



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:02 PM UTC

PDB ID : 4BTP / pdb_00004btp
Title : Structure of the capsid protein P1 of the bacteriophage phi8
Authors : El Omari, K.; Sutton, G.; Ravantti, J.J.; Zhang, H.; Walter, T.S.; Grimes, J.M.; Bamford, D.H.; Stuart, D.I.; Mancini, E.J.
Deposited on : 2013-06-18
Resolution : 3.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

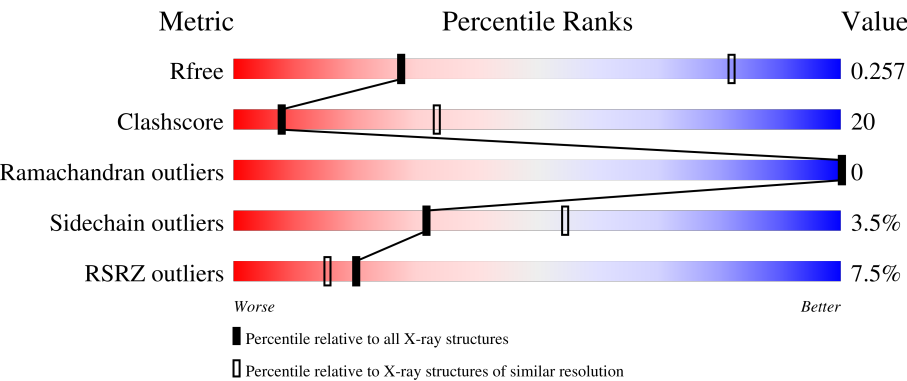
MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1131 (3.80-3.60)
Clashscore	190562	1171 (3.80-3.60)
Ramachandran outliers	187476	1129 (3.80-3.60)
Sidechain outliers	187428	1126 (3.80-3.60)
RSRZ outliers	180081	1130 (3.80-3.60)

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

Mol	Chain	Length	Quality of chain
1	A	792	7% 61% 32% • 5%
1	B	792	8% 61% 33% • 5%
1	C	792	6% 62% 31% • 5%
1	D	792	7% 61% 32% • 5%
1	E	792	7% 61% 32% • 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	792	8% 61% 32% • 5%
1	G	792	7% 61% 32% • 5%
1	H	792	7% 61% 32% • 5%
1	I	792	8% 62% 31% • 5%
1	J	792	7% 61% 32% • 5%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 57630 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 p1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	B	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	C	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	D	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	E	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	F	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	G	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	H	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	I	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			
1	J	749	Total	C	N	O	S	0	0	0
			5763	3634	998	1107	24			

There are 30 discrepancies between the modelled and reference sequences:

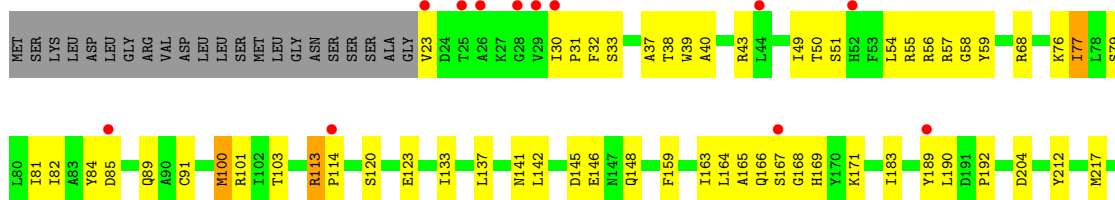
Chain	Residue	Modelled	Actual	Comment	Reference
A	419	ALA	GLY	engineered mutation	UNP Q9MC13
A	691	ASP	GLU	engineered mutation	UNP Q9MC13
A	716	ALA	GLY	conflict	UNP Q9MC13
B	419	ALA	GLY	engineered mutation	UNP Q9MC13
B	691	ASP	GLU	engineered mutation	UNP Q9MC13
B	716	ALA	GLY	conflict	UNP Q9MC13
C	419	ALA	GLY	engineered mutation	UNP Q9MC13
C	691	ASP	GLU	engineered mutation	UNP Q9MC13
C	716	ALA	GLY	conflict	UNP Q9MC13

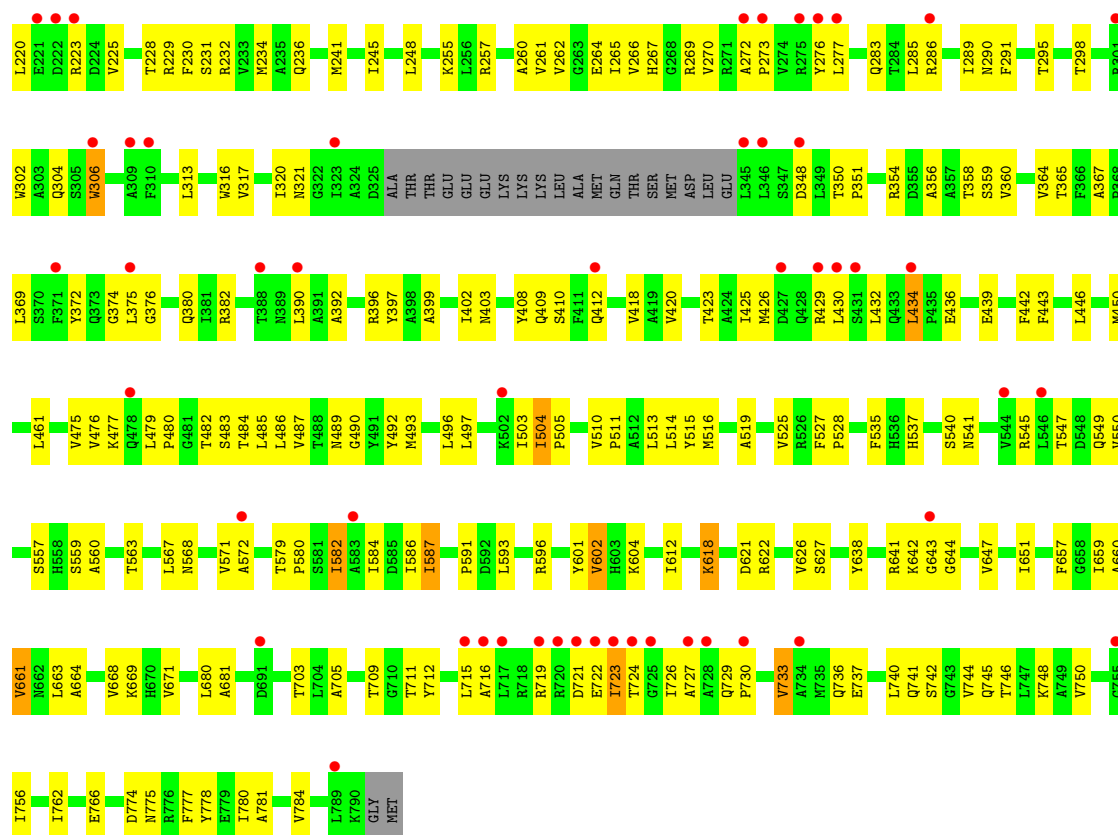
Continued on next page...

Continued from previous page...

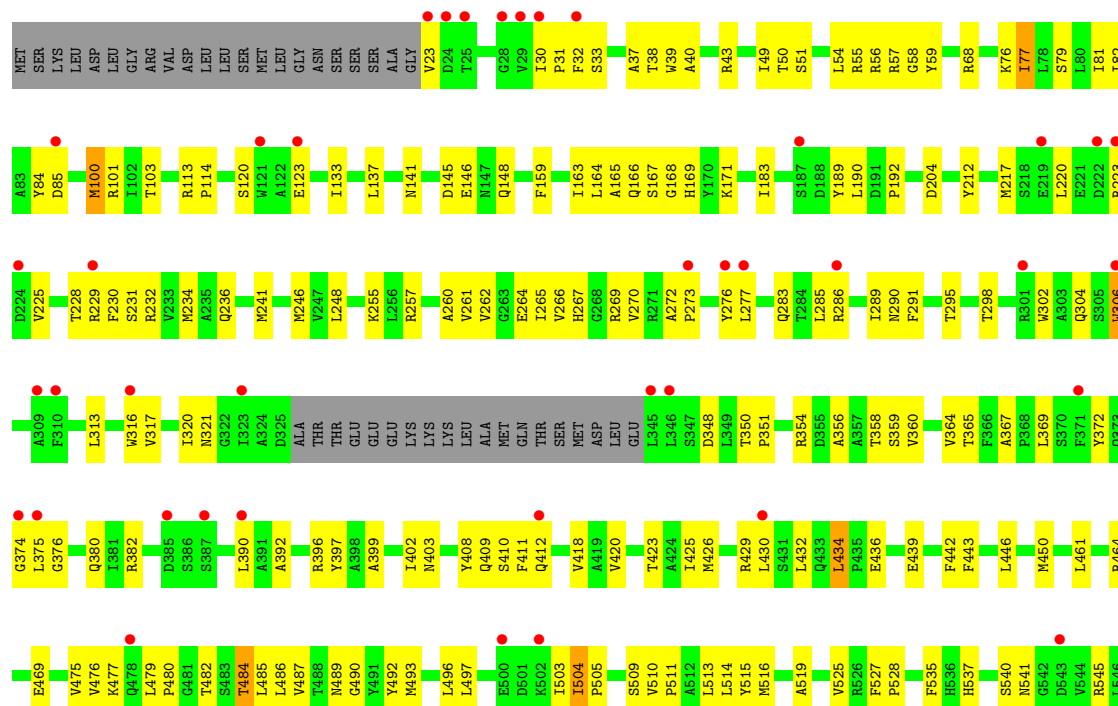
Chain	Residue	Modelled	Actual	Comment	Reference
D	419	ALA	GLY	engineered mutation	UNP Q9MC13
D	691	ASP	GLU	engineered mutation	UNP Q9MC13
D	716	ALA	GLY	conflict	UNP Q9MC13
E	419	ALA	GLY	engineered mutation	UNP Q9MC13
E	691	ASP	GLU	engineered mutation	UNP Q9MC13
E	716	ALA	GLY	conflict	UNP Q9MC13
F	419	ALA	GLY	engineered mutation	UNP Q9MC13
F	691	ASP	GLU	engineered mutation	UNP Q9MC13
F	716	ALA	GLY	conflict	UNP Q9MC13
G	419	ALA	GLY	engineered mutation	UNP Q9MC13
G	691	ASP	GLU	engineered mutation	UNP Q9MC13
G	716	ALA	GLY	conflict	UNP Q9MC13
H	419	ALA	GLY	engineered mutation	UNP Q9MC13
H	691	ASP	GLU	engineered mutation	UNP Q9MC13
H	716	ALA	GLY	conflict	UNP Q9MC13
I	419	ALA	GLY	engineered mutation	UNP Q9MC13
I	691	ASP	GLU	engineered mutation	UNP Q9MC13
I	716	ALA	GLY	conflict	UNP Q9MC13
J	419	ALA	GLY	engineered mutation	UNP Q9MC13
J	691	ASP	GLU	engineered mutation	UNP Q9MC13
J	716	ALA	GLY	conflict	UNP Q9MC13

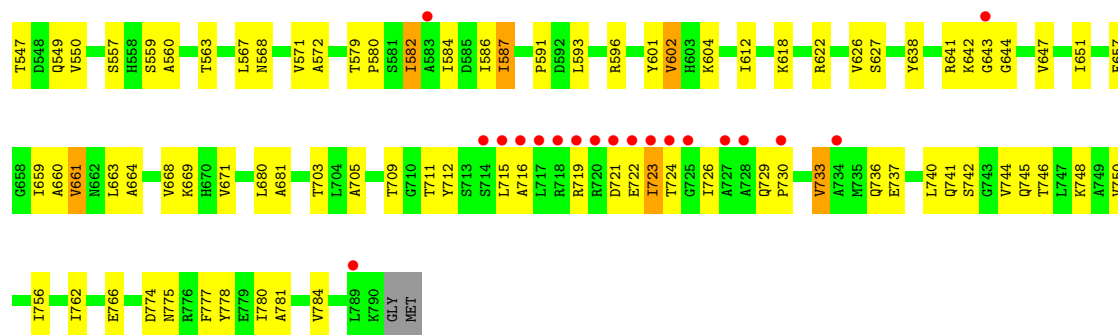




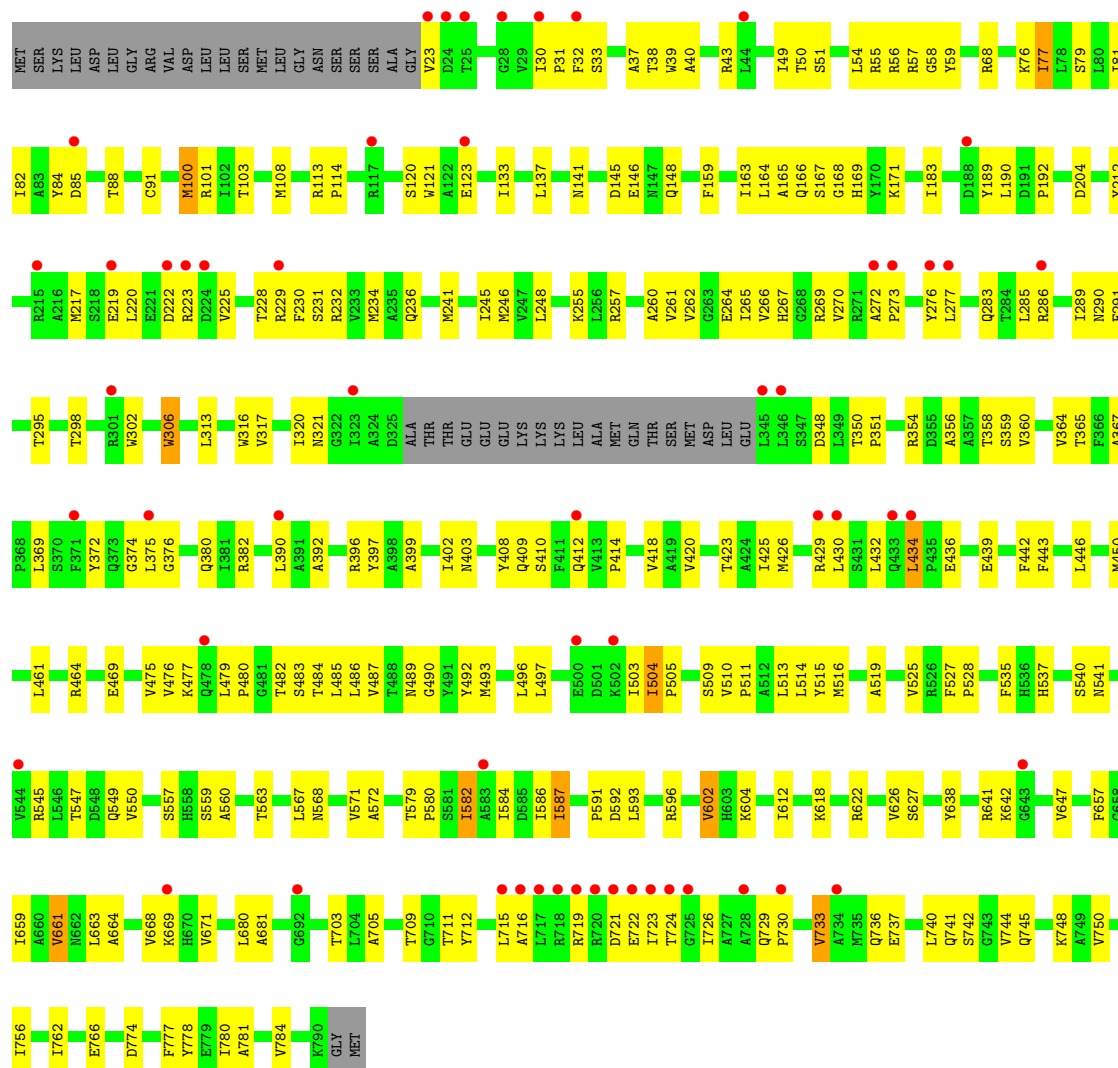


• Molecule 1: p1



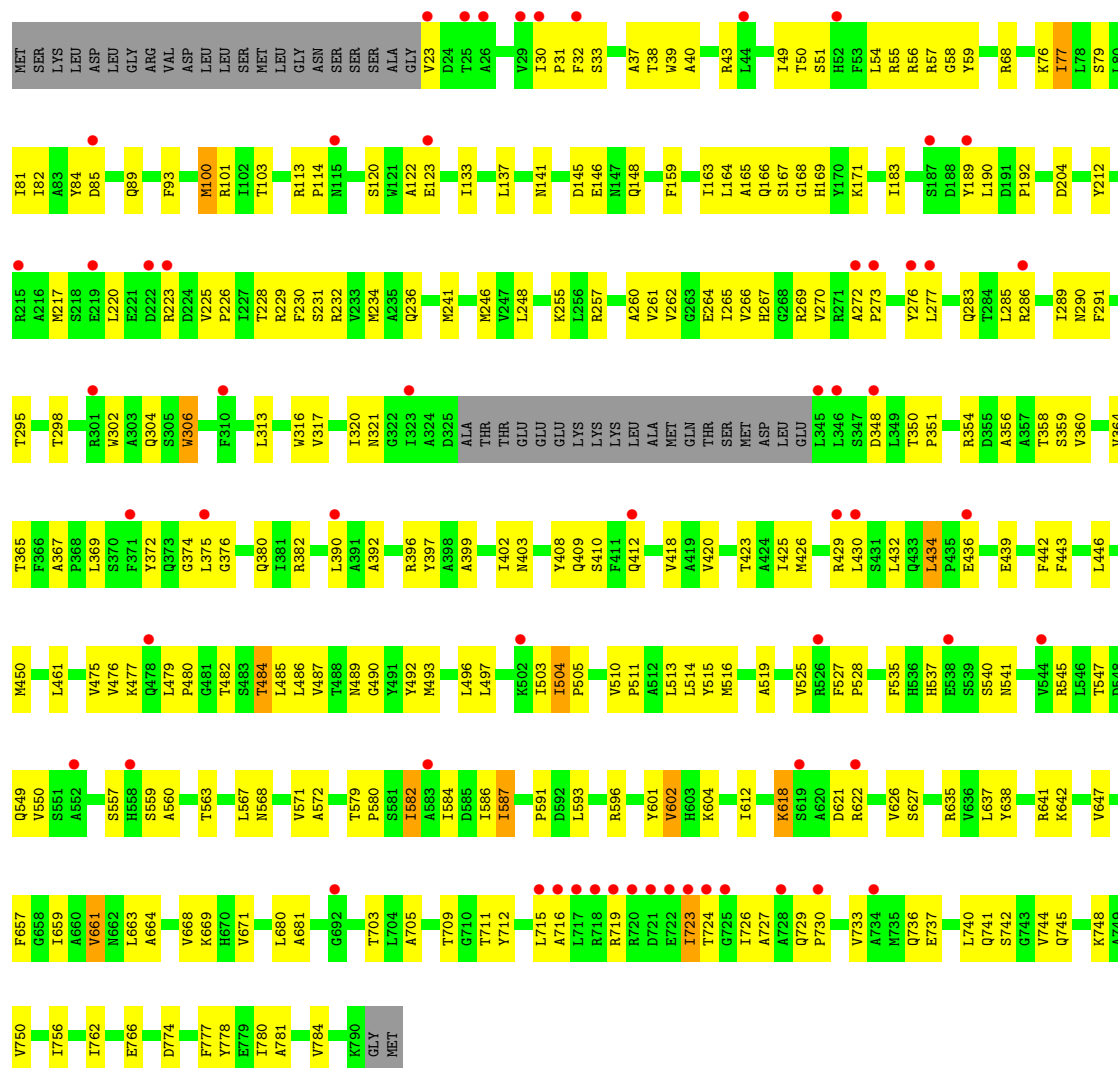


• Molecule 1: p1

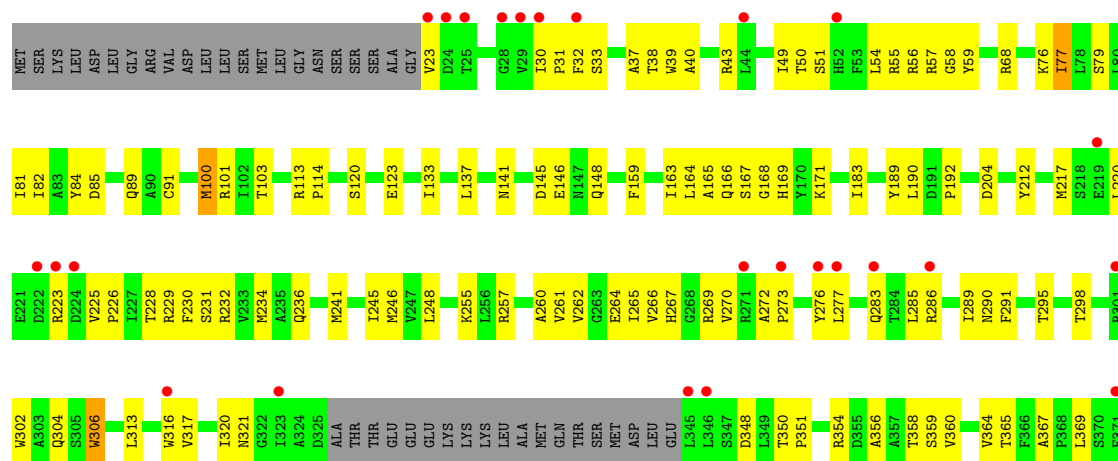


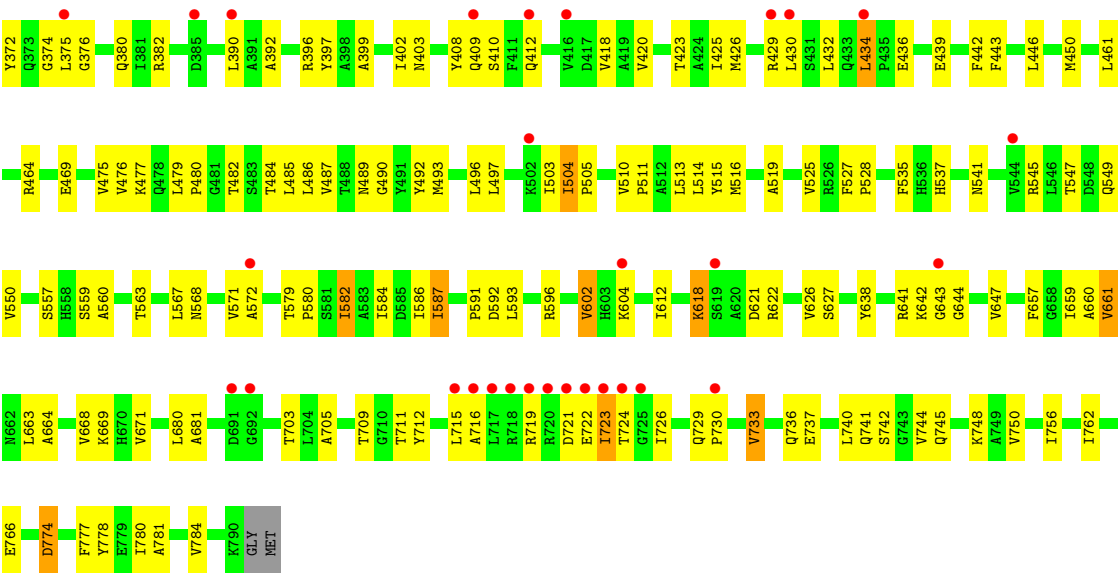
• Molecule 1: p1





• Molecule 1: p1





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	314.35Å 314.35Å 527.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.01 – 3.70 30.01 – 3.70	Depositor EDS
% Data completeness (in resolution range)	97.0 (30.01-3.70) 97.0 (30.01-3.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.75Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.244 , 0.258 0.244 , 0.257	Depositor DCC
R_{free} test set	13636 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	126.2	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 92.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	57630	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/5865	0.90	5/7957 (0.1%)
1	B	0.52	0/5865	0.90	5/7957 (0.1%)
1	C	0.51	0/5865	0.90	5/7957 (0.1%)
1	D	0.52	0/5865	0.90	5/7957 (0.1%)
1	E	0.52	0/5865	0.90	6/7957 (0.1%)
1	F	0.52	0/5865	0.89	5/7957 (0.1%)
1	G	0.52	0/5865	0.90	5/7957 (0.1%)
1	H	0.52	0/5865	0.90	5/7957 (0.1%)
1	I	0.52	0/5865	0.89	5/7957 (0.1%)
1	J	0.51	0/5865	0.89	5/7957 (0.1%)
All	All	0.52	0/58650	0.90	51/79570 (0.1%)

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	504	ILE	CA-C-N	-5.74	114.70	120.21
1	J	504	ILE	C-N-CA	-5.74	114.70	120.21
1	A	504	ILE	CA-C-N	-5.66	114.78	120.21
1	A	504	ILE	C-N-CA	-5.66	114.78	120.21
1	H	504	ILE	CA-C-N	-5.64	114.80	120.21
1	H	504	ILE	C-N-CA	-5.64	114.80	120.21
1	B	504	ILE	CA-C-N	-5.61	114.83	120.21
1	B	504	ILE	C-N-CA	-5.61	114.83	120.21
1	A	434	LEU	CA-C-N	5.59	124.78	118.97
1	A	434	LEU	C-N-CA	5.59	124.78	118.97
1	D	504	ILE	CA-C-N	-5.59	114.84	120.21
1	D	504	ILE	C-N-CA	-5.59	114.84	120.21
1	G	504	ILE	CA-C-N	-5.58	114.86	120.21
1	G	504	ILE	C-N-CA	-5.58	114.86	120.21
1	C	504	ILE	CA-C-N	-5.56	114.87	120.21
1	C	504	ILE	C-N-CA	-5.56	114.87	120.21
1	B	434	LEU	CA-C-N	5.54	124.74	118.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	LEU	C-N-CA	5.54	124.74	118.97
1	D	434	LEU	CA-C-N	5.54	124.73	118.97
1	D	434	LEU	C-N-CA	5.54	124.73	118.97
1	F	434	LEU	CA-C-N	5.52	124.71	118.97
1	F	434	LEU	C-N-CA	5.52	124.71	118.97
1	E	504	ILE	CA-C-N	-5.50	114.93	120.21
1	E	504	ILE	C-N-CA	-5.50	114.93	120.21
1	I	434	LEU	CA-C-N	5.50	124.69	118.97
1	I	434	LEU	C-N-CA	5.50	124.69	118.97
1	E	434	LEU	CA-C-N	5.48	124.67	118.97
1	E	434	LEU	C-N-CA	5.48	124.67	118.97
1	D	661	VAL	N-CA-C	5.48	116.38	108.48
1	C	434	LEU	CA-C-N	5.47	124.66	118.97
1	C	434	LEU	C-N-CA	5.47	124.66	118.97
1	F	504	ILE	CA-C-N	-5.47	114.96	120.21
1	F	504	ILE	C-N-CA	-5.47	114.96	120.21
1	G	434	LEU	CA-C-N	5.46	124.65	118.97
1	G	434	LEU	C-N-CA	5.46	124.65	118.97
1	F	661	VAL	N-CA-C	5.43	116.30	108.48
1	E	661	VAL	N-CA-C	5.43	116.30	108.48
1	H	434	LEU	CA-C-N	5.42	124.61	118.97
1	H	434	LEU	C-N-CA	5.42	124.61	118.97
1	J	434	LEU	CA-C-N	5.42	124.60	118.97
1	J	434	LEU	C-N-CA	5.42	124.60	118.97
1	I	661	VAL	N-CA-C	5.37	116.21	108.48
1	A	661	VAL	N-CA-C	5.37	116.21	108.48
1	J	661	VAL	N-CA-C	5.35	116.19	108.48
1	H	661	VAL	N-CA-C	5.35	116.19	108.48
1	I	504	ILE	CA-C-N	-5.35	115.07	120.21
1	I	504	ILE	C-N-CA	-5.35	115.07	120.21
1	C	661	VAL	N-CA-C	5.31	116.13	108.48
1	B	661	VAL	N-CA-C	5.30	116.11	108.48
1	G	661	VAL	N-CA-C	5.18	115.94	108.48
1	E	503	ILE	N-CA-C	5.09	116.55	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5763	0	5773	239	0
1	B	5763	0	5773	241	0
1	C	5763	0	5773	230	0
1	D	5763	0	5773	237	6
1	E	5763	0	5773	237	0
1	F	5763	0	5773	236	0
1	G	5763	0	5773	237	0
1	H	5763	0	5773	243	6
1	I	5763	0	5773	237	0
1	J	5763	0	5773	242	0
All	All	57630	0	57730	2269	6

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 20.

