



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:29 PM UTC

PDB ID : 1R4M / pdb_00001r4m
Title : APPBP1-UBA3-NEDD8, an E1-ubiquitin-like protein complex
Authors : Walden, H.; Podgorski, M.S.; Holton, J.M.; Schulman, B.A.
Deposited on : 2003-10-07
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

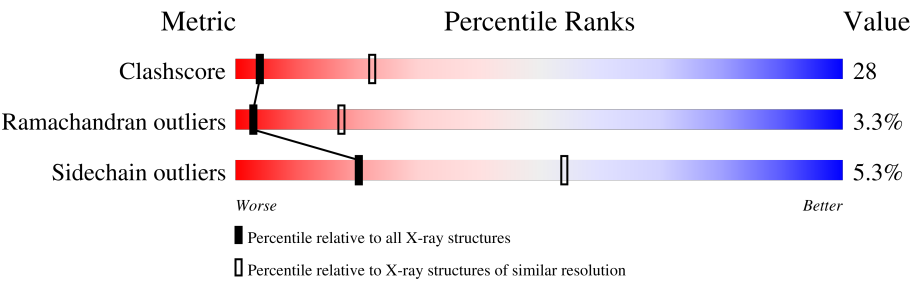
1 Overall quality at a glance i

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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	529	58%33%6% ..
1	C	529	59%32%6% ..
1	E	529	59%32%6% ..
1	G	529	58%32%6% ..
2	B	431	49%41%5% ..
2	D	431	49%41%5% ..
2	F	431	51%39%5% ..
2	H	431	48%43%6% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	I	76	49% 45% 7%
3	J	76	51% 43% 5%
3	K	76	50% 42% 8%
3	L	76	46% 47% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 31620 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 amyloid beta precursor protein-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4105	2602	699	789	15			
1	C	516	Total	C	N	O	S	0	0	0
			4105	2602	699	789	15			
1	E	516	Total	C	N	O	S	0	0	0
			4105	2602	699	789	15			
1	G	516	Total	C	N	O	S	0	0	0
			4105	2602	699	789	15			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLU	deletion	UNP Q13564
A	?	-	ASN	deletion	UNP Q13564
A	?	-	GLY	deletion	UNP Q13564
A	?	-	ALA	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLU	deletion	UNP Q13564
C	?	-	ASN	deletion	UNP Q13564
C	?	-	GLY	deletion	UNP Q13564
C	?	-	ALA	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLU	deletion	UNP Q13564
E	?	-	ASN	deletion	UNP Q13564
E	?	-	GLY	deletion	UNP Q13564
E	?	-	ALA	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLU	deletion	UNP Q13564
G	?	-	ASN	deletion	UNP Q13564
G	?	-	GLY	deletion	UNP Q13564
G	?	-	ALA	deletion	UNP Q13564

- Molecule 2 is a protein called ubiquitin-activating enzyme E1C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	418	Total	C	N	O	S	0	0	0
			3199	2038	549	595	17			
2	D	418	Total	C	N	O	S	0	0	0
			3199	2038	549	595	17			
2	F	418	Total	C	N	O	S	0	0	0
			3199	2038	549	595	17			
2	H	418	Total	C	N	O	S	0	0	0
			3199	2038	549	595	17			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	216	ALA	CYS	engineered mutation	UNP Q8TBC4
D	216	ALA	CYS	engineered mutation	UNP Q8TBC4
F	216	ALA	CYS	engineered mutation	UNP Q8TBC4
H	216	ALA	CYS	engineered mutation	UNP Q8TBC4

- Molecule 3 is a protein called Ubiquitin-like protein NEDD8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			
3	J	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			
3	K	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			
3	L	76	Total	C	N	O	S	0	0	0
			600	378	104	116	2			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

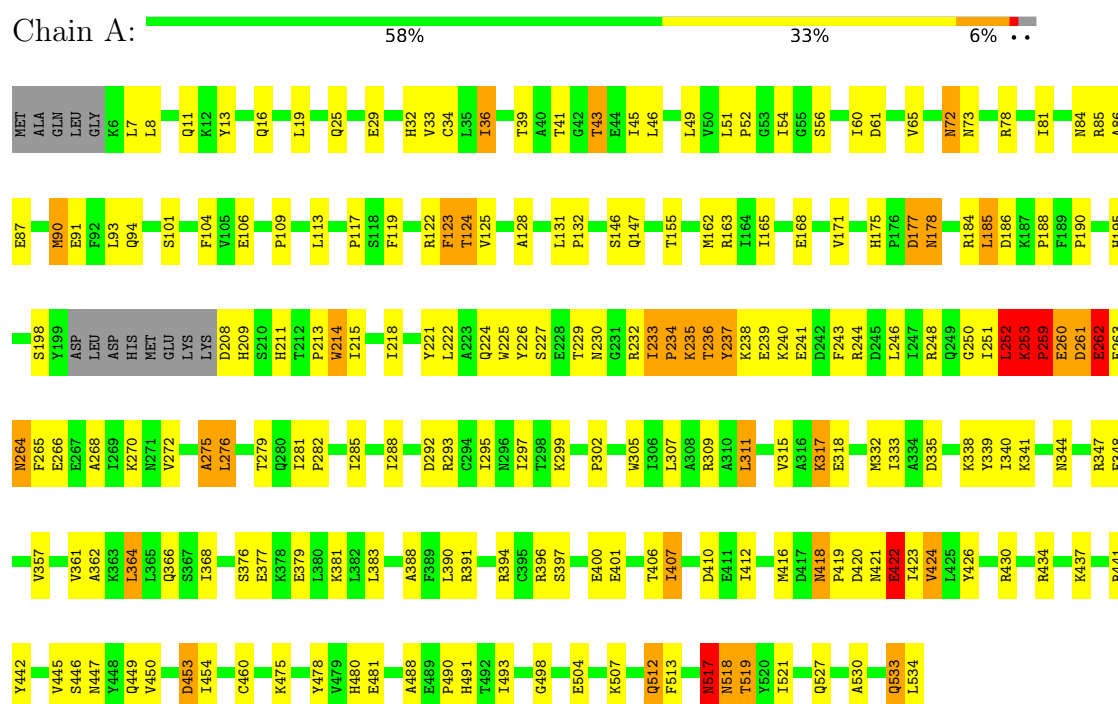
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	J	1	Total	Zn	0	0
			1	1		
4	F	1	Total	Zn	0	0
			1	1		
4	H	2	Total	Zn	0	0
			2	2		

3 Residue-property plots

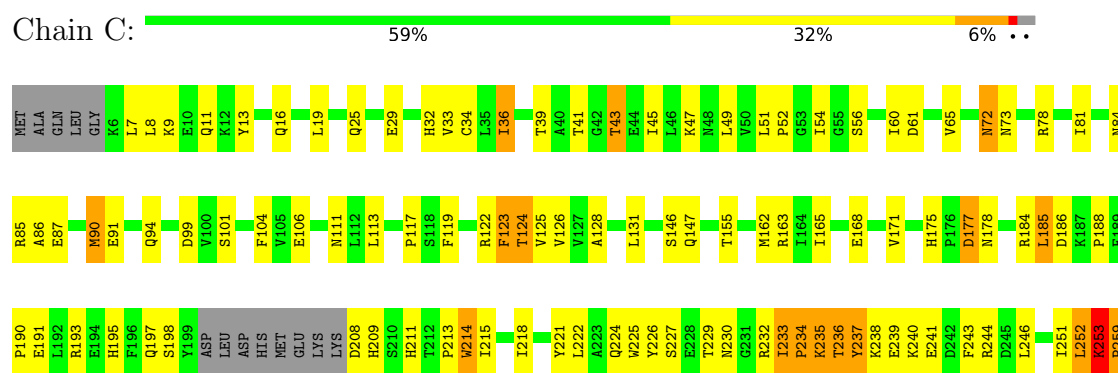
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

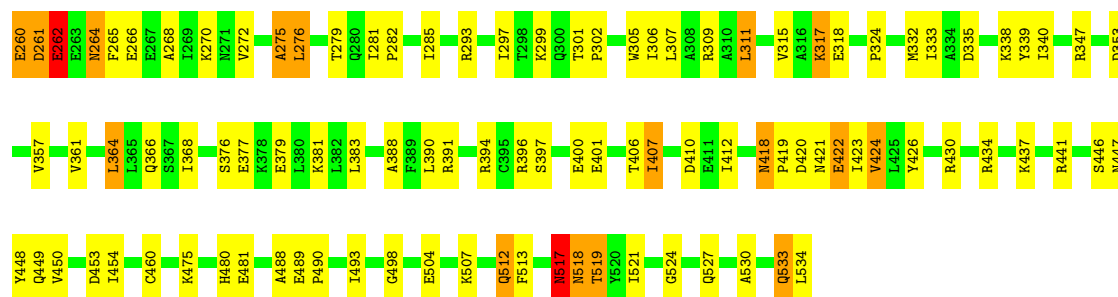
Note EDS was not executed.

- Molecule 1: amyloid beta precursor protein-binding protein 1



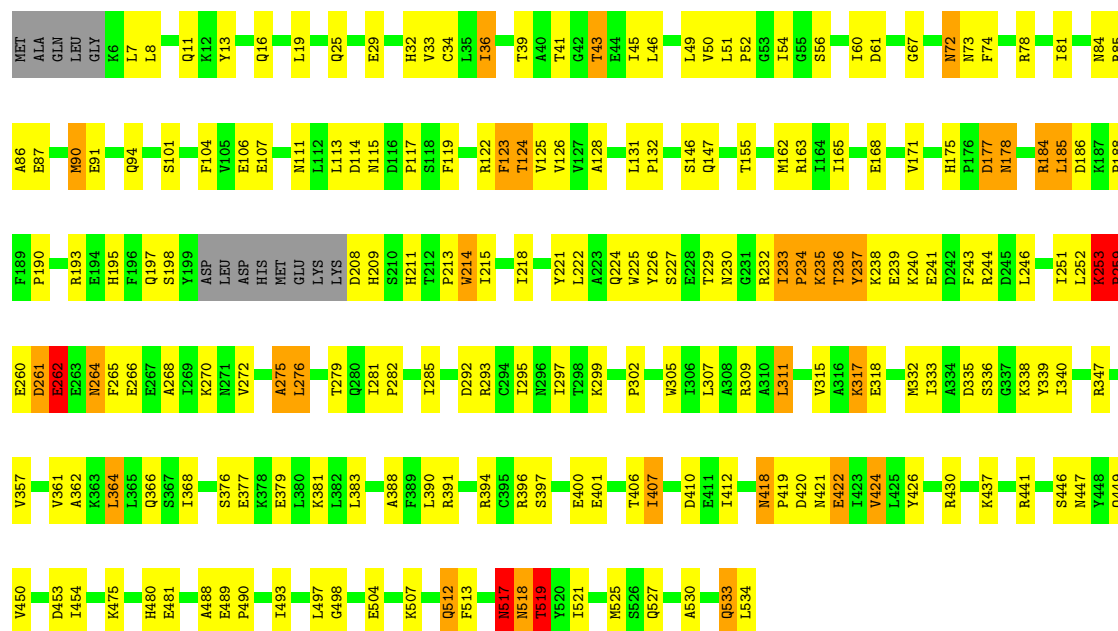
- Molecule 1: amyloid beta precursor protein-binding protein 1





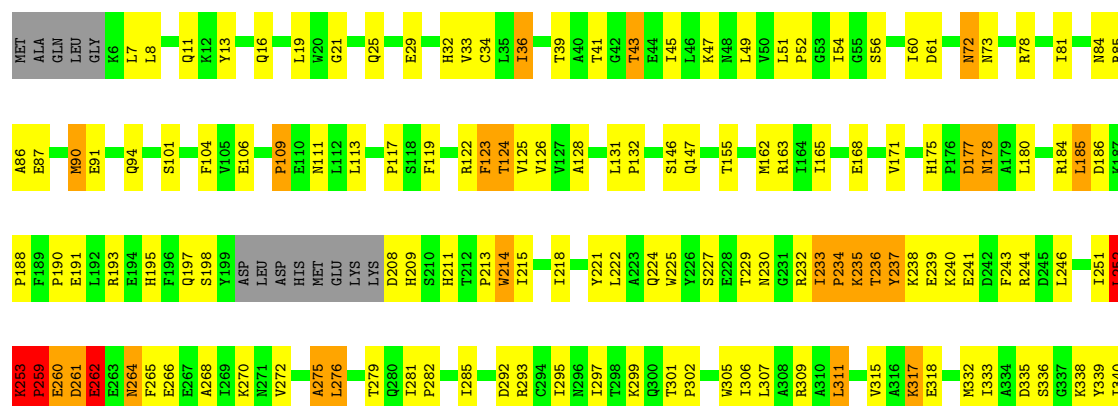
- Molecule 1: amyloid beta precursor protein-binding protein 1

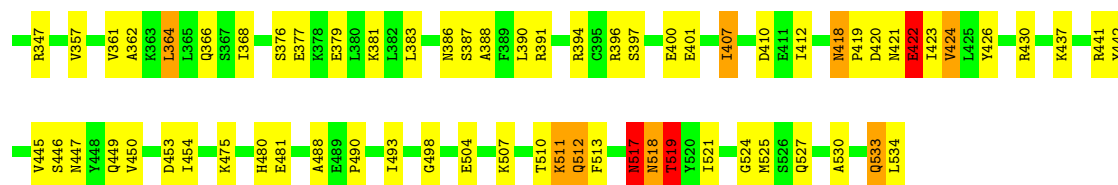
Chain E: 59% 32% 6% ..



- Molecule 1: amyloid beta precursor protein-binding protein 1

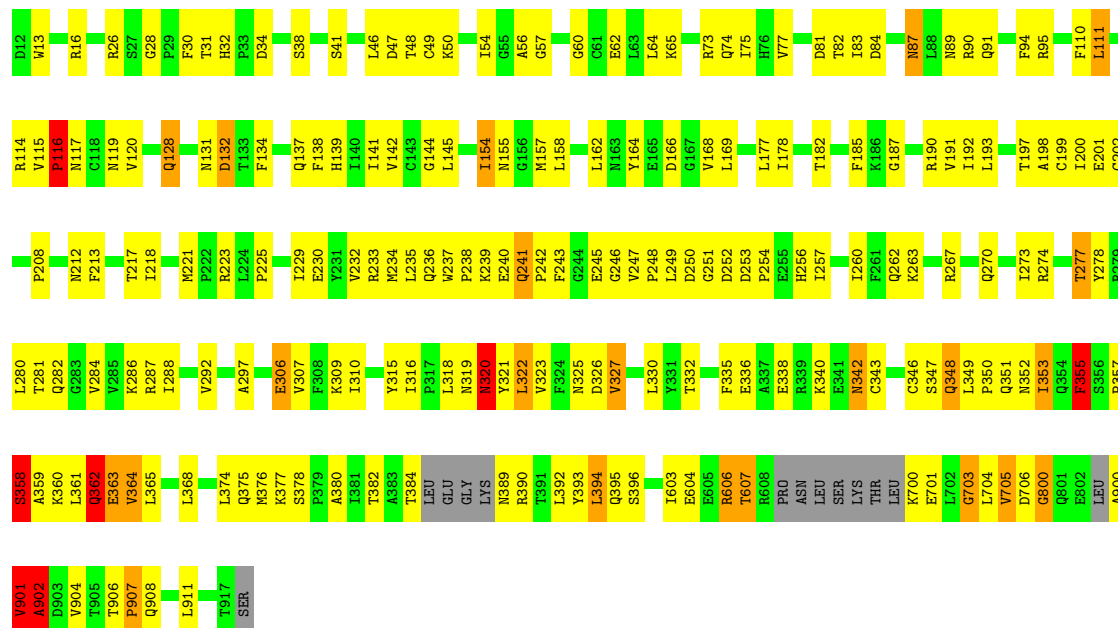
Chain G: 58% 32% 6% ..





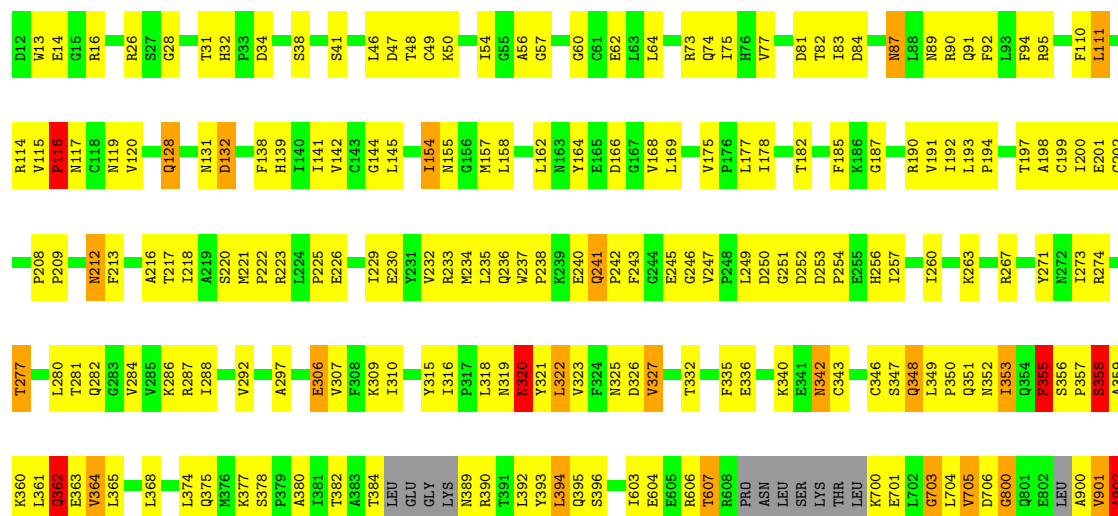
• Molecule 2: ubiquitin-activating enzyme E1C

Chain B: 49% 41% 5% . .



• Molecule 2: ubiquitin-activating enzyme E1C

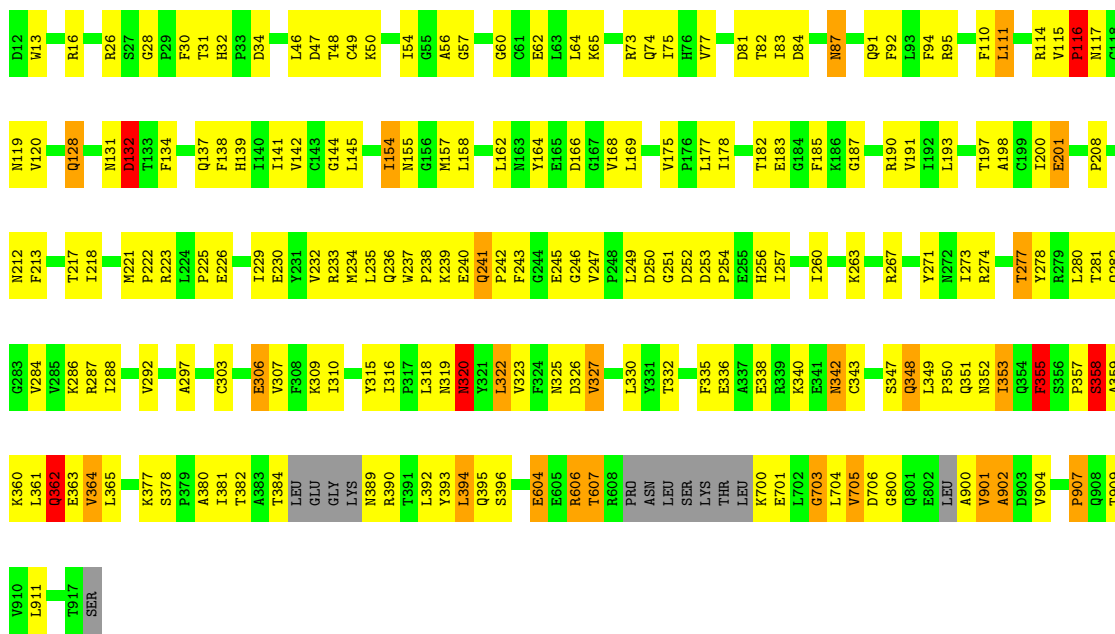
Chain D: 49% 41% 5% . .





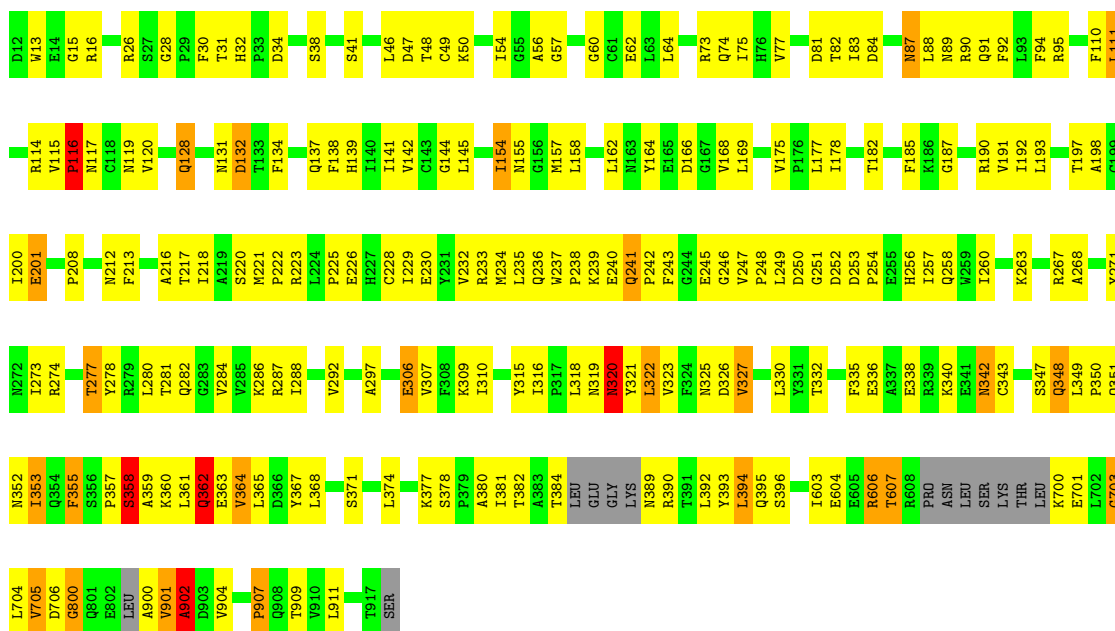
• Molecule 2: ubiquitin-activating enzyme E1C

Chain F: 51% 39% 5% ..



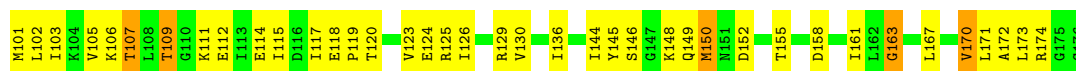
• Molecule 2: ubiquitin-activating enzyme E1C

Chain H: 48% 43% 6% ..



