Full wwPDB X-ray Structure Validation Report (i)

Sep 28, 2024 – 07:22 pm BST

PDB ID	:	4ATW
Title	:	The crystal structure of Arabinofuranosidase
Authors	:	Dumbrepatil, A.; Song, H.-N.; Jung, T.-Y.; Kim, T.-J.; Woo, E.-J.
Deposited on	:	2012-05-10
Resolution	:	3.00 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 (i) 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 (1)) were used in the production of this report:

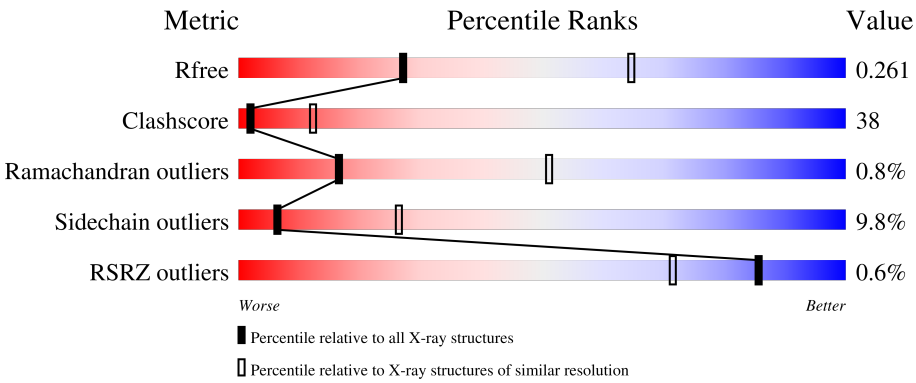
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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 <=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	482	51% 39% 8% •
1	B	482	% 51% 39% 8% •
1	C	482	50% 40% 9% •
1	D	482	50% 39% 9% •
1	E	482	% 50% 42% 7% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	482	% 53% 39% 7%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 23256 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	481	3876	2486	646	729	15	0	0	0
1	B	481	3876	2486	646	729	15	0	0	0
1	C	481	3876	2486	646	729	15	0	0	0
1	D	481	3876	2486	646	729	15	0	0	0
1	E	481	3876	2486	646	729	15	0	0	0
1	F	481	3876	2486	646	729	15	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

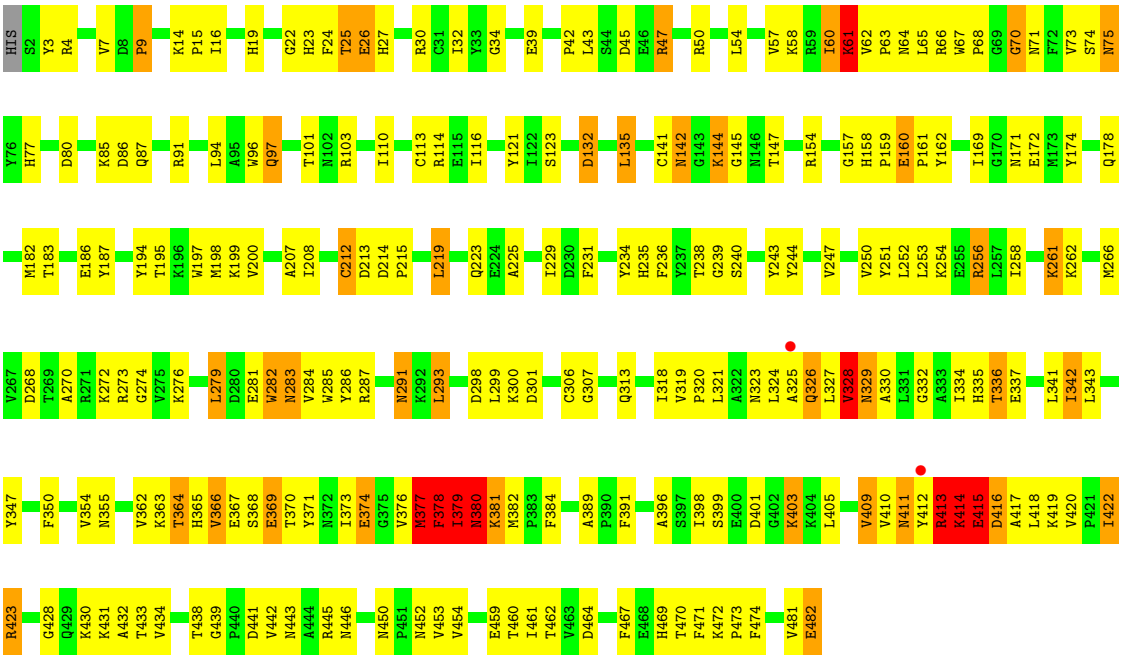
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP G4FHJ5
B	1	HIS	-	expression tag	UNP G4FHJ5
C	1	HIS	-	expression tag	UNP G4FHJ5
D	1	HIS	-	expression tag	UNP G4FHJ5
E	1	HIS	-	expression tag	UNP G4FHJ5
F	1	HIS	-	expression tag	UNP G4FHJ5

3 Residue-property plots (i)

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

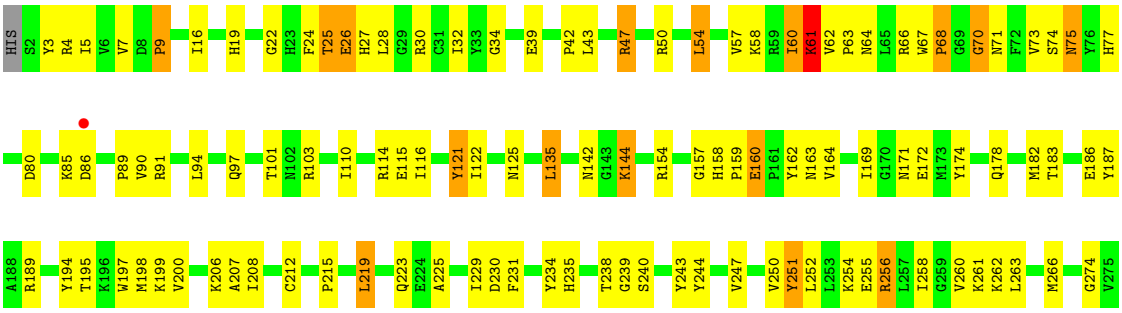
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

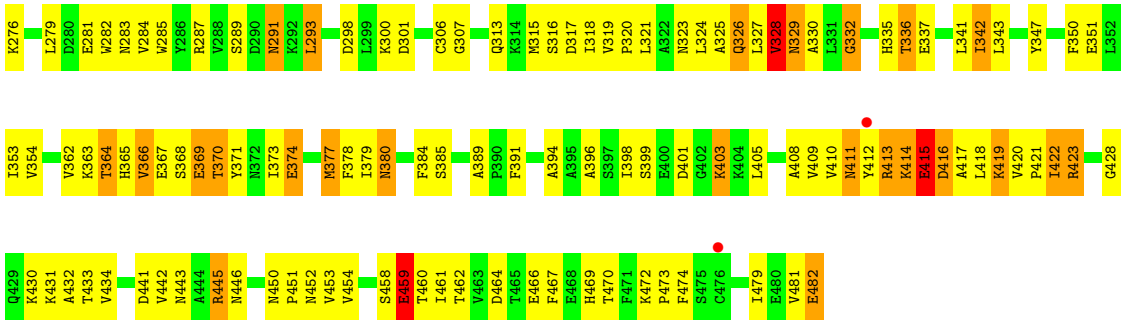
Chain A:



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

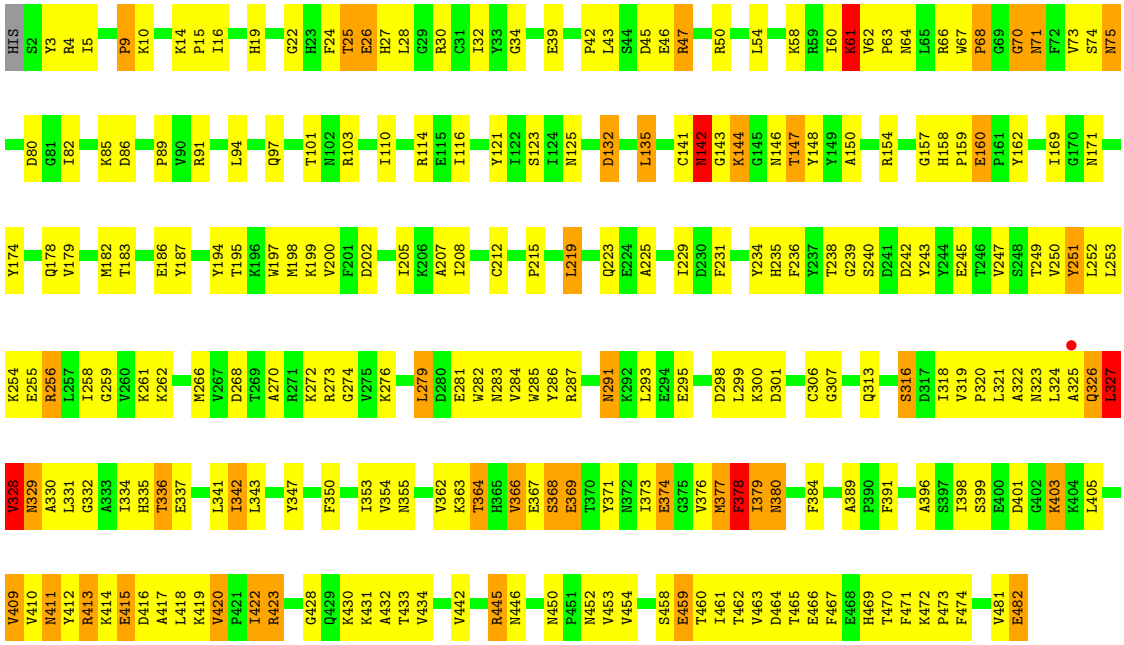
Chain B:





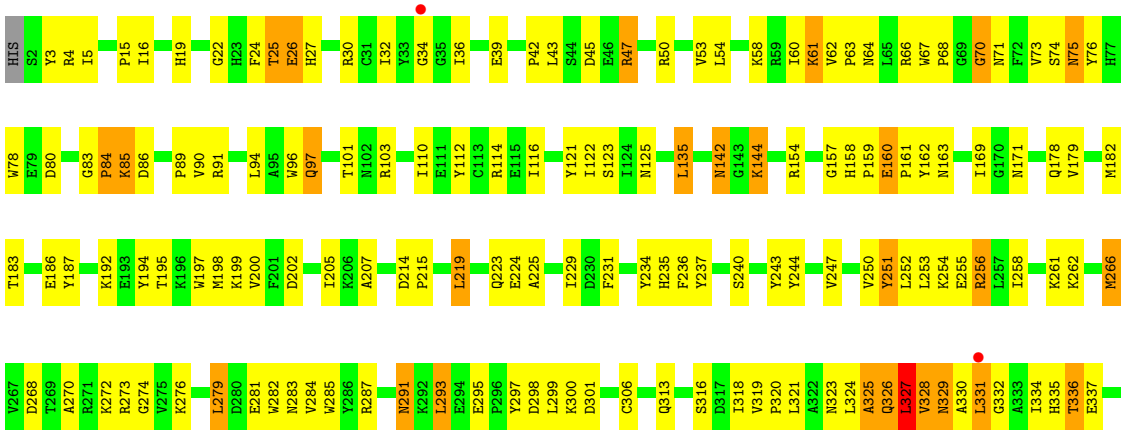
- Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

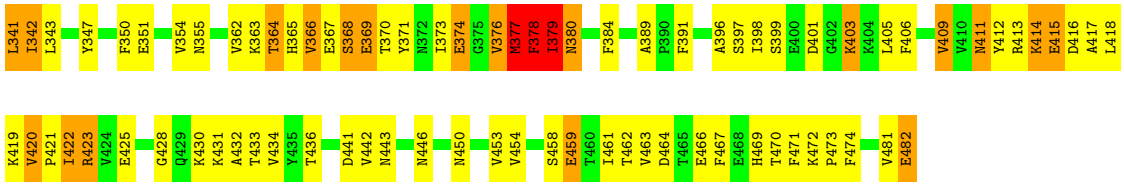
Chain C:



- Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

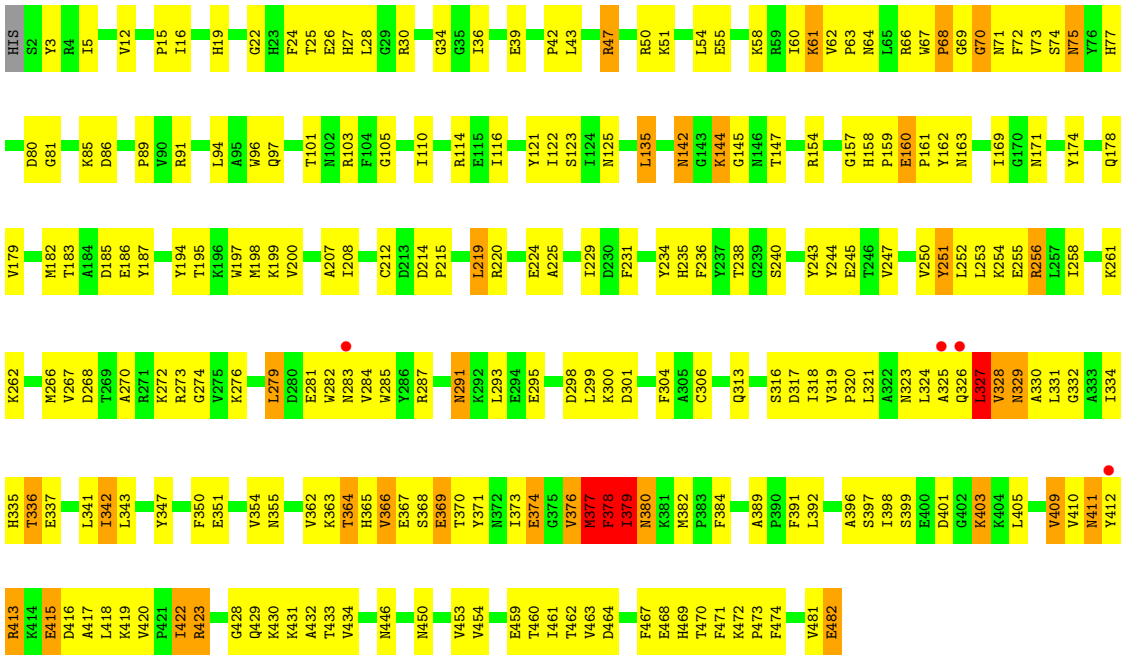
Chain D:





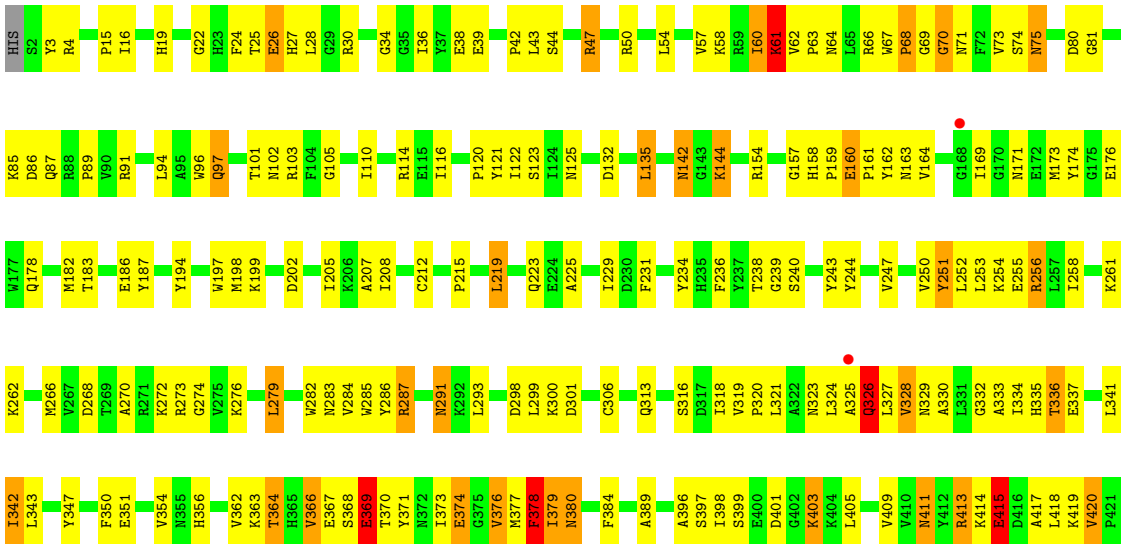
• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

Chain E:



• Molecule 1: ALPHA-L-ARABINOFURANOSIDASE DOMAIN PROTEIN

Chain F:



I422
R423
G428
Q429
K430
K431
A432
T433
V434
V442
R445
N446
N450
V453
V454
E459
T460
I461
T462
V463
D464
F467
E468
H469
T470
F471
K472
P473
F474
V478
I479
E480
V481
E482

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	103.71Å 161.54Å 112.60Å 90.00° 106.30° 90.00°	Depositor
Resolution (Å)	29.94 – 3.00 29.94 – 3.00	Depositor EDS
% Data completeness (in resolution range)	84.5 (29.94-3.00) 84.4 (29.94-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.24 (at 3.00Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.227 , 0.262 0.227 , 0.261	Depositor DCC
R_{free} test set	4430 reflections (7.37%)	wwPDB-VP
Wilson B-factor (Å^2)	45.1	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	23256	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.04	21/3971 (0.5%)	1.01	31/5383 (0.6%)
1	B	0.73	5/3971 (0.1%)	0.98	22/5383 (0.4%)
1	C	0.99	24/3971 (0.6%)	0.96	24/5383 (0.4%)
1	D	1.10	37/3971 (0.9%)	1.04	31/5383 (0.6%)
1	E	0.84	16/3971 (0.4%)	0.95	17/5383 (0.3%)
1	F	0.81	11/3971 (0.3%)	0.91	16/5383 (0.3%)
All	All	0.93	114/23826 (0.5%)	0.97	141/32298 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	1
1	F	0	3
All	All	1	9

All (114) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	328	VAL	CB-CG1	-19.15	1.12	1.52
1	A	328	VAL	CA-CB	-18.55	1.15	1.54
1	D	26	GLU	C-N	-17.58	0.93	1.34
1	A	378	PHE	CE2-CZ	-16.47	1.06	1.37
1	D	328	VAL	CB-CG2	-16.30	1.18	1.52
1	D	328	VAL	CB-CG1	-15.48	1.20	1.52
1	E	376	VAL	CA-CB	-15.41	1.22	1.54
1	A	328	VAL	CB-CG2	-14.88	1.21	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	328	VAL	CB-CG2	-14.40	1.22	1.52
1	E	378	PHE	CE2-CZ	-14.12	1.10	1.37
1	F	376	VAL	CB-CG2	-13.75	1.24	1.52
1	D	376	VAL	CB-CG2	-13.41	1.24	1.52
1	C	328	VAL	CA-CB	-13.33	1.26	1.54
1	A	377	MET	C-O	-13.32	0.98	1.23
1	C	328	VAL	CB-CG2	-13.32	1.24	1.52
1	F	376	VAL	CA-CB	-13.27	1.26	1.54
1	A	378	PHE	CD1-CE1	-12.64	1.14	1.39
1	C	147	THR	C-O	-12.14	1.00	1.23
1	B	328	VAL	CB-CG1	-12.02	1.27	1.52
1	C	368	SER	C-O	-11.99	1.00	1.23
1	C	26	GLU	C-N	-11.78	1.06	1.34
1	A	378	PHE	CD2-CE2	-11.68	1.15	1.39
1	F	369	GLU	CD-OE1	-11.34	1.13	1.25
1	F	376	VAL	CB-CG1	-11.18	1.29	1.52
1	D	377	MET	C-O	-11.17	1.02	1.23
1	E	378	PHE	CG-CD1	-11.13	1.22	1.38
1	C	328	VAL	CB-CG1	-11.03	1.29	1.52
1	C	147	THR	N-CA	-10.90	1.24	1.46
1	D	378	PHE	CD2-CE2	-10.74	1.17	1.39
1	D	328	VAL	CA-CB	-10.49	1.32	1.54
1	F	369	GLU	CB-CG	-10.18	1.32	1.52
1	D	377	MET	N-CA	-10.13	1.26	1.46
1	A	328	VAL	C-O	-9.97	1.04	1.23
1	C	414	LYS	CB-CG	-9.97	1.25	1.52
1	A	378	PHE	CE1-CZ	-9.86	1.18	1.37
1	F	376	VAL	C-O	-9.86	1.04	1.23
1	C	329	ASN	C-O	-9.85	1.04	1.23
1	A	378	PHE	CG-CD1	-9.80	1.24	1.38
1	D	370	THR	CB-CG2	-9.66	1.20	1.52
1	D	327	LEU	C-O	-9.62	1.05	1.23
1	F	369	GLU	CG-CD	-9.57	1.37	1.51
1	B	328	VAL	C-O	-9.55	1.05	1.23
1	D	378	PHE	CE1-CZ	-9.44	1.19	1.37
1	C	147	THR	CB-CG2	-9.38	1.21	1.52
1	E	378	PHE	C-O	-9.37	1.05	1.23
1	C	329	ASN	CG-OD1	-9.32	1.03	1.24
1	E	376	VAL	CB-CG1	-9.19	1.33	1.52
1	D	369	GLU	CD-OE1	-9.06	1.15	1.25
1	D	370	THR	CA-CB	-8.92	1.30	1.53
1	D	376	VAL	CB-CG1	-8.88	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	414	LYS	C-O	-8.88	1.06	1.23
1	E	378	PHE	CE1-CZ	-8.82	1.20	1.37
1	D	327	LEU	CG-CD1	-8.78	1.19	1.51
1	D	378	PHE	CD1-CE1	-8.76	1.21	1.39
1	B	328	VAL	CA-CB	-8.74	1.36	1.54
1	D	327	LEU	CG-CD2	-8.66	1.19	1.51
1	D	370	THR	C-O	-8.57	1.07	1.23
1	B	26	GLU	C-N	-8.54	1.14	1.34
1	A	378	PHE	CG-CD2	-8.44	1.26	1.38
1	C	414	LYS	CD-CE	-8.19	1.30	1.51
1	E	378	PHE	CA-C	-8.14	1.31	1.52
1	D	377	MET	CG-SD	-8.11	1.60	1.81
1	F	378	PHE	CD1-CE1	-8.10	1.23	1.39
1	D	378	PHE	C-O	-8.09	1.07	1.23
1	D	376	VAL	CA-CB	-8.01	1.38	1.54
1	C	414	LYS	CE-NZ	-8.00	1.29	1.49
1	A	378	PHE	C-O	-7.97	1.08	1.23
1	D	369	GLU	N-CA	-7.79	1.30	1.46
1	D	377	MET	CB-CG	-7.71	1.26	1.51
1	A	415	GLU	CG-CD	7.49	1.63	1.51
1	C	368	SER	CB-OG	-7.41	1.32	1.42
1	A	26	GLU	C-N	-7.38	1.17	1.34
1	F	369	GLU	C-O	-7.37	1.09	1.23
1	E	377	MET	C-O	-7.30	1.09	1.23
1	D	376	VAL	C-O	-7.14	1.09	1.23
1	E	378	PHE	CG-CD2	-7.05	1.28	1.38
1	D	328	VAL	C-O	-6.99	1.10	1.23
1	C	328	VAL	N-CA	-6.91	1.32	1.46
1	E	378	PHE	CD2-CE2	-6.83	1.25	1.39
1	A	377	MET	CG-SD	-6.80	1.63	1.81
1	D	377	MET	CA-CB	-6.79	1.39	1.53
1	E	378	PHE	CB-CG	-6.78	1.39	1.51
1	C	147	THR	CA-CB	-6.76	1.35	1.53
1	C	329	ASN	CA-C	-6.76	1.35	1.52
1	C	329	ASN	CG-ND2	-6.67	1.16	1.32
1	D	370	THR	CB-OG1	-6.57	1.30	1.43
1	E	378	PHE	CA-CB	-6.56	1.39	1.53
1	E	377	MET	CG-SD	-6.55	1.64	1.81
1	D	377	MET	CA-C	-6.54	1.35	1.52
1	C	368	SER	CA-CB	-6.52	1.43	1.52
1	F	378	PHE	CE1-CZ	-6.52	1.25	1.37
1	D	369	GLU	CD-OE2	-6.42	1.18	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	376	VAL	CB-CG2	-6.18	1.39	1.52
1	C	414	LYS	CA-CB	-6.17	1.40	1.53
1	D	329	ASN	C-O	-6.07	1.11	1.23
1	F	369	GLU	CD-OE2	-6.01	1.19	1.25
1	A	141	CYS	CB-SG	-5.81	1.72	1.81
1	D	370	THR	CA-C	-5.81	1.37	1.52
1	E	376	VAL	C-O	-5.67	1.12	1.23
1	C	328	VAL	CA-C	-5.65	1.38	1.52
1	C	329	ASN	CB-CG	-5.64	1.38	1.51
1	A	9	PRO	N-CD	-5.62	1.40	1.47
1	D	368	SER	C-N	-5.50	1.21	1.34
1	C	414	LYS	N-CA	-5.47	1.35	1.46
1	A	212	CYS	CB-SG	-5.43	1.73	1.81
1	D	378	PHE	CG-CD1	-5.41	1.30	1.38
1	A	113	CYS	CB-SG	-5.39	1.73	1.81
1	E	376	VAL	N-CA	-5.33	1.35	1.46
1	D	377	MET	SD-CE	-5.24	1.48	1.77
1	D	15	PRO	N-CD	-5.23	1.40	1.47
1	D	369	GLU	CG-CD	-5.22	1.44	1.51
1	D	376	VAL	N-CA	-5.09	1.36	1.46
1	A	377	MET	N-CA	-5.02	1.36	1.46
1	A	377	MET	CB-CG	-5.01	1.35	1.51

