Full wwPDB X-ray Structure Validation Report (i)

Oct 25, 2023 – 01:43 PM EDT

PDB ID	:	3F5N
Title	:	Structure of native human neuroserpin
Authors	:	Ricagno, S.; Caccia, S.; Sorrentino, G.; Bolognesi, M.
Deposited on	:	2008-11-04
Resolution	:	3.15 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

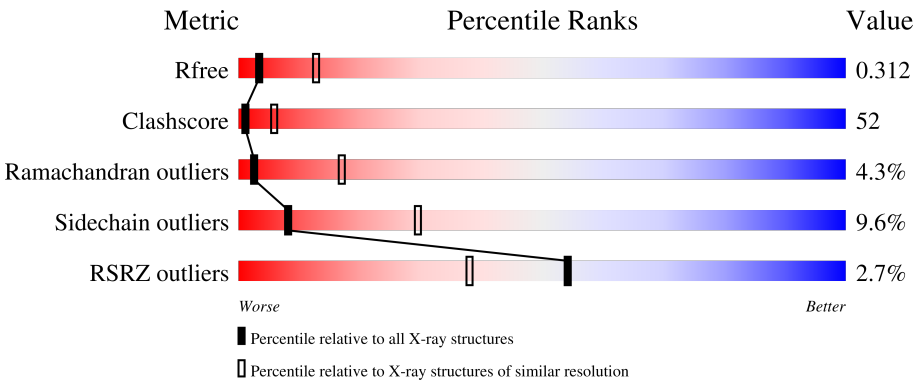
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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

Mol	Chain	Length	Quality of chain
1	A	407	% 43% 39% 7% 11%
1	B	407	3% 40% 39% 10% • 8%
1	C	407	40% 38% 9% • 12%
1	D	407	3% 48% 36% 5% 11%
1	E	407	4% 43% 33% 5% • 16%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 14513 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 Neuroserpin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	364	2925	1872	478	558	17	0	0	0
1	B	376	3012	1924	495	575	18	0	0	0
1	C	358	2889	1852	474	546	17	0	0	0
1	D	363	2924	1874	478	555	17	0	0	0
1	E	340	2763	1778	451	518	16	0	0	0

There are 65 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MET	-	initiating methionine	UNP Q99574
A	5	ARG	-	expression tag	UNP Q99574
A	6	GLY	-	expression tag	UNP Q99574
A	7	SER	-	expression tag	UNP Q99574
A	8	HIS	-	expression tag	UNP Q99574
A	9	HIS	-	expression tag	UNP Q99574
A	10	HIS	-	expression tag	UNP Q99574
A	11	HIS	-	expression tag	UNP Q99574
A	12	HIS	-	expression tag	UNP Q99574
A	13	HIS	-	expression tag	UNP Q99574
A	14	THR	-	expression tag	UNP Q99574
A	15	ASP	-	expression tag	UNP Q99574
A	16	PRO	-	expression tag	UNP Q99574
B	4	MET	-	initiating methionine	UNP Q99574
B	5	ARG	-	expression tag	UNP Q99574
B	6	GLY	-	expression tag	UNP Q99574
B	7	SER	-	expression tag	UNP Q99574
B	8	HIS	-	expression tag	UNP Q99574
B	9	HIS	-	expression tag	UNP Q99574

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	HIS	-	expression tag	UNP Q99574
B	11	HIS	-	expression tag	UNP Q99574
B	12	HIS	-	expression tag	UNP Q99574
B	13	HIS	-	expression tag	UNP Q99574
B	14	THR	-	expression tag	UNP Q99574
B	15	ASP	-	expression tag	UNP Q99574
B	16	PRO	-	expression tag	UNP Q99574
C	4	MET	-	initiating methionine	UNP Q99574
C	5	ARG	-	expression tag	UNP Q99574
C	6	GLY	-	expression tag	UNP Q99574
C	7	SER	-	expression tag	UNP Q99574
C	8	HIS	-	expression tag	UNP Q99574
C	9	HIS	-	expression tag	UNP Q99574
C	10	HIS	-	expression tag	UNP Q99574
C	11	HIS	-	expression tag	UNP Q99574
C	12	HIS	-	expression tag	UNP Q99574
C	13	HIS	-	expression tag	UNP Q99574
C	14	THR	-	expression tag	UNP Q99574
C	15	ASP	-	expression tag	UNP Q99574
C	16	PRO	-	expression tag	UNP Q99574
D	4	MET	-	initiating methionine	UNP Q99574
D	5	ARG	-	expression tag	UNP Q99574
D	6	GLY	-	expression tag	UNP Q99574
D	7	SER	-	expression tag	UNP Q99574
D	8	HIS	-	expression tag	UNP Q99574
D	9	HIS	-	expression tag	UNP Q99574
D	10	HIS	-	expression tag	UNP Q99574
D	11	HIS	-	expression tag	UNP Q99574
D	12	HIS	-	expression tag	UNP Q99574
D	13	HIS	-	expression tag	UNP Q99574
D	14	THR	-	expression tag	UNP Q99574
D	15	ASP	-	expression tag	UNP Q99574
D	16	PRO	-	expression tag	UNP Q99574
E	4	MET	-	initiating methionine	UNP Q99574
E	5	ARG	-	expression tag	UNP Q99574
E	6	GLY	-	expression tag	UNP Q99574
E	7	SER	-	expression tag	UNP Q99574
E	8	HIS	-	expression tag	UNP Q99574
E	9	HIS	-	expression tag	UNP Q99574
E	10	HIS	-	expression tag	UNP Q99574
E	11	HIS	-	expression tag	UNP Q99574
E	12	HIS	-	expression tag	UNP Q99574

Continued on next page...

Continued from previous page...

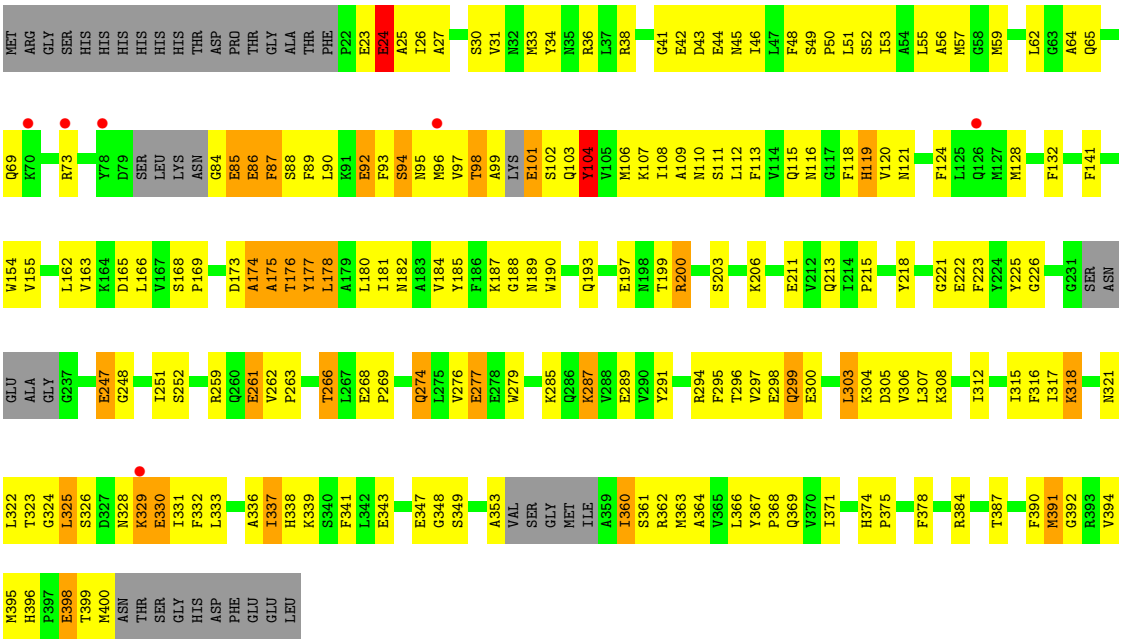
Chain	Residue	Modelled	Actual	Comment	Reference
E	13	HIS	-	expression tag	UNP Q99574
E	14	THR	-	expression tag	UNP Q99574
E	15	ASP	-	expression tag	UNP Q99574
E	16	PRO	-	expression tag	UNP Q99574

3 Residue-property plots (i)

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

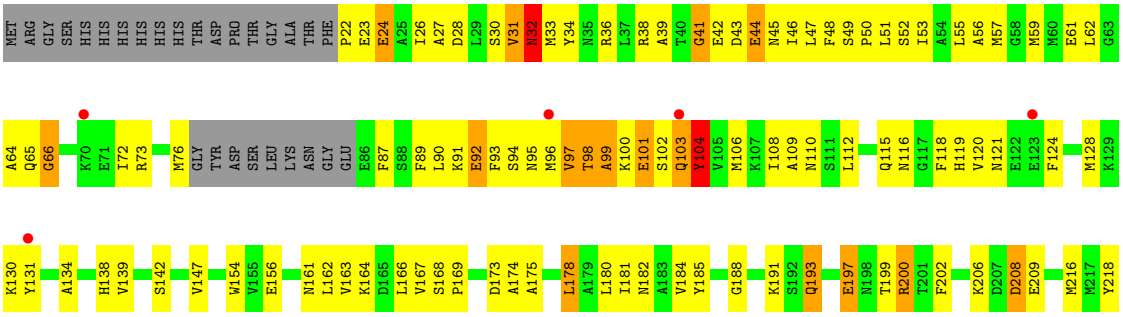
• Molecule 1: Neuroserpin

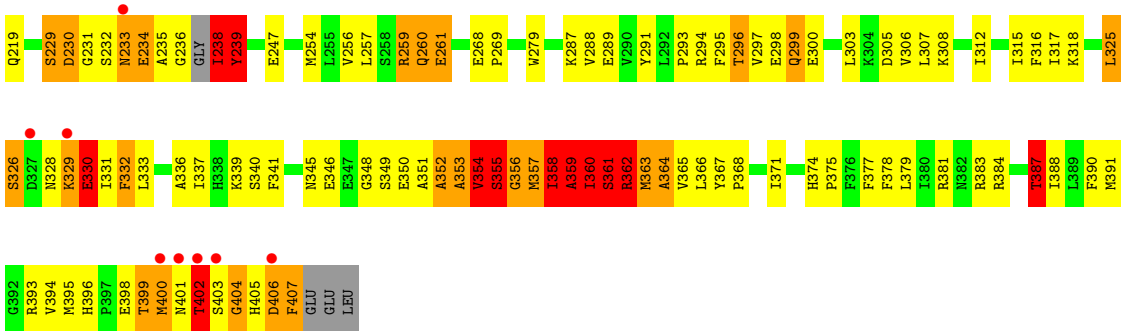
Chain A:



• Molecule 1: Neuroserpin

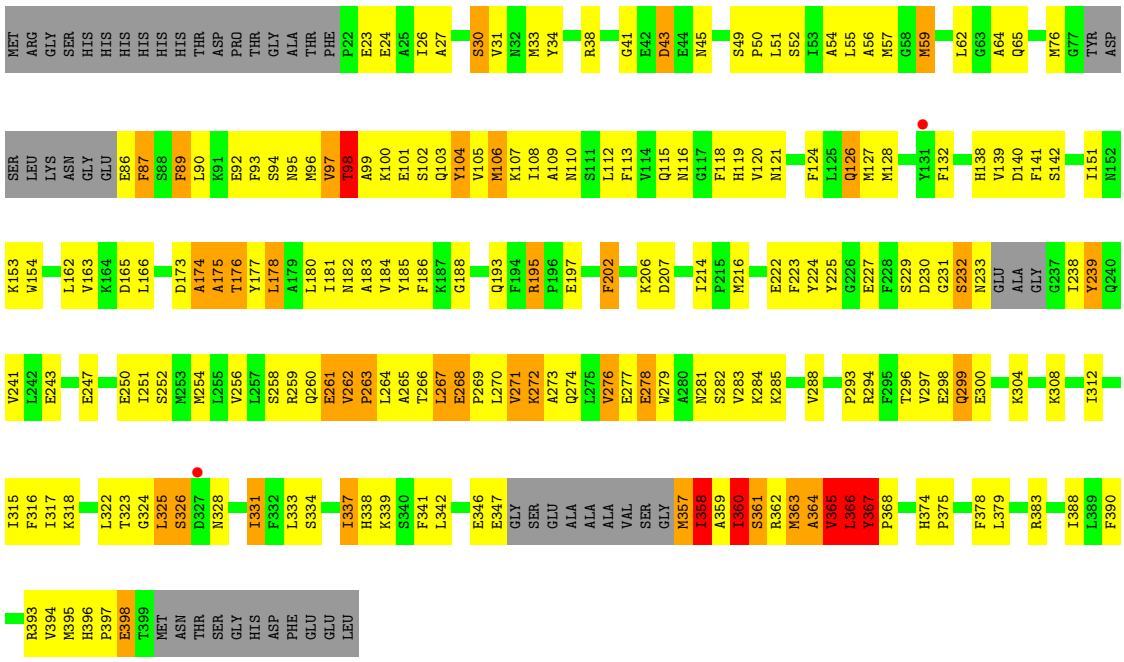
Chain B:





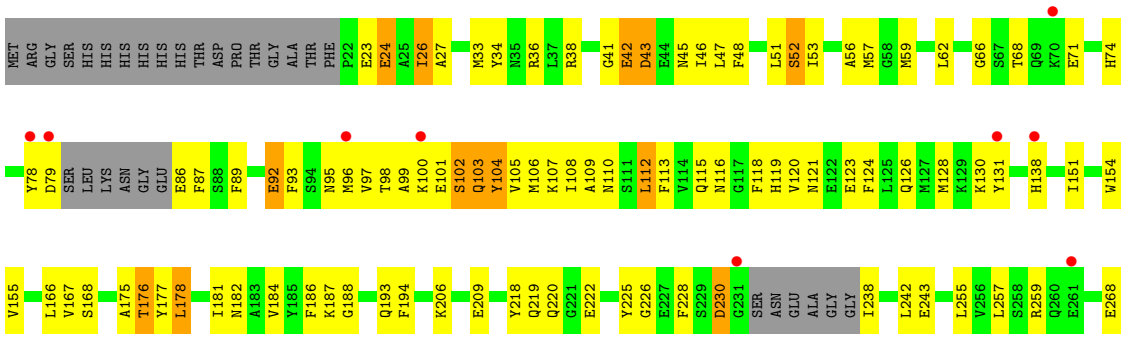
- Molecule 1: Neuroserpin

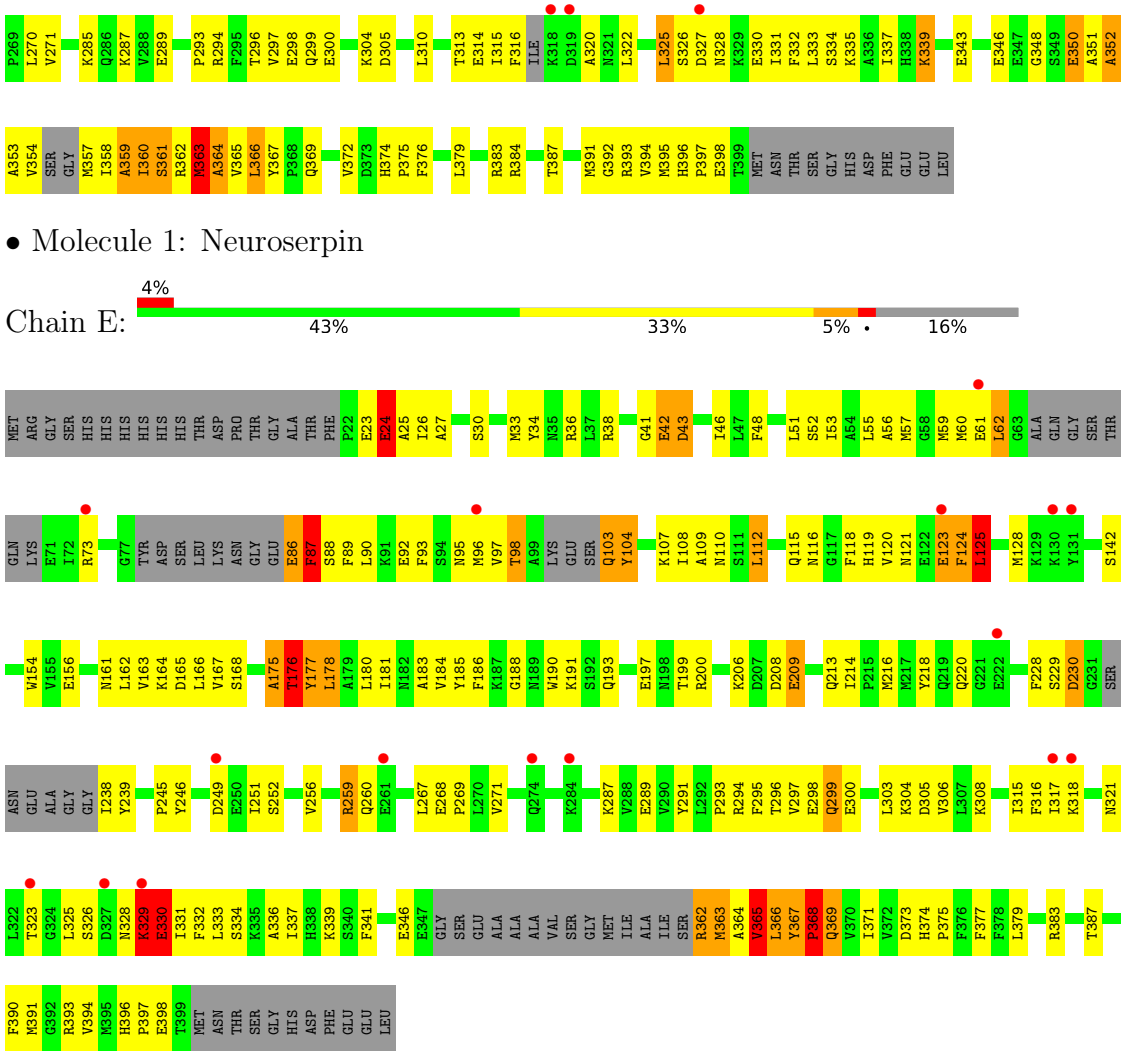
Chain C: 40% 38% 9% • 12%



- Molecule 1: Neuroserpin

Chain D: 3% 48% 36% 5% 11%





• Molecule 1: Neuroserpin

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	171.80Å 179.18Å 248.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.15 19.98 – 3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-3.15) 100.0 (19.98-3.15)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	2.10 (at 3.15Å)	Xtriage
Refinement program	REFMAC 5.4.0069	Depositor
R, R_{free}	0.234 , 0.283 0.265 , 0.312	Depositor DCC
R_{free} test set	3356 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	83.3	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.012 for -1/2*h+1/2*k+1/2*l,1/2*h-1/2*k+1/2*l,h+k 0.024 for -1/2*h+1/2*k-1/2*l,1/2*h-1/2*k-1/2*l,-h-k 0.025 for k,h,-l 0.021 for -1/2*h-1/2*k+1/2*l,-1/2*h-1/2*k-1/2*l,h-k 0.034 for -1/2*h-1/2*k-1/2*l,-1/2*h-1/2*k+1/2*l,-h+k	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	14513	wwPDB-VP
Average B, all atoms (Å^2)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.53	0/2982	0.73	5/4022 (0.1%)
1	B	0.47	0/3072	0.77	5/4146 (0.1%)
1	C	0.52	0/2946	0.72	4/3974 (0.1%)
1	D	0.42	0/2981	0.61	0/4021
1	E	0.41	0/2818	0.68	2/3801 (0.1%)
All	All	0.47	0/14799	0.71	16/19964 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	8
1	C	0	4
1	E	0	6
All	All	0	19

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	359	ALA	CB-CA-C	-12.93	90.71	110.10
1	B	359	ALA	N-CA-C	11.46	141.94	111.00
1	A	176	THR	N-CA-C	-8.66	87.61	111.00
1	B	32	ASN	N-CA-C	-8.44	88.21	111.00
1	A	174	ALA	CB-CA-C	7.31	121.07	110.10
1	B	359	ALA	C-N-CA	6.89	138.93	121.70
1	C	365	VAL	N-CA-C	6.83	129.45	111.00
1	C	268	GLU	CB-CA-C	-6.80	96.81	110.40
1	A	360	ILE	CB-CA-C	-6.48	98.63	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	398	GLU	CB-CA-C	-5.92	98.56	110.40
1	A	329	LYS	C-N-CA	5.84	136.29	121.70
1	E	177	TYR	N-CA-C	-5.81	95.31	111.00
1	A	329	LYS	N-CA-C	5.59	126.09	111.00
1	E	125	LEU	N-CA-C	-5.54	96.05	111.00
1	C	102	SER	N-CA-C	5.31	125.34	111.00
1	B	329	LYS	C-N-CA	5.30	134.95	121.70

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	175	ALA	Peptide
1	B	238	ILE	Peptide
1	B	31	VAL	Peptide
1	B	358	ILE	Peptide
1	B	359	ALA	Peptide
1	B	360	ILE	Peptide
1	B	362	ARG	Peptide
1	B	387	THR	Peptide
1	B	44	GLU	Peptide
1	C	175	ALA	Peptide
1	C	364	ALA	Peptide
1	C	366	LEU	Peptide
1	C	367	TYR	Peptide
1	E	124	PHE	Peptide
1	E	175	ALA	Peptide
1	E	176	THR	Peptide
1	E	329	LYS	Peptide
1	E	366	LEU	Peptide
1	E	368	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2925	0	2864	288	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3012	0	2954	355	0
1	C	2889	0	2849	354	0
1	D	2924	0	2874	249	0
1	E	2763	0	2719	287	0
All	All	14513	0	14260	1503	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 52.

All (1503) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HG2	1:A:128:MET:CE	1.37	1.54
1:E:364:ALA:CA	1:E:365:VAL:HG23	1.38	1.50
1:B:354:VAL:HB	1:B:355:SER:CA	1.42	1.48
1:E:364:ALA:HA	1:E:365:VAL:CG2	1.43	1.48
1:C:357:MET:C	1:C:358:ILE:HD12	1.33	1.46
1:D:304:LYS:HG3	1:D:316:PHE:CE1	1.58	1.38
1:D:357:MET:CB	1:D:358:ILE:HA	1.51	1.37
1:B:260:GLN:NE2	1:B:261:GLU:H	1.23	1.35
1:D:357:MET:HB3	1:D:358:ILE:CA	1.62	1.29
1:E:364:ALA:CB	1:E:366:LEU:HB2	1.60	1.29
1:A:84:GLY:HA2	1:A:85:GLU:CB	1.61	1.28
1:C:367:TYR:CB	1:C:368:PRO:HA	1.64	1.27
1:B:354:VAL:CB	1:B:355:SER:C	2.07	1.23
1:B:119:HIS:O	1:B:326:SER:HB2	1.26	1.23
1:A:84:GLY:CA	1:A:85:GLU:HB2	1.61	1.23
1:B:356:GLY:O	1:B:360:ILE:HB	1.14	1.23
1:C:263:PRO:O	1:C:264:LEU:HD23	1.35	1.23
1:A:287:LYS:NZ	1:A:353:ALA:HB1	1.55	1.22
1:E:287:LYS:HD3	1:E:367:TYR:OH	1.38	1.22
1:E:364:ALA:HB1	1:E:365:VAL:C	1.58	1.21
1:A:59:MET:HE1	1:A:110:ASN:CG	1.61	1.21
1:B:354:VAL:HB	1:B:355:SER:C	1.58	1.19
1:B:354:VAL:CG1	1:B:355:SER:C	2.11	1.18
1:C:119:HIS:O	1:C:326:SER:HB2	1.42	1.17
1:A:59:MET:HE1	1:A:110:ASN:OD1	1.39	1.17
1:C:268:GLU:HB2	1:C:269:PRO:HD3	1.20	1.17
1:C:367:TYR:HB3	1:C:368:PRO:CA	1.75	1.17
1:E:86:GLU:HG2	1:E:87:PHE:N	1.51	1.17
1:D:238:ILE:HD11	1:D:259:ARG:NH1	1.60	1.16

