
1	E	144	VAL
1	E	153	ASP
1	E	164	ARG
1	E	178	VAL
1	E	188	LYS
1	E	198	LEU
1	E	199	SER
1	E	200	ARG
1	E	204	MET
1	E	207	ILE
1	E	214	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	216	THR
1	E	218	VAL
1	E	220	ARG
1	E	226	ARG
1	E	237	GLU
1	E	238	VAL
1	E	241	GLU
1	E	250	VAL
1	E	251	LEU
1	E	254	SER
1	E	260	LEU
1	E	264	VAL
1	E	269	ASP
1	E	272	ILE
1	E	277	THR
1	E	278	LEU
1	E	280	GLN
1	E	285	TYR
1	E	286	LEU
1	E	289	LYS
1	E	291	VAL
1	E	293	SER
1	E	302	VAL
1	E	306	HIS
1	E	307	ARG
1	E	320	LEU
1	E	329	GLU
1	E	350	LYS
1	E	385	SER
1	E	387	LEU
1	E	390	ILE
1	E	395	ILE
1	E	406	GLN
1	E	412	THR
1	E	417	ASP
1	E	436	THR
1	E	437	GLU
1	E	440	GLN
1	A	6	ILE
1	A	10	THR
1	A	12	ILE
1	A	13	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	18	LEU
1	A	27	VAL
1	A	28	GLU
1	A	31	ARG
1	A	45	GLU
1	A	49	VAL
1	A	57	MET
1	A	58	VAL
1	A	66	VAL
1	A	75	MET
1	A	93	GLU
1	A	97	GLU
1	A	121	LEU
1	A	126	ARG
1	A	160	THR
1	A	180	HIS
1	A	184	LEU
1	A	206	LYS
1	A	218	VAL
1	A	237	GLU
1	A	251	LEU
1	A	266	LEU
1	A	271	LEU
1	A	272	ILE
1	A	285	TYR
1	A	287	ILE
1	A	293	SER
1	A	300	GLN
1	A	301	THR
1	A	303	HIS
1	A	304	ASP
1	A	315	SER
1	A	325	TYR
1	A	329	GLU
1	A	341	LEU
1	A	343	THR
1	A	361	ARG
1	A	362	GLU
1	A	364	ARG
1	A	376	THR
1	A	387	LEU
1	A	390	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	395	ILE
1	A	397	VAL
1	A	399	ARG
1	A	405	ASP
1	A	407	ILE
1	A	409	SER
1	A	410	VAL
1	A	411	GLU
1	A	412	THR
1	A	435	ILE
1	A	447	ARG
1	A	451	PRO
1	A	457	THR
1	A	459	HIS
1	B	4	ILE
1	B	13	ASP
1	B	18	LEU
1	B	20	ARG
1	B	23	THR
1	B	30	ASP
1	B	31	ARG
1	B	39	ASP
1	B	43	VAL
1	B	45	GLU
1	B	49	VAL
1	B	53	ASN
1	B	68	LEU
1	B	75	MET
1	B	92	VAL
1	B	100	GLN
1	B	121	LEU
1	B	146	MET
1	B	155	HIS
1	B	164	ARG
1	B	165	THR
1	B	170	ILE
1	B	184	LEU
1	B	185	LEU
1	B	188	LYS
1	B	195	ARG
1	B	198	LEU
1	B	199	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	204	MET
1	B	206	LYS
1	B	210	SER
1	B	214	VAL
1	B	222	VAL
1	B	226	ARG
1	B	229	GLN
1	B	232	SER
1	B	236	LEU
1	B	242	GLU
1	B	252	THR
1	B	254	SER
1	B	255	VAL
1	B	271	LEU
1	B	278	LEU
1	B	281	GLU
1	B	284	ASN
1	B	285	TYR
1	B	287	ILE
1	B	300	GLN
1	B	311	GLU
1	B	350	LYS
1	B	376	THR
1	B	377	GLN
1	B	382	LYS
1	B	384	MET
1	B	387	LEU
1	B	396	ASN
1	B	397	VAL
1	B	420	LEU
1	B	423	GLN
1	B	424	ASP
1	B	426	VAL
1	B	430	ARG
1	B	437	GLU
1	B	447	ARG
1	B	452	THR
1	B	456	VAL
1	B	457	THR
1	B	459	HIS
1	C	9	VAL
1	C	23	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	25	VAL
1	C	26	ILE
1	C	28	GLU
1	C	30	ASP
1	C	39	ASP
1	C	49	VAL
1	C	58	VAL
1	C	72	TRP
1	C	75	MET
1	C	90	ARG
1	C	118	GLU
1	C	121	LEU
1	C	124	ARG
1	C	131	ILE
1	C	137	ILE