All (141) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	329	ASN	N-CA-C	15.22	152.09	111.00
1	D	25	THR	O-C-N	-13.37	101.31	122.70
1	A	379	ILE	CB-CA-C	-12.96	85.69	111.60
1	D	325	ALA	CB-CA-C	12.94	129.50	110.10
1	E	376	VAL	CB-CA-C	-12.41	87.82	111.40
1	E	378	PHE	N-CA-CB	-12.31	88.44	110.60
1	B	329	ASN	N-CA-CB	-12.17	88.70	110.60
1	E	377	MET	N-CA-C	12.06	143.56	111.00
1	F	328	VAL	N-CA-CB	-11.83	85.48	111.50
1	A	369	GLU	N-CA-C	-11.48	80.01	111.00
1	B	419	LYS	CB-CA-C	-11.37	87.66	110.40
1	D	25	THR	C-N-CA	10.47	147.87	121.70
1	C	9	PRO	CA-N-CD	-10.33	97.04	111.50
1	B	328	VAL	N-CA-CB	-10.31	88.81	111.50
1	C	328	VAL	N-CA-CB	-10.12	89.23	111.50
1	E	370	THR	N-CA-CB	-10.04	91.23	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	370	THR	N-CA-CB	-9.94	91.42	110.30
1	E	341	LEU	CB-CA-C	-9.92	91.36	110.20
1	D	377	MET	N-CA-C	9.88	137.69	111.00
1	B	60	ILE	N-CA-C	-9.86	84.39	111.00
1	A	9	PRO	CA-N-CD	-9.73	97.88	111.50
1	F	60	ILE	N-CA-C	-9.66	84.92	111.00
1	B	9	PRO	CA-N-CD	-9.52	98.17	111.50
1	D	341	LEU	CB-CA-C	-9.33	92.48	110.20
1	A	377	MET	N-CA-C	9.28	136.05	111.00
1	A	60	ILE	N-CA-C	-9.18	86.22	111.00
1	D	326	GLN	N-CA-CB	-9.12	94.18	110.60
1	C	25	THR	O-C-N	-9.01	108.29	122.70
1	C	377	MET	CB-CA-C	8.93	128.27	110.40
1	D	370	THR	N-CA-CB	-8.93	93.33	110.30
1	D	369	GLU	N-CA-C	-8.91	86.93	111.00
1	D	327	LEU	CA-CB-CG	8.89	135.76	115.30
1	A	413	ARG	CB-CA-C	8.89	128.18	110.40
1	E	327	LEU	N-CA-C	-8.85	87.11	111.00
1	D	15	PRO	CA-N-CD	-8.66	99.37	111.50
1	C	15	PRO	CA-N-CD	-8.64	99.40	111.50
1	E	15	PRO	CA-N-CD	-8.61	99.45	111.50
1	D	325	ALA	N-CA-C	-8.50	88.04	111.00
1	A	15	PRO	CA-N-CD	-8.49	99.61	111.50
1	B	142	ASN	N-CA-C	8.46	133.85	111.00
1	B	369	GLU	CB-CA-C	-8.46	93.48	110.40
1	E	377	MET	N-CA-CB	-8.45	95.39	110.60
1	A	326	GLN	CB-CA-C	8.42	127.25	110.40
1	E	369	GLU	CB-CA-C	-8.37	93.66	110.40
1	E	369	GLU	N-CA-C	-8.37	88.41	111.00
1	D	25	THR	CA-C-N	8.33	135.52	117.20
1	D	370	THR	CB-CA-C	-8.31	89.17	111.60
1	D	327	LEU	N-CA-C	8.27	133.32	111.00
1	D	328	VAL	CB-CA-C	-8.24	95.75	111.40
1	C	341	LEU	CB-CA-C	-8.22	94.58	110.20
1	F	341	LEU	CB-CA-C	-8.21	94.60	110.20
1	A	341	LEU	CB-CA-C	-8.16	94.70	110.20
1	D	376	VAL	CB-CA-C	-8.16	95.90	111.40
1	F	369	GLU	C-N-CA	8.13	142.02	121.70
1	A	380	ASN	N-CA-C	-8.12	89.07	111.00
1	B	415	GLU	CB-CA-C	-8.04	94.32	110.40
1	C	25	THR	C-N-CA	8.02	141.74	121.70
1	B	328	VAL	C-N-CA	-8.01	101.68	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	376	VAL	CB-CA-C	-7.99	96.22	111.40
1	C	378	PHE	N-CA-C	7.88	132.26	111.00
1	C	147	THR	OG1-CB-CG2	-7.86	91.92	110.00
1	E	142	ASN	N-CA-C	7.86	132.21	111.00
1	F	15	PRO	CA-N-CD	-7.85	100.50	111.50
1	E	329	ASN	N-CA-C	7.70	131.79	111.00
1	A	282	TRP	CB-CA-C	-7.55	95.30	110.40
1	D	326	GLN	CB-CA-C	-7.53	95.34	110.40
1	B	369	GLU	N-CA-C	-7.48	90.80	111.00
1	D	328	VAL	CG1-CB-CG2	-7.39	99.08	110.90
1	A	142	ASN	N-CA-C	7.38	130.92	111.00
1	F	378	PHE	CB-CA-C	7.36	125.11	110.40
1	B	341	LEU	CB-CA-C	-7.35	96.23	110.20
1	D	377	MET	CA-C-N	7.30	133.25	117.20
1	A	70	GLY	N-CA-C	-7.23	95.02	113.10
1	C	147	THR	CA-CB-CG2	-7.18	102.35	112.40
1	E	70	GLY	N-CA-C	-7.08	95.39	113.10
1	A	283	ASN	N-CA-CB	-6.97	98.06	110.60
1	A	377	MET	O-C-N	-6.96	111.57	122.70
1	F	142	ASN	N-CA-C	6.91	129.66	111.00
1	F	376	VAL	CB-CA-C	-6.89	98.31	111.40
1	F	415	GLU	N-CA-CB	-6.89	98.20	110.60
1	C	414	LYS	N-CA-CB	-6.86	98.25	110.60
1	F	286	TYR	CB-CA-C	6.86	124.11	110.40
1	C	14	LYS	C-N-CD	-6.77	105.70	120.60
1	A	25	THR	O-C-N	-6.77	111.87	122.70
1	D	142	ASN	N-CA-C	6.73	129.18	111.00
1	F	326	GLN	N-CA-CB	-6.68	98.58	110.60
1	A	329	ASN	N-CA-CB	6.65	122.57	110.60
1	C	70	GLY	N-CA-C	-6.64	96.51	113.10
1	C	420	VAL	N-CA-CB	-6.61	96.97	111.50
1	D	85	LYS	N-CA-C	-6.60	93.19	111.00
1	E	420	VAL	N-CA-CB	-6.59	97.00	111.50
1	A	420	VAL	N-CA-CB	-6.59	97.00	111.50
1	D	84	PRO	CB-CA-C	6.58	128.44	112.00
1	C	377	MET	N-CA-CB	-6.47	98.95	110.60
1	D	379	ILE	CB-CA-C	-6.47	98.66	111.60
1	B	70	GLY	N-CA-C	-6.46	96.96	113.10
1	F	370	THR	N-CA-CB	-6.42	98.10	110.30
1	A	379	ILE	N-CA-C	6.41	128.32	111.00
1	E	327	LEU	N-CA-CB	6.38	123.16	110.40
1	C	327	LEU	N-CA-C	6.36	128.18	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	377	MET	N-CA-CB	-6.31	99.25	110.60
1	D	70	GLY	N-CA-C	-6.25	97.47	113.10
1	D	326	GLN	N-CA-C	6.23	127.81	111.00
1	A	61	LYS	N-CA-CB	-6.22	99.41	110.60
1	B	61	LYS	N-CA-CB	-6.20	99.44	110.60
1	F	61	LYS	N-CA-CB	-6.16	99.51	110.60
1	D	420	VAL	N-CA-CB	-6.16	97.95	111.50
1	C	142	ASN	CB-CA-C	-6.15	98.10	110.40
1	A	25	THR	C-N-CA	6.05	136.82	121.70
1	A	370	THR	N-CA-CB	-5.98	98.94	110.30
1	F	287	ARG	N-CA-C	5.98	127.14	111.00
1	B	459	GLU	CB-CA-C	5.90	122.19	110.40
1	B	420	VAL	N-CA-CB	-5.87	98.58	111.50
1	D	266	MET	CG-SD-CE	5.81	109.49	100.20
1	F	70	GLY	N-CA-C	-5.80	98.60	113.10
1	D	379	ILE	N-CA-C	5.80	126.65	111.00
1	C	25	THR	CA-C-N	5.79	129.93	117.20
1	B	25	THR	C-N-CA	5.74	136.05	121.70
1	A	377	MET	CG-SD-CE	5.71	109.34	100.20
1	A	377	MET	CA-CB-CG	5.66	122.92	113.30
1	C	142	ASN	N-CA-C	5.53	125.93	111.00
1	A	14	LYS	C-N-CD	-5.44	108.64	120.60
1	F	379	ILE	N-CA-CB	-5.40	98.37	110.80
1	C	328	VAL	N-CA-C	5.40	125.58	111.00
1	A	415	GLU	OE1-CD-OE2	-5.38	116.84	123.30
1	A	413	ARG	N-CA-C	-5.33	96.61	111.00
1	B	332	GLY	N-CA-C	5.32	126.40	113.10
1	A	326	GLN	N-CA-CB	-5.31	101.05	110.60
1	D	331	LEU	N-CA-C	-5.30	96.68	111.00
1	A	378	PHE	CB-CG-CD1	5.26	124.48	120.80
1	A	414	LYS	CB-CA-C	-5.25	99.90	110.40
1	C	378	PHE	N-CA-CB	-5.23	101.18	110.60
1	A	282	TRP	N-CA-C	5.21	125.06	111.00
1	B	459	GLU	N-CA-C	-5.21	96.95	111.00
1	E	379	ILE	N-CA-C	5.20	125.05	111.00
1	B	25	THR	O-C-N	-5.16	114.44	122.70
1	D	369	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	E	329	ASN	N-CA-CB	-5.11	101.40	110.60
1	B	328	VAL	CB-CA-C	5.06	121.01	111.40
1	C	68	PRO	C-N-CA	-5.04	111.70	122.30
1	C	146	ASN	N-CA-CB	-5.01	101.59	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	377	MET	CA