All (2269) 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:B:270:VAL:HG21	1:B:317:VAL:HG12	1.19	1.17
1:J:270:VAL:HG21	1:J:317:VAL:HG12	1.19	1.17
1:B:270:VAL:CG2	1:B:317:VAL:HG12	1.76	1.15
1:C:270:VAL:CG2	1:C:317:VAL:HG12	1.76	1.15
1:D:270:VAL:CG2	1:D:317:VAL:HG12	1.77	1.15
1:A:270:VAL:HG21	1:A:317:VAL:HG12	1.19	1.15
1:G:270:VAL:CG2	1:G:317:VAL:HG12	1.76	1.14
1:H:270:VAL:HG21	1:H:317:VAL:HG12	1.19	1.14
1:H:270:VAL:CG2	1:H:317:VAL:HG12	1.76	1.14
1:I:270:VAL:CG2	1:I:317:VAL:HG12	1.77	1.14
1:A:270:VAL:CG2	1:A:317:VAL:HG12	1.76	1.14
1:E:270:VAL:CG2	1:E:317:VAL:HG12	1.76	1.14
1:C:270:VAL:HG21	1:C:317:VAL:HG12	1.19	1.13
1:F:270:VAL:CG2	1:F:317:VAL:HG12	1.77	1.13
1:J:270:VAL:CG2	1:J:317:VAL:HG12	1.76	1.13
1:E:270:VAL:HG21	1:E:317:VAL:HG12	1.19	1.12
1:G:270:VAL:HG21	1:G:317:VAL:HG12	1.19	1.11
1:F:270:VAL:HG21	1:F:317:VAL:HG12	1.19	1.10
1:I:270:VAL:HG21	1:I:317:VAL:HG12	1.19	1.09
1:D:270:VAL:HG21	1:D:317:VAL:HG12	1.19	1.09
1:J:255:LYS:NZ	1:J:359:SER:OG	2.02	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:255:LYS:NZ	1:G:359:SER:OG	2.02	0.93
1:F:255:LYS:NZ	1:F:359:SER:OG	2.02	0.93
1:A:255:LYS:NZ	1:A:359:SER:OG	2.02	0.93
1:E:255:LYS:NZ	1:E:359:SER:OG	2.02	0.93
1:A:23:VAL:HG21	1:A:32:PHE:HB3	1.51	0.92
1:E:23:VAL:HG21	1:E:32:PHE:HB3	1.52	0.92
1:C:255:LYS:NZ	1:C:359:SER:OG	2.02	0.92
1:D:255:LYS:NZ	1:D:359:SER:OG	2.01	0.91
1:C:23:VAL:HG21	1:C:32:PHE:HB3	1.52	0.91
1:D:23:VAL:HG21	1:D:32:PHE:HB3	1.52	0.91
1:H:255:LYS:NZ	1:H:359:SER:OG	2.02	0.91
1:B:255:LYS:NZ	1:B:359:SER:OG	2.02	0.91
1:F:23:VAL:HG21	1:F:32:PHE:HB3	1.52	0.91
1:J:23:VAL:HG21	1:J:32:PHE:HB3	1.52	0.91
1:H:23:VAL:HG21	1:H:32:PHE:HB3	1.52	0.91
1:I:255:LYS:NZ	1:I:359:SER:OG	2.02	0.91
1:I:23:VAL:HG21	1:I:32:PHE:HB3	1.51	0.90
1:B:23:VAL:HG21	1:B:32:PHE:HB3	1.51	0.90
1:I:270:VAL:HG21	1:I:317:VAL:CG1	2.03	0.89
1:G:23:VAL:HG21	1:G:32:PHE:HB3	1.52	0.89
1:G:270:VAL:HG21	1:G:317:VAL:CG1	2.03	0.89
1:B:270:VAL:HG21	1:B:317:VAL:CG1	2.03	0.89
1:D:270:VAL:HG21	1:D:317:VAL:CG1	2.03	0.88
1:F:270:VAL:HG21	1:F:317:VAL:CG1	2.03	0.88
1:E:270:VAL:HG21	1:E:317:VAL:CG1	2.03	0.88
1:H:270:VAL:HG21	1:H:317:VAL:CG1	2.03	0.88
1:E:306:TRP:HD1	1:E:313:LEU:HD13	1.39	0.88
1:B:306:TRP:HD1	1:B:313:LEU:HD13	1.40	0.87
1:A:270:VAL:HG21	1:A:317:VAL:CG1	2.03	0.87
1:C:270:VAL:HG21	1:C:317:VAL:CG1	2.03	0.87
1:J:306:TRP:HD1	1:J:313:LEU:HD13	1.39	0.87
1:H:306:TRP:HD1	1:H:313:LEU:HD13	1.39	0.87
1:F:306:TRP:HD1	1:F:313:LEU:HD13	1.39	0.86
1:D:306:TRP:HD1	1:D:313:LEU:HD13	1.39	0.86
1:I:306:TRP:HD1	1:I:313:LEU:HD13	1.39	0.86
1:A:306:TRP:HD1	1:A:313:LEU:HD13	1.39	0.86
1:C:306:TRP:HD1	1:C:313:LEU:HD13	1.39	0.85
1:D:403:ASN:OD1	1:D:436:GLU:HG2	1.77	0.85
1:J:403:ASN:OD1	1:J:436:GLU:HG2	1.77	0.85
1:J:270:VAL:HG21	1:J:317:VAL:CG1	2.03	0.85
1:G:306:TRP:HD1	1:G:313:LEU:HD13	1.39	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:403:ASN:OD1	1:G:436:GLU:HG2	1.77	0.85
1:E:403:ASN:OD1	1:E:436:GLU:HG2	1.77	0.84
1:B:403:ASN:OD1	1:B:436:GLU:HG2	1.77	0.84
1:A:403:ASN:OD1	1:A:436:GLU:HG2	1.77	0.84
1:C:270:VAL:CG2	1:C:317:VAL:CG1	2.56	0.84
1:D:270:VAL:CG2	1:D:317:VAL:CG1	2.56	0.84
1:B:23:VAL:CG2	1:B:32:PHE:HB3	2.08	0.83
1:A:270:VAL:CG2	1:A:317:VAL:CG1	2.56	0.83
1:C:316:TRP:CE2	1:C:320:ILE:HD11	2.14	0.83
1:F:403:ASN:OD1	1:F:436:GLU:HG2	1.77	0.83
1:C:403:ASN:OD1	1:C:436:GLU:HG2	1.77	0.83
1:E:270:VAL:CG2	1:E:317:VAL:CG1	2.56	0.83
1:E:316:TRP:CE2	1:E:320:ILE:HD11	2.14	0.83
1:I:23:VAL:CG2	1:I:32:PHE:HB3	2.08	0.83
1:J:23:VAL:CG2	1:J:32:PHE:HB3	2.09	0.83
1:C:23:VAL:CG2	1:C:32:PHE:HB3	2.09	0.83
1:D:316:TRP:CE2	1:D:320:ILE:HD11	2.13	0.83
1:G:316:TRP:CE2	1:G:320:ILE:HD11	2.13	0.83
1:H:123:GLU:CD	1:I:229:ARG:HH12	1.86	0.83
1:H:403:ASN:OD1	1:H:436:GLU:HG2	1.77	0.83
1:J:316:TRP:CE2	1:J:320:ILE:HD11	2.13	0.83
1:E:306:TRP:CD1	1:E:313:LEU:HD13	2.13	0.83
1:G:306:TRP:CD1	1:G:313:LEU:HD13	2.13	0.83
1:I:403:ASN:OD1	1:I:436:GLU:HG2	1.77	0.83
1:A:306:TRP:CD1	1:A:313:LEU:HD13	2.13	0.83
1:F:316:TRP:CE2	1:F:320:ILE:HD11	2.13	0.83
1:A:23:VAL:CG2	1:A:32:PHE:HB3	2.08	0.83
1:A:316:TRP:CE2	1:A:320:ILE:HD11	2.13	0.83
1:B:270:VAL:CG2	1:B:317:VAL:CG1	2.56	0.83
1:F:270:VAL:CG2	1:F:317:VAL:CG1	2.56	0.83
1:I:306:TRP:CD1	1:I:313:LEU:HD13	2.13	0.83
1:H:270:VAL:CG2	1:H:317:VAL:CG1	2.56	0.83
1:B:306:TRP:CD1	1:B:313:LEU:HD13	2.14	0.82
1:D:306:TRP:CD1	1:D:313:LEU:HD13	2.13	0.82
1:I:316:TRP:CE2	1:I:320:ILE:HD11	2.13	0.82
1:E:23:VAL:CG2	1:E:32:PHE:HB3	2.08	0.82
1:I:270:VAL:CG2	1:I:317:VAL:CG1	2.56	0.82
1:J:270:VAL:CG2	1:J:317:VAL:CG1	2.56	0.82
1:H:316:TRP:CE2	1:H:320:ILE:HD11	2.13	0.82
1:J:306:TRP:CD1	1:J:313:LEU:HD13	2.13	0.82
1:H:23:VAL:CG2	1:H:32:PHE:HB3	2.09	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:TRP:CE2	1:B:320:ILE:HD11	2.14	0.82
1:F:306:TRP:CD1	1:F:313:LEU:HD13	2.13	0.82
1:D:23:VAL:CG2	1:D:32:PHE:HB3	2.09	0.82
1:H:306:TRP:CD1	1:H:313:LEU:HD13	2.13	0.81
1:C:306:TRP:CD1	1:C:313:LEU:HD13	2.13	0.81
1:F:23:VAL:CG2	1:F:32:PHE:HB3	2.09	0.81
1:G:270:VAL:CG2	1:G:317:VAL:CG1	2.56	0.81
1:H:171:LYS:O	1:I:232:ARG:NH2	2.13	0.81
1:C:39:TRP:CZ3	1:C:516:MET:HG2	2.17	0.81
1:G:23:VAL:CG2	1:G:32:PHE:HB3	2.09	0.81
1:B:228:THR:O	1:B:232:ARG:HG2	1.82	0.80
1:H:273:PRO:HB3	1:H:276:TYR:CD2	2.17	0.80
1:J:273:PRO:HB3	1:J:276:TYR:CD2	2.17	0.80
1:E:39:TRP:CZ3	1:E:516:MET:HG2	2.16	0.80
1:F:228:THR:O	1:F:232:ARG:HG2	1.82	0.80
1:F:504:ILE:HG13	1:F:510:VAL:HG21	1.64	0.80
1:G:273:PRO:HB3	1:G:276:TYR:CD2	2.17	0.80
1:G:39:TRP:CZ3	1:G:516:MET:HG2	2.17	0.80
1:I:228:THR:O	1:I:232:ARG:HG2	1.82	0.80
1:D:273:PRO:HB3	1:D:276:TYR:CD2	2.17	0.80
1:G:228:THR:O	1:G:232:ARG:HG2	1.82	0.80
1:I:504:ILE:HG13	1:I:510:VAL:HG21	1.64	0.79
1:C:228:THR:O	1:C:232:ARG:HG2	1.82	0.79
1:F:273:PRO:HB3	1:F:276:TYR:CD2	2.17	0.79
1:C:273:PRO:HB3	1:C:276:TYR:CD2	2.17	0.79
1:H:228:THR:O	1:H:232:ARG:HG2	1.82	0.79
1:A:228:THR:O	1:A:232:ARG:HG2	1.82	0.79
1:F:39:TRP:CZ3	1:F:516:MET:HG2	2.17	0.79
1:I:273:PRO:HB3	1:I:276:TYR:CD2	2.17	0.79
1:A:273:PRO:HB3	1:A:276:TYR:CD2	2.17	0.79
1:D:228:THR:O	1:D:232:ARG:HG2	1.81	0.79
1:H:39:TRP:CZ3	1:H:516:MET:HG2	2.18	0.79
1:J:39:TRP:CZ3	1:J:516:MET:HG2	2.18	0.79
1:D:504:ILE:HG13	1:D:510:VAL:HG21	1.64	0.78
1:B:504:ILE:HG13	1:B:510:VAL:HG21	1.65	0.78
1:I:39:TRP:CZ3	1:I:516:MET:HG2	2.17	0.78
1:A:39:TRP:CZ3	1:A:516:MET:HG2	2.18	0.78
1:D:39:TRP:CZ3	1:D:516:MET:HG2	2.18	0.78
1:E:273:PRO:HB3	1:E:276:TYR:CD2	2.19	0.78
1:A:504:ILE:HG13	1:A:510:VAL:HG21	1.64	0.78
1:B:39:TRP:CZ3	1:B:516:MET:HG2	2.17	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:504:ILE:HG13	1:J:510:VAL:HG21	1.65	0.78
1:C:504:ILE:HG13	1:C:510:VAL:HG21	1.64	0.78
1:E:228:THR:O	1:E:232:ARG:HG2	1.82	0.77
1:E:504:ILE:HG13	1:E:510:VAL:HG21	1.65	0.77
1:B:273:PRO:HB3	1:B:276:TYR:CD2	2.19	0.77
1:J:228:THR:O	1:J:232:ARG:HG2	1.83	0.77
1:G:504:ILE:HG13	1:G:510:VAL:HG21	1.64	0.77
1:D:171:LYS:O	1:J:232:ARG:NH2	2.17	0.77
1:D:123:GLU:CD	1:J:229:ARG:HH12	1.93	0.77
1:C:123:GLU:HG2	1:C:171:LYS:HD2	1.68	0.76
1:H:504:ILE:HG13	1:H:510:VAL:HG21	1.65	0.76
1:A:123:GLU:HG2	1:A:171:LYS:HD2	1.68	0.76
1:D:123:GLU:HG2	1:D:171:LYS:HD2	1.68	0.76
1:B:123:GLU:HG2	1:B:171:LYS:HD2	1.68	0.76
1:I:123:GLU:HG2	1:I:171:LYS:HD2	1.68	0.75
1:J:123:GLU:HG2	1:J:171:LYS:HD2	1.67	0.75
1:D:418:VAL:HG12	1:J:141:ASN:HD21	1.52	0.74
1:H:123:GLU:HG2	1:H:171:LYS:HD2	1.68	0.74
1:I:40:ALA:HB3	1:I:290:ASN:OD1	1.88	0.74
1:F:40:ALA:HB3	1:F:290:ASN:OD1	1.87	0.74
1:C:270:VAL:HG23	1:C:317:VAL:HG12	1.70	0.74
1:B:40:ALA:HB3	1:B:290:ASN:OD1	1.88	0.74
1:E:40:ALA:HB3	1:E:290:ASN:OD1	1.88	0.74
1:G:123:GLU:HG2	1:G:171:LYS:HD2	1.68	0.74
1:A:270:VAL:HG23	1:A:317:VAL:HG12	1.70	0.74
1:E:123:GLU:HG2	1:E:171:LYS:HD2	1.68	0.74
1:A:40:ALA:HB3	1:A:290:ASN:OD1	1.88	0.73
1:C:40:ALA:HB3	1:C:290:ASN:OD1	1.88	0.73
1:F:123:GLU:HG2	1:F:171:LYS:HD2	1.68	0.73
1:G:545:ARG:HD2	1:G:572:ALA:HB1	1.71	0.73
1:H:40:ALA:HB3	1:H:290:ASN:OD1	1.88	0.73
1:D:270:VAL:HG23	1:D:317:VAL:HG12	1.70	0.73
1:E:545:ARG:HD2	1:E:572:ALA:HB1	1.71	0.73
1:A:123:GLU:CD	1:B:229:ARG:HH12	1.96	0.72
1:D:40:ALA:HB3	1:D:290:ASN:OD1	1.88	0.72
1:J:270:VAL:HG23	1:J:317:VAL:HG12	1.70	0.72
1:H:270:VAL:HG23	1:H:317:VAL:HG12	1.70	0.72
1:G:40:ALA:HB3	1:G:290:ASN:OD1	1.88	0.72
1:F:545:ARG:HD2	1:F:572:ALA:HB1	1.71	0.72
1:H:545:ARG:HD2	1:H:572:ALA:HB1	1.71	0.72
1:G:270:VAL:HG23	1:G:317:VAL:HG12	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:545:ARG:HD2	1:I:572:ALA:HB1	1.71	0.72
1:E:123:GLU:CD	1:F:229:ARG:HH12	1.97	0.72
1:C:306:TRP:CD1	1:C:313:LEU:CD1	2.73	0.71
1:G:306:TRP:CD1	1:G:313:LEU:CD1	2.73	0.71
1:H:39:TRP:CE3	1:H:289:ILE:HD11	2.25	0.71
1:J:40:ALA:HB3	1:J:290:ASN:OD1	1.88	0.71
1:E:270:VAL:HG23	1:E:317:VAL:HG12	1.70	0.71
1:B:545:ARG:HD2	1:B:572:ALA:HB1	1.71	0.71
1:A:306:TRP:CD1	1:A:313:LEU:CD1	2.74	0.71
1:C:545:ARG:HD2	1:C:572:ALA:HB1	1.71	0.71
1:D:306:TRP:CD1	1:D:313:LEU:CD1	2.73	0.71
1:G:39:TRP:CE3	1:G:289:ILE:HD11	2.25	0.71
1:H:306:TRP:CD1	1:H:313:LEU:CD1	2.74	0.71
1:C:39:TRP:CE3	1:C:289:ILE:HD11	2.26	0.71
1:E:306:TRP:CD1	1:E:313:LEU:CD1	2.74	0.71
1:F:306:TRP:CD1	1:F:313:LEU:CD1	2.73	0.71
1:I:39:TRP:CE3	1:I:289:ILE:HD11	2.26	0.71
1:E:145:ASP:HB3	1:E:148:GLN:HE21	1.56	0.71
1:F:39:TRP:CE3	1:F:289:ILE:HD11	2.26	0.71
1:H:418:VAL:HG12	1:I:141:ASN:HD21	1.55	0.71
1:D:39:TRP:CE3	1:D:289:ILE:HD11	2.25	0.70
1:J:39:TRP:CE3	1:J:289:ILE:HD11	2.25	0.70
1:B:306:TRP:CD1	1:B:313:LEU:CD1	2.74	0.70
1:D:316:TRP:CD2	1:D:320:ILE:HD11	2.26	0.70
1:I:270:VAL:HG23	1:I:317:VAL:HG12	1.70	0.70
1:J:316:TRP:CD2	1:J:320:ILE:HD11	2.26	0.70
1:I:306:TRP:CD1	1:I:313:LEU:CD1	2.74	0.70
1:I:316:TRP:CD2	1:I:320:ILE:HD11	2.27	0.70
1:A:145:ASP:HB3	1:A:148:GLN:HE21	1.56	0.70
1:C:412:GLN:HG2	1:C:423:THR:HG22	1.73	0.70
1:G:418:VAL:HG12	1:H:141:ASN:HD21	1.57	0.70
1:J:306:TRP:CD1	1:J:313:LEU:CD1	2.74	0.70
1:A:545:ARG:HD2	1:A:572:ALA:HB1	1.71	0.70
1:E:39:TRP:CE3	1:E:289:ILE:HD11	2.26	0.70
1:G:145:ASP:HB3	1:G:148:GLN:HE21	1.57	0.70
1:G:316:TRP:CD2	1:G:320:ILE:HD11	2.27	0.70
1:A:39:TRP:CE3	1:A:289:ILE:HD11	2.25	0.70
1:F:145:ASP:HB3	1:F:148:GLN:HE21	1.57	0.70
1:B:145:ASP:HB3	1:B:148:GLN:HE21	1.56	0.70
1:D:545:ARG:HD2	1:D:572:ALA:HB1	1.71	0.70
1:E:316:TRP:CD2	1:E:320:ILE:HD11	2.27	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:TRP:CD2	1:A:320:ILE:HD11	2.27	0.70
1:B:270:VAL:HG22	1:B:321:ASN:ND2	2.07	0.70
1:B:316:TRP:CD2	1:B:320:ILE:HD11	2.27	0.70
1:H:145:ASP:HB3	1:H:148:GLN:HE21	1.56	0.70
1:B:39:TRP:CE3	1:B:289:ILE:HD11	2.26	0.70
1:B:412:GLN:HG2	1:B:423:THR:HG22	1.73	0.70
1:J:545:ARG:HD2	1:J:572:ALA:HB1	1.71	0.70
1:A:412:GLN:HG2	1:A:423:THR:HG22	1.73	0.69
1:C:270:VAL:HG22	1:C:321:ASN:ND2	2.07	0.69
1:E:270:VAL:HG22	1:E:321:ASN:ND2	2.07	0.69
1:E:412:GLN:HG2	1:E:423:THR:HG22	1.73	0.69
1:A:418:VAL:HG12	1:B:141:ASN:HD21	1.58	0.69
1:D:270:VAL:HG22	1:D:321:ASN:ND2	2.07	0.69
1:C:316:TRP:CD2	1:C:320:ILE:HD11	2.27	0.69
1:D:412:GLN:HG2	1:D:423:THR:HG22	1.74	0.69
1:F:316:TRP:CD2	1:F:320:ILE:HD11	2.27	0.69
1:H:316:TRP:CD2	1:H:320:ILE:HD11	2.27	0.69
1:B:270:VAL:HG23	1:B:317:VAL:HG12	1.70	0.69
1:F:270:VAL:HG22	1:F:321:ASN:ND2	2.07	0.69
1:J:270:VAL:HG22	1:J:321:ASN:ND2	2.08	0.69
1:D:145:ASP:HB3	1:D:148:GLN:HE21	1.56	0.69
1:A:270:VAL:HG22	1:A:321:ASN:ND2	2.08	0.69
1:J:412:GLN:HG2	1:J:423:THR:HG22	1.73	0.69
1:H:412:GLN:HG2	1:H:423:THR:HG22	1.74	0.69
1:I:145:ASP:HB3	1:I:148:GLN:HE21	1.57	0.69
1:E:171:LYS:O	1:F:232:ARG:NH2	2.25	0.69
1:F:270:VAL:HG23	1:F:317:VAL:HG12	1.70	0.69
1:G:270:VAL:HG22	1:G:321:ASN:ND2	2.07	0.69
1:J:145:ASP:HB3	1:J:148:GLN:HE21	1.57	0.69
1:D:262:VAL:HG11	1:D:285:LEU:HD12	1.76	0.69
1:H:267:HIS:NE2	1:H:295:THR:HG23	2.09	0.68
1:I:267:HIS:NE2	1:I:295:THR:HG23	2.09	0.68
1:I:412:GLN:HG2	1:I:423:THR:HG22	1.73	0.68
1:A:262:VAL:HG11	1:A:285:LEU:HD12	1.76	0.68
1:D:267:HIS:NE2	1:D:295:THR:HG23	2.09	0.68
1:F:412:GLN:HG2	1:F:423:THR:HG22	1.74	0.68
1:I:270:VAL:HG22	1:I:321:ASN:ND2	2.07	0.68
1:J:267:HIS:NE2	1:J:295:THR:HG23	2.09	0.68
1:A:171:LYS:O	1:B:232:ARG:NH2	2.26	0.68
1:G:267:HIS:NE2	1:G:295:THR:HG23	2.09	0.68
1:G:412:GLN:HG2	1:G:423:THR:HG22	1.73	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:270:VAL:HG22	1:H:321:ASN:ND2	2.07	0.68
1:I:267:HIS:HE2	1:I:295:THR:HG23	1.58	0.68
1:B:262:VAL:HG11	1:B:285:LEU:HD12	1.76	0.68
1:E:267:HIS:NE2	1:E:295:THR:HG23	2.09	0.68
1:F:267:HIS:NE2	1:F:295:THR:HG23	2.09	0.68
1:C:145:ASP:HB3	1:C:148:GLN:HE21	1.56	0.68
1:F:545:ARG:HB2	1:F:572:ALA:HB3	1.76	0.67
1:H:262:VAL:HG11	1:H:285:LEU:HD12	1.76	0.67
1:H:545:ARG:HB2	1:H:572:ALA:HB3	1.77	0.67
1:A:545:ARG:HB2	1:A:572:ALA:HB3	1.76	0.67
1:B:267:HIS:NE2	1:B:295:THR:HG23	2.09	0.67
1:G:545:ARG:HB2	1:G:572:ALA:HB3	1.76	0.67
1:J:262:VAL:HG11	1:J:285:LEU:HD12	1.76	0.67
1:B:171:LYS:O	1:C:232:ARG:NH2	2.27	0.67
1:I:593:LEU:O	1:I:596:ARG:HB3	1.95	0.67
1:J:593:LEU:O	1:J:596:ARG:HB3	1.95	0.67
1:A:267:HIS:NE2	1:A:295:THR:HG23	2.09	0.67
1:C:262:VAL:HG11	1:C:285:LEU:HD12	1.76	0.67
1:G:262:VAL:HG11	1:G:285:LEU:HD12	1.76	0.67
1:I:545:ARG:HB2	1:I:572:ALA:HB3	1.76	0.67
1:A:593:LEU:O	1:A:596:ARG:HB3	1.95	0.67
1:B:123:GLU:CD	1:C:229:ARG:HH12	2.03	0.67
1:D:545:ARG:HB2	1:D:572:ALA:HB3	1.76	0.67
1:E:593:LEU:O	1:E:596:ARG:HB3	1.95	0.67
1:C:593:LEU:O	1:C:596:ARG:HB3	1.95	0.67
1:E:545:ARG:HB2	1:E:572:ALA:HB3	1.76	0.67
1:C:267:HIS:NE2	1:C:295:THR:HG23	2.09	0.67
1:J:545:ARG:HB2	1:J:572:ALA:HB3	1.77	0.66
1:E:262:VAL:HG11	1:E:285:LEU:HD12	1.76	0.66
1:B:545:ARG:HB2	1:B:572:ALA:HB3	1.77	0.66
1:H:593:LEU:O	1:H:596:ARG:HB3	1.95	0.66
1:I:262:VAL:HG11	1:I:285:LEU:HD12	1.76	0.66
1:B:593:LEU:O	1:B:596:ARG:HB3	1.95	0.66
1:B:266:VAL:HG13	1:B:286:ARG:HD2	1.78	0.65
1:F:262:VAL:HG11	1:F:285:LEU:HD12	1.76	0.65
1:G:266:VAL:HG13	1:G:286:ARG:HD2	1.78	0.65
1:F:593:LEU:O	1:F:596:ARG:HB3	1.95	0.65
1:A:266:VAL:HG13	1:A:286:ARG:HD2	1.78	0.65
1:D:593:LEU:O	1:D:596:ARG:HB3	1.95	0.65
1:G:593:LEU:O	1:G:596:ARG:HB3	1.95	0.65
1:C:266:VAL:HG13	1:C:286:ARG:HD2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:ARG:HB2	1:C:572:ALA:HB3	1.77	0.65
1:J:266:VAL:HG13	1:J:286:ARG:HD2	1.79	0.65
1:B:272:ALA:N	1:B:273:PRO:CD	2.60	0.65
1:A:272:ALA:N	1:A:273:PRO:CD	2.60	0.64
1:D:272:ALA:N	1:D:273:PRO:CD	2.60	0.64
1:E:272:ALA:N	1:E:273:PRO:CD	2.60	0.64
1:F:418:VAL:HG12	1:G:141:ASN:HD21	1.61	0.64
1:H:266:VAL:HG13	1:H:286:ARG:HD2	1.79	0.64
1:I:272:ALA:N	1:I:273:PRO:CD	2.60	0.64
1:J:272:ALA:N	1:J:273:PRO:CD	2.60	0.64
1:F:230:PHE:O	1:F:234:MET:HG3	1.98	0.64
1:G:230:PHE:O	1:G:234:MET:HG3	1.98	0.64
1:G:272:ALA:N	1:G:273:PRO:CD	2.61	0.64
1:H:272:ALA:N	1:H:273:PRO:CD	2.61	0.64
1:E:230:PHE:O	1:E:234:MET:HG3	1.98	0.64
1:F:513:LEU:HD23	1:F:516:MET:HE3	1.80	0.64
1:H:230:PHE:O	1:H:234:MET:HG3	1.97	0.64
1:C:230:PHE:O	1:C:234:MET:HG3	1.98	0.64
1:F:266:VAL:HG13	1:F:286:ARG:HD2	1.78	0.64
1:D:230:PHE:O	1:D:234:MET:HG3	1.98	0.64
1:J:39:TRP:CH2	1:J:516:MET:HA	2.33	0.64
1:A:513:LEU:HD23	1:A:516:MET:HE3	1.79	0.64
1:B:513:LEU:HD23	1:B:516:MET:HE3	1.79	0.64
1:C:39:TRP:CH2	1:C:516:MET:HA	2.33	0.64
1:D:266:VAL:HG13	1:D:286:ARG:HD2	1.78	0.64
1:F:547:THR:HG21	1:F:571:VAL:HG12	1.80	0.64
1:I:513:LEU:HD23	1:I:516:MET:HE3	1.80	0.64
1:B:547:THR:HG21	1:B:571:VAL:HG12	1.80	0.63
1:C:272:ALA:N	1:C:273:PRO:CD	2.60	0.63
1:I:266:VAL:HG13	1:I:286:ARG:HD2	1.78	0.63
1:E:266:VAL:HG13	1:E:286:ARG:HD2	1.79	0.63
1:E:547:THR:HG21	1:E:571:VAL:HG12	1.80	0.63
1:G:39:TRP:CH2	1:G:516:MET:HA	2.33	0.63
1:A:232:ARG:NH2	1:J:171:LYS:O	2.30	0.63
1:A:547:THR:HG21	1:A:571:VAL:HG12	1.80	0.63
1:F:39:TRP:CH2	1:F:516:MET:HA	2.33	0.63
1:J:230:PHE:O	1:J:234:MET:HG3	1.98	0.63
1:B:716:ALA:HA	1:B:742:SER:OG	1.99	0.63
1:F:272:ALA:N	1:F:273:PRO:CD	2.61	0.63
1:H:513:LEU:HD23	1:H:516:MET:HE3	1.80	0.63
1:D:39:TRP:CH2	1:D:516:MET:HA	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:GLN:OE1	1:I:429:ARG:NE	2.28	0.63
1:I:230:PHE:O	1:I:234:MET:HG3	1.98	0.63
1:J:547:THR:HG21	1:J:571:VAL:HG12	1.80	0.63
1:B:230:PHE:O	1:B:234:MET:HG3	1.98	0.63
1:E:513:LEU:HD23	1:E:516:MET:HE3	1.79	0.63
1:H:716:ALA:HA	1:H:742:SER:OG	1.99	0.63
1:I:39:TRP:CH2	1:I:516:MET:HA	2.34	0.63
1:A:39:TRP:CH2	1:A:516:MET:HA	2.34	0.63
1:A:230:PHE:O	1:A:234:MET:HG3	1.98	0.63
1:B:39:TRP:CH2	1:B:516:MET:HA	2.33	0.63
1:D:513:LEU:HD23	1:D:516:MET:HE3	1.80	0.63
1:E:716:ALA:HA	1:E:742:SER:OG	1.99	0.63
1:E:39:TRP:CH2	1:E:516:MET:HA	2.33	0.63
1:I:716:ALA:HA	1:I:742:SER:OG	1.99	0.63
1:H:547:THR:HG21	1:H:571:VAL:HG12	1.80	0.63
1:C:547:THR:HG21	1:C:571:VAL:HG12	1.80	0.62
1:A:39:TRP:CZ3	1:A:289:ILE:HD11	2.35	0.62
1:C:30:ILE:HG23	1:C:31:PRO:HD2	1.82	0.62
1:C:716:ALA:HA	1:C:742:SER:OG	2.00	0.62
1:G:716:ALA:HA	1:G:742:SER:OG	1.99	0.62
1:H:123:GLU:OE2	1:I:229:ARG:NH2	2.32	0.62
1:E:232:ARG:NH2	1:I:171:LYS:O	2.32	0.62
1:J:513:LEU:HD23	1:J:516:MET:HE3	1.80	0.62
1:A:229:ARG:HH12	1:J:123:GLU:CD	2.08	0.62
1:G:513:LEU:HD23	1:G:516:MET:HE3	1.80	0.62
1:I:547:THR:HG21	1:I:571:VAL:HG12	1.80	0.62
1:F:716:ALA:HA	1:F:742:SER:OG	1.99	0.62
1:G:547:THR:HG21	1:G:571:VAL:HG12	1.80	0.62
1:H:39:TRP:CZ3	1:H:289:ILE:HD11	2.35	0.62
1:E:30:ILE:HG23	1:E:31:PRO:HD2	1.82	0.62
1:G:39:TRP:CZ3	1:G:289:ILE:HD11	2.35	0.62
1:A:429:ARG:NE	1:B:304:GLN:OE1	2.32	0.62
1:A:716:ALA:HA	1:A:742:SER:OG	1.99	0.62
1:B:51:SER:HB2	1:B:56:ARG:HA	1.82	0.62
1:D:716:ALA:HA	1:D:742:SER:OG	1.99	0.62
1:D:39:TRP:CZ3	1:D:289:ILE:HD11	2.35	0.61
1:G:30:ILE:HG23	1:G:31:PRO:HD2	1.82	0.61
1:G:426:MET:HE1	1:H:246:MET:HG2	1.82	0.61
1:C:51:SER:HB2	1:C:56:ARG:HA	1.82	0.61
1:H:39:TRP:CH2	1:H:516:MET:HA	2.34	0.61
1:I:51:SER:HB2	1:I:56:ARG:HA	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:30:ILE:HG23	1:J:31:PRO:HD2	1.82	0.61
1:C:348:ASP:C	1:C:351:PRO:HD2	2.26	0.61
1:C:513:LEU:HD23	1:C:516:MET:HE3	1.80	0.61
1:D:547:THR:HG21	1:D:571:VAL:HG12	1.80	0.61
1:J:716:ALA:HA	1:J:742:SER:OG	1.99	0.61
1:A:30:ILE:HG23	1:A:31:PRO:HD2	1.83	0.61
1:B:39:TRP:CZ3	1:B:289:ILE:HD11	2.35	0.61
1:D:30:ILE:HG23	1:D:31:PRO:HD2	1.82	0.61
1:B:30:ILE:HG23	1:B:31:PRO:HD2	1.83	0.61
1:C:39:TRP:CZ3	1:C:289:ILE:HD11	2.36	0.61
1:D:51:SER:HB2	1:D:56:ARG:HA	1.82	0.61
1:E:51:SER:HB2	1:E:56:ARG:HA	1.82	0.61
1:H:30:ILE:HG23	1:H:31:PRO:HD2	1.82	0.61
1:I:39:TRP:CZ3	1:I:289:ILE:HD11	2.35	0.61
1:B:76:LYS:O	1:B:79:SER:HB3	2.01	0.61
1:D:348:ASP:C	1:D:351:PRO:HD2	2.26	0.61
1:A:76:LYS:O	1:A:79:SER:HB3	2.01	0.61
1:E:76:LYS:O	1:E:79:SER:HB3	2.01	0.61
1:F:30:ILE:HG23	1:F:31:PRO:HD2	1.82	0.61
1:F:51:SER:HB2	1:F:56:ARG:HA	1.82	0.61
1:H:348:ASP:C	1:H:351:PRO:HD2	2.26	0.61
1:A:141:ASN:HD21	1:J:418:VAL:HG12	1.66	0.61
1:E:39:TRP:CZ3	1:E:289:ILE:HD11	2.36	0.61
1:F:39:TRP:CZ3	1:F:289:ILE:HD11	2.35	0.61
1:I:348:ASP:C	1:I:351:PRO:HD2	2.26	0.61
1:J:39:TRP:CZ3	1:J:289:ILE:HD11	2.35	0.61
1:J:348:ASP:C	1:J:351:PRO:HD2	2.26	0.61
1:I:76:LYS:O	1:I:79:SER:HB3	2.01	0.60
1:B:418:VAL:HG12	1:C:141:ASN:HD21	1.66	0.60
1:D:76:LYS:O	1:D:79:SER:HB3	2.01	0.60
1:A:51:SER:HB2	1:A:56:ARG:HA	1.82	0.60
1:B:348:ASP:C	1:B:351:PRO:HD2	2.26	0.60
1:E:229:ARG:HH12	1:I:123:GLU:CD	2.09	0.60
1:E:348:ASP:C	1:E:351:PRO:HD2	2.26	0.60
1:G:51:SER:HB2	1:G:56:ARG:HA	1.82	0.60
1:G:348:ASP:C	1:G:351:PRO:HD2	2.25	0.60
1:H:76:LYS:O	1:H:79:SER:HB3	2.01	0.60
1:F:348:ASP:C	1:F:351:PRO:HD2	2.26	0.60
1:H:51:SER:HB2	1:H:56:ARG:HA	1.83	0.60
1:F:740:LEU:HD23	1:F:784:VAL:HG21	1.84	0.60
1:J:76:LYS:O	1:J:79:SER:HB3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:76:LYS:O	1:F:79:SER:HB3	2.01	0.60
1:G:76:LYS:O	1:G:79:SER:HB3	2.01	0.60
1:H:480:PRO:HD2	1:H:567:LEU:CD2	2.32	0.60
1:C:480:PRO:HD2	1:C:567:LEU:CD2	2.32	0.60
1:E:740:LEU:HD23	1:E:784:VAL:HG21	1.84	0.60
1:J:51:SER:HB2	1:J:56:ARG:HA	1.82	0.60
1:E:141:ASN:HD21	1:I:418:VAL:HG12	1.66	0.60
1:I:30:ILE:HG23	1:I:31:PRO:HD2	1.82	0.60
1:A:348:ASP:C	1:A:351:PRO:HD2	2.26	0.59
1:C:740:LEU:HD23	1:C:784:VAL:HG21	1.84	0.59
1:I:480:PRO:HD2	1:I:567:LEU:CD2	2.32	0.59
1:I:740:LEU:HD23	1:I:784:VAL:HG21	1.84	0.59
1:A:740:LEU:HD23	1:A:784:VAL:HG21	1.84	0.59
1:B:480:PRO:HD2	1:B:567:LEU:CD2	2.32	0.59
1:F:480:PRO:HD2	1:F:567:LEU:CD2	2.32	0.59
1:A:50:THR:HG22	1:A:183:ILE:HB	1.85	0.59
1:B:740:LEU:HD23	1:B:784:VAL:HG21	1.84	0.59
1:C:418:VAL:HG12	1:D:141:ASN:HD21	1.66	0.59
1:E:480:PRO:HD2	1:E:567:LEU:CD2	2.32	0.59
1:I:50:THR:HG22	1:I:183:ILE:HB	1.85	0.59