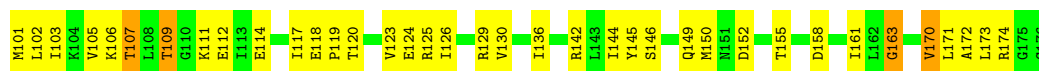
• Molecule 3: Ubiquitin-like protein NEDD8

Chain I:  49% 45% 7%



- Molecule 3: Ubiquitin-like protein NEDD8

Chain J:  51% 43% 5%

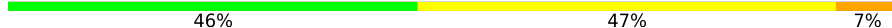


- Molecule 3: Ubiquitin-like protein NEDD8

Chain K:  50% 42% 8%



- Molecule 3: Ubiquitin-like protein NEDD8

Chain L:  46% 47% 7%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	135.40Å 198.90Å 209.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00	Depositor
% Data completeness (in resolution range)	99.9 (50.00-3.00)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.240 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	31620	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	4/4185 (0.1%)	1.04	21/5661 (0.4%)
1	C	0.56	5/4185 (0.1%)	1.02	14/5661 (0.2%)
1	E	0.53	0/4185	1.02	15/5661 (0.3%)
1	G	0.57	5/4185 (0.1%)	1.05	22/5661 (0.4%)
2	B	0.56	0/3268	1.09	21/4447 (0.5%)
2	D	0.55	1/3268 (0.0%)	1.08	19/4447 (0.4%)
2	F	0.57	1/3268 (0.0%)	1.08	21/4447 (0.5%)
2	H	0.55	0/3268	1.11	22/4447 (0.5%)
3	I	0.48	0/605	1.08	3/808 (0.4%)
3	J	0.46	0/605	1.08	3/808 (0.4%)
3	K	0.47	0/605	1.07	3/808 (0.4%)
3	L	0.43	0/605	1.07	3/808 (0.4%)
All	All	0.55	16/32232 (0.0%)	1.06	167/43664 (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
2	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	253	LYS	CA-C	11.72	1.67	1.52
1	G	253	LYS	CA-C	9.22	1.64	1.52
1	A	259	PRO	N-CA	8.76	1.58	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	259	PRO	N-CA	8.46	1.58	1.47
1	A	253	LYS	CA-C	8.42	1.63	1.52
1	G	259	PRO	N-CA	7.83	1.57	1.47
1	G	252	LEU	CA-C	7.63	1.63	1.52
1	C	253	LYS	N-CA	7.04	1.56	1.46
1	A	253	LYS	N-CA	6.01	1.54	1.46
1	G	253	LYS	N-CA	5.90	1.54	1.46
1	G	252	LEU	N-CA	5.78	1.53	1.46
1	C	253	LYS	C-N	5.76	1.47	1.33
1	C	259	PRO	C-N	-5.67	1.26	1.33
2	D	607	THR	N-CA	5.34	1.53	1.46
2	F	607	THR	C-N	5.18	1.40	1.33
1	A	253	LYS	C-N	5.08	1.45	1.33

All (167) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	355	PHE	CA-CB-CG	-16.85	96.95	113.80
1	G	259	PRO	CA-N-CD	-16.19	89.34	112.00
1	E	259	PRO	CA-N-CD	-14.75	91.35	112.00
2	D	800	GLY	N-CA-C	-14.53	92.78	112.82
2	B	800	GLY	N-CA-C	-12.78	92.69	113.02
2	H	800	GLY	N-CA-C	-12.76	92.74	113.02
1	A	259	PRO	CA-N-CD	-12.65	94.29	112.00
1	C	252	LEU	O-C-N	-9.90	109.42	122.59
2	F	800	GLY	N-CA-C	-9.57	94.68	111.62
1	A	252	LEU	O-C-N	-9.27	110.27	122.59
1	C	517	ASN	N-CA-C	9.07	122.85	111.69
1	G	517	ASN	N-CA-C	9.01	122.77	111.69
1	A	517	ASN	N-CA-C	8.92	122.66	111.69
2	F	115	VAL	CA-C-N	8.87	130.93	119.84
2	F	115	VAL	C-N-CA	8.87	130.93	119.84
2	H	115	VAL	CA-C-N	8.62	130.62	119.84
2	H	115	VAL	C-N-CA	8.62	130.62	119.84
1	E	517	ASN	N-CA-C	8.62	122.30	111.69
2	D	115	VAL	CA-C-N	8.54	130.51	119.84
2	D	115	VAL	C-N-CA	8.54	130.51	119.84
2	B	115	VAL	CA-C-N	8.51	130.48	119.84
2	B	115	VAL	C-N-CA	8.51	130.48	119.84
2	F	902	ALA	N-CA-C	-8.34	93.04	110.80
1	C	424	VAL	N-CA-C	-8.29	102.46	110.42
1	C	259	PRO	CA-C-N	8.14	131.51	120.44

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	259	PRO	C-N-CA	8.14	131.51	120.44
1	E	424	VAL	N-CA-C	-7.85	102.88	110.42
1	A	424	VAL	N-CA-C	-7.77	102.96	110.42
2	H	87	ASN	N-CA-C	-7.76	104.33	113.88
1	G	424	VAL	N-CA-C	-7.73	103.00	110.42
2	F	87	ASN	N-CA-C	-7.65	104.56	114.04
2	H	902	ALA	N-CA-C	-7.61	94.59	110.80
1	G	259	PRO	N-CA-C	7.32	127.56	112.47
2	B	87	ASN	N-CA-C	-7.28	104.93	113.88
2	D	607	THR	CA-C-N	7.04	134.38	121.70
2	D	607	THR	C-N-CA	7.04	134.38	121.70
2	D	87	ASN	N-CA-C	-6.91	105.39	113.88
2	B	907	PRO	N-CA-CB	6.77	110.36	103.25
2	F	907	PRO	N-CA-CB	6.77	110.36	103.25
2	H	907	PRO	N-CA-CB	6.72	110.31	103.25
1	A	259	PRO	CA-C-N	6.69	131.88	120.71
1	A	259	PRO	C-N-CA	6.69	131.88	120.71
2	F	607	THR	CA-C-N	6.66	133.69	121.70
2	F	607	THR	C-N-CA	6.66	133.69	121.70
1	G	123	PHE	N-CA-C	6.63	120.29	110.48
1	A	123	PHE	N-CA-C	6.61	120.26	110.48
2	B	902	ALA	N-CA-C	-6.59	96.76	110.80
2	D	907	PRO	N-CA-CB	6.55	110.13	103.25
1	C	123	PHE	N-CA-C	6.55	120.17	110.48
2	B	48	THR	N-CA-C	6.47	122.25	113.97
2	H	607	THR	CA-C-N	6.46	133.32	121.70
2	H	607	THR	C-N-CA	6.46	133.32	121.70
1	A	259	PRO	CA-CB-CG	-6.43	92.28	104.50
3	K	109	THR	N-CA-C	-6.42	103.57	112.30
3	L	150	MET	N-CA-C	6.40	120.11	110.64
2	F	48	THR	N-CA-C	6.39	122.16	113.97
2	H	48	THR	N-CA-C	6.34	122.09	113.97
1	A	259	PRO	N-CA-C	6.32	125.49	112.47
2	D	48	THR	N-CA-C	6.30	122.04	113.97
3	K	150	MET	N-CA-C	6.22	119.84	110.64
3	I	109	THR	N-CA-C	-6.20	103.87	112.30
1	A	177	ASP	N-CA-C	-6.19	99.78	109.25
2	F	320	ASN	N-CA-C	6.18	123.97	110.80
1	A	512	GLN	N-CA-C	6.18	120.95	113.17
2	B	320	ASN	N-CA-C	6.18	123.95	110.80
1	E	177	ASP	N-CA-C	-6.15	99.83	109.25
1	E	123	PHE	N-CA-C	6.10	119.51	110.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	320	ASN	N-CA-C	6.09	123.77	110.80
3	J	150	MET	N-CA-C	6.08	119.64	110.64
1	C	259	PRO	N-CA-C	6.06	124.95	112.47
3	L	109	THR	N-CA-C	-6.06	104.06	112.30
2	D	902	ALA	N-CA-C	-6.04	97.94	110.80
2	H	320	ASN	N-CA-C	6.02	123.62	110.80
1	G	185	LEU	N-CA-C	-6.00	105.04	112.90
1	E	512	GLN	N-CA-C	6.00	120.73	113.17
3	I	150	MET	N-CA-C	6.00	119.52	110.64
1	E	185	LEU	N-CA-C	-5.98	105.06	112.90
2	F	355	PHE	N-CA-C	5.96	119.86	112.59
2	B	901	VAL	O-C-N	5.90	129.95	122.57
2	H	390	ARG	N-CA-C	5.90	119.29	110.14
2	H	138	PHE	N-CA-C	5.89	119.69	110.32
1	A	185	LEU	N-CA-C	-5.86	105.22	112.90
2	B	607	THR	CA-C-N	5.85	132.23	121.70
2	B	607	THR	C-N-CA	5.85	132.23	121.70
1	G	124	THR	N-CA-C	-5.84	104.50	111.69
2	B	390	ARG	N-CA-C	5.83	119.18	110.14
1	C	504	GLU	N-CA-C	-5.82	105.02	111.36
1	C	185	LEU	N-CA-C	-5.80	105.30	112.90
1	G	518	ASN	N-CA-C	-5.78	99.52	108.42
1	G	253	LYS	CA-C-O	-5.77	112.25	120.16
1	A	184	ARG	N-CA-C	5.74	118.20	111.02
1	C	512	GLN	N-CA-C	5.74	120.41	113.17
3	J	109	THR	N-CA-C	-5.74	104.50	112.30
2	D	390	ARG	N-CA-C	5.74	119.03	110.14
2	B	355	PHE	N-CA-C	5.73	119.58	112.59
2	D	355	PHE	N-CA-C	5.72	119.57	112.59
2	H	703	GLY	N-CA-C	-5.71	105.30	113.86
3	L	174	ARG	N-CA-C	5.70	118.35	111.40
1	A	124	THR	N-CA-C	-5.68	105.17	111.36
2	D	703	GLY	N-CA-C	-5.65	105.38	113.86
2	F	138	PHE	N-CA-C	5.65	119.31	110.32
1	E	124	THR	N-CA-C	-5.65	105.20	111.36
2	F	703	GLY	N-CA-C	-5.63	105.41	113.86
3	I	174	ARG	N-CA-C	5.62	118.26	111.40
1	G	512	GLN	N-CA-C	5.61	120.24	113.17
2	B	138	PHE	N-CA-C	5.60	119.22	110.32
1	C	124	THR	N-CA-C	-5.59	105.27	111.36
1	G	259	PRO	CA-CB-CG	-5.58	93.89	104.50
2	B	703	GLY	N-CA-C	-5.56	105.52	113.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	288	ILE	N-CA-C	5.54	117.61	109.63
1	G	177	ASP	N-CA-C	-5.54	100.08	108.67
3	K	174	ARG	N-CA-C	5.52	118.14	111.40
1	G	504	GLU	N-CA-C	-5.51	105.36	111.36
1	E	519	THR	N-CA-C	5.50	122.52	110.80
1	E	518	ASN	N-CA-C	-5.49	99.97	108.42
2	F	390	ARG	N-CA-C	5.48	118.64	110.14
2	F	81	ASP	N-CA-C	5.47	118.53	110.59
2	H	144	GLY	N-CA-C	-5.47	100.21	113.18
2	H	909	THR	N-CA-C	-5.47	105.32	111.28
2	B	81	ASP	N-CA-C	5.44	118.48	110.59
2	F	909	THR	N-CA-C	-5.43	105.36	111.28
2	F	144	GLY	N-CA-C	-5.42	100.32	113.18
2	B	606	ARG	N-CA-C	-5.42	106.51	113.23
1	G	295	ILE	N-CA-C	5.41	115.62	110.53
2	B	911	LEU	N-CA-C	-5.41	105.41	112.23
1	C	518	ASN	N-CA-C	-5.39	100.11	108.42
3	J	174	ARG	N-CA-C	5.38	117.96	111.40
2	F	47	ASP	N-CA-C	5.37	118.30	111.69
1	A	295	ILE	N-CA-C	5.37	115.58	110.53
2	D	909	THR	N-CA-C	-5.37	105.43	111.28
2	F	606	ARG	N-CA-C	-5.36	106.58	113.23
2	D	47	ASP	N-CA-C	5.34	118.26	111.69
2	H	606	ARG	N-CA-C	-5.34	106.61	113.23
1	G	253	LYS	O-C-N	-5.33	115.19	121.32
2	F	288	ILE	N-CA-C	5.32	117.29	109.63
1	G	511	LYS	N-CA-C	-5.30	105.45	112.24
2	H	911	LEU	N-CA-C	-5.30	105.55	112.23
1	G	259	PRO	CA-C-N	5.30	127.65	120.44
1	G	259	PRO	C-N-CA	5.30	127.65	120.44
1	A	518	ASN	N-CA-C	-5.29	100.28	108.42
1	G	252	LEU	O-C-N	-5.28	115.56	122.59
2	H	288	ILE	N-CA-C	5.28	117.23	109.63
2	H	47	ASP	N-CA-C	5.27	118.17	111.69
2	F	911	LEU	N-CA-C	-5.26	105.60	112.23
2	B	47	ASP	N-CA-C	5.25	118.14	111.69
2	H	81	ASP	N-CA-C	5.23	118.18	110.59
2	D	144	GLY	N-CA-C	-5.23	100.78	113.18
2	B	144	GLY	N-CA-C	-5.22	100.81	113.18
1	E	504	GLU	N-CA-C	-5.22	105.59	111.28
1	A	453	ASP	N-CA-C	5.18	117.66	111.71
1	G	519	THR	N-CA-C	5.17	121.81	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	288	ILE	N-CA-C	5.17	117.07	109.63
2	D	138	PHE	N-CA-C	5.16	118.52	110.32
2	H	88	LEU	N-CA-C	5.15	119.05	112.87
1	A	504	GLU	N-CA-C	-5.15	105.75	111.36
1	E	424	VAL	CB-CA-C	-5.14	105.39	111.97
2	D	81	ASP	N-CA-C	5.13	118.03	110.59
1	G	524	GLY	N-CA-C	-5.12	107.96	114.16
1	C	177	ASP	N-CA-C	-5.12	100.17	108.41
1	A	253	LYS	CA-C-N	5.12	126.24	119.84
1	A	253	LYS	C-N-CA	5.12	126.24	119.84
1	G	109	PRO	N-CA-C	-5.12	106.16	113.47
1	A	288	ILE	N-CA-C	-5.09	105.74	110.53
1	E	295	ILE	N-CA-C	5.07	115.30	110.53
1	E	259	PRO	CA-CB-CG	-5.06	94.89	104.50
1	E	184	ARG	N-CA-C	5.03	117.31	111.02
1	C	524	GLY	N-CA-C	-5.03	108.08	114.16

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	355	PHE	Sidechain
2	D	355	PHE	Sidechain
2	F	355	PHE	Sidechain