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	377	MET	Mainchain
1	B	251	TYR	Sidechain
1	C	251	TYR	Sidechain
1	D	251	TYR	Sidechain
1	D	327	LEU	Mainchain
1	E	251	TYR	Sidechain
1	F	251	TYR	Sidechain
1	F	369	GLU	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3876	0	3788	292	0
1	B	3876	0	3788	290	0
1	C	3876	0	3788	276	2
1	D	3876	0	3787	308	0
1	E	3876	0	3789	300	2
1	F	3876	0	3788	302	0
All	All	23256	0	22728	1727	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (1727) 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:E:24:PHE:CD2	1:E:325:ALA:HB1	1.34	1.62
1:E:419:LYS:CG	1:E:470:THR:CG2	1.80	1.58
1:B:410:VAL:HG11	1:B:412:TYR:CZ	1.23	1.57
1:F:419:LYS:CG	1:F:470:THR:CG2	1.77	1.57
1:E:24:PHE:HD2	1:E:325:ALA:CB	1.17	1.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:LYS:CG	1:C:470:THR:CG2	1.83	1.53
1:F:24:PHE:HD2	1:F:325:ALA:CB	1.17	1.52
1:D:419:LYS:HG2	1:D:470:THR:CG2	1.40	1.51
1:E:24:PHE:CD2	1:E:325:ALA:CB	1.90	1.51
1:F:419:LYS:HG3	1:F:470:THR:CG2	1.37	1.51
1:D:419:LYS:CG	1:D:470:THR:CG2	1.89	1.50
1:A:419:LYS:CG	1:A:470:THR:CG2	1.92	1.47
1:F:24:PHE:CD2	1:F:325:ALA:CB	1.98	1.47
1:F:24:PHE:CD2	1:F:325:ALA:HB1	1.49	1.46
1:A:410:VAL:HG11	1:A:412:TYR:CZ	1.49	1.45
1:B:410:VAL:CG1	1:B:412:TYR:CZ	2.00	1.44
1:E:24:PHE:CB	1:E:325:ALA:HB2	1.49	1.40
1:B:410:VAL:HG11	1:B:412:TYR:CE2	1.55	1.40
1:E:419:LYS:HG2	1:E:470:THR:CG2	1.39	1.39
1:A:419:LYS:HG2	1:A:470:THR:CG2	1.47	1.39
1:C:419:LYS:HG3	1:C:470:THR:CG2	1.46	1.36
1:D:411:ASN:HD21	1:D:413:ARG:CB	1.39	1.35
1:C:419:LYS:HG2	1:C:470:THR:CG2	1.50	1.32
1:D:411:ASN:ND2	1:D:413:ARG:HB2	1.44	1.32
1:F:419:LYS:HG2	1:F:470:THR:CG2	1.48	1.29
1:E:24:PHE:HB3	1:E:325:ALA:CB	1.62	1.28
1:D:419:LYS:CG	1:D:470:THR:HG22	1.57	1.23
1:E:419:LYS:CG	1:E:470:THR:HG22	1.52	1.22
1:A:379:ILE:HG22	1:A:379:ILE:O	1.41	1.19
1:A:419:LYS:CG	1:A:470:THR:HG22	1.61	1.18
1:E:419:LYS:HG3	1:E:470:THR:CG2	1.51	1.17
1:A:410:VAL:CG1	1:A:412:TYR:CZ	2.26	1.17
1:A:419:LYS:HG3	1:A:470:THR:CG2	1.65	1.16
1:D:419:LYS:HG3	1:D:470:THR:CG2	1.65	1.16
1:F:481:VAL:HG22	1:F:482:GLU:H	1.12	1.15
1:B:285:TRP:CE2	1:B:379:ILE:HD11	1.81	1.14
1:F:326:GLN:NE2	1:F:330:ALA:HB3	1.59	1.14
1:B:410:VAL:CG1	1:B:412:TYR:CE1	2.30	1.14
1:F:419:LYS:CG	1:F:470:THR:HG22	1.49	1.14
1:A:410:VAL:HG11	1:A:412:TYR:CE1	1.82	1.13
1:A:239:GLY:O	1:A:377:MET:O	1.67	1.12
1:B:415:GLU:H	1:B:473:PRO:HB2	1.12	1.12
1:F:411:ASN:HD21	1:F:413:ARG:HB2	1.06	1.11
1:B:481:VAL:HG22	1:B:482:GLU:H	1.13	1.11
1:C:411:ASN:HD21	1:C:413:ARG:HB2	1.03	1.11
1:E:378:PHE:CD1	1:E:379:ILE:N	2.18	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:419:LYS:HG3	1:F:470:THR:HG21	1.29	1.10
1:C:481:VAL:HG22	1:C:482:GLU:H	1.14	1.10
1:F:24:PHE:CD2	1:F:325:ALA:HB2	1.85	1.10
1:E:24:PHE:CG	1:E:325:ALA:HB2	1.85	1.09
1:F:327:LEU:O	1:F:333:ALA:N	1.85	1.09
1:C:286:TYR:CB	1:C:378:PHE:O	2.00	1.09
1:F:326:GLN:HE22	1:F:330:ALA:HB3	0.98	1.08
1:C:419:LYS:HG3	1:C:470:THR:HG21	1.28	1.08
1:E:481:VAL:HG22	1:E:482:GLU:H	1.11	1.08
1:D:481:VAL:HG22	1:D:482:GLU:H	1.09	1.07
1:C:419:LYS:CG	1:C:470:THR:HG22	1.62	1.06
1:E:24:PHE:HB3	1:E:325:ALA:HB2	1.10	1.06
1:C:141:CYS:O	1:C:142:ASN:OD1	1.74	1.05
1:A:282:TRP:CD2	1:A:282:TRP:O	2.09	1.05
1:E:24:PHE:CG	1:E:325:ALA:CB	2.39	1.05
1:F:26:GLU:HB2	1:F:69:GLY:HA2	1.36	1.05
1:A:419:LYS:HG2	1:A:470:THR:HG23	1.11	1.04
1:A:481:VAL:HG22	1:A:482:GLU:H	1.14	1.04
1:D:135:LEU:HD21	1:F:94:LEU:HD21	1.38	1.04
1:D:414:LYS:O	1:D:473:PRO:HB2	1.57	1.03
1:E:419:LYS:HG3	1:E:470:THR:HG21	1.36	1.03
1:F:24:PHE:HB3	1:F:325:ALA:CA	1.88	1.03
1:D:419:LYS:HG2	1:D:470:THR:HG23	1.08	1.03
1:C:9:PRO:HD2	1:C:10:LYS:H	1.24	1.02
1:B:369:GLU:O	1:B:391:PHE:HD2	1.43	1.02
1:D:376:VAL:HG23	1:D:376:VAL:O	1.27	1.01
1:C:286:TYR:HB2	1:C:378:PHE:O	1.60	1.00
1:E:376:VAL:O	1:E:376:VAL:CG2	1.91	1.00
1:C:26:GLU:HB3	1:C:326:GLN:HE22	1.22	1.00
1:E:19:HIS:HD2	1:E:64:ASN:HD22	1.04	1.00
1:F:26:GLU:HB2	1:F:69:GLY:CA	1.90	1.00
1:A:419:LYS:HG3	1:A:470:THR:HG21	1.44	0.99
1:F:419:LYS:HG2	1:F:470:THR:HG23	1.01	0.99
1:F:362:VAL:O	1:F:364:THR:HG22	1.62	0.99
1:D:419:LYS:HG3	1:D:470:THR:HG21	1.43	0.98
1:E:24:PHE:HB3	1:E:325:ALA:CA	1.92	0.98
1:A:413:ARG:HD3	1:A:415:GLU:OE1	1.62	0.98
1:F:34:GLY:O	1:F:336:THR:HG21	1.63	0.98
1:E:328:VAL:HG12	1:E:329:ASN:H	1.28	0.98
1:C:328:VAL:HG12	1:C:329:ASN:N	1.77	0.98
1:C:411:ASN:ND2	1:C:413:ARG:HB2	1.77	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:PHE:O	1:D:326:GLN:HA	1.64	0.97
1:C:419:LYS:HG2	1:C:470:THR:HG23	0.98	0.97
1:C:327:LEU:HG	1:C:327:LEU:O	1.62	0.96
1:E:369:GLU:O	1:E:391:PHE:HD2	1.45	0.96
1:B:7:VAL:HG12	1:B:9:PRO:CD	1.94	0.96
1:A:410:VAL:CG1	1:A:412:TYR:CE2	2.48	0.96
1:F:239:GLY:O	1:F:377:MET:O	1.84	0.96
1:A:413:ARG:HD2	1:A:416:ASP:HB2	1.47	0.95
1:F:327:LEU:HG	1:F:328:VAL:HG23	1.45	0.95
1:C:26:GLU:HB3	1:C:326:GLN:NE2	1.81	0.95
1:F:71:ASN:HA	1:F:178:GLN:HE22	1.28	0.95
1:E:419:LYS:HG2	1:E:470:THR:HG23	0.97	0.95
1:A:380:ASN:HD22	1:A:380:ASN:N	1.60	0.95
1:B:391:PHE:CD1	1:B:413:ARG:HG3	2.02	0.95
1:B:7:VAL:HG12	1:B:9:PRO:HD3	1.45	0.95
1:B:410:VAL:CG1	1:B:412:TYR:CE2	2.37	0.95
1:E:19:HIS:CD2	1:E:64:ASN:HD22	1.83	0.95
1:C:247:VAL:O	1:C:250:VAL:HG12	1.66	0.95
1:C:19:HIS:HD2	1:C:64:ASN:HD22	1.11	0.94
1:C:446:ASN:HD21	1:C:454:VAL:H	1.13	0.94
1:C:286:TYR:HA	1:C:378:PHE:O	1.68	0.94
1:E:378:PHE:HD1	1:E:379:ILE:H	1.16	0.94
1:A:7:VAL:HG12	1:A:9:PRO:HD3	1.50	0.93
1:B:446:ASN:HD21	1:B:454:VAL:H	1.10	0.93
1:C:411:ASN:HD21	1:C:413:ARG:CB	1.81	0.93
1:A:380:ASN:H	1:A:380:ASN:ND2	1.67	0.93
1:F:326:GLN:HE22	1:F:330:ALA:CB	1.81	0.93
1:C:419:LYS:CG	1:C:470:THR:HG23	1.72	0.93
1:C:19:HIS:CD2	1:C:64:ASN:HD22	1.86	0.92
1:D:330:ALA:C	1:D:332:GLY:H	1.69	0.92
1:A:7:VAL:HG12	1:A:9:PRO:CD	1.99	0.92
1:A:19:HIS:HD2	1:A:64:ASN:HD22	1.07	0.92
1:C:24:PHE:HD2	1:C:325:ALA:O	1.50	0.92
1:E:446:ASN:HD21	1:E:454:VAL:H	1.13	0.92
1:C:60:ILE:HG13	1:C:60:ILE:O	1.68	0.92
1:D:376:VAL:O	1:D:376:VAL:CG2	2.05	0.92
1:B:378:PHE:HB3	1:B:380:ASN:ND2	1.84	0.92
1:D:411:ASN:ND2	1:D:413:ARG:H	1.68	0.92
1:C:369:GLU:O	1:C:391:PHE:HD2	1.51	0.92
1:D:19:HIS:HD2	1:D:64:ASN:HD22	1.12	0.92
1:B:34:GLY:O	1:B:336:THR:HG21	1.70	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:GLY:O	1:C:336:THR:HG21	1.70	0.91
1:C:286:TYR:CA	1:C:378:PHE:O	2.19	0.91
1:D:419:LYS:CG	1:D:470:THR:HG21	1.98	0.91
1:A:282:TRP:O	1:A:282:TRP:CE3	2.23	0.91
1:A:415:GLU:O	1:A:416:ASP:OD1	1.86	0.91
1:A:379:ILE:O	1:A:379:ILE:CG2	2.15	0.91
1:E:34:GLY:O	1:E:336:THR:HG21	1.71	0.91
1:E:376:VAL:O	1:E:376:VAL:HG23	1.10	0.91
1:F:411:ASN:ND2	1:F:413:ARG:HB2	1.86	0.91
1:E:411:ASN:HD21	1:E:413:ARG:HB2	1.34	0.91
1:F:481:VAL:HG22	1:F:482:GLU:N	1.85	0.90
1:B:410:VAL:HG12	1:B:412:TYR:CE1	2.06	0.90
1:D:326:GLN:NE2	1:D:330:ALA:HB3	1.86	0.90
1:E:328:VAL:HG12	1:E:329:ASN:N	1.86	0.90
1:F:282:TRP:CD1	1:F:323:ASN:O	2.25	0.90
1:F:19:HIS:HD2	1:F:64:ASN:HD22	1.17	0.90
1:D:411:ASN:ND2	1:D:413:ARG:N	2.19	0.90
1:F:327:LEU:HD23	1:F:327:LEU:H	1.36	0.90
1:D:411:ASN:HD21	1:D:413:ARG:HB2	0.75	0.90
1:F:24:PHE:HB3	1:F:325:ALA:HA	1.52	0.89
1:F:446:ASN:HD21	1:F:454:VAL:H	1.17	0.89
1:B:19:HIS:HD2	1:B:64:ASN:HD22	1.20	0.89
1:A:94:LEU:HD21	1:C:135:LEU:HD21	1.55	0.89
1:B:71:ASN:HA	1:B:178:GLN:HE22	1.38	0.89
1:C:141:CYS:C	1:C:142:ASN:OD1	2.11	0.89
1:A:328:VAL:HG12	1:A:329:ASN:N	1.84	0.89
1:C:411:ASN:ND2	1:C:413:ARG:H	1.70	0.88
1:A:19:HIS:CD2	1:A:64:ASN:HD22	1.91	0.88
1:E:324:LEU:HD22	1:E:350:PHE:CE1	2.08	0.88
1:E:419:LYS:CG	1:E:470:THR:HG23	1.72	0.88
1:D:34:GLY:O	1:D:336:THR:HG21	1.72	0.87
1:F:419:LYS:CG	1:F:470:THR:HG23	1.69	0.87
1:B:415:GLU:N	1:B:473:PRO:HB2	1.90	0.87
1:E:94:LEU:HD21	1:F:135:LEU:HD21	1.56	0.87
1:A:378:PHE:CG	1:A:378:PHE:O	2.25	0.87
1:D:446:ASN:HD21	1:D:454:VAL:H	1.18	0.87
1:C:401:ASP:OD2	1:C:403:LYS:HG2	1.73	0.87
1:E:419:LYS:HG3	1:E:470:THR:HG22	1.24	0.87
1:D:325:ALA:HB1	1:D:331:LEU:HD13	1.56	0.86
1:A:30:ARG:HH12	1:A:336:THR:HG22	1.40	0.86
1:F:285:TRP:CE2	1:F:379:ILE:HD11	2.10	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:LYS:HG3	1:D:470:THR:HG22	1.35	0.86
1:B:378:PHE:HB3	1:B:380:ASN:HD21	1.38	0.86
1:D:401:ASP:OD2	1:D:403:LYS:HG2	1.75	0.86
1:A:135:LEU:HD21	1:B:94:LEU:HD21	1.58	0.86
1:D:47:ARG:HH11	1:D:47:ARG:HG3	1.40	0.86
1:E:481:VAL:HG22	1:E:482:GLU:N	1.90	0.86
1:F:419:LYS:HG3	1:F:470:THR:HG22	1.10	0.86
1:C:47:ARG:HG3	1:C:47:ARG:HH11	1.41	0.86
1:C:71:ASN:HA	1:C:178:GLN:HE22	1.39	0.86
1:B:62:VAL:HG11	1:B:116:ILE:HD12	1.58	0.86
1:D:481:VAL:HG22	1:D:482:GLU:N	1.87	0.86
1:E:54:LEU:O	1:E:58:LYS:HG3	1.76	0.86
1:A:380:ASN:HD22	1:A:380:ASN:H	0.86	0.85
1:E:247:VAL:O	1:E:250:VAL:HG12	1.76	0.85
1:A:446:ASN:HD21	1:A:454:VAL:H	1.21	0.85
1:A:481:VAL:HG22	1:A:482:GLU:N	1.91	0.85
1:B:410:VAL:HB	1:B:412:TYR:CE1	2.12	0.85
1:A:282:TRP:O	1:A:282:TRP:CG	2.26	0.85
1:B:362:VAL:O	1:B:364:THR:HG22	1.76	0.85
1:A:34:GLY:O	1:A:336:THR:HG21	1.75	0.85
1:B:481:VAL:HG22	1:B:482:GLU:N	1.92	0.85
1:A:401:ASP:OD2	1:A:403:LYS:HG2	1.76	0.85
1:C:9:PRO:HD2	1:C:10:LYS:N	1.91	0.85
1:E:401:ASP:OD2	1:E:403:LYS:HG2	1.75	0.85
1:D:19:HIS:CD2	1:D:64:ASN:HD22	1.95	0.85
1:D:326:GLN:HE21	1:D:330:ALA:HB3	1.42	0.85
1:E:71:ASN:HA	1:E:178:GLN:HE22	1.42	0.85
1:B:19:HIS:CD2	1:B:64:ASN:HD22	1.94	0.84
1:F:350:PHE:O	1:F:354:VAL:HG22	1.77	0.84
1:F:19:HIS:CD2	1:F:64:ASN:HD22	1.96	0.84
1:F:415:GLU:H	1:F:415:GLU:CD	1.81	0.84
1:B:401:ASP:OD2	1:B:403:LYS:HG2	1.77	0.84
1:C:419:LYS:HG3	1:C:470:THR:HG22	1.27	0.84
1:D:26:GLU:HB3	1:D:326:GLN:OE1	1.75	0.84
1:D:42:PRO:HG2	1:D:43:LEU:HD12	1.60	0.83
1:F:401:ASP:OD2	1:F:403:LYS:HG2	1.77	0.83
1:D:334:ILE:HD11	1:D:347:TYR:CE2	2.12	0.83
1:E:328:VAL:O	1:E:332:GLY:HA3	1.77	0.83
1:F:24:PHE:HD2	1:F:325:ALA:HB1	0.68	0.83
1:A:368:SER:OG	1:A:369:GLU:O	1.95	0.83
1:D:71:ASN:HA	1:D:178:GLN:HE22	1.43	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:481:VAL:CG2	1:D:482:GLU:H	1.91	0.83
1:E:481:VAL:CG2	1:E:482:GLU:H	1.92	0.83
1:C:481:VAL:HG22	1:C:482:GLU:N	1.92	0.83
1:E:183:THR:OG1	1:E:186:GLU:HG3	1.78	0.83
1:E:324:LEU:HG	1:E:324:LEU:O	1.79	0.83
1:D:247:VAL:O	1:D:250:VAL:HG12	1.79	0.82
1:A:419:LYS:HG3	1:A:470:THR:HG22	1.35	0.82
1:E:362:VAL:O	1:E:364:THR:HG22	1.79	0.82
1:B:415:GLU:H	1:B:473:PRO:CB	1.91	0.82
1:B:481:VAL:CG2	1:B:482:GLU:H	1.92	0.82
1:F:62:VAL:HG11	1:F:116:ILE:HD12	1.61	0.82
1:A:71:ASN:HA	1:A:178:GLN:HE22	1.42	0.82
1:A:183:THR:OG1	1:A:186:GLU:HG3	1.80	0.81
1:A:481:VAL:CG2	1:A:482:GLU:H	1.93	0.81
1:E:419:LYS:CG	1:E:470:THR:HG21	1.96	0.81
1:B:247:VAL:O	1:B:250:VAL:HG12	1.80	0.81
1:E:378:PHE:CE1	1:E:379:ILE:HG13	2.15	0.81
1:F:481:VAL:CG2	1:F:482:GLU:H	1.91	0.81
1:D:325:ALA:CB	1:D:331:LEU:HD13	2.11	0.81
1:F:247:VAL:O	1:F:250:VAL:HG12	1.81	0.81
1:A:413:ARG:CD	1:A:415:GLU:OE1	2.28	0.81
1:A:419:LYS:CG	1:A:470:THR:HG21	2.02	0.81
1:D:411:ASN:HD22	1:D:413:ARG:H	1.27	0.81
1:F:24:PHE:CG	1:F:325:ALA:HB2	2.15	0.81
1:A:50:ARG:NH2	1:A:337:GLU:O	2.15	0.80
1:A:362:VAL:O	1:A:364:THR:HG22	1.82	0.80
1:C:326:GLN:HB3	1:C:330:ALA:O	1.81	0.80
1:B:410:VAL:CB	1:B:412:TYR:CE1	2.63	0.80
1:F:335:HIS:HB3	1:F:342:ILE:HG23	1.62	0.80
1:C:30:ARG:HH12	1:C:336:THR:HG22	1.46	0.80
1:B:369:GLU:O	1:B:391:PHE:CD2	2.34	0.80
1:B:410:VAL:HG12	1:B:412:TYR:CD1	2.16	0.80
1:D:362:VAL:O	1:D:364:THR:HG22	1.82	0.80
1:C:362:VAL:O	1:C:364:THR:HG22	1.81	0.79
1:F:24:PHE:CB	1:F:325:ALA:HB2	2.12	0.79
1:A:335:HIS:HB3	1:A:342:ILE:HG23	1.64	0.79
1:D:330:ALA:C	1:D:332:GLY:N	2.25	0.79
1:A:327:LEU:O	1:A:328:VAL:HG23	1.83	0.79
1:B:417:ALA:O	1:B:418:LEU:HD12	1.81	0.79
1:D:413:ARG:HG3	1:D:418:LEU:CD1	2.13	0.79
1:F:376:VAL:O	1:F:376:VAL:HG23	1.78	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:335:HIS:HB3	1:E:342:ILE:CG2	2.13	0.79
1:E:50:ARG:NH2	1:E:337:GLU:O	2.16	0.79
1:C:24:PHE:CD2	1:C:325:ALA:O	2.37	0.78
1:B:350:PHE:O	1:B:354:VAL:HG22	1.84	0.78
1:B:410:VAL:CB	1:B:412:TYR:CZ	2.65	0.78
1:F:47:ARG:HG3	1:F:47:ARG:HH11	1.49	0.78
1:A:378:PHE:C	1:A:379:ILE:HG13	2.04	0.78
1:E:42:PRO:HG2	1:E:43:LEU:HD12	1.66	0.78
1:F:411:ASN:ND2	1:F:413:ARG:H	1.81	0.78
1:B:415:GLU:HG2	1:B:416:ASP:N	1.98	0.78
1:F:4:ARG:HA	1:F:420:VAL:HG23	1.66	0.78
1:B:422:ILE:HD12	1:B:423:ARG:N	1.99	0.77
1:C:183:THR:OG1	1:C:186:GLU:HG3	1.83	0.77
1:D:413:ARG:O	1:D:473:PRO:HA	1.84	0.77
1:E:335:HIS:HB3	1:E:342:ILE:HG23	1.66	0.77
1:B:135:LEU:HD21	1:C:94:LEU:HD21	1.66	0.77
1:D:335:HIS:HB3	1:D:342:ILE:HG23	1.66	0.77
1:B:154:ARG:HG2	1:B:159:PRO:HA	1.66	0.77
1:C:239:GLY:O	1:C:377:MET:HA	1.84	0.77
1:C:350:PHE:O	1:C:354:VAL:HG22	1.85	0.77
1:A:42:PRO:HG2	1:A:43:LEU:HD12	1.67	0.77
1:A:378:PHE:O	1:A:379:ILE:HG13	1.83	0.77
1:F:369:GLU:O	1:F:369:GLU:HG2	1.84	0.77
1:A:247:VAL:O	1:A:250:VAL:HG12	1.84	0.77
1:A:350:PHE:O	1:A:354:VAL:HG22	1.84	0.77
1:D:50:ARG:NH2	1:D:337:GLU:O	2.18	0.77
1:A:47:ARG:HH11	1:A:47:ARG:HG3	1.49	0.77
1:B:239:GLY:O	1:B:377:MET:O	2.02	0.77
1:D:285:TRP:CE2	1:D:379:ILE:HD11	2.20	0.77
1:D:326:GLN:NE2	1:D:330:ALA:CB	2.48	0.77
1:E:47:ARG:HH11	1:E:47:ARG:HG3	1.50	0.77
1:D:62:VAL:HG11	1:D:116:ILE:HD12	1.67	0.77
1:D:144:LYS:H	1:D:144:LYS:HD3	1.49	0.77
1:B:285:TRP:NE1	1:B:379:ILE:HD11	1.99	0.76
1:A:378:PHE:O	1:A:379:ILE:CG1	2.33	0.76
1:E:369:GLU:O	1:E:391:PHE:CD2	2.34	0.76
1:A:335:HIS:HB3	1:A:342:ILE:CG2	2.15	0.76
1:D:417:ALA:O	1:D:418:LEU:HD12	1.85	0.76
1:F:25:THR:HG23	1:F:25:THR:O	1.85	0.76
1:A:62:VAL:HG11	1:A:116:ILE:HD12	1.67	0.76
1:A:318:ILE:HG13	1:A:319:VAL:HG23	1.68	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:THR:OG1	1:C:103:ARG:HG3	1.86	0.76
1:D:413:ARG:HG3	1:D:418:LEU:HD11	1.66	0.76
1:E:254:LYS:O	1:E:258:ILE:HG23	1.85	0.76
1:E:62:VAL:HG11	1:E:116:ILE:HD12	1.68	0.76
1:C:422:ILE:HD12	1:C:423:ARG:N	2.01	0.76
1:B:183:THR:OG1	1:B:186:GLU:HG3	1.85	0.75
1:D:335:HIS:HB3	1:D:342:ILE:CG2	2.16	0.75
1:F:16:ILE:HD13	1:F:313:GLN:HG3	1.67	0.75
1:A:410:VAL:HG12	1:A:412:TYR:CE2	2.20	0.75
1:E:24:PHE:CB	1:E:325:ALA:CB	2.28	0.75
1:B:285:TRP:CZ2	1:B:379:ILE:HD11	2.21	0.75
1:F:335:HIS:HB3	1:F:342:ILE:CG2	2.17	0.75
1:D:61:LYS:HE2	1:D:355:ASN:OD1	1.85	0.75
1:E:30:ARG:HH12	1:E:336:THR:HG22	1.50	0.75
1:A:415:GLU:O	1:A:416:ASP:CG	2.25	0.75
1:A:417:ALA:O	1:A:418:LEU:HD12	1.86	0.75
1:A:154:ARG:HG2	1:A:159:PRO:HA	1.67	0.75
1:B:318:ILE:HG13	1:B:319:VAL:HG23	1.67	0.74
1:D:411:ASN:CG	1:D:413:ARG:HB2	2.06	0.74
1:A:157:GLY:C	1:A:158:HIS:HB2	2.08	0.74
1:D:157:GLY:C	1:D:158:HIS:HB2	2.07	0.74
1:B:7:VAL:HG12	1:B:9:PRO:HD2	1.69	0.74
1:D:318:ILE:HG13	1:D:319:VAL:HG23	1.69	0.74
1:F:42:PRO:HG2	1:F:43:LEU:HD12	1.69	0.74
1:D:54:LEU:O	1:D:58:LYS:HG3	1.87	0.74
1:E:411:ASN:HD21	1:E:413:ARG:CB	1.99	0.74
1:F:154:ARG:HG2	1:F:159:PRO:HA	1.69	0.74
1:A:24:PHE:HD2	1:A:325:ALA:O	1.70	0.74
1:E:422:ILE:HD12	1:E:423:ARG:N	2.02	0.74
1:B:329:ASN:HD21	1:B:336:THR:HB	1.53	0.74
1:E:157:GLY:C	1:E:158:HIS:HB2	2.09	0.74
1:B:446:ASN:ND2	1:B:454:VAL:H	1.85	0.73
1:A:328:VAL:CG1	1:A:329:ASN:N	2.43	0.73
1:C:318:ILE:HG13	1:C:319:VAL:HG23	1.70	0.73
1:D:101:THR:OG1	1:D:103:ARG:HG3	1.88	0.73
1:E:24:PHE:HD2	1:E:325:ALA:HB1	0.64	0.73
1:E:61:LYS:HE2	1:E:355:ASN:OD1	1.88	0.73
1:E:154:ARG:HG2	1:E:159:PRO:HA	1.69	0.73
1:F:417:ALA:O	1:F:418:LEU:HD12	1.88	0.73
1:F:422:ILE:HD11	1:F:467:PHE:CE1	2.23	0.73
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.54	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ARG:NH2	1:B:337:GLU:O	2.21	0.73
1:D:325:ALA:HB1	1:D:331:LEU:CD1	2.16	0.73
1:A:23:HIS:HB3	1:A:327:LEU:HD22	1.69	0.73
1:F:30:ARG:HH12	1:F:336:THR:HG22	1.52	0.73
1:B:197:TRP:HB3	1:C:94:LEU:HD23	1.70	0.73
1:A:410:VAL:CG1	1:A:412:TYR:CE1	2.62	0.73
1:D:350:PHE:O	1:D:354:VAL:HG22	1.88	0.73
1:F:24:PHE:HD2	1:F:325:ALA:CA	2.01	0.73
1:A:26:GLU:HB3	1:A:326:GLN:NE2	2.03	0.73
1:B:419:LYS:HA	1:B:470:THR:HG22	1.71	0.73
1:E:350:PHE:O	1:E:354:VAL:HG22	1.89	0.72
1:C:16:ILE:HD13	1:C:313:GLN:HG3	1.71	0.72
1:E:318:ILE:HG13	1:E:319:VAL:HG23	1.71	0.72
1:D:282:TRP:O	1:D:324:LEU:HD12	1.89	0.72
1:E:417:ALA:O	1:E:418:LEU:HD12	1.89	0.72
1:F:24:PHE:CG	1:F:325:ALA:CB	2.72	0.72
1:F:50:ARG:NH2	1:F:337:GLU:O	2.22	0.72
1:C:335:HIS:HB3	1:C:342:ILE:CG2	2.19	0.72
1:F:26:GLU:CB	1:F:69:GLY:HA2	2.18	0.72
1:F:157:GLY:C	1:F:158:HIS:HB2	2.10	0.72
1:F:328:VAL:HG12	1:F:329:ASN:N	2.05	0.72
1:B:291:ASN:HD22	1:B:291:ASN:H	1.34	0.71
1:C:422:ILE:HD11	1:C:467:PHE:CE2	2.25	0.71
1:C:481:VAL:CG2	1:C:482:GLU:H	1.96	0.71
1:F:413:ARG:O	1:F:474:PHE:N	2.23	0.71
1:D:422:ILE:HD12	1:D:423:ARG:N	2.03	0.71
1:E:94:LEU:HD23	1:F:197:TRP:HB3	1.71	0.71
1:A:422:ILE:HD12	1:A:423:ARG:N	2.04	0.71
1:B:7:VAL:CG1	1:B:9:PRO:HD3	2.20	0.71
1:D:16:ILE:HD13	1:D:313:GLN:HG3	1.73	0.71
1:D:411:ASN:HD21	1:D:413:ARG:CA	2.03	0.71
1:C:283:ASN:HB2	1:C:325:ALA:HB2	1.73	0.71
1:D:144:LYS:HD3	1:D:144:LYS:N	2.05	0.71
1:F:24:PHE:HB3	1:F:325:ALA:CB	2.21	0.71
1:F:24:PHE:O	1:F:326:GLN:HB3	1.90	0.71
1:A:61:LYS:HE2	1:A:355:ASN:OD1	1.90	0.71
1:C:291:ASN:H	1:C:291:ASN:HD22	1.36	0.71
1:E:378:PHE:CG	1:E:379:ILE:N	2.54	0.71
1:B:157:GLY:C	1:B:158:HIS:HB2	2.11	0.71
1:B:254:LYS:O	1:B:258:ILE:HG23	1.91	0.71
1:A:24:PHE:O	1:A:326:GLN:HA	1.89	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:THR:HG23	1:B:25:THR:O	1.90	0.70
1:C:42:PRO:HG2	1:C:43:LEU:HD12	1.73	0.70
1:A:7:VAL:HG12	1:A:9:PRO:HD2	1.74	0.70
1:C:62:VAL:HG11	1:C:116:ILE:HD12	1.73	0.70
1:C:335:HIS:HB3	1:C:342:ILE:HG23	1.74	0.70
1:A:101:THR:OG1	1:A:103:ARG:HG3	1.91	0.70
1:B:414:LYS:O	1:B:414:LYS:HG2	1.91	0.70
1:F:419:LYS:CG	1:F:470:THR:HG21	1.96	0.70
1:C:417:ALA:O	1:C:418:LEU:HD12	1.91	0.70
1:C:328:VAL:CG1	1:C:329:ASN:N	2.47	0.70
1:D:291:ASN:HD22	1:D:291:ASN:H	1.37	0.70
1:B:327:LEU:C	1:B:328:VAL:HG23	2.12	0.70
1:B:415:GLU:N	1:B:473:PRO:CB	2.52	0.70
1:B:410:VAL:HG11	1:B:412:TYR:OH	1.87	0.70
1:C:328:VAL:HG12	1:C:329:ASN:H	1.57	0.70
1:E:24:PHE:CG	1:E:325:ALA:HB1	2.14	0.70
1:F:369:GLU:O	1:F:369:GLU:CG	2.33	0.70
1:D:36:ILE:HG23	1:D:328:VAL:HG21	1.73	0.69
1:E:24:PHE:HB3	1:E:325:ALA:HA	1.72	0.69
1:E:197:TRP:O	1:E:199:LYS:N	2.24	0.69
1:A:197:TRP:HB3	1:B:94:LEU:HD23	1.72	0.69
1:E:285:TRP:CE2	1:E:379:ILE:HD11	2.27	0.69
1:F:422:ILE:HD12	1:F:423:ARG:N	2.07	0.69
1:A:410:VAL:HG12	1:A:412:TYR:CD2	2.27	0.69
1:E:144:LYS:HD3	1:E:144:LYS:N	2.07	0.69
1:B:419:LYS:HG2	1:B:470:THR:CG2	2.22	0.69
1:E:25:THR:HG23	1:E:25:THR:O	1.91	0.69
1:A:234:TYR:OH	1:A:256:ARG:HG2	1.91	0.69
1:E:24:PHE:CD2	1:E:325:ALA:HB2	1.92	0.69
1:A:378:PHE:O	1:A:379:ILE:CB	2.39	0.69
1:B:54:LEU:O	1:B:58:LYS:HG3	1.92	0.69
1:C:50:ARG:NH2	1:C:337:GLU:O	2.24	0.69
1:F:70:GLY:O	1:F:73:VAL:HG12	1.93	0.69
1:A:7:VAL:CG1	1:A:9:PRO:HD3	2.23	0.69
1:A:414:LYS:O	1:A:473:PRO:CB	2.41	0.69
1:B:410:VAL:HG21	1:B:412:TYR:OH	1.92	0.69
1:D:379:ILE:HG22	1:D:379:ILE:O	1.92	0.69
1:A:422:ILE:HD11	1:A:467:PHE:CE2	2.28	0.69
1:B:42:PRO:HG2	1:B:43:LEU:HD12	1.74	0.69
1:C:197:TRP:O	1:C:199:LYS:N	2.24	0.68
1:E:422:ILE:HD11	1:E:467:PHE:CE1	2.28	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:329:ASN:HD21	1:F:336:THR:HB	1.58	0.68
1:C:432:ALA:HB2	1:C:481:VAL:HG23	1.76	0.68
1:D:234:TYR:OH	1:D:256:ARG:HG2	1.94	0.68
1:E:329:ASN:HD21	1:E:336:THR:HB	1.58	0.68
1:F:24:PHE:HB3	1:F:325:ALA:N	2.09	0.68
1:B:328:VAL:HG12	1:B:329:ASN:N	2.09	0.68
1:D:414:LYS:O	1:D:473:PRO:CB	2.36	0.68
1:A:24:PHE:CD2	1:A:325:ALA:O	2.47	0.68
1:F:110:ILE:HG13	1:F:162:TYR:CD2	2.29	0.68
1:A:291:ASN:H	1:A:291:ASN:HD22	1.41	0.68
1:B:422:ILE:HD11	1:B:467:PHE:CE2	2.28	0.68
1:C:411:ASN:HD22	1:C:413:ARG:H	1.38	0.68
1:D:328:VAL:O	1:D:329:ASN:HB2	1.92	0.68
1:B:16:ILE:HD13	1:B:313:GLN:HG3	1.76	0.68
1:B:335:HIS:HB3	1:B:342:ILE:HG23	1.76	0.68
1:F:327:LEU:H	1:F:327:LEU:CD2	2.05	0.68
1:E:245:GLU:OE1	1:E:376:VAL:HG22	1.95	0.67
1:D:154:ARG:HG2	1:D:159:PRO:HA	1.75	0.67
1:F:291:ASN:H	1:F:291:ASN:HD22	1.41	0.67
1:E:428:GLY:O	1:E:464:ASP:HA	1.95	0.67
1:F:54:LEU:O	1:F:58:LYS:HG3	1.93	0.67
1:B:194:TYR:O	1:B:198:MET:HB2	1.95	0.67
1:E:291:ASN:HD22	1:E:291:ASN:H	1.40	0.67
1:E:446:ASN:ND2	1:E:454:VAL:H	1.88	0.67
1:A:158:HIS:O	1:A:159:PRO:N	2.26	0.67
1:D:254:LYS:O	1:D:258:ILE:HG23	1.94	0.67
1:D:422:ILE:HD11	1:D:467:PHE:CE2	2.30	0.67
1:E:183:THR:HG1	1:E:186:GLU:HG3	1.59	0.67
1:A:325:ALA:O	1:A:326:GLN:HG3	1.95	0.66
1:B:414:LYS:O	1:B:415:GLU:CD	2.33	0.66
1:D:30:ARG:HH12	1:D:336:THR:HG22	1.60	0.66
1:E:24:PHE:HD2	1:E:325:ALA:HB3	1.46	0.66
1:B:335:HIS:HB3	1:B:342:ILE:CG2	2.25	0.66
1:B:26:GLU:HB3	1:B:326:GLN:NE2	2.10	0.66
1:E:250:VAL:HG13	1:E:251:TYR:CD2	2.30	0.66
1:B:62:VAL:CG1	1:B:116:ILE:HD12	2.25	0.66
1:F:183:THR:OG1	1:F:186:GLU:HG3	1.94	0.66
1:B:450:ASN:HB3	1:B:453:VAL:HG23	1.77	0.66
1:C:446:ASN:ND2	1:C:454:VAL:H	1.91	0.66
1:D:47:ARG:HG3	1:D:47:ARG:NH1	2.09	0.66
1:E:415:GLU:O	1:E:416:ASP:OD1	2.14	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:LEU:O	1:C:328:VAL:HG23	1.95	0.66
1:E:16:ILE:HD13	1:E:313:GLN:HG3	1.77	0.66
1:D:110:ILE:HG13	1:D:162:TYR:CD2	2.30	0.66
1:A:67:TRP:CD1	1:A:68:PRO:HA	2.31	0.66
1:F:101:THR:OG1	1:F:103:ARG:HG3	1.96	0.66
1:F:318:ILE:HG13	1:F:319:VAL:HG23	1.78	0.66
1:C:422:ILE:HD12	1:C:422:ILE:C	2.17	0.66
1:D:94:LEU:HD21	1:E:135:LEU:HD21	1.78	0.66
1:B:30:ARG:HH12	1:B:336:THR:HG22	1.61	0.65
1:B:158:HIS:C	1:B:159:PRO:N	2.49	0.65
1:E:36:ILE:HG23	1:E:328:VAL:HG21	1.78	0.65
1:B:197:TRP:O	1:B:199:LYS:N	2.28	0.65
1:B:67:TRP:CD1	1:B:68:PRO:HA	2.32	0.65
1:B:391:PHE:CD1	1:B:413:ARG:CG	2.78	0.65
1:A:158:HIS:C	1:A:159:PRO:N	2.50	0.65
1:E:287:ARG:NH2	1:E:301:ASP:OD2	2.26	0.65
1:E:450:ASN:HB3	1:E:453:VAL:HG23	1.78	0.65
1:A:362:VAL:HG22	1:A:396:ALA:O	1.96	0.65
1:D:194:TYR:O	1:D:198:MET:HB2	1.96	0.65
1:E:24:PHE:HB2	1:E:325:ALA:HB2	1.72	0.65
1:B:283:ASN:ND2	1:B:325:ALA:O	2.26	0.65
1:B:380:ASN:HD22	1:B:380:ASN:H	1.42	0.65
1:C:54:LEU:O	1:C:58:LYS:HG3	1.96	0.65
1:A:24:PHE:O	1:A:327:LEU:HD23	1.97	0.65
1:B:160:GLU:OE1	1:B:160:GLU:HA	1.95	0.65
1:C:282:TRP:O	1:C:324:LEU:HD12	1.96	0.65
1:C:39:GLU:OE2	1:C:103:ARG:HD3	1.96	0.65
1:C:369:GLU:O	1:C:391:PHE:CD2	2.43	0.65
1:F:419:LYS:CB	1:F:470:THR:HG22	2.26	0.65
1:A:182:MET:CE	1:A:187:TYR:HD1	2.10	0.65
1:D:368:SER:OG	1:D:369:GLU:N	2.26	0.65
1:F:234:TYR:OH	1:F:256:ARG:HG2	1.97	0.65
1:A:414:LYS:O	1:A:473:PRO:HB2	1.97	0.64
1:C:60:ILE:O	1:C:60:ILE:CG1	2.44	0.64
1:B:158:HIS:O	1:B:159:PRO:N	2.30	0.64
1:B:250:VAL:HG13	1:B:251:TYR:CD2	2.32	0.64
1:E:26:GLU:HB2	1:E:69:GLY:HA2	1.78	0.64
1:F:24:PHE:CD2	1:F:325:ALA:CA	2.78	0.64
1:A:197:TRP:O	1:A:199:LYS:N	2.29	0.64
1:E:160:GLU:OE1	1:E:160:GLU:HA	1.95	0.64
1:C:450:ASN:HB3	1:C:453:VAL:HG23	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:450:ASN:HB3	1:D:453:VAL:HG23	1.79	0.64
1:E:431:LYS:NZ	1:E:462:THR:HG22	2.13	0.64
1:A:286:TYR:HA	1:A:379:ILE:HG13	1.79	0.64
1:C:410:VAL:CG1	1:C:412:TYR:CE1	2.80	0.64
1:F:26:GLU:HB2	1:F:69:GLY:HA3	1.77	0.64
1:A:380:ASN:N	1:A:380:ASN:ND2	2.31	0.64
1:A:54:LEU:O	1:A:58:LYS:HG3	1.98	0.64
1:E:110:ILE:HG13	1:E:162:TYR:CD2	2.32	0.64
1:C:194:TYR:O	1:C:198:MET:HB2	1.97	0.64
1:C:287:ARG:NH2	1:C:301:ASP:OD2	2.28	0.64
1:C:411:ASN:HD22	1:C:411:ASN:C	2.01	0.64
1:E:432:ALA:HB2	1:E:481:VAL:HG23	1.80	0.64
1:F:24:PHE:CE2	1:F:325:ALA:HB1	2.28	0.64
1:F:325:ALA:C	1:F:326:GLN:HG3	2.18	0.64
1:C:182:MET:CE	1:C:187:TYR:HD1	2.11	0.63
1:A:16:ILE:HD13	1:A:313:GLN:HG3	1.80	0.63
1:F:285:TRP:CZ2	1:F:379:ILE:HD11	2.34	0.63
1:A:144:LYS:HD3	1:A:144:LYS:N	2.13	0.63
1:B:283:ASN:OD1	1:B:284:VAL:N	2.30	0.63
1:D:411:ASN:HD22	1:D:411:ASN:C	2.02	0.63
1:A:60:ILE:O	1:A:60:ILE:HG13	1.98	0.63
1:A:450:ASN:HB3	1:A:453:VAL:HG23	1.79	0.63
1:C:160:GLU:OE1	1:C:160:GLU:HA	1.98	0.63
1:D:183:THR:OG1	1:D:186:GLU:HG3	1.99	0.63
1:D:336:THR:CG2	1:D:337:GLU:N	2.62	0.63
1:E:70:GLY:O	1:E:73:VAL:HG12	1.98	0.63
1:E:274:GLY:O	1:E:276:LYS:HG3	1.99	0.63
1:C:254:LYS:O	1:C:258:ILE:HG23	1.98	0.63
1:A:160:GLU:OE1	1:A:160:GLU:HA	1.98	0.63
1:C:307:GLY:HA3	1:C:412:TYR:OH	1.99	0.63
1:A:446:ASN:ND2	1:A:454:VAL:H	1.94	0.63
1:B:234:TYR:OH	1:B:256:ARG:HG2	1.99	0.63
1:A:328:VAL:O	1:A:334:ILE:O	2.17	0.63
1:C:243:TYR:HA	1:C:300:LYS:HD2	1.81	0.63
1:F:24:PHE:HB3	1:F:325:ALA:HB2	1.81	0.63
1:F:160:GLU:OE1	1:F:160:GLU:HA	1.99	0.63
1:A:243:TYR:HA	1:A:300:LYS:HD2	1.81	0.62
1:E:101:THR:OG1	1:E:103:ARG:HG3	1.99	0.62
1:B:215:PRO:O	1:B:219:LEU:HB2	1.98	0.62
1:D:415:GLU:CD	1:D:415:GLU:H	2.02	0.62
1:B:328:VAL:HG12	1:B:329:ASN:H	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:ILE:HG12	1:D:343:LEU:HD22	1.79	0.62
1:B:39:GLU:OE2	1:B:103:ARG:HD3	1.99	0.62
1:E:144:LYS:HD3	1:E:144:LYS:H	1.63	0.62
1:F:450:ASN:HB3	1:F:453:VAL:HG23	1.81	0.62
1:A:286:TYR:HA	1:A:379:ILE:CG1	2.30	0.62
1:B:3:TYR:HA	1:B:367:GLU:O	2.00	0.62
1:D:282:TRP:O	1:D:282:TRP:CG	2.53	0.62
1:E:336:THR:CG2	1:E:337:GLU:N	2.62	0.62
1:A:419:LYS:CG	1:A:470:THR:HG23	1.91	0.62
1:D:419:LYS:HG2	1:D:470:THR:HG22	1.33	0.62
1:E:182:MET:CE	1:E:187:TYR:HD1	2.13	0.62
1:E:342:ILE:C	1:E:342:ILE:HD13	2.20	0.62
1:C:67:TRP:CD1	1:C:68:PRO:HA	2.35	0.62
1:C:419:LYS:CB	1:C:470:THR:HG22	2.29	0.62
1:D:432:ALA:HB2	1:D:481:VAL:HG23	1.81	0.62
1:E:285:TRP:O	1:E:378:PHE:CD1	2.53	0.62
1:A:328:VAL:HG12	1:A:329:ASN:H	1.60	0.62
1:D:160:GLU:OE1	1:D:160:GLU:HA	2.00	0.62
1:F:287:ARG:NH2	1:F:301:ASP:OD2	2.32	0.62
1:A:410:VAL:HB	1:A:412:TYR:CE2	2.35	0.61
1:B:144:LYS:HD3	1:B:144:LYS:N	2.14	0.61
1:B:364:THR:HG21	1:B:396:ALA:H	1.65	0.61
1:B:377:MET:HG2	1:B:384:PHE:HD2	1.65	0.61
1:C:9:PRO:CD	1:C:10:LYS:H	2.07	0.61
1:E:22:GLY:O	1:E:323:ASN:HA	2.00	0.61