1:C:76:LYS:O	1:C:79:SER:HB3	2.01	0.59
1:J:740:LEU:HD23	1:J:784:VAL:HG21	1.84	0.59
1:C:39:TRP:CD2	1:C:289:ILE:HD11	2.38	0.59
1:E:50:THR:HG22	1:E:183:ILE:HB	1.85	0.59
1:G:480:PRO:HD2	1:G:567:LEU:CD2	2.32	0.59
1:H:740:LEU:HD23	1:H:784:VAL:HG21	1.83	0.59
1:G:39:TRP:CD2	1:G:289:ILE:HD11	2.38	0.59
1:J:480:PRO:HD2	1:J:567:LEU:CD2	2.32	0.59
1:D:480:PRO:HD2	1:D:567:LEU:CD2	2.32	0.59
1:H:39:TRP:CD2	1:H:289:ILE:HD11	2.38	0.59
1:C:50:THR:HG22	1:C:183:ILE:HB	1.85	0.58
1:G:740:LEU:HD23	1:G:784:VAL:HG21	1.84	0.58
1:A:480:PRO:HD2	1:A:567:LEU:CD2	2.33	0.58
1:H:50:THR:HG22	1:H:183:ILE:HB	1.85	0.58
1:J:50:THR:HG22	1:J:183:ILE:HB	1.84	0.58
1:E:39:TRP:CD2	1:E:289:ILE:HD11	2.38	0.58
1:I:39:TRP:CD2	1:I:289:ILE:HD11	2.38	0.58
1:B:354:ARG:NH1	1:B:358:THR:HG22	2.19	0.58
1:C:30:ILE:HG23	1:C:31:PRO:CD	2.33	0.58
1:D:30:ILE:HG23	1:D:31:PRO:CD	2.34	0.58
1:D:120:SER:OG	1:D:223:ARG:N	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:740:LEU:HD23	1:D:784:VAL:HG21	1.84	0.58
1:A:39:TRP:CD2	1:A:289:ILE:HD11	2.38	0.58
1:E:30:ILE:HG23	1:E:31:PRO:CD	2.34	0.58
1:H:354:ARG:NH1	1:H:358:THR:HG22	2.19	0.58
1:C:723:ILE:HD11	1:D:509:SER:OG	2.03	0.58
1:F:30:ILE:HG23	1:F:31:PRO:CD	2.34	0.58
1:J:30:ILE:HG23	1:J:31:PRO:CD	2.34	0.58
1:F:354:ARG:NH1	1:F:358:THR:HG22	2.19	0.58
1:B:557:SER:OG	1:B:560:ALA:HB3	2.04	0.58
1:F:39:TRP:CD2	1:F:289:ILE:HD11	2.38	0.58
1:G:660:ALA:HB1	1:H:85:ASP:OD2	2.03	0.58
1:H:30:ILE:CG2	1:H:31:PRO:HD2	2.34	0.58
1:A:354:ARG:NH1	1:A:358:THR:HG22	2.19	0.57
1:B:30:ILE:HG23	1:B:31:PRO:CD	2.34	0.57
1:B:50:THR:HG22	1:B:183:ILE:HB	1.85	0.57
1:B:103:THR:HG22	1:B:133:ILE:HA	1.86	0.57
1:D:39:TRP:CD2	1:D:289:ILE:HD11	2.38	0.57
1:D:50:THR:HG22	1:D:183:ILE:HB	1.85	0.57
1:G:50:THR:HG22	1:G:183:ILE:HB	1.85	0.57
1:I:354:ARG:NH1	1:I:358:THR:HG22	2.19	0.57
1:B:39:TRP:CD2	1:B:289:ILE:HD11	2.39	0.57
1:B:285:LEU:HD13	1:B:291:PHE:CE2	2.39	0.57
1:B:375:LEU:HB2	1:B:582:ILE:O	2.05	0.57
1:E:30:ILE:CG2	1:E:31:PRO:HD2	2.34	0.57
1:F:50:THR:HG22	1:F:183:ILE:HB	1.85	0.57
1:F:375:LEU:HB2	1:F:582:ILE:O	2.04	0.57
1:G:375:LEU:HB2	1:G:582:ILE:O	2.05	0.57
1:H:120:SER:OG	1:H:223:ARG:N	2.37	0.57
1:J:30:ILE:CG2	1:J:31:PRO:HD2	2.34	0.57
1:A:30:ILE:HG23	1:A:31:PRO:CD	2.34	0.57
1:A:30:ILE:CG2	1:A:31:PRO:HD2	2.34	0.57
1:A:103:THR:HG22	1:A:133:ILE:HA	1.87	0.57
1:A:712:TYR:HE2	1:A:750:VAL:HG21	1.70	0.57
1:D:30:ILE:CG2	1:D:31:PRO:HD2	2.34	0.57
1:F:120:SER:OG	1:F:223:ARG:N	2.37	0.57
1:G:30:ILE:CG2	1:G:31:PRO:HD2	2.34	0.57
1:G:557:SER:OG	1:G:560:ALA:HB3	2.05	0.57
1:H:375:LEU:HB2	1:H:582:ILE:O	2.05	0.57
1:H:557:SER:OG	1:H:560:ALA:HB3	2.05	0.57
1:J:557:SER:OG	1:J:560:ALA:HB3	2.04	0.57
1:B:120:SER:OG	1:B:223:ARG:N	2.37	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:557:SER:OG	1:I:560:ALA:HB3	2.05	0.57
1:J:270:VAL:HG11	1:J:320:ILE:HB	1.86	0.57
1:D:123:GLU:OE2	1:J:229:ARG:NH2	2.35	0.57
1:E:123:GLU:CG	1:E:171:LYS:HD2	2.35	0.57
1:I:120:SER:OG	1:I:223:ARG:N	2.38	0.57
1:I:375:LEU:HB2	1:I:582:ILE:O	2.05	0.57
1:J:39:TRP:CD2	1:J:289:ILE:HD11	2.38	0.57
1:A:55:ARG:NE	1:A:587:ILE:HD11	2.20	0.57
1:B:30:ILE:CG2	1:B:31:PRO:HD2	2.34	0.57
1:C:30:ILE:CG2	1:C:31:PRO:HD2	2.34	0.57
1:C:103:THR:HG22	1:C:133:ILE:HA	1.87	0.57
1:I:164:LEU:O	1:I:168:GLY:HA2	2.05	0.57
1:B:164:LEU:O	1:B:168:GLY:HA2	2.05	0.57
1:E:55:ARG:NE	1:E:587:ILE:HD11	2.20	0.57
1:E:164:LEU:O	1:E:168:GLY:HA2	2.05	0.57
1:E:354:ARG:NH1	1:E:358:THR:HG22	2.19	0.57
1:F:557:SER:OG	1:F:560:ALA:HB3	2.05	0.57
1:H:30:ILE:HG23	1:H:31:PRO:CD	2.34	0.57
1:I:123:GLU:CG	1:I:171:LYS:HD2	2.35	0.57
1:J:354:ARG:NH1	1:J:358:THR:HG22	2.19	0.57
1:G:164:LEU:O	1:G:168:GLY:HA2	2.05	0.57
1:G:354:ARG:NH1	1:G:358:THR:HG22	2.19	0.57
1:I:270:VAL:HG11	1:I:320:ILE:HB	1.87	0.57
1:I:285:LEU:HD13	1:I:291:PHE:CE2	2.40	0.57
1:A:285:LEU:HD13	1:A:291:PHE:CE2	2.40	0.57
1:C:712:TYR:HE2	1:C:750:VAL:HG21	1.70	0.57
1:D:164:LEU:O	1:D:168:GLY:HA2	2.05	0.57
1:E:375:LEU:HB2	1:E:582:ILE:O	2.05	0.57
1:F:171:LYS:O	1:G:232:ARG:NH2	2.38	0.57
1:G:712:TYR:HE2	1:G:750:VAL:HG21	1.70	0.57
1:D:123:GLU:CG	1:D:171:LYS:HD2	2.35	0.57
1:E:712:TYR:HE2	1:E:750:VAL:HG21	1.70	0.57
1:G:30:ILE:HG23	1:G:31:PRO:CD	2.34	0.57
1:H:285:LEU:HD13	1:H:291:PHE:CE2	2.39	0.57
1:B:123:GLU:CG	1:B:171:LYS:HD2	2.35	0.56
1:C:164:LEU:O	1:C:168:GLY:HA2	2.05	0.56
1:C:557:SER:OG	1:C:560:ALA:HB3	2.05	0.56
1:D:55:ARG:NE	1:D:587:ILE:HD11	2.20	0.56
1:D:354:ARG:NH1	1:D:358:THR:HG22	2.19	0.56
1:E:285:LEU:HD13	1:E:291:PHE:CE2	2.39	0.56
1:E:557:SER:OG	1:E:560:ALA:HB3	2.04	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:164:LEU:O	1:F:168:GLY:HA2	2.04	0.56
1:A:375:LEU:HB2	1:A:582:ILE:O	2.05	0.56
1:A:557:SER:OG	1:A:560:ALA:HB3	2.05	0.56
1:B:146:GLU:CD	1:B:604:LYS:HZ1	2.12	0.56
1:C:123:GLU:CG	1:C:171:LYS:HD2	2.35	0.56
1:C:270:VAL:HG11	1:C:320:ILE:HB	1.87	0.56
1:D:103:THR:HG22	1:D:133:ILE:HA	1.87	0.56
1:D:285:LEU:HD13	1:D:291:PHE:CE2	2.40	0.56
1:D:659:ILE:H	1:D:659:ILE:HD12	1.70	0.56
1:F:30:ILE:CG2	1:F:31:PRO:HD2	2.34	0.56
1:G:120:SER:OG	1:G:223:ARG:N	2.38	0.56
1:J:285:LEU:HD13	1:J:291:PHE:CE2	2.40	0.56
1:J:375:LEU:HB2	1:J:582:ILE:O	2.05	0.56
1:A:123:GLU:CG	1:A:171:LYS:HD2	2.35	0.56
1:A:316:TRP:CZ2	1:A:320:ILE:HD11	2.41	0.56
1:C:120:SER:OG	1:C:223:ARG:N	2.39	0.56
1:D:375:LEU:HB2	1:D:582:ILE:O	2.04	0.56
1:D:557:SER:OG	1:D:560:ALA:HB3	2.05	0.56
1:E:103:THR:HG22	1:E:133:ILE:HA	1.87	0.56
1:E:120:SER:OG	1:E:223:ARG:N	2.38	0.56
1:E:659:ILE:H	1:E:659:ILE:HD12	1.70	0.56
1:F:659:ILE:H	1:F:659:ILE:HD12	1.70	0.56
1:G:103:THR:HG22	1:G:133:ILE:HA	1.86	0.56
1:H:164:LEU:O	1:H:168:GLY:HA2	2.04	0.56
1:I:30:ILE:HG23	1:I:31:PRO:CD	2.34	0.56
1:I:30:ILE:CG2	1:I:31:PRO:HD2	2.34	0.56
1:B:167:SER:OG	1:B:169:HIS:CD2	2.59	0.56
1:C:354:ARG:NH1	1:C:358:THR:HG22	2.19	0.56
1:E:270:VAL:HG11	1:E:320:ILE:HB	1.87	0.56
1:F:49:ILE:HG23	1:F:50:THR:HG23	1.88	0.56
1:F:270:VAL:HG11	1:F:320:ILE:HB	1.87	0.56
1:G:55:ARG:NE	1:G:587:ILE:HD11	2.20	0.56
1:G:270:VAL:HG11	1:G:320:ILE:HB	1.87	0.56
1:D:270:VAL:HG11	1:D:320:ILE:HB	1.87	0.56
1:F:285:LEU:HD13	1:F:291:PHE:CE2	2.40	0.56
1:G:503:ILE:HG22	1:G:515:TYR:CE1	2.40	0.56
1:H:55:ARG:NE	1:H:587:ILE:HD11	2.20	0.56
1:J:120:SER:OG	1:J:223:ARG:N	2.38	0.56
1:C:49:ILE:HG23	1:C:50:THR:HG23	1.87	0.56
1:C:285:LEU:HD13	1:C:291:PHE:CE2	2.40	0.56
1:D:49:ILE:HG23	1:D:50:THR:HG23	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:123:GLU:CG	1:F:171:LYS:HD2	2.35	0.56
1:F:712:TYR:HE2	1:F:750:VAL:HG21	1.70	0.56
1:I:103:THR:HG22	1:I:133:ILE:HA	1.88	0.56
1:I:167:SER:OG	1:I:169:HIS:CD2	2.59	0.56
1:I:659:ILE:H	1:I:659:ILE:HD12	1.70	0.56
1:B:55:ARG:NE	1:B:587:ILE:HD11	2.20	0.56
1:C:55:ARG:NE	1:C:587:ILE:HD11	2.20	0.56
1:H:712:TYR:HE2	1:H:750:VAL:HG21	1.70	0.56
1:J:659:ILE:H	1:J:659:ILE:HD12	1.71	0.56
1:C:375:LEU:HB2	1:C:582:ILE:O	2.04	0.56
1:D:316:TRP:CZ2	1:D:320:ILE:HD11	2.41	0.56
1:D:503:ILE:HG22	1:D:515:TYR:CE1	2.41	0.56
1:D:712:TYR:HE2	1:D:750:VAL:HG21	1.70	0.56
1:E:503:ILE:HG22	1:E:515:TYR:CE1	2.41	0.56
1:G:659:ILE:H	1:G:659:ILE:HD12	1.71	0.56
1:H:270:VAL:HG11	1:H:320:ILE:HB	1.87	0.56
1:I:712:TYR:HE2	1:I:750:VAL:HG21	1.70	0.56
1:A:120:SER:OG	1:A:223:ARG:N	2.38	0.56
1:A:167:SER:OG	1:A:169:HIS:CD2	2.59	0.56
1:A:270:VAL:HG11	1:A:320:ILE:HB	1.87	0.56
1:G:316:TRP:CZ2	1:G:320:ILE:HD11	2.41	0.56
1:H:49:ILE:HG23	1:H:50:THR:HG23	1.87	0.56
1:J:49:ILE:HG23	1:J:50:THR:HG23	1.88	0.56
1:J:164:LEU:O	1:J:168:GLY:HA2	2.05	0.56
1:J:375:LEU:HD12	1:J:375:LEU:O	2.06	0.56
1:A:503:ILE:HG22	1:A:515:TYR:CE1	2.41	0.56
1:I:55:ARG:NE	1:I:587:ILE:HD11	2.20	0.56
1:J:123:GLU:CG	1:J:171:LYS:HD2	2.35	0.56
1:B:270:VAL:HG11	1:B:320:ILE:HB	1.87	0.55
1:C:291:PHE:O	1:C:295:THR:HG22	2.07	0.55
1:H:503:ILE:HG22	1:H:515:TYR:CE1	2.41	0.55
1:H:659:ILE:HD12	1:H:659:ILE:H	1.71	0.55
1:I:316:TRP:CZ2	1:I:320:ILE:HD11	2.41	0.55
1:J:103:THR:HG22	1:J:133:ILE:HA	1.87	0.55
1:A:164:LEU:O	1:A:168:GLY:HA2	2.05	0.55
1:A:291:PHE:O	1:A:295:THR:HG22	2.07	0.55
1:B:375:LEU:HD12	1:B:375:LEU:O	2.06	0.55
1:B:712:TYR:HE2	1:B:750:VAL:HG21	1.70	0.55
1:D:375:LEU:HD12	1:D:375:LEU:O	2.06	0.55
1:F:103:THR:HG22	1:F:133:ILE:HA	1.87	0.55
1:G:167:SER:OG	1:G:169:HIS:CD2	2.60	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:285:LEU:HD13	1:G:291:PHE:CE2	2.40	0.55
1:H:123:GLU:CG	1:H:171:LYS:HD2	2.35	0.55
1:H:375:LEU:HD12	1:H:375:LEU:O	2.06	0.55
1:I:49:ILE:HG23	1:I:50:THR:HG23	1.87	0.55
1:J:291:PHE:O	1:J:295:THR:HG22	2.07	0.55
1:J:316:TRP:CZ2	1:J:320:ILE:HD11	2.41	0.55
1:C:503:ILE:HG22	1:C:515:TYR:CE1	2.42	0.55
1:D:204:ASP:O	1:D:248:LEU:HD11	2.06	0.55
1:D:291:PHE:O	1:D:295:THR:HG22	2.06	0.55
1:E:412:GLN:O	1:F:89:GLN:NE2	2.37	0.55
1:I:375:LEU:HD12	1:I:375:LEU:O	2.06	0.55
1:B:49:ILE:HG23	1:B:50:THR:HG23	1.88	0.55
1:H:103:THR:HG22	1:H:133:ILE:HA	1.86	0.55
1:J:503:ILE:HG22	1:J:515:TYR:CE1	2.41	0.55
1:J:712:TYR:HE2	1:J:750:VAL:HG21	1.70	0.55
1:A:49:ILE:HG23	1:A:50:THR:HG23	1.87	0.55
1:A:659:ILE:H	1:A:659:ILE:HD12	1.71	0.55
1:C:204:ASP:O	1:C:248:LEU:HD11	2.07	0.55
1:F:316:TRP:CZ2	1:F:320:ILE:HD11	2.41	0.55
1:I:291:PHE:O	1:I:295:THR:HG22	2.07	0.55
1:J:55:ARG:NE	1:J:587:ILE:HD11	2.21	0.55
1:J:380:GLN:HB3	1:J:390:LEU:HD23	1.88	0.55
1:C:375:LEU:O	1:C:375:LEU:HD12	2.06	0.55
1:C:659:ILE:HD12	1:C:659:ILE:H	1.70	0.55
1:E:316:TRP:CZ2	1:E:320:ILE:HD11	2.41	0.55
1:F:426:MET:HE1	1:G:246:MET:HG2	1.89	0.55
1:H:291:PHE:O	1:H:295:THR:HG22	2.07	0.55
1:D:380:GLN:HB3	1:D:390:LEU:HD23	1.89	0.55
1:E:204:ASP:O	1:E:248:LEU:HD11	2.07	0.55
1:E:375:LEU:HD12	1:E:375:LEU:O	2.07	0.55
1:G:49:ILE:HG23	1:G:50:THR:HG23	1.88	0.55
1:H:380:GLN:HB3	1:H:390:LEU:HD23	1.89	0.55
1:I:380:GLN:HB3	1:I:390:LEU:HD23	1.89	0.55
1:J:167:SER:OG	1:J:169:HIS:CD2	2.59	0.55
1:A:418:VAL:CG1	1:B:141:ASN:HD21	2.19	0.55
1:B:503:ILE:HG22	1:B:515:TYR:CE1	2.42	0.55
1:C:316:TRP:CZ2	1:C:320:ILE:HD11	2.41	0.55
1:F:167:SER:OG	1:F:169:HIS:CD2	2.60	0.55
1:G:375:LEU:HD12	1:G:375:LEU:O	2.07	0.55
1:H:167:SER:OG	1:H:169:HIS:CD2	2.60	0.55
1:H:204:ASP:O	1:H:248:LEU:HD11	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:204:ASP:O	1:J:248:LEU:HD11	2.07	0.55
1:A:204:ASP:O	1:A:248:LEU:HD11	2.07	0.55
1:A:375:LEU:HD12	1:A:375:LEU:O	2.06	0.55
1:B:291:PHE:O	1:B:295:THR:HG22	2.06	0.55
1:C:313:LEU:O	1:C:317:VAL:HG23	2.07	0.55
1:E:380:GLN:HB3	1:E:390:LEU:HD23	1.89	0.55
1:F:123:GLU:CD	1:G:229:ARG:HH12	2.15	0.55
1:F:313:LEU:O	1:F:317:VAL:HG23	2.07	0.55
1:G:380:GLN:HB3	1:G:390:LEU:HD23	1.89	0.55
1:B:316:TRP:CZ2	1:B:320:ILE:HD11	2.41	0.54
1:B:659:ILE:H	1:B:659:ILE:HD12	1.70	0.54
1:D:476:VAL:HG13	1:D:485:LEU:HD13	1.89	0.54
1:F:55:ARG:NE	1:F:587:ILE:HD11	2.20	0.54
1:F:204:ASP:O	1:F:248:LEU:HD11	2.07	0.54
1:F:375:LEU:O	1:F:375:LEU:HD12	2.06	0.54
1:F:476:VAL:HG13	1:F:485:LEU:HD13	1.89	0.54
1:G:313:LEU:O	1:G:317:VAL:HG23	2.07	0.54
1:I:204:ASP:O	1:I:248:LEU:HD11	2.07	0.54
1:I:313:LEU:O	1:I:317:VAL:HG23	2.07	0.54
1:A:146:GLU:CD	1:A:604:LYS:HZ1	2.15	0.54
1:A:476:VAL:HG13	1:A:485:LEU:HD13	1.90	0.54
1:E:429:ARG:NE	1:F:304:GLN:OE1	2.40	0.54
1:E:476:VAL:HG13	1:E:485:LEU:HD13	1.89	0.54
1:A:313:LEU:O	1:A:317:VAL:HG23	2.07	0.54
1:A:412:GLN:O	1:B:89:GLN:NE2	2.39	0.54
1:C:167:SER:OG	1:C:169:HIS:CD2	2.60	0.54
1:E:167:SER:OG	1:E:169:HIS:CD2	2.60	0.54
1:F:291:PHE:O	1:F:295:THR:HG22	2.07	0.54
1:F:503:ILE:HG22	1:F:515:TYR:CE1	2.42	0.54
1:H:316:TRP:CZ2	1:H:320:ILE:HD11	2.41	0.54
1:H:418:VAL:CG1	1:I:141:ASN:HD21	2.19	0.54
1:I:146:GLU:CD	1:I:604:LYS:HZ1	2.16	0.54
1:A:123:GLU:OE2	1:B:229:ARG:NH2	2.40	0.54
1:A:380:GLN:HB3	1:A:390:LEU:HD23	1.89	0.54
1:D:313:LEU:O	1:D:317:VAL:HG23	2.07	0.54
1:E:49:ILE:HG23	1:E:50:THR:HG23	1.88	0.54
1:E:291:PHE:O	1:E:295:THR:HG22	2.06	0.54
1:G:660:ALA:HB1	1:H:85:ASP:CG	2.32	0.54
1:B:204:ASP:O	1:B:248:LEU:HD11	2.07	0.54
1:B:476:VAL:HG13	1:B:485:LEU:HD13	1.89	0.54
1:G:204:ASP:O	1:G:248:LEU:HD11	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:476:VAL:HG13	1:G:485:LEU:HD13	1.89	0.54
1:D:167:SER:OG	1:D:169:HIS:CD2	2.60	0.54
1:J:313:LEU:O	1:J:317:VAL:HG23	2.07	0.54
1:C:146:GLU:OE2	1:C:604:LYS:NZ	2.38	0.54
1:C:476:VAL:HG13	1:C:485:LEU:HD13	1.89	0.54
1:E:313:LEU:O	1:E:317:VAL:HG23	2.07	0.54
1:B:313:LEU:O	1:B:317:VAL:HG23	2.07	0.54
1:G:291:PHE:O	1:G:295:THR:HG22	2.07	0.54
1:G:723:ILE:HD11	1:H:509:SER:OG	2.08	0.54
1:I:503:ILE:HG22	1:I:515:TYR:CE1	2.42	0.54
1:B:429:ARG:NE	1:C:304:GLN:OE1	2.40	0.54
1:D:418:VAL:CG1	1:J:141:ASN:HD21	2.19	0.54
1:E:270:VAL:HG23	1:E:317:VAL:CG1	2.34	0.54
1:F:380:GLN:HB3	1:F:390:LEU:HD23	1.89	0.54
1:I:56:ARG:HD2	1:I:671:VAL:HG22	1.90	0.54
1:B:380:GLN:HB3	1:B:390:LEU:HD23	1.89	0.54
1:J:476:VAL:HG13	1:J:485:LEU:HD13	1.89	0.54
1:A:497:LEU:HD12	1:A:511:PRO:HB2	1.91	0.53
1:C:40:ALA:HB1	1:C:192:PRO:HG3	1.91	0.53
1:E:418:VAL:HG12	1:F:141:ASN:HD21	1.73	0.53
1:F:56:ARG:HD2	1:F:671:VAL:HG22	1.90	0.53
1:H:313:LEU:O	1:H:317:VAL:HG23	2.07	0.53
1:H:476:VAL:HG13	1:H:485:LEU:HD13	1.89	0.53
1:B:270:VAL:HG23	1:B:317:VAL:CG1	2.34	0.53
1:G:568:ASN:O	1:G:571:VAL:O	2.26	0.53
1:I:145:ASP:OD1	1:I:146:GLU:N	2.41	0.53
1:J:40:ALA:HB1	1:J:192:PRO:HG3	1.90	0.53
1:D:497:LEU:HD12	1:D:511:PRO:HB2	1.90	0.53
1:F:58:GLY:O	1:F:669:LYS:HE2	2.09	0.53
1:G:270:VAL:HG23	1:G:317:VAL:CG1	2.34	0.53
1:A:736:GLN:O	1:A:781:ALA:HB1	2.09	0.53
1:B:40:ALA:HB1	1:B:192:PRO:HG3	1.91	0.53
1:C:426:MET:HE1	1:D:246:MET:HG2	1.90	0.53
1:B:568:ASN:O	1:B:571:VAL:O	2.26	0.53
1:C:380:GLN:HB3	1:C:390:LEU:HD23	1.89	0.53
1:D:568:ASN:O	1:D:571:VAL:O	2.26	0.53
1:I:58:GLY:O	1:I:669:LYS:HE2	2.08	0.53
1:A:40:ALA:HB1	1:A:192:PRO:HG3	1.91	0.53
1:A:568:ASN:O	1:A:571:VAL:O	2.26	0.53
1:G:40:ALA:HB1	1:G:192:PRO:HG3	1.90	0.53
1:G:56:ARG:HD2	1:G:671:VAL:HG22	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:568:ASN:O	1:H:571:VAL:O	2.26	0.53
1:I:568:ASN:O	1:I:571:VAL:O	2.27	0.53
1:J:56:ARG:HD2	1:J:671:VAL:HG22	1.91	0.53
1:A:56:ARG:HD2	1:A:671:VAL:HG22	1.90	0.53
1:D:40:ALA:HB1	1:D:192:PRO:HG3	1.90	0.53
1:H:146:GLU:OE2	1:H:604:LYS:NZ	2.39	0.53
1:H:736:GLN:O	1:H:781:ALA:HB1	2.09	0.53
1:B:490:GLY:HA2	1:B:493:MET:HG2	1.91	0.53
1:C:497:LEU:HD12	1:C:511:PRO:HB2	1.91	0.53
1:C:736:GLN:O	1:C:781:ALA:HB1	2.09	0.53
1:D:56:ARG:HD2	1:D:671:VAL:HG22	1.91	0.53
1:F:568:ASN:O	1:F:571:VAL:O	2.26	0.53
1:J:736:GLN:O	1:J:781:ALA:HB1	2.09	0.53
1:B:497:LEU:HD12	1:B:511:PRO:HB2	1.91	0.53
1:B:736:GLN:O	1:B:781:ALA:HB1	2.09	0.53
1:D:145:ASP:OD1	1:D:146:GLU:N	2.42	0.53
1:E:56:ARG:HD2	1:E:671:VAL:HG22	1.90	0.53
1:E:58:GLY:O	1:E:669:LYS:HE2	2.09	0.53
1:I:476:VAL:HG13	1:I:485:LEU:HD13	1.89	0.53
1:C:486:LEU:CD1	1:C:514:LEU:HD11	2.40	0.53
1:D:58:GLY:O	1:D:669:LYS:HE2	2.09	0.53
1:G:736:GLN:O	1:G:781:ALA:HB1	2.09	0.53
1:H:270:VAL:HG23	1:H:317:VAL:CG1	2.34	0.53
1:J:270:VAL:HG23	1:J:317:VAL:CG1	2.34	0.53
1:J:497:LEU:HD12	1:J:511:PRO:HB2	1.91	0.53
1:A:490:GLY:HA2	1:A:493:MET:HG2	1.91	0.52
1:B:58:GLY:O	1:B:669:LYS:HE2	2.09	0.52
1:D:740:LEU:HD12	1:D:777:PHE:CE2	2.44	0.52
1:E:568:ASN:O	1:E:571:VAL:O	2.26	0.52
1:B:56:ARG:HD2	1:B:671:VAL:HG22	1.90	0.52
1:B:145:ASP:OD1	1:B:146:GLU:N	2.42	0.52
1:B:547:THR:OG1	1:B:549:GLN:OE1	2.28	0.52
1:B:715:LEU:HA	1:B:719:ARG:H	1.75	0.52
1:D:547:THR:OG1	1:D:549:GLN:OE1	2.28	0.52
1:E:490:GLY:HA2	1:E:493:MET:HG2	1.91	0.52
1:F:547:THR:OG1	1:F:549:GLN:OE1	2.28	0.52
1:G:123:GLU:CG	1:G:171:LYS:HD2	2.35	0.52
1:H:145:ASP:OD1	1:H:146:GLU:N	2.42	0.52
1:I:490:GLY:HA2	1:I:493:MET:HG2	1.91	0.52
1:A:740:LEU:HD12	1:A:777:PHE:CE2	2.44	0.52
1:C:56:ARG:HD2	1:C:671:VAL:HG22	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:58:GLY:O	1:C:669:LYS:HE2	2.09	0.52
1:C:740:LEU:HD12	1:C:777:PHE:CE2	2.44	0.52
1:F:264:GLU:OE2	1:F:298:THR:OG1	2.26	0.52
1:H:40:ALA:HB1	1:H:192:PRO:HG3	1.90	0.52
1:I:736:GLN:O	1:I:781:ALA:HB1	2.09	0.52
1:A:547:THR:OG1	1:A:549:GLN:OE1	2.28	0.52
1:C:490:GLY:HA2	1:C:493:MET:HG2	1.91	0.52
1:D:490:GLY:HA2	1:D:493:MET:HG2	1.91	0.52
1:D:736:GLN:O	1:D:781:ALA:HB1	2.09	0.52
1:E:736:GLN:O	1:E:781:ALA:HB1	2.09	0.52
1:G:740:LEU:HD12	1:G:777:PHE:CE2	2.44	0.52
1:J:380:GLN:HB3	1:J:390:LEU:CD2	2.40	0.52
1:A:58:GLY:O	1:A:669:LYS:HE2	2.09	0.52
1:D:380:GLN:HB3	1:D:390:LEU:CD2	2.40	0.52
1:E:497:LEU:HD12	1:E:511:PRO:HB2	1.90	0.52
1:F:145:ASP:OD1	1:F:146:GLU:N	2.43	0.52
1:F:723:ILE:HD11	1:G:509:SER:OG	2.09	0.52
1:F:736:GLN:O	1:F:781:ALA:HB1	2.09	0.52
1:H:58:GLY:O	1:H:669:LYS:HE2	2.09	0.52
1:H:285:LEU:HD13	1:H:291:PHE:CD2	2.45	0.52
1:D:409:GLN:HG3	1:D:661:VAL:HG13	1.92	0.52
1:E:30:ILE:CG2	1:E:31:PRO:CD	2.88	0.52
1:E:145:ASP:OD1	1:E:146:GLU:N	2.42	0.52
1:E:285:LEU:HD13	1:E:291:PHE:CD2	2.45	0.52
1:E:409:GLN:HG3	1:E:661:VAL:HG13	1.92	0.52
1:E:740:LEU:HD12	1:E:777:PHE:CE2	2.44	0.52
1:F:40:ALA:HB1	1:F:192:PRO:HG3	1.90	0.52
1:F:490:GLY:HA2	1:F:493:MET:HG2	1.91	0.52
1:H:39:TRP:CZ3	1:H:289:ILE:CD1	2.93	0.52
1:H:56:ARG:HD2	1:H:671:VAL:HG22	1.91	0.52
1:H:740:LEU:HD12	1:H:777:PHE:CE2	2.45	0.52
1:J:58:GLY:O	1:J:669:LYS:HE2	2.09	0.52
1:A:145:ASP:OD1	1:A:146:GLU:N	2.43	0.52
1:A:715:LEU:HA	1:A:719:ARG:H	1.75	0.52
1:B:285:LEU:HD13	1:B:291:PHE:CD2	2.45	0.52
1:B:486:LEU:CD1	1:B:514:LEU:HD11	2.40	0.52
1:C:568:ASN:O	1:C:571:VAL:O	2.27	0.52
1:D:659:ILE:HD12	1:D:659:ILE:N	2.25	0.52
1:E:486:LEU:CD1	1:E:514:LEU:HD11	2.40	0.52
1:E:547:THR:OG1	1:E:549:GLN:OE1	2.28	0.52
1:F:30:ILE:CG2	1:F:31:PRO:CD	2.88	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:380:GLN:HB3	1:F:390:LEU:CD2	2.40	0.52
1:G:39:TRP:CZ3	1:G:289:ILE:CD1	2.93	0.52
1:J:490:GLY:HA2	1:J:493:MET:HG2	1.91	0.52
1:A:659:ILE:HD12	1:A:659:ILE:N	2.25	0.52
1:D:146:GLU:CD	1:D:604:LYS:HZ1	2.18	0.52
1:E:380:GLN:HB3	1:E:390:LEU:CD2	2.40	0.52
1:G:145:ASP:OD1	1:G:146:GLU:N	2.43	0.52
1:G:486:LEU:CD1	1:G:514:LEU:HD11	2.40	0.52
1:G:715:LEU:HA	1:G:719:ARG:H	1.75	0.52
1:H:380:GLN:HB3	1:H:390:LEU:CD2	2.40	0.52
1:H:547:THR:OG1	1:H:549:GLN:OE1	2.28	0.52
1:I:380:GLN:HB3	1:I:390:LEU:CD2	2.40	0.52
1:J:409:GLN:HG3	1:J:661:VAL:HG13	1.92	0.52
1:J:568:ASN:O	1:J:571:VAL:O	2.26	0.52
1:J:715:LEU:HA	1:J:719:ARG:H	1.75	0.52
1:B:30:ILE:CG2	1:B:31:PRO:CD	2.88	0.52
1:B:409:GLN:HG3	1:B:661:VAL:HG13	1.92	0.52
1:D:30:ILE:CG2	1:D:31:PRO:CD	2.88	0.52
1:D:426:MET:HE1	1:J:246:MET:HG2	1.92	0.52
1:F:285:LEU:HD13	1:F:291:PHE:CD2	2.45	0.52
1:G:146:GLU:OE2	1:G:604:LYS:NZ	2.38	0.52
1:G:380:GLN:HB3	1:G:390:LEU:CD2	2.40	0.52
1:G:490:GLY:HA2	1:G:493:MET:HG2	1.91	0.52
1:H:497:LEU:HD12	1:H:511:PRO:HB2	1.91	0.52
1:I:486:LEU:CD1	1:I:514:LEU:HD11	2.40	0.52
1:I:740:LEU:HD12	1:I:777:PHE:CE2	2.45	0.52
1:J:145:ASP:OD1	1:J:146:GLU:N	2.42	0.52
1:J:740:LEU:HD12	1:J:777:PHE:CE2	2.45	0.52
1:E:40:ALA:HB1	1:E:192:PRO:HG3	1.91	0.52
1:F:146:GLU:OE2	1:F:604:LYS:NZ	2.38	0.52
1:F:486:LEU:CD1	1:F:514:LEU:HD11	2.39	0.52
1:H:264:GLU:OE2	1:H:298:THR:OG1	2.26	0.52
1:J:30:ILE:CG2	1:J:31:PRO:CD	2.88	0.52
1:J:264:GLU:OE2	1:J:298:THR:OG1	2.26	0.52
1:B:740:LEU:HD12	1:B:777:PHE:CE2	2.44	0.51
1:F:642:LYS:HZ2	1:F:733:VAL:HG21	1.75	0.51
1:G:497:LEU:HD12	1:G:511:PRO:HB2	1.91	0.51
1:H:741:GLN:O	1:H:745:GLN:HG3	2.10	0.51
1:A:350:THR:OG1	1:A:351:PRO:HD3	2.11	0.51
1:B:380:GLN:HB3	1:B:390:LEU:CD2	2.40	0.51
1:D:715:LEU:HA	1:D:719:ARG:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:659:ILE:HD12	1:F:659:ILE:N	2.25	0.51
1:G:58:GLY:O	1:G:669:LYS:HE2	2.09	0.51
1:G:659:ILE:HD12	1:G:659:ILE:N	2.25	0.51
1:H:409:GLN:HG3	1:H:661:VAL:HG13	1.92	0.51
1:H:490:GLY:HA2	1:H:493:MET:HG2	1.90	0.51
1:I:40:ALA:HB1	1:I:192:PRO:HG3	1.90	0.51
1:J:547:THR:OG1	1:J:549:GLN:OE1	2.28	0.51
1:A:30:ILE:CG2	1:A:31:PRO:CD	2.89	0.51
1:A:39:TRP:CZ3	1:A:289:ILE:CD1	2.93	0.51
1:C:145:ASP:OD1	1:C:146:GLU:N	2.43	0.51
1:C:285:LEU:HD13	1:C:291:PHE:CD2	2.45	0.51
1:D:285:LEU:HD13	1:D:291:PHE:CD2	2.46	0.51
1:F:741:GLN:O	1:F:745:GLN:HG3	2.10	0.51
1:I:780:ILE:O	1:I:784:VAL:HG23	2.11	0.51
1:J:741:GLN:O	1:J:745:GLN:HG3	2.11	0.51
1:C:659:ILE:HD12	1:C:659:ILE:N	2.25	0.51
1:G:409:GLN:HG3	1:G:661:VAL:HG13	1.92	0.51
1:G:641:ARG:HG3	1:G:777:PHE:CE1	2.46	0.51
1:H:429:ARG:NE	1:I:304:GLN:OE1	2.40	0.51
1:I:659:ILE:HD12	1:I:659:ILE:N	2.25	0.51
1:J:350:THR:OG1	1:J:351:PRO:HD3	2.11	0.51
1:A:380:GLN:HB3	1:A:390:LEU:CD2	2.40	0.51
1:A:741:GLN:O	1:A:745:GLN:HG3	2.11	0.51
1:A:780:ILE:O	1:A:784:VAL:HG23	2.11	0.51
1:B:350:THR:OG1	1:B:351:PRO:HD3	2.10	0.51