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	4105	0	4063	213	0
1	C	4105	0	4063	217	0
1	E	4105	0	4063	235	0
1	G	4105	0	4063	220	0
2	B	3199	0	3066	206	0
2	D	3199	0	3066	202	0
2	F	3199	0	3062	196	0
2	H	3199	0	3062	202	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	600	0	635	46	0
3	J	600	0	635	45	0
3	K	600	0	635	47	0
3	L	600	0	635	48	0
4	F	1	0	0	0	0
4	H	2	0	0	0	0
4	J	1	0	0	0	0
All	All	31620	0	31048	1749	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (1749) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:LEU:O	1:A:253:LYS:C	1.90	1.14
1:G:252:LEU:O	1:G:253:LYS:C	1.93	1.12
3:K:123:VAL:HB	3:K:152:ASP:HA	1.31	1.11
3:J:123:VAL:HB	3:J:152:ASP:HA	1.33	1.08
3:I:123:VAL:HB	3:I:152:ASP:HA	1.30	1.08
2:B:274:ARG:HH22	1:E:107:GLU:HA	1.18	1.07
3:L:107:THR:HG22	3:L:111:LYS:H	1.21	1.06
3:L:123:VAL:HB	3:L:152:ASP:HA	1.35	1.05
1:E:211:HIS:HB3	1:E:335:ASP:HB2	1.39	1.05
1:A:211:HIS:HB3	1:A:335:ASP:HB2	1.39	1.03
1:G:211:HIS:HB3	1:G:335:ASP:HB2	1.38	1.03
1:C:211:HIS:HB3	1:C:335:ASP:HB2	1.40	1.02
3:K:107:THR:HG22	3:K:111:LYS:H	1.23	1.02
2:B:262:GLN:NE2	1:E:67:GLY:H	1.59	1.01
3:J:107:THR:HG22	3:J:111:LYS:H	1.22	1.01
2:D:323:VAL:HG21	3:J:170:VAL:HG22	1.44	0.99
3:I:107:THR:HG22	3:I:111:LYS:H	1.26	0.98
2:H:323:VAL:HG21	3:L:170:VAL:HG22	1.46	0.97
1:A:344:ASN:ND2	1:E:111:ASN:HD22	1.63	0.97
2:H:342:ASN:H	2:H:342:ASN:HD22	0.95	0.95
1:E:213:PRO:HB3	1:E:332:MET:HE2	1.49	0.94
1:A:213:PRO:HB3	1:A:332:MET:HE2	1.49	0.93
2:F:323:VAL:HG21	3:K:170:VAL:HG22	1.49	0.92
2:F:342:ASN:HD22	2:F:342:ASN:H	0.93	0.92
1:G:213:PRO:HB3	1:G:332:MET:HE2	1.50	0.91
1:A:421:ASN:O	1:A:424:VAL:HG23	1.71	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:421:ASN:O	1:E:424:VAL:HG23	1.71	0.91
1:A:344:ASN:HD22	1:E:111:ASN:ND2	1.68	0.90
1:C:213:PRO:HB3	1:C:332:MET:HE2	1.52	0.90
1:A:252:LEU:O	1:A:253:LYS:O	1.88	0.90
2:H:901:VAL:C	2:H:902:ALA:O	2.04	0.90
2:B:274:ARG:NH2	1:E:107:GLU:HA	1.86	0.90
2:B:342:ASN:HD22	2:B:342:ASN:N	1.68	0.90
1:G:421:ASN:O	1:G:424:VAL:HG23	1.72	0.90
2:D:342:ASN:HD22	2:D:342:ASN:H	0.92	0.89
2:H:64:LEU:HB3	2:H:111:LEU:CD1	2.02	0.89
2:F:342:ASN:HD22	2:F:342:ASN:N	1.70	0.88
1:E:253:LYS:O	1:E:260:GLU:N	2.06	0.88
2:D:901:VAL:C	2:D:902:ALA:O	2.13	0.88
2:B:342:ASN:HD22	2:B:342:ASN:H	0.92	0.88
1:C:421:ASN:O	1:C:424:VAL:HG23	1.75	0.87
2:D:342:ASN:HD22	2:D:342:ASN:N	1.70	0.87
1:E:215:ILE:HG13	1:E:332:MET:HE1	1.54	0.87
2:B:323:VAL:HG21	3:I:170:VAL:HG22	1.55	0.87
2:F:342:ASN:H	2:F:342:ASN:ND2	1.74	0.86
2:H:342:ASN:HD22	2:H:342:ASN:N	1.72	0.86
2:B:352:ASN:C	2:B:353:ILE:HD13	2.00	0.86
1:E:297:ILE:HG22	1:E:368:ILE:HD11	1.58	0.86
2:D:64:LEU:HB3	2:D:111:LEU:CD1	2.05	0.86
2:F:64:LEU:HB3	2:F:111:LEU:CD1	2.05	0.86
2:D:352:ASN:C	2:D:353:ILE:HD13	2.01	0.86
2:H:352:ASN:C	2:H:353:ILE:HD13	2.02	0.85
1:G:297:ILE:HG22	1:G:368:ILE:HD11	1.58	0.85
2:B:64:LEU:HB3	2:B:111:LEU:CD1	2.07	0.84
1:A:297:ILE:HG22	1:A:368:ILE:HD11	1.58	0.84
2:H:141:ILE:HD12	2:H:158:LEU:HD21	1.59	0.84
2:B:262:GLN:HE22	1:E:67:GLY:N	1.74	0.84
2:B:262:GLN:HE22	1:E:67:GLY:H	0.88	0.84
2:D:393:TYR:CE1	2:D:607:THR:HA	2.13	0.84
2:H:342:ASN:H	2:H:342:ASN:ND2	1.76	0.84
2:B:128:GLN:HE21	2:B:128:GLN:H	1.26	0.84
1:G:215:ILE:HG13	1:G:332:MET:HE1	1.57	0.84
2:F:141:ILE:HD12	2:F:158:LEU:HD21	1.60	0.84
2:F:352:ASN:C	2:F:353:ILE:HD13	2.02	0.83
2:H:128:GLN:HE21	2:H:128:GLN:H	1.26	0.83
2:B:208:PRO:HG3	3:I:171:LEU:HD11	1.61	0.82
2:D:141:ILE:HD12	2:D:158:LEU:HD21	1.60	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:128:GLN:HE21	2:F:128:GLN:H	1.27	0.82
1:A:215:ILE:HG13	1:A:332:MET:HE1	1.62	0.82
1:C:236:THR:HG23	1:C:237:TYR:H	1.45	0.82
1:C:297:ILE:HG22	1:C:368:ILE:HD11	1.62	0.82
2:D:128:GLN:HE21	2:D:128:GLN:H	1.28	0.82
2:B:361:LEU:O	2:B:363:GLU:N	2.13	0.82
2:D:342:ASN:H	2:D:342:ASN:ND2	1.73	0.82
1:C:215:ILE:HG13	1:C:332:MET:HE1	1.60	0.81
2:D:213:PHE:HB2	2:D:218:ILE:HD11	1.63	0.81
1:A:236:THR:HG23	1:A:237:TYR:H	1.45	0.81
2:D:14:GLU:HG3	2:H:258:GLN:HG3	1.62	0.81
3:L:107:THR:HG23	3:L:109:THR:H	1.46	0.81
2:B:141:ILE:HD12	2:B:158:LEU:HD21	1.61	0.81
1:E:236:THR:HG23	1:E:237:TYR:H	1.45	0.81
1:G:236:THR:HG23	1:G:237:TYR:H	1.44	0.80
2:H:393:TYR:CE1	2:H:607:THR:HA	2.17	0.79
3:K:107:THR:HG23	3:K:109:THR:H	1.49	0.78
3:L:155:THR:HG23	3:L:158:ASP:H	1.48	0.78
2:B:213:PHE:HB2	2:B:218:ILE:HD11	1.64	0.78
2:H:213:PHE:HB2	2:H:218:ILE:HD11	1.66	0.77
2:D:241:GLN:HE21	2:D:246:GLY:H	1.31	0.77
2:D:208:PRO:HG3	3:J:171:LEU:HD11	1.66	0.77
3:K:155:THR:HG22	3:K:158:ASP:OD2	1.84	0.77
2:B:128:GLN:H	2:B:128:GLN:NE2	1.82	0.77
2:D:128:GLN:H	2:D:128:GLN:NE2	1.82	0.77
2:B:241:GLN:HE21	2:B:246:GLY:H	1.32	0.77
3:J:107:THR:HG23	3:J:109:THR:H	1.49	0.77
3:K:155:THR:HG23	3:K:158:ASP:H	1.50	0.77
3:I:107:THR:HG23	3:I:109:THR:H	1.50	0.76
2:F:241:GLN:HE21	2:F:246:GLY:H	1.31	0.76
2:H:241:GLN:HE21	2:H:246:GLY:H	1.30	0.76
2:H:703:GLY:C	2:H:705:VAL:H	1.93	0.76
3:J:155:THR:HG23	3:J:158:ASP:H	1.49	0.76
2:F:213:PHE:HB2	2:F:218:ILE:HD11	1.67	0.76
1:E:376:SER:OG	1:E:379:GLU:HG3	1.86	0.76
2:D:351:GLN:HG3	2:D:353:ILE:HD11	1.68	0.76
2:D:703:GLY:C	2:D:705:VAL:H	1.93	0.76
2:F:703:GLY:C	2:F:705:VAL:H	1.94	0.76
2:B:342:ASN:H	2:B:342:ASN:ND2	1.73	0.75
1:G:297:ILE:CG2	1:G:368:ILE:HD11	2.15	0.75
1:A:376:SER:OG	1:A:379:GLU:HG3	1.86	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:348:GLN:HE21	2:H:348:GLN:C	1.94	0.75
2:H:208:PRO:HG3	3:L:171:LEU:HD11	1.67	0.75
1:A:224:GLN:NE2	1:A:246:LEU:HD11	2.02	0.75
3:I:155:THR:HG23	3:I:158:ASP:H	1.49	0.74
2:H:128:GLN:H	2:H:128:GLN:NE2	1.83	0.74
1:A:297:ILE:CG2	1:A:368:ILE:HD11	2.16	0.74
1:E:297:ILE:CG2	1:E:368:ILE:HD11	2.17	0.74
2:F:901:VAL:C	2:F:902:ALA:O	2.23	0.74
1:A:262:GLU:HB3	1:A:265:PHE:HB2	1.69	0.74
2:D:348:GLN:HE21	2:D:348:GLN:C	1.95	0.74
2:H:353:ILE:HB	2:H:355:PHE:CE1	2.23	0.74
3:I:155:THR:HG22	3:I:158:ASP:OD2	1.86	0.74
1:C:376:SER:OG	1:C:379:GLU:HG3	1.87	0.74
1:C:297:ILE:CG2	1:C:368:ILE:HD11	2.18	0.74
2:F:208:PRO:HG3	3:K:171:LEU:HD11	1.70	0.74
2:H:185:PHE:HB3	2:H:326:ASP:HB2	1.68	0.74
2:D:185:PHE:HB3	2:D:326:ASP:HB2	1.69	0.74
3:J:155:THR:HG22	3:J:158:ASP:OD2	1.88	0.73
2:F:128:GLN:H	2:F:128:GLN:NE2	1.84	0.73
2:B:348:GLN:C	2:B:348:GLN:HE21	1.95	0.73
2:F:348:GLN:HE21	2:F:348:GLN:C	1.95	0.73
2:F:353:ILE:HB	2:F:355:PHE:CE1	2.24	0.73
2:B:703:GLY:C	2:B:705:VAL:H	1.95	0.73
2:B:393:TYR:CE1	2:B:607:THR:HA	2.23	0.73
1:E:224:GLN:NE2	1:E:246:LEU:HD11	2.04	0.73
1:E:264:ASN:HD22	1:E:264:ASN:N	1.85	0.73
1:G:252:LEU:O	1:G:253:LYS:O	2.06	0.73
1:G:262:GLU:HB3	1:G:265:PHE:HB2	1.70	0.73
1:G:376:SER:OG	1:G:379:GLU:HG3	1.87	0.73
2:D:361:LEU:O	2:D:363:GLU:N	2.21	0.73
1:E:262:GLU:HB3	1:E:265:PHE:HB2	1.71	0.73
1:A:264:ASN:HD22	1:A:264:ASN:N	1.84	0.73
2:B:267:ARG:HG2	2:B:267:ARG:HH11	1.53	0.73
2:D:322:LEU:HD12	2:D:323:VAL:N	2.04	0.73
1:G:264:ASN:N	1:G:264:ASN:HD22	1.86	0.73
1:C:224:GLN:NE2	1:C:246:LEU:HD11	2.04	0.72
1:C:264:ASN:HD22	1:C:264:ASN:N	1.85	0.72
1:E:317:LYS:HB3	1:E:318:GLU:OE1	1.89	0.72
2:B:185:PHE:HB3	2:B:326:ASP:HB2	1.70	0.72
2:F:361:LEU:O	2:F:364:VAL:HG22	1.89	0.72
2:H:322:LEU:HD12	2:H:323:VAL:N	2.05	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:262:GLU:HB3	1:C:265:PHE:HB2	1.70	0.72
2:D:267:ARG:HG2	2:D:267:ARG:HH11	1.55	0.72
2:F:351:GLN:HG3	2:F:353:ILE:HD11	1.71	0.72
2:H:351:GLN:HG3	2:H:353:ILE:HD11	1.70	0.72
3:L:155:THR:HG22	3:L:158:ASP:OD2	1.89	0.72
2:F:361:LEU:O	2:F:363:GLU:N	2.22	0.72
2:H:267:ARG:HG2	2:H:267:ARG:HH11	1.55	0.72
2:D:361:LEU:O	2:D:364:VAL:HG22	1.90	0.72
2:F:393:TYR:CE1	2:F:607:THR:HA	2.24	0.72
2:B:351:GLN:HG3	2:B:353:ILE:HD11	1.71	0.71
2:H:901:VAL:O	2:H:902:ALA:O	2.07	0.71
2:H:361:LEU:O	2:H:363:GLU:N	2.23	0.71
1:A:317:LYS:HB3	1:A:318:GLU:OE1	1.90	0.71
1:G:224:GLN:NE2	1:G:246:LEU:HD11	2.06	0.71
3:J:124:GLU:HB2	3:J:152:ASP:O	1.90	0.71
1:E:340:ILE:HD11	2:F:273:ILE:HG12	1.73	0.71
1:G:61:ASP:HB3	1:G:86:ALA:HB2	1.73	0.71
2:B:50:LYS:H	2:B:139:HIS:CD2	2.09	0.71
2:H:62:GLU:HG2	2:H:297:ALA:HA	1.73	0.71
1:A:61:ASP:HB3	1:A:86:ALA:HB2	1.72	0.70
2:B:353:ILE:HB	2:B:355:PHE:CE1	2.26	0.70
1:A:224:GLN:HE22	1:A:246:LEU:HD11	1.55	0.70
1:E:251:ILE:HG23	1:E:262:GLU:HB2	1.73	0.70
2:H:322:LEU:HD12	2:H:322:LEU:C	2.16	0.70
3:I:101:MET:HB3	3:I:117:ILE:O	1.92	0.70
2:D:50:LYS:H	2:D:139:HIS:CD2	2.10	0.70
2:F:185:PHE:HB3	2:F:326:ASP:HB2	1.72	0.70
1:G:251:ILE:HG23	1:G:262:GLU:HB2	1.74	0.70
1:C:61:ASP:HB3	1:C:86:ALA:HB2	1.74	0.70
1:C:251:ILE:HG23	1:C:262:GLU:HB2	1.72	0.70
2:D:322:LEU:HD12	2:D:322:LEU:C	2.17	0.70
2:D:187:GLY:HA2	3:J:173:LEU:HD13	1.72	0.70
2:H:361:LEU:O	2:H:364:VAL:HG22	1.92	0.70
3:L:101:MET:HB3	3:L:117:ILE:O	1.90	0.70
2:B:54:ILE:HG22	2:B:145:LEU:HD21	1.73	0.70
3:I:124:GLU:HB2	3:I:152:ASP:O	1.92	0.70
2:D:393:TYR:HE1	2:D:607:THR:HA	1.55	0.70
3:L:124:GLU:HB2	3:L:152:ASP:O	1.92	0.70
3:K:123:VAL:CB	3:K:152:ASP:HA	2.17	0.70
2:H:50:LYS:H	2:H:139:HIS:CD2	2.10	0.70
2:H:901:VAL:O	2:H:902:ALA:C	2.30	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:ARG:HG2	1:A:163:ARG:HH11	1.56	0.70
1:A:61:ASP:OD2	1:A:85:ARG:HD2	1.92	0.69
2:F:62:GLU:HG2	2:F:297:ALA:HA	1.74	0.69
1:G:317:LYS:HB3	1:G:318:GLU:OE1	1.92	0.69
2:B:202:CYS:SG	2:B:343:CYS:SG	2.90	0.69
1:E:224:GLN:HE22	1:E:246:LEU:HD11	1.58	0.69
1:C:224:GLN:HE22	1:C:246:LEU:HD11	1.58	0.69
2:F:322:LEU:C	2:F:322:LEU:HD12	2.18	0.69
1:C:517:ASN:O	1:C:517:ASN:ND2	2.26	0.69
1:E:61:ASP:HB3	1:E:86:ALA:HB2	1.75	0.69
1:E:517:ASN:ND2	1:E:517:ASN:O	2.26	0.69
2:F:54:ILE:HG22	2:F:145:LEU:HD21	1.74	0.69
2:F:267:ARG:HG2	2:F:267:ARG:HH11	1.57	0.69
3:K:124:GLU:HB2	3:K:152:ASP:O	1.93	0.69
2:B:199:CYS:SG	2:B:346:CYS:SG	2.91	0.69
2:B:322:LEU:C	2:B:322:LEU:HD12	2.18	0.69
3:J:123:VAL:CB	3:J:152:ASP:HA	2.18	0.69
1:A:251:ILE:HG23	1:A:262:GLU:HB2	1.75	0.68
1:C:163:ARG:HG2	1:C:163:ARG:HH11	1.59	0.68
1:E:49:LEU:C	1:E:52:PRO:HD2	2.18	0.68
2:F:241:GLN:NE2	2:F:246:GLY:H	1.91	0.68
1:A:178:ASN:HD22	3:I:136:ILE:HG12	1.57	0.68
2:D:187:GLY:CA	3:J:173:LEU:HD13	2.23	0.68
2:F:322:LEU:HD12	2:F:323:VAL:N	2.09	0.68
1:G:61:ASP:OD2	1:G:85:ARG:HD2	1.93	0.68
2:D:901:VAL:O	2:D:902:ALA:O	2.10	0.68
1:A:235:LYS:HB3	1:A:239:GLU:HB2	1.76	0.68
2:F:50:LYS:H	2:F:139:HIS:CD2	2.11	0.68
2:H:187:GLY:HA2	3:L:173:LEU:HD13	1.75	0.68
3:I:123:VAL:CB	3:I:152:ASP:HA	2.17	0.68
1:G:340:ILE:HD11	2:H:273:ILE:HG12	1.75	0.68
2:B:322:LEU:HD12	2:B:323:VAL:N	2.08	0.68
3:K:101:MET:HB3	3:K:117:ILE:O	1.93	0.68
2:H:241:GLN:NE2	2:H:246:GLY:H	1.92	0.68
1:A:264:ASN:HD22	1:A:264:ASN:H	1.42	0.68
1:A:517:ASN:O	1:A:517:ASN:ND2	2.26	0.68
1:C:61:ASP:OD2	1:C:85:ARG:HD2	1.93	0.68
1:C:235:LYS:HB3	1:C:239:GLU:HB2	1.74	0.68
2:D:62:GLU:HG2	2:D:297:ALA:HA	1.76	0.68
1:G:224:GLN:HE22	1:G:246:LEU:HD11	1.59	0.68
1:A:240:LYS:HE2	1:A:276:LEU:HD12	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:GLU:HG2	2:B:297:ALA:HA	1.75	0.67
1:C:317:LYS:HB3	1:C:318:GLU:OE1	1.94	0.67
1:E:163:ARG:HH11	1:E:163:ARG:HG2	1.58	0.67
1:C:264:ASN:HD22	1:C:264:ASN:H	1.42	0.67
3:J:101:MET:HB3	3:J:117:ILE:O	1.94	0.67
1:G:517:ASN:O	1:G:517:ASN:ND2	2.26	0.67
1:A:195:HIS:O	1:A:198:SER:HB3	1.94	0.67
2:D:241:GLN:NE2	2:D:246:GLY:H	1.92	0.67
2:F:900:ALA:O	2:F:901:VAL:CB	2.43	0.67
1:C:177:ASP:OD2	2:D:327:VAL:HG21	1.95	0.67
1:A:344:ASN:ND2	1:E:111:ASN:ND2	2.31	0.66
1:C:260:GLU:O	1:C:261:ASP:HB2	1.94	0.66
1:G:8:LEU:HD12	1:G:11:GLN:OE1	1.96	0.66
2:B:241:GLN:NE2	2:B:246:GLY:H	1.93	0.66
2:F:393:TYR:HE1	2:F:607:THR:HA	1.59	0.66
1:A:307:LEU:HB3	1:A:383:LEU:HD22	1.78	0.66
1:E:235:LYS:HB3	1:E:239:GLU:HB2	1.77	0.66
1:E:307:LEU:HB3	1:E:383:LEU:HD22	1.75	0.66
2:H:54:ILE:HG22	2:H:145:LEU:HD21	1.78	0.66
1:G:41:THR:O	1:G:45:ILE:HG13	1.96	0.66
1:G:347:ARG:HH22	2:H:274:ARG:HD2	1.59	0.66
1:A:49:LEU:C	1:A:52:PRO:HD2	2.21	0.66
2:B:705:VAL:O	2:B:800:GLY:O	2.14	0.66
2:D:901:VAL:O	2:D:902:ALA:C	2.39	0.66
2:D:54:ILE:HG22	2:D:145:LEU:HD21	1.78	0.66
1:G:163:ARG:HG2	1:G:163:ARG:HH11	1.59	0.66
2:B:901:VAL:C	2:B:902:ALA:O	2.32	0.66
2:F:384:THR:HA	2:F:389:ASN:HA	1.77	0.66
1:G:235:LYS:HB3	1:G:239:GLU:HB2	1.77	0.66
1:A:401:GLU:HG3	1:A:533:GLN:HE22	1.61	0.65
1:A:517:ASN:HD22	1:A:517:ASN:C	2.04	0.65
2:B:384:THR:HA	2:B:389:ASN:HA	1.78	0.65
1:C:45:ILE:HG12	1:C:498:GLY:HA2	1.78	0.65
2:D:705:VAL:O	2:D:800:GLY:O	2.14	0.65
2:H:237:TRP:HB3	2:H:238:PRO:HD3	1.78	0.65
1:A:285:ILE:HD11	1:A:388:ALA:HA	1.79	0.65
2:B:900:ALA:O	2:B:901:VAL:CB	2.44	0.65
2:H:187:GLY:CA	3:L:173:LEU:HD13	2.26	0.65
2:D:384:THR:HA	2:D:389:ASN:HA	1.78	0.65
3:K:117:ILE:HD13	3:K:126:ILE:HG12	1.78	0.65
2:B:361:LEU:O	2:B:364:VAL:HG22	1.97	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:384:THR:HA	2:H:389:ASN:HA	1.78	0.65
1:C:195:HIS:O	1:C:198:SER:HB3	1.96	0.65
2:D:353:ILE:HB	2:D:355:PHE:CE1	2.31	0.65
1:E:61:ASP:OD2	1:E:85:ARG:HD2	1.97	0.65
1:G:297:ILE:HD11	1:G:309:ARG:HG2	1.78	0.65
2:H:393:TYR:HE1	2:H:607:THR:HA	1.57	0.65
1:E:240:LYS:HE2	1:E:276:LEU:HD12	1.78	0.65
2:B:199:CYS:SG	2:B:202:CYS:SG	2.94	0.65
2:B:16:ARG:NH2	2:B:116:PRO:HB2	2.13	0.64
1:G:401:GLU:HG3	1:G:533:GLN:HE22	1.62	0.64
1:C:297:ILE:HD11	1:C:309:ARG:HG2	1.80	0.64
2:D:900:ALA:O	2:D:901:VAL:CB	2.45	0.64
1:E:264:ASN:HD22	1:E:264:ASN:H	1.45	0.64
1:E:397:SER:OG	1:E:400:GLU:HG3	1.97	0.64
3:K:155:THR:HG22	3:K:158:ASP:CG	2.22	0.64
1:C:422:GLU:HG3	1:C:530:ALA:HB3	1.79	0.64
2:D:202:CYS:HG	2:D:343:CYS:HG	1.42	0.64
2:F:235:LEU:O	2:F:238:PRO:HD2	1.97	0.64
1:G:240:LYS:HE2	1:G:276:LEU:HD12	1.78	0.64
1:G:264:ASN:HD22	1:G:264:ASN:H	1.45	0.64
1:G:397:SER:OG	1:G:400:GLU:HG3	1.98	0.64
2:B:235:LEU:O	2:B:238:PRO:HD2	1.98	0.64
1:C:51:LEU:HB2	1:C:52:PRO:HD3	1.80	0.64
1:E:45:ILE:HG12	1:E:498:GLY:HA2	1.80	0.64
2:B:277:THR:HG23	2:B:280:LEU:H	1.63	0.64
1:C:8:LEU:HD12	1:C:11:GLN:OE1	1.98	0.64
1:E:195:HIS:O	1:E:198:SER:HB3	1.98	0.64
1:C:307:LEU:HB3	1:C:383:LEU:HD22	1.80	0.63
1:E:8:LEU:HD12	1:E:11:GLN:OE1	1.98	0.63
1:G:49:LEU:C	1:G:52:PRO:HD2	2.22	0.63
1:G:422:GLU:HG3	1:G:530:ALA:HB3	1.80	0.63
1:A:33:VAL:CG2	1:A:54:ILE:HD11	2.29	0.63
2:B:358:SER:O	2:B:358:SER:OG	2.14	0.63
1:C:390:LEU:O	1:C:391:ARG:HG2	1.97	0.63
1:C:41:THR:O	1:C:45:ILE:HG13	1.97	0.63
1:C:235:LYS:HB3	1:C:239:GLU:CG	2.28	0.63
1:G:260:GLU:O	1:G:261:ASP:HB2	1.97	0.63
2:F:187:GLY:HA2	3:K:173:LEU:HD13	1.81	0.63
2:H:229:ILE:HD13	2:H:281:THR:HA	1.80	0.63
2:D:235:LEU:O	2:D:238:PRO:HD2	1.99	0.63
2:B:95:ARG:HH11	2:B:95:ARG:HG3	1.64	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:TYR:HE1	2:B:607:THR:HA	1.62	0.63
2:F:229:ILE:HD13	2:F:281:THR:HA	1.80	0.63
2:H:335:PHE:CZ	3:L:144:ILE:HD13	2.34	0.63
1:A:8:LEU:HD12	1:A:11:GLN:OE1	1.98	0.63
1:C:235:LYS:HD3	1:C:239:GLU:HG3	1.80	0.63
2:F:95:ARG:HH11	2:F:95:ARG:HG3	1.63	0.63
1:A:45:ILE:HG12	1:A:498:GLY:HA2	1.81	0.63
2:B:237:TRP:HB3	2:B:238:PRO:HD3	1.79	0.63
1:C:448:TYR:CE2	2:H:240:GLU:OE2	2.52	0.63
2:D:393:TYR:CD1	2:D:607:THR:HA	2.34	0.63
3:J:117:ILE:HD13	3:J:126:ILE:HG12	1.81	0.63
1:G:285:ILE:HD11	1:G:388:ALA:HA	1.81	0.63
2:H:95:ARG:HH11	2:H:95:ARG:HG3	1.63	0.63
1:G:195:HIS:O	1:G:198:SER:HB3	1.99	0.62
2:H:277:THR:HG23	2:H:280:LEU:H	1.64	0.62
1:E:401:GLU:HG3	1:E:533:GLN:HE22	1.64	0.62
2:B:252:ASP:O	2:B:254:PRO:HD3	1.99	0.62
1:C:241:GLU:HA	1:C:244:ARG:HH11	1.65	0.62
2:F:277:THR:HG23	2:F:280:LEU:H	1.65	0.62
1:C:446:SER:HB2	1:C:449:GLN:HG3	1.79	0.62
1:G:45:ILE:HG12	1:G:498:GLY:HA2	1.80	0.62
3:L:155:THR:HG22	3:L:158:ASP:CG	2.24	0.62
1:A:297:ILE:HD11	1:A:309:ARG:HG2	1.81	0.62
2:F:237:TRP:HB3	2:F:238:PRO:HD3	1.82	0.62
1:G:307:LEU:HB3	1:G:383:LEU:HD22	1.79	0.62
1:G:517:ASN:C	1:G:517:ASN:HD22	2.08	0.62
2:B:306:GLU:OE2	2:B:309:LYS:HD2	1.98	0.62
2:D:95:ARG:HG3	2:D:95:ARG:HH11	1.64	0.62
2:D:229:ILE:HD13	2:D:281:THR:HA	1.81	0.62
3:J:155:THR:HG22	3:J:158:ASP:CG	2.25	0.62
1:E:41:THR:O	1:E:45:ILE:HG13	2.00	0.62
1:A:396:ARG:HG3	1:A:534:LEU:HD11	1.81	0.62
3:I:155:THR:HG22	3:I:158:ASP:CG	2.25	0.62
3:K:106:LYS:HG3	3:K:112:GLU:HB2	1.81	0.62
1:A:51:LEU:HB2	1:A:52:PRO:HD3	1.81	0.62
1:E:309:ARG:HG3	1:E:364:LEU:HD21	1.82	0.62
3:K:125:ARG:HD3	3:K:129:ARG:NH2	2.15	0.62
1:A:241:GLU:HA	1:A:244:ARG:HH11	1.65	0.62
2:D:252:ASP:O	2:D:254:PRO:HD3	2.00	0.62
3:J:125:ARG:HD3	3:J:129:ARG:NH2	2.15	0.62
3:K:170:VAL:HG13	3:K:171:LEU:N	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:285:ILE:HD11	1:C:388:ALA:HA	1.82	0.62
1:E:297:ILE:HD11	1:E:309:ARG:HG2	1.81	0.61
1:E:347:ARG:HH22	2:F:274:ARG:HD2	1.65	0.61
1:G:241:GLU:HA	1:G:244:ARG:HH11	1.65	0.61
1:C:397:SER:OG	1:C:400:GLU:HG3	1.99	0.61
1:E:56:SER:HB3	1:E:101:SER:OG	2.01	0.61
1:E:422:GLU:HG3	1:E:530:ALA:HB3	1.82	0.61
1:G:51:LEU:HB2	1:G:52:PRO:HD3	1.82	0.61
1:C:517:ASN:HD22	1:C:517:ASN:C	2.08	0.61
1:G:124:THR:HG22	1:G:125:VAL:HG23	1.81	0.61
1:G:235:LYS:HD3	1:G:239:GLU:HG3	1.82	0.61
2:H:338:GLU:HG3	3:L:148:LYS:HD3	1.82	0.61
1:A:285:ILE:CD1	1:A:388:ALA:HA	2.31	0.61
1:C:49:LEU:C	1:C:52:PRO:HD2	2.25	0.61
1:C:340:ILE:HD11	2:D:273:ILE:HG12	1.82	0.61
1:C:448:TYR:HE2	2:H:240:GLU:OE2	1.84	0.61
1:E:235:LYS:HB3	1:E:239:GLU:CG	2.30	0.61
1:E:235:LYS:HD3	1:E:239:GLU:HG3	1.82	0.61
3:L:106:LYS:HG3	3:L:112:GLU:HB2	1.82	0.61
2:H:252:ASP:O	2:H:254:PRO:HD3	2.00	0.61
3:L:125:ARG:HD3	3:L:129:ARG:NH2	2.15	0.61
1:A:446:SER:HB2	1:A:449:GLN:HG3	1.81	0.61
2:B:237:TRP:O	2:B:242:PRO:HD3	2.01	0.61
1:E:241:GLU:HA	1:E:244:ARG:HH11	1.66	0.61
1:E:390:LEU:O	1:E:391:ARG:HG2	2.01	0.61
2:B:187:GLY:HA2	3:I:173:LEU:HD13	1.81	0.61
1:E:285:ILE:HD11	1:E:388:ALA:HA	1.83	0.61
1:E:396:ARG:HG3	1:E:534:LEU:HD11	1.83	0.61
1:E:517:ASN:C	1:E:517:ASN:HD22	2.08	0.61
2:H:193:LEU:H	2:H:197:THR:HB	1.65	0.61
1:C:214:TRP:CZ3	1:C:332:MET:HB3	2.36	0.61
1:C:396:ARG:HG3	1:C:534:LEU:HD11	1.83	0.61
2:B:64:LEU:HD21	2:B:77:VAL:CG2	2.30	0.61
2:D:351:GLN:CG	2:D:353:ILE:HD11	2.30	0.61
3:L:123:VAL:CB	3:L:152:ASP:HA	2.22	0.61
1:A:235:LYS:HD3	1:A:239:GLU:HG3	1.83	0.60
2:H:237:TRP:O	2:H:242:PRO:HD3	2.01	0.60
1:A:260:GLU:O	1:A:261:ASP:HB2	2.00	0.60
3:I:106:LYS:HG3	3:I:112:GLU:HB2	1.84	0.60
1:C:235:LYS:HE2	1:C:238:LYS:HB3	1.83	0.60
2:D:237:TRP:HB3	2:D:238:PRO:HD3	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:705:VAL:O	2:H:800:GLY:O	2.19	0.60
1:A:311:LEU:O	1:A:315:VAL:HG23	2.00	0.60
1:C:178:ASN:HD22	3:J:136:ILE:HG12	1.66	0.60
1:G:235:LYS:HE2	1:G:238:LYS:HB3	1.82	0.60
1:G:396:ARG:HG3	1:G:534:LEU:HD11	1.82	0.60
3:J:106:LYS:HG3	3:J:112:GLU:HB2	1.82	0.60
2:F:237:TRP:O	2:F:242:PRO:HD3	2.01	0.60
1:G:390:LEU:O	1:G:391:ARG:HG2	2.02	0.60
3:L:125:ARG:HD3	3:L:129:ARG:HH21	1.66	0.60
1:A:397:SER:OG	1:A:400:GLU:HG3	2.00	0.60
3:I:117:ILE:HD13	3:I:126:ILE:HG12	1.83	0.60
2:D:343:CYS:O	2:D:347:SER:HB3	2.01	0.60
1:E:333:ILE:HA	2:F:223:ARG:NH2	2.15	0.60
1:E:446:SER:HB2	1:E:449:GLN:HG3	1.83	0.60
1:A:104:PHE:HE1	1:A:106:GLU:HG3	1.66	0.60
1:E:450:VAL:O	1:E:454:ILE:HG13	2.00	0.60
1:G:517:ASN:ND2	1:G:534:LEU:HD12	2.16	0.60
2:H:318:LEU:HD12	2:H:319:ASN:H	1.66	0.60
2:H:362:GLN:OE1	2:H:362:GLN:HA	2.01	0.60
1:A:390:LEU:O	1:A:391:ARG:HG2	2.02	0.60
2:B:54:ILE:CG2	2:B:145:LEU:HD21	2.31	0.60
3:I:125:ARG:HD3	3:I:129:ARG:NH2	2.16	0.60
2:F:343:CYS:O	2:F:347:SER:HB3	2.01	0.60
1:C:33:VAL:CG2	1:C:54:ILE:HD11	2.31	0.60
2:D:16:ARG:NH2	2:D:116:PRO:HB2	2.17	0.60
2:D:64:LEU:HD21	2:D:77:VAL:CG2	2.32	0.60
1:E:33:VAL:CG2	1:E:54:ILE:HD11	2.32	0.60
1:E:178:ASN:HD22	3:K:136:ILE:HG12	1.66	0.60
1:G:446:SER:HB2	1:G:449:GLN:HG3	1.83	0.60