1:E:243:TYR:HA	1:E:300:LYS:HD2	1.82	0.61
1:D:297:TYR:OH	1:D:331:LEU:HD23	2.01	0.61
1:E:194:TYR:O	1:E:198:MET:HB2	2.00	0.61
1:B:422:ILE:HD12	1:B:422:ILE:C	2.20	0.61
1:D:169:ILE:CD1	1:D:207:ALA:HB1	2.30	0.61
1:D:414:LYS:C	1:D:473:PRO:HB2	2.20	0.61
1:A:39:GLU:OE2	1:A:103:ARG:HD3	1.99	0.61
1:C:9:PRO:CD	1:C:10:LYS:N	2.63	0.61
1:D:342:ILE:C	1:D:342:ILE:HD13	2.21	0.61
1:B:22:GLY:O	1:B:323:ASN:HA	2.00	0.61
1:B:101:THR:OG1	1:B:103:ARG:HG3	1.99	0.61
1:B:414:LYS:O	1:B:415:GLU:CB	2.49	0.61
1:C:298:ASP:OD1	1:C:300:LYS:HB3	2.01	0.61
1:E:24:PHE:HD1	1:E:66:ARG:HB3	1.66	0.61
1:A:428:GLY:O	1:A:464:ASP:HA	2.00	0.61
1:B:328:VAL:O	1:B:332:GLY:HA3	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:250:VAL:HG13	1:D:251:TYR:CD2	2.36	0.61
1:D:411:ASN:ND2	1:D:413:ARG:CA	2.63	0.61
1:A:47:ARG:HG3	1:A:47:ARG:NH1	2.15	0.60
1:A:368:SER:OG	1:A:369:GLU:N	2.32	0.60
1:B:182:MET:CE	1:B:187:TYR:HD1	2.14	0.60
1:D:157:GLY:CA	1:D:158:HIS:HB2	2.31	0.60
1:B:197:TRP:HB3	1:C:94:LEU:CD2	2.31	0.60
1:F:328:VAL:O	1:F:334:ILE:O	2.19	0.60
1:C:274:GLY:O	1:C:276:LYS:HG3	2.02	0.60
1:B:428:GLY:O	1:B:464:ASP:HA	2.02	0.60
1:D:67:TRP:CD1	1:D:68:PRO:HA	2.36	0.60
1:F:231:PHE:HE2	1:F:320:PRO:HG2	1.67	0.60
1:A:194:TYR:O	1:A:198:MET:HB2	2.02	0.60
1:E:327:LEU:HG	1:E:328:VAL:HG23	1.84	0.60
1:B:419:LYS:HG2	1:B:470:THR:HG22	1.82	0.60
1:F:144:LYS:HD3	1:F:144:LYS:N	2.17	0.60
1:E:415:GLU:H	1:E:415:GLU:CD	2.05	0.60
1:F:254:LYS:O	1:F:258:ILE:HG23	2.00	0.60
1:A:70:GLY:O	1:A:73:VAL:HG12	2.00	0.60
1:B:231:PHE:HE2	1:B:320:PRO:HG2	1.66	0.60
1:D:411:ASN:HD22	1:D:413:ARG:N	1.91	0.60
1:F:67:TRP:CD1	1:F:68:PRO:HA	2.37	0.60
1:B:414:LYS:O	1:B:415:GLU:CG	2.49	0.59
1:E:24:PHE:CD2	1:E:325:ALA:HB3	2.26	0.59
1:E:47:ARG:HG3	1:E:47:ARG:NH1	2.14	0.59
1:C:336:THR:CG2	1:C:337:GLU:N	2.65	0.59
1:D:25:THR:O	1:D:25:THR:HG23	2.02	0.59
1:E:411:ASN:HD22	1:E:411:ASN:C	2.05	0.59
1:A:413:ARG:O	1:A:474:PHE:N	2.23	0.59
1:C:371:TYR:CD1	1:C:389:ALA:O	2.56	0.59
1:D:411:ASN:ND2	1:D:413:ARG:CB	2.22	0.59
1:F:26:GLU:HG3	1:F:27:HIS:N	2.17	0.59
1:C:157:GLY:C	1:C:158:HIS:HB2	2.21	0.59
1:D:158:HIS:C	1:D:159:PRO:N	2.56	0.59
1:E:234:TYR:OH	1:E:256:ARG:HG2	2.00	0.59
1:D:298:ASP:OD1	1:D:300:LYS:HB3	2.02	0.59
1:B:380:ASN:ND2	1:B:380:ASN:H	2.00	0.59
1:D:297:TYR:OH	1:D:331:LEU:CD2	2.51	0.59
1:E:283:ASN:OD1	1:E:284:VAL:N	2.34	0.59
1:A:250:VAL:HG13	1:A:251:TYR:CD2	2.38	0.59
1:D:414:LYS:HG2	1:D:415:GLU:N	2.16	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:169:ILE:CD1	1:F:207:ALA:HB1	2.33	0.59
1:A:197:TRP:HB3	1:B:94:LEU:CD2	2.33	0.59
1:C:410:VAL:HG11	1:C:412:TYR:CE1	2.38	0.59
1:D:231:PHE:HE2	1:D:320:PRO:HG2	1.68	0.59
1:D:378:PHE:CG	1:D:379:ILE:N	2.71	0.59
1:E:36:ILE:CG2	1:E:328:VAL:HG21	2.32	0.59
1:B:287:ARG:NH2	1:B:301:ASP:OD2	2.35	0.59
1:D:158:HIS:O	1:D:159:PRO:N	2.36	0.59
1:F:24:PHE:CB	1:F:325:ALA:CB	2.78	0.59
1:C:231:PHE:HE2	1:C:320:PRO:HG2	1.68	0.58
1:D:334:ILE:HD11	1:D:347:TYR:CD2	2.37	0.58
1:E:169:ILE:CD1	1:E:207:ALA:HB1	2.33	0.58
1:E:362:VAL:HG22	1:E:396:ALA:O	2.02	0.58
1:F:411:ASN:HD22	1:F:413:ARG:H	1.50	0.58
1:C:74:SER:CB	1:C:178:GLN:HE21	2.15	0.58
1:E:378:PHE:O	1:E:379:ILE:C	2.30	0.58
1:F:327:LEU:HD23	1:F:327:LEU:N	2.12	0.58
1:E:91:ARG:HH11	1:E:91:ARG:HG3	1.68	0.58
1:E:158:HIS:C	1:E:159:PRO:N	2.57	0.58
1:E:231:PHE:HE2	1:E:320:PRO:HG2	1.67	0.58
1:A:80:ASP:OD2	1:A:91:ARG:NH1	2.36	0.58
1:C:67:TRP:CG	1:C:68:PRO:HA	2.39	0.58
1:E:24:PHE:CD1	1:E:66:ARG:HB3	2.38	0.58
1:E:70:GLY:HA2	1:E:171:ASN:OD1	2.04	0.58
1:E:380:ASN:HD22	1:E:380:ASN:N	2.00	0.58
1:C:26:GLU:CB	1:C:326:GLN:HE22	2.08	0.58
1:C:154:ARG:HG2	1:C:159:PRO:HA	1.85	0.58
1:D:169:ILE:HD11	1:D:207:ALA:HB1	1.86	0.58
1:D:197:TRP:O	1:D:199:LYS:N	2.34	0.58
1:D:282:TRP:O	1:D:282:TRP:CD2	2.57	0.58
1:D:419:LYS:CG	1:D:470:THR:HG23	1.90	0.58
1:D:419:LYS:CB	1:D:470:THR:HG22	2.32	0.58
1:E:67:TRP:CD1	1:E:68:PRO:HA	2.39	0.58
1:F:282:TRP:O	1:F:324:LEU:HD12	2.03	0.58
1:B:398:ILE:HG22	1:B:399:SER:O	2.03	0.58
1:D:24:PHE:O	1:D:326:GLN:CA	2.47	0.58
1:E:26:GLU:HG2	1:E:27:HIS:N	2.17	0.58
1:E:285:TRP:O	1:E:378:PHE:HD1	1.85	0.58
1:F:158:HIS:C	1:F:159:PRO:N	2.57	0.58
1:F:158:HIS:O	1:F:159:PRO:N	2.37	0.58
1:A:25:THR:O	1:A:25:THR:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:398:ILE:HG22	1:A:399:SER:O	2.03	0.58
1:B:57:VAL:O	1:B:60:ILE:O	2.21	0.58
1:B:243:TYR:HA	1:B:300:LYS:HD2	1.84	0.58
1:D:413:ARG:O	1:D:473:PRO:CA	2.51	0.58
1:E:364:THR:HG21	1:E:396:ALA:H	1.69	0.58
1:A:391:PHE:CD1	1:A:413:ARG:HG3	2.38	0.58
1:B:169:ILE:HG22	1:B:169:ILE:O	2.03	0.58
1:D:26:GLU:HA	1:D:68:PRO:O	2.04	0.58
1:F:243:TYR:HA	1:F:300:LYS:HD2	1.85	0.58
1:A:410:VAL:CB	1:A:412:TYR:CE2	2.87	0.57
1:D:431:LYS:NZ	1:D:462:THR:HG22	2.19	0.57
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.68	0.57
1:A:169:ILE:O	1:A:169:ILE:HG22	2.04	0.57
1:B:182:MET:HB3	1:B:186:GLU:HB2	1.86	0.57
1:D:80:ASP:OD2	1:D:91:ARG:NH1	2.37	0.57
1:A:3:TYR:HA	1:A:367:GLU:O	2.05	0.57
1:B:417:ALA:C	1:B:418:LEU:HD12	2.24	0.57
1:C:47:ARG:HG3	1:C:47:ARG:NH1	2.10	0.57
1:C:91:ARG:HG3	1:C:91:ARG:HH11	1.69	0.57
1:D:274:GLY:O	1:D:276:LYS:HG3	2.04	0.57
1:D:285:TRP:CZ2	1:D:379:ILE:HD11	2.40	0.57
1:F:398:ILE:HG22	1:F:399:SER:O	2.04	0.57
1:A:70:GLY:HA2	1:A:171:ASN:OD1	2.04	0.57
1:B:336:THR:CG2	1:B:337:GLU:N	2.66	0.57
1:D:270:ALA:O	1:D:273:ARG:O	2.23	0.57
1:D:285:TRP:HB2	1:D:331:LEU:HD21	1.86	0.57
1:F:274:GLY:O	1:F:276:LYS:HG3	2.04	0.57
1:D:3:TYR:HA	1:D:367:GLU:O	2.05	0.57
1:D:19:HIS:HD2	1:D:64:ASN:ND2	1.94	0.57
1:E:19:HIS:CD2	1:E:64:ASN:ND2	2.65	0.57
1:A:342:ILE:HD13	1:A:342:ILE:C	2.25	0.57
1:B:377:MET:HG2	1:B:384:PHE:CD2	2.40	0.57
1:D:380:ASN:ND2	1:D:380:ASN:H	2.03	0.57
1:F:22:GLY:O	1:F:323:ASN:HA	2.04	0.57
1:F:328:VAL:HA	1:F:334:ILE:O	2.04	0.57
1:D:252:LEU:HD21	1:D:256:ARG:CZ	2.35	0.57
1:E:80:ASP:OD2	1:E:91:ARG:NH1	2.38	0.57
1:E:157:GLY:CA	1:E:158:HIS:HB2	2.34	0.57
1:A:231:PHE:HE2	1:A:320:PRO:HG2	1.69	0.57
1:C:380:ASN:HD22	1:C:380:ASN:N	2.02	0.57
1:F:50:ARG:O	1:F:54:LEU:HB2	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:GLY:O	1:B:158:HIS:HB2	2.03	0.57
1:B:298:ASP:OD1	1:B:300:LYS:HB3	2.05	0.57
1:B:472:LYS:HB3	1:B:473:PRO:HD2	1.87	0.57
1:C:328:VAL:O	1:C:334:ILE:O	2.22	0.57
1:C:415:GLU:OE1	1:C:415:GLU:N	2.35	0.57
1:F:194:TYR:O	1:F:198:MET:HB2	2.04	0.57
1:C:169:ILE:O	1:C:169:ILE:HG22	2.05	0.56
1:D:243:TYR:HA	1:D:300:LYS:HD2	1.87	0.56
1:A:336:THR:CG2	1:A:337:GLU:N	2.69	0.56
1:A:411:ASN:C	1:A:411:ASN:HD22	2.09	0.56
1:C:411:ASN:ND2	1:C:413:ARG:N	2.50	0.56
1:C:431:LYS:HD3	1:C:462:THR:HG22	1.86	0.56
1:D:287:ARG:NH2	1:D:301:ASP:OD2	2.35	0.56
1:F:157:GLY:CA	1:F:158:HIS:HB2	2.35	0.56
1:D:422:ILE:HD12	1:D:422:ILE:C	2.26	0.56
1:E:154:ARG:HA	1:E:158:HIS:O	2.05	0.56
1:A:376:VAL:HG12	1:A:381:LYS:O	2.05	0.56
1:C:25:THR:HG23	1:C:25:THR:O	2.04	0.56
1:C:378:PHE:CE1	1:C:379:ILE:HG12	2.40	0.56
1:F:446:ASN:ND2	1:F:454:VAL:H	1.96	0.56
1:A:62:VAL:CG1	1:A:116:ILE:HD12	2.35	0.56
1:C:24:PHE:CD1	1:C:66:ARG:HB3	2.40	0.56
1:C:169:ILE:CD1	1:C:207:ALA:HB1	2.35	0.56
1:D:70:GLY:O	1:D:73:VAL:HG12	2.05	0.56
1:E:39:GLU:OE2	1:E:103:ARG:HD3	2.05	0.56
1:E:174:TYR:CE2	1:E:212:CYS:HB3	2.41	0.56
1:C:380:ASN:ND2	1:C:380:ASN:H	2.04	0.56
1:D:157:GLY:HA3	1:D:158:HIS:ND1	2.20	0.56
1:F:24:PHE:HD1	1:F:66:ARG:HB3	1.70	0.56
1:B:285:TRP:CZ2	1:B:379:ILE:CD1	2.89	0.56
1:C:342:ILE:HD13	1:C:342:ILE:C	2.26	0.56
1:C:362:VAL:HG11	1:C:398:ILE:CD1	2.36	0.56
1:A:274:GLY:O	1:A:276:LYS:HG3	2.06	0.56
1:B:70:GLY:O	1:B:73:VAL:HG12	2.06	0.56
1:B:158:HIS:CD2	1:B:158:HIS:N	2.73	0.56
1:B:378:PHE:CE1	1:B:379:ILE:HG13	2.40	0.56
1:C:283:ASN:CB	1:C:325:ALA:HB2	2.35	0.56
1:C:291:ASN:H	1:C:291:ASN:ND2	2.04	0.56
1:E:158:HIS:O	1:E:159:PRO:N	2.39	0.56
1:E:377:MET:O	1:E:378:PHE:HB2	2.06	0.56
1:E:422:ILE:HD12	1:E:422:ILE:C	2.25	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:414:LYS:HG3	1:F:442:VAL:HG11	1.87	0.56
1:D:24:PHE:CD1	1:D:66:ARG:HB3	2.41	0.56
1:D:428:GLY:O	1:D:464:ASP:HA	2.05	0.56
1:D:39:GLU:OE2	1:D:103:ARG:HD3	2.06	0.55
1:D:179:VAL:HA	1:E:197:TRP:CZ2	2.41	0.55
1:E:328:VAL:HA	1:E:334:ILE:O	2.06	0.55
1:E:415:GLU:CD	1:E:415:GLU:N	2.60	0.55
1:E:419:LYS:CB	1:E:470:THR:HG22	2.30	0.55
1:F:47:ARG:HG3	1:F:47:ARG:NH1	2.16	0.55
1:F:71:ASN:HA	1:F:178:GLN:NE2	2.11	0.55
1:A:461:ILE:CG2	1:A:462:THR:N	2.69	0.55
1:B:60:ILE:O	1:B:60:ILE:HG13	2.07	0.55
1:C:419:LYS:CG	1:C:470:THR:HG21	1.96	0.55
1:C:431:LYS:NZ	1:C:462:THR:HG22	2.21	0.55
1:E:378:PHE:CD1	1:E:379:ILE:HG13	2.42	0.55
1:F:36:ILE:HG23	1:F:328:VAL:HG21	1.88	0.55
1:A:22:GLY:O	1:A:323:ASN:HA	2.06	0.55
1:B:291:ASN:H	1:B:291:ASN:ND2	2.03	0.55
1:C:3:TYR:HA	1:C:367:GLU:O	2.06	0.55
1:C:413:ARG:O	1:C:474:PHE:N	2.37	0.55
1:D:446:ASN:ND2	1:D:454:VAL:H	1.96	0.55
1:F:327:LEU:HG	1:F:328:VAL:CG2	2.28	0.55
1:F:366:VAL:CG2	1:F:367:GLU:N	2.69	0.55
1:D:22:GLY:O	1:D:323:ASN:HA	2.06	0.55
1:D:197:TRP:O	1:D:198:MET:HB2	2.07	0.55
1:F:283:ASN:OD1	1:F:284:VAL:N	2.37	0.55
1:F:422:ILE:HD12	1:F:422:ILE:C	2.27	0.55
1:A:24:PHE:HD1	1:A:66:ARG:HB3	1.72	0.55
1:A:30:ARG:CB	1:A:329:ASN:HD22	2.19	0.55
1:C:85:LYS:O	1:C:86:ASP:HB2	2.07	0.55
1:D:252:LEU:HD21	1:D:256:ARG:NH1	2.22	0.55
1:F:34:GLY:O	1:F:336:THR:CG2	2.45	0.55
1:F:262:LYS:O	1:F:266:MET:HG3	2.06	0.55
1:A:30:ARG:HB2	1:A:329:ASN:HD22	1.70	0.55
1:A:422:ILE:HD12	1:A:422:ILE:C	2.26	0.55
1:D:75:ASN:C	1:D:75:ASN:HD22	2.08	0.55
1:D:91:ARG:HH11	1:D:91:ARG:HG3	1.70	0.55
1:D:182:MET:HB3	1:D:186:GLU:HB2	1.88	0.55
1:E:336:THR:HG23	1:E:337:GLU:N	2.21	0.55
1:E:398:ILE:HG22	1:E:399:SER:O	2.06	0.55
1:A:67:TRP:CG	1:A:68:PRO:HA	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:VAL:O	1:E:147:THR:HA	2.07	0.55
1:D:157:GLY:O	1:D:158:HIS:HB2	2.07	0.55
1:E:3:TYR:HA	1:E:367:GLU:O	2.07	0.55
1:F:67:TRP:CG	1:F:68:PRO:HA	2.42	0.55
1:A:157:GLY:HA3	1:A:158:HIS:ND1	2.21	0.55
1:A:215:PRO:O	1:A:219:LEU:HB2	2.07	0.55
1:C:398:ILE:HG22	1:C:399:SER:O	2.07	0.55
1:D:24:PHE:HD1	1:D:66:ARG:HB3	1.71	0.55
1:A:3:TYR:OH	1:A:413:ARG:NH2	2.40	0.54
1:A:24:PHE:CD1	1:A:66:ARG:HB3	2.41	0.54
1:B:47:ARG:HG3	1:B:47:ARG:NH1	2.19	0.54
1:C:287:ARG:HB2	1:C:295:GLU:OE2	2.07	0.54
1:D:50:ARG:O	1:D:54:LEU:HB2	2.07	0.54
1:F:285:TRP:O	1:F:378:PHE:HB2	2.07	0.54
1:A:94:LEU:HD23	1:C:197:TRP:HB3	1.88	0.54
1:A:254:LYS:O	1:A:258:ILE:HG23	2.08	0.54
1:B:342:ILE:C	1:B:342:ILE:HD13	2.26	0.54
1:C:371:TYR:CE1	1:C:389:ALA:O	2.61	0.54
1:F:24:PHE:O	1:F:326:GLN:CB	2.56	0.54
1:F:182:MET:CE	1:F:187:TYR:HD1	2.20	0.54
1:F:197:TRP:O	1:F:198:MET:HB2	2.06	0.54
1:F:255:GLU:OE1	1:F:258:ILE:HD11	2.06	0.54
1:F:368:SER:OG	1:F:369:GLU:N	2.38	0.54
1:A:283:ASN:OD1	1:A:284:VAL:N	2.35	0.54
1:A:378:PHE:O	1:A:379:ILE:HB	2.07	0.54
1:B:431:LYS:NZ	1:B:462:THR:HG22	2.22	0.54
1:C:242:ASP:OD2	1:C:245:GLU:HG3	2.07	0.54
1:D:67:TRP:CG	1:D:68:PRO:HA	2.43	0.54
1:D:417:ALA:C	1:D:418:LEU:HD12	2.27	0.54
1:E:362:VAL:O	1:E:363:LYS:C	2.45	0.54
1:F:208:ILE:HD12	1:F:208:ILE:N	2.22	0.54
1:A:157:GLY:CA	1:A:158:HIS:HB2	2.36	0.54
1:B:373:ILE:HG12	1:B:374:GLU:N	2.22	0.54
1:C:195:THR:O	1:C:199:LYS:HB2	2.07	0.54
1:D:283:ASN:OD1	1:D:284:VAL:N	2.36	0.54
1:A:431:LYS:NZ	1:A:462:THR:HG22	2.23	0.54
1:B:158:HIS:C	1:B:159:PRO:CA	2.76	0.54
1:C:419:LYS:CA	1:C:470:THR:HG22	2.38	0.54
1:D:262:LYS:O	1:D:266:MET:HG3	2.07	0.54
1:D:413:ARG:O	1:D:474:PHE:N	2.37	0.54
1:E:73:VAL:HG21	1:E:123:SER:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:431:LYS:HD3	1:E:462:THR:HG22	1.89	0.54
1:F:380:ASN:HD22	1:F:380:ASN:N	2.04	0.54
1:A:19:HIS:HD2	1:A:64:ASN:ND2	1.91	0.54
1:B:289:SER:HB3	1:B:379:ILE:HG21	1.90	0.54
1:D:80:ASP:HB3	1:D:89:PRO:HG2	1.90	0.54
1:F:24:PHE:CD1	1:F:66:ARG:HB3	2.43	0.54
1:F:411:ASN:HD22	1:F:411:ASN:C	2.10	0.54
1:A:26:GLU:HB3	1:A:326:GLN:HE22	1.72	0.54
1:A:110:ILE:HG13	1:A:162:TYR:CD2	2.42	0.54
1:C:182:MET:HE1	1:C:187:TYR:HD1	1.73	0.54
1:E:291:ASN:H	1:E:291:ASN:ND2	2.05	0.54
1:F:364:THR:HG21	1:F:396:ALA:H	1.72	0.54
1:B:26:GLU:HG2	1:B:27:HIS:N	2.23	0.54
1:C:259:GLY:HA2	1:F:262:LYS:HD3	1.90	0.54
1:C:336:THR:HG23	1:C:337:GLU:N	2.23	0.54
1:D:297:TYR:OH	1:D:331:LEU:HA	2.08	0.54
1:F:36:ILE:CG2	1:F:328:VAL:HG21	2.38	0.54
1:A:262:LYS:O	1:A:266:MET:HG3	2.08	0.54
1:D:380:ASN:HD22	1:D:380:ASN:N	2.04	0.54
1:E:343:LEU:HD13	1:E:347:TYR:CE1	2.43	0.54
1:B:28:LEU:HD22	1:B:330:ALA:CB	2.38	0.53
1:F:144:LYS:HD3	1:F:144:LYS:H	1.73	0.53
1:F:219:LEU:O	1:F:223:GLN:HB2	2.08	0.53
1:F:327:LEU:O	1:F:334:ILE:N	2.36	0.53
1:A:391:PHE:CE1	1:A:413:ARG:HG3	2.43	0.53
1:F:26:GLU:CG	1:F:27:HIS:N	2.72	0.53
1:A:71:ASN:HA	1:A:178:GLN:NE2	2.20	0.53
1:A:373:ILE:HG12	1:A:374:GLU:N	2.23	0.53
1:C:431:LYS:CD	1:C:462:THR:HG22	2.37	0.53
1:D:197:TRP:HB3	1:F:94:LEU:HD23	1.89	0.53
1:D:215:PRO:O	1:D:219:LEU:HB2	2.09	0.53
1:E:328:VAL:CG1	1:E:329:ASN:N	2.60	0.53
1:E:431:LYS:CD	1:E:462:THR:HG22	2.38	0.53
1:D:336:THR:HG23	1:D:337:GLU:N	2.23	0.53
1:A:142:ASN:O	1:A:161:PRO:HB2	2.09	0.53
1:A:144:LYS:HD3	1:A:144:LYS:H	1.73	0.53
1:B:144:LYS:HD3	1:B:144:LYS:H	1.73	0.53
1:B:410:VAL:CG1	1:B:412:TYR:CD2	2.91	0.53
1:E:26:GLU:CG	1:E:27:HIS:N	2.71	0.53
1:A:182:MET:HB3	1:A:186:GLU:HB2	1.91	0.53
1:E:50:ARG:O	1:E:54:LEU:HB2	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LYS:HD3	1:A:462:THR:HG22	1.91	0.53
1:B:362:VAL:HG11	1:B:398:ILE:CD1	2.38	0.53
1:F:154:ARG:HA	1:F:158:HIS:O	2.08	0.53
1:A:225:ALA:HB1	1:A:229:ILE:HG23	1.90	0.53
1:B:208:ILE:N	1:B:208:ILE:HD12	2.24	0.53
1:D:334:ILE:HG23	1:D:343:LEU:HD23	1.91	0.53
1:E:28:LEU:HD22	1:E:330:ALA:CB	2.39	0.53
1:F:431:LYS:NZ	1:F:462:THR:HG22	2.23	0.53
1:B:431:LYS:HD3	1:B:462:THR:HG22	1.91	0.53
1:C:158:HIS:C	1:C:159:PRO:N	2.62	0.53
1:C:362:VAL:HG11	1:C:398:ILE:HD12	1.90	0.53
1:C:371:TYR:CZ	1:C:389:ALA:HB3	2.43	0.53
1:C:428:GLY:O	1:C:464:ASP:HA	2.09	0.53
1:E:67:TRP:CG	1:E:68:PRO:HA	2.43	0.53
1:F:291:ASN:HD22	1:F:291:ASN:N	2.03	0.53
1:A:283:ASN:HB2	1:A:325:ALA:HB2	1.91	0.53
1:A:287:ARG:NH2	1:A:301:ASP:OD2	2.36	0.53
1:A:405:LEU:HB3	1:A:481:VAL:CG1	2.39	0.53
1:C:413:ARG:HD2	1:C:416:ASP:HB2	1.90	0.53
1:D:75:ASN:C	1:D:75:ASN:ND2	2.60	0.53
1:D:368:SER:OG	1:D:369:GLU:O	2.26	0.53
1:E:252:LEU:HD21	1:E:256:ARG:CZ	2.38	0.53
1:F:80:ASP:OD2	1:F:91:ARG:NH1	2.42	0.53
1:F:282:TRP:O	1:F:282:TRP:CG	2.62	0.53
1:F:356:HIS:HB3	1:F:478:VAL:HG11	1.91	0.53
1:A:307:GLY:HA2	1:A:412:TYR:OH	2.09	0.52
1:E:244:TYR:HA	1:E:247:VAL:HG22	1.90	0.52
1:F:91:ARG:HG3	1:F:91:ARG:HH11	1.74	0.52
1:F:157:GLY:HA3	1:F:158:HIS:ND1	2.24	0.52
1:A:423:ARG:O	1:A:423:ARG:HG3	2.09	0.52
1:C:291:ASN:HD22	1:C:291:ASN:N	1.99	0.52
1:D:373:ILE:HG12	1:D:374:GLU:N	2.25	0.52
1:F:39:GLU:OE2	1:F:103:ARG:HD3	2.09	0.52
1:F:250:VAL:HG13	1:F:251:TYR:CD2	2.44	0.52
1:A:19:HIS:CD2	1:A:64:ASN:ND2	2.69	0.52
1:A:158:HIS:CD2	1:A:158:HIS:N	2.77	0.52
1:B:67:TRP:CG	1:B:68:PRO:HA	2.45	0.52
1:B:411:ASN:HD22	1:B:411:ASN:C	2.11	0.52
1:C:410:VAL:HG12	1:C:412:TYR:CD1	2.44	0.52
1:D:182:MET:CE	1:D:187:TYR:HD1	2.22	0.52
1:E:19:HIS:HD2	1:E:64:ASN:ND2	1.89	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:380:ASN:H	1:E:380:ASN:ND2	2.07	0.52
1:A:157:GLY:O	1:A:158:HIS:HB2	2.09	0.52
1:B:74:SER:CB	1:B:178:GLN:HE21	2.22	0.52
1:B:419:LYS:CA	1:B:470:THR:HG22	2.38	0.52
1:C:262:LYS:O	1:C:266:MET:HG3	2.10	0.52
1:C:474:PHE:O	1:C:474:PHE:CD1	2.63	0.52
1:E:240:SER:O	1:E:300:LYS:HE3	2.09	0.52
1:A:298:ASP:OD1	1:A:300:LYS:HB3	2.09	0.52
1:D:142:ASN:O	1:D:161:PRO:CB	2.58	0.52
1:E:371:TYR:CD1	1:E:389:ALA:O	2.63	0.52
1:C:80:ASP:HB3	1:C:89:PRO:HG2	1.92	0.52
1:D:364:THR:HG21	1:D:396:ALA:H	1.75	0.52
1:D:398:ILE:HG22	1:D:399:SER:O	2.10	0.52
1:A:336:THR:HG23	1:A:337:GLU:N	2.24	0.52
1:B:110:ILE:HG13	1:B:162:TYR:CD2	2.45	0.52
1:C:371:TYR:CE1	1:C:389:ALA:HB3	2.44	0.52
1:B:431:LYS:CD	1:B:462:THR:HG22	2.39	0.52
1:C:24:PHE:HD1	1:C:66:ARG:HB3	1.74	0.52
1:D:235:HIS:CD2	1:D:281:GLU:HB2	2.45	0.52
1:E:157:GLY:O	1:E:158:HIS:HB2	2.10	0.52
1:F:415:GLU:CD	1:F:415:GLU:N	2.56	0.52
1:A:376:VAL:HG11	1:A:381:LYS:HB3	1.92	0.52
1:B:307:GLY:HA2	1:B:412:TYR:OH	2.09	0.52
1:D:380:ASN:H	1:D:380:ASN:HD22	1.57	0.52
1:E:197:TRP:HA	1:E:200:VAL:HG13	1.92	0.52
1:E:380:ASN:N	1:E:380:ASN:ND2	2.58	0.52
1:C:283:ASN:HB2	1:C:325:ALA:CB	2.39	0.52
1:C:474:PHE:O	1:C:474:PHE:HD1	1.93	0.52
1:D:368:SER:HG	1:D:369:GLU:H	1.53	0.52
1:D:461:ILE:CG2	1:D:462:THR:N	2.72	0.52
1:A:461:ILE:HG22	1:A:462:THR:N	2.25	0.51
1:C:110:ILE:HG13	1:C:162:TYR:CD2	2.45	0.51
1:C:225:ALA:HB1	1:C:229:ILE:HG23	1.92	0.51
1:F:3:TYR:HA	1:F:367:GLU:O	2.11	0.51
1:F:85:LYS:O	1:F:86:ASP:HB2	2.10	0.51
1:F:432:ALA:HB2	1:F:481:VAL:HG23	1.92	0.51
1:F:472:LYS:HB3	1:F:473:PRO:HD2	1.91	0.51
1:B:80:ASP:HB3	1:B:89:PRO:HG2	1.92	0.51
1:C:26:GLU:CB	1:C:326:GLN:NE2	2.66	0.51
1:F:380:ASN:N	1:F:380:ASN:ND2	2.58	0.51
1:B:225:ALA:HB1	1:B:229:ILE:HG23	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:HIS:C	1:C:159:PRO:CA	2.79	0.51
1:C:174:TYR:CE2	1:C:212:CYS:HB3	2.46	0.51
1:C:197:TRP:HA	1:C:200:VAL:HG13	1.91	0.51
1:C:262:LYS:HD2	1:F:258:ILE:HG13	1.92	0.51
1:E:291:ASN:HD22	1:E:291:ASN:N	2.04	0.51
1:E:373:ILE:HG12	1:E:374:GLU:N	2.26	0.51
1:B:80:ASP:OD2	1:B:91:ARG:NH1	2.43	0.51
1:E:298:ASP:OD1	1:E:300:LYS:HB3	2.10	0.51
1:E:299:LEU:HD21	1:E:474:PHE:CD1	2.45	0.51
1:F:285:TRP:NE1	1:F:379:ILE:HD11	2.25	0.51
1:A:219:LEU:O	1:A:223:GLN:HB2	2.10	0.51
1:B:197:TRP:O	1:B:198:MET:HB2	2.10	0.51
1:B:380:ASN:HD22	1:B:380:ASN:N	2.01	0.51
1:C:252:LEU:HD21	1:C:256:ARG:CZ	2.40	0.51
1:C:330:ALA:C	1:C:332:GLY:N	2.62	0.51
1:D:74:SER:CB	1:D:178:GLN:HE21	2.22	0.51
1:D:419:LYS:CA	1:D:470:THR:HG22	2.41	0.51
1:E:157:GLY:HA3	1:E:158:HIS:ND1	2.25	0.51
1:E:366:VAL:CG2	1:E:367:GLU:N	2.73	0.51
1:F:282:TRP:HD1	1:F:323:ASN:O	1.87	0.51
1:B:423:ARG:HG3	1:B:423:ARG:O	2.10	0.51
1:D:326:GLN:HE22	1:D:330:ALA:CB	2.22	0.51
1:E:431:LYS:HZ3	1:E:462:THR:HG22	1.74	0.51
1:F:240:SER:O	1:F:300:LYS:HE3	2.11	0.51
1:F:327:LEU:CG	1:F:328:VAL:HG23	2.28	0.51
1:F:342:ILE:HD13	1:F:342:ILE:C	2.30	0.51
1:C:70:GLY:O	1:C:73:VAL:HG12	2.11	0.51
1:D:362:VAL:O	1:D:363:LYS:C	2.49	0.51
1:B:262:LYS:O	1:B:266:MET:HG3	2.10	0.51
1:B:362:VAL:O	1:B:363:LYS:C	2.48	0.51
1:C:26:GLU:HA	1:C:68:PRO:O	2.10	0.51
1:D:142:ASN:O	1:D:161:PRO:HB2	2.10	0.51
1:E:461:ILE:CG2	1:E:462:THR:N	2.74	0.51
1:F:291:ASN:H	1:F:291:ASN:ND2	2.08	0.51
1:F:373:ILE:HG12	1:F:374:GLU:N	2.26	0.51
1:A:182:MET:HE1	1:A:187:TYR:HD1	1.76	0.51
1:C:182:MET:HB3	1:C:186:GLU:HB2	1.92	0.51
1:E:182:MET:HB3	1:E:186:GLU:HB2	1.91	0.51
1:F:182:MET:HB3	1:F:186:GLU:HB2	1.93	0.51
1:A:85:LYS:O	1:A:86:ASP:HB2	2.11	0.51
1:A:330:ALA:C	1:A:332:GLY:N	2.61	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:410:VAL:HG11	1:A:412:TYR:OH	2.05	0.51
1:B:85:LYS:O	1:B:86:ASP:HB2	2.10	0.51
1:B:410:VAL:HG12	1:B:412:TYR:CG	2.45	0.51
1:B:474:PHE:O	1:B:474:PHE:CD1	2.64	0.51
1:C:250:VAL:HG13	1:C:251:TYR:CD2	2.46	0.51
1:C:417:ALA:C	1:C:418:LEU:HD12	2.31	0.51
1:D:19:HIS:CD2	1:D:64:ASN:ND2	2.73	0.51
1:E:74:SER:CB	1:E:178:GLN:HE21	2.24	0.51
1:E:287:ARG:HB2	1:E:295:GLU:OE2	2.11	0.51
1:E:169:ILE:HD11	1:E:207:ALA:HB1	1.93	0.50
1:F:57:VAL:O	1:F:60:ILE:O	2.29	0.50
1:F:244:TYR:HA	1:F:247:VAL:HG22	1.93	0.50
1:F:336:THR:CG2	1:F:337:GLU:N	2.74	0.50
1:F:414:LYS:O	1:F:473:PRO:HB2	2.11	0.50
1:A:235:HIS:CD2	1:A:281:GLU:HB2	2.46	0.50
1:C:70:GLY:HA2	1:C:171:ASN:OD1	2.11	0.50
1:D:342:ILE:HD13	1:D:343:LEU:N	2.27	0.50
1:E:179:VAL:HG22	1:F:197:TRP:CZ2	2.47	0.50
1:A:57:VAL:O	1:A:60:ILE:O	2.29	0.50
1:A:362:VAL:O	1:A:363:LYS:C	2.47	0.50
1:C:368:SER:OG	1:C:369:GLU:N	2.44	0.50
1:A:30:ARG:HB2	1:A:329:ASN:ND2	2.26	0.50
1:B:174:TYR:CE2	1:B:212:CYS:HB3	2.46	0.50
1:D:299:LEU:HD21	1:D:474:PHE:CD1	2.47	0.50
1:E:236:PHE:CG	1:E:253:LEU:HD13	2.46	0.50
1:B:75:ASN:ND2	1:B:75:ASN:C	2.65	0.50
1:B:291:ASN:HD22	1:B:291:ASN:N	1.98	0.50
1:B:330:ALA:C	1:B:332:GLY:N	2.63	0.50
1:C:22:GLY:O	1:C:323:ASN:HA	2.11	0.50
1:D:362:VAL:HG22	1:D:396:ALA:O	2.12	0.50
1:D:421:PRO:O	1:D:421:PRO:HG2	2.12	0.50
1:F:62:VAL:CG1	1:F:116:ILE:HD12	2.37	0.50
1:F:298:ASP:OD1	1:F:300:LYS:HB3	2.11	0.50
1:F:461:ILE:CG2	1:F:462:THR:N	2.73	0.50
1:D:158:HIS:C	1:D:159:PRO:CA	2.80	0.50
1:D:158:HIS:CD2	1:D:158:HIS:N	2.80	0.50
1:D:434:VAL:O	1:D:434:VAL:HG23	2.11	0.50
1:B:342:ILE:HD13	1:B:343:LEU:N	2.27	0.50
1:D:169:ILE:CD1	1:D:195:THR:OG1	2.60	0.50
1:E:342:ILE:HD13	1:E:343:LEU:N	2.27	0.50
1:A:50:ARG:O	1:A:54:LEU:HB2	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:LEU:HD13	1:B:347:TYR:CE1	2.47	0.50
1:C:158:HIS:N	1:C:158:HIS:CD2	2.80	0.50
1:D:154:ARG:HA	1:D:158:HIS:O	2.11	0.50
1:D:318:ILE:CG1	1:D:319:VAL:HG23	2.41	0.50
1:E:85:LYS:O	1:E:86:ASP:HB2	2.12	0.50
1:F:415:GLU:N	1:F:415:GLU:OE1	2.39	0.50
1:B:432:ALA:HB2	1:B:481:VAL:HG23	1.94	0.50
1:C:283:ASN:OD1	1:C:284:VAL:N	2.41	0.50
1:C:380:ASN:HD22	1:C:380:ASN:H	1.57	0.50
1:D:482:GLU:OE1	1:D:482:GLU:O	2.30	0.50
1:E:279:LEU:HD22	1:E:282:TRP:HB3	1.94	0.50
1:F:239:GLY:N	1:F:377:MET:O	2.44	0.50
1:B:474:PHE:O	1:B:474:PHE:HD1	1.95	0.49
1:E:70:GLY:HA2	1:E:171:ASN:CG	2.33	0.49
1:E:94:LEU:CD2	1:F:197:TRP:HB3	2.39	0.49
1:E:417:ALA:C	1:E:418:LEU:HD12	2.32	0.49
1:B:446:ASN:HD21	1:B:454:VAL:N	1.93	0.49
1:C:411:ASN:ND2	1:C:411:ASN:C	2.66	0.49
1:C:423:ARG:HG3	1:C:423:ARG:O	2.11	0.49
1:E:324:LEU:HD22	1:E:350:PHE:HE1	1.72	0.49
1:F:74:SER:CB	1:F:178:GLN:HE21	2.25	0.49
1:A:132:ASP:OD2	1:B:77:HIS:CE1	2.65	0.49
1:C:236:PHE:CG	1:C:253:LEU:HD13	2.47	0.49
1:F:28:LEU:HD22	1:F:330:ALA:CB	2.43	0.49
1:F:158:HIS:C	1:F:159:PRO:CA	2.80	0.49
1:F:169:ILE:HD11	1:F:207:ALA:HB1	1.94	0.49
1:F:417:ALA:C	1:F:418:LEU:HD12	2.32	0.49
1:A:158:HIS:C	1:A:159:PRO:CA	2.81	0.49
1:C:73:VAL:O	1:C:125:ASN:HB2	2.11	0.49
1:C:270:ALA:O	1:C:273:ARG:O	2.30	0.49
1:A:432:ALA:HB2	1:A:481:VAL:HG23	1.93	0.49
1:D:334:ILE:HD11	1:D:347:TYR:HE2	1.69	0.49
1:F:428:GLY:O	1:F:464:ASP:HA	2.12	0.49
1:C:238:THR:O	1:C:284:VAL:HA	2.12	0.49
1:C:366:VAL:CG2	1:C:367:GLU:N	2.76	0.49
1:D:70:GLY:HA2	1:D:171:ASN:OD1	2.12	0.49
1:D:328:VAL:O	1:D:328:VAL:HG12	1.96	0.49
1:E:169:ILE:HG22	1:E:169:ILE:O	2.11	0.49
1:A:376:VAL:CG1	1:A:381:LYS:O	2.60	0.49
1:E:423:ARG:HG3	1:E:423:ARG:O	2.11	0.49
1:F:252:LEU:HD12	1:F:384:PHE:CD1	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASN:C	1:B:75:ASN:HD22	2.16	0.49
1:B:91:ARG:HH11	1:B:91:ARG:HG3	1.78	0.49
1:B:169:ILE:CD1	1:B:207:ALA:HB1	2.43	0.49
1:B:328:VAL:O	1:B:332:GLY:CA	2.61	0.49
1:C:154:ARG:HA	1:C:158:HIS:O	2.12	0.49
1:D:327:LEU:HG	1:D:328:VAL:HG23	1.94	0.49
1:D:472:LYS:HB3	1:D:473:PRO:HD2	1.95	0.49
1:A:431:LYS:HZ3	1:A:462:THR:HG22	1.78	0.49
1:B:252:LEU:HD13	1:B:377:MET:HE1	1.95	0.49
1:C:157:GLY:HA3	1:C:158:HIS:ND1	2.28	0.49
1:D:219:LEU:O	1:D:223:GLN:HB2	2.13	0.49
1:F:255:GLU:O	1:F:258:ILE:HG12	2.12	0.49
1:A:142:ASN:O	1:A:161:PRO:CB	2.61	0.49
1:C:28:LEU:HD22	1:C:330:ALA:CB	2.42	0.49
1:C:169:ILE:CD1	1:C:195:THR:OG1	2.61	0.49
1:E:158:HIS:C	1:E:159:PRO:CA	2.81	0.49
1:E:225:ALA:HB1	1:E:229:ILE:HG23	1.95	0.49
1:F:376:VAL:H	1:F:376:VAL:HG22	1.29	0.49
1:B:379:ILE:HG22	1:B:379:ILE:O	2.13	0.48
1:C:26:GLU:HG2	1:C:27:HIS:N	2.27	0.48
1:D:225:ALA:HB1	1:D:229:ILE:HG23	1.95	0.48
1:E:330:ALA:C	1:E:332:GLY:N	2.66	0.48
1:F:70:GLY:HA2	1:F:171:ASN:OD1	2.12	0.48
1:F:343:LEU:HD13	1:F:347:TYR:CE1	2.47	0.48
1:A:364:THR:HG21	1:A:396:ALA:H	1.78	0.48
1:B:26:GLU:CG	1:B:27:HIS:N	2.75	0.48
1:E:411:ASN:C	1:E:411:ASN:ND2	2.67	0.48
1:C:258:ILE:HG13	1:F:262:LYS:HD2	1.95	0.48
1:C:327:LEU:O	1:C:327:LEU:CG	2.45	0.48
1:D:297:TYR:HH	1:D:331:LEU:CD2	2.26	0.48
1:D:411:ASN:ND2	1:D:411:ASN:C	2.66	0.48
1:F:75:ASN:C	1:F:75:ASN:ND2	2.66	0.48
1:F:419:LYS:CA	1:F:470:THR:HG22	2.43	0.48
1:A:366:VAL:CG2	1:A:367:GLU:N	2.76	0.48
1:B:461:ILE:CG2	1:B:462:THR:N	2.75	0.48
1:C:343:LEU:HD13	1:C:347:TYR:CE1	2.49	0.48
1:D:291:ASN:N	1:D:291:ASN:ND2	2.61	0.48
1:E:335:HIS:O	1:E:342:ILE:HG22	2.13	0.48
1:F:380:ASN:ND2	1:F:380:ASN:H	2.11	0.48
1:E:419:LYS:CA	1:E:470:THR:HG22	2.44	0.48
1:A:60:ILE:O	1:A:60:ILE:CG1	2.61	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:LYS:CD	1:A:462:THR:HG22	2.43	0.48
1:A:434:VAL:O	1:A:434:VAL:HG23	2.14	0.48
1:A:472:LYS:HB3	1:A:473:PRO:HD2	1.96	0.48
1:B:318:ILE:CG1	1:B:319:VAL:HG23	2.39	0.48
1:D:287:ARG:HB2	1:D:295:GLU:OE2	2.13	0.48
1:D:379:ILE:O	1:D:379:ILE:CG2	2.61	0.48
1:E:235:HIS:CD2	1:E:281:GLU:HB2	2.49	0.48
1:F:157:GLY:O	1:F:158:HIS:HB2	2.13	0.48
1:F:431:LYS:HD3	1:F:462:THR:HG22	1.94	0.48
1:B:481:VAL:CG2	1:B:482:GLU:N	2.63	0.48
1:D:22:GLY:HA2	1:D:63:PRO:HD2	1.96	0.48
1:D:73:VAL:HG21	1:D:123:SER:O	2.14	0.48
1:E:197:TRP:C	1:E:199:LYS:N	2.66	0.48
1:F:24:PHE:CB	1:F:325:ALA:HA	2.35	0.48
1:F:197:TRP:O	1:F:199:LYS:N	2.41	0.48
1:A:197:TRP:O	1:A:198:MET:HB2	2.12	0.48
1:A:419:LYS:CB	1:A:470:THR:HG22	2.36	0.48
1:C:169:ILE:HD12	1:C:207:ALA:HB1	1.95	0.48
1:D:291:ASN:H	1:D:291:ASN:ND2	2.06	0.48
1:F:461:ILE:HD11	1:F:469:HIS:CE1	2.48	0.48
1:A:238:THR:O	1:A:284:VAL:HA	2.13	0.48
1:B:4:ARG:HH11	1:B:4:ARG:HG3	1.79	0.48
1:E:73:VAL:O	1:E:125:ASN:HB2	2.13	0.48
1:F:60:ILE:O	1:F:60:ILE:HG13	2.13	0.48
1:F:158:HIS:N	1:F:158:HIS:CD2	2.82	0.48
1:A:236:PHE:CG	1:A:253:LEU:HD13	2.49	0.47
1:B:377:MET:SD	1:B:384:PHE:HB3	2.53	0.47
1:B:434:VAL:CG1	1:B:479:ILE:HG12	2.44	0.47
1:D:431:LYS:HD3	1:D:462:THR:HG22	1.96	0.47
1:F:279:LEU:HD22	1:F:282:TRP:HB3	1.95	0.47
1:B:410:VAL:HB	1:B:412:TYR:HE1	1.76	0.47
1:C:262:LYS:CD	1:F:258:ILE:HG13	2.44	0.47
1:D:144:LYS:N	1:D:144:LYS:CD	2.71	0.47
1:D:380:ASN:ND2	1:D:380:ASN:N	2.62	0.47