1:B:780:ILE:O	1:B:784:VAL:HG23	2.11	0.51
1:C:741:GLN:O	1:C:745:GLN:HG3	2.11	0.51
1:E:659:ILE:HD12	1:E:659:ILE:N	2.25	0.51
1:E:741:GLN:O	1:E:745:GLN:HG3	2.10	0.51
1:F:409:GLN:HG3	1:F:661:VAL:HG13	1.92	0.51
1:F:497:LEU:HD12	1:F:511:PRO:HB2	1.91	0.51
1:F:740:LEU:HD12	1:F:777:PHE:CE2	2.45	0.51
1:I:39:TRP:CZ3	1:I:289:ILE:CD1	2.94	0.51
1:I:547:THR:OG1	1:I:549:GLN:OE1	2.28	0.51
1:J:442:PHE:CE2	1:J:681:ALA:HB1	2.46	0.51
1:J:486:LEU:CD1	1:J:514:LEU:HD11	2.40	0.51
1:C:442:PHE:CE2	1:C:681:ALA:HB1	2.46	0.51
1:E:429:ARG:HD2	1:E:661:VAL:HG11	1.93	0.51
1:E:641:ARG:HG3	1:E:777:PHE:CE1	2.46	0.51
1:F:350:THR:OG1	1:F:351:PRO:HD3	2.11	0.51
1:G:285:LEU:HD13	1:G:291:PHE:CD2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:ILE:CG2	1:H:31:PRO:CD	2.88	0.51
1:H:68:ARG:HH12	1:H:166:GLN:HG2	1.76	0.51
1:H:350:THR:OG1	1:H:351:PRO:HD3	2.11	0.51
1:H:486:LEU:CD1	1:H:514:LEU:HD11	2.40	0.51
1:I:497:LEU:HD12	1:I:511:PRO:HB2	1.91	0.51
1:A:486:LEU:CD1	1:A:514:LEU:HD11	2.41	0.51
1:B:641:ARG:HG3	1:B:777:PHE:CE1	2.46	0.51
1:E:146:GLU:CD	1:E:604:LYS:HZ1	2.18	0.51
1:E:442:PHE:CE2	1:E:681:ALA:HB1	2.45	0.51
1:G:547:THR:OG1	1:G:549:GLN:OE1	2.28	0.51
1:C:715:LEU:HA	1:C:719:ARG:H	1.75	0.51
1:C:780:ILE:O	1:C:784:VAL:HG23	2.11	0.51
1:F:39:TRP:CZ3	1:F:289:ILE:CD1	2.94	0.51
1:H:641:ARG:HG3	1:H:777:PHE:CE1	2.46	0.51
1:J:780:ILE:O	1:J:784:VAL:HG23	2.11	0.51
1:A:31:PRO:HB3	1:A:528:PRO:HA	1.93	0.51
1:A:146:GLU:OE2	1:A:604:LYS:NZ	2.38	0.51
1:A:285:LEU:HD13	1:A:291:PHE:CD2	2.46	0.51
1:B:39:TRP:CZ3	1:B:289:ILE:CD1	2.94	0.51
1:C:145:ASP:CB	1:C:148:GLN:HE21	2.24	0.51
1:C:429:ARG:NE	1:D:304:GLN:OE1	2.42	0.51
1:C:547:THR:OG1	1:C:549:GLN:OE1	2.28	0.51
1:C:660:ALA:HB1	1:D:85:ASP:OD2	2.10	0.51
1:D:39:TRP:CZ3	1:D:289:ILE:CD1	2.93	0.51
1:I:270:VAL:HG23	1:I:317:VAL:CG1	2.34	0.51
1:I:409:GLN:HG3	1:I:661:VAL:HG13	1.91	0.51
1:I:641:ARG:HG3	1:I:777:PHE:CE1	2.45	0.51
1:I:741:GLN:O	1:I:745:GLN:HG3	2.10	0.51
1:A:409:GLN:HG3	1:A:661:VAL:HG13	1.92	0.51
1:I:442:PHE:CE2	1:I:681:ALA:HB1	2.46	0.51
1:B:31:PRO:HB3	1:B:528:PRO:HA	1.93	0.50
1:B:741:GLN:O	1:B:745:GLN:HG3	2.10	0.50
1:D:486:LEU:CD1	1:D:514:LEU:HD11	2.40	0.50
1:D:519:ALA:HB1	1:D:535:PHE:CE2	2.46	0.50
1:H:659:ILE:HD12	1:H:659:ILE:N	2.25	0.50
1:J:39:TRP:CZ3	1:J:289:ILE:CD1	2.93	0.50
1:J:68:ARG:HH12	1:J:166:GLN:HG2	1.76	0.50
1:A:89:GLN:NE2	1:J:412:GLN:O	2.44	0.50
1:B:519:ALA:HB1	1:B:535:PHE:CE2	2.46	0.50
1:B:659:ILE:HD12	1:B:659:ILE:N	2.25	0.50
1:C:380:GLN:HB3	1:C:390:LEU:CD2	2.40	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:642:LYS:HZ2	1:C:733:VAL:HG21	1.76	0.50
1:D:166:GLN:HB3	1:D:217:MET:HE2	1.93	0.50
1:F:68:ARG:HH12	1:F:166:GLN:HG2	1.77	0.50
1:F:519:ALA:HB1	1:F:535:PHE:CE2	2.47	0.50
1:F:641:ARG:HG3	1:F:777:PHE:CE1	2.47	0.50
1:G:31:PRO:HB3	1:G:528:PRO:HA	1.93	0.50
1:H:108:MET:HA	1:I:114:PRO:CG	2.42	0.50
1:H:429:ARG:HD2	1:H:661:VAL:HG11	1.93	0.50
1:H:442:PHE:CE2	1:H:681:ALA:HB1	2.46	0.50
1:I:30:ILE:CG2	1:I:31:PRO:CD	2.88	0.50
1:I:68:ARG:HH12	1:I:166:GLN:HG2	1.76	0.50
1:J:285:LEU:HD13	1:J:291:PHE:CD2	2.45	0.50
1:B:492:TYR:CE2	1:B:680:LEU:HA	2.46	0.50
1:C:350:THR:OG1	1:C:351:PRO:HD3	2.11	0.50
1:D:442:PHE:CE2	1:D:681:ALA:HB1	2.46	0.50
1:D:741:GLN:O	1:D:745:GLN:HG3	2.10	0.50
1:F:715:LEU:HA	1:F:719:ARG:H	1.75	0.50
1:F:745:GLN:HG2	1:F:766:GLU:OE2	2.12	0.50
1:G:30:ILE:CG2	1:G:31:PRO:CD	2.88	0.50
1:G:442:PHE:CE2	1:G:681:ALA:HB1	2.47	0.50
1:G:741:GLN:O	1:G:745:GLN:HG3	2.11	0.50
1:H:780:ILE:O	1:H:784:VAL:HG23	2.11	0.50
1:J:641:ARG:HG3	1:J:777:PHE:CE1	2.46	0.50
1:C:39:TRP:CZ3	1:C:289:ILE:CD1	2.94	0.50
1:C:429:ARG:HD2	1:C:661:VAL:HG11	1.93	0.50
1:D:492:TYR:CE2	1:D:680:LEU:HA	2.47	0.50
1:E:39:TRP:CZ3	1:E:289:ILE:CD1	2.94	0.50
1:E:780:ILE:O	1:E:784:VAL:HG23	2.11	0.50
1:G:166:GLN:HB3	1:G:217:MET:HE2	1.94	0.50
1:G:420:VAL:CG1	1:G:602:VAL:HG13	2.42	0.50
1:I:519:ALA:HB1	1:I:535:PHE:CE2	2.47	0.50
1:B:418:VAL:CG1	1:C:141:ASN:HD21	2.25	0.50
1:B:429:ARG:HD2	1:B:661:VAL:HG11	1.93	0.50
1:C:31:PRO:HB3	1:C:528:PRO:HA	1.94	0.50
1:F:780:ILE:O	1:F:784:VAL:HG23	2.11	0.50
1:G:68:ARG:HH12	1:G:166:GLN:HG2	1.77	0.50
1:G:145:ASP:CB	1:G:148:GLN:HE21	2.24	0.50
1:G:492:TYR:CE2	1:G:680:LEU:HA	2.47	0.50
1:I:285:LEU:HD13	1:I:291:PHE:CD2	2.45	0.50
1:I:350:THR:OG1	1:I:351:PRO:HD3	2.11	0.50
1:J:382:ARG:HA	1:J:390:LEU:HA	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:492:TYR:CE2	1:A:680:LEU:HA	2.47	0.50
1:C:409:GLN:HG3	1:C:661:VAL:HG13	1.92	0.50
1:D:641:ARG:HG3	1:D:777:PHE:CE1	2.47	0.50
1:D:780:ILE:O	1:D:784:VAL:HG23	2.11	0.50
1:E:220:LEU:HD23	1:E:230:PHE:CD1	2.46	0.50
1:G:475:VAL:HG22	1:G:680:LEU:HD12	1.94	0.50
1:G:780:ILE:O	1:G:784:VAL:HG23	2.11	0.50
1:H:31:PRO:HB3	1:H:528:PRO:HA	1.93	0.50
1:J:659:ILE:HD12	1:J:659:ILE:N	2.25	0.50
1:C:270:VAL:HG23	1:C:317:VAL:CG1	2.34	0.50
1:C:475:VAL:HG22	1:C:680:LEU:HD12	1.94	0.50
1:C:492:TYR:CE2	1:C:680:LEU:HA	2.47	0.50
1:D:31:PRO:HB3	1:D:528:PRO:HA	1.94	0.50
1:D:429:ARG:HD2	1:D:661:VAL:HG11	1.93	0.50
1:E:350:THR:OG1	1:E:351:PRO:HD3	2.10	0.50
1:F:270:VAL:HG23	1:F:317:VAL:CG1	2.34	0.50
1:F:429:ARG:HD2	1:F:661:VAL:HG11	1.94	0.50
1:G:220:LEU:HD23	1:G:230:PHE:CD1	2.47	0.50
1:G:264:GLU:OE2	1:G:298:THR:OG1	2.26	0.50
1:I:31:PRO:HB3	1:I:528:PRO:HA	1.93	0.50
1:A:475:VAL:HG22	1:A:680:LEU:HD12	1.94	0.50
1:A:519:ALA:HB1	1:A:535:PHE:CE2	2.46	0.50
1:B:412:GLN:O	1:C:89:GLN:NE2	2.42	0.50
1:C:30:ILE:CG2	1:C:31:PRO:CD	2.88	0.50
1:D:350:THR:OG1	1:D:351:PRO:HD3	2.11	0.50
1:D:642:LYS:HZ2	1:D:733:VAL:HG21	1.77	0.50
1:E:68:ARG:HH12	1:E:166:GLN:HG2	1.76	0.50
1:H:715:LEU:HA	1:H:719:ARG:H	1.75	0.50
1:I:145:ASP:CB	1:I:148:GLN:HE21	2.24	0.50
1:I:264:GLU:OE2	1:I:298:THR:OG1	2.26	0.50
1:I:715:LEU:HA	1:I:719:ARG:H	1.76	0.50
1:J:420:VAL:CG1	1:J:602:VAL:HG13	2.42	0.50
1:J:429:ARG:HD2	1:J:661:VAL:HG11	1.93	0.50
1:B:442:PHE:CE2	1:B:681:ALA:HB1	2.46	0.50
1:C:220:LEU:HD23	1:C:230:PHE:CD1	2.47	0.50
1:D:382:ARG:HA	1:D:390:LEU:HA	1.94	0.50
1:E:492:TYR:CE2	1:E:680:LEU:HA	2.46	0.50
1:E:519:ALA:HB1	1:E:535:PHE:CE2	2.47	0.50
1:E:715:LEU:HA	1:E:719:ARG:H	1.76	0.50
1:H:166:GLN:HB3	1:H:217:MET:HE2	1.94	0.50
1:J:519:ALA:HB1	1:J:535:PHE:CE2	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:VAL:CG1	1:A:602:VAL:HG13	2.42	0.49
1:B:420:VAL:CG1	1:B:602:VAL:HG13	2.42	0.49
1:C:264:GLU:OE2	1:C:298:THR:OG1	2.26	0.49
1:D:420:VAL:CG1	1:D:602:VAL:HG13	2.42	0.49
1:E:166:GLN:HB3	1:E:217:MET:HE2	1.94	0.49
1:H:220:LEU:HD23	1:H:230:PHE:CD1	2.47	0.49
1:H:492:TYR:CE2	1:H:680:LEU:HA	2.47	0.49
1:A:442:PHE:CE2	1:A:681:ALA:HB1	2.46	0.49
1:B:642:LYS:HZ2	1:B:733:VAL:HG21	1.77	0.49
1:C:68:ARG:HH12	1:C:166:GLN:HG2	1.76	0.49
1:C:541:ASN:HA	1:C:559:SER:HB3	1.95	0.49
1:D:745:GLN:HG2	1:D:766:GLU:OE2	2.12	0.49
1:I:492:TYR:CE2	1:I:680:LEU:HA	2.47	0.49
1:J:475:VAL:HG22	1:J:680:LEU:HD12	1.94	0.49
1:A:68:ARG:HH12	1:A:166:GLN:HG2	1.77	0.49
1:D:403:ASN:O	1:D:434:LEU:HB2	2.13	0.49
1:E:31:PRO:HB3	1:E:528:PRO:HA	1.93	0.49
1:G:350:THR:OG1	1:G:351:PRO:HD3	2.11	0.49
1:G:593:LEU:HD13	1:G:596:ARG:HD2	1.95	0.49
1:I:420:VAL:CG1	1:I:602:VAL:HG13	2.42	0.49
1:I:429:ARG:HD2	1:I:661:VAL:HG11	1.93	0.49
1:I:745:GLN:HG2	1:I:766:GLU:OE2	2.12	0.49
1:J:745:GLN:HG2	1:J:766:GLU:OE2	2.12	0.49
1:A:429:ARG:HD2	1:A:661:VAL:HG11	1.93	0.49
1:C:641:ARG:HG3	1:C:777:PHE:CE1	2.47	0.49
1:D:145:ASP:CB	1:D:148:GLN:HE21	2.24	0.49
1:F:442:PHE:CE2	1:F:681:ALA:HB1	2.46	0.49
1:F:492:TYR:CE2	1:F:680:LEU:HA	2.47	0.49
1:G:429:ARG:HD2	1:G:661:VAL:HG11	1.93	0.49
1:G:745:GLN:HG2	1:G:766:GLU:OE2	2.12	0.49
1:J:31:PRO:HB3	1:J:528:PRO:HA	1.93	0.49
1:J:166:GLN:HB3	1:J:217:MET:HE2	1.94	0.49
1:J:390:LEU:O	1:J:484:THR:HG22	2.13	0.49
1:C:403:ASN:O	1:C:434:LEU:HB2	2.13	0.49
1:D:475:VAL:HG22	1:D:680:LEU:HD12	1.94	0.49
1:C:519:ALA:HB1	1:C:535:PHE:CE2	2.47	0.49
1:D:68:ARG:HH12	1:D:166:GLN:HG2	1.77	0.49
1:D:537:HIS:O	1:D:560:ALA:HA	2.13	0.49
1:G:537:HIS:O	1:G:560:ALA:HA	2.13	0.49
1:H:745:GLN:HG2	1:H:766:GLU:OE2	2.12	0.49
1:A:403:ASN:O	1:A:434:LEU:HB2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:541:ASN:HA	1:A:559:SER:HB3	1.95	0.49
1:A:641:ARG:HG3	1:A:777:PHE:CE1	2.47	0.49
1:A:745:GLN:HG2	1:A:766:GLU:OE2	2.12	0.49
1:B:382:ARG:HA	1:B:390:LEU:HA	1.94	0.49
1:B:745:GLN:HG2	1:B:766:GLU:OE2	2.12	0.49
1:C:166:GLN:HB3	1:C:217:MET:HE2	1.93	0.49
1:D:541:ASN:HA	1:D:559:SER:HB3	1.94	0.49
1:F:475:VAL:HG22	1:F:680:LEU:HD12	1.94	0.49
1:H:412:GLN:O	1:I:89:GLN:NE2	2.42	0.49
1:H:420:VAL:CG1	1:H:602:VAL:HG13	2.42	0.49
1:H:519:ALA:HB1	1:H:535:PHE:CE2	2.47	0.49
1:J:541:ASN:HA	1:J:559:SER:HB3	1.95	0.49
1:A:166:GLN:HB3	1:A:217:MET:HE2	1.94	0.49
1:A:593:LEU:HD13	1:A:596:ARG:HD2	1.95	0.49
1:C:390:LEU:O	1:C:484:THR:HG22	2.13	0.49
1:E:420:VAL:CG1	1:E:602:VAL:HG13	2.42	0.49
1:E:745:GLN:HG2	1:E:766:GLU:OE2	2.12	0.49
1:F:420:VAL:CG1	1:F:602:VAL:HG13	2.42	0.49
1:G:418:VAL:CG1	1:H:141:ASN:HD21	2.25	0.49
1:H:475:VAL:HG22	1:H:680:LEU:HD12	1.94	0.49
1:J:220:LEU:HD23	1:J:230:PHE:CD1	2.48	0.49
1:C:420:VAL:CG1	1:C:602:VAL:HG13	2.42	0.49
1:D:264:GLU:OE2	1:D:298:THR:OG1	2.26	0.49
1:E:264:GLU:OE2	1:E:298:THR:OG1	2.26	0.49
1:F:612:ILE:HD11	1:F:657:PHE:CD2	2.48	0.49
1:F:660:ALA:HB1	1:G:85:ASP:OD2	2.13	0.49
1:H:537:HIS:O	1:H:560:ALA:HA	2.13	0.49
1:I:612:ILE:HD11	1:I:657:PHE:CD2	2.47	0.49
1:J:492:TYR:CE2	1:J:680:LEU:HA	2.47	0.49
1:A:220:LEU:HD23	1:A:230:PHE:CD1	2.47	0.49
1:B:432:LEU:HD13	1:B:756:ILE:HD11	1.95	0.49
1:B:475:VAL:HG22	1:B:680:LEU:HD12	1.94	0.49
1:E:141:ASN:HD21	1:I:418:VAL:CG1	2.26	0.49
1:E:593:LEU:HD13	1:E:596:ARG:HD2	1.95	0.49
1:F:403:ASN:O	1:F:434:LEU:HB2	2.13	0.49
1:F:418:VAL:CG1	1:G:141:ASN:HD21	2.25	0.49
1:F:537:HIS:O	1:F:560:ALA:HA	2.13	0.49
1:G:519:ALA:HB1	1:G:535:PHE:CE2	2.47	0.49
1:I:166:GLN:HB3	1:I:217:MET:HE2	1.94	0.49
1:I:392:ALA:HB2	1:I:450:MET:HE2	1.95	0.49
1:I:475:VAL:HG22	1:I:680:LEU:HD12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:612:ILE:HD11	1:J:657:PHE:CD2	2.48	0.49
1:A:382:ARG:HA	1:A:390:LEU:HA	1.95	0.48
1:B:68:ARG:HH12	1:B:166:GLN:HG2	1.76	0.48
1:B:166:GLN:HB3	1:B:217:MET:HE2	1.94	0.48
1:B:408:TYR:HB3	1:B:425:ILE:HG23	1.95	0.48
1:C:432:LEU:HD13	1:C:756:ILE:HD11	1.95	0.48
1:C:593:LEU:HD13	1:C:596:ARG:HD2	1.95	0.48
1:D:660:ALA:HB1	1:J:85:ASP:OD2	2.13	0.48
1:F:31:PRO:HB3	1:F:528:PRO:HA	1.94	0.48
1:F:390:LEU:O	1:F:484:THR:HG22	2.13	0.48
1:G:146:GLU:CD	1:G:604:LYS:HZ1	2.18	0.48
1:G:390:LEU:O	1:G:484:THR:HG22	2.13	0.48
1:G:403:ASN:O	1:G:434:LEU:HB2	2.13	0.48
1:G:432:LEU:HD13	1:G:756:ILE:HD11	1.95	0.48
1:I:220:LEU:HD23	1:I:230:PHE:CD1	2.48	0.48
1:I:537:HIS:O	1:I:560:ALA:HA	2.13	0.48
1:J:432:LEU:HD13	1:J:756:ILE:HD11	1.95	0.48
1:A:432:LEU:HD13	1:A:756:ILE:HD11	1.95	0.48
1:B:403:ASN:O	1:B:434:LEU:HB2	2.13	0.48
1:B:541:ASN:HA	1:B:559:SER:HB3	1.95	0.48
1:C:382:ARG:HA	1:C:390:LEU:HA	1.94	0.48
1:D:390:LEU:O	1:D:484:THR:HG22	2.13	0.48
1:E:475:VAL:HG22	1:E:680:LEU:HD12	1.94	0.48
1:H:612:ILE:HD11	1:H:657:PHE:CD2	2.48	0.48
1:A:270:VAL:HG23	1:A:317:VAL:CG1	2.34	0.48
1:C:537:HIS:O	1:C:560:ALA:HA	2.13	0.48
1:E:390:LEU:O	1:E:484:THR:HG22	2.13	0.48
1:G:382:ARG:HA	1:G:390:LEU:HA	1.94	0.48
1:I:382:ARG:HA	1:I:390:LEU:HA	1.95	0.48
1:I:403:ASN:O	1:I:434:LEU:HB2	2.13	0.48
1:B:390:LEU:O	1:B:484:THR:HG22	2.13	0.48
1:C:745:GLN:HG2	1:C:766:GLU:OE2	2.12	0.48
1:E:146:GLU:OE2	1:E:604:LYS:NZ	2.38	0.48
1:E:382:ARG:HA	1:E:390:LEU:HA	1.94	0.48
1:H:121:TRP:CE3	1:I:226:PRO:HG3	2.48	0.48
1:I:541:ASN:HA	1:I:559:SER:HB3	1.95	0.48
1:B:537:HIS:O	1:B:560:ALA:HA	2.13	0.48
1:D:392:ALA:HB2	1:D:450:MET:HE2	1.96	0.48
1:E:122:ALA:HB1	1:F:114:PRO:HB2	1.95	0.48
1:F:541:ASN:HA	1:F:559:SER:HB3	1.95	0.48
1:G:721:ASP:HA	1:G:722:GLU:HA	1.57	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:541:ASN:HA	1:H:559:SER:HB3	1.94	0.48
1:I:432:LEU:HD13	1:I:756:ILE:HD11	1.95	0.48
1:J:392:ALA:HB2	1:J:450:MET:HE2	1.96	0.48
1:J:403:ASN:O	1:J:434:LEU:HB2	2.13	0.48
1:B:220:LEU:HD23	1:B:230:PHE:CD1	2.47	0.48
1:E:612:ILE:HD11	1:E:657:PHE:CD2	2.48	0.48
1:F:220:LEU:HD23	1:F:230:PHE:CD1	2.48	0.48
1:F:593:LEU:HD13	1:F:596:ARG:HD2	1.96	0.48
1:H:382:ARG:HA	1:H:390:LEU:HA	1.95	0.48
1:H:390:LEU:O	1:H:484:THR:HG22	2.13	0.48
1:H:392:ALA:HB2	1:H:450:MET:HE2	1.96	0.48
1:A:390:LEU:O	1:A:484:THR:HG22	2.13	0.48
1:A:426:MET:HE1	1:B:246:MET:HG2	1.96	0.48
1:A:612:ILE:HD11	1:A:657:PHE:CD2	2.48	0.48
1:B:612:ILE:HD11	1:B:657:PHE:CD2	2.48	0.48
1:C:612:ILE:HD11	1:C:657:PHE:CD2	2.48	0.48
1:E:403:ASN:O	1:E:434:LEU:HB2	2.13	0.48
1:F:146:GLU:CD	1:F:604:LYS:HZ1	2.18	0.48
1:F:382:ARG:HA	1:F:390:LEU:HA	1.95	0.48
1:H:121:TRP:CZ3	1:I:226:PRO:HG3	2.49	0.48
1:H:408:TYR:HB3	1:H:425:ILE:HG23	1.96	0.48
1:A:509:SER:OG	1:J:723:ILE:HD11	2.13	0.48
1:A:537:HIS:O	1:A:560:ALA:HA	2.13	0.48
1:E:432:LEU:HD13	1:E:756:ILE:HD11	1.95	0.48
1:G:408:TYR:HB3	1:G:425:ILE:HG23	1.95	0.48
1:H:426:MET:HE1	1:I:246:MET:HG2	1.96	0.48
1:I:612:ILE:HD11	1:I:657:PHE:HD2	1.79	0.48
1:J:146:GLU:OE2	1:J:604:LYS:NZ	2.38	0.48
1:B:593:LEU:HD13	1:B:596:ARG:HD2	1.96	0.48
1:E:541:ASN:HA	1:E:559:SER:HB3	1.95	0.48
1:H:432:LEU:HD13	1:H:756:ILE:HD11	1.95	0.48
1:J:537:HIS:O	1:J:560:ALA:HA	2.13	0.48
1:A:145:ASP:CB	1:A:148:GLN:HE21	2.23	0.48
1:D:220:LEU:HD23	1:D:230:PHE:CD1	2.48	0.48
1:E:145:ASP:CB	1:E:148:GLN:HE21	2.23	0.48
1:G:392:ALA:HB2	1:G:450:MET:HE2	1.96	0.48
1:G:612:ILE:HD11	1:G:657:PHE:CD2	2.49	0.48
1:H:403:ASN:O	1:H:434:LEU:HB2	2.13	0.48
1:J:612:ILE:HD11	1:J:657:PHE:HD2	1.79	0.48
1:A:612:ILE:HD11	1:A:657:PHE:HD2	1.79	0.47
1:B:145:ASP:CB	1:B:148:GLN:HE21	2.24	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:ALA:HB2	1:C:450:MET:HE2	1.96	0.47
1:E:537:HIS:O	1:E:560:ALA:HA	2.13	0.47
1:F:432:LEU:HD13	1:F:756:ILE:HD11	1.95	0.47
1:H:108:MET:HA	1:I:114:PRO:HG2	1.96	0.47
1:J:642:LYS:HZ2	1:J:733:VAL:HG21	1.78	0.47
1:B:260:ALA:HB2	1:B:302:TRP:HB3	1.96	0.47
1:B:264:GLU:OE2	1:B:298:THR:OG1	2.26	0.47
1:C:493:MET:HG3	1:C:496:LEU:HD12	1.96	0.47
1:D:260:ALA:HB2	1:D:302:TRP:HB3	1.96	0.47
1:E:408:TYR:HB3	1:E:425:ILE:HG23	1.96	0.47
1:F:166:GLN:HB3	1:F:217:MET:HE2	1.94	0.47
1:F:396:ARG:HD3	1:F:443:PHE:CG	2.49	0.47
1:J:114:PRO:HA	1:J:228:THR:CG2	2.45	0.47
1:C:396:ARG:HD3	1:C:443:PHE:CG	2.49	0.47
1:D:593:LEU:HD13	1:D:596:ARG:HD2	1.95	0.47
1:D:705:ALA:O	1:D:709:THR:HG22	2.15	0.47
1:F:429:ARG:NE	1:G:304:GLN:OE1	2.42	0.47
1:I:390:LEU:O	1:I:484:THR:HG22	2.13	0.47
1:I:477:LYS:O	1:I:486:LEU:HD23	2.15	0.47
1:A:392:ALA:HB2	1:A:450:MET:HE2	1.95	0.47
1:A:493:MET:HG3	1:A:496:LEU:HD12	1.96	0.47
1:C:114:PRO:HA	1:C:228:THR:CG2	2.45	0.47
1:C:705:ALA:O	1:C:709:THR:HG22	2.14	0.47
1:F:392:ALA:HB2	1:F:450:MET:HE2	1.95	0.47
1:I:408:TYR:HB3	1:I:425:ILE:HG23	1.95	0.47
1:B:146:GLU:OE2	1:B:604:LYS:NZ	2.39	0.47
1:B:477:LYS:O	1:B:486:LEU:HD23	2.15	0.47
1:B:493:MET:HG3	1:B:496:LEU:HD12	1.97	0.47
1:C:260:ALA:HB2	1:C:302:TRP:HB3	1.97	0.47
1:D:396:ARG:HD3	1:D:443:PHE:CG	2.49	0.47
1:D:612:ILE:HD11	1:D:657:PHE:CD2	2.49	0.47
1:F:705:ALA:O	1:F:709:THR:HG22	2.14	0.47
1:F:721:ASP:HA	1:F:722:GLU:HA	1.57	0.47
1:G:477:LYS:O	1:G:486:LEU:HD23	2.14	0.47
1:H:123:GLU:CD	1:I:229:ARG:NH1	2.65	0.47
1:H:612:ILE:HD11	1:H:657:PHE:HD2	1.79	0.47
1:H:705:ALA:O	1:H:709:THR:HG22	2.15	0.47
1:I:114:PRO:HA	1:I:228:THR:CG2	2.44	0.47
1:A:396:ARG:HD3	1:A:443:PHE:CG	2.49	0.47
1:A:705:ALA:O	1:A:709:THR:HG22	2.15	0.47
1:B:33:SER:HA	1:B:525:VAL:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ALA:HB2	1:B:450:MET:HE2	1.95	0.47
1:C:33:SER:HA	1:C:525:VAL:O	2.15	0.47
1:C:477:LYS:O	1:C:486:LEU:HD23	2.14	0.47
1:D:100:MET:HE2	1:D:100:MET:HA	1.97	0.47
1:D:262:VAL:O	1:D:266:VAL:HG23	2.15	0.47
1:D:432:LEU:HD13	1:D:756:ILE:HD11	1.95	0.47
1:D:477:LYS:O	1:D:486:LEU:HD23	2.14	0.47
1:E:396:ARG:HD3	1:E:443:PHE:CG	2.49	0.47
1:E:493:MET:HG3	1:E:496:LEU:HD12	1.96	0.47
1:F:100:MET:HE2	1:F:100:MET:HA	1.97	0.47
1:F:262:VAL:O	1:F:266:VAL:HG23	2.15	0.47
1:F:408:TYR:HB3	1:F:425:ILE:HG23	1.96	0.47
1:G:493:MET:HG3	1:G:496:LEU:HD12	1.96	0.47
1:G:705:ALA:O	1:G:709:THR:HG22	2.15	0.47
1:H:145:ASP:CB	1:H:148:GLN:HE21	2.23	0.47
1:I:55:ARG:CZ	1:I:587:ILE:HD11	2.45	0.47
1:I:396:ARG:HD3	1:I:443:PHE:CG	2.50	0.47
1:I:705:ALA:O	1:I:709:THR:HG22	2.15	0.47
1:J:33:SER:HA	1:J:525:VAL:O	2.15	0.47
1:J:260:ALA:HB2	1:J:302:TRP:HB3	1.97	0.47
1:J:262:VAL:O	1:J:266:VAL:HG23	2.15	0.47
1:J:374:GLY:HA3	1:J:375:LEU:HA	1.73	0.47
1:J:721:ASP:HA	1:J:722:GLU:HA	1.57	0.47
1:A:264:GLU:OE2	1:A:298:THR:OG1	2.26	0.47
1:A:460:GLU:OE1	1:G:775:ASN:ND2	2.41	0.47
1:B:100:MET:HA	1:B:100:MET:HE2	1.97	0.47
1:B:612:ILE:HD11	1:B:657:PHE:HD2	1.80	0.47
1:D:277:LEU:O	1:D:283:GLN:HG2	2.15	0.47
1:D:612:ILE:HD11	1:D:657:PHE:HD2	1.80	0.47
1:E:477:LYS:O	1:E:486:LEU:HD23	2.14	0.47
1:E:612:ILE:HD11	1:E:657:PHE:HD2	1.80	0.47
1:F:277:LEU:O	1:F:283:GLN:HG2	2.15	0.47
1:F:493:MET:HG3	1:F:496:LEU:HD12	1.96	0.47
1:I:390:LEU:O	1:I:549:GLN:NE2	2.48	0.47
1:J:114:PRO:HA	1:J:228:THR:HG21	1.97	0.47
1:J:396:ARG:HD3	1:J:443:PHE:CG	2.50	0.47
1:J:545:ARG:HB2	1:J:572:ALA:CB	2.45	0.47
1:J:593:LEU:HD13	1:J:596:ARG:HD2	1.96	0.47
1:A:100:MET:HE2	1:A:100:MET:HA	1.96	0.47
1:A:477:LYS:O	1:A:486:LEU:HD23	2.15	0.47
1:A:642:LYS:HZ2	1:A:733:VAL:HG21	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:MET:HE2	1:C:100:MET:HA	1.97	0.47
1:C:277:LEU:O	1:C:283:GLN:HG2	2.15	0.47
1:E:545:ARG:HB2	1:E:572:ALA:CB	2.45	0.47
1:F:145:ASP:CB	1:F:148:GLN:HE21	2.24	0.47
1:F:477:LYS:O	1:F:486:LEU:HD23	2.15	0.47
1:G:33:SER:HA	1:G:525:VAL:O	2.15	0.47
1:G:277:LEU:O	1:G:283:GLN:HG2	2.15	0.47
1:G:541:ASN:HA	1:G:559:SER:HB3	1.95	0.47
1:C:354:ARG:HH12	1:C:358:THR:HG22	1.80	0.47
1:D:721:ASP:HA	1:D:722:GLU:HA	1.57	0.47
1:F:114:PRO:HA	1:F:228:THR:CG2	2.45	0.47
1:F:612:ILE:HD11	1:F:657:PHE:HD2	1.80	0.47
1:G:114:PRO:HA	1:G:228:THR:CG2	2.45	0.47
1:G:262:VAL:O	1:G:266:VAL:HG23	2.15	0.47
1:H:354:ARG:HH12	1:H:358:THR:HG22	1.80	0.47
1:J:257:ARG:O	1:J:261:VAL:HG23	2.15	0.47
1:J:477:LYS:O	1:J:486:LEU:HD23	2.15	0.47
1:J:493:MET:HG3	1:J:496:LEU:HD12	1.96	0.47
1:J:705:ALA:O	1:J:709:THR:HG22	2.15	0.47
1:B:396:ARG:HD3	1:B:443:PHE:CG	2.49	0.46
1:D:33:SER:HA	1:D:525:VAL:O	2.15	0.46
1:E:55:ARG:CZ	1:E:587:ILE:HD11	2.45	0.46
1:E:114:PRO:HA	1:E:228:THR:CG2	2.45	0.46
1:E:257:ARG:O	1:E:261:VAL:HG23	2.16	0.46
1:F:737:GLU:HG3	1:F:777:PHE:CZ	2.50	0.46
1:H:33:SER:HA	1:H:525:VAL:O	2.15	0.46
1:I:100:MET:HE2	1:I:100:MET:HA	1.96	0.46
1:I:260:ALA:HB2	1:I:302:TRP:HB3	1.96	0.46
1:J:100:MET:HA	1:J:100:MET:HE2	1.97	0.46
1:J:145:ASP:CB	1:J:148:GLN:HE21	2.24	0.46
1:C:612:ILE:HD11	1:C:657:PHE:HD2	1.80	0.46
1:D:429:ARG:NE	1:J:304:GLN:OE1	2.45	0.46
1:H:277:LEU:O	1:H:283:GLN:HG2	2.15	0.46
1:H:396:ARG:HD3	1:H:443:PHE:CG	2.50	0.46
1:I:277:LEU:O	1:I:283:GLN:HG2	2.15	0.46
1:I:593:LEU:HD13	1:I:596:ARG:HD2	1.95	0.46
1:A:33:SER:HA	1:A:525:VAL:O	2.15	0.46
1:A:257:ARG:O	1:A:261:VAL:HG23	2.16	0.46
1:A:262:VAL:O	1:A:266:VAL:HG23	2.15	0.46
1:B:262:VAL:O	1:B:266:VAL:HG23	2.15	0.46
1:B:390:LEU:O	1:B:549:GLN:NE2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:ALA:O	1:B:709:THR:HG22	2.15	0.46
1:C:262:VAL:O	1:C:266:VAL:HG23	2.15	0.46
1:D:270:VAL:HG23	1:D:317:VAL:CG1	2.34	0.46
1:D:493:MET:HG3	1:D:496:LEU:HD12	1.96	0.46
1:E:317:VAL:HA	1:E:320:ILE:HD12	1.97	0.46
1:G:55:ARG:CZ	1:G:587:ILE:HD11	2.46	0.46
1:G:100:MET:HE2	1:G:100:MET:HA	1.97	0.46
1:G:171:LYS:O	1:H:232:ARG:NH2	2.48	0.46
1:H:257:ARG:O	1:H:261:VAL:HG23	2.15	0.46
1:H:477:LYS:O	1:H:486:LEU:HD23	2.14	0.46
1:I:748:LYS:HA	1:I:762:ILE:HD13	1.97	0.46
1:J:408:TYR:HB3	1:J:425:ILE:HG23	1.96	0.46
1:A:260:ALA:HB2	1:A:302:TRP:HB3	1.97	0.46
1:A:354:ARG:HH12	1:A:358:THR:HG22	1.80	0.46
1:A:408:TYR:HB3	1:A:425:ILE:HG23	1.96	0.46
1:C:408:TYR:HB3	1:C:425:ILE:HG23	1.96	0.46
1:D:114:PRO:HA	1:D:228:THR:CG2	2.45	0.46
1:D:286:ARG:HH12	1:D:527:PHE:HB3	1.81	0.46
1:E:277:LEU:O	1:E:283:GLN:HG2	2.16	0.46
1:E:392:ALA:HB2	1:E:450:MET:HE2	1.96	0.46
1:F:270:VAL:HG22	1:F:321:ASN:HD21	1.81	0.46
1:F:354:ARG:HH12	1:F:358:THR:HG22	1.80	0.46
1:H:260:ALA:HB2	1:H:302:TRP:HB3	1.96	0.46
1:H:286:ARG:HH12	1:H:527:PHE:HB3	1.81	0.46
1:H:493:MET:HG3	1:H:496:LEU:HD12	1.97	0.46
1:A:737:GLU:HG3	1:A:777:PHE:CZ	2.50	0.46
1:B:114:PRO:HA	1:B:228:THR:CG2	2.45	0.46
1:B:317:VAL:HA	1:B:320:ILE:HD12	1.97	0.46
1:C:114:PRO:HA	1:C:228:THR:HG21	1.97	0.46
1:D:257:ARG:O	1:D:261:VAL:HG23	2.16	0.46