2:B:362:GLN:OE1	2:B:362:GLN:HA	2.01	0.60
2:D:50:LYS:H	2:D:139:HIS:HD2	1.49	0.60
2:F:252:ASP:O	2:F:254:PRO:HD3	2.02	0.60
1:G:235:LYS:HB3	1:G:239:GLU:CG	2.31	0.60
2:F:358:SER:O	2:F:358:SER:OG	2.17	0.60
2:B:229:ILE:HD13	2:B:281:THR:HA	1.83	0.59
1:E:177:ASP:OD2	2:F:327:VAL:HG21	2.02	0.59
1:G:422:GLU:HG3	1:G:530:ALA:CB	2.32	0.59
2:B:325:ASN:HD21	2:B:327:VAL:HG22	1.68	0.59
1:C:517:ASN:ND2	1:C:534:LEU:HD12	2.16	0.59
1:E:214:TRP:CZ3	1:E:332:MET:HB3	2.38	0.59
2:H:306:GLU:OE2	2:H:309:LYS:HD2	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:362:GLN:HA	2:D:362:GLN:OE1	2.01	0.59
3:J:125:ARG:HD3	3:J:129:ARG:HH21	1.67	0.59
2:F:193:LEU:H	2:F:197:THR:HB	1.68	0.59
2:H:358:SER:O	2:H:358:SER:OG	2.17	0.59
1:A:422:GLU:HG3	1:A:530:ALA:HB3	1.83	0.59
1:C:235:LYS:HB3	1:C:239:GLU:CB	2.32	0.59
2:D:306:GLU:OE2	2:D:309:LYS:HD2	2.02	0.59
3:K:125:ARG:HD3	3:K:129:ARG:HH21	1.68	0.59
1:A:235:LYS:HB3	1:A:239:GLU:CG	2.31	0.59
2:F:54:ILE:CG2	2:F:145:LEU:HD21	2.32	0.59
1:C:401:GLU:HG3	1:C:533:GLN:HE22	1.68	0.59
2:D:193:LEU:H	2:D:197:THR:HB	1.68	0.59
1:G:507:LYS:HG2	1:G:513:PHE:HB2	1.84	0.59
1:A:178:ASN:ND2	3:I:136:ILE:HG12	2.17	0.59
2:B:16:ARG:HH22	2:B:116:PRO:HB2	1.67	0.59
1:E:104:PHE:HE1	1:E:106:GLU:HG3	1.66	0.59
2:F:335:PHE:CZ	3:K:144:ILE:HD13	2.38	0.59
2:H:64:LEU:HD21	2:H:77:VAL:CG2	2.33	0.59
1:A:517:ASN:ND2	1:A:534:LEU:HD12	2.17	0.59
1:G:285:ILE:CD1	1:G:388:ALA:HA	2.33	0.59
2:B:187:GLY:CA	3:I:173:LEU:HD13	2.32	0.58
1:E:309:ARG:CG	1:E:364:LEU:HD21	2.32	0.58
1:E:488:ALA:O	1:E:490:PRO:HD3	2.03	0.58
2:F:187:GLY:CA	3:K:173:LEU:HD13	2.33	0.58
3:K:149:GLN:HG3	3:K:149:GLN:O	2.02	0.58
1:G:377:GLU:OE2	1:G:381:LYS:HE3	2.03	0.58
3:I:125:ARG:HD3	3:I:129:ARG:HH21	1.68	0.58
1:E:285:ILE:CD1	1:E:388:ALA:HA	2.33	0.58
1:A:60:ILE:HD11	1:A:119:PHE:HE2	1.68	0.58
2:B:351:GLN:CG	2:B:353:ILE:HD11	2.33	0.58
2:D:277:THR:HG23	2:D:280:LEU:H	1.67	0.58
2:D:335:PHE:CZ	3:J:144:ILE:HD13	2.39	0.58
3:J:170:VAL:HG13	3:J:171:LEU:N	2.18	0.58
1:E:235:LYS:HE2	1:E:238:LYS:HB3	1.84	0.58
2:F:306:GLU:OE2	2:F:309:LYS:HD2	2.02	0.58
1:A:214:TRP:C	1:A:214:TRP:CD1	2.81	0.58
3:I:149:GLN:O	3:I:149:GLN:HG3	2.02	0.58
1:C:309:ARG:HG3	1:C:364:LEU:HD21	1.85	0.58
1:E:218:ILE:O	1:E:222:LEU:HB2	2.03	0.58
1:E:377:GLU:OE2	1:E:381:LYS:HE3	2.03	0.58
1:G:309:ARG:HG3	1:G:364:LEU:HD21	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:TRP:O	2:D:242:PRO:HD3	2.02	0.58
2:H:701:GLU:HA	2:H:704:LEU:CB	2.34	0.58
1:A:309:ARG:HG3	1:A:364:LEU:HD21	1.85	0.58
1:C:104:PHE:HE1	1:C:106:GLU:HG3	1.68	0.58
1:E:311:LEU:O	1:E:315:VAL:HG23	2.04	0.58
2:F:362:GLN:OE1	2:F:362:GLN:HA	2.03	0.58
1:C:25:GLN:O	1:C:29:GLU:HG3	2.04	0.58
1:C:285:ILE:CD1	1:C:388:ALA:HA	2.34	0.58
1:E:260:GLU:O	1:E:261:ASP:HB2	2.03	0.58
1:G:450:VAL:O	1:G:454:ILE:HG13	2.02	0.58
2:H:318:LEU:HD12	2:H:319:ASN:N	2.19	0.58
1:A:124:THR:HG22	1:A:125:VAL:HG23	1.84	0.58
3:I:170:VAL:HG13	3:I:171:LEU:N	2.18	0.58
1:C:454:ILE:HD13	1:C:480:HIS:ND1	2.19	0.58
2:D:325:ASN:HD21	2:D:327:VAL:HG22	1.67	0.58
2:F:325:ASN:HD21	2:F:327:VAL:HG22	1.69	0.58
1:G:78:ARG:O	1:G:81:ILE:HG13	2.03	0.58
1:A:177:ASP:OD2	2:B:327:VAL:HG21	2.04	0.58
1:C:178:ASN:ND2	3:J:136:ILE:HG12	2.18	0.58
1:C:218:ILE:O	1:C:222:LEU:HB2	2.04	0.58
1:C:240:LYS:HE2	1:C:276:LEU:HD12	1.85	0.58
1:C:377:GLU:OE2	1:C:381:LYS:HE3	2.03	0.58
2:H:235:LEU:O	2:H:238:PRO:HD2	2.03	0.58
2:H:343:CYS:O	2:H:347:SER:HB3	2.04	0.58
1:C:214:TRP:CE3	1:C:332:MET:HB3	2.39	0.58
1:E:517:ASN:ND2	1:E:534:LEU:HD12	2.18	0.58
1:G:214:TRP:CZ3	1:G:332:MET:HB3	2.39	0.58
2:B:335:PHE:CZ	3:I:144:ILE:HD13	2.38	0.57
2:D:164:TYR:CE2	2:D:169:LEU:HB2	2.39	0.57
2:F:64:LEU:HD21	2:F:77:VAL:CG2	2.33	0.57
1:G:33:VAL:CG2	1:G:54:ILE:HD11	2.34	0.57
1:G:454:ILE:HD13	1:G:480:HIS:ND1	2.18	0.57
2:H:217:THR:HA	2:H:221:MET:HG2	1.86	0.57
2:H:351:GLN:CG	2:H:353:ILE:HD11	2.33	0.57
1:A:235:LYS:HE2	1:A:238:LYS:HB3	1.84	0.57
1:A:454:ILE:HD13	1:A:480:HIS:ND1	2.19	0.57
2:D:325:ASN:ND2	2:D:327:VAL:HG22	2.18	0.57
1:E:507:LYS:HG2	1:E:513:PHE:HB2	1.85	0.57
1:E:481:GLU:HB2	2:F:30:PHE:HE1	1.69	0.57
1:A:450:VAL:O	1:A:454:ILE:HG13	2.04	0.57
2:D:243:PHE:O	2:D:247:VAL:HG21	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:351:GLN:CG	2:F:353:ILE:HD11	2.33	0.57
2:H:325:ASN:HD21	2:H:327:VAL:HG22	1.70	0.57
2:H:393:TYR:CD1	2:H:607:THR:HA	2.39	0.57
1:E:488:ALA:C	1:E:490:PRO:HD3	2.29	0.57
1:G:214:TRP:CD1	1:G:214:TRP:C	2.81	0.57
1:G:418:ASN:ND2	1:G:420:ASP:H	2.03	0.57
1:A:56:SER:HB3	1:A:101:SER:OG	2.05	0.57
2:B:208:PRO:HG3	3:I:171:LEU:CD1	2.32	0.57
1:E:33:VAL:HG23	1:E:54:ILE:HD11	1.85	0.57
2:H:164:TYR:CE2	2:H:169:LEU:HB2	2.39	0.57
3:L:170:VAL:HG13	3:L:171:LEU:N	2.19	0.57
1:A:218:ILE:O	1:A:222:LEU:HB2	2.03	0.57
2:D:202:CYS:SG	2:D:343:CYS:SG	2.91	0.57
1:E:124:THR:HG22	1:E:125:VAL:HG23	1.86	0.57
2:H:64:LEU:HB3	2:H:111:LEU:HD13	1.86	0.57
1:A:33:VAL:HG23	1:A:54:ILE:HD11	1.86	0.57
1:G:104:PHE:HE1	1:G:106:GLU:HG3	1.69	0.57
1:C:124:THR:HG22	1:C:125:VAL:HG23	1.86	0.57
1:C:214:TRP:CD1	1:C:214:TRP:C	2.82	0.57
1:C:309:ARG:CG	1:C:364:LEU:HD21	2.35	0.57
1:E:214:TRP:CD1	1:E:214:TRP:C	2.82	0.57
1:G:218:ILE:O	1:G:222:LEU:HB2	2.04	0.57
1:E:39:THR:O	1:E:43:THR:HB	2.05	0.57
3:K:118:GLU:O	3:K:120:THR:N	2.38	0.57
1:A:377:GLU:OE2	1:A:381:LYS:HE3	2.05	0.56
1:C:347:ARG:HH22	2:D:274:ARG:HD2	1.70	0.56
2:D:84:ASP:H	2:D:87:ASN:ND2	2.03	0.56
2:D:701:GLU:HA	2:D:704:LEU:CB	2.35	0.56
2:H:50:LYS:H	2:H:139:HIS:HD2	1.51	0.56
2:H:178:ILE:HD11	2:H:310:ILE:HD12	1.86	0.56
2:B:164:TYR:CE2	2:B:169:LEU:HB2	2.40	0.56
2:B:193:LEU:H	2:B:197:THR:HB	1.68	0.56
1:E:235:LYS:HB3	1:E:239:GLU:CB	2.36	0.56
2:F:132:ASP:HA	2:F:157:MET:HE2	1.87	0.56
3:L:118:GLU:O	3:L:120:THR:N	2.39	0.56
1:A:36:ILE:HB	1:A:128:ALA:HA	1.87	0.56
1:E:113:LEU:O	1:E:117:PRO:HG3	2.06	0.56
2:F:392:LEU:O	2:F:606:ARG:CB	2.54	0.56
3:L:149:GLN:HG3	3:L:149:GLN:O	2.05	0.56
1:A:418:ASN:ND2	1:A:420:ASP:H	2.01	0.56
2:B:325:ASN:ND2	2:B:327:VAL:HG22	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:SER:HB3	1:C:101:SER:OG	2.04	0.56
1:C:418:ASN:ND2	1:C:420:ASP:H	2.03	0.56
1:C:450:VAL:O	1:C:454:ILE:HG13	2.06	0.56
1:E:527:GLN:OE1	1:E:527:GLN:HA	2.05	0.56
1:E:51:LEU:HB2	1:E:52:PRO:HD3	1.87	0.56
1:A:25:GLN:O	1:A:29:GLU:HG3	2.06	0.56
1:A:104:PHE:CE1	1:A:106:GLU:HG3	2.41	0.56
1:A:235:LYS:HB3	1:A:239:GLU:CB	2.35	0.56
1:C:422:GLU:HG3	1:C:530:ALA:CB	2.35	0.56
3:J:118:GLU:O	3:J:120:THR:N	2.39	0.56
1:G:235:LYS:HB3	1:G:239:GLU:CB	2.36	0.56
1:G:418:ASN:C	1:G:418:ASN:HD22	2.14	0.56
2:H:243:PHE:O	2:H:247:VAL:HG21	2.05	0.56
2:B:217:THR:HA	2:B:221:MET:HG2	1.88	0.56
2:B:217:THR:HG21	2:B:223:ARG:HH22	1.70	0.56
2:B:251:GLY:O	2:B:286:LYS:HE3	2.05	0.56
3:J:155:THR:O	3:J:158:ASP:HB2	2.06	0.56
1:E:104:PHE:CE1	1:E:106:GLU:HG3	2.41	0.56
1:E:422:GLU:HG3	1:E:530:ALA:CB	2.36	0.56
1:C:39:THR:O	1:C:43:THR:HB	2.06	0.56
1:C:60:ILE:HD11	1:C:119:PHE:HE2	1.71	0.56
2:D:208:PRO:HG3	3:J:171:LEU:CD1	2.36	0.56
2:F:164:TYR:CE2	2:F:169:LEU:HB2	2.41	0.56
1:G:56:SER:HB3	1:G:101:SER:OG	2.06	0.56
2:H:16:ARG:NH2	2:H:116:PRO:HB2	2.21	0.56
3:L:107:THR:HG22	3:L:111:LYS:N	2.06	0.56
1:C:260:GLU:HG3	1:C:261:ASP:N	2.21	0.56
1:C:507:LYS:HG2	1:C:513:PHE:HB2	1.87	0.56
1:G:25:GLN:O	1:G:29:GLU:HG3	2.06	0.56
2:D:251:GLY:O	2:D:257:ILE:HD11	2.06	0.56
2:D:377:LYS:O	2:D:378:SER:C	2.49	0.56
3:J:149:GLN:HG3	3:J:149:GLN:O	2.06	0.56
1:E:441:ARG:NH2	1:E:453:ASP:OD2	2.39	0.56
2:F:178:ILE:HD11	2:F:310:ILE:HD12	1.87	0.56
2:H:54:ILE:CG2	2:H:145:LEU:HD21	2.35	0.56
1:A:309:ARG:CG	1:A:364:LEU:HD21	2.36	0.55
1:A:527:GLN:OE1	1:A:527:GLN:HA	2.05	0.55
1:C:113:LEU:O	1:C:117:PRO:HG3	2.06	0.55
1:E:418:ASN:ND2	1:E:420:ASP:H	2.04	0.55
2:F:325:ASN:ND2	2:F:327:VAL:HG22	2.21	0.55
3:K:155:THR:O	3:K:158:ASP:HB2	2.04	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:900:ALA:O	2:H:901:VAL:CB	2.53	0.55
1:A:430:ARG:HB3	1:A:430:ARG:NH1	2.21	0.55
1:A:447:ASN:ND2	2:B:26:ARG:HH21	2.03	0.55
3:I:118:GLU:O	3:I:120:THR:N	2.39	0.55
1:C:488:ALA:C	1:C:490:PRO:HD3	2.31	0.55
2:D:54:ILE:CG2	2:D:145:LEU:HD21	2.36	0.55
3:L:155:THR:O	3:L:158:ASP:HB2	2.04	0.55
1:C:418:ASN:HD22	1:C:419:PRO:CD	2.19	0.55
1:G:60:ILE:HD11	1:G:119:PHE:HE2	1.71	0.55
1:G:488:ALA:C	1:G:490:PRO:HD3	2.31	0.55
1:E:25:GLN:O	1:E:29:GLU:HG3	2.06	0.55
1:G:233:ILE:N	1:G:234:PRO:HD3	2.21	0.55
1:A:78:ARG:O	1:A:81:ILE:HG13	2.05	0.55
1:A:418:ASN:HD22	1:A:418:ASN:C	2.15	0.55
1:A:41:THR:O	1:A:45:ILE:HG13	2.05	0.55
1:A:215:ILE:CG1	1:A:332:MET:HE1	2.36	0.55
1:C:419:PRO:HB2	1:C:475:LYS:HE3	1.88	0.55
2:F:50:LYS:H	2:F:139:HIS:HD2	1.52	0.55
1:A:233:ILE:N	1:A:234:PRO:HD3	2.21	0.55
1:A:251:ILE:O	1:A:252:LEU:C	2.50	0.55
1:A:441:ARG:NH2	1:A:453:ASP:OD2	2.40	0.55
1:C:33:VAL:HG23	1:C:54:ILE:HD11	1.87	0.55
1:C:36:ILE:HB	1:C:128:ALA:HA	1.89	0.55
1:E:347:ARG:HH12	2:F:274:ARG:HD2	1.71	0.55
2:F:217:THR:HA	2:F:221:MET:HG2	1.89	0.55
2:F:703:GLY:C	2:F:705:VAL:N	2.64	0.55
1:G:177:ASP:OD2	2:H:327:VAL:HG21	2.07	0.55
1:A:332:MET:HG2	1:A:339:TYR:HE1	1.72	0.55
1:A:422:GLU:HG3	1:A:530:ALA:CB	2.36	0.55
1:A:488:ALA:O	1:A:490:PRO:HD3	2.07	0.55
3:I:155:THR:O	3:I:158:ASP:HB2	2.07	0.55
1:C:233:ILE:N	1:C:234:PRO:HD3	2.22	0.55
1:C:311:LEU:O	1:C:315:VAL:HG23	2.07	0.55
3:J:102:LEU:HD11	3:J:114:GLU:HG2	1.88	0.55
1:G:311:LEU:O	1:G:315:VAL:HG23	2.07	0.55
1:G:332:MET:HG2	1:G:339:TYR:HE1	1.71	0.55
2:F:64:LEU:HB3	2:F:111:LEU:HD13	1.86	0.55
3:L:117:ILE:HD13	3:L:126:ILE:HG12	1.87	0.55
1:A:507:LYS:HG2	1:A:513:PHE:HB2	1.88	0.54
2:B:225:PRO:HG3	2:B:274:ARG:O	2.07	0.54
1:C:527:GLN:HA	1:C:527:GLN:OE1	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:ILE:N	1:E:234:PRO:HD3	2.21	0.54
2:F:243:PHE:O	2:F:247:VAL:HG21	2.06	0.54
1:G:309:ARG:CG	1:G:364:LEU:HD21	2.37	0.54
2:H:84:ASP:H	2:H:87:ASN:ND2	2.05	0.54
1:A:214:TRP:CZ3	1:A:332:MET:HB3	2.42	0.54
2:B:178:ILE:HD11	2:B:310:ILE:HD12	1.89	0.54
2:D:217:THR:HA	2:D:221:MET:HG2	1.89	0.54
1:E:332:MET:HG2	1:E:339:TYR:HE1	1.72	0.54
2:F:701:GLU:HA	2:F:704:LEU:CB	2.37	0.54
2:H:232:VAL:HG11	2:H:263:LYS:HB2	1.89	0.54
1:A:419:PRO:HB2	1:A:475:LYS:HE3	1.89	0.54
2:B:132:ASP:HA	2:B:157:MET:HE2	1.89	0.54
2:B:701:GLU:HA	2:B:704:LEU:CB	2.37	0.54
2:D:16:ARG:HH22	2:D:116:PRO:HB2	1.72	0.54
1:E:214:TRP:CE3	1:E:332:MET:HB3	2.43	0.54
2:B:377:LYS:O	2:B:378:SER:C	2.49	0.54
2:D:257:ILE:HD13	2:D:282:GLN:HG2	1.89	0.54
3:J:172:ALA:C	3:J:173:LEU:HG	2.32	0.54
2:F:73:ARG:HD3	2:F:117:ASN:O	2.06	0.54
2:B:49:CYS:HA	2:B:139:HIS:HD2	1.73	0.54
2:B:50:LYS:H	2:B:139:HIS:HD2	1.51	0.54
2:B:233:ARG:HH12	2:B:234:MET:HB2	1.73	0.54
1:E:36:ILE:HB	1:E:128:ALA:HA	1.90	0.54
2:F:377:LYS:O	2:F:378:SER:C	2.50	0.54
2:H:256:HIS:O	2:H:260:ILE:HG13	2.08	0.54
2:H:392:LEU:O	2:H:606:ARG:CB	2.55	0.54
1:A:39:THR:O	1:A:43:THR:HB	2.06	0.54
1:A:340:ILE:HD11	2:B:273:ILE:HG12	1.89	0.54
2:F:232:VAL:HG11	2:F:263:LYS:HB2	1.90	0.54
1:C:441:ARG:NH2	1:C:453:ASP:OD1	2.40	0.54
2:D:703:GLY:C	2:D:705:VAL:N	2.63	0.54
1:E:215:ILE:CG1	1:E:332:MET:HE1	2.32	0.54
2:F:251:GLY:O	2:F:286:LYS:HE3	2.07	0.54
1:G:214:TRP:CE3	1:G:332:MET:HB3	2.43	0.54
2:F:251:GLY:O	2:F:257:ILE:HD11	2.07	0.54
2:B:49:CYS:HA	2:B:139:HIS:CD2	2.43	0.54
2:B:257:ILE:HD13	2:B:282:GLN:HG2	1.90	0.54
2:B:392:LEU:O	2:B:606:ARG:CB	2.55	0.54
1:C:208:ASP:OD1	1:C:211:HIS:HB2	2.08	0.54
1:C:441:ARG:NH2	1:C:453:ASP:OD2	2.40	0.54
2:F:16:ARG:NH2	2:F:116:PRO:HB2	2.23	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:132:ASP:HA	2:H:157:MET:HE2	1.90	0.54
3:I:102:LEU:HD11	3:I:114:GLU:HG2	1.89	0.54
2:D:132:ASP:HA	2:D:157:MET:HE2	1.89	0.54
2:D:233:ARG:HH12	2:D:234:MET:HB2	1.73	0.54
1:E:418:ASN:C	1:E:418:ASN:HD22	2.16	0.54
1:G:33:VAL:HG23	1:G:54:ILE:HD11	1.90	0.54
1:E:178:ASN:ND2	3:K:136:ILE:HG12	2.23	0.53
2:H:32:HIS:CD2	2:H:34:ASP:H	2.26	0.53
1:A:447:ASN:HD22	2:B:26:ARG:HH21	1.56	0.53
3:I:172:ALA:C	3:I:173:LEU:HG	2.33	0.53
2:D:199:CYS:SG	2:D:202:CYS:SG	2.95	0.53
2:D:361:LEU:O	2:D:364:VAL:CG2	2.56	0.53
1:E:49:LEU:O	1:E:52:PRO:HD2	2.08	0.53
1:E:454:ILE:HD13	1:E:480:HIS:ND1	2.23	0.53
2:F:241:GLN:HG3	2:F:245:GLU:HA	1.90	0.53
1:G:447:ASN:ND2	2:H:26:ARG:HH21	2.07	0.53
1:A:229:THR:O	1:A:230:ASN:CB	2.57	0.53
2:B:243:PHE:O	2:B:247:VAL:HG21	2.08	0.53
1:C:418:ASN:HD22	1:C:418:ASN:C	2.14	0.53
1:E:78:ARG:O	1:E:81:ILE:HG13	2.08	0.53
1:E:175:HIS:HD2	1:E:512:GLN:O	1.92	0.53
3:K:102:LEU:HD11	3:K:114:GLU:HG2	1.90	0.53
3:L:172:ALA:C	3:L:173:LEU:HG	2.32	0.53
1:A:264:ASN:N	1:A:264:ASN:ND2	2.55	0.53
1:A:488:ALA:C	1:A:490:PRO:HD3	2.32	0.53
2:B:128:GLN:NE2	2:B:128:GLN:N	2.56	0.53
2:B:131:ASN:HB3	2:D:131:ASN:HD22	1.74	0.53
1:C:488:ALA:O	1:C:490:PRO:HD3	2.08	0.53
2:D:353:ILE:HB	2:D:355:PHE:CZ	2.43	0.53
1:E:163:ARG:HG3	1:E:519:THR:H	1.73	0.53
1:G:419:PRO:HB2	1:G:475:LYS:HE3	1.90	0.53
1:A:163:ARG:NH2	1:A:518:ASN:HD21	2.06	0.53
1:C:262:GLU:OE1	1:C:262:GLU:HA	2.09	0.53
2:D:318:LEU:HD12	2:D:319:ASN:H	1.74	0.53
2:H:353:ILE:HB	2:H:355:PHE:CZ	2.42	0.53
2:B:251:GLY:O	2:B:257:ILE:HD11	2.08	0.53
1:C:104:PHE:CE1	1:C:106:GLU:HG3	2.43	0.53
2:D:225:PRO:HG3	2:D:274:ARG:O	2.09	0.53
2:D:241:GLN:HG3	2:D:245:GLU:HA	1.90	0.53
1:G:488:ALA:O	1:G:490:PRO:HD3	2.08	0.53
1:A:232:ARG:C	1:A:233:ILE:HG13	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:ARG:HD3	2:B:117:ASN:O	2.09	0.53
1:C:407:ILE:HG23	1:C:407:ILE:O	2.08	0.53
1:C:430:ARG:NH1	1:C:430:ARG:HB3	2.23	0.53
2:D:49:CYS:HA	2:D:139:HIS:HD2	1.74	0.53
1:E:418:ASN:HD22	1:E:419:PRO:CD	2.22	0.53
2:F:208:PRO:HG3	3:K:171:LEU:CD1	2.39	0.53
2:F:256:HIS:O	2:F:260:ILE:HG13	2.09	0.53
1:G:185:LEU:O	1:G:188:PRO:HD3	2.09	0.53
1:G:215:ILE:CG1	1:G:332:MET:HE1	2.34	0.53
2:H:325:ASN:ND2	2:H:327:VAL:HG22	2.23	0.53
1:A:208:ASP:OD1	1:A:211:HIS:HB2	2.08	0.53
1:C:78:ARG:O	1:C:81:ILE:HG13	2.09	0.53
1:C:264:ASN:N	1:C:264:ASN:ND2	2.57	0.53
2:D:49:CYS:HA	2:D:139:HIS:CD2	2.44	0.53
2:D:351:GLN:CD	2:D:353:ILE:HD11	2.33	0.53
1:E:264:ASN:N	1:E:264:ASN:ND2	2.57	0.53
2:F:49:CYS:HA	2:F:139:HIS:CD2	2.43	0.53
2:F:318:LEU:HD12	2:F:319:ASN:H	1.73	0.53
3:K:117:ILE:HD11	3:K:126:ILE:HG23	1.90	0.53
1:A:262:GLU:OE1	1:A:262:GLU:HA	2.08	0.53
2:F:64:LEU:HD11	2:F:77:VAL:HG21	1.90	0.53
2:H:251:GLY:O	2:H:257:ILE:HD11	2.08	0.53
2:H:340:LYS:HB3	2:H:342:ASN:ND2	2.24	0.53
2:F:32:HIS:CD2	2:F:34:ASP:H	2.26	0.53
2:H:349:LEU:HB3	2:H:350:PRO:CD	2.38	0.53
1:A:119:PHE:O	1:A:122:ARG:HG3	2.08	0.52
1:C:175:HIS:HD2	1:C:512:GLN:O	1.92	0.52
1:C:264:ASN:H	1:C:264:ASN:ND2	2.08	0.52
2:F:280:LEU:O	2:F:284:VAL:HG23	2.09	0.52
2:F:318:LEU:HD12	2:F:319:ASN:N	2.25	0.52
1:G:34:CYS:HB2	1:G:123:PHE:CG	2.43	0.52
1:G:36:ILE:HB	1:G:128:ALA:HA	1.91	0.52
1:G:208:ASP:OD1	1:G:211:HIS:HB2	2.09	0.52
1:G:264:ASN:N	1:G:264:ASN:ND2	2.57	0.52
2:H:225:PRO:HG3	2:H:274:ARG:O	2.09	0.52
2:B:64:LEU:HB3	2:B:111:LEU:HD13	1.88	0.52
1:C:119:PHE:O	1:C:122:ARG:HG3	2.10	0.52
1:C:418:ASN:HD22	1:C:419:PRO:N	2.08	0.52
1:E:307:LEU:HB3	1:E:383:LEU:CD2	2.39	0.52
2:F:225:PRO:HG3	2:F:274:ARG:O	2.09	0.52
1:A:348:GLU:HG3	1:E:115:ASN:CG	2.34	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:OE2	2:B:315:TYR:HE2	1.92	0.52
2:B:202:CYS:HG	2:B:343:CYS:HG	1.51	0.52
1:E:419:PRO:HB2	1:E:475:LYS:HE3	1.90	0.52
2:H:377:LYS:O	2:H:378:SER:C	2.52	0.52
2:B:131:ASN:HD22	2:D:131:ASN:HB3	1.75	0.52
2:D:73:ARG:HD3	2:D:117:ASN:O	2.09	0.52
2:F:361:LEU:O	2:F:364:VAL:CG2	2.56	0.52
1:G:104:PHE:CE1	1:G:106:GLU:HG3	2.44	0.52
2:H:249:LEU:CD1	2:H:260:ILE:HD11	2.40	0.52
2:D:343:CYS:SG	2:D:346:CYS:SG	3.08	0.52
2:F:249:LEU:CD1	2:F:260:ILE:HD11	2.40	0.52
1:G:113:LEU:O	1:G:117:PRO:HG3	2.10	0.52
2:H:217:THR:HG21	2:H:223:ARG:HH22	1.75	0.52
2:H:257:ILE:HD13	2:H:282:GLN:HG2	1.91	0.52
2:B:232:VAL:HG11	2:B:263:LYS:HB2	1.92	0.52
1:C:253:LYS:O	1:C:260:GLU:N	2.42	0.52
2:D:240:GLU:O	2:D:241:GLN:C	2.53	0.52
2:F:232:VAL:HA	2:F:236:GLN:HB3	1.91	0.52
1:G:235:LYS:NZ	1:G:238:LYS:HD3	2.25	0.52
2:H:73:ARG:HD3	2:H:117:ASN:O	2.09	0.52
2:B:240:GLU:O	2:B:241:GLN:C	2.53	0.52
2:B:361:LEU:O	2:B:362:GLN:C	2.52	0.52
2:D:46:LEU:O	2:D:73:ARG:HB2	2.10	0.52
3:J:107:THR:HG22	3:J:111:LYS:N	2.07	0.52
2:H:155:ASN:CG	2:H:200:ILE:HB	2.35	0.52
2:H:351:GLN:HA	2:H:351:GLN:HE21	1.75	0.52
1:A:61:ASP:CB	1:A:86:ALA:HB2	2.37	0.52
2:D:318:LEU:HD12	2:D:319:ASN:N	2.25	0.52
1:G:336:SER:HB2	2:H:221:MET:HA	1.92	0.52
2:H:240:GLU:O	2:H:241:GLN:C	2.53	0.52
1:C:215:ILE:CG1	1:C:332:MET:HE1	2.37	0.52
2:D:351:GLN:HE21	2:D:351:GLN:HA	1.75	0.52
1:G:215:ILE:H	1:G:332:MET:HE1	1.75	0.52
2:H:49:CYS:HA	2:H:139:HIS:CD2	2.44	0.52
2:H:142:VAL:HG21	2:H:307:VAL:HG21	1.91	0.52
1:A:264:ASN:H	1:A:264:ASN:ND2	2.06	0.52
1:A:348:GLU:HG3	1:E:115:ASN:ND2	2.24	0.52
2:B:318:LEU:HD12	2:B:319:ASN:H	1.75	0.52
1:E:441:ARG:NH2	1:E:453:ASP:OD1	2.42	0.52
2:F:49:CYS:HA	2:F:139:HIS:HD2	1.73	0.52
1:A:175:HIS:HD2	1:A:512:GLN:O	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:234:PRO:O	1:E:235:LYS:C	2.53	0.51
1:G:61:ASP:CB	1:G:86:ALA:HB2	2.39	0.51
1:G:262:GLU:OE1	1:G:262:GLU:HA	2.08	0.51
1:A:214:TRP:CE3	1:A:332:MET:HB3	2.46	0.51
2:B:343:CYS:O	2:B:347:SER:HB3	2.10	0.51
2:D:233:ARG:NH1	2:D:233:ARG:HG2	2.25	0.51
1:E:163:ARG:NH1	1:E:165:ILE:HG12	2.25	0.51
1:G:264:ASN:H	1:G:264:ASN:ND2	2.09	0.51
2:B:393:TYR:CD1	2:B:607:THR:HA	2.45	0.51
2:D:232:VAL:HG11	2:D:263:LYS:HB2	1.92	0.51
1:E:34:CYS:HB2	1:E:123:PHE:CG	2.45	0.51
2:F:349:LEU:HB3	2:F:350:PRO:CD	2.40	0.51
1:G:7:LEU:O	1:G:11:GLN:HG3	2.11	0.51
1:G:39:THR:O	1:G:43:THR:HB	2.11	0.51
1:G:418:ASN:HD22	1:G:419:PRO:CD	2.23	0.51
2:H:251:GLY:O	2:H:286:LYS:HE3	2.10	0.51
1:A:418:ASN:HD22	1:A:419:PRO:CD	2.23	0.51
1:C:61:ASP:CB	1:C:86:ALA:HB2	2.39	0.51
1:C:221:TYR:HD2	1:C:246:LEU:HG	1.76	0.51
2:F:351:GLN:CD	2:F:353:ILE:HD11	2.36	0.51
1:G:441:ARG:NH2	1:G:453:ASP:OD2	2.42	0.51
2:B:351:GLN:HE21	2:B:351:GLN:HA	1.76	0.51
1:G:481:GLU:HB2	2:H:30:PHE:HE1	1.76	0.51
2:H:361:LEU:O	2:H:364:VAL:CG2	2.57	0.51
3:I:111:LYS:O	3:I:112:GLU:HB3	2.11	0.51
1:C:332:MET:HG2	1:C:339:TYR:HE1	1.76	0.51
1:E:60:ILE:HD11	1:E:119:PHE:HE2	1.76	0.51
1:E:235:LYS:NZ	1:E:238:LYS:HD3	2.26	0.51
1:E:264:ASN:H	1:E:264:ASN:ND2	2.09	0.51
1:G:232:ARG:C	1:G:233:ILE:HG13	2.35	0.51
2:H:49:CYS:HA	2:H:139:HIS:HD2	1.74	0.51
2:H:232:VAL:HA	2:H:236:GLN:HB3	1.91	0.51
1:A:113:LEU:O	1:A:117:PRO:HG3	2.10	0.51
2:B:351:GLN:CD	2:B:353:ILE:HD11	2.36	0.51
2:D:178:ILE:HD11	2:D:310:ILE:HD12	1.93	0.51
1:E:347:ARG:HH12	2:F:274:ARG:CD	2.23	0.51
1:A:208:ASP:OD1	1:A:208:ASP:O	2.29	0.51
2:B:249:LEU:CD1	2:B:260:ILE:HD11	2.41	0.51
1:C:163:ARG:NH2	1:C:518:ASN:HD21	2.09	0.51
1:G:84:ASN:OD1	1:G:86:ALA:HB3	2.11	0.51
1:G:333:ILE:HA	2:H:223:ARG:NH2	2.24	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:280:LEU:O	2:H:284:VAL:HG23	2.10	0.51
1:C:163:ARG:NH1	1:C:165:ILE:HG12	2.26	0.51
1:C:447:ASN:ND2	2:D:26:ARG:HH21	2.08	0.51
2:D:142:VAL:HG21	2:D:307:VAL:HG21	1.92	0.51
2:D:232:VAL:HA	2:D:236:GLN:HB3	1.93	0.51
1:E:221:TYR:HD2	1:E:246:LEU:HG	1.76	0.51
2:F:340:LYS:HB3	2:F:342:ASN:ND2	2.26	0.51
3:L:102:LEU:HD11	3:L:114:GLU:HG2	1.92	0.51
1:C:34:CYS:HB2	1:C:123:PHE:CG	2.46	0.51
1:C:208:ASP:OD1	1:C:208:ASP:O	2.29	0.51
2:D:361:LEU:O	2:D:362:GLN:C	2.54	0.51
1:E:232:ARG:C	1:E:233:ILE:HG13	2.35	0.51
1:E:262:GLU:OE1	1:E:262:GLU:HA	2.10	0.51
1:G:307:LEU:HB3	1:G:383:LEU:CD2	2.40	0.51
1:C:7:LEU:O	1:C:11:GLN:HG3	2.11	0.50
2:H:191:VAL:H	2:H:320:ASN:HA	1.76	0.50
2:B:142:VAL:HG21	2:B:307:VAL:HG21	1.93	0.50
1:E:229:THR:O	1:E:230:ASN:CB	2.60	0.50