1:E:279:LEU:CD2	1:E:282:TRP:HB3	2.43	0.47
1:B:378:PHE:CG	1:B:379:ILE:N	2.81	0.47
1:F:431:LYS:CD	1:F:462:THR:HG22	2.44	0.47
1:A:419:LYS:CA	1:A:470:THR:HG22	2.44	0.47
1:C:373:ILE:HG12	1:C:374:GLU:N	2.29	0.47
1:C:415:GLU:N	1:C:415:GLU:CD	2.67	0.47
1:D:71:ASN:OD1	1:D:71:ASN:N	2.43	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:TRP:NE1	1:D:379:ILE:HD11	2.29	0.47
1:D:343:LEU:HD13	1:D:347:TYR:CE1	2.50	0.47
1:E:255:GLU:O	1:E:258:ILE:HG12	2.14	0.47
1:F:434:VAL:HG12	1:F:479:ILE:HG12	1.96	0.47
1:A:26:GLU:HG2	1:A:27:HIS:N	2.27	0.47
1:B:274:GLY:O	1:B:276:LYS:HG3	2.14	0.47
1:C:70:GLY:HA2	1:C:171:ASN:CG	2.34	0.47
1:C:291:ASN:ND2	1:C:291:ASN:N	2.61	0.47
1:E:25:THR:O	1:E:25:THR:CG2	2.61	0.47
1:E:197:TRP:O	1:E:198:MET:HB2	2.14	0.47
1:B:24:PHE:CD1	1:B:66:ARG:HB3	2.50	0.47
1:B:244:TYR:HA	1:B:247:VAL:HG22	1.95	0.47
1:B:336:THR:HG23	1:B:337:GLU:N	2.29	0.47
1:C:197:TRP:O	1:C:198:MET:HB2	2.14	0.47
1:C:364:THR:HG21	1:C:396:ALA:H	1.80	0.47
1:E:158:HIS:N	1:E:158:HIS:CD2	2.83	0.47
1:F:252:LEU:HD21	1:F:256:ARG:CZ	2.45	0.47
1:B:197:TRP:HA	1:B:200:VAL:HG13	1.96	0.47
1:B:235:HIS:CD2	1:B:281:GLU:HB2	2.49	0.47
1:C:472:LYS:HB3	1:C:473:PRO:HD2	1.97	0.47
1:D:419:LYS:HE2	1:D:419:LYS:HB3	1.68	0.47
1:E:75:ASN:ND2	1:E:75:ASN:C	2.68	0.47
1:F:120:PRO:HG2	1:F:164:VAL:HG13	1.97	0.47
1:A:214:ASP:C	1:A:214:ASP:OD1	2.53	0.47
1:C:464:ASP:O	1:C:466:GLU:N	2.47	0.47
1:D:268:ASP:O	1:D:272:LYS:HD3	2.15	0.47
1:E:75:ASN:C	1:E:75:ASN:HD22	2.18	0.47
1:E:285:TRP:CZ2	1:E:379:ILE:HD11	2.49	0.47
1:E:419:LYS:HE2	1:E:419:LYS:HB3	1.59	0.47
1:F:225:ALA:HB1	1:F:229:ILE:HG23	1.96	0.47
1:A:328:VAL:O	1:A:328:VAL:HG13	1.95	0.47
1:B:240:SER:O	1:B:300:LYS:HE3	2.14	0.47
1:C:27:HIS:CD2	1:C:32:ILE:HG13	2.50	0.47
1:E:142:ASN:O	1:E:161:PRO:HB2	2.15	0.47
1:E:182:MET:HE1	1:E:187:TYR:HD1	1.79	0.47
1:F:252:LEU:HD21	1:F:256:ARG:NH1	2.30	0.47
1:F:268:ASP:O	1:F:272:LYS:HD3	2.15	0.47
1:F:330:ALA:C	1:F:332:GLY:N	2.67	0.47
1:A:85:LYS:O	1:A:87:GLN:N	2.43	0.47
1:B:378:PHE:CD1	1:B:379:ILE:N	2.80	0.47
1:C:50:ARG:O	1:C:54:LEU:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:169:ILE:HD13	1:D:195:THR:OG1	2.14	0.47
1:E:362:VAL:HG11	1:E:398:ILE:CD1	2.45	0.47
1:F:142:ASN:O	1:F:161:PRO:HB2	2.15	0.47
1:C:147:THR:O	1:C:148:TYR:C	2.48	0.46
1:C:235:HIS:CD2	1:C:281:GLU:HB2	2.50	0.46
1:C:419:LYS:HB3	1:C:419:LYS:HE2	1.70	0.46
1:D:244:TYR:HA	1:D:247:VAL:HG22	1.97	0.46
1:D:279:LEU:CD2	1:D:282:TRP:HB3	2.45	0.46
1:D:419:LYS:HA	1:D:470:THR:HG22	1.97	0.46
1:E:215:PRO:O	1:E:219:LEU:HB2	2.15	0.46
1:A:25:THR:HG22	1:A:66:ARG:O	2.15	0.46
1:C:268:ASP:O	1:C:272:LYS:HD3	2.16	0.46
1:C:419:LYS:HA	1:C:470:THR:HG22	1.98	0.46
1:D:94:LEU:HD23	1:E:197:TRP:HB3	1.97	0.46
1:F:445:ARG:HH11	1:F:445:ARG:HG3	1.79	0.46
1:F:461:ILE:HG22	1:F:462:THR:N	2.30	0.46
1:A:147:THR:HA	1:B:90:VAL:HG12	1.97	0.46
1:A:169:ILE:HD13	1:A:195:THR:OG1	2.15	0.46
1:A:252:LEU:HD21	1:A:256:ARG:CZ	2.45	0.46
1:C:215:PRO:HG3	1:F:266:MET:HB3	1.96	0.46
1:D:255:GLU:OE1	1:D:258:ILE:HD11	2.15	0.46
1:D:423:ARG:O	1:D:423:ARG:HG3	2.15	0.46
1:E:77:HIS:CE1	1:F:132:ASP:OD2	2.68	0.46
1:F:75:ASN:C	1:F:75:ASN:HD22	2.18	0.46
1:F:142:ASN:O	1:F:161:PRO:CB	2.64	0.46
1:A:25:THR:HB	1:A:65:LEU:HD11	1.98	0.46
1:A:174:TYR:CE2	1:A:212:CYS:HB3	2.50	0.46
1:B:328:VAL:CG1	1:B:329:ASN:N	2.77	0.46
1:B:414:LYS:O	1:B:415:GLU:HB3	2.15	0.46
1:C:45:ASP:OD2	1:C:47:ARG:NH1	2.49	0.46
1:D:251:TYR:HE2	1:D:412:TYR:HH	1.61	0.46
1:E:125:ASN:C	1:E:125:ASN:OD1	2.54	0.46
1:E:214:ASP:C	1:E:214:ASP:OD1	2.54	0.46
1:A:24:PHE:HB3	1:A:325:ALA:O	2.15	0.46
1:A:417:ALA:C	1:A:418:LEU:HD12	2.35	0.46
1:A:445:ARG:HG3	1:A:445:ARG:HH11	1.80	0.46
1:B:50:ARG:O	1:B:54:LEU:HB2	2.15	0.46
1:C:158:HIS:O	1:C:159:PRO:N	2.48	0.46
1:E:185:ASP:OD1	1:E:220:ARG:HD3	2.15	0.46
1:E:285:TRP:NE1	1:E:379:ILE:HD11	2.31	0.46
1:A:43:LEU:HD12	1:A:43:LEU:N	2.31	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLY:O	1:B:377:MET:HA	2.15	0.46
1:B:366:VAL:CG2	1:B:367:GLU:N	2.78	0.46
1:C:143:GLY:O	1:C:150:ALA:HB1	2.15	0.46
1:D:27:HIS:CD2	1:D:32:ILE:HG13	2.50	0.46
1:D:405:LEU:HG	1:D:406:PHE:N	2.29	0.46
1:D:409:VAL:HG21	1:D:471:PHE:CE2	2.50	0.46
1:D:461:ILE:HG22	1:D:462:THR:N	2.30	0.46
1:E:51:LYS:O	1:E:55:GLU:HG3	2.16	0.46
1:F:326:GLN:NE2	1:F:330:ALA:CB	2.52	0.46
1:A:239:GLY:O	1:A:377:MET:HA	2.15	0.46
1:B:24:PHE:HD1	1:B:66:ARG:HB3	1.80	0.46
1:B:154:ARG:HA	1:B:158:HIS:O	2.15	0.46
1:C:4:ARG:HG3	1:C:4:ARG:HH11	1.80	0.46
1:C:169:ILE:HD13	1:C:195:THR:OG1	2.15	0.46
1:D:83:GLY:C	1:D:84:PRO:O	2.52	0.46
1:D:291:ASN:HD22	1:D:291:ASN:N	1.98	0.46
1:B:5:ILE:HG22	1:B:366:VAL:HG23	1.97	0.46
1:C:285:TRP:CD1	1:C:285:TRP:C	2.88	0.46
1:C:410:VAL:HG11	1:C:412:TYR:CZ	2.50	0.46
1:D:283:ASN:HB2	1:D:325:ALA:HB3	1.98	0.46
1:F:60:ILE:HG22	1:F:351:GLU:HA	1.97	0.46
1:F:327:LEU:HG	1:F:328:VAL:N	2.31	0.46
1:A:343:LEU:HD13	1:A:347:TYR:CE1	2.51	0.46
1:A:450:ASN:C	1:A:452:ASN:H	2.20	0.46
1:B:144:LYS:N	1:B:144:LYS:CD	2.78	0.46
1:D:157:GLY:HA3	1:D:158:HIS:HB2	1.97	0.46
1:D:330:ALA:O	1:D:332:GLY:N	2.49	0.46
1:F:80:ASP:HB3	1:F:89:PRO:HG2	1.98	0.46
1:F:362:VAL:HG22	1:F:396:ALA:O	2.16	0.46
1:F:434:VAL:CG1	1:F:479:ILE:HG12	2.46	0.46
1:A:410:VAL:CB	1:A:412:TYR:CZ	2.95	0.46
1:B:169:ILE:CD1	1:B:195:THR:OG1	2.64	0.46
1:D:255:GLU:O	1:D:258:ILE:HG12	2.15	0.46
1:D:434:VAL:O	1:D:434:VAL:CG2	2.63	0.46
1:A:307:GLY:CA	1:A:412:TYR:OH	2.63	0.45
1:B:329:ASN:ND2	1:B:336:THR:HB	2.27	0.45
1:B:368:SER:OG	1:B:369:GLU:N	2.50	0.45
1:C:279:LEU:HD22	1:C:282:TRP:HB3	1.99	0.45
1:C:330:ALA:O	1:C:331:LEU:C	2.55	0.45
1:C:445:ARG:HH11	1:C:445:ARG:HG3	1.81	0.45
1:D:73:VAL:O	1:D:125:ASN:HB2	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:27:HIS:HB2	1:E:72:PHE:CD2	2.50	0.45
1:E:240:SER:HB2	1:E:376:VAL:CG2	2.46	0.45
1:F:169:ILE:O	1:F:169:ILE:HG22	2.16	0.45
1:F:384:PHE:CD1	1:F:384:PHE:C	2.90	0.45
1:A:77:HIS:CE1	1:C:132:ASP:OD2	2.68	0.45
1:A:169:ILE:CD1	1:A:207:ALA:HB1	2.47	0.45
1:A:416:ASP:H	1:A:473:PRO:HB3	1.81	0.45
1:A:419:LYS:HE2	1:A:419:LYS:HB3	1.72	0.45
1:A:474:PHE:CD1	1:A:474:PHE:O	2.69	0.45
1:C:378:PHE:CG	1:C:379:ILE:N	2.84	0.45
1:D:36:ILE:CG2	1:D:328:VAL:HG21	2.43	0.45
1:D:411:ASN:HD22	1:D:412:TYR:N	2.14	0.45
1:A:270:ALA:O	1:A:273:ARG:O	2.34	0.45
1:A:384:PHE:CD1	1:A:384:PHE:C	2.89	0.45
1:B:62:VAL:HA	1:B:63:PRO:HD3	1.75	0.45
1:B:182:MET:HE3	1:B:187:TYR:HD1	1.81	0.45
1:B:252:LEU:HD23	1:B:252:LEU:C	2.37	0.45
1:D:368:SER:HG	1:D:391:PHE:H	1.64	0.45
1:E:94:LEU:HD23	1:F:197:TRP:CB	2.45	0.45
1:F:169:ILE:HD12	1:F:207:ALA:HB1	1.98	0.45
1:A:27:HIS:CD2	1:A:32:ILE:HG13	2.51	0.45
1:A:291:ASN:H	1:A:291:ASN:ND2	2.12	0.45
1:C:75:ASN:C	1:C:75:ASN:HD22	2.19	0.45
1:C:75:ASN:C	1:C:75:ASN:ND2	2.68	0.45
1:C:157:GLY:CA	1:C:158:HIS:HB2	2.47	0.45
1:F:60:ILE:HA	1:F:354:VAL:HG21	1.97	0.45
1:B:47:ARG:NH2	1:B:115:GLU:OE1	2.49	0.45
1:B:282:TRP:CG	1:B:282:TRP:O	2.70	0.45
1:C:182:MET:HE1	1:C:187:TYR:HA	1.99	0.45
1:C:318:ILE:CG1	1:C:319:VAL:HG23	2.43	0.45
1:C:326:GLN:HG2	1:C:330:ALA:HB3	1.99	0.45
1:D:26:GLU:CB	1:D:326:GLN:OE1	2.56	0.45
1:D:169:ILE:O	1:D:169:ILE:HG22	2.17	0.45
1:D:214:ASP:C	1:D:214:ASP:OD1	2.55	0.45
1:E:262:LYS:O	1:E:266:MET:HG3	2.16	0.45
1:F:25:THR:O	1:F:25:THR:CG2	2.56	0.45
1:F:243:TYR:CG	1:F:414:LYS:HD2	2.52	0.45
1:A:47:ARG:HH11	1:A:47:ARG:CG	2.26	0.45
1:B:24:PHE:O	1:B:327:LEU:HB2	2.16	0.45
1:C:197:TRP:C	1:C:199:LYS:N	2.69	0.45
1:D:378:PHE:O	1:D:379:ILE:C	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:PHE:HA	1:E:276:LYS:O	2.17	0.45
1:F:329:ASN:ND2	1:F:336:THR:HB	2.30	0.45
1:A:291:ASN:HD22	1:A:291:ASN:N	2.03	0.45
1:E:460:THR:HG22	1:E:461:ILE:N	2.32	0.45
1:F:4:ARG:HG3	1:F:4:ARG:HH11	1.82	0.45
1:F:376:VAL:O	1:F:376:VAL:CG2	2.44	0.45
1:A:30:ARG:NH1	1:A:336:THR:HG22	2.21	0.45
1:A:244:TYR:HA	1:A:247:VAL:HG22	1.98	0.45
1:C:26:GLU:CG	1:C:27:HIS:N	2.79	0.45
1:C:62:VAL:HA	1:C:63:PRO:HD3	1.71	0.45
1:C:461:ILE:CG2	1:C:462:THR:N	2.80	0.45
1:E:25:THR:HA	1:E:326:GLN:HG2	1.98	0.45
1:F:282:TRP:O	1:F:282:TRP:CD2	2.70	0.45
1:A:318:ILE:CG1	1:A:319:VAL:HG23	2.43	0.45
1:B:219:LEU:O	1:B:223:GLN:HB2	2.16	0.45
1:B:260:VAL:HA	1:B:263:LEU:HD12	1.97	0.45
1:B:416:ASP:N	1:B:473:PRO:HB3	2.32	0.45
1:C:73:VAL:HG21	1:C:123:SER:O	2.17	0.45
1:D:431:LYS:CD	1:D:462:THR:HG22	2.47	0.45
1:E:318:ILE:CG1	1:E:319:VAL:HG23	2.43	0.45
1:A:75:ASN:C	1:A:75:ASN:ND2	2.71	0.44
1:B:60:ILE:O	1:B:60:ILE:CG1	2.64	0.44
1:B:60:ILE:HG22	1:B:351:GLU:HA	1.98	0.44
1:B:252:LEU:HD21	1:B:256:ARG:CZ	2.47	0.44
1:C:19:HIS:CD2	1:C:64:ASN:ND2	2.70	0.44
1:D:96:TRP:C	1:D:97:GLN:HG3	2.37	0.44
1:D:334:ILE:CG1	1:D:347:TYR:CD2	3.00	0.44
1:E:5:ILE:HG22	1:E:366:VAL:HG23	2.00	0.44
1:F:197:TRP:O	1:F:198:MET:CB	2.64	0.44
1:A:261:LYS:C	1:A:261:LYS:CD	2.86	0.44
1:A:362:VAL:HG11	1:A:398:ILE:HG13	1.98	0.44
1:B:27:HIS:CD2	1:B:32:ILE:HG13	2.52	0.44
1:B:66:ARG:HA	1:B:121:TYR:O	2.17	0.44
1:D:45:ASP:OD2	1:D:47:ARG:NH1	2.49	0.44
1:D:179:VAL:HG22	1:E:197:TRP:CZ2	2.52	0.44
1:E:28:LEU:HD22	1:E:330:ALA:HB2	1.99	0.44
1:E:28:LEU:HD22	1:E:330:ALA:HB1	2.00	0.44
1:E:81:GLY:O	1:E:105:GLY:HA3	2.18	0.44
1:F:174:TYR:CE2	1:F:212:CYS:HB3	2.53	0.44
1:F:327:LEU:C	1:F:333:ALA:H	2.12	0.44
1:A:335:HIS:O	1:A:342:ILE:HG22	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:LEU:HD23	1:B:28:LEU:C	2.37	0.44
1:B:431:LYS:HZ3	1:B:462:THR:HG22	1.80	0.44
1:C:158:HIS:C	1:C:159:PRO:HA	2.37	0.44
1:D:474:PHE:CD1	1:D:474:PHE:O	2.70	0.44
1:E:250:VAL:HG13	1:E:251:TYR:CE2	2.53	0.44
1:E:391:PHE:CD1	1:E:413:ARG:HD3	2.52	0.44
1:F:270:ALA:O	1:F:273:ARG:O	2.35	0.44
1:F:411:ASN:ND2	1:F:411:ASN:C	2.71	0.44
1:A:169:ILE:HD12	1:A:207:ALA:HB1	1.99	0.44
1:B:362:VAL:HG11	1:B:398:ILE:HD12	1.97	0.44
1:B:362:VAL:HG22	1:B:396:ALA:O	2.16	0.44
1:C:463:VAL:HB	1:C:467:PHE:CE2	2.53	0.44
1:D:4:ARG:HA	1:D:420:VAL:HG23	1.99	0.44
1:D:157:GLY:O	1:D:158:HIS:CB	2.66	0.44
1:D:197:TRP:HA	1:D:200:VAL:HG13	1.99	0.44
1:E:60:ILE:HG22	1:E:351:GLU:HA	2.00	0.44
1:E:392:LEU:HD12	1:E:410:VAL:O	2.18	0.44
1:F:202:ASP:O	1:F:205:ILE:HG12	2.16	0.44
1:F:403:LYS:O	1:F:403:LYS:HG3	2.17	0.44
1:B:70:GLY:HA2	1:B:171:ASN:OD1	2.18	0.44
1:B:325:ALA:HA	1:B:326:GLN:HA	1.75	0.44
1:B:446:ASN:HD22	1:B:446:ASN:N	2.15	0.44
1:B:450:ASN:C	1:B:452:ASN:H	2.20	0.44
1:C:327:LEU:C	1:C:328:VAL:HG23	2.38	0.44
1:D:318:ILE:HG13	1:D:319:VAL:CG2	2.44	0.44
1:E:24:PHE:O	1:E:326:GLN:HA	2.17	0.44
1:E:291:ASN:ND2	1:E:291:ASN:N	2.64	0.44
1:E:377:MET:O	1:E:377:MET:HG3	2.17	0.44
1:B:162:TYR:O	1:B:163:ASN:HB3	2.18	0.44
1:B:347:TYR:CD1	1:B:347:TYR:C	2.90	0.44
1:C:208:ILE:HD12	1:C:208:ILE:N	2.33	0.44
1:D:162:TYR:O	1:D:163:ASN:HB3	2.18	0.44
1:D:192:LYS:HE2	1:F:176:GLU:OE2	2.17	0.44
1:E:208:ILE:N	1:E:208:ILE:HD12	2.33	0.44
1:E:384:PHE:CD1	1:E:384:PHE:C	2.91	0.44
1:F:125:ASN:OD1	1:F:125:ASN:C	2.56	0.44
1:F:243:TYR:CB	1:F:414:LYS:HD2	2.48	0.44
1:A:145:GLY:O	1:A:154:ARG:NH2	2.50	0.44
1:A:240:SER:O	1:A:300:LYS:HE3	2.18	0.44
1:B:60:ILE:HA	1:B:354:VAL:HG21	2.00	0.44
1:B:182:MET:HE1	1:B:187:TYR:HD1	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:LEU:O	1:B:470:THR:HA	2.18	0.44
1:D:70:GLY:HA2	1:D:171:ASN:CG	2.37	0.44
1:D:463:VAL:HB	1:D:467:PHE:CE2	2.53	0.44
1:E:434:VAL:O	1:E:434:VAL:HG23	2.18	0.44
1:F:60:ILE:O	1:F:60:ILE:CG1	2.66	0.44
1:F:215:PRO:O	1:F:219:LEU:HB2	2.17	0.44
1:F:371:TYR:CD1	1:F:389:ALA:O	2.71	0.44
1:F:423:ARG:O	1:F:423:ARG:HG3	2.16	0.44
1:A:74:SER:CB	1:A:178:GLN:HE21	2.30	0.44
1:C:22:GLY:HA2	1:C:63:PRO:HD2	1.99	0.44
1:E:282:TRP:O	1:E:324:LEU:HD12	2.18	0.44
1:E:397:SER:O	1:E:405:LEU:HD12	2.17	0.44
1:E:472:LYS:HB3	1:E:473:PRO:HD2	1.99	0.44
1:F:24:PHE:CB	1:F:325:ALA:CA	2.78	0.44
1:F:342:ILE:HD13	1:F:343:LEU:N	2.33	0.44
1:B:197:TRP:O	1:B:198:MET:CB	2.65	0.44
1:B:255:GLU:O	1:B:258:ILE:HG12	2.18	0.44
1:B:410:VAL:CG2	1:B:412:TYR:OH	2.64	0.44
1:C:28:LEU:HD22	1:C:330:ALA:HB1	2.00	0.44
1:E:377:MET:N	1:E:382:MET:O	2.47	0.44
1:F:70:GLY:HA2	1:F:171:ASN:CG	2.38	0.44
1:B:250:VAL:HG13	1:B:251:TYR:CE2	2.53	0.43
1:B:405:LEU:HB3	1:B:481:VAL:CG1	2.48	0.43
1:C:74:SER:HB2	1:C:178:GLN:HE21	1.83	0.43
1:C:219:LEU:O	1:C:223:GLN:HB2	2.17	0.43
1:E:330:ALA:O	1:E:331:LEU:C	2.57	0.43
1:E:409:VAL:HG21	1:E:471:PHE:CE2	2.53	0.43
1:A:291:ASN:ND2	1:A:291:ASN:N	2.66	0.43
1:A:299:LEU:HD21	1:A:474:PHE:CD1	2.53	0.43
1:A:419:LYS:HG2	1:A:470:THR:HG22	1.38	0.43
1:B:318:ILE:HG13	1:B:319:VAL:CG2	2.43	0.43
1:C:282:TRP:O	1:C:282:TRP:CG	2.71	0.43
1:D:197:TRP:C	1:D:199:LYS:N	2.72	0.43
1:D:250:VAL:HG13	1:D:251:TYR:CE2	2.54	0.43
1:D:371:TYR:CD1	1:D:389:ALA:O	2.72	0.43
1:B:373:ILE:CG1	1:B:374:GLU:N	2.80	0.43
1:D:458:SER:O	1:D:459:GLU:HB2	2.18	0.43
1:E:415:GLU:N	1:E:415:GLU:OE1	2.43	0.43
1:F:22:GLY:HA2	1:F:63:PRO:HD2	2.00	0.43
1:F:328:VAL:HA	1:F:334:ILE:HB	2.00	0.43
1:A:208:ILE:HD12	1:A:208:ILE:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASP:C	1:A:443:ASN:H	2.20	0.43
1:A:474:PHE:O	1:A:474:PHE:HD1	2.01	0.43
1:E:91:ARG:HH11	1:E:91:ARG:CG	2.31	0.43
1:F:85:LYS:O	1:F:87:GLN:N	2.49	0.43
1:A:380:ASN:HD22	1:A:381:LYS:N	2.16	0.43
1:A:409:VAL:HG21	1:A:471:PHE:CE1	2.54	0.43
1:B:28:LEU:HD22	1:B:330:ALA:HB2	1.98	0.43
1:B:122:ILE:HD12	1:B:164:VAL:HG21	2.01	0.43
1:C:16:ILE:HA	1:C:316:SER:OG	2.18	0.43
1:C:30:ARG:NH1	1:C:336:THR:HG22	2.24	0.43
1:C:405:LEU:HB3	1:C:481:VAL:CG1	2.48	0.43
1:D:377:MET:O	1:D:378:PHE:CB	2.54	0.43
1:E:251:TYR:HE2	1:E:412:TYR:CZ	2.37	0.43
1:F:434:VAL:HG23	1:F:434:VAL:O	2.19	0.43
1:B:411:ASN:C	1:B:411:ASN:ND2	2.72	0.43
1:D:62:VAL:CG1	1:D:116:ILE:HD12	2.44	0.43
1:D:446:ASN:HD22	1:D:446:ASN:N	2.16	0.43
1:E:62:VAL:HA	1:E:63:PRO:HD3	1.74	0.43
1:A:73:VAL:HG21	1:A:123:SER:O	2.18	0.43
1:A:411:ASN:C	1:A:411:ASN:ND2	2.72	0.43
1:A:460:THR:HG22	1:A:461:ILE:N	2.33	0.43
1:B:157:GLY:O	1:B:158:HIS:CB	2.65	0.43
1:B:197:TRP:C	1:B:199:LYS:N	2.72	0.43
1:B:326:GLN:HB2	1:B:330:ALA:O	2.19	0.43
1:B:378:PHE:C	1:B:380:ASN:N	2.71	0.43
1:B:458:SER:O	1:B:459:GLU:HB2	2.18	0.43
1:C:255:GLU:O	1:C:258:ILE:HG12	2.18	0.43
1:D:125:ASN:C	1:D:125:ASN:OD1	2.57	0.43
1:E:411:ASN:HD22	1:E:412:TYR:N	2.16	0.43
1:F:96:TRP:C	1:F:97:GLN:HG3	2.38	0.43
1:F:157:GLY:HA3	1:F:158:HIS:HB2	2.01	0.43
1:F:291:ASN:N	1:F:291:ASN:ND2	2.64	0.43
1:B:70:GLY:HA2	1:B:171:ASN:CG	2.39	0.43
1:B:206:LYS:HA	1:B:230:ASP:OD2	2.18	0.43
1:B:215:PRO:HG3	1:E:266:MET:HB3	2.01	0.43
1:B:434:VAL:HG12	1:B:479:ILE:HG12	2.01	0.43
1:C:5:ILE:HG22	1:C:366:VAL:HG23	2.01	0.43
1:D:279:LEU:HD22	1:D:282:TRP:HB3	1.99	0.43
1:F:73:VAL:O	1:F:125:ASN:HB2	2.18	0.43
1:F:238:THR:O	1:F:284:VAL:HA	2.19	0.43
1:F:279:LEU:CD2	1:F:282:TRP:HB3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ASN:HD22	1:A:325:ALA:HB3	1.83	0.43
1:B:125:ASN:OD1	1:B:125:ASN:C	2.57	0.43
1:C:464:ASP:C	1:C:466:GLU:N	2.71	0.43
1:D:53:VAL:HG22	1:D:341:LEU:HD11	2.01	0.43
1:D:285:TRP:CD1	1:D:285:TRP:C	2.90	0.43
1:D:365:HIS:ND1	1:D:365:HIS:C	2.71	0.43
1:E:142:ASN:O	1:E:161:PRO:CB	2.67	0.43
1:F:62:VAL:HA	1:F:63:PRO:HD3	1.77	0.43
1:A:26:GLU:CG	1:A:27:HIS:N	2.81	0.43
1:B:74:SER:HB2	1:B:178:GLN:HE21	1.84	0.43
1:D:384:PHE:CD1	1:D:384:PHE:C	2.92	0.43
1:D:411:ASN:OD1	1:D:413:ARG:HB2	2.19	0.43
1:E:67:TRP:O	1:E:122:ILE:HA	2.18	0.43
1:F:70:GLY:O	1:F:71:ASN:C	2.57	0.43
1:F:199:LYS:HE2	1:F:205:ILE:O	2.18	0.43
1:F:362:VAL:HG11	1:F:398:ILE:HD12	2.00	0.43
1:F:461:ILE:HD11	1:F:469:HIS:ND1	2.34	0.43
1:A:371:TYR:CD1	1:A:389:ALA:O	2.72	0.42
1:B:285:TRP:CD1	1:B:285:TRP:C	2.90	0.42
1:B:335:HIS:O	1:B:342:ILE:HG22	2.19	0.42
1:B:394:ALA:HB1	1:B:408:ALA:O	2.19	0.42
1:F:411:ASN:ND2	1:F:413:ARG:N	2.60	0.42
1:A:30:ARG:CB	1:A:329:ASN:ND2	2.83	0.42
1:A:197:TRP:HA	1:A:200:VAL:HG13	2.00	0.42
1:B:197:TRP:CZ2	1:C:179:VAL:HG22	2.53	0.42
1:B:460:THR:HG22	1:B:461:ILE:N	2.34	0.42
1:C:202:ASP:O	1:C:205:ILE:HG12	2.18	0.42
1:C:234:TYR:OH	1:C:256:ARG:HG2	2.19	0.42
1:C:299:LEU:HD21	1:C:474:PHE:CD1	2.54	0.42
1:D:67:TRP:O	1:D:122:ILE:HA	2.19	0.42
1:E:461:ILE:HD11	1:E:469:HIS:CE1	2.54	0.42
1:F:418:LEU:O	1:F:470:THR:HA	2.18	0.42
1:A:197:TRP:O	1:A:198:MET:CB	2.66	0.42
1:B:157:GLY:CA	1:B:158:HIS:HB2	2.49	0.42
1:C:34:GLY:O	1:C:336:THR:CG2	2.56	0.42
1:D:362:VAL:HG11	1:D:398:ILE:CD1	2.50	0.42
1:E:214:ASP:HA	1:E:215:PRO:HD3	1.92	0.42
1:E:362:VAL:HG11	1:E:398:ILE:HD12	2.01	0.42
1:E:368:SER:OG	1:E:369:GLU:N	2.52	0.42
1:A:67:TRP:CE2	1:A:68:PRO:HB3	2.55	0.42
1:A:94:LEU:CD2	1:C:197:TRP:HB3	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:GLY:HA3	1:B:158:HIS:ND1	2.34	0.42
1:B:411:ASN:ND2	1:B:413:ARG:H	2.16	0.42
1:B:445:ARG:HH11	1:B:445:ARG:HG3	1.85	0.42
1:C:71:ASN:OD1	1:C:71:ASN:N	2.42	0.42
1:C:215:PRO:O	1:C:219:LEU:HB2	2.18	0.42
1:C:330:ALA:O	1:C:332:GLY:N	2.52	0.42
1:C:450:ASN:C	1:C:452:ASN:H	2.22	0.42
1:D:94:LEU:CD2	1:E:197:TRP:HB3	2.49	0.42
1:E:461:ILE:HG22	1:E:462:THR:N	2.34	0.42
1:F:236:PHE:CG	1:F:253:LEU:HD13	2.54	0.42
1:A:154:ARG:HA	1:A:158:HIS:O	2.19	0.42
1:A:434:VAL:O	1:A:434:VAL:CG2	2.67	0.42
1:B:28:LEU:HD22	1:B:330:ALA:HB1	2.00	0.42
1:B:371:TYR:CD1	1:B:389:ALA:O	2.72	0.42
1:B:461:ILE:HD11	1:B:469:HIS:ND1	2.34	0.42
1:C:45:ASP:CG	1:C:46:GLU:N	2.71	0.42
1:C:61:LYS:HE2	1:C:355:ASN:OD1	2.19	0.42
1:D:240:SER:O	1:D:300:LYS:HE3	2.19	0.42
1:D:324:LEU:O	1:D:325:ALA:C	2.58	0.42
1:D:347:TYR:CD1	1:D:347:TYR:C	2.93	0.42
1:E:169:ILE:CD1	1:E:195:THR:OG1	2.68	0.42
1:C:245:GLU:O	1:C:249:THR:HG23	2.18	0.42
1:D:158:HIS:O	1:D:159:PRO:CA	2.68	0.42
1:E:365:HIS:C	1:E:365:HIS:ND1	2.71	0.42
1:A:45:ASP:OD2	1:A:47:ARG:NH1	2.52	0.42
1:A:158:HIS:O	1:A:159:PRO:CA	2.68	0.42
1:B:362:VAL:HG11	1:B:398:ILE:HG13	2.02	0.42
1:E:179:VAL:HG22	1:F:197:TRP:CE2	2.54	0.42
1:E:299:LEU:HD21	1:E:474:PHE:HD1	1.84	0.42
1:E:378:PHE:HD1	1:E:379:ILE:N	1.84	0.42
1:F:158:HIS:O	1:F:159:PRO:CA	2.68	0.42
1:A:324:LEU:HD12	1:A:324:LEU:HA	1.91	0.42
1:D:62:VAL:HA	1:D:63:PRO:HD3	1.73	0.42
1:D:202:ASP:O	1:D:205:ILE:HG12	2.20	0.42
1:D:405:LEU:HB3	1:D:481:VAL:CG1	2.50	0.42
1:E:268:ASP:O	1:E:272:LYS:HD3	2.20	0.42
1:E:329:ASN:ND2	1:E:336:THR:HB	2.31	0.42
1:A:268:ASP:O	1:A:272:LYS:HD3	2.19	0.42
1:A:438:THR:HG23	1:A:439:GLY:N	2.35	0.42
1:B:384:PHE:CD1	1:B:384:PHE:C	2.93	0.42
1:E:250:VAL:HG11	1:E:412:TYR:OH	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:ARG:HG2	1:E:416:ASP:HB2	2.02	0.42
1:B:169:ILE:HD13	1:B:195:THR:OG1	2.19	0.42
1:B:231:PHE:HA	1:B:276:LYS:O	2.19	0.42
1:D:75:ASN:OD1	1:D:94:LEU:HD13	2.20	0.42
1:E:224:GLU:OE1	1:E:224:GLU:HA	2.19	0.42
1:F:81:GLY:O	1:F:105:GLY:HA3	2.19	0.42
1:A:197:TRP:C	1:A:199:LYS:N	2.73	0.41
1:B:238:THR:O	1:B:284:VAL:HA	2.20	0.41
1:C:409:VAL:HG21	1:C:471:PHE:CE2	2.54	0.41
1:C:410:VAL:HG12	1:C:412:TYR:CE1	2.53	0.41
1:D:112:TYR:O	1:D:116:ILE:HG12	2.20	0.41
1:A:70:GLY:HA2	1:A:171:ASN:CG	2.40	0.41
1:B:197:TRP:CB	1:C:94:LEU:HD23	2.43	0.41
1:B:293:LEU:HD12	1:B:293:LEU:HA	1.82	0.41
1:B:370:THR:H	1:B:370:THR:HG23	1.38	0.41
1:B:378:PHE:C	1:B:380:ASN:H	2.21	0.41
1:B:441:ASP:C	1:B:443:ASN:H	2.22	0.41
1:B:464:ASP:C	1:B:466:GLU:N	2.74	0.41
1:A:285:TRP:O	1:A:378:PHE:HB2	2.19	0.41
1:A:286:TYR:HA	1:A:379:ILE:HG12	1.99	0.41
1:A:342:ILE:HD13	1:A:343:LEU:N	2.36	0.41
1:A:365:HIS:ND1	1:A:365:HIS:C	2.73	0.41
1:B:365:HIS:ND1	1:B:365:HIS:C	2.73	0.41
1:B:410:VAL:CB	1:B:412:TYR:OH	2.68	0.41
1:B:434:VAL:O	1:B:434:VAL:HG23	2.19	0.41
1:B:461:ILE:HG22	1:B:462:THR:N	2.35	0.41
1:C:125:ASN:C	1:C:125:ASN:OD1	2.58	0.41
1:D:224:GLU:OE1	1:D:224:GLU:HA	2.20	0.41
1:D:283:ASN:CB	1:D:325:ALA:HB3	2.50	0.41
1:E:157:GLY:HA3	1:E:158:HIS:HB2	2.02	0.41
1:E:238:THR:HG21	1:E:304:PHE:CE1	2.55	0.41
1:E:405:LEU:HB3	1:E:481:VAL:CG1	2.50	0.41
1:E:446:ASN:HD21	1:E:454:VAL:N	1.96	0.41
1:E:463:VAL:HB	1:E:467:PHE:CE1	2.55	0.41
1:E:481:VAL:CG2	1:E:482:GLU:N	2.62	0.41
1:F:28:LEU:HD22	1:F:330:ALA:HB2	2.01	0.41
1:F:110:ILE:HG13	1:F:162:TYR:CE2	2.55	0.41
1:F:411:ASN:ND2	1:F:413:ARG:CB	2.71	0.41
1:F:431:LYS:HZ3	1:F:462:THR:HG22	1.85	0.41
1:A:373:ILE:CG1	1:A:374:GLU:N	2.82	0.41
1:A:419:LYS:HA	1:A:470:THR:HG22	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:458:SER:O	1:C:459:GLU:HB2	2.20	0.41
1:C:460:THR:HG22	1:C:461:ILE:N	2.34	0.41
1:E:144:LYS:N	1:E:144:LYS:CD	2.74	0.41
1:E:182:MET:HE3	1:E:187:TYR:HD1	1.84	0.41
1:F:378:PHE:O	1:F:379:ILE:C	2.59	0.41
1:A:4:ARG:HH11	1:A:4:ARG:HG3	1.85	0.41
1:B:197:TRP:CE2	1:C:179:VAL:HG22	2.55	0.41
1:C:4:ARG:HA	1:C:420:VAL:HG23	2.02	0.41
1:C:157:GLY:O	1:C:158:HIS:HB2	2.19	0.41
1:E:22:GLY:HA2	1:E:63:PRO:HD2	2.02	0.41
1:F:38:GLU:HB3	1:F:44:SER:HG	1.86	0.41
1:F:397:SER:O	1:F:405:LEU:HD12	2.21	0.41
1:A:22:GLY:HA2	1:A:63:PRO:HD2	2.03	0.41
1:C:182:MET:HE3	1:C:187:TYR:HD1	1.85	0.41
1:D:85:LYS:O	1:D:86:ASP:HB2	2.21	0.41
1:D:237:TYR:HE1	1:D:325:ALA:HB2	1.84	0.41
1:D:441:ASP:C	1:D:443:ASN:H	2.24	0.41
1:F:73:VAL:HG21	1:F:123:SER:O	2.20	0.41
1:F:446:ASN:N	1:F:446:ASN:HD22	2.18	0.41
1:A:250:VAL:HG13	1:A:251:TYR:CE2	2.56	0.41
1:C:431:LYS:HZ3	1:C:462:THR:HG22	1.83	0.41
1:C:434:VAL:O	1:C:434:VAL:HG23	2.20	0.41
1:D:91:ARG:HH11	1:D:91:ARG:CG	2.32	0.41
1:D:110:ILE:HG13	1:D:162:TYR:CE2	2.56	0.41
1:D:461:ILE:HD11	1:D:469:HIS:CE1	2.56	0.41
1:D:474:PHE:O	1:D:474:PHE:HD1	2.03	0.41
1:F:419:LYS:HE2	1:F:419:LYS:HB3	1.65	0.41
1:A:60:ILE:HA	1:A:354:VAL:HG21	2.03	0.41
1:B:158:HIS:O	1:B:159:PRO:CA	2.67	0.41
1:B:353:ILE:O	1:B:353:ILE:HG22	2.21	0.41
1:C:353:ILE:O	1:C:353:ILE:HG22	2.20	0.41
1:D:60:ILE:HG22	1:D:351:GLU:HA	2.01	0.41
1:D:285:TRP:HB2	1:D:331:LEU:CD2	2.48	0.41
1:E:197:TRP:C	1:E:199:LYS:H	2.16	0.41
1:E:461:ILE:HD11	1:E:469:HIS:ND1	2.36	0.41
1:F:61:LYS:H	1:F:61:LYS:HG2	1.01	0.41
1:F:231:PHE:HA	1:F:276:LYS:O	2.20	0.41
1:A:279:LEU:HD22	1:A:282:TRP:HB3	2.03	0.41
1:A:380:ASN:O	1:A:381:LYS:HB2	2.21	0.41
1:A:446:ASN:N	1:A:446:ASN:HD22	2.18	0.41
1:B:25:THR:O	1:B:25:THR:CG2	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:THR:HG22	1:B:66:ARG:O	2.21	0.41
1:C:71:ASN:HA	1:C:178:GLN:NE2	2.21	0.41
1:C:240:SER:O	1:C:300:LYS:HE3	2.21	0.41
1:C:279:LEU:O	1:C:322:ALA:HA	2.21	0.41
1:C:362:VAL:O	1:C:363:LYS:C	2.59	0.41
1:D:76:TYR:CE2	1:D:78:TRP:HA	2.55	0.41
1:D:158:HIS:C	1:D:159:PRO:HA	2.40	0.41
1:D:231:PHE:HA	1:D:276:LYS:O	2.20	0.41
1:D:362:VAL:HG11	1:D:398:ILE:HD12	2.02	0.41
1:D:413:ARG:HG3	1:D:418:LEU:HD13	1.96	0.41
1:D:423:ARG:NH1	1:D:425:GLU:OE1	2.54	0.41
1:D:464:ASP:C	1:D:466:GLU:N	2.74	0.41
1:E:28:LEU:C	1:E:28:LEU:HD23	2.41	0.41
1:E:197:TRP:O	1:E:198:MET:CB	2.69	0.41
1:E:267:VAL:O	1:E:268:ASP:C	2.60	0.41
1:E:317:ASP:OD1	1:E:317:ASP:N	2.53	0.41
1:F:336:THR:HG23	1:F:337:GLU:N	2.36	0.41
1:A:252:LEU:C	1:A:252:LEU:HD23	2.41	0.41
1:A:293:LEU:HD12	1:A:293:LEU:HA	1.88	0.41
1:A:461:ILE:HD11	1:A:469:HIS:ND1	2.36	0.41
1:C:258:ILE:HG13	1:F:262:LYS:CD	2.50	0.41
1:D:43:LEU:HD12	1:D:43:LEU:N	2.35	0.41
1:D:158:HIS:O	1:D:159:PRO:HA	2.21	0.41
1:D:179:VAL:HG22	1:E:197:TRP:CE2	2.56	0.41
1:D:377:MET:HB3	1:D:384:PHE:CD2	2.56	0.41
1:D:378:PHE:HD2	1:D:380:ASN:ND2	2.19	0.41
1:E:429:GLN:HA	1:E:463:VAL:O	2.21	0.41
1:F:80:ASP:O	1:F:102:ASN:HB3	2.21	0.41
1:A:381:LYS:O	1:A:382:MET:C	2.60	0.40
1:B:282:TRP:O	1:B:324:LEU:HD12	2.21	0.40
1:B:482:GLU:OE1	1:B:482:GLU:O	2.40	0.40
1:C:384:PHE:CD1	1:C:384:PHE:C	2.94	0.40
1:D:297:TYR:HH	1:D:331:LEU:HD22	1.84	0.40
1:D:411:ASN:HD21	1:D:413:ARG:CG	2.19	0.40
1:E:28:LEU:HD12	1:E:96:TRP:CZ2	2.56	0.40
1:E:94:LEU:HD23	1:F:197:TRP:CG	2.56	0.40
1:E:434:VAL:O	1:E:434:VAL:CG2	2.69	0.40
1:F:162:TYR:O	1:F:163:ASN:HB3	2.21	0.40
1:A:96:TRP:C	1:A:97:GLN:HG3	2.41	0.40
1:A:376:VAL:HB	1:A:381:LYS:CA	2.51	0.40
1:B:315:MET:O	1:B:317:ASP:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:VAL:O	1:C:73:VAL:HG22	2.21	0.40
1:C:318:ILE:HG13	1:C:319:VAL:CG2	2.48	0.40
1:D:197:TRP:O	1:D:198:MET:CB	2.66	0.40
1:D:366:VAL:CG2	1:D:367:GLU:N	2.83	0.40
1:E:252:LEU:HD12	1:E:384:PHE:CD1	2.57	0.40
1:F:253:LEU:O	1:F:253:LEU:HG	2.20	0.40
1:F:299:LEU:HD21	1:F:474:PHE:CD1	2.56	0.40
1:F:461:ILE:CD1	1:F:469:HIS:ND1	2.84	0.40
1:A:212:CYS:SG	1:A:213:ASP:N	2.94	0.40
1:C:158:HIS:O	1:C:159:PRO:HA	2.21	0.40
1:D:236:PHE:CG	1:D:253:LEU:HD13	2.57	0.40
1:D:293:LEU:HD12	1:D:293:LEU:HA	1.87	0.40
1:E:145:GLY:O	1:E:154:ARG:NH2	2.54	0.40
1:E:162:TYR:O	1:E:163:ASN:HB3	2.19	0.40
1:E:169:ILE:HD12	1:E:207:ALA:HB1	2.01	0.40
1:E:270:ALA:O	1:E:273:ARG:O	2.39	0.40
1:E:467:PHE:HD2	1:E:468:GLU:O	2.04	0.40
1:F:325:ALA:HA	1:F:326:GLN:HA	1.77	0.40
1:F:362:VAL:O	1:F:363:LYS:C	2.59	0.40
1:F:405:LEU:HB3	1:F:481:VAL:CG1	2.52	0.40
1:A:75:ASN:C	1:A:75:ASN:HD22	2.25	0.40
1:A:215:PRO:HB2	1:D:219:LEU:HD21	2.03	0.40
1:A:231:PHE:HA	1:A:276:LYS:O	2.20	0.40
1:A:283:ASN:CB	1:A:325:ALA:HB2	2.51	0.40
1:B:384:PHE:CD1	1:B:385:SER:N	2.90	0.40
1:B:421:PRO:O	1:B:421:PRO:HG2	2.21	0.40
1:C:461:ILE:HD11	1:C:469:HIS:ND1	2.36	0.40
1:E:62:VAL:CG1	1:E:116:ILE:HD12	2.46	0.40
1:E:80:ASP:HB3	1:E:89:PRO:HG2	2.04	0.40
1:E:240:SER:HB2	1:E:376:VAL:HG23	2.03	0.40
1:F:411:ASN:HD21	1:F:413:ARG:CB	1.99	0.40
1:A:414:LYS:O	1:A:473:PRO:HB3	2.20	0.40
1:B:158:HIS:C	1:B:159:PRO:HA	2.41	0.40
1:B:373:ILE:HG12	1:B:374:GLU:H	1.87	0.40
1:C:82:ILE:HD13	1:C:82:ILE:HG21	1.87	0.40
1:D:4:ARG:HH11	1:D:4:ARG:HG3	1.86	0.40
1:D:26:GLU:HG2	1:D:27:HIS:N	2.36	0.40
1:E:195:THR:O	1:E:199:LYS:HB2	2.22	0.40
1:E:467:PHE:CD2	1:E:468:GLU:N	2.90	0.40
1:F:67:TRP:O	1:F:122:ILE:HA	2.21	0.40
1:F:171:ASN:H	1:F:173:MET:HE3	1.86	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:LYS:CE	1:E:431:LYS:CE[1_556]	1.60	0.60
1:C:144:LYS:CE	1:E:431:LYS:NZ[1_556]	1.90	0.30