1:D:408:TYR:HB3	1:D:425:ILE:HG23	1.95	0.46
1:E:390:LEU:O	1:E:549:GLN:NE2	2.49	0.46
1:E:705:ALA:O	1:E:709:THR:HG22	2.15	0.46
1:F:55:ARG:CZ	1:F:587:ILE:HD11	2.46	0.46
1:F:748:LYS:HA	1:F:762:ILE:HD13	1.98	0.46
1:G:257:ARG:O	1:G:261:VAL:HG23	2.15	0.46
1:G:612:ILE:HD11	1:G:657:PHE:HD2	1.81	0.46
1:H:390:LEU:O	1:H:549:GLN:NE2	2.49	0.46
1:A:277:LEU:O	1:A:283:GLN:HG2	2.15	0.46
1:D:390:LEU:O	1:D:549:GLN:NE2	2.49	0.46
1:D:402:ILE:O	1:D:434:LEU:HD12	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:354:ARG:HH12	1:E:358:THR:HG22	1.81	0.46
1:E:737:GLU:HG3	1:E:777:PHE:CZ	2.50	0.46
1:F:286:ARG:HH12	1:F:527:PHE:HB3	1.81	0.46
1:G:396:ARG:HD3	1:G:443:PHE:CG	2.50	0.46
1:G:408:TYR:HB3	1:G:425:ILE:CG2	2.46	0.46
1:H:100:MET:HE2	1:H:100:MET:HA	1.98	0.46
1:H:410:SER:HB3	1:H:664:ALA:HB2	1.98	0.46
1:H:540:SER:HA	1:H:541:ASN:HA	1.75	0.46
1:I:273:PRO:CB	1:I:276:TYR:CD2	2.96	0.46
1:I:737:GLU:HG3	1:I:777:PHE:CZ	2.51	0.46
1:A:55:ARG:CZ	1:A:587:ILE:HD11	2.46	0.46
1:A:141:ASN:HD21	1:J:418:VAL:CG1	2.28	0.46
1:A:317:VAL:HA	1:A:320:ILE:HD12	1.98	0.46
1:B:114:PRO:HA	1:B:228:THR:HG21	1.98	0.46
1:B:277:LEU:O	1:B:283:GLN:HG2	2.15	0.46
1:C:55:ARG:CZ	1:C:587:ILE:HD11	2.46	0.46
1:D:55:ARG:CZ	1:D:587:ILE:HD11	2.46	0.46
1:D:410:SER:HB3	1:D:664:ALA:HB2	1.98	0.46
1:E:33:SER:HA	1:E:525:VAL:O	2.15	0.46
1:F:33:SER:HA	1:F:525:VAL:O	2.15	0.46
1:F:390:LEU:O	1:F:549:GLN:NE2	2.48	0.46
1:G:390:LEU:O	1:G:549:GLN:NE2	2.48	0.46
1:H:593:LEU:HD13	1:H:596:ARG:HD2	1.96	0.46
1:J:55:ARG:CZ	1:J:587:ILE:HD11	2.46	0.46
1:J:277:LEU:O	1:J:283:GLN:HG2	2.15	0.46
1:J:286:ARG:HH12	1:J:527:PHE:HB3	1.81	0.46
1:A:545:ARG:HB2	1:A:572:ALA:CB	2.45	0.46
1:B:264:GLU:OE1	1:B:269:ARG:HD2	2.16	0.46
1:B:374:GLY:HA3	1:B:375:LEU:HA	1.73	0.46
1:C:286:ARG:HH12	1:C:527:PHE:HB3	1.81	0.46
1:E:264:GLU:OE1	1:E:269:ARG:HD2	2.16	0.46
1:G:410:SER:HB3	1:G:664:ALA:HB2	1.98	0.46
1:H:37:ALA:O	1:H:369:LEU:HB2	2.16	0.46
1:H:737:GLU:HG3	1:H:777:PHE:CZ	2.51	0.46
1:I:262:VAL:O	1:I:266:VAL:HG23	2.15	0.46
1:J:399:ALA:HB2	1:J:584:ILE:HB	1.98	0.46
1:A:114:PRO:HA	1:A:228:THR:CG2	2.46	0.46
1:A:399:ALA:HB2	1:A:584:ILE:HB	1.98	0.46
1:A:479:LEU:HD11	1:A:567:LEU:HD23	1.98	0.46
1:B:257:ARG:O	1:B:261:VAL:HG23	2.16	0.46
1:B:402:ILE:O	1:B:434:LEU:HD12	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:737:GLU:HG3	1:B:777:PHE:CZ	2.50	0.46
1:C:317:VAL:HA	1:C:320:ILE:HD12	1.98	0.46
1:C:390:LEU:O	1:C:549:GLN:NE2	2.49	0.46
1:E:260:ALA:HB2	1:E:302:TRP:HB3	1.97	0.46
1:E:262:VAL:O	1:E:266:VAL:HG23	2.15	0.46
1:E:270:VAL:HG22	1:E:321:ASN:HD21	1.81	0.46
1:E:479:LEU:HD11	1:E:567:LEU:HD23	1.98	0.46
1:F:504:ILE:CG1	1:F:510:VAL:HG21	2.42	0.46
1:G:479:LEU:HD11	1:G:567:LEU:HD23	1.98	0.46
1:I:257:ARG:O	1:I:261:VAL:HG23	2.16	0.46
1:I:493:MET:HG3	1:I:496:LEU:HD12	1.96	0.46
1:J:410:SER:HB3	1:J:664:ALA:HB2	1.98	0.46
1:A:390:LEU:O	1:A:549:GLN:NE2	2.49	0.46
1:B:37:ALA:O	1:B:369:LEU:HB2	2.16	0.46
1:B:55:ARG:CZ	1:B:587:ILE:HD11	2.46	0.46
1:B:408:TYR:HB3	1:B:425:ILE:CG2	2.47	0.46
1:C:402:ILE:O	1:C:434:LEU:HD12	2.16	0.46
1:D:408:TYR:HB3	1:D:425:ILE:CG2	2.46	0.46
1:D:737:GLU:HG3	1:D:777:PHE:CZ	2.51	0.46
1:E:402:ILE:O	1:E:434:LEU:HD12	2.16	0.46
1:E:479:LEU:CD1	1:E:567:LEU:HD23	2.46	0.46
1:F:257:ARG:O	1:F:261:VAL:HG23	2.16	0.46
1:F:260:ALA:HB2	1:F:302:TRP:HB3	1.97	0.46
1:H:399:ALA:HB2	1:H:584:ILE:HB	1.98	0.46
1:H:408:TYR:HB3	1:H:425:ILE:CG2	2.47	0.46
1:I:374:GLY:HA3	1:I:375:LEU:HA	1.74	0.46
1:I:402:ILE:O	1:I:434:LEU:HD12	2.16	0.46
1:I:504:ILE:CG1	1:I:510:VAL:HG21	2.43	0.46
1:B:54:LEU:CD2	1:B:375:LEU:HD23	2.46	0.45
1:B:399:ALA:HB2	1:B:584:ILE:HB	1.98	0.45
1:C:146:GLU:CD	1:C:604:LYS:HZ1	2.22	0.45
1:E:100:MET:HA	1:E:100:MET:HE2	1.97	0.45
1:G:479:LEU:CD1	1:G:567:LEU:HD23	2.47	0.45
1:I:37:ALA:O	1:I:369:LEU:HB2	2.16	0.45
1:I:114:PRO:HA	1:I:228:THR:HG21	1.97	0.45
1:J:273:PRO:CB	1:J:276:TYR:CD2	2.96	0.45
1:J:479:LEU:HD11	1:J:567:LEU:HD23	1.98	0.45
1:J:740:LEU:HD21	1:J:780:ILE:HG22	1.98	0.45
1:A:410:SER:HB3	1:A:664:ALA:HB2	1.99	0.45
1:C:257:ARG:O	1:C:261:VAL:HG23	2.16	0.45
1:C:399:ALA:HB2	1:C:584:ILE:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:740:LEU:HD21	1:C:780:ILE:HG22	1.98	0.45
1:D:354:ARG:HH12	1:D:358:THR:HG22	1.81	0.45
1:D:479:LEU:HD11	1:D:567:LEU:HD23	1.98	0.45
1:F:402:ILE:O	1:F:434:LEU:HD12	2.16	0.45
1:F:545:ARG:HB2	1:F:572:ALA:CB	2.45	0.45
1:F:740:LEU:HD21	1:F:780:ILE:HG22	1.98	0.45
1:G:286:ARG:HH12	1:G:527:PHE:HB3	1.81	0.45
1:G:317:VAL:HA	1:G:320:ILE:HD12	1.98	0.45
1:G:740:LEU:HD21	1:G:780:ILE:HG22	1.99	0.45
1:H:317:VAL:HA	1:H:320:ILE:HD12	1.98	0.45
1:H:740:LEU:HD21	1:H:780:ILE:HG22	1.98	0.45
1:H:748:LYS:HA	1:H:762:ILE:HD13	1.98	0.45
1:I:33:SER:HA	1:I:525:VAL:O	2.15	0.45
1:A:85:ASP:OD2	1:J:660:ALA:HB1	2.16	0.45
1:A:246:MET:HG2	1:J:426:MET:HE1	1.98	0.45
1:A:479:LEU:CD1	1:A:567:LEU:HD23	2.47	0.45
1:B:563:THR:HG21	1:B:568:ASN:HB2	1.98	0.45
1:D:54:LEU:CD2	1:D:375:LEU:HD23	2.46	0.45
1:D:264:GLU:OE1	1:D:269:ARG:HD2	2.16	0.45
1:E:408:TYR:HB3	1:E:425:ILE:CG2	2.47	0.45
1:G:260:ALA:HB2	1:G:302:TRP:HB3	1.97	0.45
1:H:262:VAL:O	1:H:266:VAL:HG23	2.15	0.45
1:H:479:LEU:HB3	1:H:482:THR:OG1	2.17	0.45
1:J:23:VAL:HG21	1:J:32:PHE:CB	2.37	0.45
1:J:479:LEU:CD1	1:J:567:LEU:HD23	2.47	0.45
1:J:737:GLU:HG3	1:J:777:PHE:CZ	2.51	0.45
1:A:740:LEU:HD21	1:A:780:ILE:HG22	1.98	0.45
1:C:54:LEU:CD2	1:C:375:LEU:HD23	2.46	0.45
1:C:479:LEU:HB3	1:C:482:THR:OG1	2.17	0.45
1:C:737:GLU:HG3	1:C:777:PHE:CZ	2.50	0.45
1:D:412:GLN:O	1:J:89:GLN:NE2	2.48	0.45
1:E:748:LYS:HA	1:E:762:ILE:HD13	1.97	0.45
1:F:479:LEU:CD1	1:F:567:LEU:HD23	2.47	0.45
1:G:54:LEU:CD2	1:G:375:LEU:HD23	2.46	0.45
1:G:397:TYR:CE1	1:G:497:LEU:HD21	2.51	0.45
1:G:737:GLU:HG3	1:G:777:PHE:CZ	2.51	0.45
1:H:479:LEU:CD1	1:H:567:LEU:HD23	2.46	0.45
1:I:317:VAL:HA	1:I:320:ILE:HD12	1.98	0.45
1:A:37:ALA:O	1:A:369:LEU:HB2	2.16	0.45
1:A:402:ILE:O	1:A:434:LEU:HD12	2.16	0.45
1:A:479:LEU:HB3	1:A:482:THR:OG1	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:ILE:HD11	1:B:509:SER:OG	2.17	0.45
1:B:286:ARG:HH12	1:B:527:PHE:HB3	1.81	0.45
1:D:317:VAL:HA	1:D:320:ILE:HD12	1.98	0.45
1:E:37:ALA:O	1:E:369:LEU:HB2	2.17	0.45
1:E:54:LEU:CD2	1:E:375:LEU:HD23	2.46	0.45
1:G:273:PRO:CB	1:G:276:TYR:CD2	2.96	0.45
1:G:354:ARG:HH12	1:G:358:THR:HG22	1.81	0.45
1:G:402:ILE:O	1:G:434:LEU:HD12	2.16	0.45
1:I:354:ARG:HH12	1:I:358:THR:HG22	1.80	0.45
1:I:397:TYR:CE1	1:I:497:LEU:HD21	2.52	0.45
1:I:563:THR:HG21	1:I:568:ASN:HB2	1.98	0.45
1:J:390:LEU:O	1:J:549:GLN:NE2	2.49	0.45
1:A:54:LEU:CD2	1:A:375:LEU:HD23	2.46	0.45
1:A:286:ARG:HH12	1:A:527:PHE:HB3	1.81	0.45
1:B:479:LEU:HD11	1:B:567:LEU:HD23	1.98	0.45
1:B:740:LEU:HD21	1:B:780:ILE:HG22	1.99	0.45
1:C:410:SER:HB3	1:C:664:ALA:HB2	1.99	0.45
1:E:418:VAL:CG1	1:F:141:ASN:HD21	2.30	0.45
1:F:114:PRO:HA	1:F:228:THR:HG21	1.98	0.45
1:F:540:SER:HA	1:F:541:ASN:HA	1.75	0.45
1:G:748:LYS:HA	1:G:762:ILE:HD13	1.98	0.45
1:I:286:ARG:HH12	1:I:527:PHE:HB3	1.81	0.45
1:I:399:ALA:HB2	1:I:584:ILE:HB	1.98	0.45
1:I:479:LEU:CD1	1:I:567:LEU:HD23	2.46	0.45
1:J:37:ALA:O	1:J:369:LEU:HB2	2.16	0.45
1:A:145:ASP:HB3	1:A:148:GLN:HG3	1.99	0.45
1:A:748:LYS:HA	1:A:762:ILE:HD13	1.98	0.45
1:C:545:ARG:HB2	1:C:572:ALA:CB	2.45	0.45
1:D:748:LYS:HA	1:D:762:ILE:HD13	1.97	0.45
1:E:114:PRO:HA	1:E:228:THR:HG21	1.98	0.45
1:E:399:ALA:HB2	1:E:584:ILE:HB	1.99	0.45
1:F:317:VAL:HA	1:F:320:ILE:HD12	1.98	0.45
1:G:504:ILE:CG1	1:G:510:VAL:HG21	2.43	0.45
1:I:146:GLU:OE2	1:I:604:LYS:NZ	2.38	0.45
1:I:408:TYR:HB3	1:I:425:ILE:CG2	2.47	0.45
1:A:550:VAL:HG13	1:A:568:ASN:CG	2.42	0.45
1:C:563:THR:HG21	1:C:568:ASN:HB2	1.99	0.45
1:C:748:LYS:HA	1:C:762:ILE:HD13	1.98	0.45
1:D:37:ALA:O	1:D:369:LEU:HB2	2.17	0.45
1:D:114:PRO:HA	1:D:228:THR:HG21	1.98	0.45
1:D:479:LEU:CD1	1:D:567:LEU:HD23	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:563:THR:HG21	1:D:568:ASN:HB2	1.99	0.45
1:E:740:LEU:HD21	1:E:780:ILE:HG22	1.98	0.45
1:F:37:ALA:O	1:F:369:LEU:HB2	2.17	0.45
1:H:55:ARG:CZ	1:H:587:ILE:HD11	2.46	0.45
1:J:270:VAL:HG22	1:J:321:ASN:HD21	1.81	0.45
1:J:354:ARG:HH12	1:J:358:THR:HG22	1.80	0.45
1:C:260:ALA:O	1:C:264:GLU:HG2	2.17	0.45
1:C:479:LEU:CD1	1:C:567:LEU:HD23	2.47	0.45
1:D:399:ALA:HB2	1:D:584:ILE:HB	1.98	0.45
1:E:286:ARG:HH12	1:E:527:PHE:HB3	1.82	0.45
1:G:264:GLU:OE1	1:G:269:ARG:HD2	2.16	0.45
1:G:550:VAL:HG13	1:G:568:ASN:CG	2.42	0.45
1:I:264:GLU:OE1	1:I:269:ARG:HD2	2.16	0.45
1:J:748:LYS:HA	1:J:762:ILE:HD13	1.98	0.45
1:A:408:TYR:HB3	1:A:425:ILE:CG2	2.47	0.45
1:D:260:ALA:O	1:D:264:GLU:HG2	2.17	0.45
1:D:740:LEU:HD21	1:D:780:ILE:HG22	1.99	0.45
1:E:414:PRO:HB3	1:F:142:LEU:HD22	1.98	0.45
1:G:37:ALA:O	1:G:369:LEU:HB2	2.16	0.45
1:G:545:ARG:HB2	1:G:572:ALA:CB	2.45	0.45
1:H:545:ARG:HB2	1:H:572:ALA:CB	2.45	0.45
1:I:40:ALA:CB	1:I:290:ASN:OD1	2.64	0.45
1:I:54:LEU:CD2	1:I:375:LEU:HD23	2.46	0.45
1:I:410:SER:HB3	1:I:664:ALA:HB2	1.98	0.45
1:I:545:ARG:HB2	1:I:572:ALA:CB	2.45	0.45
1:A:260:ALA:O	1:A:264:GLU:HG2	2.17	0.44
1:B:410:SER:HB3	1:B:664:ALA:HB2	1.99	0.44
1:B:657:PHE:CD2	1:B:663:LEU:HD12	2.52	0.44
1:C:145:ASP:HB3	1:C:148:GLN:HG3	1.99	0.44
1:D:545:ARG:HB2	1:D:572:ALA:CB	2.45	0.44
1:D:726:ILE:HA	1:D:727:ALA:HA	1.82	0.44
1:E:563:THR:HG21	1:E:568:ASN:HB2	1.99	0.44
1:F:399:ALA:HB2	1:F:584:ILE:HB	1.99	0.44
1:H:114:PRO:HA	1:H:228:THR:CG2	2.47	0.44
1:H:397:TYR:CE1	1:H:497:LEU:HD21	2.52	0.44
1:I:159:PHE:CD2	1:I:241:MET:HE1	2.52	0.44
1:J:54:LEU:CD2	1:J:375:LEU:HD23	2.46	0.44
1:J:317:VAL:HA	1:J:320:ILE:HD12	1.98	0.44
1:J:408:TYR:HB3	1:J:425:ILE:CG2	2.47	0.44
1:A:232:ARG:O	1:A:236:GLN:HG3	2.18	0.44
1:B:40:ALA:CB	1:B:290:ASN:OD1	2.64	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ALA:O	1:B:264:GLU:HG2	2.17	0.44
1:B:748:LYS:HA	1:B:762:ILE:HD13	1.98	0.44
1:C:273:PRO:CB	1:C:276:TYR:CD2	2.96	0.44
1:D:38:THR:HA	1:D:367:ALA:O	2.17	0.44
1:D:108:MET:HA	1:J:114:PRO:CG	2.47	0.44
1:D:418:VAL:HG12	1:J:141:ASN:ND2	2.28	0.44
1:E:89:GLN:NE2	1:I:412:GLN:O	2.44	0.44
1:E:232:ARG:O	1:E:236:GLN:HG3	2.17	0.44
1:F:54:LEU:CD2	1:F:375:LEU:HD23	2.46	0.44
1:F:145:ASP:HB3	1:F:148:GLN:HG3	2.00	0.44
1:F:479:LEU:HB3	1:F:482:THR:OG1	2.17	0.44
1:H:503:ILE:HG21	1:H:515:TYR:CD2	2.53	0.44
1:I:479:LEU:HD11	1:I:567:LEU:HD23	1.98	0.44
1:B:38:THR:HA	1:B:367:ALA:O	2.18	0.44
1:B:397:TYR:CE1	1:B:497:LEU:HD21	2.51	0.44
1:F:479:LEU:HD11	1:F:567:LEU:HD23	1.98	0.44
1:G:114:PRO:HA	1:G:228:THR:HG21	1.98	0.44
1:H:264:GLU:OE1	1:H:269:ARG:HD2	2.16	0.44
1:H:479:LEU:HD11	1:H:567:LEU:HD23	1.98	0.44
1:H:642:LYS:HG3	1:H:778:TYR:OH	2.17	0.44
1:I:550:VAL:HG13	1:I:568:ASN:CG	2.42	0.44
1:I:740:LEU:HD21	1:I:780:ILE:HG22	1.99	0.44
1:A:264:GLU:OE1	1:A:269:ARG:HD2	2.16	0.44
1:C:37:ALA:O	1:C:369:LEU:HB2	2.17	0.44
1:C:418:VAL:CG1	1:D:141:ASN:HD21	2.31	0.44
1:D:550:VAL:HG13	1:D:568:ASN:CG	2.43	0.44
1:D:715:LEU:N	1:D:716:ALA:HB3	2.33	0.44
1:E:410:SER:HB3	1:E:664:ALA:HB2	1.98	0.44
1:F:264:GLU:OE1	1:F:269:ARG:HD2	2.17	0.44
1:I:38:THR:HA	1:I:367:ALA:O	2.18	0.44
1:I:232:ARG:O	1:I:236:GLN:HG3	2.17	0.44
1:J:264:GLU:OE1	1:J:269:ARG:HD2	2.16	0.44
1:J:563:THR:HG21	1:J:568:ASN:HB2	1.99	0.44
1:A:563:THR:HG21	1:A:568:ASN:HB2	1.99	0.44
1:C:408:TYR:HB3	1:C:425:ILE:CG2	2.47	0.44
1:C:571:VAL:HA	1:C:572:ALA:HA	1.80	0.44
1:D:265:ILE:HD12	1:D:273:PRO:HG3	2.00	0.44
1:E:397:TYR:CE1	1:E:497:LEU:HD21	2.53	0.44
1:F:232:ARG:O	1:F:236:GLN:HG3	2.18	0.44
1:F:397:TYR:CE1	1:F:497:LEU:HD21	2.52	0.44
1:G:265:ILE:HD12	1:G:273:PRO:HG3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:563:THR:HG21	1:G:568:ASN:HB2	1.98	0.44
1:G:642:LYS:HZ2	1:G:733:VAL:HG21	1.83	0.44
1:H:232:ARG:O	1:H:236:GLN:HG3	2.18	0.44
1:H:402:ILE:O	1:H:434:LEU:HD12	2.16	0.44
1:H:550:VAL:HG13	1:H:568:ASN:CG	2.43	0.44
1:H:715:LEU:N	1:H:716:ALA:HB3	2.33	0.44
1:J:265:ILE:HD12	1:J:273:PRO:HG3	2.00	0.44
1:J:397:TYR:CE1	1:J:497:LEU:HD21	2.52	0.44
1:J:642:LYS:HG3	1:J:778:TYR:OH	2.18	0.44
1:A:715:LEU:N	1:A:716:ALA:HB3	2.33	0.44
1:B:479:LEU:HB3	1:B:482:THR:OG1	2.17	0.44
1:C:264:GLU:OE1	1:C:269:ARG:HD2	2.16	0.44
1:C:550:VAL:HG13	1:C:568:ASN:CG	2.43	0.44
1:D:374:GLY:HA3	1:D:375:LEU:HA	1.74	0.44
1:E:479:LEU:HB3	1:E:482:THR:OG1	2.17	0.44
1:E:503:ILE:HG21	1:E:515:TYR:CD2	2.53	0.44
1:E:504:ILE:HG22	1:E:505:PRO:HD2	2.00	0.44
1:F:265:ILE:HD12	1:F:273:PRO:HG3	1.99	0.44
1:G:23:VAL:HG21	1:G:32:PHE:CB	2.36	0.44
1:G:399:ALA:HB2	1:G:584:ILE:HB	1.98	0.44
1:H:657:PHE:CD2	1:H:663:LEU:HD12	2.53	0.44
1:I:145:ASP:HB3	1:I:148:GLN:HG3	1.99	0.44
1:B:43:ARG:CG	1:B:365:THR:HG23	2.48	0.44
1:B:145:ASP:HB3	1:B:148:GLN:HG3	2.00	0.44
1:D:446:LEU:O	1:D:450:MET:HG2	2.18	0.44
1:E:657:PHE:CD2	1:E:663:LEU:HD12	2.53	0.44
1:F:260:ALA:O	1:F:264:GLU:HG2	2.17	0.44
1:F:408:TYR:HB3	1:F:425:ILE:CG2	2.47	0.44
1:F:657:PHE:CD2	1:F:663:LEU:HD12	2.53	0.44
1:G:479:LEU:HB3	1:G:482:THR:OG1	2.17	0.44
1:H:54:LEU:CD2	1:H:375:LEU:HD23	2.46	0.44
1:H:571:VAL:HA	1:H:572:ALA:HA	1.80	0.44
1:I:260:ALA:O	1:I:264:GLU:HG2	2.18	0.44
1:I:265:ILE:HD12	1:I:273:PRO:HG3	2.00	0.44
1:I:270:VAL:HG22	1:I:321:ASN:HD21	1.81	0.44
1:I:479:LEU:HB3	1:I:482:THR:OG1	2.17	0.44
1:J:402:ILE:O	1:J:434:LEU:HD12	2.17	0.44
1:J:479:LEU:HB3	1:J:482:THR:OG1	2.17	0.44
1:A:114:PRO:HA	1:A:228:THR:HG21	1.99	0.44
1:A:374:GLY:HA3	1:A:375:LEU:HA	1.73	0.44
1:B:446:LEU:O	1:B:450:MET:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:LEU:N	1:B:716:ALA:HB3	2.32	0.44
1:C:38:THR:HA	1:C:367:ALA:O	2.18	0.44
1:C:446:LEU:O	1:C:450:MET:HG2	2.18	0.44
1:E:642:LYS:HG3	1:E:778:TYR:OH	2.17	0.44
1:F:504:ILE:HG22	1:F:505:PRO:HD2	2.00	0.44
1:H:504:ILE:HG22	1:H:505:PRO:HD2	2.00	0.44
1:H:563:THR:HG21	1:H:568:ASN:HB2	1.99	0.44
1:J:190:LEU:O	1:J:190:LEU:HD13	2.18	0.44
1:J:260:ALA:O	1:J:264:GLU:HG2	2.17	0.44
1:A:38:THR:HA	1:A:367:ALA:O	2.18	0.44
1:A:642:LYS:HG3	1:A:778:TYR:OH	2.18	0.44
1:B:503:ILE:HG21	1:B:515:TYR:CD2	2.53	0.44
1:B:726:ILE:HA	1:B:727:ALA:HA	1.82	0.44
1:D:643:GLY:HA3	1:D:644:GLY:HA2	1.84	0.44
1:F:410:SER:HB3	1:F:664:ALA:HB2	1.99	0.44
1:F:446:LEU:O	1:F:450:MET:HG2	2.18	0.44
1:G:232:ARG:O	1:G:236:GLN:HG3	2.18	0.44
1:G:642:LYS:HG3	1:G:778:TYR:OH	2.17	0.44
1:H:40:ALA:CB	1:H:290:ASN:OD1	2.63	0.44
1:H:260:ALA:O	1:H:264:GLU:HG2	2.17	0.44
1:J:38:THR:HA	1:J:367:ALA:O	2.18	0.44
1:A:446:LEU:O	1:A:450:MET:HG2	2.18	0.43
1:C:479:LEU:HD11	1:C:567:LEU:HD23	1.98	0.43
1:D:121:TRP:CZ3	1:J:226:PRO:HG3	2.53	0.43
1:D:146:GLU:OE2	1:D:604:LYS:NZ	2.39	0.43
1:D:163:ILE:HD13	1:D:212:TYR:CE2	2.53	0.43
1:D:439:GLU:OE2	1:D:489:ASN:ND2	2.51	0.43
1:E:145:ASP:HB3	1:E:148:GLN:HG3	1.99	0.43
1:E:509:SER:OG	1:I:723:ILE:HD11	2.18	0.43
1:F:38:THR:HA	1:F:367:ALA:O	2.18	0.43
1:G:260:ALA:O	1:G:264:GLU:HG2	2.17	0.43
1:G:504:ILE:HG22	1:G:505:PRO:HD2	2.00	0.43
1:H:145:ASP:HB3	1:H:148:GLN:HG3	1.99	0.43
1:H:446:LEU:O	1:H:450:MET:HG2	2.18	0.43
1:I:190:LEU:O	1:I:190:LEU:HD13	2.18	0.43
1:I:715:LEU:N	1:I:716:ALA:HB3	2.33	0.43
1:A:159:PHE:CD2	1:A:241:MET:HE1	2.54	0.43
1:A:190:LEU:O	1:A:190:LEU:HD13	2.18	0.43
1:B:479:LEU:CD1	1:B:567:LEU:HD23	2.47	0.43
1:C:232:ARG:O	1:C:236:GLN:HG3	2.17	0.43
1:D:397:TYR:CE1	1:D:497:LEU:HD21	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:503:ILE:HG21	1:D:515:TYR:CD2	2.53	0.43
1:D:540:SER:HA	1:D:541:ASN:HA	1.75	0.43
1:D:642:LYS:HG3	1:D:778:TYR:OH	2.17	0.43
1:E:114:PRO:HB2	1:I:122:ALA:HB1	2.00	0.43
1:F:563:THR:HG21	1:F:568:ASN:HB2	1.99	0.43
1:G:446:LEU:O	1:G:450:MET:HG2	2.18	0.43
1:G:503:ILE:HG21	1:G:515:TYR:CD2	2.53	0.43
1:G:657:PHE:CD2	1:G:663:LEU:HD12	2.52	0.43
1:I:642:LYS:HG3	1:I:778:TYR:OH	2.18	0.43
1:J:145:ASP:HB3	1:J:148:GLN:HG3	2.00	0.43
1:J:446:LEU:O	1:J:450:MET:HG2	2.18	0.43
1:J:715:LEU:N	1:J:716:ALA:HB3	2.33	0.43
1:C:159:PHE:CD2	1:C:241:MET:HE1	2.53	0.43
1:C:642:LYS:HG3	1:C:778:TYR:OH	2.18	0.43
1:D:232:ARG:O	1:D:236:GLN:HG3	2.18	0.43
1:D:270:VAL:HG22	1:D:321:ASN:HD21	1.81	0.43
1:D:479:LEU:HB3	1:D:482:THR:OG1	2.17	0.43
1:D:657:PHE:CD2	1:D:663:LEU:HD12	2.53	0.43
1:E:260:ALA:O	1:E:264:GLU:HG2	2.17	0.43
1:H:163:ILE:HD13	1:H:212:TYR:CE2	2.54	0.43
1:H:265:ILE:HD12	1:H:273:PRO:HG3	2.00	0.43
1:I:514:LEU:HD23	1:I:514:LEU:HA	1.91	0.43
1:A:270:VAL:HG22	1:A:321:ASN:HD21	1.81	0.43
1:A:304:GLN:OE1	1:J:429:ARG:NE	2.46	0.43
1:A:397:TYR:CE1	1:A:497:LEU:HD21	2.53	0.43
1:A:504:ILE:HG22	1:A:505:PRO:HD2	2.00	0.43
1:B:190:LEU:HD13	1:B:190:LEU:O	2.18	0.43
1:C:270:VAL:HG22	1:C:321:ASN:HD21	1.81	0.43
1:C:397:TYR:CE1	1:C:497:LEU:HD21	2.53	0.43
1:E:23:VAL:HG21	1:E:32:PHE:CB	2.36	0.43
1:E:159:PHE:CD2	1:E:241:MET:HE1	2.53	0.43
1:E:715:LEU:N	1:E:716:ALA:HB3	2.33	0.43
1:F:159:PHE:CD2	1:F:241:MET:HE1	2.53	0.43
1:H:190:LEU:O	1:H:190:LEU:HD13	2.18	0.43
1:I:163:ILE:HD13	1:I:212:TYR:CE2	2.54	0.43
1:I:446:LEU:O	1:I:450:MET:HG2	2.18	0.43
1:J:232:ARG:O	1:J:236:GLN:HG3	2.18	0.43
1:J:550:VAL:HG13	1:J:568:ASN:CG	2.42	0.43
1:A:503:ILE:HG21	1:A:515:TYR:CD2	2.53	0.43
1:A:657:PHE:CD2	1:A:663:LEU:HD12	2.53	0.43
1:B:504:ILE:HG22	1:B:505:PRO:HD2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:550:VAL:HG13	1:B:568:ASN:CG	2.44	0.43
1:E:109:GLY:HA3	1:F:113:ARG:CD	2.48	0.43
1:E:374:GLY:HA3	1:E:375:LEU:HA	1.73	0.43
1:F:503:ILE:HG21	1:F:515:TYR:CD2	2.54	0.43
1:F:642:LYS:HG3	1:F:778:TYR:OH	2.18	0.43
1:F:715:LEU:N	1:F:716:ALA:HB3	2.33	0.43
1:G:38:THR:HA	1:G:367:ALA:O	2.18	0.43
1:I:356:ALA:O	1:I:360:VAL:HG23	2.19	0.43
1:I:504:ILE:HG22	1:I:505:PRO:HD2	2.00	0.43
1:J:356:ALA:O	1:J:360:VAL:HG23	2.19	0.43
1:B:159:PHE:CD2	1:B:241:MET:HE1	2.54	0.43
1:B:265:ILE:HD12	1:B:273:PRO:HG3	2.00	0.43
1:B:642:LYS:HG3	1:B:778:TYR:OH	2.18	0.43
1:C:272:ALA:N	1:C:273:PRO:HD3	2.34	0.43
1:C:715:LEU:N	1:C:716:ALA:HB3	2.33	0.43
1:C:726:ILE:HA	1:C:727:ALA:HA	1.83	0.43
1:E:434:LEU:O	1:E:711:THR:HG21	2.18	0.43
1:E:571:VAL:HA	1:E:572:ALA:HA	1.80	0.43
1:F:23:VAL:HG21	1:F:32:PHE:CB	2.36	0.43
1:G:190:LEU:O	1:G:190:LEU:HD13	2.18	0.43
1:G:356:ALA:O	1:G:360:VAL:HG23	2.19	0.43
1:G:434:LEU:O	1:G:711:THR:HG21	2.19	0.43
1:I:657:PHE:CD2	1:I:663:LEU:HD12	2.54	0.43
1:J:503:ILE:HG21	1:J:515:TYR:CG	2.54	0.43
1:A:439:GLU:OE2	1:A:489:ASN:ND2	2.52	0.43
1:A:446:LEU:CD2	1:A:487:VAL:HG11	2.49	0.43
1:B:504:ILE:CG1	1:B:510:VAL:HG21	2.43	0.43
1:B:729:GLN:O	1:B:730:PRO:C	2.62	0.43
1:C:356:ALA:O	1:C:360:VAL:HG23	2.19	0.43
1:D:145:ASP:HB3	1:D:148:GLN:HG3	2.00	0.43
1:D:434:LEU:O	1:D:711:THR:HG21	2.19	0.43
1:E:190:LEU:HD13	1:E:190:LEU:O	2.18	0.43
1:E:550:VAL:HG13	1:E:568:ASN:CG	2.44	0.43
1:F:434:LEU:O	1:F:711:THR:HG21	2.19	0.43
1:G:145:ASP:HB3	1:G:148:GLN:HG3	1.99	0.43
1:G:715:LEU:N	1:G:716:ALA:HB3	2.33	0.43
1:H:38:THR:HA	1:H:367:ALA:O	2.18	0.43
1:H:114:PRO:HA	1:H:228:THR:HG21	1.99	0.43
1:H:350:THR:N	1:H:351:PRO:CD	2.82	0.43
1:J:504:ILE:HG22	1:J:505:PRO:HD2	2.00	0.43
1:A:43:ARG:CG	1:A:365:THR:HG23	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:ILE:HD12	1:A:273:PRO:HG3	2.00	0.43
1:A:721:ASP:HA	1:A:722:GLU:HA	1.57	0.43
1:B:374:GLY:HA2	1:B:376:GLY:H	1.84	0.43
1:B:545:ARG:HB2	1:B:572:ALA:CB	2.45	0.43
1:E:249:ASN:HD22	1:I:426:MET:HE2	1.84	0.43
1:E:356:ALA:O	1:E:360:VAL:HG23	2.19	0.43
1:E:425:ILE:HD12	1:E:593:LEU:HD22	2.01	0.43
1:E:439:GLU:OE2	1:E:489:ASN:ND2	2.52	0.43
1:E:446:LEU:O	1:E:450:MET:HG2	2.18	0.43
1:F:356:ALA:O	1:F:360:VAL:HG23	2.19	0.43
1:F:550:VAL:HG13	1:F:568:ASN:CG	2.44	0.43
1:F:643:GLY:HA3	1:F:644:GLY:HA2	1.84	0.43
1:I:446:LEU:CD2	1:I:487:VAL:HG11	2.49	0.43
1:J:439:GLU:OE2	1:J:489:ASN:ND2	2.52	0.43
1:A:272:ALA:N	1:A:273:PRO:HD3	2.34	0.43
1:A:402:ILE:HD12	1:A:668:VAL:CG1	2.49	0.43
1:B:122:ALA:HB1	1:C:114:PRO:HB2	2.00	0.43
1:B:272:ALA:N	1:B:273:PRO:HD3	2.33	0.43
1:B:354:ARG:HH12	1:B:358:THR:HG22	1.80	0.43
1:C:425:ILE:HD12	1:C:593:LEU:HD22	2.01	0.43
1:D:120:SER:HB3	1:D:222:ASP:HA	2.01	0.43
1:E:77:ILE:O	1:E:81:ILE:HG13	2.19	0.43
1:E:402:ILE:HD12	1:E:668:VAL:CG1	2.49	0.43
1:F:777:PHE:HA	1:F:780:ILE:HD12	2.01	0.43
1:H:721:ASP:HA	1:H:722:GLU:HA	1.57	0.43
1:I:425:ILE:HD12	1:I:593:LEU:HD22	2.01	0.43
1:J:43:ARG:CG	1:J:365:THR:HG23	2.49	0.43
1:J:503:ILE:HG21	1:J:515:TYR:CD2	2.53	0.43
1:A:356:ALA:O	1:A:360:VAL:HG23	2.19	0.43
1:B:356:ALA:O	1:B:360:VAL:HG23	2.19	0.43
1:C:657:PHE:CD2	1:C:663:LEU:HD12	2.53	0.43
1:D:159:PHE:CD2	1:D:241:MET:HE1	2.53	0.43
1:E:43:ARG:CG	1:E:365:THR:HG23	2.48	0.43
1:E:51:SER:HB2	1:E:57:ARG:H	1.84	0.43