1	C	163	THR
1	C	180	HIS
1	C	191	ARG
1	C	205	LEU
1	C	206	LYS
1	C	207	ILE
1	C	214	VAL
1	C	218	VAL
1	C	220	ARG
1	C	224	PHE
1	C	226	ARG
1	C	230	THR
1	C	233	ARG
1	C	250	VAL
1	C	251	LEU
1	C	253	HIS
1	C	256	SER
1	C	301	THR
1	C	302	VAL
1	C	307	ARG
1	C	313	VAL
1	C	323	GLU
1	C	338	LYS
1	C	350	LYS
1	C	351	ASP
1	C	352	HIS
1	C	353	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	378	SER
1	C	390	ILE
1	C	395	ILE
1	C	407	ILE
1	C	437	GLU
1	D	6	ILE
1	D	23	THR
1	D	24	THR
1	D	30	ASP
1	D	31	ARG
1	D	35	VAL
1	D	72	TRP
1	D	74	PHE
1	D	75	MET
1	D	81	ILE
1	D	82	GLU
1	D	83	TYR
1	D	84	LEU
1	D	100	GLN
1	D	117	ILE
1	D	118	GLU
1	D	121	LEU
1	D	124	ARG
1	D	126	ARG
1	D	127	ILE
1	D	131	ILE
1	D	133	GLN
1	D	143	ILE
1	D	163	THR
1	D	171	ASP
1	D	173	MET
1	D	182	LEU
1	D	183	SER
1	D	187	ARG
1	D	195	ARG
1	D	198	LEU
1	D	199	SER
1	D	204	MET
1	D	210	SER
1	D	213	ILE
1	D	216	THR
1	D	220	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	221	SER
1	D	224	PHE
1	D	230	THR
1	D	232	SER
1	D	236	LEU
1	D	238	VAL
1	D	251	LEU
1	D	256	SER
1	D	264	VAL
1	D	272	ILE
1	D	280	GLN
1	D	282	ILE
1	D	286	LEU
1	D	289	LYS
1	D	293	SER
1	D	327	THR
1	D	333	ILE
1	D	334	SER
1	D	336	ASN
1	D	338	LYS
1	D	340	LEU
1	D	342	ASN
1	D	343	THR
1	D	350	LYS
1	D	381	GLU
1	D	391	SER
1	D	395	ILE
1	D	399	ARG
1	D	420	LEU
1	D	421	LEU
1	D	422	ASP
1	D	427	ASP
1	D	436	THR
1	D	459	HIS
1	F	26	ILE
1	F	28	GLU
1	F	38	SER
1	F	40	SER
1	F	43	VAL
1	F	48	THR
1	F	49	VAL
1	F	50	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	86	ARG
1	F	101	LEU
1	F	112	ASP
1	F	113	THR
1	F	115	ASN
1	F	117	ILE
1	F	126	ARG
1	F	151	SER
1	F	154	PHE
1	F	184	LEU
1	F	185	LEU
1	F	188	LYS
1	F	199	SER
1	F	204	MET
1	F	216	THR
1	F	219	ASP
1	F	224	PHE
1	F	226	ARG
1	F	240	VAL
1	F	251	LEU
1	F	257	VAL
1	F	263	SER
1	F	265	GLU
1	F	266	LEU
1	F	278	LEU
1	F	281	GLU
1	F	282	ILE
1	F	290	ILE
1	F	291	VAL
1	F	294	ASP
1	F	299	LEU
1	F	302	VAL
1	F	303	HIS
1	F	304	ASP
1	F	320	LEU
1	F	327	THR
1	F	328	ASN
1	F	329	GLU
1	F	333	ILE
1	F	336	ASN
1	F	347	CYS
1	F	349	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	350	LYS
1	F	351	ASP
1	F	360	GLU
1	F	362	GLU
1	F	407	ILE
1	F	409	SER
1	F	412	THR
1	F	422	ASP
1	F	424	ASP
1	F	428	ASP
1	F	429	ILE
1	F	430	ARG
1	F	435	ILE
1	F	436	THR
1	F	440	GLN
1	F	447	ARG
1	F	453	THR
1	F	455	LEU
1	F	457	THR
1	G	4	ILE
1	G	7	THR
1	G	9	VAL
1	G	11	LEU
1	G	15	LEU
1	G	20	ARG
1	G	24	THR
1	G	26	ILE
1	G	35	VAL
1	G	38	SER
1	G	43	VAL
1	G	45	GLU
1	G	48	THR
1	G	50	VAL
1	G	51	ASP
1	G	54	ARG
1	G	55	ARG
1	G	75	MET
1	G	78	PRO
1	G	80	THR
1	G	82	GLU
1	G	113	THR
1	G	118	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	124	ARG