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	476/482 (99%)	409 (86%)	62 (13%)	5 (1%)	12	44
1	B	476/482 (99%)	409 (86%)	61 (13%)	6 (1%)	10	39
1	C	476/482 (99%)	410 (86%)	61 (13%)	5 (1%)	12	44
1	D	476/482 (99%)	403 (85%)	70 (15%)	3 (1%)	22	57
1	E	476/482 (99%)	407 (86%)	66 (14%)	3 (1%)	22	57
1	F	476/482 (99%)	406 (85%)	68 (14%)	2 (0%)	30	66
All	All	2856/2892 (99%)	2444 (86%)	388 (14%)	24 (1%)	16	51

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	328	VAL
1	A	379	ILE
1	B	172	GLU
1	C	465	THR
1	E	328	VAL
1	A	172	GLU
1	B	61	LYS
1	B	316	SER
1	C	61	LYS
1	D	316	SER
1	A	61	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	71	ASN
1	C	316	SER
1	E	316	SER
1	F	316	SER
1	B	328	VAL
1	E	379	ILE
1	F	442	VAL
1	C	442	VAL
1	D	442	VAL
1	A	442	VAL
1	B	442	VAL
1	B	451	PRO
1	D	379	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	417/418 (100%)	376 (90%)	41 (10%)	6	26
1	B	417/418 (100%)	375 (90%)	42 (10%)	6	25
1	C	417/418 (100%)	374 (90%)	43 (10%)	6	24
1	D	417/418 (100%)	376 (90%)	41 (10%)	6	26
1	E	417/418 (100%)	378 (91%)	39 (9%)	7	28
1	F	417/418 (100%)	377 (90%)	40 (10%)	7	27
All	All	2502/2508 (100%)	2256 (90%)	246 (10%)	6	26