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LEU:CD1	1:D:93:PHE:CD1	2.29	1.16
1:B:260:GLN:HE21	1:B:261:GLU:N	1.43	1.15
1:A:336:ALA:O	1:A:337:ILE:HD12	1.47	1.15
1:D:304:LYS:HG3	1:D:316:PHE:CZ	1.82	1.15
1:B:354:VAL:CG1	1:B:355:SER:O	1.94	1.14
1:A:274:GLN:HE21	1:A:274:GLN:CA	1.60	1.14
1:A:94:SER:O	1:A:98:THR:HG21	1.46	1.13
1:E:176:THR:O	1:E:334:SER:HB3	1.48	1.13
1:D:51:LEU:HD11	1:D:93:PHE:HB3	1.27	1.12
1:E:86:GLU:HG2	1:E:87:PHE:H	1.02	1.12
1:C:261:GLU:O	1:C:262:VAL:HG23	1.50	1.12
1:B:181:ILE:HD11	1:B:337:ILE:HD12	1.27	1.11
1:A:59:MET:HG2	1:A:128:MET:HE1	1.28	1.11
1:E:364:ALA:HB1	1:E:365:VAL:O	1.50	1.11
1:B:358:ILE:HG22	1:B:359:ALA:N	1.59	1.10
1:A:59:MET:CG	1:A:128:MET:CE	2.28	1.10
1:B:360:ILE:HG22	1:B:361:SER:N	1.59	1.10
1:E:119:HIS:O	1:E:326:SER:HB2	1.52	1.10
1:E:362:ARG:HD2	1:E:363:MET:H	1.04	1.10
1:B:354:VAL:HG12	1:B:355:SER:C	1.68	1.09
1:C:231:GLY:O	1:C:232:SER:HB3	1.49	1.09
1:D:359:ALA:O	1:D:360:ILE:HG23	1.51	1.09
1:E:362:ARG:HD2	1:E:363:MET:N	1.67	1.09
1:A:222:GLU:CG	1:A:287:LYS:HG2	1.82	1.08
1:C:367:TYR:HB3	1:C:368:PRO:HA	1.25	1.08
1:B:354:VAL:HG12	1:B:356:GLY:CA	1.84	1.08
1:B:59:MET:HB2	1:B:128:MET:SD	1.93	1.08
1:D:26:ILE:CD1	1:D:93:PHE:HE1	1.65	1.08
1:D:314:GLU:O	1:D:320:ALA:HB2	1.54	1.08
1:B:356:GLY:HA3	1:B:360:ILE:CD1	1.83	1.08
1:B:261:GLU:OE2	1:B:261:GLU:HA	1.50	1.08
1:E:103:GLN:HE21	1:E:103:GLN:CA	1.64	1.07
1:E:259:ARG:NH1	1:E:260:GLN:HB2	1.70	1.07
1:C:163:VAL:HG13	1:C:339:LYS:HD3	1.35	1.07
1:C:268:GLU:HB2	1:C:269:PRO:CD	1.84	1.07
1:B:299:GLN:HE21	1:B:300:GLU:N	1.50	1.07
1:C:103:GLN:HG2	1:C:104:TYR:H	1.09	1.07
1:B:356:GLY:CA	1:B:360:ILE:HD12	1.84	1.06
1:D:119:HIS:O	1:D:326:SER:HB2	1.55	1.06
1:B:354:VAL:HB	1:B:355:SER:HA	1.11	1.06
1:C:195:ARG:HH12	1:C:358:ILE:CA	1.68	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:CE	1:A:110:ASN:CG	2.24	1.04
1:B:356:GLY:HA3	1:B:360:ILE:HD12	1.07	1.04
1:C:89:PHE:HD2	1:C:89:PHE:O	1.40	1.04
1:A:119:HIS:O	1:A:326:SER:HB2	1.58	1.03
1:B:354:VAL:CB	1:B:355:SER:CA	2.32	1.03
1:B:401:ASN:HA	1:B:402:THR:OG1	1.54	1.03
1:D:51:LEU:HD12	1:D:93:PHE:HD1	1.20	1.03
1:E:103:GLN:HE21	1:E:103:GLN:HA	0.91	1.03
1:E:103:GLN:HA	1:E:103:GLN:NE2	1.59	1.03
1:E:364:ALA:CB	1:E:365:VAL:O	2.07	1.03
1:A:274:GLN:HE21	1:A:274:GLN:HA	0.89	1.02
1:A:299:GLN:OE1	1:A:299:GLN:HA	1.57	1.02
1:A:59:MET:CG	1:A:128:MET:HE1	1.89	1.02
1:B:299:GLN:NE2	1:B:300:GLU:H	1.56	1.02
1:D:51:LEU:HD12	1:D:93:PHE:CD1	1.93	1.02
1:B:167:VAL:HG12	1:B:337:ILE:HD13	1.43	1.01
1:A:247:GLU:OE2	1:A:248:GLY:N	1.93	1.01
1:A:287:LYS:NZ	1:A:353:ALA:CB	2.22	1.01
1:B:360:ILE:HG22	1:B:361:SER:H	0.88	1.01
1:E:259:ARG:HD3	1:E:260:GLN:N	1.76	1.01
1:E:362:ARG:HH11	1:E:362:ARG:CG	1.73	1.01
1:A:51:LEU:HD11	1:A:93:PHE:HB3	1.42	1.01
1:A:274:GLN:HA	1:A:274:GLN:NE2	1.68	1.01
1:B:354:VAL:HG12	1:B:356:GLY:N	1.76	1.01
1:C:231:GLY:O	1:C:232:SER:CB	2.08	1.01
1:B:193:GLN:HG3	1:B:349:SER:O	1.58	1.00
1:E:364:ALA:HB1	1:E:366:LEU:HB2	1.37	1.00
1:E:51:LEU:HD11	1:E:93:PHE:CG	1.97	1.00
1:E:364:ALA:HB2	1:E:366:LEU:HB2	1.40	1.00
1:A:222:GLU:HG2	1:A:287:LYS:HG2	1.43	1.00
1:C:357:MET:C	1:C:358:ILE:CD1	2.29	1.00
1:A:336:ALA:C	1:A:337:ILE:CD1	2.31	0.99
1:E:176:THR:O	1:E:334:SER:CB	2.11	0.99
1:C:359:ALA:O	1:C:360:ILE:HB	1.61	0.99
1:B:238:ILE:HA	1:B:239:TYR:HB3	1.42	0.99
1:A:59:MET:HG2	1:A:128:MET:HE3	0.99	0.98
1:B:59:MET:CE	1:B:180:LEU:CD1	2.42	0.98
1:A:193:GLN:HG2	1:A:349:SER:O	1.63	0.98
1:A:221:GLY:HA2	1:A:287:LYS:HE2	1.45	0.98
1:B:299:GLN:NE2	1:B:299:GLN:HA	1.78	0.98
1:C:367:TYR:HB2	1:C:368:PRO:HA	1.42	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:362:ARG:O	1:C:363:MET:CB	2.11	0.98
1:B:353:ALA:HA	1:B:354:VAL:C	1.83	0.98
1:C:358:ILE:HD12	1:C:358:ILE:N	1.77	0.98
1:A:277:GLU:OE2	1:A:277:GLU:HA	1.59	0.97
1:B:356:GLY:O	1:B:360:ILE:CB	2.11	0.97
1:E:362:ARG:HG2	1:E:362:ARG:NH1	1.60	0.97
1:B:232:SER:HB2	1:B:234:GLU:O	1.64	0.97
1:B:59:MET:HE2	1:B:180:LEU:HD11	1.47	0.97
1:D:363:MET:HG3	1:D:363:MET:O	1.61	0.97
1:A:59:MET:CG	1:A:128:MET:HE3	1.90	0.96
1:B:360:ILE:CG2	1:B:361:SER:H	1.78	0.96
1:C:100:LYS:HE3	1:C:105:VAL:CG1	1.93	0.96
1:D:362:ARG:HG2	1:D:363:MET:H	1.29	0.96
1:C:263:PRO:O	1:C:264:LEU:CD2	2.11	0.96
1:B:358:ILE:HG22	1:B:359:ALA:H	1.15	0.96
1:C:103:GLN:HG2	1:C:104:TYR:N	1.76	0.96
1:E:163:VAL:CG1	1:E:339:LYS:HE2	1.94	0.96
1:C:262:VAL:O	1:C:262:VAL:HG12	1.62	0.96
1:E:51:LEU:HD11	1:E:93:PHE:HB3	1.45	0.96
1:E:362:ARG:HH11	1:E:362:ARG:HG2	0.80	0.96
1:B:401:ASN:HA	1:B:402:THR:CB	1.93	0.96
1:B:62:LEU:HD12	1:B:128:MET:HE2	1.46	0.95
1:D:360:ILE:O	1:D:361:SER:HB3	1.66	0.95
1:C:89:PHE:HD2	1:C:89:PHE:C	1.69	0.95
1:C:142:SER:OG	1:C:174:ALA:HB2	1.66	0.95
1:B:119:HIS:O	1:B:326:SER:CB	2.15	0.95
1:E:208:ASP:O	1:E:209:GLU:HG2	1.67	0.95
1:D:109:ALA:HB1	1:D:154:TRP:CZ3	2.02	0.95
1:B:260:GLN:NE2	1:B:261:GLU:N	2.06	0.94
1:A:336:ALA:C	1:A:337:ILE:HD12	1.86	0.94
1:B:59:MET:CE	1:B:180:LEU:HD11	1.98	0.94
1:C:263:PRO:HB2	1:C:266:THR:HB	1.47	0.94
1:A:261:GLU:HA	1:A:261:GLU:OE2	1.66	0.94
1:E:208:ASP:O	1:E:209:GLU:CG	2.16	0.94
1:C:93:PHE:HD2	1:C:97:VAL:HG22	1.31	0.94
1:B:247:GLU:OE2	1:B:349:SER:HB2	1.68	0.93
1:E:287:LYS:CD	1:E:367:TYR:OH	2.15	0.93
1:C:357:MET:O	1:C:358:ILE:HD12	1.66	0.93
1:E:259:ARG:HH11	1:E:260:GLN:CB	1.80	0.93
1:B:401:ASN:CA	1:B:402:THR:OG1	2.16	0.93
1:D:304:LYS:CG	1:D:316:PHE:CZ	2.51	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:GLN:HA	1:E:299:GLN:OE1	1.65	0.93
1:C:62:LEU:HG	1:C:87:PHE:HE2	1.34	0.93
1:B:299:GLN:HE21	1:B:299:GLN:CA	1.78	0.93
1:C:195:ARG:HH12	1:C:358:ILE:N	1.66	0.92
1:B:51:LEU:HD11	1:B:93:PHE:CG	2.04	0.92
1:A:103:GLN:O	1:A:104:TYR:HB3	1.66	0.92
1:D:26:ILE:CD1	1:D:93:PHE:CE1	2.53	0.92
1:C:365:VAL:HG12	1:C:366:LEU:H	1.33	0.92
1:E:59:MET:HB2	1:E:128:MET:SD	2.08	0.92
1:C:38:ARG:HH21	1:C:261:GLU:CD	1.73	0.92
1:C:163:VAL:CG1	1:C:339:LYS:HD3	2.00	0.92
1:C:93:PHE:HD2	1:C:97:VAL:CG2	1.81	0.92
1:C:358:ILE:HD13	1:C:358:ILE:O	1.70	0.92
1:E:51:LEU:HD11	1:E:93:PHE:CB	2.01	0.91
1:D:26:ILE:HD11	1:D:93:PHE:HE1	1.32	0.91
1:E:86:GLU:CG	1:E:87:PHE:N	2.30	0.91
1:C:197:GLU:CD	1:C:358:ILE:HG21	1.90	0.91
1:B:193:GLN:HE21	1:B:350:GLU:HA	1.35	0.91
1:A:222:GLU:HG3	1:A:287:LYS:HG2	1.53	0.91
1:D:51:LEU:HD11	1:D:93:PHE:CB	2.01	0.91
1:A:277:GLU:OE2	1:A:277:GLU:CA	2.17	0.90
1:A:85:GLU:C	1:A:86:GLU:HG3	1.92	0.90
1:B:352:ALA:O	1:B:353:ALA:HB2	1.69	0.90
1:B:354:VAL:HG12	1:B:355:SER:O	1.61	0.90
1:E:181:ILE:HD11	1:E:337:ILE:CD1	2.00	0.90
1:A:287:LYS:HZ3	1:A:353:ALA:HB1	1.26	0.90
1:B:181:ILE:CD1	1:B:337:ILE:HD12	2.02	0.90
1:B:104:TYR:CD1	1:B:104:TYR:O	2.25	0.90
1:B:358:ILE:CG2	1:B:359:ALA:N	2.33	0.89
1:D:24:GLU:O	1:D:27:ALA:HB3	1.72	0.89
1:A:200:ARG:HH11	1:A:200:ARG:HB2	1.36	0.89
1:C:297:VAL:HG21	1:C:394:VAL:HG22	1.51	0.89
1:D:304:LYS:CG	1:D:316:PHE:CE1	2.51	0.89
1:E:163:VAL:HG13	1:E:339:LYS:CE	2.02	0.89
1:D:359:ALA:O	1:D:360:ILE:CG2	2.20	0.89
1:B:261:GLU:OE2	1:B:261:GLU:CA	2.20	0.89
1:B:405:HIS:O	1:B:406:ASP:HB2	1.73	0.89
1:C:206:LYS:NZ	1:C:396:HIS:HD2	1.70	0.89
1:B:293:PRO:O	1:B:295:PHE:HD2	1.55	0.89
1:B:353:ALA:HB1	1:B:354:VAL:O	1.72	0.89
1:A:86:GLU:O	1:A:89:PHE:HB3	1.72	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ALA:CB	1:B:354:VAL:O	2.21	0.88
1:C:365:VAL:HG12	1:C:366:LEU:N	1.88	0.88
1:D:359:ALA:O	1:D:360:ILE:HG12	1.72	0.88
1:D:366:LEU:HD23	1:D:367:TYR:N	1.88	0.88
1:C:195:ARG:HH12	1:C:358:ILE:HA	1.37	0.88
1:C:195:ARG:NH1	1:C:358:ILE:HA	1.87	0.88
1:B:299:GLN:NE2	1:B:300:GLU:N	2.17	0.88