1:F:77:ILE:O	1:F:81:ILE:HG13	2.19	0.43
1:G:77:ILE:O	1:G:81:ILE:HG13	2.19	0.43
1:G:571:VAL:HA	1:G:572:ALA:HA	1.81	0.43
1:H:43:ARG:CG	1:H:365:THR:HG23	2.49	0.43
1:H:374:GLY:HA3	1:H:375:LEU:HA	1.73	0.43
1:H:434:LEU:O	1:H:711:THR:HG21	2.19	0.43
1:I:51:SER:HB2	1:I:57:ARG:H	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:163:ILE:HD13	1:J:212:TYR:CE2	2.54	0.43
1:A:77:ILE:O	1:A:81:ILE:HG13	2.19	0.42
1:A:350:THR:N	1:A:351:PRO:CD	2.82	0.42
1:B:503:ILE:HG21	1:B:515:TYR:CG	2.54	0.42
1:C:77:ILE:O	1:C:81:ILE:HG13	2.19	0.42
1:C:503:ILE:HG21	1:C:515:TYR:CD2	2.54	0.42
1:D:504:ILE:HG22	1:D:505:PRO:HD2	2.00	0.42
1:E:446:LEU:CD2	1:E:487:VAL:HG11	2.49	0.42
1:F:43:ARG:CG	1:F:365:THR:HG23	2.49	0.42
1:F:726:ILE:HA	1:F:727:ALA:HA	1.83	0.42
1:G:51:SER:HB2	1:G:57:ARG:H	1.84	0.42
1:G:729:GLN:O	1:G:730:PRO:C	2.62	0.42
1:H:261:VAL:HG13	1:H:316:TRP:HH2	1.85	0.42
1:A:434:LEU:O	1:A:711:THR:HG21	2.19	0.42
1:D:190:LEU:O	1:D:190:LEU:HD13	2.18	0.42
1:E:642:LYS:HZ2	1:E:733:VAL:HG21	1.84	0.42
1:F:446:LEU:CD2	1:F:487:VAL:HG11	2.49	0.42
1:G:159:PHE:CD2	1:G:241:MET:HE1	2.54	0.42
1:G:261:VAL:HG13	1:G:316:TRP:HH2	1.84	0.42
1:G:439:GLU:OE2	1:G:489:ASN:ND2	2.51	0.42
1:H:503:ILE:HG21	1:H:515:TYR:CG	2.54	0.42
1:I:434:LEU:O	1:I:711:THR:HG21	2.19	0.42
1:I:503:ILE:HG21	1:I:515:TYR:CD2	2.54	0.42
1:J:146:GLU:CD	1:J:604:LYS:HZ1	2.25	0.42
1:J:261:VAL:HG13	1:J:316:TRP:HH2	1.84	0.42
1:B:232:ARG:O	1:B:236:GLN:HG3	2.18	0.42
1:B:439:GLU:OE2	1:B:489:ASN:ND2	2.52	0.42
1:D:261:VAL:HG13	1:D:316:TRP:HH2	1.84	0.42
1:D:402:ILE:HD12	1:D:668:VAL:CG1	2.49	0.42
1:F:84:TYR:O	1:F:85:ASP:C	2.62	0.42
1:F:273:PRO:CB	1:F:276:TYR:CD2	2.96	0.42
1:F:729:GLN:O	1:F:730:PRO:C	2.62	0.42
1:G:163:ILE:HD13	1:G:212:TYR:CE2	2.53	0.42
1:H:68:ARG:HG3	1:H:165:ALA:CB	2.49	0.42
1:H:402:ILE:HD12	1:H:668:VAL:CG1	2.49	0.42
1:I:43:ARG:CG	1:I:365:THR:HG23	2.49	0.42
1:I:77:ILE:O	1:I:81:ILE:HG13	2.19	0.42
1:J:272:ALA:N	1:J:273:PRO:HD3	2.33	0.42
1:J:425:ILE:HD12	1:J:593:LEU:HD22	2.01	0.42
1:A:374:GLY:HA2	1:A:376:GLY:H	1.84	0.42
1:B:350:THR:N	1:B:351:PRO:CD	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:LEU:CD2	1:B:487:VAL:HG11	2.50	0.42
1:C:265:ILE:HD12	1:C:273:PRO:HG3	2.00	0.42
1:C:439:GLU:OE2	1:C:489:ASN:ND2	2.52	0.42
1:D:503:ILE:HG21	1:D:515:TYR:CG	2.54	0.42
1:E:38:THR:HA	1:E:367:ALA:O	2.18	0.42
1:G:350:THR:N	1:G:351:PRO:CD	2.82	0.42
1:G:418:VAL:HA	1:H:141:ASN:HD21	1.84	0.42
1:G:446:LEU:CD2	1:G:487:VAL:HG11	2.49	0.42
1:G:547:THR:HG23	1:G:550:VAL:HG23	2.02	0.42
1:G:643:GLY:HA3	1:G:644:GLY:HA2	1.84	0.42
1:J:657:PHE:CD2	1:J:663:LEU:HD12	2.54	0.42
1:A:40:ALA:CB	1:A:290:ASN:OD1	2.63	0.42
1:A:261:VAL:HG13	1:A:316:TRP:HH2	1.84	0.42
1:B:77:ILE:O	1:B:81:ILE:HG13	2.19	0.42
1:C:446:LEU:CD2	1:C:487:VAL:HG11	2.49	0.42
1:C:504:ILE:HG22	1:C:505:PRO:HD2	2.00	0.42
1:D:77:ILE:O	1:D:81:ILE:HG13	2.19	0.42
1:E:163:ILE:HD13	1:E:212:TYR:CE2	2.54	0.42
1:E:729:GLN:O	1:E:730:PRO:C	2.62	0.42
1:F:68:ARG:HG3	1:F:165:ALA:CB	2.50	0.42
1:F:190:LEU:O	1:F:190:LEU:HD13	2.18	0.42
1:H:101:ARG:HA	1:H:231:SER:HB3	2.02	0.42
1:H:273:PRO:CB	1:H:276:TYR:CD2	2.96	0.42
1:H:374:GLY:HA2	1:H:376:GLY:H	1.84	0.42
1:I:350:THR:N	1:I:351:PRO:CD	2.82	0.42
1:I:402:ILE:HD12	1:I:668:VAL:CG1	2.49	0.42
1:I:540:SER:HA	1:I:541:ASN:HA	1.74	0.42
1:A:141:ASN:HD21	1:J:418:VAL:HA	1.84	0.42
1:A:163:ILE:HD13	1:A:212:TYR:CE2	2.54	0.42
1:A:273:PRO:CB	1:A:276:TYR:CD2	2.96	0.42
1:A:547:THR:HG23	1:A:550:VAL:HG23	2.02	0.42
1:B:51:SER:HB2	1:B:57:ARG:H	1.85	0.42
1:B:425:ILE:HD12	1:B:593:LEU:HD22	2.01	0.42
1:B:434:LEU:O	1:B:711:THR:HG21	2.19	0.42
1:C:82:ILE:N	1:C:82:ILE:HD12	2.34	0.42
1:C:190:LEU:O	1:C:190:LEU:HD13	2.18	0.42
1:C:434:LEU:O	1:C:711:THR:HG21	2.19	0.42
1:D:68:ARG:HG3	1:D:165:ALA:CB	2.50	0.42
1:D:374:GLY:HA2	1:D:376:GLY:H	1.85	0.42
1:D:446:LEU:CD2	1:D:487:VAL:HG11	2.49	0.42
1:E:265:ILE:HD12	1:E:273:PRO:HG3	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:291:PHE:CE1	1:E:295:THR:HG21	2.54	0.42
1:E:374:GLY:HA2	1:E:376:GLY:H	1.84	0.42
1:E:503:ILE:HG21	1:E:515:TYR:CG	2.54	0.42
1:E:721:ASP:HA	1:E:722:GLU:HA	1.56	0.42
1:F:503:ILE:HG21	1:F:515:TYR:CG	2.55	0.42
1:G:84:TYR:O	1:G:85:ASP:C	2.63	0.42
1:G:123:GLU:CD	1:H:229:ARG:HH12	2.28	0.42
1:G:503:ILE:HG21	1:G:515:TYR:CG	2.54	0.42
1:H:82:ILE:N	1:H:82:ILE:HD12	2.35	0.42
1:J:77:ILE:O	1:J:81:ILE:HG13	2.19	0.42
1:A:68:ARG:HG3	1:A:165:ALA:CB	2.50	0.42
1:A:729:GLN:O	1:A:730:PRO:C	2.62	0.42
1:B:163:ILE:HD13	1:B:212:TYR:CE2	2.54	0.42
1:B:261:VAL:HG13	1:B:316:TRP:HH2	1.85	0.42
1:B:402:ILE:HD12	1:B:668:VAL:CG1	2.49	0.42
1:B:777:PHE:HA	1:B:780:ILE:HD12	2.02	0.42
1:C:374:GLY:HA2	1:C:376:GLY:H	1.85	0.42
1:D:291:PHE:CE1	1:D:295:THR:HG21	2.55	0.42
1:D:356:ALA:O	1:D:360:VAL:HG23	2.19	0.42
1:D:777:PHE:HA	1:D:780:ILE:HD12	2.02	0.42
1:F:82:ILE:N	1:F:82:ILE:HD12	2.35	0.42
1:F:163:ILE:HD13	1:F:212:TYR:CE2	2.54	0.42
1:G:291:PHE:CE1	1:G:295:THR:HG21	2.55	0.42
1:H:159:PHE:CD2	1:H:241:MET:HE1	2.55	0.42
1:H:446:LEU:CD2	1:H:487:VAL:HG11	2.50	0.42
1:I:23:VAL:HG21	1:I:32:PHE:CB	2.36	0.42
1:I:101:ARG:HA	1:I:231:SER:HB3	2.01	0.42
1:I:192:PRO:HB2	1:I:364:VAL:HG22	2.02	0.42
1:J:84:TYR:O	1:J:85:ASP:C	2.63	0.42
1:J:374:GLY:HA2	1:J:376:GLY:H	1.85	0.42
1:J:643:GLY:HA3	1:J:644:GLY:HA2	1.84	0.42
1:A:51:SER:HB2	1:A:57:ARG:H	1.84	0.42
1:B:68:ARG:HG3	1:B:165:ALA:CB	2.50	0.42
1:B:270:VAL:HG22	1:B:321:ASN:HD21	1.81	0.42
1:B:460:GLU:HG2	1:F:775:ASN:ND2	2.35	0.42
1:B:622:ARG:O	1:B:626:VAL:HG23	2.20	0.42
1:C:68:ARG:HG3	1:C:165:ALA:CB	2.50	0.42
1:C:402:ILE:HD12	1:C:668:VAL:CG1	2.50	0.42
1:E:101:ARG:HA	1:E:231:SER:HB3	2.01	0.42
1:F:622:ARG:O	1:F:626:VAL:HG23	2.20	0.42
1:G:374:GLY:HA2	1:G:376:GLY:H	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:777:PHE:HA	1:G:780:ILE:HD12	2.02	0.42
1:H:480:PRO:HD2	1:H:567:LEU:HD22	2.02	0.42
1:H:622:ARG:O	1:H:626:VAL:HG23	2.20	0.42
1:I:84:TYR:O	1:I:85:ASP:C	2.62	0.42
1:I:439:GLU:OE2	1:I:489:ASN:ND2	2.52	0.42
1:J:434:LEU:O	1:J:711:THR:HG21	2.19	0.42
1:J:493:MET:HG3	1:J:493:MET:O	2.20	0.42
1:B:123:GLU:OE2	1:C:229:ARG:NH2	2.52	0.42
1:B:408:TYR:CB	1:B:425:ILE:CG2	2.98	0.42
1:B:408:TYR:CB	1:B:425:ILE:HG23	2.50	0.42
1:C:503:ILE:HG21	1:C:515:TYR:CG	2.54	0.42
1:E:59:TYR:CE2	1:E:591:PRO:HD3	2.55	0.42
1:E:540:SER:HA	1:E:541:ASN:HA	1.74	0.42
1:F:291:PHE:CE1	1:F:295:THR:HG21	2.54	0.42
1:F:439:GLU:OE2	1:F:489:ASN:ND2	2.53	0.42
1:F:493:MET:HG3	1:F:493:MET:O	2.20	0.42
1:G:540:SER:HA	1:G:541:ASN:HA	1.75	0.42
1:H:356:ALA:O	1:H:360:VAL:HG23	2.19	0.42
1:H:439:GLU:OE2	1:H:489:ASN:ND2	2.52	0.42
1:I:291:PHE:CE1	1:I:295:THR:HG21	2.55	0.42
1:J:159:PHE:CD2	1:J:241:MET:HE1	2.55	0.42
1:A:503:ILE:HG21	1:A:515:TYR:CG	2.54	0.42
1:A:540:SER:HA	1:A:541:ASN:HA	1.75	0.42
1:C:43:ARG:CG	1:C:365:THR:HG23	2.49	0.42
1:C:504:ILE:CG1	1:C:510:VAL:HG21	2.43	0.42
1:D:408:TYR:CB	1:D:425:ILE:CG2	2.98	0.42
1:D:638:TYR:CE1	1:D:647:VAL:HG11	2.55	0.42
1:E:374:GLY:CA	1:E:376:GLY:H	2.33	0.42
1:F:101:ARG:HA	1:F:231:SER:HB3	2.02	0.42
1:F:261:VAL:HG13	1:F:316:TRP:HH2	1.84	0.42
1:F:350:THR:N	1:F:351:PRO:CD	2.82	0.42
1:G:622:ARG:O	1:G:626:VAL:HG23	2.20	0.42
1:I:503:ILE:HG21	1:I:515:TYR:CG	2.55	0.42
1:B:374:GLY:CA	1:B:376:GLY:H	2.33	0.41
1:C:163:ILE:HD13	1:C:212:TYR:CE2	2.55	0.41
1:C:374:GLY:HA3	1:C:375:LEU:HA	1.74	0.41
1:D:108:MET:HA	1:J:114:PRO:HG2	2.02	0.41
1:D:123:GLU:CD	1:J:229:ARG:NH1	2.71	0.41
1:E:777:PHE:HA	1:E:780:ILE:HD12	2.02	0.41
1:G:43:ARG:CG	1:G:365:THR:HG23	2.50	0.41
1:G:411:PHE:CE2	1:H:88:THR:HG21	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:408:TYR:CB	1:I:425:ILE:HG23	2.50	0.41
1:J:68:ARG:HG3	1:J:165:ALA:CB	2.50	0.41
1:J:101:ARG:HA	1:J:231:SER:HB3	2.01	0.41
1:J:192:PRO:HB2	1:J:364:VAL:HG22	2.02	0.41
1:A:425:ILE:HD12	1:A:593:LEU:HD22	2.02	0.41
1:A:638:TYR:CE1	1:A:647:VAL:HG11	2.55	0.41
1:A:777:PHE:HA	1:A:780:ILE:HD12	2.02	0.41
1:C:40:ALA:CB	1:C:290:ASN:OD1	2.64	0.41
1:C:192:PRO:HB2	1:C:364:VAL:HG22	2.02	0.41
1:C:622:ARG:O	1:C:626:VAL:HG23	2.20	0.41
1:D:43:ARG:CG	1:D:365:THR:HG23	2.49	0.41
1:E:171:LYS:HB3	1:F:232:ARG:NH2	2.35	0.41
1:E:273:PRO:CB	1:E:276:TYR:CD2	2.98	0.41
1:E:350:THR:N	1:E:351:PRO:CD	2.82	0.41
1:G:402:ILE:HD12	1:G:668:VAL:CG1	2.50	0.41
1:G:418:VAL:HG12	1:H:141:ASN:ND2	2.30	0.41
1:H:51:SER:HB2	1:H:57:ARG:H	1.85	0.41
1:H:77:ILE:O	1:H:81:ILE:HG13	2.19	0.41
1:H:192:PRO:HB2	1:H:364:VAL:HG22	2.01	0.41
1:H:291:PHE:CE1	1:H:295:THR:HG21	2.54	0.41
1:H:642:LYS:HZ2	1:H:733:VAL:HG21	1.85	0.41
1:I:82:ILE:N	1:I:82:ILE:HD12	2.35	0.41
1:A:426:MET:HE2	1:B:249:ASN:HD22	1.85	0.41
1:C:291:PHE:CE1	1:C:295:THR:HG21	2.55	0.41
1:C:350:THR:N	1:C:351:PRO:CD	2.82	0.41
1:C:408:TYR:CB	1:C:425:ILE:CG2	2.98	0.41
1:D:82:ILE:HD12	1:D:82:ILE:N	2.36	0.41
1:D:192:PRO:HB2	1:D:364:VAL:HG22	2.02	0.41
1:E:82:ILE:HD12	1:E:82:ILE:N	2.35	0.41
1:E:408:TYR:CB	1:E:425:ILE:CG2	2.99	0.41
1:E:493:MET:HG3	1:E:493:MET:O	2.20	0.41
1:F:192:PRO:HB2	1:F:364:VAL:HG22	2.02	0.41
1:G:59:TYR:CE2	1:G:591:PRO:HD3	2.56	0.41
1:G:101:ARG:HA	1:G:231:SER:HB3	2.02	0.41
1:G:425:ILE:HD12	1:G:593:LEU:HD22	2.01	0.41
1:G:579:THR:HB	1:G:580:PRO:HD2	2.02	0.41
1:H:408:TYR:CB	1:H:425:ILE:CG2	2.98	0.41
1:H:729:GLN:O	1:H:730:PRO:C	2.63	0.41
1:I:261:VAL:HG13	1:I:316:TRP:HH2	1.85	0.41
1:I:374:GLY:HA2	1:I:376:GLY:H	1.85	0.41
1:A:192:PRO:HB2	1:A:364:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:MET:HG3	1:A:493:MET:O	2.20	0.41
1:B:190:LEU:CD2	1:B:290:ASN:ND2	2.83	0.41
1:C:171:LYS:O	1:D:232:ARG:NH2	2.51	0.41
1:C:643:GLY:HA3	1:C:644:GLY:HA2	1.84	0.41
1:D:350:THR:N	1:D:351:PRO:CD	2.83	0.41
1:D:425:ILE:O	1:D:596:ARG:HG3	2.21	0.41
1:E:403:ASN:OD1	1:E:403:ASN:O	2.38	0.41
1:E:420:VAL:HG12	1:E:602:VAL:HG13	2.03	0.41
1:E:425:ILE:O	1:E:596:ARG:HG3	2.21	0.41
1:E:622:ARG:O	1:E:626:VAL:HG23	2.20	0.41
1:F:402:ILE:HD12	1:F:668:VAL:CG1	2.49	0.41
1:F:403:ASN:OD1	1:F:403:ASN:O	2.38	0.41
1:F:408:TYR:CB	1:F:425:ILE:HG23	2.51	0.41
1:F:660:ALA:HB1	1:G:85:ASP:CG	2.46	0.41
1:G:403:ASN:OD1	1:G:403:ASN:O	2.38	0.41
1:H:84:TYR:O	1:H:85:ASP:C	2.63	0.41
1:H:638:TYR:CE1	1:H:647:VAL:HG11	2.55	0.41
1:I:408:TYR:CB	1:I:425:ILE:CG2	2.98	0.41
1:I:420:VAL:HG12	1:I:602:VAL:HG13	2.03	0.41
1:I:726:ILE:HA	1:I:727:ALA:HA	1.83	0.41
1:A:101:ARG:HA	1:A:231:SER:HB3	2.02	0.41
1:A:291:PHE:CE1	1:A:295:THR:HG21	2.55	0.41
1:B:59:TYR:CE2	1:B:591:PRO:HD3	2.55	0.41
1:B:291:PHE:CE1	1:B:295:THR:HG21	2.55	0.41
1:B:403:ASN:OD1	1:B:403:ASN:O	2.38	0.41
1:B:420:VAL:HG12	1:B:602:VAL:HG13	2.03	0.41
1:B:579:THR:HB	1:B:580:PRO:HD2	2.02	0.41
1:C:84:TYR:O	1:C:85:ASP:C	2.62	0.41
1:C:408:TYR:CB	1:C:425:ILE:HG23	2.50	0.41
1:C:480:PRO:HD2	1:C:567:LEU:HD22	2.02	0.41
1:C:660:ALA:HB1	1:D:85:ASP:CG	2.45	0.41
1:C:729:GLN:O	1:C:730:PRO:C	2.62	0.41
1:E:272:ALA:N	1:E:273:PRO:HD3	2.33	0.41
1:F:420:VAL:HG12	1:F:602:VAL:HG13	2.03	0.41
1:F:579:THR:HB	1:F:580:PRO:HD2	2.02	0.41
1:G:68:ARG:HG3	1:G:165:ALA:CB	2.50	0.41
1:H:306:TRP:CE3	1:H:306:TRP:HA	2.56	0.41
1:I:777:PHE:HA	1:I:780:ILE:HD12	2.02	0.41
1:J:51:SER:HB2	1:J:57:ARG:H	1.86	0.41
1:J:402:ILE:HD12	1:J:668:VAL:CG1	2.49	0.41
1:J:729:GLN:O	1:J:730:PRO:C	2.62	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:622:ARG:O	1:A:626:VAL:HG23	2.20	0.41
1:B:82:ILE:HD12	1:B:82:ILE:N	2.35	0.41
1:D:59:TYR:CE2	1:D:591:PRO:HD3	2.56	0.41
1:D:101:ARG:HA	1:D:231:SER:HB3	2.02	0.41
1:D:374:GLY:CA	1:D:376:GLY:H	2.34	0.41
1:D:403:ASN:OD1	1:D:403:ASN:O	2.38	0.41
1:D:660:ALA:HB1	1:J:85:ASP:CG	2.46	0.41
1:E:84:TYR:O	1:E:85:ASP:C	2.63	0.41
1:E:261:VAL:HG13	1:E:316:TRP:HH2	1.84	0.41
1:E:627:SER:HB3	1:E:726:ILE:CD1	2.51	0.41
1:F:425:ILE:HD12	1:F:593:LEU:HD22	2.01	0.41
1:F:627:SER:HB3	1:F:726:ILE:CD1	2.51	0.41
1:G:374:GLY:CA	1:G:376:GLY:H	2.34	0.41
1:G:408:TYR:CB	1:G:425:ILE:CG2	2.98	0.41
1:H:120:SER:HB3	1:H:222:ASP:HA	2.02	0.41
1:H:146:GLU:CD	1:H:604:LYS:HZ1	2.25	0.41
1:H:425:ILE:O	1:H:596:ARG:HG3	2.21	0.41
1:I:59:TYR:CE2	1:I:591:PRO:HD3	2.56	0.41
1:I:622:ARG:O	1:I:626:VAL:HG23	2.20	0.41
1:J:82:ILE:HD12	1:J:82:ILE:N	2.35	0.41
1:J:350:THR:N	1:J:351:PRO:CD	2.83	0.41
1:A:579:THR:HB	1:A:580:PRO:HD2	2.02	0.41
1:B:101:ARG:HA	1:B:231:SER:HB3	2.01	0.41
1:B:638:TYR:CE1	1:B:647:VAL:HG11	2.56	0.41
1:C:374:GLY:CA	1:C:376:GLY:H	2.34	0.41
1:C:579:THR:HB	1:C:580:PRO:HD2	2.02	0.41
1:D:272:ALA:N	1:D:273:PRO:HD3	2.34	0.41
1:D:547:THR:HG23	1:D:550:VAL:HG23	2.02	0.41
1:D:627:SER:HB3	1:D:726:ILE:CD1	2.51	0.41
1:F:408:TYR:CB	1:F:425:ILE:CG2	2.98	0.41
1:F:425:ILE:O	1:F:596:ARG:HG3	2.21	0.41
1:F:547:THR:HG23	1:F:550:VAL:HG23	2.02	0.41
1:G:514:LEU:HD23	1:G:514:LEU:HA	1.91	0.41
1:H:40:ALA:CB	1:H:192:PRO:HG3	2.51	0.41
1:H:59:TYR:CE2	1:H:591:PRO:HD3	2.55	0.41
1:H:408:TYR:CB	1:H:425:ILE:HG23	2.50	0.41
1:H:547:THR:CG2	1:H:550:VAL:HG23	2.51	0.41
1:I:493:MET:HG3	1:I:493:MET:O	2.20	0.41
1:I:579:THR:HB	1:I:580:PRO:HD2	2.03	0.41
1:I:627:SER:HB3	1:I:726:ILE:CD1	2.51	0.41
1:J:59:TYR:CE2	1:J:591:PRO:HD3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:291:PHE:CE1	1:J:295:THR:HG21	2.55	0.41
1:J:408:TYR:CB	1:J:425:ILE:CG2	2.99	0.41
1:J:592:ASP:O	1:J:592:ASP:CG	2.64	0.41
1:J:622:ARG:O	1:J:626:VAL:HG23	2.20	0.41
1:A:59:TYR:CE2	1:A:591:PRO:HD3	2.56	0.41
1:A:82:ILE:HD12	1:A:82:ILE:N	2.36	0.41
1:A:403:ASN:OD1	1:A:403:ASN:O	2.39	0.41
1:B:547:THR:HG23	1:B:550:VAL:HG23	2.02	0.41
1:B:721:ASP:HA	1:B:722:GLU:HA	1.56	0.41
1:C:51:SER:HB2	1:C:57:ARG:H	1.85	0.41
1:C:627:SER:HB3	1:C:726:ILE:CD1	2.51	0.41
1:D:84:TYR:O	1:D:85:ASP:C	2.63	0.41
1:D:408:TYR:CB	1:D:425:ILE:HG23	2.50	0.41
1:D:504:ILE:CG1	1:D:510:VAL:HG21	2.43	0.41
1:E:68:ARG:HG3	1:E:165:ALA:CB	2.50	0.41
1:E:418:VAL:HA	1:F:141:ASN:HD21	1.84	0.41
1:E:638:TYR:CE1	1:E:647:VAL:HG11	2.56	0.41
1:F:547:THR:CG2	1:F:550:VAL:HG23	2.51	0.41
1:G:480:PRO:HB2	1:G:510:VAL:HG22	2.03	0.41
1:G:547:THR:CG2	1:G:550:VAL:HG23	2.51	0.41
1:H:403:ASN:OD1	1:H:403:ASN:O	2.39	0.41
1:H:425:ILE:HD12	1:H:593:LEU:HD22	2.01	0.41
1:H:514:LEU:HD23	1:H:514:LEU:HA	1.91	0.41
1:A:91:CYS:SG	1:A:245:ILE:HD11	2.61	0.41
1:A:306:TRP:HA	1:A:306:TRP:CE3	2.56	0.41
1:A:374:GLY:CA	1:A:376:GLY:H	2.34	0.41
1:A:414:PRO:HG3	1:B:93:PHE:HD1	1.86	0.41
1:B:40:ALA:CB	1:B:192:PRO:HG3	2.51	0.41
1:B:480:PRO:HD2	1:B:567:LEU:HD22	2.03	0.41
1:B:493:MET:HG3	1:B:493:MET:O	2.20	0.41
1:B:643:GLY:HA3	1:B:644:GLY:HA2	1.84	0.41
1:C:101:ARG:HA	1:C:231:SER:HB3	2.01	0.41
1:C:261:VAL:HG13	1:C:316:TRP:HH2	1.85	0.41
1:C:596:ARG:HB2	1:C:601:TYR:HE1	1.86	0.41
1:C:777:PHE:HA	1:C:780:ILE:HD12	2.02	0.41
1:D:51:SER:HB2	1:D:57:ARG:H	1.84	0.41
1:D:273:PRO:CB	1:D:276:TYR:CD2	2.96	0.41
1:D:547:THR:CG2	1:D:550:VAL:HG23	2.51	0.41
1:D:596:ARG:HB2	1:D:601:TYR:HE1	1.85	0.41
1:D:622:ARG:O	1:D:626:VAL:HG23	2.20	0.41
1:F:91:CYS:SG	1:F:245:ILE:HD11	2.61	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:480:PRO:HD2	1:F:567:LEU:HD22	2.02	0.41
1:F:596:ARG:HB2	1:F:601:TYR:HE1	1.86	0.41
1:F:638:TYR:CE1	1:F:647:VAL:HG11	2.56	0.41
1:G:82:ILE:HD12	1:G:82:ILE:N	2.35	0.41
1:G:159:PHE:CD1	1:G:159:PHE:C	2.99	0.41
1:G:408:TYR:CB	1:G:425:ILE:HG23	2.50	0.41
1:G:464:ARG:HD3	1:G:469:GLU:OE2	2.21	0.41
1:G:627:SER:HB3	1:G:726:ILE:CD1	2.51	0.41
1:H:270:VAL:HG22	1:H:321:ASN:HD21	1.81	0.41
1:H:414:PRO:HG3	1:I:93:PHE:HD1	1.86	0.41
1:H:464:ARG:HD3	1:H:469:GLU:OE2	2.21	0.41
1:H:493:MET:HG3	1:H:493:MET:O	2.20	0.41
1:H:777:PHE:HA	1:H:780:ILE:HD12	2.03	0.41
1:I:638:TYR:CE1	1:I:647:VAL:HG11	2.56	0.41
1:J:403:ASN:OD1	1:J:403:ASN:O	2.38	0.41
1:J:446:LEU:CD2	1:J:487:VAL:HG11	2.50	0.41
1:J:480:PRO:HB2	1:J:510:VAL:HG22	2.03	0.41
1:J:504:ILE:CG1	1:J:510:VAL:HG21	2.43	0.41
1:J:514:LEU:HD23	1:J:514:LEU:HA	1.91	0.41
1:J:547:THR:HG23	1:J:550:VAL:HG23	2.02	0.41
1:J:579:THR:HB	1:J:580:PRO:HD2	2.02	0.41
1:J:627:SER:HB3	1:J:726:ILE:CD1	2.51	0.41
1:J:777:PHE:HA	1:J:780:ILE:HD12	2.02	0.41
1:A:408:TYR:CB	1:A:425:ILE:CG2	2.99	0.41
1:A:514:LEU:HD23	1:A:514:LEU:HA	1.91	0.41
1:B:120:SER:HB3	1:B:222:ASP:HA	2.03	0.41
1:B:627:SER:HB3	1:B:726:ILE:CD1	2.51	0.41
1:C:592:ASP:O	1:C:592:ASP:CG	2.64	0.41
1:D:480:PRO:HB2	1:D:510:VAL:HG22	2.03	0.41
1:G:40:ALA:CB	1:G:192:PRO:HG3	2.51	0.41
1:G:192:PRO:HB2	1:G:364:VAL:HG22	2.02	0.41
1:H:91:CYS:SG	1:H:245:ILE:HD11	2.61	0.41
1:J:374:GLY:CA	1:J:376:GLY:H	2.34	0.41
1:J:547:THR:CG2	1:J:550:VAL:HG23	2.51	0.41
1:A:480:PRO:HD2	1:A:567:LEU:HD22	2.03	0.40
1:A:547:THR:CG2	1:A:550:VAL:HG23	2.51	0.40
1:B:464:ARG:HD3	1:B:469:GLU:OE2	2.22	0.40
1:B:596:ARG:HB2	1:B:601:TYR:HE1	1.86	0.40
1:C:403:ASN:OD1	1:C:403:ASN:O	2.38	0.40
1:C:540:SER:HA	1:C:541:ASN:HA	1.75	0.40
1:C:547:THR:HG23	1:C:550:VAL:HG23	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:408:TYR:CB	1:E:425:ILE:HG23	2.51	0.40
1:E:547:THR:HG23	1:E:550:VAL:HG23	2.02	0.40
1:E:579:THR:HB	1:E:580:PRO:HD2	2.03	0.40
1:F:51:SER:HB2	1:F:57:ARG:H	1.85	0.40
1:F:374:GLY:HA2	1:F:376:GLY:H	1.85	0.40
1:H:272:ALA:N	1:H:273:PRO:HD3	2.34	0.40
1:H:480:PRO:HB2	1:H:510:VAL:HG22	2.03	0.40
1:H:627:SER:HB3	1:H:726:ILE:CD1	2.51	0.40
1:I:68:ARG:HG3	1:I:165:ALA:CB	2.50	0.40
1:I:374:GLY:CA	1:I:376:GLY:H	2.34	0.40
1:I:425:ILE:O	1:I:596:ARG:HG3	2.21	0.40
1:A:108:MET:HA	1:B:114:PRO:CG	2.50	0.40
1:B:651:ILE:HG23	1:B:746:THR:HG22	2.04	0.40
1:D:425:ILE:HD12	1:D:593:LEU:HD22	2.02	0.40
1:D:514:LEU:HD23	1:D:514:LEU:HA	1.91	0.40
1:D:579:THR:HB	1:D:580:PRO:HD2	2.02	0.40
1:E:464:ARG:HD3	1:E:469:GLU:OE2	2.22	0.40
1:E:635:ARG:HE	1:E:637:LEU:HD21	1.86	0.40
1:G:493:MET:HG3	1:G:493:MET:O	2.20	0.40
1:G:651:ILE:HG23	1:G:746:THR:HG22	2.03	0.40
1:I:596:ARG:HB2	1:I:601:TYR:HE1	1.87	0.40
1:I:618:LYS:HB2	1:I:621:ASP:HB3	2.04	0.40
1:I:635:ARG:HE	1:I:637:LEU:HD21	1.86	0.40
1:J:306:TRP:HA	1:J:306:TRP:CE3	2.56	0.40
1:J:464:ARG:HD3	1:J:469:GLU:OE2	2.21	0.40
1:A:408:TYR:CB	1:A:425:ILE:HG23	2.51	0.40
1:A:618:LYS:HB2	1:A:621:ASP:HB3	2.03	0.40
1:B:84:TYR:O	1:B:85:ASP:C	2.63	0.40
1:B:192:PRO:HB2	1:B:364:VAL:HG22	2.03	0.40
1:B:273:PRO:CB	1:B:276:TYR:CD2	2.99	0.40
1:C:306:TRP:HA	1:C:306:TRP:CE3	2.56	0.40
1:E:120:SER:HB3	1:E:222:ASP:HA	2.04	0.40
1:E:480:PRO:HD2	1:E:567:LEU:HD22	2.03	0.40
1:E:592:ASP:O	1:E:592:ASP:CG	2.64	0.40
1:E:618:LYS:HB2	1:E:621:ASP:HB3	2.03	0.40
1:F:59:TYR:CE2	1:F:591:PRO:HD3	2.56	0.40
1:F:618:LYS:HB2	1:F:621:ASP:HB3	2.04	0.40
1:F:651:ILE:HG23	1:F:746:THR:HG22	2.03	0.40
1:H:547:THR:HG23	1:H:550:VAL:HG23	2.02	0.40
1:I:403:ASN:OD1	1:I:403:ASN:O	2.38	0.40
1:I:729:GLN:O	1:I:730:PRO:C	2.62	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:TYR:O	1:A:85:ASP:C	2.63	0.40
1:A:120:SER:HB3	1:A:222:ASP:HA	2.04	0.40
1:B:425:ILE:O	1:B:596:ARG:HG3	2.21	0.40
1:C:425:ILE:O	1:C:596:ARG:HG3	2.21	0.40
1:C:638:TYR:CE1	1:C:647:VAL:HG11	2.56	0.40
1:D:493:MET:HG3	1:D:493:MET:O	2.20	0.40
1:E:547:THR:CG2	1:E:550:VAL:HG23	2.51	0.40
1:G:272:ALA:N	1:G:273:PRO:HD3	2.34	0.40
1:G:306:TRP:CE3	1:G:306:TRP:HA	2.56	0.40
1:G:596:ARG:HB2	1:G:601:TYR:HE1	1.86	0.40
1:H:374:GLY:CA	1:H:376:GLY:H	2.34	0.40
1:H:592:ASP:O	1:H:592:ASP:CG	2.64	0.40
1:J:425:ILE:O	1:J:596:ARG:HG3	2.21	0.40
1:J:638:TYR:CE1	1:J:647:VAL:HG11	2.55	0.40
1:J:641:ARG:NH1	1:J:774:ASP:HA	2.36	0.40
1:A:425:ILE:O	1:A:596:ARG:HG3	2.21	0.40
1:A:627:SER:HB3	1:A:726:ILE:CD1	2.51	0.40
1:A:641:ARG:NH1	1:A:774:ASP:HA	2.36	0.40
1:A:651:ILE:HG23	1:A:746:THR:HG22	2.03	0.40
1:B:23:VAL:HG21	1:B:32:PHE:CB	2.36	0.40
1:B:306:TRP:HA	1:B:306:TRP:CE3	2.57	0.40
1:B:480:PRO:HB2	1:B:510:VAL:HG22	2.03	0.40
1:C:493:MET:HG3	1:C:493:MET:O	2.20	0.40
1:C:641:ARG:NH1	1:C:774:ASP:HA	2.37	0.40
1:D:121:TRP:CE3	1:J:226:PRO:HG3	2.56	0.40
1:E:190:LEU:CD2	1:E:290:ASN:ND2	2.85	0.40
1:E:461:LEU:HD23	1:E:485:LEU:CD2	2.52	0.40
1:F:272:ALA:N	1:F:273:PRO:HD3	2.34	0.40
1:G:638:TYR:CE1	1:G:647:VAL:HG11	2.56	0.40
1:H:579:THR:HB	1:H:580:PRO:HD2	2.03	0.40
1:I:190:LEU:CD2	1:I:290:ASN:ND2	2.84	0.40
1:I:547:THR:HG23	1:I:550:VAL:HG23	2.02	0.40
1:J:91:CYS:SG	1:J:245:ILE:HD11	2.61	0.40
1:J:618:LYS:HB2	1:J:621:ASP:HB3	2.03	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:GLU:OE1	1:H:219:GLU:OE2[6_476]	1.30	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:219:GLU:OE1	1:H:219:GLU:CD[6_476]	1.35	0.85
1:D:219:GLU:OE1	1:H:219:GLU:OE1[6_476]	1.40	0.80
1:D:219:GLU:OE2	1:H:219:GLU:OE1[6_476]	1.40	0.80
1:D:219:GLU:CD	1:H:219:GLU:OE1[6_476]	1.43	0.77
1:D:219:GLU:CD	1:H:219:GLU:CD[6_476]	1.93	0.27