All (246) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	ARG
1	A	61	LYS
1	A	75	ASN
1	A	97	GLN
1	A	114	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	121	TYR
1	A	132	ASP
1	A	135	LEU
1	A	144	LYS
1	A	160	GLU
1	A	219	LEU
1	A	256	ARG
1	A	261	LYS
1	A	279	LEU
1	A	291	ASN
1	A	293	LEU
1	A	306	CYS
1	A	321	LEU
1	A	328	VAL
1	A	336	THR
1	A	342	ILE
1	A	364	THR
1	A	366	VAL
1	A	374	GLU
1	A	377	MET
1	A	378	PHE
1	A	380	ASN
1	A	381	LYS
1	A	403	LYS
1	A	409	VAL
1	A	411	ASN
1	A	413	ARG
1	A	414	LYS
1	A	415	GLU
1	A	416	ASP
1	A	422	ILE
1	A	423	ARG
1	A	430	LYS
1	A	433	THR
1	A	459	GLU
1	A	482	GLU
1	B	47	ARG
1	B	54	LEU
1	B	61	LYS
1	B	68	PRO
1	B	75	ASN
1	B	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	114	ARG
1	B	121	TYR
1	B	135	LEU
1	B	144	LYS
1	B	160	GLU
1	B	189	ARG
1	B	219	LEU
1	B	256	ARG
1	B	261	LYS
1	B	279	LEU
1	B	291	ASN
1	B	293	LEU
1	B	306	CYS
1	B	321	LEU
1	B	326	GLN
1	B	336	THR
1	B	342	ILE
1	B	364	THR
1	B	366	VAL
1	B	374	GLU
1	B	377	MET
1	B	380	ASN
1	B	403	LYS
1	B	409	VAL
1	B	411	ASN
1	B	413	ARG
1	B	414	LYS
1	B	415	GLU
1	B	416	ASP
1	B	422	ILE
1	B	423	ARG
1	B	430	LYS
1	B	433	THR
1	B	445	ARG
1	B	459	GLU
1	B	482	GLU
1	C	47	ARG
1	C	61	LYS
1	C	75	ASN
1	C	97	GLN
1	C	114	ARG
1	C	121	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	132	ASP
1	C	135	LEU
1	C	142	ASN
1	C	144	LYS
1	C	160	GLU
1	C	219	LEU
1	C	256	ARG
1	C	261	LYS
1	C	279	LEU
1	C	291	ASN
1	C	293	LEU
1	C	306	CYS
1	C	321	LEU
1	C	326	GLN
1	C	327	LEU
1	C	328	VAL
1	C	336	THR
1	C	342	ILE
1	C	364	THR
1	C	366	VAL
1	C	369	GLU
1	C	374	GLU
1	C	378	PHE
1	C	379	ILE
1	C	380	ASN
1	C	403	LYS
1	C	409	VAL
1	C	411	ASN
1	C	413	ARG
1	C	415	GLU
1	C	422	ILE
1	C	423	ARG
1	C	430	LYS
1	C	433	THR
1	C	445	ARG
1	C	459	GLU
1	C	482	GLU
1	D	5	ILE
1	D	47	ARG
1	D	61	LYS
1	D	75	ASN
1	D	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	114	ARG
1	D	121	TYR
1	D	135	LEU
1	D	144	LYS
1	D	160	GLU
1	D	219	LEU
1	D	256	ARG
1	D	261	LYS
1	D	279	LEU
1	D	291	ASN
1	D	293	LEU
1	D	306	CYS
1	D	321	LEU
1	D	327	LEU
1	D	336	THR
1	D	342	ILE
1	D	364	THR
1	D	366	VAL
1	D	374	GLU
1	D	377	MET
1	D	378	PHE
1	D	380	ASN
1	D	397	SER
1	D	403	LYS
1	D	409	VAL
1	D	411	ASN
1	D	414	LYS
1	D	415	GLU
1	D	416	ASP
1	D	422	ILE
1	D	423	ARG
1	D	430	LYS
1	D	433	THR
1	D	436	THR
1	D	459	GLU
1	D	482	GLU
1	E	12	VAL
1	E	47	ARG
1	E	61	LYS
1	E	68	PRO
1	E	75	ASN
1	E	97	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	114	ARG
1	E	121	TYR
1	E	135	LEU
1	E	144	LYS
1	E	160	GLU
1	E	219	LEU
1	E	256	ARG
1	E	261	LYS
1	E	279	LEU
1	E	291	ASN
1	E	293	LEU
1	E	306	CYS
1	E	321	LEU
1	E	327	LEU
1	E	336	THR
1	E	342	ILE
1	E	364	THR
1	E	366	VAL
1	E	374	GLU
1	E	377	MET
1	E	378	PHE
1	E	380	ASN
1	E	403	LYS
1	E	409	VAL
1	E	411	ASN
1	E	413	ARG
1	E	415	GLU
1	E	422	ILE
1	E	423	ARG
1	E	430	LYS
1	E	433	THR
1	E	459	GLU
1	E	482	GLU
1	F	26	GLU
1	F	47	ARG
1	F	61	LYS
1	F	68	PRO
1	F	75	ASN
1	F	97	GLN
1	F	114	ARG
1	F	121	TYR
1	F	135	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	144	LYS
1	F	160	GLU
1	F	219	LEU
1	F	256	ARG
1	F	261	LYS
1	F	279	LEU
1	F	291	ASN
1	F	293	LEU
1	F	306	CYS
1	F	321	LEU
1	F	326	GLN
1	F	336	THR
1	F	342	ILE
1	F	364	THR
1	F	366	VAL
1	F	374	GLU
1	F	378	PHE
1	F	380	ASN
1	F	403	LYS
1	F	409	VAL
1	F	411	ASN
1	F	413	ARG
1	F	415	GLU
1	F	420	VAL
1	F	422	ILE
1	F	423	ARG
1	F	430	LYS
1	F	433	THR
1	F	445	ARG
1	F	459	GLU
1	F	482	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	19	HIS
1	A	77	HIS
1	A	87	GLN
1	A	97	GLN
1	A	178	GLN
1	A	291	ASN
1	A	326	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	380	ASN
1	A	388	ASN
1	A	411	ASN
1	A	429	GLN
1	A	446	ASN
1	A	452	ASN
1	B	19	HIS
1	B	77	HIS
1	B	87	GLN
1	B	97	GLN
1	B	178	GLN
1	B	291	ASN
1	B	326	GLN
1	B	380	ASN
1	B	388	ASN
1	B	411	ASN
1	B	429	GLN
1	B	446	ASN
1	B	452	ASN
1	C	19	HIS
1	C	77	HIS
1	C	87	GLN
1	C	97	GLN
1	C	178	GLN
1	C	291	ASN
1	C	326	GLN
1	C	380	ASN
1	C	388	ASN
1	C	411	ASN
1	C	429	GLN
1	C	446	ASN
1	C	452	ASN
1	D	19	HIS
1	D	77	HIS
1	D	87	GLN
1	D	97	GLN
1	D	178	GLN
1	D	291	ASN
1	D	380	ASN
1	D	388	ASN
1	D	411	ASN
1	D	429	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	446	ASN
1	D	452	ASN
1	E	19	HIS
1	E	77	HIS
1	E	87	GLN
1	E	97	GLN
1	E	178	GLN
1	E	291	ASN
1	E	326	GLN
1	E	380	ASN
1	E	388	ASN
1	E	411	ASN
1	E	429	GLN
1	E	446	ASN
1	E	452	ASN
1	F	19	HIS
1	F	77	HIS
1	F	87	GLN
1	F	97	GLN
1	F	178	GLN
1	F	291	ASN
1	F	326	GLN
1	F	380	ASN
1	F	388	ASN
1	F	411	ASN
1	F	429	GLN
1	F	446	ASN
1	F	452	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	3
1	A	3
1	B	3
1	D	3
1	F	2
1	E	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	157:GLY	C	158:HIS	N	3.85
1	F	157:GLY	C	158:HIS	N	3.82
1	A	157:GLY	C	158:HIS	N	3.80
1	B	157:GLY	C	158:HIS	N	3.80
1	E	157:GLY	C	158:HIS	N	3.79
1	D	157:GLY	C	158:HIS	N	3.76
1	C	158:HIS	C	159:PRO	N	2.62
1	E	158:HIS	C	159:PRO	N	2.57
1	F	158:HIS	C	159:PRO	N	2.57
1	D	158:HIS	C	159:PRO	N	2.56
1	A	158:HIS	C	159:PRO	N	2.50
1	B	158:HIS	C	159:PRO	N	2.49
1	A	26:GLU	C	27:HIS	N	1.17
1	B	26:GLU	C	27:HIS	N	1.14
1	C	26:GLU	C	27:HIS	N	1.07
1	D	26:GLU	C	27:HIS	N	0.93