1:B:57:MET:HE2	1:B:57:MET:HA	1.55	0.88
1:C:62:LEU:CD2	1:C:87:PHE:HE2	1.85	0.88
1:C:56:ALA:HA	1:C:59:MET:HE2	1.56	0.88
1:C:367:TYR:CB	1:C:368:PRO:CA	2.39	0.88
1:B:193:GLN:CG	1:B:349:SER:O	2.20	0.87
1:A:55:LEU:HD23	1:A:90:LEU:HD22	1.56	0.87
1:C:62:LEU:HG	1:C:87:PHE:CE2	2.09	0.87
1:C:93:PHE:CD2	1:C:97:VAL:HG22	2.08	0.87
1:E:156:GLU:OE2	1:E:164:LYS:HG3	1.75	0.86
1:A:94:SER:C	1:A:98:THR:HG21	1.96	0.86
1:D:118:PHE:HB3	1:D:331:ILE:HD11	1.58	0.86
1:E:119:HIS:O	1:E:326:SER:CB	2.24	0.86
1:C:268:GLU:CB	1:C:269:PRO:HD3	2.06	0.86
1:A:104:TYR:O	1:A:104:TYR:CD1	2.29	0.86
1:C:357:MET:O	1:C:357:MET:SD	2.34	0.86
1:E:109:ALA:HB1	1:E:154:TRP:CZ3	2.11	0.86
1:E:181:ILE:HD11	1:E:337:ILE:HD12	1.55	0.85
1:C:89:PHE:C	1:C:89:PHE:CD2	2.45	0.85
1:B:407:PHE:C	1:B:407:PHE:CD2	2.48	0.85
1:A:62:LEU:HD21	1:A:87:PHE:CE2	2.12	0.85
1:C:263:PRO:HB2	1:C:266:THR:CB	2.06	0.85
1:A:103:GLN:HG3	1:A:247:GLU:HB3	1.59	0.85
1:B:51:LEU:HD11	1:B:93:PHE:HB3	1.56	0.85
1:B:238:ILE:O	1:B:238:ILE:HG13	1.74	0.85
1:E:120:VAL:HG22	1:E:325:LEU:CD1	2.07	0.85
1:C:267:LEU:CD1	1:C:267:LEU:C	2.44	0.84
1:B:354:VAL:CB	1:B:355:SER:HA	2.03	0.84
1:B:356:GLY:C	1:B:360:ILE:HB	1.97	0.84
1:E:362:ARG:CD	1:E:363:MET:H	1.88	0.84
1:D:42:GLU:O	1:D:43:ASP:HB3	1.76	0.84
1:A:106:MET:CE	1:A:108:ILE:HD11	2.07	0.84
1:C:118:PHE:CD2	1:C:331:ILE:HG13	2.13	0.84
1:D:362:ARG:CG	1:D:363:MET:H	1.89	0.84
1:C:89:PHE:O	1:C:89:PHE:CD2	2.29	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:ARG:NH1	1:E:260:GLN:CB	2.39	0.84
1:A:94:SER:O	1:A:98:THR:CG2	2.25	0.84
1:D:304:LYS:HD3	1:D:316:PHE:CG	2.13	0.84
1:E:87:PHE:H	1:E:87:PHE:HD1	1.20	0.84
1:E:163:VAL:HG12	1:E:339:LYS:HE2	1.58	0.84
1:A:104:TYR:HA	1:A:188:GLY:HA2	1.57	0.83
1:B:299:GLN:HE21	1:B:299:GLN:C	1.80	0.83
1:E:364:ALA:CB	1:E:365:VAL:C	2.43	0.83
1:A:51:LEU:HD11	1:A:93:PHE:CB	2.09	0.83
1:D:362:ARG:HG2	1:D:363:MET:N	1.93	0.83
1:B:354:VAL:HG11	1:B:355:SER:O	1.79	0.83
1:A:336:ALA:C	1:A:337:ILE:HD13	1.98	0.83
1:C:362:ARG:O	1:C:363:MET:HB3	1.76	0.83
1:C:229:SER:HB2	1:D:365:VAL:HG22	1.61	0.83
1:E:191:LYS:HE2	1:E:249:ASP:OD1	1.78	0.82
1:D:304:LYS:HE2	1:D:316:PHE:CD1	2.15	0.82
1:B:353:ALA:CA	1:B:354:VAL:O	2.28	0.82
1:E:364:ALA:HB1	1:E:366:LEU:CB	2.09	0.82
1:B:406:ASP:OD1	1:B:407:PHE:N	2.12	0.82
1:C:261:GLU:O	1:C:262:VAL:CG2	2.26	0.82
1:E:181:ILE:CD1	1:E:337:ILE:HD12	2.09	0.82
1:C:62:LEU:CG	1:C:87:PHE:HE2	1.91	0.81
1:B:120:VAL:HG22	1:B:325:LEU:CD1	2.09	0.81
1:C:175:ALA:HB3	1:C:176:THR:HA	1.62	0.81
1:E:124:PHE:CZ	1:E:128:MET:HE3	2.15	0.81
1:E:259:ARG:HD3	1:E:260:GLN:H	1.41	0.81
1:A:24:GLU:O	1:A:27:ALA:HB3	1.80	0.81
1:A:399:THR:OG1	1:A:400:MET:N	2.06	0.81
1:C:195:ARG:NH1	1:C:358:ILE:CA	2.44	0.81
1:B:109:ALA:HB1	1:B:154:TRP:CZ3	2.16	0.81
1:B:299:GLN:NE2	1:B:299:GLN:CA	2.38	0.81
1:C:100:LYS:HE3	1:C:105:VAL:HG11	1.62	0.81
1:A:337:ILE:CD1	1:A:337:ILE:N	2.44	0.81
1:A:85:GLU:O	1:A:86:GLU:HG3	1.80	0.81
1:B:206:LYS:NZ	1:B:396:HIS:HD2	1.78	0.81
1:E:121:ASN:N	1:E:325:LEU:O	2.13	0.80
1:E:289:GLU:OE1	1:E:369:GLN:NE2	2.14	0.80
1:B:166:LEU:HD23	1:B:181:ILE:HG13	1.64	0.80
1:B:51:LEU:HD11	1:B:93:PHE:CB	2.12	0.80
1:A:31:VAL:HA	1:A:391:MET:HE1	1.63	0.80
1:B:353:ALA:HA	1:B:354:VAL:O	1.80	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:PHE:CD2	1:B:407:PHE:O	2.34	0.80
1:C:100:LYS:HE3	1:C:105:VAL:HG13	1.62	0.80
1:E:362:ARG:O	1:E:363:MET:O	2.00	0.80
1:B:166:LEU:CD2	1:B:181:ILE:HG13	2.11	0.80
1:E:287:LYS:HB3	1:E:367:TYR:CE2	2.17	0.80
1:A:366:LEU:C	1:A:366:LEU:HD23	2.02	0.80
1:D:359:ALA:O	1:D:360:ILE:CG1	2.29	0.80
1:E:191:LYS:HE3	1:E:245:PRO:HB2	1.62	0.80
1:E:315:ILE:HD11	1:E:316:PHE:CE2	2.16	0.80
1:A:215:PRO:HG2	1:A:294:ARG:HB3	1.63	0.80
1:C:56:ALA:HA	1:C:59:MET:CE	2.11	0.80
1:B:104:TYR:HA	1:B:188:GLY:HA2	1.62	0.79
1:D:374:HIS:HB2	1:D:375:PRO:HD2	1.64	0.79
1:A:62:LEU:CD2	1:A:87:PHE:CE2	2.65	0.79
1:A:176:THR:O	1:A:177:TYR:HB2	1.82	0.79
1:B:103:GLN:O	1:B:104:TYR:HB3	1.81	0.79
1:B:358:ILE:CG2	1:B:359:ALA:H	1.95	0.79
1:D:26:ILE:HD12	1:D:93:PHE:CE1	2.15	0.79
1:B:354:VAL:CA	1:B:356:GLY:N	2.46	0.79
1:C:267:LEU:HD13	1:C:267:LEU:O	1.83	0.79
1:E:364:ALA:CB	1:E:366:LEU:CB	2.53	0.79
1:D:121:ASN:N	1:D:325:LEU:O	2.15	0.79
1:C:142:SER:OG	1:C:174:ALA:CB	2.31	0.79
1:A:289:GLU:HG3	1:A:369:GLN:NE2	1.97	0.79
1:A:287:LYS:HZ1	1:A:353:ALA:CB	1.94	0.78
1:B:315:ILE:HD11	1:B:316:PHE:CE2	2.17	0.78
1:C:265:ALA:O	1:C:269:PRO:HD2	1.82	0.78
1:A:43:ASP:OD1	1:A:43:ASP:O	2.01	0.78
1:D:62:LEU:HD21	1:D:87:PHE:CE2	2.17	0.78
1:E:362:ARG:CD	1:E:363:MET:N	2.46	0.78
1:B:352:ALA:O	1:B:353:ALA:CB	2.31	0.78
1:C:195:ARG:HH12	1:C:358:ILE:H	1.30	0.78
1:D:314:GLU:O	1:D:320:ALA:CB	2.32	0.78
1:A:289:GLU:HG3	1:A:369:GLN:HE22	1.49	0.78
1:B:357:MET:O	1:B:358:ILE:O	2.01	0.78
1:D:119:HIS:O	1:D:326:SER:CB	2.31	0.78
1:C:43:ASP:CG	1:C:43:ASP:O	2.22	0.78
1:B:28:ASP:O	1:B:32:ASN:HB2	1.83	0.77
1:B:368:PRO:HD3	1:D:360:ILE:HG22	1.66	0.77
1:D:104:TYR:HA	1:D:188:GLY:HA2	1.63	0.77
1:B:354:VAL:HG12	1:B:356:GLY:HA3	1.66	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLU:CB	1:C:269:PRO:CD	2.53	0.77
1:B:351:ALA:O	1:B:352:ALA:HB2	1.84	0.77
1:B:23:GLU:N	1:B:89:PHE:HZ	1.82	0.77
1:C:315:ILE:HD11	1:C:316:PHE:CE2	2.19	0.77
1:B:362:ARG:HG3	1:C:367:TYR:HD1	1.49	0.77
1:B:206:LYS:NZ	1:B:396:HIS:CD2	2.53	0.77
1:B:405:HIS:O	1:B:406:ASP:CB	2.33	0.77
1:E:86:GLU:HG2	1:E:87:PHE:HD1	1.50	0.77
1:B:59:MET:HE3	1:B:180:LEU:HD13	1.67	0.76
1:B:360:ILE:CG2	1:B:361:SER:N	2.33	0.76
1:D:51:LEU:CD1	1:D:93:PHE:HD1	1.84	0.76
1:E:97:VAL:HA	1:E:104:TYR:OH	1.85	0.76
1:B:57:MET:HA	1:B:57:MET:CE	2.16	0.76
1:A:374:HIS:HB2	1:A:375:PRO:CD	2.15	0.76
1:C:97:VAL:HA	1:C:104:TYR:OH	1.85	0.76
1:E:287:LYS:HD3	1:E:367:TYR:CZ	2.21	0.76
1:A:51:LEU:CD1	1:A:93:PHE:HB3	2.16	0.76
1:B:121:ASN:N	1:B:325:LEU:O	2.18	0.76
1:C:283:VAL:HG23	1:C:283:VAL:O	1.84	0.76
1:C:265:ALA:O	1:C:269:PRO:CD	2.34	0.76
1:C:118:PHE:CD2	1:C:328:ASN:ND2	2.54	0.76
1:C:265:ALA:O	1:C:269:PRO:HG2	1.86	0.76
1:C:120:VAL:HG22	1:C:325:LEU:HD12	1.68	0.76
1:D:120:VAL:HG22	1:D:325:LEU:CD1	2.15	0.76
1:C:62:LEU:CD2	1:C:87:PHE:CE2	2.70	0.75
1:C:197:GLU:OE2	1:C:358:ILE:HG21	1.85	0.75
1:D:358:ILE:O	1:D:359:ALA:HB2	1.83	0.75
1:A:106:MET:HE1	1:A:108:ILE:HD11	1.69	0.75
1:C:362:ARG:O	1:C:363:MET:HB2	1.84	0.75
1:A:86:GLU:O	1:A:89:PHE:CB	2.34	0.75
1:B:36:ARG:NH2	1:B:305:ASP:OD1	2.18	0.75
1:E:115:GLN:HG3	1:E:116:ASN:N	2.02	0.75
1:A:59:MET:CE	1:A:110:ASN:ND2	2.49	0.75
1:D:59:MET:CE	1:D:110:ASN:OD1	2.35	0.75
1:D:62:LEU:CD2	1:D:87:PHE:CE2	2.69	0.75
1:E:259:ARG:HH11	1:E:260:GLN:HB3	1.52	0.74
1:D:178:LEU:CD1	1:D:333:LEU:HA	2.17	0.74
1:A:103:GLN:HB2	1:A:189:ASN:HB2	1.69	0.74
1:A:120:VAL:HG22	1:A:325:LEU:CD1	2.17	0.74
1:B:33:MET:HE1	1:B:53:ILE:HD12	1.68	0.74
1:D:297:VAL:HG21	1:D:394:VAL:HG22	1.68	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:186:PHE:HD2	1:C:342:LEU:HD11	1.52	0.74
1:D:101:GLU:O	1:D:102:SER:CB	2.34	0.74
1:D:108:ILE:HD12	1:D:108:ILE:O	1.87	0.74
1:A:222:GLU:HG3	1:A:287:LYS:HE3	1.70	0.74
1:D:104:TYR:O	1:D:104:TYR:CD1	2.40	0.74
1:B:315:ILE:HD13	1:B:333:LEU:HD23	1.68	0.74
1:C:365:VAL:O	1:C:366:LEU:HG	1.88	0.74
1:C:267:LEU:C	1:C:267:LEU:HD13	2.08	0.74
1:A:109:ALA:HB1	1:A:154:TRP:CZ3	2.23	0.73
1:A:206:LYS:NZ	1:A:396:HIS:HD2	1.86	0.73
1:C:120:VAL:HG22	1:C:325:LEU:CD1	2.18	0.73
1:D:124:PHE:CZ	1:D:128:MET:HE3	2.23	0.73
1:E:86:GLU:OE1	1:E:87:PHE:CE1	2.41	0.73
1:E:206:LYS:NZ	1:E:396:HIS:HD2	1.86	0.73
1:A:34:TYR:HB2	1:A:391:MET:CE	2.18	0.73
1:D:59:MET:HB2	1:D:128:MET:SD	2.27	0.73