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	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	B	745/792 (94%)	711 (95%)	34 (5%)	0	100	100
1	C	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	D	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	E	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	F	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	G	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	H	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	I	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
1	J	745/792 (94%)	712 (96%)	33 (4%)	0	100	100
All	All	7450/7920 (94%)	7119 (96%)	331 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	622/663 (94%)	600 (96%)	22 (4%)	32	54
1	B	622/663 (94%)	600 (96%)	22 (4%)	32	54
1	C	622/663 (94%)	601 (97%)	21 (3%)	32	55
1	D	622/663 (94%)	599 (96%)	23 (4%)	30	54
1	E	622/663 (94%)	600 (96%)	22 (4%)	32	54
1	F	622/663 (94%)	600 (96%)	22 (4%)	32	54
1	G	622/663 (94%)	600 (96%)	22 (4%)	32	54
1	H	622/663 (94%)	600 (96%)	22 (4%)	32	54
1	I	622/663 (94%)	600 (96%)	22 (4%)	32	54
1	J	622/663 (94%)	601 (97%)	21 (3%)	32	55
All	All	6220/6630 (94%)	6001 (96%)	219 (4%)	32	54

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ILE
1	A	100	MET
1	A	113	ARG
1	A	137	LEU
1	A	189	TYR
1	A	225	VAL
1	A	306	TRP
1	A	372	TYR
1	A	430	LEU
1	A	461	LEU
1	A	483	SER
1	A	582	ILE
1	A	586	ILE
1	A	587	ILE
1	A	602	VAL
1	A	618	LYS
1	A	703	THR
1	A	723	ILE
1	A	724	THR
1	A	733	VAL
1	A	744	VAL
1	A	774	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	77	ILE
1	B	100	MET
1	B	113	ARG
1	B	137	LEU
1	B	189	TYR
1	B	225	VAL
1	B	306	TRP
1	B	372	TYR
1	B	430	LEU
1	B	461	LEU
1	B	483	SER
1	B	582	ILE
1	B	586	ILE
1	B	587	ILE
1	B	602	VAL
1	B	618	LYS
1	B	703	THR
1	B	723	ILE
1	B	724	THR
1	B	733	VAL
1	B	744	VAL
1	B	774	ASP
1	C	77	ILE
1	C	100	MET
1	C	113	ARG
1	C	137	LEU
1	C	189	TYR
1	C	225	VAL
1	C	306	TRP
1	C	372	TYR
1	C	430	LEU
1	C	461	LEU
1	C	582	ILE
1	C	586	ILE
1	C	587	ILE
1	C	602	VAL
1	C	618	LYS
1	C	703	THR
1	C	723	ILE
1	C	724	THR
1	C	733	VAL
1	C	744	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	774	ASP
1	D	77	ILE
1	D	100	MET
1	D	113	ARG
1	D	137	LEU
1	D	189	TYR
1	D	225	VAL
1	D	306	TRP
1	D	372	TYR
1	D	430	LEU
1	D	461	LEU
1	D	483	SER
1	D	484	THR
1	D	582	ILE
1	D	586	ILE
1	D	587	ILE
1	D	602	VAL
1	D	618	LYS
1	D	703	THR
1	D	723	ILE
1	D	724	THR
1	D	733	VAL
1	D	744	VAL
1	D	774	ASP
1	E	77	ILE
1	E	100	MET
1	E	113	ARG
1	E	137	LEU
1	E	189	TYR
1	E	225	VAL
1	E	306	TRP
1	E	372	TYR
1	E	430	LEU
1	E	461	LEU
1	E	483	SER
1	E	582	ILE
1	E	586	ILE
1	E	587	ILE
1	E	602	VAL
1	E	618	LYS
1	E	703	THR
1	E	723	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	724	THR
1	E	733	VAL
1	E	744	VAL
1	E	774	ASP
1	F	77	ILE
1	F	100	MET
1	F	113	ARG
1	F	137	LEU
1	F	189	TYR
1	F	225	VAL
1	F	306	TRP
1	F	372	TYR
1	F	430	LEU
1	F	461	LEU
1	F	483	SER
1	F	582	ILE
1	F	586	ILE
1	F	587	ILE
1	F	602	VAL
1	F	618	LYS
1	F	703	THR
1	F	723	ILE
1	F	724	THR
1	F	733	VAL
1	F	744	VAL
1	F	774	ASP
1	G	77	ILE
1	G	100	MET
1	G	113	ARG
1	G	137	LEU
1	G	189	TYR
1	G	225	VAL
1	G	306	TRP
1	G	372	TYR
1	G	430	LEU
1	G	461	LEU
1	G	484	THR
1	G	582	ILE
1	G	586	ILE
1	G	587	ILE
1	G	602	VAL
1	G	618	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	703	THR
1	G	723	ILE
1	G	724	THR
1	G	733	VAL
1	G	744	VAL
1	G	774	ASP
1	H	77	ILE
1	H	100	MET
1	H	113	ARG
1	H	137	LEU
1	H	189	TYR
1	H	225	VAL
1	H	306	TRP
1	H	372	TYR
1	H	430	LEU
1	H	461	LEU
1	H	483	SER
1	H	582	ILE
1	H	586	ILE
1	H	587	ILE
1	H	602	VAL
1	H	618	LYS
1	H	703	THR
1	H	723	ILE
1	H	724	THR
1	H	733	VAL
1	H	744	VAL
1	H	774	ASP
1	I	77	ILE
1	I	100	MET
1	I	113	ARG
1	I	137	LEU
1	I	189	TYR
1	I	225	VAL
1	I	306	TRP
1	I	372	TYR
1	I	430	LEU
1	I	461	LEU
1	I	484	THR
1	I	582	ILE
1	I	586	ILE
1	I	587	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	602	VAL
1	I	618	LYS
1	I	703	THR
1	I	723	ILE
1	I	724	THR
1	I	733	VAL
1	I	744	VAL
1	I	774	ASP
1	J	77	ILE
1	J	100	MET
1	J	113	ARG
1	J	137	LEU
1	J	189	TYR
1	J	225	VAL
1	J	306	TRP
1	J	372	TYR
1	J	430	LEU
1	J	461	LEU
1	J	582	ILE
1	J	586	ILE
1	J	587	ILE
1	J	602	VAL
1	J	618	LYS
1	J	703	THR
1	J	723	ILE
1	J	724	THR
1	J	733	VAL
1	J	744	VAL
1	J	774	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	130	ASN
1	A	141	ASN
1	A	148	GLN
1	A	169	HIS
1	A	239	ASN
1	A	409	GLN
1	A	489	ASN
1	A	541	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	549	GLN
1	A	729	GLN
1	B	130	ASN
1	B	141	ASN
1	B	148	GLN
1	B	169	HIS
1	B	239	ASN
1	B	409	GLN
1	B	478	GLN
1	B	541	ASN
1	B	549	GLN
1	B	729	GLN
1	C	119	ASN
1	C	130	ASN
1	C	141	ASN
1	C	148	GLN
1	C	169	HIS
1	C	239	ASN
1	C	409	GLN
1	C	478	GLN
1	C	541	ASN
1	C	549	GLN
1	C	729	GLN
1	C	775	ASN
1	D	119	ASN
1	D	130	ASN
1	D	141	ASN
1	D	148	GLN
1	D	169	HIS
1	D	239	ASN
1	D	380	GLN
1	D	409	GLN
1	D	478	GLN
1	D	541	ASN
1	D	549	GLN
1	D	729	GLN
1	E	130	ASN
1	E	141	ASN
1	E	148	GLN
1	E	169	HIS
1	E	239	ASN
1	E	249	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	409	GLN
1	E	489	ASN
1	E	541	ASN
1	E	549	GLN
1	E	729	GLN
1	F	119	ASN
1	F	130	ASN
1	F	141	ASN
1	F	148	GLN
1	F	169	HIS
1	F	380	GLN
1	F	409	GLN
1	F	478	GLN
1	F	489	ASN
1	F	537	HIS
1	F	541	ASN
1	F	549	GLN
1	F	729	GLN
1	F	741	GLN
1	F	775	ASN
1	G	130	ASN
1	G	141	ASN
1	G	148	GLN
1	G	169	HIS
1	G	239	ASN
1	G	409	GLN
1	G	478	GLN
1	G	537	HIS
1	G	541	ASN
1	G	549	GLN
1	G	729	GLN
1	H	119	ASN
1	H	130	ASN
1	H	141	ASN
1	H	148	GLN
1	H	169	HIS
1	H	239	ASN
1	H	409	GLN
1	H	489	ASN
1	H	541	ASN
1	H	549	GLN
1	H	729	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	130	ASN
1	I	141	ASN
1	I	148	GLN
1	I	169	HIS
1	I	239	ASN
1	I	409	GLN
1	I	489	ASN
1	I	537	HIS
1	I	541	ASN
1	I	549	GLN
1	I	729	GLN
1	J	119	ASN
1	J	130	ASN
1	J	141	ASN
1	J	148	GLN
1	J	169	HIS
1	J	239	ASN
1	J	380	GLN
1	J	409	GLN
1	J	541	ASN
1	J	549	GLN
1	J	729	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	749/792 (94%)	0.46	53 (7%)	22	16	85, 134, 194, 235	0
1	B	749/792 (94%)	0.48	60 (8%)	18	14	79, 127, 189, 230	0
1	C	749/792 (94%)	0.49	48 (6%)	25	18	86, 144, 202, 250	0
1	D	749/792 (94%)	0.60	55 (7%)	21	16	88, 138, 198, 241	0
1	E	749/792 (94%)	0.50	57 (7%)	20	15	86, 131, 189, 231	0
1	F	749/792 (94%)	0.54	63 (8%)	17	14	88, 146, 206, 239	0
1	G	749/792 (94%)	0.57	59 (7%)	18	15	85, 140, 199, 240	0
1	H	749/792 (94%)	0.45	56 (7%)	20	15	83, 136, 199, 238	0
1	I	749/792 (94%)	0.52	60 (8%)	18	14	86, 134, 199, 246	0
1	J	749/792 (94%)	0.45	54 (7%)	21	16	87, 138, 199, 235	0
All	All	7490/7920 (94%)	0.51	565 (7%)	20	15	79, 137, 198, 250	0