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	481/482 (99%)	-0.50	2 (0%)	89	77	14, 42, 75, 115	0
1	B	481/482 (99%)	-0.31	3 (0%)	85	71	15, 47, 92, 117	0
1	C	481/482 (99%)	-0.52	1 (0%)	92	84	17, 40, 66, 88	0
1	D	481/482 (99%)	-0.27	2 (0%)	89	77	17, 54, 85, 110	0
1	E	481/482 (99%)	0.11	4 (0%)	82	66	31, 67, 93, 115	0
1	F	481/482 (99%)	0.04	4 (0%)	82	66	33, 64, 91, 129	0
All	All	2886/2892 (99%)	-0.24	16 (0%)	85	71	14, 52, 88, 129	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	412	TYR	5.5
1	A	412	TYR	5.0
1	E	325	ALA	4.6
1	A	325	ALA	4.1
1	F	325	ALA	4.0
1	E	326	GLN	3.6
1	C	325	ALA	3.4
1	F	431	LYS	3.2
1	E	412	TYR	2.8
1	B	86	ASP	2.7
1	D	331	LEU	2.6
1	B	476	CYS	2.4
1	F	168	GLY	2.4
1	E	283	ASN	2.3
1	D	34	GLY	2.3
1	F	429	GLN	2.2

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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.