1:C:357:MET:O	1:C:358:ILE:CD1	2.34	0.73
1:E:124:PHE:CZ	1:E:128:MET:CE	2.70	0.73
1:E:163:VAL:HG13	1:E:339:LYS:HE3	1.69	0.73
1:A:337:ILE:HD13	1:A:337:ILE:N	2.01	0.73
1:C:178:LEU:CD1	1:C:333:LEU:HA	2.18	0.73
1:C:193:GLN:OE1	1:C:347:GLU:C	2.26	0.73
1:A:104:TYR:CD1	1:A:104:TYR:C	2.62	0.73
1:B:297:VAL:HG21	1:B:394:VAL:HG22	1.71	0.73
1:D:360:ILE:O	1:D:361:SER:CB	2.36	0.73
1:A:193:GLN:HG3	1:A:193:GLN:O	1.86	0.73
1:E:163:VAL:HG13	1:E:339:LYS:HE2	1.61	0.73
1:C:100:LYS:CG	1:C:105:VAL:HG13	2.19	0.72
1:C:175:ALA:CB	1:C:176:THR:HA	2.18	0.72
1:B:206:LYS:HZ3	1:B:396:HIS:CD2	2.06	0.72
1:E:118:PHE:HZ	1:E:177:TYR:CD2	2.07	0.72
1:C:59:MET:HB2	1:C:128:MET:SD	2.28	0.72
1:A:274:GLN:CA	1:A:274:GLN:NE2	2.35	0.72
1:E:86:GLU:OE1	1:E:87:PHE:HE1	1.71	0.72
1:D:26:ILE:HD11	1:D:93:PHE:CE1	2.22	0.72
1:D:238:ILE:HD11	1:D:259:ARG:CZ	2.18	0.72
1:D:304:LYS:HG3	1:D:316:PHE:CD1	2.24	0.72
1:E:176:THR:HG22	1:E:334:SER:OG	1.90	0.72
1:B:33:MET:CE	1:B:53:ILE:HD12	2.20	0.72
1:C:365:VAL:O	1:C:366:LEU:CB	2.37	0.72
1:E:104:TYR:O	1:E:104:TYR:CD1	2.42	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:GLN:HG3	1:E:116:ASN:H	1.54	0.72
1:B:354:VAL:HA	1:B:356:GLY:N	2.05	0.72
1:C:59:MET:HE1	1:C:110:ASN:OD1	1.90	0.72
1:C:365:VAL:CG1	1:C:366:LEU:H	2.03	0.71
1:E:298:GLU:HG3	1:E:341:PHE:HD1	1.56	0.71
1:B:362:ARG:CG	1:C:367:TYR:HD1	2.03	0.71
1:C:178:LEU:HD11	1:C:333:LEU:HA	1.72	0.71
1:A:34:TYR:HB2	1:A:391:MET:HE2	1.72	0.71
1:B:181:ILE:HD11	1:B:337:ILE:CD1	2.15	0.71
1:C:360:ILE:O	1:C:361:SER:O	2.08	0.71
1:D:52:SER:HB3	1:D:184:VAL:HG21	1.72	0.71
1:E:321:ASN:OD1	1:E:323:THR:HG23	1.90	0.71
1:A:57:MET:HA	1:A:57:MET:CE	2.20	0.71
1:A:299:GLN:OE1	1:A:299:GLN:CA	2.34	0.71
1:A:315:ILE:HD11	1:A:316:PHE:CE2	2.25	0.71
1:E:299:GLN:OE1	1:E:299:GLN:CA	2.36	0.71
1:E:51:LEU:CD1	1:E:93:PHE:CG	2.74	0.71
1:B:407:PHE:C	1:B:407:PHE:HD2	1.94	0.71
1:B:61:GLU:OE2	1:B:73:ARG:HG2	1.91	0.70
1:C:206:LYS:HZ3	1:C:396:HIS:HD2	1.38	0.70
1:E:191:LYS:CE	1:E:249:ASP:OD1	2.39	0.70
1:B:51:LEU:CD1	1:B:93:PHE:CD1	2.74	0.70
1:A:106:MET:HE3	1:A:108:ILE:HD11	1.73	0.70
1:C:195:ARG:NH1	1:C:358:ILE:CG2	2.54	0.70
1:C:239:TYR:CD1	1:C:239:TYR:N	2.56	0.70
1:D:109:ALA:HB1	1:D:154:TRP:HZ3	1.55	0.70
1:D:118:PHE:CB	1:D:331:ILE:HD11	2.22	0.70
1:D:359:ALA:O	1:D:360:ILE:CB	2.39	0.70
1:E:176:THR:N	1:E:177:TYR:HA	2.06	0.70
1:A:259:ARG:HH21	1:B:362:ARG:NH1	1.89	0.70
1:D:359:ALA:C	1:D:360:ILE:HG23	2.10	0.70
1:A:59:MET:CB	1:A:128:MET:HE1	2.21	0.70
1:E:364:ALA:CA	1:E:365:VAL:CG2	2.28	0.70
1:A:99:ALA:O	1:A:101:GLU:OE2	2.10	0.70
1:B:102:SER:O	1:B:103:GLN:CB	2.40	0.70
1:B:351:ALA:O	1:B:352:ALA:CB	2.39	0.70
1:B:356:GLY:CA	1:B:360:ILE:CD1	2.58	0.70
1:C:206:LYS:HZ3	1:C:396:HIS:CD2	2.09	0.70
1:E:176:THR:H	1:E:177:TYR:HA	1.55	0.70
1:C:315:ILE:HD13	1:C:333:LEU:HD23	1.74	0.70
1:D:52:SER:CB	1:D:184:VAL:HG21	2.22	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:O	1:A:392:GLY:CA	2.40	0.70
1:A:101:GLU:OE2	1:A:101:GLU:N	2.24	0.70
1:B:93:PHE:O	1:B:97:VAL:HG23	1.91	0.69
1:B:260:GLN:HE21	1:B:261:GLU:H	0.72	0.69
1:C:283:VAL:O	1:C:283:VAL:CG2	2.40	0.69
1:D:315:ILE:HD11	1:D:316:PHE:CE2	2.27	0.69
1:B:404:GLY:O	1:B:405:HIS:HD2	1.75	0.69
1:D:104:TYR:CD1	1:D:104:TYR:C	2.65	0.69
1:E:24:GLU:O	1:E:27:ALA:HB3	1.91	0.69
1:C:315:ILE:CD1	1:C:316:PHE:CE2	2.75	0.69
1:A:291:TYR:HB2	1:A:371:ILE:HA	1.75	0.69
1:E:118:PHE:CZ	1:E:177:TYR:CD2	2.80	0.69
1:C:365:VAL:O	1:C:366:LEU:HB2	1.92	0.69
1:D:118:PHE:CD2	1:D:328:ASN:ND2	2.60	0.69
1:A:178:LEU:HD13	1:A:333:LEU:HD12	1.75	0.69
1:C:239:TYR:CE2	1:C:266:THR:HG21	2.28	0.69
1:B:353:ALA:CA	1:B:354:VAL:C	2.57	0.69
1:D:351:ALA:O	1:D:352:ALA:HB3	1.92	0.69
1:A:94:SER:C	1:A:98:THR:CG2	2.61	0.69
1:A:221:GLY:HA2	1:A:287:LYS:CE	2.23	0.69
1:B:109:ALA:HB1	1:B:154:TRP:HZ3	1.57	0.69
1:B:178:LEU:CD1	1:B:333:LEU:HA	2.22	0.69
1:B:234:GLU:HG2	1:B:235:ALA:HB2	1.73	0.69
1:E:56:ALA:HA	1:E:110:ASN:HD21	1.55	0.69
1:E:86:GLU:HG2	1:E:87:PHE:CD1	2.27	0.69
1:E:104:TYR:HA	1:E:188:GLY:HA2	1.75	0.69
1:C:55:LEU:HD23	1:C:90:LEU:HD22	1.73	0.69
1:D:238:ILE:CD1	1:D:259:ARG:NH1	2.49	0.69
1:C:239:TYR:CZ	1:C:266:THR:HG21	2.28	0.68
1:C:94:SER:O	1:C:98:THR:HG21	1.94	0.68
1:B:354:VAL:CB	1:B:356:GLY:N	2.56	0.68
1:C:173:ASP:O	1:C:176:THR:HG23	1.92	0.68
1:D:178:LEU:HD11	1:D:333:LEU:HA	1.76	0.68
1:C:173:ASP:O	1:C:175:ALA:N	2.26	0.68
1:D:357:MET:CB	1:D:358:ILE:CA	2.39	0.68
1:A:86:GLU:C	1:A:88:SER:H	1.97	0.68
1:A:222:GLU:HB3	1:A:285:LYS:HE2	1.75	0.68
1:E:259:ARG:CD	1:E:260:GLN:H	2.06	0.68
1:A:120:VAL:HG13	1:A:325:LEU:HD12	1.75	0.68
1:A:206:LYS:HZ2	1:A:396:HIS:HD2	1.42	0.68
1:C:195:ARG:NH1	1:C:358:ILE:HG23	2.07	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:MET:HE3	1:B:180:LEU:CD1	2.23	0.68
1:B:178:LEU:HD11	1:B:333:LEU:HA	1.76	0.68
1:E:206:LYS:HZ1	1:E:396:HIS:HD2	1.41	0.68
1:A:62:LEU:CD2	1:A:87:PHE:HE2	2.05	0.68
1:A:89:PHE:CD2	1:A:93:PHE:HZ	2.12	0.68
1:C:364:ALA:O	1:C:367:TYR:CE2	2.46	0.68
1:E:86:GLU:O	1:E:88:SER:N	2.27	0.68
1:A:178:LEU:HD11	1:A:333:LEU:HA	1.76	0.67
1:A:193:GLN:CG	1:A:349:SER:O	2.39	0.67
1:E:120:VAL:HG22	1:E:325:LEU:HD12	1.74	0.67
1:B:293:PRO:O	1:B:295:PHE:CD2	2.45	0.67
1:C:186:PHE:HD2	1:C:342:LEU:CD1	2.05	0.67
1:C:262:VAL:O	1:C:262:VAL:CG1	2.36	0.67
1:D:103:GLN:HE21	1:D:104:TYR:H	1.42	0.67
1:E:57:MET:HE2	1:E:57:MET:HA	1.76	0.67
1:E:104:TYR:CD1	1:E:104:TYR:C	2.67	0.67
1:B:166:LEU:CD1	1:B:339:LYS:HB3	2.24	0.67
1:C:271:VAL:O	1:C:274:GLN:HG3	1.93	0.67
1:D:51:LEU:HD11	1:D:93:PHE:CG	2.29	0.67
1:D:74:HIS:HA	1:D:78:TYR:HB2	1.75	0.67
1:C:93:PHE:CD2	1:C:97:VAL:CG2	2.72	0.67
1:E:175:ALA:O	1:E:177:TYR:CD1	2.48	0.67
1:D:175:ALA:O	1:D:177:TYR:N	2.28	0.67
1:B:115:GLN:HG3	1:B:116:ASN:N	2.10	0.67
1:C:365:VAL:CG1	1:C:366:LEU:N	2.58	0.67
1:D:358:ILE:O	1:D:359:ALA:CB	2.43	0.67
1:E:191:LYS:CE	1:E:245:PRO:HB2	2.24	0.67
1:A:178:LEU:CD1	1:A:333:LEU:HA	2.25	0.66
1:D:366:LEU:HD23	1:D:366:LEU:C	2.15	0.66
1:D:71:GLU:OE2	1:D:314:GLU:CG	2.43	0.66
1:E:166:LEU:CD1	1:E:339:LYS:HB3	2.25	0.66
1:A:118:PHE:HB3	1:A:331:ILE:HD11	1.76	0.66
1:D:51:LEU:HD11	1:D:93:PHE:CD1	2.28	0.66
1:E:87:PHE:C	1:E:89:PHE:H	1.98	0.66
1:E:364:ALA:HB1	1:E:366:LEU:N	2.11	0.66
1:C:358:ILE:CD1	1:C:358:ILE:O	2.43	0.66
1:D:68:THR:HG23	1:D:314:GLU:HB3	1.78	0.66
1:B:124:PHE:CZ	1:B:128:MET:CE	2.78	0.66
1:E:62:LEU:HD12	1:E:128:MET:HE1	1.76	0.66
1:B:354:VAL:CG1	1:B:356:GLY:N	2.48	0.66
1:C:277:GLU:O	1:C:279:TRP:N	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:LYS:NZ	1:A:396:HIS:CD2	2.62	0.66
1:B:50:PRO:HG3	1:B:388:ILE:HG22	1.77	0.66
1:C:24:GLU:O	1:C:27:ALA:HB3	1.96	0.66
1:C:206:LYS:NZ	1:C:396:HIS:CD2	2.59	0.66
1:C:271:VAL:HG12	1:C:272:LYS:N	2.10	0.66
1:C:357:MET:C	1:C:357:MET:SD	2.73	0.66
1:A:287:LYS:HZ2	1:A:353:ALA:HB1	1.59	0.65
1:B:356:GLY:CA	1:B:360:ILE:CG1	2.74	0.65
1:C:26:ILE:O	1:C:30:SER:OG	2.13	0.65
1:C:173:ASP:C	1:C:175:ALA:H	1.99	0.65
1:D:51:LEU:CD1	1:D:93:PHE:CG	2.78	0.65
1:D:366:LEU:C	1:D:366:LEU:CD2	2.65	0.65
1:A:124:PHE:O	1:A:128:MET:HG2	1.96	0.65
1:B:401:ASN:HA	1:B:402:THR:CG2	2.25	0.65
1:C:362:ARG:NH1	1:E:371:ILE:HG21	2.10	0.65
1:B:62:LEU:CD1	1:B:128:MET:HE2	2.24	0.65
1:A:121:ASN:N	1:A:325:LEU:O	2.28	0.65
1:C:197:GLU:CD	1:C:358:ILE:CG2	2.65	0.65
1:C:265:ALA:O	1:C:269:PRO:CG	2.44	0.65
1:C:367:TYR:HB3	1:C:368:PRO:C	2.16	0.65
1:E:43:ASP:CG	1:E:43:ASP:O	2.35	0.65
1:A:57:MET:HA	1:A:57:MET:HE2	1.79	0.65
1:A:247:GLU:OE2	1:A:247:GLU:C	2.34	0.65
1:B:102:SER:O	1:B:103:GLN:HB2	1.94	0.65
1:B:206:LYS:NZ	1:B:398:GLU:OE2	2.30	0.65