3:K:172:ALA:C	3:K:173:LEU:HG	2.34	0.50
1:G:221:TYR:HD2	1:G:246:LEU:HG	1.76	0.50
1:C:235:LYS:NZ	1:C:238:LYS:HD3	2.26	0.50
3:K:111:LYS:O	3:K:112:GLU:HB3	2.11	0.50
1:G:19:LEU:HD12	2:H:292:VAL:HG13	1.93	0.50
2:H:277:THR:HG23	2:H:280:LEU:CB	2.41	0.50
1:A:87:GLU:O	1:A:91:GLU:HG3	2.11	0.50
1:A:430:ARG:HB3	1:A:430:ARG:HH11	1.77	0.50
3:J:111:LYS:O	3:J:112:GLU:HB3	2.10	0.50
1:E:32:HIS:HA	1:E:56:SER:O	2.12	0.50
1:E:61:ASP:CB	1:E:86:ALA:HB2	2.40	0.50
1:E:208:ASP:OD1	1:E:211:HIS:HB2	2.10	0.50
1:E:357:VAL:O	1:E:361:VAL:HG23	2.11	0.50
1:G:163:ARG:HG3	1:G:519:THR:H	1.77	0.50
1:G:234:PRO:O	1:G:235:LYS:C	2.54	0.50
1:A:235:LYS:NZ	1:A:238:LYS:HD3	2.26	0.50
1:A:441:ARG:NH2	1:A:453:ASP:OD1	2.45	0.50
2:B:262:GLN:NE2	1:E:67:GLY:N	2.42	0.50
2:B:349:LEU:HB3	2:B:350:PRO:CD	2.40	0.50
1:C:185:LEU:O	1:C:188:PRO:HD3	2.12	0.50
2:D:64:LEU:HB3	2:D:111:LEU:HD13	1.88	0.50
2:D:349:LEU:HB3	2:D:350:PRO:CD	2.42	0.50
2:D:360:LYS:HA	2:D:700:LYS:O	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:118:GLU:C	3:K:120:THR:H	2.20	0.50
2:H:351:GLN:CD	2:H:353:ILE:HD11	2.36	0.50
1:A:163:ARG:HG2	1:A:163:ARG:NH1	2.27	0.50
2:B:64:LEU:HD11	2:B:77:VAL:HG21	1.94	0.50
2:B:241:GLN:HG3	2:B:245:GLU:HA	1.93	0.50
1:E:7:LEU:O	1:E:11:GLN:HG3	2.12	0.50
1:E:447:ASN:ND2	2:F:26:ARG:HH21	2.10	0.50
2:F:257:ILE:HD13	2:F:282:GLN:HG2	1.93	0.50
3:K:107:THR:HG22	3:K:111:LYS:N	2.08	0.50
1:G:178:ASN:HD22	3:L:136:ILE:HG12	1.76	0.50
1:G:527:GLN:OE1	1:G:527:GLN:HA	2.10	0.50
1:A:7:LEU:O	1:A:11:GLN:HG3	2.11	0.50
1:A:33:VAL:HG21	1:A:54:ILE:HD11	1.94	0.50
1:A:418:ASN:HD22	1:A:419:PRO:N	2.09	0.50
2:B:232:VAL:HA	2:B:236:GLN:HB3	1.93	0.50
2:B:394:LEU:C	2:B:396:SER:H	2.20	0.50
1:E:119:PHE:O	1:E:122:ARG:HG3	2.11	0.50
2:F:240:GLU:O	2:F:241:GLN:C	2.55	0.50
2:H:241:GLN:HG3	2:H:245:GLU:HA	1.92	0.50
2:B:54:ILE:HG22	2:B:145:LEU:CD2	2.42	0.50
1:E:43:THR:HG21	1:E:73:ASN:OD1	2.12	0.50
2:F:353:ILE:HB	2:F:355:PHE:CZ	2.45	0.50
1:G:236:THR:HG23	1:G:237:TYR:CD2	2.47	0.50
1:G:418:ASN:HD22	1:G:419:PRO:N	2.10	0.50
1:A:229:THR:O	1:A:230:ASN:HB2	2.12	0.50
1:A:481:GLU:HB2	2:B:30:PHE:HE1	1.77	0.50
2:B:233:ARG:NH1	2:B:234:MET:HB2	2.26	0.50
1:C:236:THR:HG23	1:C:237:TYR:N	2.22	0.50
1:C:243:PHE:O	1:C:246:LEU:HB3	2.12	0.50
1:C:251:ILE:HG23	1:C:262:GLU:CB	2.41	0.50
2:D:233:ARG:NH1	2:D:234:MET:HB2	2.26	0.50
2:F:46:LEU:O	2:F:73:ARG:HB2	2.12	0.50
2:F:84:ASP:H	2:F:87:ASN:ND2	2.10	0.50
2:F:351:GLN:HA	2:F:351:GLN:HE21	1.77	0.50
2:H:132:ASP:OD1	2:H:132:ASP:N	2.45	0.50
1:A:233:ILE:O	1:A:233:ILE:HG22	2.11	0.49
1:C:225:TRP:NE1	1:C:233:ILE:HG12	2.27	0.49
1:C:232:ARG:C	1:C:233:ILE:HG13	2.37	0.49
2:D:199:CYS:SG	2:D:346:CYS:SG	3.07	0.49
2:F:361:LEU:O	2:F:362:GLN:C	2.55	0.49
1:G:229:THR:O	1:G:230:ASN:CB	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:GLU:HG3	1:A:394:ARG:HE	1.77	0.49
2:D:217:THR:HG21	2:D:223:ARG:HH22	1.77	0.49
2:F:197:THR:CG2	2:F:198:ALA:N	2.75	0.49
2:B:280:LEU:O	2:B:284:VAL:HG23	2.11	0.49
1:C:441:ARG:NH2	1:C:453:ASP:CG	2.70	0.49
2:F:128:GLN:HE21	2:F:128:GLN:N	2.04	0.49
2:F:217:THR:HG21	2:F:223:ARG:HH22	1.76	0.49
1:G:430:ARG:HB3	1:G:430:ARG:NH1	2.28	0.49
2:H:233:ARG:HG2	2:H:233:ARG:NH1	2.26	0.49
2:H:361:LEU:O	2:H:362:GLN:C	2.56	0.49
1:C:229:THR:O	1:C:230:ASN:CB	2.59	0.49
1:C:234:PRO:O	1:C:235:LYS:C	2.55	0.49
1:C:236:THR:HG23	1:C:237:TYR:CD2	2.47	0.49
1:E:19:LEU:HD12	2:F:292:VAL:HG13	1.94	0.49
1:G:72:ASN:ND2	1:G:72:ASN:C	2.69	0.49
1:G:155:THR:HG23	1:G:493:ILE:HG22	1.95	0.49
2:H:360:LYS:HA	2:H:700:LYS:O	2.12	0.49
2:B:267:ARG:HG2	2:B:267:ARG:NH1	2.25	0.49
2:B:361:LEU:C	2:B:363:GLU:N	2.69	0.49
2:D:251:GLY:O	2:D:286:LYS:HE3	2.12	0.49
1:E:407:ILE:O	1:E:407:ILE:HG23	2.12	0.49
2:B:46:LEU:O	2:B:73:ARG:HB2	2.12	0.49
2:D:361:LEU:C	2:D:363:GLU:N	2.70	0.49
3:J:117:ILE:HD11	3:J:126:ILE:HG23	1.94	0.49
2:B:32:HIS:CD2	2:B:34:ASP:H	2.30	0.49
2:B:233:ARG:NH1	2:B:233:ARG:HG2	2.28	0.49
1:C:84:ASN:OD1	1:C:86:ALA:HB3	2.12	0.49
1:E:441:ARG:NH2	1:E:453:ASP:CG	2.70	0.49
1:G:163:ARG:NH1	1:G:165:ILE:HG12	2.28	0.49
2:B:318:LEU:HD12	2:B:319:ASN:N	2.27	0.49
1:C:186:ASP:HB2	1:C:232:ARG:NH2	2.28	0.49
1:E:208:ASP:OD1	1:E:208:ASP:O	2.31	0.49
3:L:107:THR:HG23	3:L:109:THR:N	2.22	0.49
1:G:447:ASN:HD22	2:H:26:ARG:HH21	1.60	0.49
3:L:117:ILE:HD11	3:L:126:ILE:HG23	1.94	0.49
2:B:155:ASN:CG	2:B:200:ILE:HB	2.38	0.49
2:B:353:ILE:HB	2:B:355:PHE:CZ	2.48	0.49
1:C:163:ARG:HG3	1:C:519:THR:H	1.76	0.49
1:C:418:ASN:HD22	1:C:419:PRO:HD2	1.78	0.49
2:D:340:LYS:HB3	2:D:342:ASN:ND2	2.28	0.49
2:F:360:LYS:HA	2:F:700:LYS:O	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:208:PRO:HG3	3:L:171:LEU:CD1	2.38	0.49
1:A:34:CYS:HB2	1:A:123:PHE:CG	2.47	0.48
2:B:197:THR:CG2	2:B:198:ALA:N	2.76	0.48
2:D:351:GLN:HG3	2:D:353:ILE:CD1	2.40	0.48
2:F:142:VAL:HG21	2:F:307:VAL:HG21	1.95	0.48
2:F:233:ARG:NH1	2:F:233:ARG:HG2	2.28	0.48
1:G:211:HIS:O	1:G:338:LYS:HD2	2.13	0.48
2:H:154:ILE:O	2:H:154:ILE:HD13	2.12	0.48
2:H:603:ILE:O	2:H:607:THR:N	2.35	0.48
1:A:299:LYS:HA	1:A:368:ILE:HG23	1.95	0.48
2:B:84:ASP:H	2:B:87:ASN:ND2	2.10	0.48
1:E:78:ARG:CZ	2:F:13:TRP:HB3	2.43	0.48
1:E:185:LEU:O	1:E:188:PRO:HD3	2.14	0.48
1:G:186:ASP:HB2	1:G:232:ARG:NH2	2.27	0.48
2:H:361:LEU:C	2:H:363:GLU:N	2.71	0.48
1:A:186:ASP:HB2	1:A:232:ARG:NH2	2.28	0.48
1:A:236:THR:HG23	1:A:237:TYR:CD2	2.47	0.48
2:D:392:LEU:O	2:D:606:ARG:CB	2.62	0.48
1:G:208:ASP:OD1	1:G:208:ASP:O	2.31	0.48
2:H:64:LEU:HB3	2:H:111:LEU:HD12	1.91	0.48
3:L:118:GLU:C	3:L:120:THR:H	2.22	0.48
2:B:277:THR:HG23	2:B:280:LEU:CB	2.43	0.48
1:C:225:TRP:CE2	1:C:233:ILE:HG12	2.48	0.48
2:D:249:LEU:CD1	2:D:260:ILE:HD11	2.42	0.48
2:D:351:GLN:HA	2:D:351:GLN:NE2	2.28	0.48
1:E:252:LEU:HB2	1:E:260:GLU:HG2	1.95	0.48
2:F:361:LEU:C	2:F:363:GLU:N	2.71	0.48
1:G:441:ARG:NH2	1:G:453:ASP:OD1	2.45	0.48
2:B:128:GLN:HE21	2:B:128:GLN:N	2.03	0.48
2:B:351:GLN:HA	2:B:351:GLN:NE2	2.29	0.48
2:B:901:VAL:O	2:B:902:ALA:C	2.53	0.48
3:I:101:MET:HG3	3:I:163:GLY:H	1.79	0.48
3:I:118:GLU:C	3:I:120:THR:H	2.22	0.48
1:C:34:CYS:HB2	1:C:123:PHE:CD2	2.48	0.48
2:D:213:PHE:CB	2:D:218:ILE:HD11	2.40	0.48
2:D:236:GLN:HE22	2:D:263:LYS:HB3	1.78	0.48
1:G:119:PHE:O	1:G:122:ARG:HG3	2.13	0.48
1:A:234:PRO:O	1:A:235:LYS:C	2.55	0.48
1:A:447:ASN:HD22	2:B:26:ARG:NH2	2.11	0.48
2:B:191:VAL:H	2:B:320:ASN:HA	1.78	0.48
2:D:277:THR:HG23	2:D:280:LEU:CB	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:393:TYR:HE1	2:D:607:THR:CA	2.24	0.48
1:E:418:ASN:HD22	1:E:419:PRO:N	2.11	0.48
1:G:51:LEU:HD11	2:H:92:PHE:HB3	1.95	0.48
1:A:163:ARG:NH1	1:A:165:ILE:HG12	2.29	0.48
2:B:236:GLN:HE22	2:B:263:LYS:HB3	1.79	0.48
1:E:236:THR:HG23	1:E:237:TYR:CD2	2.48	0.48
1:E:481:GLU:OE2	2:F:315:TYR:HE2	1.97	0.48
2:F:277:THR:HG23	2:F:280:LEU:CB	2.43	0.48
2:F:353:ILE:HB	2:F:355:PHE:HE1	1.77	0.48
1:G:155:THR:HG23	1:G:493:ILE:CG2	2.44	0.48
1:G:175:HIS:HD2	1:G:512:GLN:O	1.96	0.48
2:H:158:LEU:CD1	2:H:177:LEU:HB2	2.44	0.48
1:A:307:LEU:HB3	1:A:383:LEU:CD2	2.42	0.48
2:B:322:LEU:C	2:B:322:LEU:CD1	2.87	0.48
2:B:360:LYS:HA	2:B:700:LYS:O	2.14	0.48
1:C:238:LYS:O	1:C:239:GLU:C	2.56	0.48
2:D:197:THR:CG2	2:D:198:ALA:N	2.77	0.48
1:E:186:ASP:HB2	1:E:232:ARG:NH2	2.28	0.48
1:E:418:ASN:HD22	1:E:419:PRO:HD2	1.79	0.48
2:F:191:VAL:H	2:F:320:ASN:HA	1.79	0.48
3:L:111:LYS:O	3:L:112:GLU:HB3	2.13	0.48
1:A:215:ILE:H	1:A:332:MET:HE1	1.79	0.48
2:D:32:HIS:CD2	2:D:34:ASP:H	2.32	0.48
2:D:394:LEU:C	2:D:396:SER:H	2.21	0.48
1:E:34:CYS:HB2	1:E:123:PHE:CD2	2.49	0.48
2:F:16:ARG:HH22	2:F:116:PRO:HB2	1.77	0.48
2:F:75:ILE:O	2:F:120:VAL:HA	2.13	0.48
2:H:267:ARG:HG2	2:H:267:ARG:NH1	2.27	0.48
1:A:211:HIS:O	1:A:338:LYS:HD2	2.14	0.48
2:B:351:GLN:HG3	2:B:353:ILE:CD1	2.44	0.48
1:C:43:THR:HG21	1:C:73:ASN:OD1	2.14	0.48
1:C:215:ILE:H	1:C:332:MET:HE1	1.79	0.48
1:C:299:LYS:HA	1:C:368:ILE:HG23	1.96	0.48
1:C:447:ASN:HD22	2:D:26:ARG:HH21	1.62	0.48
2:D:191:VAL:H	2:D:320:ASN:HA	1.79	0.48
1:G:211:HIS:NE2	2:H:221:MET:HE1	2.27	0.48
1:G:299:LYS:HA	1:G:368:ILE:HG23	1.96	0.48
1:G:407:ILE:HG23	1:G:407:ILE:O	2.13	0.48
2:H:75:ILE:O	2:H:120:VAL:HA	2.14	0.48
2:H:89:ASN:OD1	2:H:90:ARG:NH1	2.46	0.48
1:C:19:LEU:HD12	2:D:292:VAL:HG13	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:LEU:HD11	2:D:92:PHE:HB3	1.96	0.47
2:D:357:PRO:O	2:D:358:SER:CB	2.62	0.47
1:E:146:SER:O	1:E:147:GLN:HB2	2.13	0.47
1:E:215:ILE:H	1:E:332:MET:HE1	1.78	0.47
1:E:229:THR:O	1:E:230:ASN:HB2	2.14	0.47
2:F:394:LEU:C	2:F:396:SER:H	2.21	0.47
1:A:185:LEU:O	1:A:188:PRO:HD3	2.14	0.47
2:B:338:GLU:HG3	3:I:148:LYS:HD3	1.97	0.47
3:I:107:THR:HG23	3:I:109:THR:N	2.23	0.47
2:D:358:SER:O	2:D:358:SER:OG	2.19	0.47
1:E:211:HIS:O	1:E:338:LYS:HD2	2.14	0.47
2:F:158:LEU:CD1	2:F:177:LEU:HB2	2.44	0.47
1:A:36:ILE:HG21	1:A:131:LEU:HD21	1.96	0.47
1:A:221:TYR:HD2	1:A:246:LEU:HG	1.78	0.47
1:A:347:ARG:HH22	2:B:274:ARG:HD2	1.78	0.47
1:A:441:ARG:NH2	1:A:453:ASP:CG	2.72	0.47
2:D:13:TRP:HZ3	2:D:116:PRO:HG2	1.79	0.47
3:J:118:GLU:C	3:J:120:THR:H	2.22	0.47
1:G:437:LYS:HA	1:G:437:LYS:HD2	1.75	0.47
1:A:225:TRP:NE1	1:A:233:ILE:HG12	2.28	0.47
1:A:238:LYS:O	1:A:239:GLU:C	2.57	0.47
1:C:208:ASP:CG	1:C:211:HIS:HB2	2.39	0.47
1:C:229:THR:O	1:C:230:ASN:HB2	2.14	0.47
3:J:101:MET:HG3	3:J:163:GLY:H	1.79	0.47
1:E:72:ASN:C	1:E:72:ASN:ND2	2.72	0.47
1:G:236:THR:HG23	1:G:237:TYR:N	2.22	0.47
3:L:101:MET:HG3	3:L:163:GLY:H	1.79	0.47
1:A:243:PHE:O	1:A:246:LEU:HB3	2.14	0.47
2:D:320:ASN:HD21	2:D:336:GLU:HG3	1.79	0.47
1:E:238:LYS:O	1:E:239:GLU:C	2.57	0.47
2:F:233:ARG:HH12	2:F:234:MET:HB2	1.78	0.47
3:K:107:THR:CG2	3:K:109:THR:H	2.24	0.47
1:G:233:ILE:HG22	1:G:233:ILE:O	2.15	0.47
1:G:307:LEU:HD22	1:G:383:LEU:HD22	1.97	0.47
2:H:197:THR:CG2	2:H:198:ALA:N	2.78	0.47
1:A:227:SER:C	1:A:229:THR:H	2.22	0.47
2:B:158:LEU:HD12	2:B:177:LEU:HD22	1.96	0.47
2:D:14:GLU:HG3	2:H:258:GLN:CG	2.40	0.47
2:D:132:ASP:OD1	2:D:132:ASP:N	2.48	0.47
2:D:233:ARG:HG2	2:D:233:ARG:HH11	1.78	0.47
2:F:154:ILE:HD13	2:F:154:ILE:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:106:LYS:HA	3:K:112:GLU:HA	1.97	0.47
2:H:351:GLN:HA	2:H:351:GLN:NE2	2.28	0.47
1:A:163:ARG:HG3	1:A:519:THR:H	1.80	0.47
1:A:186:ASP:OD2	1:A:279:THR:HB	2.15	0.47
1:A:341:LYS:HE3	1:E:114:ASP:OD1	2.15	0.47
3:I:145:TYR:O	3:I:146:SER:C	2.58	0.47
1:C:430:ARG:HB3	1:C:430:ARG:HH11	1.79	0.47
2:D:75:ILE:O	2:D:120:VAL:HA	2.15	0.47
2:D:155:ASN:CG	2:D:200:ILE:HB	2.39	0.47
3:J:107:THR:HG23	3:J:109:THR:N	2.24	0.47
2:F:155:ASN:CG	2:F:200:ILE:HB	2.39	0.47
2:F:357:PRO:O	2:F:358:SER:CB	2.62	0.47
1:G:225:TRP:NE1	1:G:233:ILE:HG12	2.29	0.47
1:G:243:PHE:O	1:G:246:LEU:HB3	2.14	0.47
1:G:362:ALA:O	1:G:366:GLN:HG3	2.14	0.47
2:H:46:LEU:O	2:H:73:ARG:HB2	2.14	0.47
1:A:208:ASP:CG	1:A:211:HIS:HB2	2.39	0.47
2:B:13:TRP:HZ3	2:B:116:PRO:HG2	1.78	0.47
1:E:233:ILE:O	1:E:233:ILE:HG22	2.15	0.47
1:G:34:CYS:HB2	1:G:123:PHE:CD2	2.50	0.47
1:G:238:LYS:O	1:G:241:GLU:N	2.48	0.47
1:G:481:GLU:OE2	2:H:315:TYR:HE2	1.98	0.47
2:H:16:ARG:HH22	2:H:116:PRO:HB2	1.77	0.47
2:H:128:GLN:NE2	2:H:128:GLN:N	2.59	0.47
2:H:233:ARG:HG2	2:H:233:ARG:HH11	1.78	0.47
1:C:357:VAL:O	1:C:361:VAL:HG23	2.15	0.47
1:G:268:ALA:O	1:G:272:VAL:HG23	2.15	0.47
2:H:249:LEU:HD11	2:H:260:ILE:HD11	1.96	0.47
2:D:236:GLN:NE2	2:D:263:LYS:HB3	2.30	0.47
2:D:280:LEU:O	2:D:284:VAL:HG23	2.14	0.47
1:E:430:ARG:NH1	1:E:430:ARG:HB3	2.30	0.47
2:F:351:GLN:HA	2:F:351:GLN:NE2	2.30	0.47
3:K:101:MET:HG3	3:K:163:GLY:H	1.80	0.47
1:G:208:ASP:CG	1:G:211:HIS:HB2	2.39	0.47
1:G:229:THR:O	1:G:230:ASN:HB2	2.15	0.47
1:A:43:THR:HG21	1:A:73:ASN:OD1	2.15	0.46
1:A:72:ASN:ND2	1:A:72:ASN:C	2.73	0.46
1:C:252:LEU:HB2	1:C:260:GLU:HG2	1.96	0.46
2:D:64:LEU:HB3	2:D:111:LEU:HD12	1.93	0.46
1:E:184:ARG:HB3	1:E:279:THR:OG1	2.15	0.46
1:E:243:PHE:O	1:E:246:LEU:HB3	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:251:ILE:O	1:G:252:LEU:C	2.59	0.46
3:I:101:MET:CG	3:I:163:GLY:H	2.28	0.46
1:E:155:THR:HG23	1:E:493:ILE:HG22	1.98	0.46
1:E:299:LYS:HA	1:E:368:ILE:HG23	1.97	0.46
2:F:233:ARG:NH1	2:F:234:MET:HB2	2.30	0.46
2:F:235:LEU:C	2:F:238:PRO:HD2	2.40	0.46
2:F:703:GLY:HA2	2:F:706:ASP:CB	2.45	0.46
1:G:441:ARG:NH2	1:G:453:ASP:CG	2.73	0.46
2:H:38:SER:HB3	2:H:41:SER:OG	2.15	0.46
1:A:268:ALA:O	1:A:272:VAL:HG23	2.14	0.46
1:C:260:GLU:CG	1:C:261:ASP:N	2.77	0.46
2:D:158:LEU:CD1	2:D:177:LEU:HB2	2.44	0.46
2:D:267:ARG:HG2	2:D:267:ARG:NH1	2.26	0.46
2:F:128:GLN:NE2	2:F:128:GLN:N	2.59	0.46
2:B:901:VAL:O	2:B:902:ALA:O	2.32	0.46
3:I:117:ILE:HD11	3:I:126:ILE:HG23	1.97	0.46
1:E:225:TRP:NE1	1:E:233:ILE:HG12	2.30	0.46
1:G:238:LYS:O	1:G:239:GLU:C	2.58	0.46
2:H:233:ARG:HH12	2:H:234:MET:HB2	1.80	0.46
2:B:320:ASN:HD21	2:B:336:GLU:HG3	1.79	0.46
1:C:119:PHE:CE1	1:C:122:ARG:NE	2.82	0.46
2:D:128:GLN:HE21	2:D:128:GLN:N	2.06	0.46
1:E:168:GLU:HG3	1:E:394:ARG:HE	1.80	0.46
1:E:238:LYS:O	1:E:241:GLU:N	2.48	0.46
1:E:268:ALA:O	1:E:272:VAL:HG23	2.16	0.46
1:G:72:ASN:HD22	1:G:72:ASN:H	1.64	0.46
2:H:28:GLY:O	2:H:31:THR:HG22	2.16	0.46
3:L:103:ILE:HA	3:L:163:GLY:O	2.15	0.46
3:L:103:ILE:HG21	3:L:161:ILE:CG2	2.46	0.46
1:A:155:THR:HG23	1:A:493:ILE:HG22	1.98	0.46
1:A:32:HIS:HA	1:A:56:SER:O	2.15	0.46
2:B:603:ILE:O	2:B:607:THR:N	2.35	0.46
1:C:72:ASN:C	1:C:72:ASN:ND2	2.71	0.46
1:E:215:ILE:HG13	1:E:332:MET:CE	2.37	0.46
2:F:132:ASP:OD1	2:F:132:ASP:N	2.48	0.46
2:H:95:ARG:HH11	2:H:95:ARG:CG	2.28	0.46
2:H:381:ILE:CG2	2:H:902:ALA:HB1	2.45	0.46
1:C:146:SER:O	1:C:147:GLN:HB2	2.16	0.46
1:C:260:GLU:HG3	1:C:261:ASP:H	1.78	0.46
1:C:418:ASN:ND2	1:C:418:ASN:C	2.74	0.46
1:E:125:VAL:HG12	1:E:126:VAL:N	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:347:ARG:NH2	2:F:274:ARG:HD2	2.31	0.46
1:E:347:ARG:NH2	2:F:274:ARG:NH1	2.63	0.46
2:F:338:GLU:HG3	3:K:148:LYS:HD3	1.97	0.46
1:G:525:MET:HE3	2:H:30:PHE:CG	2.51	0.46
3:L:106:LYS:HA	3:L:112:GLU:HA	1.98	0.46
1:A:34:CYS:HB2	1:A:123:PHE:CD2	2.51	0.46
1:A:84:ASN:OD1	1:A:86:ALA:HB3	2.16	0.46
1:A:307:LEU:HD22	1:A:383:LEU:HD22	1.97	0.46
1:C:32:HIS:HA	1:C:56:SER:O	2.16	0.46
2:D:162:LEU:HD22	2:D:169:LEU:HD11	1.98	0.46
1:E:36:ILE:O	1:E:60:ILE:O	2.33	0.46
3:K:107:THR:HG23	3:K:109:THR:N	2.23	0.46
2:H:394:LEU:C	2:H:396:SER:H	2.22	0.46
1:A:266:GLU:O	1:A:270:LYS:HG3	2.16	0.46
1:A:407:ILE:HG23	1:A:407:ILE:O	2.16	0.46
2:B:74:GLN:HE22	2:B:119:ASN:HD22	1.64	0.46
2:B:235:LEU:C	2:B:238:PRO:HD2	2.40	0.46
2:B:340:LYS:HB3	2:B:342:ASN:ND2	2.30	0.46
2:D:212:ASN:HD22	2:D:212:ASN:HA	1.54	0.46
2:D:235:LEU:C	2:D:238:PRO:HD2	2.40	0.46
3:J:103:ILE:HG21	3:J:161:ILE:CG2	2.46	0.46
1:A:418:ASN:ND2	1:A:418:ASN:C	2.74	0.45
1:A:418:ASN:HD22	1:A:419:PRO:HD2	1.81	0.45
2:B:162:LEU:HD22	2:B:169:LEU:HD11	1.98	0.45
2:B:166:ASP:C	2:B:168:VAL:H	2.24	0.45
1:C:87:GLU:O	1:C:91:GLU:HG3	2.16	0.45
1:E:236:THR:HG23	1:E:237:TYR:N	2.22	0.45
1:G:36:ILE:O	1:G:60:ILE:O	2.34	0.45
2:H:226:GLU:OE1	2:H:226:GLU:N	2.48	0.45
1:A:518:ASN:O	1:A:519:THR:C	2.59	0.45
2:B:236:GLN:NE2	2:B:263:LYS:HB3	2.31	0.45
2:D:380:ALA:O	2:D:904:VAL:HA	2.17	0.45
2:F:197:THR:HG22	2:F:198:ALA:N	2.31	0.45
2:H:232:VAL:O	2:H:232:VAL:HG12	2.16	0.45
1:A:185:LEU:HD12	1:A:275:ALA:HB1	1.99	0.45
2:D:232:VAL:O	2:D:232:VAL:HG12	2.16	0.45
3:J:106:LYS:HA	3:J:112:GLU:HA	1.97	0.45
1:E:163:ARG:HG2	1:E:163:ARG:NH1	2.29	0.45
1:G:32:HIS:HA	1:G:56:SER:O	2.17	0.45
1:G:266:GLU:O	1:G:270:LYS:HG3	2.17	0.45
1:A:481:GLU:HA	1:A:481:GLU:OE1	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:LEU:CD1	2:B:177:LEU:HB2	2.47	0.45
2:F:322:LEU:C	2:F:322:LEU:CD1	2.86	0.45
1:G:178:ASN:ND2	3:L:136:ILE:HG12	2.31	0.45
2:H:357:PRO:O	2:H:358:SER:CB	2.65	0.45
1:A:13:TYR:O	1:A:16:GLN:HG2	2.16	0.45
2:B:50:LYS:N	2:B:139:HIS:HD2	2.14	0.45
2:D:166:ASP:C	2:D:168:VAL:H	2.25	0.45
1:E:266:GLU:O	1:E:270:LYS:HG3	2.17	0.45
2:F:162:LEU:HD22	2:F:169:LEU:HD11	1.98	0.45
2:F:213:PHE:CB	2:F:218:ILE:HD11	2.43	0.45
1:G:213:PRO:CB	1:G:332:MET:HE2	2.35	0.45
1:G:418:ASN:ND2	1:G:418:ASN:C	2.73	0.45
2:H:64:LEU:HD11	2:H:77:VAL:HG21	1.99	0.45
2:H:233:ARG:NH1	2:H:234:MET:HB2	2.32	0.45
2:H:349:LEU:HB3	2:H:350:PRO:HD2	1.98	0.45
1:A:238:LYS:O	1:A:241:GLU:N	2.49	0.45
1:C:268:ALA:O	1:C:272:VAL:HG23	2.17	0.45
2:D:64:LEU:HD11	2:D:77:VAL:HG21	1.98	0.45
3:J:101:MET:CG	3:J:163:GLY:H	2.29	0.45
2:F:249:LEU:HD11	2:F:260:ILE:HD11	1.98	0.45
2:F:267:ARG:HG2	2:F:267:ARG:NH1	2.28	0.45
2:F:365:LEU:HD11	2:F:395:GLN:NE2	2.31	0.45
3:K:101:MET:CG	3:K:163:GLY:H	2.29	0.45
2:H:13:TRP:HZ3	2:H:116:PRO:HG2	1.81	0.45
1:A:155:THR:HG23	1:A:493:ILE:CG2	2.46	0.45
2:B:703:GLY:HA2	2:B:706:ASP:CB	2.47	0.45
2:D:256:HIS:O	2:D:260:ILE:HG13	2.16	0.45
1:E:178:ASN:ND2	3:K:136:ILE:HG23	2.32	0.45
2:F:13:TRP:HZ3	2:F:116:PRO:HG2	1.82	0.45
1:G:227:SER:C	1:G:229:THR:H	2.24	0.45
1:G:447:ASN:HD22	2:H:26:ARG:NH2	2.14	0.45
2:B:256:HIS:O	2:B:260:ILE:HG13	2.17	0.45
3:I:103:ILE:HA	3:I:163:GLY:O	2.17	0.45
3:I:106:LYS:HA	3:I:112:GLU:HA	1.99	0.45
1:C:163:ARG:HG2	1:C:163:ARG:NH1	2.28	0.45
1:C:186:ASP:OD2	1:C:279:THR:HB	2.17	0.45
1:E:211:HIS:NE2	2:F:221:MET:HE1	2.31	0.45
1:E:251:ILE:HG23	1:E:262:GLU:CB	2.42	0.45
1:E:336:SER:HB2	2:F:221:MET:HA	1.99	0.45
2:F:226:GLU:OE1	2:F:226:GLU:N	2.49	0.45
3:K:118:GLU:C	3:K:120:THR:N	2.73	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:184:ARG:HB3	1:G:279:THR:OG1	2.17	0.45
1:G:481:GLU:OE1	1:G:481:GLU:HA	2.16	0.45
2:B:142:VAL:CG2	2:B:307:VAL:HG21	2.47	0.45
2:B:233:ARG:HG2	2:B:233:ARG:HH11	1.81	0.45
2:B:274:ARG:NH1	1:E:106:GLU:O	2.49	0.45
1:C:13:TYR:O	1:C:16:GLN:HG2	2.17	0.45
1:C:437:LYS:HA	1:C:437:LYS:HD2	1.75	0.45
2:D:249:LEU:HD11	2:D:260:ILE:HD11	1.98	0.45
3:J:118:GLU:C	3:J:120:THR:N	2.75	0.45
1:E:302:PRO:HG2	1:E:305:TRP:HD1	1.82	0.45
1:E:447:ASN:HD22	2:F:26:ARG:NH2	2.14	0.45
1:G:146:SER:O	1:G:147:GLN:HB2	2.16	0.45
2:H:236:GLN:HE22	2:H:263:LYS:HB3	1.81	0.45
2:H:267:ARG:HH11	2:H:267:ARG:CG	2.28	0.45
2:H:320:ASN:HD21	2:H:336:GLU:HG3	1.81	0.45
3:L:101:MET:CG	3:L:163:GLY:H	2.30	0.45
1:A:90:MET:O	1:A:94:GLN:HB2	2.17	0.45
1:A:225:TRP:CE2	1:A:233:ILE:HG12	2.52	0.45
1:A:236:THR:HG23	1:A:237:TYR:N	2.22	0.45
1:A:357:VAL:O	1:A:361:VAL:HG23	2.17	0.45
1:C:33:VAL:HG21	1:C:54:ILE:HD11	1.98	0.45
1:C:90:MET:O	1:C:94:GLN:HB2	2.17	0.45
1:C:235:LYS:HB2	1:C:239:GLU:OE2	2.17	0.45
1:C:251:ILE:HG23	1:C:262:GLU:HG2	1.98	0.45
1:C:407:ILE:HD11	1:C:412:ILE:HD12	1.98	0.45
1:E:84:ASN:OD1	1:E:86:ALA:HB3	2.17	0.45
1:E:119:PHE:CE1	1:E:122:ARG:NE	2.83	0.45
1:E:213:PRO:CB	1:E:332:MET:HE2	2.35	0.45
1:E:235:LYS:HB3	1:E:239:GLU:HG3	1.98	0.45
1:E:347:ARG:HH22	2:F:274:ARG:CD	2.29	0.45
1:E:418:ASN:ND2	1:E:418:ASN:C	2.74	0.45
2:F:233:ARG:HG2	2:F:233:ARG:HH11	1.82	0.45
1:G:357:VAL:O	1:G:361:VAL:HG23	2.16	0.45
2:H:162:LEU:HD22	2:H:169:LEU:HD11	1.99	0.45
2:H:197:THR:HG22	2:H:198:ALA:N	2.32	0.45
2:H:236:GLN:NE2	2:H:263:LYS:HB3	2.32	0.45
1:A:119:PHE:CE1	1:A:122:ARG:NE	2.84	0.44
2:D:57:GLY:C	2:D:91:GLN:HG2	2.41	0.44
1:E:155:THR:HG23	1:E:493:ILE:CG2	2.47	0.44
1:E:208:ASP:CG	1:E:211:HIS:HB2	2.41	0.44
3:K:101:MET:HG3	3:K:163:GLY:HA2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:GLU:O	1:G:91:GLU:HG3	2.18	0.44
1:G:163:ARG:NH2	1:G:518:ASN:HD21	2.13	0.44
1:A:49:LEU:O	1:A:52:PRO:HD2	2.18	0.44
1:A:235:LYS:HB2	1:A:239:GLU:OE2	2.17	0.44
2:D:164:TYR:CE2	2:D:348:GLN:HG2	2.52	0.44
2:D:603:ILE:O	2:D:607:THR:N	2.38	0.44
1:E:227:SER:C	1:E:229:THR:H	2.25	0.44
1:E:251:ILE:HG23	1:E:262:GLU:HG2	1.99	0.44
2:F:95:ARG:HH11	2:F:95:ARG:CG	2.29	0.44