1	G	137	ILE
1	G	155	HIS
1	G	164	ARG
1	G	170	ILE
1	G	172	SER
1	G	180	HIS
1	G	182	LEU
1	G	193	ARG
1	G	205	LEU
1	G	207	ILE
1	G	219	ASP
1	G	220	ARG
1	G	222	VAL
1	G	225	ASP
1	G	230	THR
1	G	266	LEU
1	G	269	ASP
1	G	272	ILE
1	G	275	ASN
1	G	285	TYR
1	G	286	LEU
1	G	293	SER
1	G	300	GLN
1	G	301	THR
1	G	302	VAL
1	G	320	LEU
1	G	324	PRO
1	G	327	THR
1	G	329	GLU
1	G	342	ASN
1	G	347	CYS
1	G	349	SER
1	G	350	LYS
1	G	382	LYS
1	G	388	GLU
1	G	390	ILE
1	G	391	SER
1	G	395	ILE
1	G	429	ILE
1	G	430	ARG
1	G	437	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	440	GLN
1	G	453	THR
1	G	457	THR
1	G	459	HIS
1	H	11	LEU
1	H	13	ASP
1	H	15	LEU
1	H	18	LEU
1	H	30	ASP
1	H	39	ASP
1	H	45	GLU
1	H	48	THR
1	H	54	ARG
1	H	67	HIS
1	H	101	LEU
1	H	113	THR
1	H	118	GLU
1	H	126	ARG
1	H	151	SER
1	H	167	VAL
1	H	180	HIS
1	H	181	GLN
1	H	193	ARG
1	H	195	ARG
1	H	199	SER
1	H	204	MET
1	H	205	LEU
1	H	216	THR
1	H	217	LEU
1	H	218	VAL
1	H	220	ARG
1	H	224	PHE
1	H	226	ARG
1	H	229	GLN
1	H	233	ARG
1	H	256	SER
1	H	257	VAL
1	H	271	LEU
1	H	273	HIS
1	H	275	ASN
1	H	285	TYR
1	H	286	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	295	SER
1	H	306	HIS
1	H	310	LEU
1	H	312	ASP
1	H	327	THR
1	H	328	ASN
1	H	330	ARG
1	H	331	ASN
1	H	333	ILE
1	H	338	LYS
1	H	339	ILE
1	H	340	LEU
1	H	343	THR
1	H	360	GLU
1	H	377	GLN
1	H	378	SER
1	H	380	VAL
1	H	381	GLU
1	H	382	LYS
1	H	385	SER
1	H	395	ILE
1	H	406	GLN
1	H	411	GLU
1	H	412	THR
1	H	432	LEU
1	H	436	THR
1	H	445	VAL
1	H	447	ARG
1	H	452	THR
1	H	453	THR
1	H	455	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	67	HIS
1	E	273	HIS
1	E	352	HIS
1	A	63	ASN
1	A	212	HIS
1	A	370	ASN
1	A	406	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	440	GLN
1	B	328	ASN
1	B	352	HIS
1	B	440	GLN
1	C	331	ASN
1	C	431	ASN
1	D	331	ASN
1	F	8	ASN
1	F	105	ASN
1	F	114	HIS
1	F	212	HIS
1	F	253	HIS
1	F	440	GLN
1	G	273	HIS
1	G	300	GLN
1	G	303	HIS
1	H	100	GLN
1	H	377	GLN
1	H	440	GLN
1	H	459	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	459/461 (99%)	-1.54	0 100 100	21, 44, 63, 101	0
1	B	459/461 (99%)	-1.63	0 100 100	10, 29, 48, 75	1 (0%)
1	C	459/461 (99%)	-1.55	0 100 100	18, 42, 66, 86	1 (0%)
1	D	459/461 (99%)	-1.63	0 100 100	9, 30, 53, 82	0
1	E	459/461 (99%)	-1.59	0 100 100	9, 35, 61, 95	0
1	F	459/461 (99%)	-1.47	0 100 100	24, 52, 75, 94	0
1	G	459/461 (99%)	-1.56	0 100 100	10, 37, 70, 97	0
1	H	459/461 (99%)	-1.52	0 100 100	22, 47, 64, 91	0
All	All	3672/3688 (99%)	-1.56	0 100 100	9, 40, 65, 101	2 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	501	1/1	1.00	0.02	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.