1:B:296:THR:HG21	1:B:400:MET:HE2	1.78	0.65
1:C:124:PHE:CZ	1:C:128:MET:CE	2.80	0.65
1:D:23:GLU:HG2	1:D:387:THR:OG1	1.97	0.65
1:D:101:GLU:O	1:D:102:SER:HB2	1.96	0.65
1:A:120:VAL:HG22	1:A:325:LEU:HD12	1.79	0.65
1:D:23:GLU:CD	1:D:89:PHE:HZ	1.99	0.65
1:A:304:LYS:HE2	1:A:316:PHE:CD1	2.32	0.65
1:C:95:ASN:HA	1:C:98:THR:HG22	1.77	0.65
1:D:92:GLU:HG3	1:D:96:MET:CG	2.27	0.65
1:B:236:GLY:O	1:B:238:ILE:HG23	1.96	0.65
1:C:315:ILE:HD12	1:C:316:PHE:CD2	2.32	0.65
1:D:71:GLU:OE2	1:D:314:GLU:HG2	1.95	0.65
1:E:167:VAL:CG1	1:E:337:ILE:HD13	2.26	0.65
1:A:182:ASN:O	1:A:338:HIS:HA	1.96	0.64
1:A:287:LYS:HZ3	1:A:353:ALA:CB	1.99	0.64
1:A:104:TYR:O	1:A:104:TYR:CG	2.50	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:CG	1:B:235:ALA:HB2	2.27	0.64
1:E:315:ILE:CD1	1:E:316:PHE:CE2	2.80	0.64
1:D:59:MET:HE1	1:D:110:ASN:OD1	1.95	0.64
1:E:55:LEU:HD23	1:E:90:LEU:HD22	1.78	0.64
1:E:363:MET:HG3	1:E:364:ALA:N	2.11	0.64
1:C:52:SER:OG	1:C:182:ASN:OD1	2.16	0.64
1:C:278:GLU:O	1:C:281:ASN:HB2	1.98	0.64
1:A:277:GLU:OE2	1:A:277:GLU:N	2.31	0.64
1:B:98:THR:O	1:B:100:LYS:N	2.26	0.64
1:E:175:ALA:CB	1:E:176:THR:HA	2.27	0.64
1:C:374:HIS:HB2	1:C:375:PRO:HD2	1.80	0.64
1:D:166:LEU:O	1:D:300:GLU:OE2	2.15	0.64
1:E:36:ARG:NH2	1:E:305:ASP:OD1	2.30	0.64
1:A:33:MET:HG2	1:A:306:VAL:CG1	2.28	0.64
1:B:139:VAL:HB	1:B:147:VAL:HG23	1.80	0.64
1:A:297:VAL:HG21	1:A:394:VAL:HG22	1.78	0.63
1:B:51:LEU:HD11	1:B:93:PHE:CD1	2.33	0.63
1:C:224:TYR:HB2	1:C:243:GLU:HB3	1.80	0.63
1:B:404:GLY:O	1:B:405:HIS:CD2	2.51	0.63
1:D:23:GLU:CD	1:D:89:PHE:CZ	2.72	0.63
1:D:238:ILE:HD11	1:D:259:ARG:HH12	1.60	0.63
1:E:178:LEU:HD12	1:E:332:PHE:O	1.97	0.63
1:E:362:ARG:O	1:E:363:MET:C	2.36	0.63
1:E:365:VAL:O	1:E:367:TYR:HB2	1.98	0.63
1:D:315:ILE:HD11	1:D:316:PHE:CZ	2.33	0.63
1:E:56:ALA:CA	1:E:110:ASN:HD21	2.10	0.63
1:C:107:LYS:O	1:C:184:VAL:HA	1.99	0.63
1:A:42:GLU:O	1:A:43:ASP:HB3	1.98	0.63
1:A:193:GLN:HB3	1:A:348:GLY:C	2.18	0.63
1:C:87:PHE:HD1	1:C:87:PHE:H	1.43	0.63
1:C:264:LEU:O	1:C:267:LEU:N	2.32	0.63
1:D:68:THR:HG23	1:D:314:GLU:CB	2.28	0.63
1:B:118:PHE:CG	1:B:331:ILE:HD11	2.34	0.63
1:C:124:PHE:CZ	1:C:128:MET:HE3	2.34	0.63
1:C:267:LEU:C	1:C:267:LEU:HD12	2.18	0.63
1:B:45:ASN:H	1:B:395:MET:HG2	1.64	0.62
1:D:120:VAL:HG22	1:D:325:LEU:HD12	1.81	0.62
1:D:124:PHE:CZ	1:D:128:MET:CE	2.82	0.62
1:E:57:MET:HA	1:E:57:MET:CE	2.29	0.62
1:C:121:ASN:N	1:C:325:LEU:O	2.32	0.62
1:D:98:THR:O	1:D:99:ALA:C	2.36	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:GLN:OE1	1:E:300:GLU:N	2.30	0.62
1:B:162:LEU:HD13	1:B:185:TYR:CE2	2.34	0.62
1:A:52:SER:OG	1:A:182:ASN:OD1	2.18	0.62
1:C:109:ALA:HB1	1:C:154:TRP:CZ3	2.35	0.62
1:B:51:LEU:CD1	1:B:93:PHE:CG	2.82	0.62
1:B:233:ASN:O	1:B:234:GLU:HB2	1.99	0.62
1:D:176:THR:O	1:D:177:TYR:HB2	2.00	0.62
1:B:356:GLY:HA2	1:B:360:ILE:CG1	2.29	0.62
1:B:356:GLY:HA2	1:B:360:ILE:HG13	1.80	0.62
1:C:365:VAL:O	1:C:366:LEU:CG	2.48	0.62
1:A:46:ILE:O	1:A:392:GLY:HA3	1.99	0.62
1:C:357:MET:SD	1:C:357:MET:N	2.73	0.62
1:B:291:TYR:HB2	1:B:371:ILE:HA	1.81	0.61
1:D:92:GLU:HG3	1:D:96:MET:HG3	1.82	0.61
1:B:403:SER:O	1:B:405:HIS:N	2.33	0.61
1:A:26:ILE:HD12	1:A:387:THR:HG23	1.83	0.61
1:A:103:GLN:O	1:A:104:TYR:CB	2.44	0.61
1:A:113:PHE:O	1:A:178:LEU:HA	2.00	0.61
1:B:124:PHE:CZ	1:B:128:MET:HE3	2.36	0.61
1:C:357:MET:O	1:C:358:ILE:C	2.39	0.61
1:A:36:ARG:NH2	1:A:305:ASP:OD1	2.33	0.61
1:B:400:MET:O	1:B:401:ASN:HB2	2.01	0.61
1:C:267:LEU:CD1	1:C:267:LEU:O	2.46	0.61
1:D:33:MET:HE1	1:D:53:ILE:CD1	2.31	0.61
1:B:355:SER:O	1:B:357:MET:HG3	2.01	0.61
1:B:354:VAL:CG1	1:B:356:GLY:HA3	2.31	0.61
1:C:232:SER:O	1:C:233:ASN:HB2	2.00	0.61
1:A:118:PHE:CB	1:A:331:ILE:HD11	2.31	0.61
1:B:354:VAL:CG1	1:B:356:GLY:CA	2.72	0.61
1:B:361:SER:HB2	1:B:363:MET:HG2	1.80	0.61
1:A:368:PRO:HA	1:D:364:ALA:HA	1.81	0.60
1:D:42:GLU:O	1:D:43:ASP:CB	2.49	0.60
1:D:120:VAL:HG13	1:D:325:LEU:HD12	1.82	0.60
1:B:362:ARG:HB2	1:C:367:TYR:CD1	2.36	0.60
1:E:115:GLN:HB3	1:E:118:PHE:CD1	2.36	0.60
1:E:364:ALA:C	1:E:365:VAL:CG2	2.68	0.60
1:A:62:LEU:CD1	1:A:132:PHE:HE2	2.14	0.60
1:E:59:MET:HG2	1:E:60:MET:H	1.67	0.60
1:E:287:LYS:CB	1:E:367:TYR:CE2	2.84	0.60
1:B:118:PHE:CD2	1:B:328:ASN:ND2	2.70	0.60
1:E:191:LYS:NZ	1:E:249:ASP:OD1	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:ILE:HD12	1:E:316:PHE:CD2	2.35	0.60
1:D:268:GLU:O	1:D:271:VAL:HG23	2.01	0.60
1:E:23:GLU:HG2	1:E:387:THR:OG1	2.02	0.60
1:E:103:GLN:CA	1:E:103:GLN:NE2	2.37	0.60
1:C:186:PHE:CD2	1:C:342:LEU:HD11	2.35	0.60
1:C:267:LEU:O	1:C:270:LEU:HB2	2.02	0.60
1:D:33:MET:CE	1:D:53:ILE:HD13	2.32	0.60
1:D:304:LYS:CD	1:D:316:PHE:CD1	2.84	0.60
1:C:195:ARG:NH1	1:C:358:ILE:H	1.98	0.59
1:B:166:LEU:HD23	1:B:181:ILE:CG1	2.31	0.59
1:C:62:LEU:HD21	1:C:127:MET:HG2	1.83	0.59
1:C:214:ILE:HD13	1:C:293:PRO:HB3	1.84	0.59
1:C:300:GLU:HB2	1:C:339:LYS:HG3	1.84	0.59
1:E:397:PRO:HD2	1:E:398:GLU:OE1	2.02	0.59
1:A:85:GLU:O	1:A:86:GLU:CG	2.48	0.59
1:B:254:MET:HE3	1:B:381:ARG:HD3	1.83	0.59
1:B:362:ARG:HG3	1:C:367:TYR:CD1	2.35	0.59
1:A:103:GLN:CG	1:A:247:GLU:HB3	2.32	0.59
1:E:86:GLU:O	1:E:89:PHE:N	2.35	0.59
1:A:85:GLU:C	1:A:86:GLU:CG	2.68	0.59
1:B:52:SER:OG	1:B:182:ASN:OD1	2.19	0.59
1:B:59:MET:CB	1:B:128:MET:SD	2.81	0.59
1:B:193:GLN:HB3	1:B:348:GLY:CA	2.32	0.59
1:A:118:PHE:CD2	1:A:328:ASN:ND2	2.71	0.59
1:B:104:TYR:CD1	1:B:104:TYR:C	2.75	0.59
1:B:238:ILE:CA	1:B:239:TYR:HB3	2.27	0.59
1:C:45:ASN:OD1	1:C:395:MET:N	2.31	0.59
1:B:22:PRO:C	1:B:89:PHE:HZ	2.06	0.59
1:D:361:SER:O	1:D:362:ARG:HB2	2.03	0.59
1:E:87:PHE:C	1:E:89:PHE:N	2.55	0.59
1:A:374:HIS:HB2	1:A:375:PRO:HD2	1.84	0.59
1:B:232:SER:CB	1:B:234:GLU:O	2.47	0.59
1:C:100:LYS:HG3	1:C:105:VAL:HG13	1.84	0.59
1:B:355:SER:O	1:B:357:MET:CG	2.50	0.58
1:A:59:MET:HE1	1:A:110:ASN:ND2	2.15	0.58
1:C:264:LEU:C	1:C:267:LEU:H	2.07	0.58
1:E:208:ASP:O	1:E:209:GLU:HG3	2.03	0.58
1:A:173:ASP:O	1:A:175:ALA:N	2.35	0.58
1:A:261:GLU:OE2	1:A:261:GLU:CA	2.47	0.58
1:E:362:ARG:CG	1:E:362:ARG:NH1	2.43	0.58
1:C:86:GLU:O	1:C:87:PHE:C	2.40	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:239:TYR:N	1:C:239:TYR:HD1	2.01	0.58
1:B:202:PHE:CD1	1:B:216:MET:HB3	2.39	0.58
1:C:115:GLN:HG3	1:C:116:ASN:N	2.17	0.58
1:C:166:LEU:CD2	1:C:181:ILE:HG13	2.33	0.58
1:C:359:ALA:O	1:C:360:ILE:CB	2.43	0.58
1:E:379:LEU:HD23	1:E:391:MET:HB2	1.86	0.58
1:E:165:ASP:CG	1:E:165:ASP:O	2.42	0.58
1:A:251:ILE:HG22	1:A:252:SER:N	2.18	0.58
1:B:208:ASP:O	1:B:209:GLU:HB2	2.04	0.58
1:C:104:TYR:O	1:C:104:TYR:CD1	2.57	0.58
1:C:277:GLU:C	1:C:279:TRP:N	2.56	0.58
1:D:115:GLN:HB3	1:D:118:PHE:CD1	2.39	0.58
1:E:199:THR:HG21	1:E:294:ARG:HH12	1.68	0.58
1:A:89:PHE:CD2	1:A:93:PHE:CZ	2.91	0.58
1:B:199:THR:OG1	1:B:346:GLU:OE2	2.19	0.58
1:E:118:PHE:CZ	1:E:177:TYR:HD2	2.22	0.58
1:A:206:LYS:HE2	1:A:396:HIS:HA	1.85	0.57
1:B:400:MET:SD	1:B:400:MET:N	2.77	0.57
1:A:175:ALA:CB	1:A:176:THR:HA	2.34	0.57
1:A:185:TYR:HE1	1:A:341:PHE:CE2	2.22	0.57
1:C:104:TYR:CD1	1:C:104:TYR:C	2.78	0.57
1:C:185:TYR:CD1	1:C:341:PHE:CD2	2.92	0.57
1:D:105:VAL:O	1:D:186:PHE:HA	2.04	0.57
1:D:304:LYS:HG2	1:D:316:PHE:CZ	2.38	0.57
1:D:351:ALA:O	1:D:352:ALA:CB	2.51	0.57
1:B:112:LEU:HD13	1:B:180:LEU:HD13	1.85	0.57
1:C:100:LYS:CE	1:C:105:VAL:CG1	2.77	0.57
1:B:56:ALA:O	1:B:59:MET:HG2	2.05	0.57
1:B:166:LEU:CD1	1:B:339:LYS:CB	2.83	0.57
1:B:399:THR:C	1:B:400:MET:SD	2.83	0.57
1:E:33:MET:HE1	1:E:53:ILE:CD1	2.34	0.57
1:E:36:ARG:NE	1:E:305:ASP:OD2	2.31	0.57
1:A:175:ALA:HB3	1:A:176:THR:HA	1.85	0.57
1:B:362:ARG:CB	1:C:367:TYR:CD1	2.87	0.57
1:A:43:ASP:O	1:A:43:ASP:CG	2.43	0.57