2:F:236:GLN:NE2	2:F:263:LYS:HB3	2.32	0.44
1:G:430:ARG:HB3	1:G:430:ARG:HH11	1.83	0.44
1:G:442:TYR:O	1:G:445:VAL:HG23	2.17	0.44
1:G:510:THR:O	1:G:511:LYS:HB2	2.18	0.44
2:B:64:LEU:HB3	2:B:111:LEU:HD12	1.97	0.44
1:C:447:ASN:HD22	2:D:26:ARG:NH2	2.14	0.44
2:D:703:GLY:HA2	2:D:706:ASP:CB	2.48	0.44
1:E:481:GLU:OE1	1:E:481:GLU:HA	2.17	0.44
1:E:525:MET:HE3	2:F:30:PHE:CG	2.52	0.44
2:F:236:GLN:HE22	2:F:263:LYS:HB3	1.81	0.44
2:F:604:GLU:HA	2:F:607:THR:CB	2.47	0.44
3:K:103:ILE:HG21	3:K:161:ILE:CG2	2.47	0.44
3:K:103:ILE:HA	3:K:163:GLY:O	2.17	0.44
1:G:49:LEU:O	1:G:52:PRO:HD2	2.17	0.44
1:A:162:MET:HE1	2:B:330:LEU:HD11	1.99	0.44
2:B:13:TRP:CZ3	2:B:116:PRO:HG2	2.52	0.44
2:B:132:ASP:OD1	2:B:132:ASP:N	2.48	0.44
1:C:238:LYS:O	1:C:241:GLU:N	2.50	0.44
1:C:419:PRO:CB	1:C:475:LYS:HE3	2.47	0.44
2:D:54:ILE:HG22	2:D:145:LEU:CD2	2.46	0.44
2:F:351:GLN:HG3	2:F:353:ILE:CD1	2.43	0.44
1:G:168:GLU:HG3	1:G:394:ARG:HE	1.82	0.44
1:G:252:LEU:C	1:G:253:LYS:O	2.58	0.44
2:H:322:LEU:C	2:H:322:LEU:CD1	2.85	0.44
1:A:281:ILE:HA	1:A:282:PRO:HD3	1.86	0.44
1:A:442:TYR:O	1:A:445:VAL:HG23	2.17	0.44
2:B:197:THR:HG22	2:B:198:ALA:N	2.32	0.44
1:C:177:ASP:O	1:C:178:ASN:HB2	2.17	0.44
1:C:251:ILE:O	1:C:252:LEU:C	2.60	0.44
1:C:266:GLU:O	1:C:270:LYS:HG3	2.16	0.44
1:E:46:LEU:O	1:E:50:VAL:HG23	2.18	0.44
1:E:407:ILE:HD11	1:E:412:ILE:HD12	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:426:TYR:HB2	1:E:521:ILE:HD11	1.99	0.44
2:F:54:ILE:HG22	2:F:145:LEU:CD2	2.44	0.44
2:F:56:ALA:HA	2:F:60:GLY:HA3	2.00	0.44
3:K:150:MET:HE1	3:K:167:LEU:HD13	2.00	0.44
1:G:162:MET:HE1	2:H:330:LEU:HD11	2.00	0.44
1:G:251:ILE:HG23	1:G:262:GLU:HG2	2.00	0.44
2:H:703:GLY:HA2	2:H:706:ASP:CB	2.47	0.44
1:C:227:SER:C	1:C:229:THR:H	2.25	0.44
1:C:347:ARG:NH2	2:D:274:ARG:NH1	2.66	0.44
2:D:199:CYS:HG	2:D:346:CYS:HG	1.63	0.44
2:D:226:GLU:OE1	2:D:226:GLU:N	2.48	0.44
1:E:51:LEU:HD11	2:F:92:PHE:HB3	1.99	0.44
1:E:419:PRO:CB	1:E:475:LYS:HE3	2.48	0.44
1:G:163:ARG:HG2	1:G:163:ARG:NH1	2.29	0.44
2:H:132:ASP:HA	2:H:157:MET:CE	2.48	0.44
1:C:235:LYS:HB3	1:C:239:GLU:HG3	1.97	0.44
1:E:518:ASN:O	1:E:519:THR:C	2.61	0.44
1:G:47:LYS:C	1:G:47:LYS:HD2	2.43	0.44
1:G:225:TRP:CE2	1:G:233:ILE:HG12	2.52	0.44
1:G:347:ARG:HH12	2:H:274:ARG:HD2	1.83	0.44
3:L:136:ILE:O	3:L:141:GLN:NE2	2.49	0.44
1:E:185:LEU:HD12	1:E:275:ALA:HB1	1.99	0.44
1:G:235:LYS:HB3	1:G:239:GLU:HG3	2.00	0.44
2:H:95:ARG:HD3	2:H:95:ARG:HA	1.74	0.44
2:B:28:GLY:O	2:B:31:THR:HG22	2.18	0.44
2:B:110:PHE:C	2:B:110:PHE:CD2	2.96	0.44
2:B:178:ILE:HD12	2:B:178:ILE:N	2.33	0.44
1:C:185:LEU:HD12	1:C:275:ALA:HB1	1.99	0.44
1:C:489:GLU:HG2	1:C:489:GLU:O	2.18	0.44
2:D:64:LEU:HD21	2:D:77:VAL:HG21	2.00	0.44
2:F:131:ASN:O	2:F:132:ASP:C	2.61	0.44
2:H:166:ASP:C	2:H:168:VAL:H	2.26	0.44
2:B:380:ALA:O	2:B:904:VAL:HA	2.18	0.43
3:I:103:ILE:HG21	3:I:161:ILE:CG2	2.48	0.43
1:E:87:GLU:O	1:E:91:GLU:HG3	2.18	0.43
2:F:393:TYR:CD1	2:F:607:THR:HA	2.52	0.43
1:A:252:LEU:HB2	1:A:260:GLU:HG2	1.99	0.43
1:A:366:GLN:C	1:A:368:ILE:H	2.25	0.43
2:B:323:VAL:O	2:B:332:THR:HA	2.18	0.43
3:I:118:GLU:C	3:I:120:THR:N	2.75	0.43
1:C:36:ILE:HG21	1:C:131:LEU:HD21	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:ALA:HA	2:D:60:GLY:HA3	2.00	0.43
1:E:347:ARG:HH22	2:F:274:ARG:NH1	2.17	0.43
1:E:437:LYS:HD2	1:E:437:LYS:HA	1.75	0.43
2:F:50:LYS:N	2:F:139:HIS:HD2	2.15	0.43
2:H:131:ASN:O	2:H:132:ASP:C	2.61	0.43
2:H:134:PHE:O	2:H:137:GLN:HG3	2.18	0.43
2:D:74:GLN:HE22	2:D:119:ASN:HD22	1.65	0.43
2:D:89:ASN:OD1	2:D:90:ARG:NH1	2.49	0.43
2:D:110:PHE:C	2:D:110:PHE:CD2	2.96	0.43
1:E:264:ASN:ND2	1:E:265:PHE:H	2.16	0.43
1:G:131:LEU:HA	1:G:132:PRO:HD3	1.81	0.43
1:G:251:ILE:HG23	1:G:262:GLU:CB	2.43	0.43
2:H:56:ALA:HA	2:H:60:GLY:HA3	2.01	0.43
2:H:74:GLN:HE22	2:H:119:ASN:HD22	1.67	0.43
2:H:213:PHE:CB	2:H:218:ILE:HD11	2.43	0.43
2:H:222:PRO:HD2	2:H:271:TYR:CD2	2.54	0.43
1:A:36:ILE:HG23	1:A:109:PRO:HG3	2.00	0.43
1:A:348:GLU:HG3	1:E:115:ASN:CB	2.47	0.43
1:A:362:ALA:O	1:A:366:GLN:HG3	2.19	0.43
1:A:518:ASN:O	1:A:519:THR:O	2.37	0.43
2:B:230:GLU:OE2	2:B:234:MET:HE3	2.18	0.43
1:G:186:ASP:HB2	1:G:232:ARG:CZ	2.49	0.43
1:G:260:GLU:HG3	1:G:261:ASP:N	2.33	0.43
1:G:302:PRO:HG2	1:G:305:TRP:HD1	1.84	0.43
2:H:228:CYS:SG	2:H:268:ALA:HA	2.59	0.43
2:H:250:ASP:HB3	2:H:253:ASP:HB2	1.99	0.43
1:A:33:VAL:HG21	1:A:54:ILE:CD1	2.48	0.43
2:B:249:LEU:HD11	2:B:260:ILE:HD11	2.00	0.43
1:C:72:ASN:H	1:C:72:ASN:HD22	1.67	0.43
1:C:168:GLU:HG3	1:C:394:ARG:HE	1.84	0.43
1:C:307:LEU:HB3	1:C:383:LEU:CD2	2.46	0.43
2:D:28:GLY:O	2:D:31:THR:HG22	2.18	0.43
2:F:132:ASP:HA	2:F:157:MET:CE	2.49	0.43
1:G:128:ALA:HB1	1:G:131:LEU:HD11	2.01	0.43
2:H:158:LEU:HD22	2:H:175:VAL:HB	2.01	0.43
2:H:320:ASN:O	2:H:321:TYR:HB2	2.18	0.43
2:B:75:ILE:O	2:B:120:VAL:HA	2.18	0.43
3:I:103:ILE:C	3:I:103:ILE:HD12	2.44	0.43
1:C:426:TYR:HB2	1:C:521:ILE:HD11	2.01	0.43
1:C:481:GLU:OE2	2:D:315:TYR:HE2	2.01	0.43
2:D:907:PRO:C	2:D:909:THR:H	2.27	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:131:LEU:HA	1:E:132:PRO:HD3	1.85	0.43
1:E:186:ASP:HB2	1:E:232:ARG:CZ	2.49	0.43
1:E:347:ARG:HH22	2:F:274:ARG:HH11	1.66	0.43
2:F:166:ASP:C	2:F:168:VAL:H	2.27	0.43
2:F:323:VAL:O	2:F:332:THR:HA	2.19	0.43
1:G:185:LEU:HD12	1:G:275:ALA:HB1	2.00	0.43
1:G:418:ASN:HD22	1:G:419:PRO:HD2	1.81	0.43
2:H:323:VAL:O	2:H:332:THR:HA	2.18	0.43
1:A:146:SER:O	1:A:147:GLN:HB2	2.18	0.43
1:A:213:PRO:CB	1:A:332:MET:HE2	2.35	0.43
1:A:251:ILE:HG23	1:A:262:GLU:CB	2.45	0.43
1:A:419:PRO:CB	1:A:475:LYS:HE3	2.49	0.43
2:B:131:ASN:O	2:B:132:ASP:C	2.62	0.43
2:B:361:LEU:O	2:B:364:VAL:CG2	2.65	0.43
1:C:186:ASP:HB2	1:C:232:ARG:CZ	2.49	0.43
1:C:211:HIS:O	1:C:338:LYS:HD2	2.19	0.43
2:D:353:ILE:HD13	2:D:353:ILE:N	2.33	0.43
1:E:90:MET:O	1:E:94:GLN:HB2	2.18	0.43
1:E:111:ASN:OD1	1:E:111:ASN:C	2.62	0.43
1:E:235:LYS:HB2	1:E:239:GLU:OE2	2.19	0.43
1:E:253:LYS:O	1:E:259:PRO:C	2.60	0.43
1:G:33:VAL:HG21	1:G:54:ILE:HD11	2.00	0.43
1:G:90:MET:O	1:G:94:GLN:HB2	2.18	0.43
2:H:235:LEU:C	2:H:238:PRO:HD2	2.43	0.43
2:B:357:PRO:O	2:B:358:SER:CB	2.65	0.43
3:I:115:ILE:HD13	3:I:129:ARG:HB2	2.01	0.43
2:H:351:GLN:HG3	2:H:353:ILE:CD1	2.43	0.43
2:B:54:ILE:CD1	2:B:154:ILE:HG13	2.49	0.43
2:B:154:ILE:O	2:B:154:ILE:HD13	2.18	0.43
2:B:213:PHE:CB	2:B:218:ILE:HD11	2.41	0.43
3:J:101:MET:HG3	3:J:163:GLY:HA2	2.01	0.43
1:E:281:ILE:HA	1:E:282:PRO:HD3	1.87	0.43
2:F:158:LEU:HD12	2:F:177:LEU:HD22	2.01	0.43
2:F:303:CYS:O	2:F:307:VAL:HG23	2.19	0.43
3:K:119:PRO:O	3:K:157:ALA:HB2	2.19	0.43
1:G:72:ASN:C	1:G:72:ASN:HD22	2.26	0.43
2:B:349:LEU:HB3	2:B:350:PRO:HD2	1.99	0.43
3:I:107:THR:CG2	3:I:109:THR:H	2.23	0.43
1:C:324:PRO:HB3	1:C:353:ASP:HB3	2.01	0.43
1:C:333:ILE:HA	2:D:223:ARG:NH2	2.33	0.43
2:D:13:TRP:CZ3	2:D:116:PRO:HG2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:197:THR:HG22	2:D:198:ALA:N	2.33	0.43
2:D:284:VAL:O	2:D:287:ARG:NH1	2.52	0.43
3:J:103:ILE:HA	3:J:163:GLY:O	2.18	0.43
1:E:186:ASP:OD2	1:E:279:THR:HB	2.18	0.43
1:E:311:LEU:HD12	1:E:311:LEU:HA	1.85	0.43
1:A:229:THR:O	1:A:230:ASN:ND2	2.52	0.42
1:A:235:LYS:HB3	1:A:239:GLU:HG3	2.00	0.42
2:B:250:ASP:HB3	2:B:253:ASP:HB2	2.01	0.42
2:B:353:ILE:HB	2:B:355:PHE:HE1	1.80	0.42
2:D:349:LEU:HB3	2:D:350:PRO:HD2	2.00	0.42
1:E:33:VAL:HG21	1:E:54:ILE:HD11	2.01	0.42
2:F:250:ASP:HB3	2:F:253:ASP:HB2	2.01	0.42
2:F:353:ILE:HD13	2:F:353:ILE:N	2.34	0.42
1:G:43:THR:HG21	1:G:73:ASN:OD1	2.19	0.42
1:G:426:TYR:HB2	1:G:521:ILE:HD11	2.00	0.42
2:H:50:LYS:N	2:H:139:HIS:HD2	2.15	0.42
2:H:365:LEU:HD11	2:H:395:GLN:NE2	2.34	0.42
3:L:103:ILE:C	3:L:103:ILE:HD12	2.44	0.42
2:D:162:LEU:HD21	2:D:194:PRO:O	2.19	0.42
1:E:307:LEU:HD22	1:E:383:LEU:HD22	2.02	0.42
1:E:497:LEU:HD12	1:E:497:LEU:HA	1.91	0.42
2:F:57:GLY:C	2:F:91:GLN:HG2	2.43	0.42
2:F:74:GLN:HE22	2:F:119:ASN:HD22	1.68	0.42
2:F:164:TYR:CE2	2:F:348:GLN:HG2	2.54	0.42
2:H:54:ILE:HG22	2:H:145:LEU:CD2	2.47	0.42
2:H:201:GLU:HB3	2:H:343:CYS:SG	2.59	0.42
1:A:396:ARG:HD2	1:A:534:LEU:HD21	2.01	0.42
2:D:158:LEU:HD22	2:D:175:VAL:HB	2.02	0.42
1:E:163:ARG:NH2	1:E:518:ASN:HD21	2.16	0.42
3:K:145:TYR:O	3:K:146:SER:C	2.61	0.42
1:G:111:ASN:OD1	1:G:111:ASN:C	2.62	0.42
1:G:215:ILE:HG13	1:G:332:MET:CE	2.40	0.42
2:H:284:VAL:O	2:H:287:ARG:NH1	2.51	0.42
1:A:347:ARG:HH22	2:B:274:ARG:NH1	2.17	0.42
2:B:284:VAL:O	2:B:287:ARG:NH1	2.52	0.42
3:I:150:MET:HE1	3:I:167:LEU:HD13	2.02	0.42
1:C:155:THR:HG23	1:C:493:ILE:CG2	2.49	0.42
1:C:426:TYR:HB2	1:C:521:ILE:CD1	2.49	0.42
2:D:154:ILE:O	2:D:154:ILE:HD13	2.19	0.42
2:D:250:ASP:HB3	2:D:253:ASP:HB2	2.01	0.42
1:E:225:TRP:CE2	1:E:233:ILE:HG12	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:LYS:HB2	1:G:239:GLU:OE2	2.20	0.42
1:G:311:LEU:HD12	1:G:311:LEU:HA	1.83	0.42
2:H:216:ALA:O	2:H:220:SER:HB2	2.20	0.42
2:B:164:TYR:CE2	2:B:348:GLN:HG2	2.55	0.42
2:B:267:ARG:HH11	2:B:267:ARG:CG	2.24	0.42
2:B:393:TYR:CZ	2:B:395:GLN:HG2	2.54	0.42
3:I:101:MET:HG3	3:I:163:GLY:HA2	2.01	0.42
1:C:454:ILE:HD13	1:C:480:HIS:CE1	2.55	0.42
2:D:132:ASP:HA	2:D:157:MET:CE	2.50	0.42
2:D:323:VAL:O	2:D:332:THR:HA	2.19	0.42
2:F:158:LEU:HD22	2:F:175:VAL:HB	2.02	0.42
1:G:366:GLN:C	1:G:368:ILE:H	2.26	0.42
2:H:257:ILE:HG22	2:H:278:TYR:CE1	2.55	0.42
3:L:118:GLU:C	3:L:120:THR:N	2.75	0.42
1:E:362:ALA:O	1:E:366:GLN:HG3	2.18	0.42
2:F:145:LEU:O	3:K:176:GLY:HA3	2.20	0.42
2:F:320:ASN:HD21	2:F:336:GLU:HG3	1.84	0.42
2:F:380:ALA:O	2:F:904:VAL:HA	2.19	0.42
1:A:426:TYR:HB2	1:A:521:ILE:CD1	2.50	0.42
2:B:64:LEU:HD21	2:B:77:VAL:HG21	2.00	0.42
2:B:83:ILE:HD13	2:B:94:PHE:HB3	2.02	0.42
2:B:89:ASN:OD1	2:B:90:ARG:NH1	2.48	0.42
1:C:236:THR:O	1:C:237:TYR:C	2.62	0.42
1:C:347:ARG:HH22	2:D:274:ARG:NH1	2.16	0.42
1:C:347:ARG:HH12	2:D:274:ARG:HD2	1.85	0.42
1:C:518:ASN:O	1:C:519:THR:C	2.62	0.42
2:D:74:GLN:NE2	2:D:119:ASN:HD22	2.17	0.42
1:E:234:PRO:HB2	1:E:235:LYS:H	1.71	0.42
1:E:426:TYR:HB2	1:E:521:ILE:CD1	2.49	0.42
2:F:178:ILE:N	2:F:178:ILE:HD12	2.35	0.42
1:G:281:ILE:HA	1:G:282:PRO:HD3	1.87	0.42
2:H:368:LEU:HA	2:H:374:LEU:HD12	2.01	0.42
2:B:74:GLN:NE2	2:B:119:ASN:HD22	2.17	0.42
2:B:134:PHE:O	2:B:137:GLN:HG3	2.19	0.42
2:B:368:LEU:HA	2:B:374:LEU:HD12	2.00	0.42
1:C:155:THR:HG23	1:C:493:ILE:HG22	2.02	0.42
1:C:366:GLN:C	1:C:368:ILE:N	2.78	0.42
1:C:517:ASN:ND2	1:C:517:ASN:C	2.71	0.42
2:D:83:ILE:HD13	2:D:94:PHE:HB3	2.01	0.42
1:E:33:VAL:CG2	1:E:54:ILE:CD1	2.98	0.42
2:F:83:ILE:HD13	2:F:94:PHE:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:183:GLU:HB2	3:K:173:LEU:HB3	2.02	0.42
2:F:284:VAL:O	2:F:287:ARG:NH1	2.53	0.42
3:L:101:MET:HG3	3:L:163:GLY:HA2	2.02	0.42
1:A:407:ILE:HD11	1:A:412:ILE:HD12	2.02	0.42
2:D:199:CYS:HG	2:D:343:CYS:HG	1.61	0.42
2:F:241:GLN:CG	2:F:245:GLU:HA	2.49	0.42
2:F:257:ILE:HG22	2:F:278:TYR:CE1	2.55	0.42
1:G:297:ILE:HG21	1:G:368:ILE:HD11	2.00	0.42
1:G:412:ILE:HA	1:G:423:ILE:HD13	2.02	0.42
1:G:426:TYR:HB2	1:G:521:ILE:CD1	2.49	0.42
2:B:705:VAL:C	2:B:800:GLY:O	2.63	0.42
1:C:33:VAL:HG21	1:C:54:ILE:CD1	2.50	0.42
1:C:125:VAL:HG12	1:C:126:VAL:N	2.34	0.42
2:D:131:ASN:O	2:D:132:ASP:C	2.62	0.42
2:D:222:PRO:HD2	2:D:271:TYR:CD2	2.55	0.42
2:D:241:GLN:CG	2:D:245:GLU:HA	2.49	0.42
1:G:386:ASN:O	1:G:387:SER:C	2.63	0.42
1:A:517:ASN:ND2	1:A:517:ASN:C	2.67	0.41
2:B:132:ASP:HA	2:B:157:MET:CE	2.49	0.41
1:C:518:ASN:O	1:C:519:THR:O	2.38	0.41
2:D:54:ILE:CD1	2:D:154:ILE:HG13	2.50	0.41
3:J:145:TYR:O	3:J:146:SER:C	2.62	0.41
1:G:264:ASN:ND2	1:G:265:PHE:H	2.17	0.41
1:G:318:GLU:H	1:G:318:GLU:CD	2.27	0.41
1:G:332:MET:HG2	1:G:339:TYR:CE1	2.53	0.41
2:H:340:LYS:HB3	2:H:342:ASN:HD21	1.85	0.41
1:A:33:VAL:CG2	1:A:54:ILE:CD1	2.97	0.41
1:A:248:ARG:C	1:A:250:GLY:H	2.28	0.41
2:B:365:LEU:HD11	2:B:395:GLN:NE2	2.35	0.41
1:C:233:ILE:O	1:C:233:ILE:HG22	2.20	0.41
3:J:103:ILE:C	3:J:103:ILE:HD12	2.45	0.41
1:E:517:ASN:ND2	1:E:517:ASN:C	2.70	0.41
2:F:95:ARG:HD3	2:F:95:ARG:HA	1.73	0.41
2:F:236:GLN:HE22	2:F:263:LYS:HD2	1.85	0.41
2:F:349:LEU:HB3	2:F:350:PRO:HD2	2.00	0.41
2:F:381:ILE:CG2	2:F:902:ALA:HB1	2.50	0.41
1:G:180:LEU:HD23	3:L:135:GLY:CA	2.49	0.41
1:G:193:ARG:O	1:G:197:GLN:HG3	2.20	0.41
1:G:407:ILE:HD11	1:G:412:ILE:HD12	2.01	0.41
2:H:54:ILE:CD1	2:H:154:ILE:HG13	2.50	0.41
2:H:57:GLY:C	2:H:91:GLN:HG2	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:VAL:CG2	2:H:307:VAL:HG21	2.50	0.41
2:H:178:ILE:N	2:H:178:ILE:HD12	2.36	0.41
2:B:95:ARG:HD3	2:B:95:ARG:HA	1.73	0.41
1:C:191:GLU:H	1:C:191:GLU:CD	2.26	0.41
1:C:226:TYR:O	1:C:230:ASN:N	2.53	0.41
1:C:307:LEU:HD22	1:C:383:LEU:HD22	2.01	0.41
2:D:50:LYS:N	2:D:139:HIS:HD2	2.14	0.41
2:D:368:LEU:HA	2:D:374:LEU:HD12	2.02	0.41
1:E:72:ASN:H	1:E:72:ASN:HD22	1.68	0.41
1:E:366:GLN:C	1:E:368:ILE:N	2.79	0.41
1:E:422:GLU:CD	1:E:422:GLU:H	2.27	0.41
2:F:201:GLU:HB3	2:F:343:CYS:SG	2.61	0.41
1:G:119:PHE:CE1	1:G:122:ARG:NE	2.85	0.41
1:G:186:ASP:OD2	1:G:279:THR:HB	2.20	0.41
1:G:419:PRO:CB	1:G:475:LYS:HE3	2.50	0.41
2:H:230:GLU:OE2	2:H:234:MET:HE3	2.20	0.41
1:A:19:LEU:HD12	2:B:292:VAL:HG13	2.01	0.41
1:A:131:LEU:HA	1:A:132:PRO:HD3	1.84	0.41
1:A:235:LYS:O	1:A:236:THR:C	2.63	0.41
1:A:236:THR:O	1:A:237:TYR:C	2.64	0.41
1:C:47:LYS:HD2	1:C:47:LYS:C	2.45	0.41
1:C:225:TRP:CD1	1:C:225:TRP:C	2.98	0.41
1:C:302:PRO:HG2	1:C:305:TRP:HD1	1.84	0.41
1:G:454:ILE:HD13	1:G:480:HIS:CE1	2.55	0.41
2:H:13:TRP:CZ3	2:H:116:PRO:HG2	2.55	0.41
2:H:335:PHE:CZ	3:L:144:ILE:CD1	3.02	0.41
1:A:186:ASP:HB2	1:A:232:ARG:CZ	2.51	0.41
1:A:426:TYR:HB2	1:A:521:ILE:HD11	2.02	0.41
2:B:38:SER:HB3	2:B:41:SER:OG	2.19	0.41
2:B:57:GLY:C	2:B:91:GLN:HG2	2.44	0.41
2:B:232:VAL:O	2:B:232:VAL:HG12	2.19	0.41
1:C:184:ARG:HB3	1:C:279:THR:OG1	2.19	0.41
1:C:281:ILE:HA	1:C:282:PRO:HD3	1.86	0.41
2:D:209:PRO:HD3	3:J:142:ARG:HH21	1.86	0.41
2:D:320:ASN:O	2:D:321:TYR:HB2	2.19	0.41
1:E:396:ARG:HD2	1:E:534:LEU:HD21	2.02	0.41
2:F:222:PRO:HD2	2:F:271:TYR:CD2	2.55	0.41
1:G:191:GLU:H	1:G:191:GLU:CD	2.27	0.41
3:L:145:TYR:O	3:L:146:SER:C	2.62	0.41
1:A:406:THR:O	1:A:407:ILE:C	2.63	0.41
1:A:412:ILE:HA	1:A:423:ILE:HD13	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:MET:C	1:A:418:ASN:N	2.78	0.41
2:B:217:THR:CG2	2:B:223:ARG:HH22	2.33	0.41
2:B:267:ARG:O	2:B:270:GLN:HB2	2.21	0.41
1:C:481:GLU:OE1	1:C:481:GLU:HA	2.20	0.41
1:E:162:MET:HE1	2:F:330:LEU:HD11	2.03	0.41
2:F:13:TRP:CZ3	2:F:116:PRO:HG2	2.56	0.41
2:F:393:TYR:CZ	2:F:395:GLN:HG2	2.56	0.41
1:G:225:TRP:CD1	1:G:225:TRP:C	2.98	0.41
2:H:15:GLY:O	2:H:16:ARG:C	2.64	0.41
2:H:110:PHE:C	2:H:110:PHE:CD2	2.99	0.41
2:H:353:ILE:HD13	2:H:353:ILE:N	2.36	0.41
3:L:115:ILE:HD13	3:L:129:ARG:HB2	2.02	0.41
1:A:46:LEU:HD23	1:A:93:LEU:HD13	2.02	0.41
1:A:424:VAL:HG11	1:A:478:TYR:CD1	2.55	0.41
1:A:434:ARG:HD3	1:A:460:CYS:HB3	2.03	0.41
2:B:192:ILE:CD1	2:B:200:ILE:HG12	2.50	0.41
1:C:65:VAL:CG2	1:C:85:ARG:HA	2.51	0.41
1:C:434:ARG:HD3	1:C:460:CYS:HB3	2.03	0.41
2:D:192:ILE:CD1	2:D:200:ILE:HG12	2.51	0.41
1:E:226:TYR:O	1:E:230:ASN:N	2.54	0.41
1:E:336:SER:OG	2:F:271:TYR:HD2	2.04	0.41
2:F:54:ILE:CD1	2:F:154:ILE:HG13	2.50	0.41
2:F:232:VAL:O	2:F:232:VAL:HG12	2.19	0.41
2:B:87:ASN:HB3	2:B:91:GLN:CD	2.46	0.41
1:C:111:ASN:OD1	1:C:111:ASN:C	2.63	0.41
1:C:235:LYS:O	1:C:236:THR:C	2.63	0.41
1:C:366:GLN:C	1:C:368:ILE:H	2.26	0.41
1:E:489:GLU:O	1:E:489:GLU:HG2	2.20	0.41
1:G:396:ARG:HD2	1:G:534:LEU:HD21	2.03	0.41
2:H:380:ALA:O	2:H:904:VAL:HA	2.19	0.41
1:A:65:VAL:CG2	1:A:85:ARG:HA	2.51	0.41
1:A:226:TYR:O	1:A:230:ASN:N	2.54	0.41
1:A:407:ILE:C	1:A:407:ILE:HD13	2.46	0.41
1:A:437:LYS:HD2	1:A:437:LYS:HA	1.75	0.41
1:C:9:LYS:HE2	1:C:99:ASP:OD1	2.21	0.41
1:C:162:MET:O	1:C:519:THR:HA	2.21	0.41
1:C:396:ARG:HD2	1:C:534:LEU:HD21	2.02	0.41
1:C:407:ILE:HD13	1:C:407:ILE:C	2.46	0.41
1:C:412:ILE:HA	1:C:423:ILE:HD13	2.03	0.41
2:D:237:TRP:CZ2	2:D:249:LEU:HA	2.56	0.41
2:D:908:GLN:O	2:D:909:THR:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:105:VAL:HG11	3:J:130:VAL:HG22	2.02	0.41
1:E:33:VAL:HG21	1:E:54:ILE:CD1	2.51	0.41
2:F:74:GLN:NE2	2:F:74:GLN:HA	2.36	0.41
1:G:125:VAL:HG12	1:G:126:VAL:N	2.36	0.41
1:G:252:LEU:HD12	1:G:260:GLU:HG2	2.02	0.41
1:G:301:THR:HG22	1:G:306:ILE:HG13	2.03	0.41
1:G:347:ARG:NH2	2:H:274:ARG:HD2	2.30	0.41
1:G:366:GLN:C	1:G:368:ILE:N	2.79	0.41
2:H:64:LEU:HD21	2:H:77:VAL:HG21	2.01	0.41
2:H:164:TYR:CE2	2:H:348:GLN:HG2	2.56	0.41
2:H:367:TYR:O	2:H:371:SER:HB2	2.21	0.41
3:L:105:VAL:HG11	3:L:130:VAL:HG22	2.03	0.41
3:L:119:PRO:O	3:L:157:ALA:HB2	2.21	0.41
1:A:263:GLU:OE1	1:A:333:ILE:HD13	2.21	0.41
2:B:257:ILE:HG22	2:B:278:TYR:CE1	2.55	0.41
3:I:105:VAL:HG11	3:I:130:VAL:HG22	2.03	0.41
3:I:107:THR:HG22	3:I:111:LYS:N	2.10	0.41
1:C:33:VAL:CG2	1:C:54:ILE:CD1	2.99	0.41
1:C:234:PRO:HB2	1:C:235:LYS:H	1.73	0.41
1:E:236:THR:O	1:E:237:TYR:C	2.64	0.41
1:E:297:ILE:HG21	1:E:368:ILE:HD11	2.02	0.41
1:E:318:GLU:H	1:E:318:GLU:CD	2.28	0.41
1:G:36:ILE:HG23	1:G:109:PRO:HG3	2.03	0.41
1:G:72:ASN:HD22	1:G:72:ASN:N	2.19	0.41
1:G:518:ASN:O	1:G:519:THR:C	2.64	0.41
2:B:56:ALA:HA	2:B:60:GLY:HA3	2.03	0.40
2:B:221:MET:HG2	2:B:221:MET:H	1.80	0.40
2:B:267:ARG:NH1	2:B:267:ARG:CG	2.83	0.40
1:C:282:PRO:HD2	1:C:285:ILE:HD12	2.03	0.40
2:D:216:ALA:O	2:D:220:SER:HB2	2.21	0.40
2:D:374:LEU:O	2:D:375:GLN:C	2.64	0.40
2:D:705:VAL:C	2:D:800:GLY:O	2.64	0.40
1:E:193:ARG:O	1:E:197:GLN:HG3	2.22	0.40
1:A:264:ASN:ND2	1:A:265:PHE:H	2.19	0.40
1:A:333:ILE:HA	2:B:223:ARG:NH2	2.36	0.40
2:B:247:VAL:HA	2:B:248:PRO:HD3	1.77	0.40
2:B:320:ASN:O	2:B:321:TYR:HB2	2.20	0.40
1:C:33:VAL:CG1	1:C:34:CYS:N	2.85	0.40
1:C:193:ARG:O	1:C:197:GLN:HG3	2.21	0.40
2:D:74:GLN:NE2	2:D:74:GLN:HA	2.35	0.40
2:D:230:GLU:OE2	2:D:234:MET:HE3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:ASN:C	1:E:72:ASN:HD22	2.29	0.40
2:F:110:PHE:C	2:F:110:PHE:CD2	2.99	0.40
2:H:83:ILE:HD13	2:H:94:PHE:HB3	2.03	0.40
1:A:302:PRO:HG2	1:A:305:TRP:HD1	1.86	0.40
2:B:361:LEU:C	2:B:363:GLU:H	2.29	0.40
2:B:374:LEU:O	2:B:375:GLN:C	2.64	0.40
2:B:376:MET:HE2	2:B:906:THR:CB	2.51	0.40
1:C:301:THR:HG22	1:C:306:ILE:HG13	2.04	0.40
1:C:407:ILE:O	1:C:407:ILE:CG2	2.69	0.40
2:D:95:ARG:HA	2:D:95:ARG:HD3	1.76	0.40
2:D:365:LEU:HD11	2:D:395:GLN:NE2	2.36	0.40
1:E:13:TYR:O	1:E:16:GLN:HG2	2.20	0.40
2:F:241:GLN:CB	2:F:245:GLU:HA	2.52	0.40
1:G:407:ILE:C	1:G:407:ILE:HD13	2.47	0.40
1:G:422:GLU:CD	1:G:422:GLU:H	2.29	0.40
1:G:507:LYS:O	1:G:511:LYS:N	2.52	0.40
1:A:128:ALA:HB1	1:A:131:LEU:HD11	2.02	0.40
1:A:491:HIS:NE2	2:B:65:LYS:NZ	2.62	0.40
1:C:262:GLU:HG3	1:C:265:PHE:CD1	2.56	0.40
2:D:38:SER:HB3	2:D:41:SER:OG	2.21	0.40
2:D:356:SER:HA	2:D:357:PRO:HD3	1.93	0.40
3:J:102:LEU:CD1	3:J:114:GLU:HG2	2.52	0.40
3:J:107:THR:CG2	3:J:109:THR:H	2.26	0.40
1:E:128:ALA:HB1	1:E:131:LEU:HD11	2.04	0.40
1:E:366:GLN:C	1:E:368:ILE:H	2.29	0.40
2:F:28:GLY:O	2:F:31:THR:HG22	2.21	0.40
2:F:230:GLU:OE2	2:F:234:MET:HE3	2.21	0.40
1:G:13:TYR:O	1:G:16:GLN:HG2	2.21	0.40
1:G:33:VAL:HG21	1:G:54:ILE:CD1	2.52	0.40
2:H:74:GLN:HA	2:H:74:GLN:NE2	2.36	0.40
2:H:247:VAL:HA	2:H:248:PRO:HD3	1.81	0.40
1:A:252:LEU:C	1:A:253:LYS:O	2.61	0.40
1:C:406:THR:O	1:C:407:ILE:C	2.65	0.40
2:D:236:GLN:O	2:D:240:GLU:HG2	2.22	0.40
1:E:74:PHE:CD1	2:F:65:LYS:HG3	2.57	0.40
1:E:229:THR:O	1:E:230:ASN:ND2	2.55	0.40
1:E:235:LYS:O	1:E:236:THR:C	2.63	0.40
1:E:332:MET:HG2	1:E:339:TYR:CE1	2.54	0.40
1:E:406:THR:O	1:E:407:ILE:C	2.65	0.40
2:F:134:PHE:O	2:F:137:GLN:HG3	2.21	0.40
2:H:192:ILE:CD1	2:H:200:ILE:HG12	2.52	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:343:CYS:O	2:H:347:SER:CB	2.70	0.40