All (565) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	720	ARG	15.1
1	G	720	ARG	12.1
1	C	720	ARG	11.6
1	H	720	ARG	11.2
1	F	720	ARG	11.2
1	I	720	ARG	10.0
1	E	720	ARG	9.6
1	A	720	ARG	9.4
1	B	720	ARG	8.0
1	F	716	ALA	7.8
1	J	720	ARG	7.8
1	D	719	ARG	7.6
1	B	715	LEU	7.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	719	ARG	7.3
1	C	719	ARG	6.9
1	D	717	LEU	6.7
1	C	716	ALA	6.6
1	J	222	ASP	6.6
1	F	719	ARG	6.6
1	F	715	LEU	6.5
1	E	716	ALA	6.5
1	G	719	ARG	6.3
1	D	716	ALA	6.3
1	G	716	ALA	6.1
1	I	719	ARG	6.1
1	D	219	GLU	6.1
1	A	717	LEU	6.0
1	B	345	LEU	5.9
1	D	223	ARG	5.7
1	J	719	ARG	5.7
1	J	716	ALA	5.7
1	H	716	ALA	5.7
1	G	717	LEU	5.6
1	H	223	ARG	5.6
1	I	723	ILE	5.6
1	A	716	ALA	5.5
1	I	222	ASP	5.5
1	G	721	ASP	5.4
1	D	222	ASP	5.4
1	E	719	ARG	5.4
1	F	345	LEU	5.4
1	I	345	LEU	5.4
1	F	721	ASP	5.4
1	H	715	LEU	5.3
1	D	117	ARG	5.3
1	J	715	LEU	5.3
1	C	721	ASP	5.3
1	H	721	ASP	5.2
1	A	715	LEU	5.2
1	F	222	ASP	5.2
1	F	723	ILE	5.1
1	H	719	ARG	5.1
1	J	345	LEU	5.0
1	A	724	THR	5.0
1	E	724	THR	5.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	117	ARG	5.0
1	I	23	VAL	5.0
1	I	717	LEU	4.9
1	G	222	ASP	4.9
1	E	723	ILE	4.9
1	D	715	LEU	4.9
1	A	345	LEU	4.9
1	C	345	LEU	4.9
1	E	345	LEU	4.9
1	E	717	LEU	4.8
1	H	219	GLU	4.8
1	D	723	ILE	4.8
1	B	719	ARG	4.8
1	H	44	LEU	4.8
1	E	24	ASP	4.8
1	H	345	LEU	4.8
1	B	23	VAL	4.7
1	G	715	LEU	4.7
1	E	715	LEU	4.7
1	B	723	ILE	4.7
1	I	724	THR	4.6
1	F	724	THR	4.6
1	C	222	ASP	4.5
1	F	286	ARG	4.5
1	C	715	LEU	4.5
1	I	716	ALA	4.5
1	D	301	ARG	4.5
1	E	272	ALA	4.4
1	C	717	LEU	4.4
1	G	345	LEU	4.4
1	I	301	ARG	4.4
1	D	345	LEU	4.3
1	H	25	THR	4.3
1	D	721	ASP	4.3
1	E	727	ALA	4.3
1	A	723	ILE	4.3
1	J	723	ILE	4.3
1	B	24	ASP	4.3
1	B	222	ASP	4.3
1	A	721	ASP	4.3
1	B	346	LEU	4.3
1	J	286	ARG	4.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	23	VAL	4.2
1	B	716	ALA	4.2
1	D	23	VAL	4.1
1	C	724	THR	4.1
1	G	23	VAL	4.1
1	J	23	VAL	4.1
1	G	286	ARG	4.1
1	H	23	VAL	4.0
1	D	286	ARG	4.0
1	H	286	ARG	4.0
1	E	275	ARG	4.0
1	F	717	LEU	4.0
1	D	224	ASP	4.0
1	E	278	ASN	4.0
1	B	717	LEU	4.0
1	A	286	ARG	4.0
1	F	375	LEU	3.9
1	G	390	LEU	3.9
1	H	346	LEU	3.9
1	H	224	ASP	3.9
1	C	346	LEU	3.9
1	G	724	THR	3.9
1	G	323	ILE	3.9
1	E	371	PHE	3.8
1	B	301	ARG	3.8
1	E	52	HIS	3.8
1	G	346	LEU	3.8
1	A	728	ALA	3.8
1	B	272	ALA	3.8
1	J	724	THR	3.8
1	D	371	PHE	3.8
1	F	390	LEU	3.8
1	C	301	ARG	3.8
1	C	727	ALA	3.8
1	B	371	PHE	3.7
1	E	44	LEU	3.7
1	J	346	LEU	3.7
1	E	274	VAL	3.7
1	C	722	GLU	3.7
1	A	23	VAL	3.7
1	F	301	ARG	3.7
1	E	721	ASP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	32	PHE	3.6
1	I	721	ASP	3.6
1	B	354	ARG	3.6
1	A	727	ALA	3.6
1	A	301	ARG	3.6
1	G	25	THR	3.6
1	F	346	LEU	3.6
1	H	723	ILE	3.6
1	D	724	THR	3.6
1	J	25	THR	3.6
1	D	412	GLN	3.6
1	J	30	ILE	3.6
1	D	44	LEU	3.5
1	D	722	GLU	3.5
1	H	734	ALA	3.5
1	E	43	ARG	3.5
1	E	542	GLY	3.5
1	J	375	LEU	3.5
1	C	286	ARG	3.5
1	E	354	ARG	3.5
1	I	502	LYS	3.5
1	H	722	GLU	3.4
1	F	544	VAL	3.4
1	B	375	LEU	3.4
1	E	390	LEU	3.4
1	J	502	LYS	3.4
1	E	32	PHE	3.4
1	H	222	ASP	3.4
1	D	390	LEU	3.4
1	B	724	THR	3.4
1	E	301	ARG	3.4
1	F	44	LEU	3.4
1	J	430	LEU	3.4
1	J	301	ARG	3.3
1	J	219	GLU	3.3
1	I	715	LEU	3.3
1	I	722	GLU	3.3
1	C	544	VAL	3.3
1	G	30	ILE	3.3
1	C	725	GLY	3.3
1	A	722	GLU	3.3
1	A	718	ARG	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	721	ASP	3.3
1	B	390	LEU	3.3
1	H	301	ARG	3.3
1	J	721	ASP	3.3
1	C	375	LEU	3.2
1	J	717	LEU	3.2
1	F	29	VAL	3.2
1	G	24	ASP	3.2
1	I	25	THR	3.2
1	A	430	LEU	3.2
1	B	277	LEU	3.2
1	H	724	THR	3.2
1	J	544	VAL	3.2
1	F	412	GLN	3.2
1	H	412	GLN	3.2
1	G	722	GLU	3.2
1	I	286	ARG	3.2
1	I	544	VAL	3.2
1	H	390	LEU	3.2
1	B	304	GLN	3.2
1	I	430	LEU	3.2
1	J	429	ARG	3.2
1	J	385	ASP	3.2
1	A	274	VAL	3.2
1	E	430	LEU	3.2
1	F	28	GLY	3.1
1	H	24	ASP	3.1
1	A	643	GLY	3.1
1	I	725	GLY	3.1
1	B	714	SER	3.1
1	D	323	ILE	3.1
1	A	25	THR	3.1
1	D	25	THR	3.1
1	H	30	ILE	3.1
1	B	722	GLU	3.1
1	F	371	PHE	3.1
1	F	722	GLU	3.1
1	J	371	PHE	3.0
1	A	412	GLN	3.0
1	I	32	PHE	3.0
1	I	728	ALA	3.0
1	D	276	TYR	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	30	ILE	3.0
1	I	371	PHE	3.0
1	F	276	TYR	3.0
1	J	730	PRO	3.0
1	B	544	VAL	3.0
1	H	371	PHE	3.0
1	A	44	LEU	3.0
1	D	28	GLY	3.0
1	B	583	ALA	3.0
1	F	583	ALA	3.0
1	J	44	LEU	2.9
1	E	280	SER	2.9
1	G	727	ALA	2.9
1	B	430	LEU	2.9
1	A	28	GLY	2.9
1	G	725	GLY	2.9
1	I	692	GLY	2.9
1	B	274	VAL	2.9
1	D	372	TYR	2.9
1	I	189	TYR	2.9
1	A	371	PHE	2.9
1	A	189	TYR	2.9
1	I	223	ARG	2.9
1	E	692	GLY	2.9
1	G	219	GLU	2.9
1	D	544	VAL	2.9
1	A	30	ILE	2.9
1	A	734	ALA	2.9
1	B	286	ARG	2.9
1	A	725	GLY	2.8
1	J	692	GLY	2.8
1	H	375	LEU	2.8
1	J	722	GLU	2.8
1	G	28	GLY	2.8
1	D	583	ALA	2.8
1	D	32	PHE	2.8
1	G	371	PHE	2.8
1	C	723	ILE	2.8
1	I	277	LEU	2.8
1	B	52	HIS	2.8
1	F	348	ASP	2.8
1	I	272	ALA	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	429	ARG	2.8
1	C	44	LEU	2.8
1	G	375	LEU	2.8
1	G	276	TYR	2.8
1	G	723	ILE	2.8
1	H	583	ALA	2.8
1	A	429	ARG	2.8
1	D	29	VAL	2.8
1	B	278	ASN	2.8
1	E	728	ALA	2.8
1	C	302	TRP	2.8
1	I	390	LEU	2.8
1	G	223	ARG	2.7
1	G	718	ARG	2.7
1	F	277	LEU	2.7
1	C	30	ILE	2.7
1	G	412	GLN	2.7
1	G	309	ALA	2.7
1	A	32	PHE	2.7
1	A	502	LYS	2.7
1	B	223	ARG	2.7
1	I	558	HIS	2.7
1	D	691	ASP	2.7
1	E	85	ASP	2.7
1	F	427	ASP	2.7
1	F	478	GLN	2.7
1	E	286	ARG	2.7
1	F	734	ALA	2.7
1	B	502	LYS	2.7
1	A	24	ASP	2.7
1	A	385	ASP	2.7
1	B	348	ASP	2.7
1	I	412	GLN	2.7
1	E	734	ALA	2.7
1	F	727	ALA	2.7
1	J	323	ILE	2.7
1	H	502	LYS	2.7
1	G	430	LEU	2.7
1	H	434	LEU	2.7
1	G	273	PRO	2.7
1	D	718	ARG	2.7
1	B	25	THR	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	219	GLU	2.7
1	B	619	SER	2.7
1	C	23	VAL	2.6
1	G	29	VAL	2.6
1	H	323	ILE	2.6
1	H	272	ALA	2.6
1	G	277	LEU	2.6
1	G	730	PRO	2.6
1	C	502	LYS	2.6
1	J	725	GLY	2.6
1	A	85	ASP	2.6
1	B	385	ASP	2.6
1	C	189	TYR	2.6
1	C	371	PHE	2.6
1	J	223	ARG	2.6
1	A	273	PRO	2.6
1	E	730	PRO	2.6
1	B	572	ALA	2.6
1	F	572	ALA	2.6
1	E	277	LEU	2.6
1	E	346	LEU	2.6
1	G	85	ASP	2.6
1	A	436	GLU	2.6
1	B	347	SER	2.6
1	F	273	PRO	2.6
1	B	44	LEU	2.6
1	D	692	GLY	2.6
1	G	301	ARG	2.6
1	J	718	ARG	2.6
1	I	44	LEU	2.6
1	E	643	GLY	2.6
1	H	28	GLY	2.6
1	H	229	ARG	2.6
1	B	280	SER	2.5
1	G	123	GLU	2.5
1	A	375	LEU	2.5
1	F	430	LEU	2.5
1	A	619	SER	2.5
1	B	43	ARG	2.5
1	F	23	VAL	2.5
1	A	346	LEU	2.5
1	E	434	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	730	PRO	2.5
1	H	478	GLN	2.5
1	H	643	GLY	2.5
1	J	643	GLY	2.5
1	D	215	ARG	2.5
1	I	429	ARG	2.5
1	C	277	LEU	2.5
1	I	85	ASP	2.5
1	J	412	GLN	2.5
1	I	526	ARG	2.5
1	A	390	LEU	2.5
1	E	544	VAL	2.5
1	D	528	PRO	2.5
1	F	691	ASP	2.5
1	D	375	LEU	2.5
1	I	29	VAL	2.5
1	G	32	PHE	2.5
1	G	121	TRP	2.5
1	I	115	ASN	2.5
1	I	734	ALA	2.5
1	E	223	ARG	2.5
1	F	725	GLY	2.5
1	H	215	ARG	2.4
1	G	224	ASP	2.4
1	A	29	VAL	2.4
1	C	276	TYR	2.4
1	C	323	ILE	2.4
1	H	123	GLU	2.4
1	J	409	GLN	2.4
1	E	619	SER	2.4
1	F	25	THR	2.4
1	C	694	LYS	2.4
1	G	502	LYS	2.4
1	F	189	TYR	2.4
1	I	276	TYR	2.4
1	C	583	ALA	2.4
1	F	730	PRO	2.4
1	I	348	ASP	2.4
1	F	272	ALA	2.4
1	G	583	ALA	2.4
1	A	374	GLY	2.4
1	H	544	VAL	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	30	ILE	2.4
1	C	54	LEU	2.4
1	D	430	LEU	2.4
1	E	375	LEU	2.4
1	A	223	ARG	2.4
1	C	223	ARG	2.4
1	C	718	ARG	2.4
1	B	362	LYS	2.4
1	A	311	GLY	2.4
1	F	643	GLY	2.4
1	B	312	SER	2.4
1	H	717	LEU	2.4
1	J	390	LEU	2.4
1	A	276	TYR	2.4
1	F	85	ASP	2.4
1	H	500	GLU	2.4
1	F	114	PRO	2.3
1	B	117	ARG	2.3
1	F	223	ARG	2.3
1	I	718	ARG	2.3
1	A	277	LEU	2.3
1	F	52	HIS	2.3
1	J	277	LEU	2.3
1	J	604	LYS	2.3
1	D	728	ALA	2.3
1	G	734	ALA	2.3
1	D	30	ILE	2.3
1	I	346	LEU	2.3
1	G	728	ALA	2.3
1	J	28	GLY	2.3
1	F	388	THR	2.3
1	E	502	LYS	2.3
1	H	32	PHE	2.3
1	J	572	ALA	2.3
1	B	361	GLU	2.3
1	G	385	ASP	2.3
1	H	85	ASP	2.3
1	H	692	GLY	2.3
1	I	273	PRO	2.3
1	J	691	ASP	2.3
1	F	502	LYS	2.3
1	E	541	ASN	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	H	718	ARG	2.3
1	J	32	PHE	2.3
1	D	572	ALA	2.3
1	D	478	GLN	2.3
1	C	123	GLU	2.3
1	C	374	GLY	2.3
1	J	224	ASP	2.3
1	C	390	LEU	2.2
1	G	316	TRP	2.2
1	F	323	ILE	2.2
1	I	30	ILE	2.2
1	A	544	VAL	2.2
1	E	229	ARG	2.2
1	C	734	ALA	2.2
1	I	552	ALA	2.2
1	G	187	SER	2.2
1	H	276	TYR	2.2
1	E	622	ARG	2.2
1	D	388	THR	2.2
1	C	691	ASP	2.2
1	I	52	HIS	2.2
1	B	727	ALA	2.2
1	F	728	ALA	2.2
1	H	430	LEU	2.2
1	I	215	ARG	2.2
1	F	221	GLU	2.2
1	G	500	GLU	2.2
1	I	436	GLU	2.2
1	A	528	PRO	2.2
1	E	348	ASP	2.2
1	E	691	ASP	2.2
1	J	52	HIS	2.2
1	I	619	SER	2.2
1	J	619	SER	2.2
1	B	275	ARG	2.2
1	I	583	ALA	2.2
1	G	789	LEU	2.2
1	I	375	LEU	2.2
1	B	429	ARG	2.2
1	F	429	ARG	2.2
1	I	622	ARG	2.2
1	J	276	TYR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	53	PHE	2.2
1	E	219	GLU	2.2
1	E	401	GLU	2.2
1	G	310	PHE	2.2
1	H	730	PRO	2.2
1	C	388	THR	2.2
1	D	421	LYS	2.2
1	G	229	ARG	2.1
1	H	188	ASP	2.1
1	H	429	ARG	2.1
1	F	306	TRP	2.1
1	G	306	TRP	2.1
1	C	420	VAL	2.1
1	E	53	PHE	2.1
1	H	273	PRO	2.1
1	I	123	GLU	2.1
1	C	55	ARG	2.1
1	B	30	ILE	2.1
1	B	188	ASP	2.1
1	I	323	ILE	2.1
1	J	24	ASP	2.1
1	B	173	VAL	2.1
1	J	29	VAL	2.1
1	G	643	GLY	2.1
1	F	434	LEU	2.1
1	F	546	LEU	2.1
1	J	434	LEU	2.1
1	D	429	ARG	2.1
1	D	734	ALA	2.1
1	E	412	GLN	2.1
1	E	729	GLN	2.1
1	G	478	GLN	2.1
1	C	53	PHE	2.1
1	C	85	ASP	2.1
1	D	502	LYS	2.1
1	J	416	VAL	2.1
1	E	192	PRO	2.1
1	J	271	ARG	2.1
1	F	26	ALA	2.1
1	G	387	SER	2.1
1	B	85	ASP	2.1
1	C	427	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	789	LEU	2.1
1	J	316	TRP	2.1
1	D	42	PRO	2.1
1	I	730	PRO	2.1
1	A	309	ALA	2.1
1	H	433	GLN	2.1
1	I	478	GLN	2.1
1	A	542	GLY	2.1
1	B	276	TYR	2.1
1	D	385	ASP	2.1
1	I	26	ALA	2.1
1	A	278	ASN	2.1
1	B	412	GLN	2.1
1	F	310	PHE	2.1
1	H	725	GLY	2.0
1	B	617	PRO	2.0
1	J	273	PRO	2.0
1	B	229	ARG	2.0
1	C	25	THR	2.0
1	D	689	GLU	2.0
1	H	669	LYS	2.0
1	D	727	ALA	2.0
1	H	728	ALA	2.0
1	B	785	VAL	2.0
1	J	283	GLN	2.0
1	F	755	GLY	2.0
1	G	374	GLY	2.0
1	B	271	ARG	2.0
1	C	429	ARG	2.0
1	D	273	PRO	2.0
1	F	275	ARG	2.0
1	D	24	ASP	2.0
1	G	543	ASP	2.0
1	D	53	PHE	2.0
1	E	508	ALA	2.0
1	F	167	SER	2.0
1	F	431	SER	2.0
1	G	714	SER	2.0
1	A	314	LYS	2.0
1	C	421	LYS	2.0
1	E	84	TYR	2.0
1	C	272	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	417	ASP	2.0
1	H	277	LEU	2.0
1	I	310	PHE	2.0
1	I	538	GLU	2.0
1	F	309	ALA	2.0
1	I	187	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.