1:A:163:VAL:CG1	1:A:339:LYS:HD3	2.34	0.57
1:D:257:LEU:HD11	1:D:374:HIS:CE1	2.39	0.57
1:E:364:ALA:HB2	1:E:366:LEU:CB	2.26	0.57
1:A:364:ALA:HB1	1:D:366:LEU:HD21	1.86	0.57
1:B:162:LEU:HD13	1:B:185:TYR:CZ	2.40	0.57
1:D:118:PHE:CD2	1:D:331:ILE:CG1	2.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLU:OE2	1:C:358:ILE:CG2	2.51	0.56
1:C:278:GLU:O	1:C:281:ASN:N	2.38	0.56
1:E:328:ASN:C	1:E:328:ASN:OD1	2.43	0.56
1:B:206:LYS:CE	1:B:396:HIS:HD2	2.18	0.56
1:B:355:SER:O	1:B:357:MET:N	2.33	0.56
1:D:120:VAL:HG22	1:D:325:LEU:HD11	1.85	0.56
1:E:178:LEU:CD1	1:E:178:LEU:C	2.74	0.56
1:A:59:MET:HE2	1:A:110:ASN:CG	2.22	0.56
1:B:92:GLU:HG3	1:B:96:MET:HB2	1.86	0.56
1:B:260:GLN:HG2	1:B:261:GLU:OE2	2.05	0.56
1:C:89:PHE:HE2	1:C:93:PHE:CD1	2.23	0.56
1:D:47:LEU:HD22	1:D:297:VAL:HG12	1.87	0.56
1:D:62:LEU:CD2	1:D:87:PHE:HE2	2.18	0.56
1:D:304:LYS:CD	1:D:316:PHE:CG	2.87	0.56
1:D:304:LYS:CE	1:D:316:PHE:CD1	2.86	0.56
1:A:45:ASN:OD1	1:A:395:MET:N	2.37	0.56
1:D:36:ARG:NH2	1:D:305:ASP:OD1	2.26	0.56
1:A:23:GLU:N	1:A:89:PHE:HZ	2.02	0.56
1:A:175:ALA:O	1:A:177:TYR:CD1	2.58	0.56
1:E:59:MET:O	1:E:62:LEU:HB2	2.05	0.56
1:B:36:ARG:HH21	1:B:305:ASP:CG	2.07	0.56
1:C:100:LYS:CE	1:C:105:VAL:HG13	2.33	0.56
1:D:166:LEU:CD1	1:D:339:LYS:HB2	2.36	0.56
1:E:175:ALA:O	1:E:177:TYR:CE1	2.59	0.56
1:B:142:SER:OG	1:B:174:ALA:HB2	2.05	0.56
1:C:166:LEU:HG	1:C:337:ILE:HG21	1.86	0.56
1:A:84:GLY:HA2	1:A:85:GLU:HB2	0.71	0.56
1:A:118:PHE:CD2	1:A:331:ILE:HG13	2.41	0.56
1:E:33:MET:HE1	1:E:53:ILE:HD12	1.88	0.56
1:E:230:ASP:N	1:E:230:ASP:OD2	2.39	0.56
1:E:175:ALA:HB3	1:E:176:THR:HG23	1.88	0.56
1:E:363:MET:HG3	1:E:364:ALA:H	1.71	0.56
1:A:366:LEU:HD23	1:A:367:TYR:N	2.21	0.56
1:E:109:ALA:HB1	1:E:154:TRP:HZ3	1.65	0.56
1:E:328:ASN:OD1	1:E:330:GLU:CB	2.54	0.56
1:C:93:PHE:HD2	1:C:97:VAL:HG21	1.66	0.55
1:B:104:TYR:O	1:B:104:TYR:CG	2.60	0.55
1:B:115:GLN:HB3	1:B:118:PHE:CD1	2.42	0.55
1:B:167:VAL:CG1	1:B:337:ILE:HD13	2.28	0.55
1:B:356:GLY:C	1:B:360:ILE:HD12	2.25	0.55
1:B:401:ASN:HA	1:B:402:THR:HG23	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:393:ARG:O	1:C:393:ARG:HG3	2.04	0.55
1:E:315:ILE:CD1	1:E:316:PHE:CD2	2.89	0.55
1:E:366:LEU:C	1:E:367:TYR:O	2.43	0.55
1:B:315:ILE:CD1	1:B:316:PHE:CE2	2.88	0.55
1:D:379:LEU:HD23	1:D:391:MET:HB3	1.88	0.55
1:C:298:GLU:OE2	1:C:339:LYS:HE3	2.06	0.55
1:D:166:LEU:CD2	1:D:181:ILE:HG23	2.37	0.55
1:D:374:HIS:HB2	1:D:375:PRO:CD	2.32	0.55
1:A:42:GLU:O	1:A:42:GLU:CG	2.54	0.55
1:A:274:GLN:HE21	1:A:274:GLN:C	2.10	0.55
1:B:102:SER:O	1:B:103:GLN:CG	2.55	0.55
1:B:357:MET:HB2	1:C:259:ARG:HH21	1.72	0.55
1:D:51:LEU:HD13	1:D:93:PHE:CD1	2.31	0.55
1:E:363:MET:CG	1:E:364:ALA:H	2.18	0.55
1:B:193:GLN:NE2	1:B:350:GLU:HA	2.15	0.55
1:D:393:ARG:O	1:D:393:ARG:HG3	2.04	0.55
1:E:303:LEU:HB3	1:E:336:ALA:CB	2.37	0.55
1:E:61:GLU:OE2	1:E:87:PHE:CZ	2.60	0.55
1:B:317:ILE:HG22	1:B:318:LYS:N	2.21	0.55
1:D:193:GLN:NE2	1:D:350:GLU:HA	2.21	0.55
1:D:230:ASP:HB3	1:D:270:LEU:HD11	1.87	0.55
1:C:263:PRO:HB2	1:C:266:THR:OG1	2.06	0.55
1:A:206:LYS:HZ3	1:A:396:HIS:CD2	2.23	0.55
1:C:38:ARG:HH21	1:C:261:GLU:CG	2.20	0.55
1:E:176:THR:O	1:E:334:SER:HB2	2.01	0.55
1:C:261:GLU:O	1:C:262:VAL:CB	2.54	0.54
1:E:368:PRO:O	1:E:368:PRO:CD	2.51	0.54
1:E:62:LEU:HD12	1:E:128:MET:CE	2.37	0.54
1:C:374:HIS:HB2	1:C:375:PRO:CD	2.38	0.54
1:A:162:LEU:HD13	1:A:185:TYR:CZ	2.43	0.54
1:B:166:LEU:HD21	1:B:181:ILE:HG13	1.89	0.54
1:D:71:GLU:OE2	1:D:314:GLU:HG3	2.07	0.54
1:E:115:GLN:HB3	1:E:118:PHE:HD1	1.72	0.54
1:C:115:GLN:HA	1:C:139:VAL:O	2.07	0.54
1:C:118:PHE:CZ	1:C:177:TYR:CD1	2.95	0.54
1:C:357:MET:CA	1:C:358:ILE:HD12	2.34	0.54
1:A:185:TYR:CD1	1:A:341:PHE:CD2	2.95	0.54
1:B:120:VAL:HG22	1:B:325:LEU:HD12	1.87	0.54
1:C:118:PHE:O	1:C:138:HIS:HE1	1.89	0.54
1:E:59:MET:CG	1:E:60:MET:N	2.70	0.54
1:E:95:ASN:CA	1:E:98:THR:HG22	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:LEU:C	1:E:178:LEU:HD13	2.27	0.54
1:E:259:ARG:HH12	1:E:260:GLN:HB2	1.67	0.54
1:A:176:THR:O	1:A:177:TYR:CB	2.56	0.54
1:B:387:THR:HG22	1:B:388:ILE:O	2.07	0.54
1:C:195:ARG:NH1	1:C:358:ILE:N	2.48	0.54
1:D:56:ALA:HA	1:D:110:ASN:HD21	1.71	0.54
1:A:185:TYR:CE1	1:A:341:PHE:CD2	2.95	0.54
1:C:178:LEU:CD1	1:C:178:LEU:C	2.76	0.54
1:C:277:GLU:O	1:C:278:GLU:C	2.47	0.54
1:D:178:LEU:CD1	1:D:178:LEU:C	2.75	0.54
1:E:374:HIS:HB2	1:E:375:PRO:HD2	1.90	0.54
1:A:225:TYR:CG	1:A:226:GLY:N	2.76	0.54
1:B:328:ASN:OD1	1:B:330:GLU:CB	2.55	0.54
1:C:262:VAL:O	1:C:263:PRO:C	2.47	0.53
1:C:357:MET:HB2	1:E:213:GLN:HE22	1.72	0.53
1:E:34:TYR:HE2	1:E:38:ARG:HD2	1.73	0.53
1:E:364:ALA:HA	1:E:365:VAL:CB	2.27	0.53
1:E:368:PRO:O	1:E:368:PRO:HD2	2.08	0.53
1:B:328:ASN:OD1	1:B:330:GLU:HB2	2.07	0.53
1:C:52:SER:HB2	1:C:184:VAL:HG21	1.89	0.53
1:C:57:MET:HE2	1:C:57:MET:HA	1.90	0.53
1:C:264:LEU:O	1:C:267:LEU:HB3	2.08	0.53
1:E:206:LYS:NZ	1:E:396:HIS:CD2	2.73	0.53
1:C:308:LYS:HA	1:C:312:ILE:O	2.08	0.53
1:C:124:PHE:CZ	1:C:128:MET:HE1	2.43	0.53
1:E:124:PHE:CZ	1:E:128:MET:HE2	2.43	0.53
1:E:303:LEU:HB3	1:E:336:ALA:HB1	1.91	0.53
1:B:365:VAL:HA	1:D:362:ARG:CB	2.38	0.53
1:D:59:MET:HE2	1:D:110:ASN:CG	2.29	0.53
1:D:357:MET:HB3	1:D:358:ILE:HA	0.65	0.53
1:E:328:ASN:OD1	1:E:330:GLU:HB3	2.08	0.53
1:E:329:LYS:CA	1:E:330:GLU:HB2	2.39	0.53
1:B:31:VAL:O	1:B:34:TYR:HB3	2.09	0.53
1:B:178:LEU:HD12	1:B:332:PHE:O	2.08	0.53
1:C:186:PHE:O	1:C:342:LEU:HD12	2.09	0.53
1:A:175:ALA:O	1:A:177:TYR:CE1	2.62	0.53
1:B:33:MET:CE	1:B:53:ILE:CD1	2.86	0.53
1:C:108:ILE:O	1:C:108:ILE:HD12	2.09	0.53
1:C:239:TYR:OH	1:C:263:PRO:HG2	2.07	0.53
1:D:33:MET:CE	1:D:53:ILE:CD1	2.87	0.53
1:E:176:THR:N	1:E:177:TYR:CA	2.71	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:MET:HB3	1:A:128:MET:HE1	1.91	0.53
1:A:247:GLU:OE2	1:A:247:GLU:CA	2.57	0.53
1:B:124:PHE:CZ	1:B:128:MET:HE1	2.44	0.53
1:C:163:VAL:HG11	1:C:183:ALA:HB1	1.91	0.53
1:C:315:ILE:HG22	1:C:322:LEU:HD21	1.89	0.53
1:A:86:GLU:C	1:A:88:SER:N	2.61	0.53
1:A:93:PHE:HA	1:A:97:VAL:HG22	1.91	0.53
1:A:185:TYR:CD1	1:A:341:PHE:HD2	2.26	0.53
1:A:329:LYS:N	1:A:330:GLU:HB2	2.24	0.53
1:B:232:SER:C	1:B:234:GLU:N	2.62	0.53
1:B:374:HIS:HB2	1:B:375:PRO:CD	2.39	0.53
1:B:403:SER:O	1:B:404:GLY:C	2.46	0.53
1:D:206:LYS:NZ	1:D:396:HIS:HD2	2.06	0.53
1:E:26:ILE:O	1:E:30:SER:OG	2.24	0.53
1:B:26:ILE:O	1:B:30:SER:OG	2.24	0.53
1:D:43:ASP:CG	1:D:43:ASP:O	2.46	0.53
1:E:43:ASP:O	1:E:43:ASP:OD1	2.27	0.53
1:E:163:VAL:CG1	1:E:339:LYS:CE	2.67	0.53
1:B:120:VAL:HG22	1:B:325:LEU:HD11	1.90	0.52
1:C:178:LEU:C	1:C:178:LEU:HD13	2.29	0.52
1:C:263:PRO:C	1:C:264:LEU:HG	2.28	0.52
1:D:353:ALA:O	1:D:354:VAL:CG2	2.57	0.52
1:E:289:GLU:O	1:E:369:GLN:HA	2.09	0.52
1:B:101:GLU:O	1:B:102:SER:HB3	2.09	0.52
1:B:178:LEU:CD1	1:B:178:LEU:C	2.77	0.52
1:C:262:VAL:O	1:C:263:PRO:O	2.27	0.52
1:E:191:LYS:HG3	1:E:246:TYR:O	2.10	0.52
1:A:120:VAL:HA	1:A:325:LEU:O	2.10	0.52
1:A:93:PHE:O	1:A:95:ASN:N	2.43	0.52
1:B:315:ILE:HD12	1:B:316:PHE:CG	2.43	0.52
1:B:356:GLY:HA2	1:B:360:ILE:H	1.74	0.52
1:C:261:GLU:C	1:C:262:VAL:HG23	2.27	0.52
1:D:45:ASN:OD1	1:D:395:MET:N	2.32	0.52
1:D:304:LYS:CG	1:D:316:PHE:CE2	2.91	0.52
1:E:364:ALA:HB3	1:E:365:VAL:O	2.07	0.52
1:A:115:GLN:HG3	1:A:116:ASN:N	2.24	0.52
1:D:107:LYS:O	1:D:184:VAL:HA	2.08	0.52
1:E:259:ARG:CD	1:E:260:GLN:N	2.60	0.52
1:B:178:LEU:C	1:B:178:LEU:HD13	2.30	0.52
1:C:104:TYR:HA	1:C:188:GLY:CA	2.40	0.52
1:C:106:MET:HG2	1:C:186:PHE:HD1	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:176:THR:H	1:C:177:TYR:HA	1.73	0.52
1:D:26:ILE:HD12	1:D:93:PHE:CZ	2.45	0.52