There are no symmetry-related clashes.

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	512/529 (97%)	459 (90%)	34 (7%)	19 (4%)	2	15
1	C	512/529 (97%)	458 (90%)	38 (7%)	16 (3%)	3	19
1	E	512/529 (97%)	459 (90%)	36 (7%)	17 (3%)	3	17
1	G	512/529 (97%)	460 (90%)	32 (6%)	20 (4%)	2	14
2	B	408/431 (95%)	342 (84%)	52 (13%)	14 (3%)	3	17
2	D	408/431 (95%)	341 (84%)	55 (14%)	12 (3%)	3	20
2	F	408/431 (95%)	342 (84%)	54 (13%)	12 (3%)	3	20
2	H	408/431 (95%)	345 (85%)	51 (12%)	12 (3%)	3	20
3	I	74/76 (97%)	63 (85%)	9 (12%)	2 (3%)	4	22
3	J	74/76 (97%)	64 (86%)	8 (11%)	2 (3%)	4	22
3	K	74/76 (97%)	64 (86%)	8 (11%)	2 (3%)	4	22
3	L	74/76 (97%)	64 (86%)	8 (11%)	2 (3%)	4	22
All	All	3976/4144 (96%)	3461 (87%)	385 (10%)	130 (3%)	3	17

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	PRO
1	A	235	LYS
1	A	236	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	259	PRO
1	A	261	ASP
1	A	519	THR
2	B	116	PRO
2	B	358	SER
2	B	362	GLN
2	B	901	VAL
1	C	234	PRO
1	C	235	LYS
1	C	236	THR
1	C	253	LYS
1	C	261	ASP
1	C	519	THR
2	D	116	PRO
2	D	358	SER
2	D	362	GLN
2	D	901	VAL
2	D	902	ALA
1	E	234	PRO
1	E	235	LYS
1	E	236	THR
1	E	253	LYS
1	E	259	PRO
1	E	261	ASP
1	E	519	THR
2	F	116	PRO
2	F	358	SER
2	F	362	GLN
2	F	901	VAL
1	G	234	PRO
1	G	235	LYS
1	G	236	THR
1	G	259	PRO
1	G	261	ASP
1	G	519	THR
2	H	116	PRO
2	H	358	SER
2	H	362	GLN
2	H	901	VAL
2	H	902	ALA
1	A	237	TYR
1	A	533	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	902	ALA
3	I	163	GLY
1	C	237	TYR
1	C	259	PRO
1	C	275	ALA
1	C	533	GLN
2	D	604	GLU
3	J	163	GLY
1	E	237	TYR
1	E	275	ALA
1	E	533	GLN
3	K	163	GLY
1	G	237	TYR
1	G	275	ALA
1	G	533	GLN
3	L	163	GLY
1	A	252	LEU
1	A	253	LYS
1	A	275	ALA
1	A	276	LEU
2	B	320	ASN
2	B	604	GLU
3	I	119	PRO
1	C	36	ILE
1	C	276	LEU
2	D	320	ASN
3	J	119	PRO
1	E	276	LEU
2	F	320	ASN
2	F	604	GLU
3	K	119	PRO
1	G	252	LEU
1	G	276	LEU
2	H	320	ASN
2	H	604	GLU
3	L	119	PRO
1	A	36	ILE
1	A	178	ASN
1	A	233	ILE
1	A	262	GLU
1	A	317	LYS
1	A	422	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	359	ALA
2	B	907	PRO
2	B	908	GLN
2	D	359	ALA
2	D	907	PRO
2	D	908	GLN
1	E	317	LYS
2	F	359	ALA
2	F	907	PRO
1	G	36	ILE
1	G	253	LYS
2	H	359	ALA
2	H	705	VAL
2	H	907	PRO
2	B	239	LYS
2	B	241	GLN
2	B	705	VAL
1	C	233	ILE
1	C	262	GLU
1	C	317	LYS
2	D	241	GLN
2	D	705	VAL
1	E	36	ILE
1	E	178	ASN
1	E	233	ILE
1	E	262	GLU
2	F	239	LYS
2	F	241	GLN
2	F	705	VAL
1	G	233	ILE
1	G	262	GLU
1	G	317	LYS
1	G	422	GLU
2	H	239	LYS
2	H	241	GLN
2	B	363	GLU
2	F	132	ASP
1	G	178	ASN
1	E	190	PRO
1	G	190	PRO
1	C	190	PRO
1	G	21	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	190	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	450/461 (98%)	430 (96%)	20 (4%)	25	60
1	C	450/461 (98%)	432 (96%)	18 (4%)	28	62
1	E	450/461 (98%)	431 (96%)	19 (4%)	26	61
1	G	450/461 (98%)	431 (96%)	19 (4%)	26	61
2	B	334/379 (88%)	310 (93%)	24 (7%)	13	43
2	D	334/379 (88%)	310 (93%)	24 (7%)	13	43
2	F	334/379 (88%)	310 (93%)	24 (7%)	13	43
2	H	334/379 (88%)	310 (93%)	24 (7%)	13	43
3	I	66/66 (100%)	64 (97%)	2 (3%)	36	69
3	J	66/66 (100%)	64 (97%)	2 (3%)	36	69
3	K	66/66 (100%)	64 (97%)	2 (3%)	36	69
3	L	66/66 (100%)	64 (97%)	2 (3%)	36	69
All	All	3400/3624 (94%)	3220 (95%)	180 (5%)	20	54

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	72	ASN
1	A	90	MET
1	A	171	VAL
1	A	209	HIS
1	A	214	TRP
1	A	253	LYS
1	A	259	PRO
1	A	260	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	262	GLU
1	A	264	ASN
1	A	292	ASP
1	A	293	ARG
1	A	311	LEU
1	A	364	LEU
1	A	407	ILE
1	A	410	ASP
1	A	418	ASN
1	A	422	GLU
1	A	517	ASN
2	B	82	THR
2	B	111	LEU
2	B	114	ARG
2	B	116	PRO
2	B	128	GLN
2	B	132	ASP
2	B	154	ILE
2	B	182	THR
2	B	190	ARG
2	B	201	GLU
2	B	212	ASN
2	B	277	THR
2	B	306	GLU
2	B	316	ILE
2	B	322	LEU
2	B	327	VAL
2	B	342	ASN
2	B	348	GLN
2	B	353	ILE
2	B	358	SER
2	B	362	GLN
2	B	364	VAL
2	B	382	THR
2	B	394	LEU
3	I	107	THR
3	I	170	VAL
1	C	43	THR
1	C	72	ASN
1	C	90	MET
1	C	171	VAL
1	C	209	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	214	TRP
1	C	253	LYS
1	C	260	GLU
1	C	262	GLU
1	C	264	ASN
1	C	293	ARG
1	C	311	LEU
1	C	364	LEU
1	C	407	ILE
1	C	410	ASP
1	C	418	ASN
1	C	422	GLU
1	C	517	ASN
2	D	82	THR
2	D	111	LEU
2	D	114	ARG
2	D	116	PRO
2	D	128	GLN
2	D	132	ASP
2	D	154	ILE
2	D	182	THR
2	D	190	ARG
2	D	201	GLU
2	D	212	ASN
2	D	277	THR
2	D	306	GLU
2	D	316	ILE
2	D	322	LEU
2	D	327	VAL
2	D	342	ASN
2	D	348	GLN
2	D	353	ILE
2	D	358	SER
2	D	362	GLN
2	D	364	VAL
2	D	382	THR
2	D	394	LEU
3	J	107	THR
3	J	170	VAL
1	E	43	THR
1	E	72	ASN
1	E	90	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	171	VAL
1	E	209	HIS
1	E	214	TRP
1	E	253	LYS
1	E	259	PRO
1	E	262	GLU
1	E	264	ASN
1	E	292	ASP
1	E	293	ARG
1	E	311	LEU
1	E	364	LEU
1	E	407	ILE
1	E	410	ASP
1	E	418	ASN
1	E	422	GLU
1	E	517	ASN
2	F	82	THR
2	F	111	LEU
2	F	114	ARG
2	F	116	PRO
2	F	128	GLN
2	F	132	ASP
2	F	154	ILE
2	F	182	THR
2	F	190	ARG
2	F	201	GLU
2	F	212	ASN
2	F	277	THR
2	F	306	GLU
2	F	316	ILE
2	F	322	LEU
2	F	327	VAL
2	F	342	ASN
2	F	348	GLN
2	F	353	ILE
2	F	358	SER
2	F	362	GLN
2	F	364	VAL
2	F	382	THR
2	F	394	LEU
3	K	107	THR
3	K	170	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	43	THR
1	G	72	ASN
1	G	90	MET
1	G	171	VAL
1	G	209	HIS
1	G	214	TRP
1	G	259	PRO
1	G	260	GLU
1	G	262	GLU
1	G	264	ASN
1	G	292	ASP
1	G	293	ARG
1	G	311	LEU
1	G	364	LEU
1	G	407	ILE
1	G	410	ASP
1	G	418	ASN
1	G	422	GLU
1	G	517	ASN
2	H	82	THR
2	H	111	LEU
2	H	114	ARG
2	H	116	PRO
2	H	128	GLN
2	H	132	ASP
2	H	154	ILE
2	H	182	THR
2	H	190	ARG
2	H	201	GLU
2	H	212	ASN
2	H	277	THR
2	H	306	GLU
2	H	316	ILE
2	H	322	LEU
2	H	327	VAL
2	H	342	ASN
2	H	348	GLN
2	H	353	ILE
2	H	358	SER
2	H	362	GLN
2	H	364	VAL
2	H	382	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	394	LEU
3	L	107	THR
3	L	170	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	72	ASN
1	A	77	GLN
1	A	178	ASN
1	A	197	GLN
1	A	209	HIS
1	A	224	GLN
1	A	230	ASN
1	A	264	ASN
1	A	271	ASN
1	A	277	ASN
1	A	320	GLN
1	A	343	GLN
1	A	344	ASN
1	A	359	ASN
1	A	366	GLN
1	A	418	ASN
1	A	439	GLN
1	A	447	ASN
1	A	449	GLN
1	A	533	GLN
2	B	74	GLN
2	B	87	ASN
2	B	128	GLN
2	B	131	ASN
2	B	139	HIS
2	B	212	ASN
2	B	236	GLN
2	B	241	GLN
2	B	262	GLN
2	B	325	ASN
2	B	342	ASN
2	B	348	GLN
2	B	351	GLN
2	B	370	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	141	GLN
1	C	37	ASN
1	C	72	ASN
1	C	77	GLN
1	C	178	ASN
1	C	197	GLN
1	C	209	HIS
1	C	224	GLN
1	C	230	ASN
1	C	264	ASN
1	C	271	ASN
1	C	277	ASN
1	C	320	GLN
1	C	359	ASN
1	C	366	GLN
1	C	418	ASN
1	C	439	GLN
1	C	447	ASN
1	C	518	ASN
1	C	533	GLN
2	D	74	GLN
2	D	87	ASN
2	D	128	GLN
2	D	131	ASN
2	D	139	HIS
2	D	212	ASN
2	D	236	GLN
2	D	241	GLN
2	D	325	ASN
2	D	342	ASN
2	D	348	GLN
2	D	351	GLN
2	D	370	ASN
3	J	141	GLN
1	E	37	ASN
1	E	72	ASN
1	E	77	GLN
1	E	178	ASN
1	E	197	GLN
1	E	209	HIS
1	E	224	GLN
1	E	230	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	264	ASN
1	E	271	ASN
1	E	277	ASN
1	E	320	GLN
1	E	359	ASN
1	E	366	GLN
1	E	418	ASN
1	E	439	GLN
1	E	447	ASN
1	E	533	GLN
2	F	74	GLN
2	F	87	ASN
2	F	128	GLN
2	F	139	HIS
2	F	212	ASN
2	F	236	GLN
2	F	241	GLN
2	F	325	ASN
2	F	342	ASN
2	F	348	GLN
2	F	351	GLN
2	F	370	ASN
3	K	141	GLN
1	G	37	ASN
1	G	72	ASN
1	G	77	GLN
1	G	178	ASN
1	G	197	GLN
1	G	224	GLN
1	G	230	ASN
1	G	264	ASN
1	G	271	ASN
1	G	277	ASN
1	G	320	GLN
1	G	343	GLN
1	G	359	ASN
1	G	366	GLN
1	G	418	ASN
1	G	436	HIS
1	G	439	GLN
1	G	447	ASN
1	G	517	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	533	GLN
2	H	74	GLN
2	H	87	ASN
2	H	128	GLN
2	H	139	HIS
2	H	212	ASN
2	H	236	GLN
2	H	241	GLN
2	H	325	ASN
2	H	342	ASN
2	H	348	GLN
2	H	351	GLN
2	H	370	ASN
3	L	141	GLN

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	1
2	H	1
2	D	1
2	F	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	396:SER	C	600:VAL	N	3.82
1	H	396:SER	C	600:VAL	N	3.80
1	D	396:SER	C	600:VAL	N	3.78
1	F	396:SER	C	600:VAL	N	3.78

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.