1:D:57:MET:CE	1:D:57:MET:HA	2.40	0.52
1:D:304:LYS:HD3	1:D:316:PHE:CD2	2.44	0.52
1:A:69:GLN:OE1	1:A:73:ARG:NH2	2.43	0.52
1:A:93:PHE:C	1:A:95:ASN:H	2.11	0.52
1:D:33:MET:HE3	1:D:53:ILE:HD13	1.91	0.52
1:D:397:PRO:HD2	1:D:398:GLU:OE1	2.10	0.52
1:A:23:GLU:HG2	1:A:387:THR:OG1	2.09	0.52
1:C:206:LYS:HZ1	1:C:396:HIS:HD2	1.55	0.52
1:C:263:PRO:CB	1:C:266:THR:OG1	2.58	0.52
1:A:46:ILE:O	1:A:392:GLY:HA2	2.10	0.51
1:A:64:ALA:C	1:A:65:GLN:HG2	2.30	0.51
1:A:162:LEU:HD13	1:A:185:TYR:CE1	2.44	0.51
1:B:294:ARG:HG3	1:B:345:ASN:HA	1.91	0.51
1:C:193:GLN:HG2	1:C:347:GLU:C	2.30	0.51
1:C:256:VAL:HG21	1:C:270:LEU:HD13	1.91	0.51
1:A:222:GLU:CG	1:A:287:LYS:CG	2.73	0.51
1:D:42:GLU:O	1:D:42:GLU:HG3	2.09	0.51
1:B:118:PHE:CD2	1:B:331:ILE:HG13	2.45	0.51
1:E:62:LEU:CD1	1:E:128:MET:HE1	2.40	0.51
1:E:363:MET:CG	1:E:364:ALA:N	2.72	0.51
1:B:260:GLN:CG	1:B:261:GLU:N	2.73	0.51
1:B:364:ALA:O	1:D:362:ARG:HB3	2.10	0.51
1:C:89:PHE:HE2	1:C:93:PHE:HD1	1.57	0.51
1:A:178:LEU:CD1	1:A:178:LEU:C	2.79	0.51
1:C:100:LYS:CE	1:C:105:VAL:HG11	2.36	0.51
1:C:113:PHE:O	1:C:178:LEU:HA	2.11	0.51
1:C:195:ARG:HH22	1:C:358:ILE:H	1.57	0.51
1:E:41:GLY:O	1:E:42:GLU:C	2.49	0.51
1:E:61:GLU:OE2	1:E:87:PHE:HZ	1.94	0.51
1:B:46:ILE:HG13	1:B:393:ARG:HE	1.76	0.51
1:B:98:THR:HG23	1:B:99:ALA:N	2.26	0.51
1:D:304:LYS:HG2	1:D:316:PHE:CE2	2.45	0.51
1:A:90:LEU:HD23	1:A:93:PHE:CD1	2.45	0.51
1:C:230:ASP:OD1	1:C:231:GLY:N	2.44	0.51
1:E:120:VAL:HA	1:E:325:LEU:O	2.11	0.51
1:E:364:ALA:HB1	1:E:366:LEU:CA	2.40	0.51
1:A:62:LEU:HD12	1:A:128:MET:SD	2.50	0.51
1:A:85:GLU:O	1:A:86:GLU:CB	2.59	0.51
1:A:328:ASN:OD1	1:A:330:GLU:CB	2.59	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLU:OE2	1:B:73:ARG:CG	2.59	0.51
1:C:346:GLU:O	1:C:347:GLU:C	2.49	0.51
1:C:360:ILE:HD11	1:E:291:TYR:CD1	2.46	0.51
1:D:56:ALA:CA	1:D:110:ASN:HD21	2.24	0.51
1:D:108:ILE:HG22	1:D:184:VAL:HG22	1.93	0.51
1:A:218:TYR:C	1:A:218:TYR:CD2	2.83	0.51
1:A:315:ILE:HD12	1:A:316:PHE:CG	2.46	0.51
1:C:141:PHE:CE2	1:C:177:TYR:O	2.63	0.51
1:C:239:TYR:OH	1:C:266:THR:HG21	2.10	0.51
1:D:118:PHE:CD2	1:D:331:ILE:HG13	2.45	0.51
1:E:118:PHE:CE2	1:E:328:ASN:ND2	2.79	0.51
1:A:317:ILE:CG2	1:A:318:LYS:N	2.74	0.51
1:A:328:ASN:OD1	1:A:330:GLU:HB2	2.10	0.51
1:B:22:PRO:C	1:B:89:PHE:CZ	2.84	0.51
1:D:71:GLU:OE1	1:D:313:THR:N	2.33	0.51
1:E:175:ALA:HB3	1:E:176:THR:HA	1.93	0.51
1:A:307:LEU:HD22	1:A:312:ILE:HD12	1.93	0.50
1:E:185:TYR:CD1	1:E:341:PHE:HD2	2.29	0.50
1:A:374:HIS:HB2	1:A:375:PRO:HD3	1.93	0.50
1:A:103:GLN:N	1:A:103:GLN:OE1	2.44	0.50
1:A:378:PHE:CD1	1:A:378:PHE:C	2.83	0.50
1:B:98:THR:C	1:B:100:LYS:H	2.10	0.50
1:C:317:ILE:HG22	1:C:318:LYS:N	2.26	0.50
1:D:52:SER:OG	1:D:182:ASN:OD1	2.20	0.50
1:E:191:LYS:CE	1:E:249:ASP:HA	2.42	0.50
1:A:200:ARG:HH11	1:A:200:ARG:CB	2.16	0.50
1:B:130:LYS:HE3	1:B:131:TYR:CE1	2.47	0.50
1:B:379:LEU:HD23	1:B:391:MET:HB2	1.93	0.50
1:C:86:GLU:O	1:C:89:PHE:N	2.45	0.50
1:C:269:PRO:O	1:C:273:ALA:N	2.32	0.50
1:D:57:MET:HA	1:D:57:MET:HE2	1.92	0.50
1:E:120:VAL:HG13	1:E:325:LEU:CD1	2.41	0.50
1:A:52:SER:HB2	1:A:184:VAL:HG21	1.92	0.50
1:A:90:LEU:HD13	1:A:132:PHE:HE1	1.77	0.50
1:A:118:PHE:CD2	1:A:331:ILE:CG1	2.94	0.50
1:C:358:ILE:CD1	1:C:358:ILE:N	2.50	0.50
1:A:274:GLN:NE2	1:A:274:GLN:O	2.45	0.50
1:B:56:ALA:CA	1:B:110:ASN:HD21	2.25	0.50
1:B:193:GLN:HG2	1:B:349:SER:O	2.05	0.50
1:E:46:ILE:HB	1:E:393:ARG:HG2	1.94	0.50
1:A:178:LEU:CD1	1:A:332:PHE:O	2.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:ILE:HD12	1:B:316:PHE:CD2	2.47	0.50
1:C:166:LEU:HD21	1:C:181:ILE:HG13	1.94	0.50
1:C:297:VAL:HG21	1:C:394:VAL:CG2	2.34	0.50
1:E:120:VAL:HG13	1:E:325:LEU:HD12	1.94	0.50
1:A:111:SER:HB2	1:A:154:TRP:CH2	2.47	0.50
1:A:120:VAL:HG22	1:A:325:LEU:HD11	1.90	0.50
1:B:36:ARG:O	1:B:39:ALA:HB3	2.12	0.50
1:B:59:MET:HE1	1:B:180:LEU:CD1	2.37	0.50
1:C:357:MET:O	1:C:358:ILE:O	2.28	0.50
1:A:317:ILE:HG22	1:A:318:LYS:N	2.26	0.50
1:B:23:GLU:N	1:B:89:PHE:CZ	2.73	0.50
1:B:53:ILE:HD13	1:B:303:LEU:HD11	1.94	0.50
1:B:299:GLN:HE22	1:B:300:GLU:H	1.52	0.50
1:C:162:LEU:HD13	1:C:185:TYR:CZ	2.47	0.50
1:D:187:LYS:HG3	1:D:343:GLU:HB3	1.94	0.50
1:B:142:SER:OG	1:B:174:ALA:CB	2.60	0.49
1:B:173:ASP:C	1:B:175:ALA:H	2.15	0.49
1:E:156:GLU:HB3	1:E:161:ASN:HD22	1.76	0.49
1:C:264:LEU:HA	1:C:267:LEU:HB2	1.94	0.49
1:E:120:VAL:HA	1:E:326:SER:HB3	1.93	0.49
1:B:50:PRO:CG	1:B:388:ILE:HG22	2.41	0.49
1:C:185:TYR:CD1	1:C:341:PHE:HD2	2.29	0.49
1:C:185:TYR:HD1	1:C:341:PHE:CD2	2.30	0.49
1:E:315:ILE:HD12	1:E:316:PHE:CG	2.47	0.49
1:B:398:GLU:O	1:B:399:THR:O	2.30	0.49
1:C:38:ARG:NH2	1:C:261:GLU:CD	2.53	0.49
1:C:264:LEU:O	1:C:267:LEU:CB	2.60	0.49
1:B:399:THR:OG1	1:B:400:MET:N	2.44	0.49
1:B:234:GLU:CD	1:B:235:ALA:HB2	2.33	0.49
1:B:354:VAL:C	1:B:356:GLY:H	2.16	0.49
1:B:398:GLU:OE1	1:B:398:GLU:N	2.28	0.49
1:B:401:ASN:CB	1:B:402:THR:OG1	2.59	0.49
1:C:118:PHE:CD2	1:C:328:ASN:CG	2.85	0.49
1:E:166:LEU:HD13	1:E:339:LYS:HB3	1.93	0.49
1:E:206:LYS:HZ1	1:E:396:HIS:CD2	2.24	0.49
1:B:156:GLU:HG2	1:B:164:LYS:HG2	1.95	0.49
1:C:207:ASP:OD1	1:C:207:ASP:O	2.31	0.49
1:C:304:LYS:O	1:C:308:LYS:HG3	2.12	0.49
1:D:304:LYS:CG	1:D:316:PHE:CD1	2.91	0.49
1:E:199:THR:HG21	1:E:294:ARG:NH1	2.28	0.49
1:A:185:TYR:CE1	1:A:341:PHE:CE2	3.00	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:193:GLN:HG2	1:B:349:SER:C	2.33	0.49
1:C:366:LEU:N	1:C:366:LEU:HD23	2.27	0.49
1:D:178:LEU:HD13	1:D:333:LEU:HD12	1.95	0.49
1:E:178:LEU:CD1	1:E:332:PHE:O	2.61	0.49
1:A:86:GLU:O	1:A:88:SER:N	2.45	0.49
1:A:115:GLN:HB3	1:A:118:PHE:CD1	2.48	0.49
1:D:175:ALA:O	1:D:177:TYR:CD1	2.66	0.49
1:E:33:MET:HG2	1:E:306:VAL:CG1	2.43	0.49
1:E:366:LEU:O	1:E:367:TYR:O	2.31	0.49
1:A:303:LEU:HB3	1:A:336:ALA:HB1	1.94	0.49
1:A:366:LEU:C	1:A:366:LEU:CD2	2.77	0.49
1:B:354:VAL:C	1:B:356:GLY:N	2.65	0.49
1:C:34:TYR:CE2	1:C:38:ARG:HD2	2.48	0.49
1:C:120:VAL:HG13	1:C:325:LEU:HD12	1.93	0.49
1:D:228:PHE:O	1:D:238:ILE:HA	2.13	0.49
1:B:363:MET:O	1:C:227:GLU:OE2	2.30	0.48
1:C:357:MET:HB2	1:E:213:GLN:NE2	2.27	0.48
1:D:298:GLU:OE2	1:D:339:LYS:HE3	2.13	0.48
1:E:191:LYS:CD	1:E:245:PRO:HB2	2.42	0.48
1:A:93:PHE:O	1:A:97:VAL:HG23	2.12	0.48
1:A:336:ALA:O	1:A:337:ILE:CD1	2.31	0.48
1:B:128:MET:HG3	1:B:134:ALA:HB3	1.95	0.48
1:C:362:ARG:HH12	1:E:371:ILE:HG21	1.76	0.48
1:A:118:PHE:CD2	1:A:328:ASN:CG	2.87	0.48
1:B:91:LYS:O	1:B:95:ASN:HB2	2.12	0.48
1:A:89:PHE:O	1:A:92:GLU:N	2.43	0.48
1:B:298:GLU:HG2	1:B:341:PHE:HD1	1.77	0.48
1:D:103:GLN:NE2	1:D:104:TYR:H	2.08	0.48
1:A:315:ILE:CD1	1:A:316:PHE:CE2	2.96	0.48
1:B:64:ALA:C	1:B:65:GLN:HG2	2.33	0.48
1:B:166:LEU:HG	1:B:337:ILE:HG21	1.95	0.48
1:C:89:PHE:CE2	1:C:93:PHE:CD1	3.01	0.48
1:E:95:ASN:HA	1:E:98:THR:HG22	1.96	0.48
1:E:107:LYS:HB2	1:E:185:TYR:HB3	1.96	0.48
1:E:118:PHE:CD2	1:E:328:ASN:ND2	2.82	0.48
1:A:23:GLU:O	1:A:24:GLU:C	2.51	0.48
1:B:315:ILE:CD1	1:B:316:PHE:CD2	2.96	0.48
1:C:100:LYS:HG2	1:C:105:VAL:HG13	1.92	0.48
1:C:113:PHE:CE2	1:C:151:ILE:HG12	2.48	0.48
1:C:299:GLN:OE1	1:C:300:GLU:N	2.37	0.48
1:D:220:GLN:HB2	1:D:289:GLU:OE2	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:LEU:HD12	1:C:128:MET:HE2	1.96	0.48
1:C:315:ILE:CD1	1:C:316:PHE:CZ	2.97	0.48
1:C:364:ALA:HB1	1:C:367:TYR:HA	1.95	0.48
1:D:363:MET:O	1:D:364:ALA:HB3	2.14	0.48
1:E:52:SER:HB2	1:E:184:VAL:HG21	1.95	0.48
1:B:118:PHE:CE2	1:B:328:ASN:ND2	2.82	0.48
1:B:166:LEU:HD12	1:B:339:LYS:HB2	1.94	0.48
1:C:118:PHE:CD1	1:C:118:PHE:N	2.80	0.48
1:D:222:GLU:CD	1:D:285:LYS:HE2	2.34	0.48
1:A:187:LYS:NZ	1:A:347:GLU:OE2	2.45	0.48
1:B:260:GLN:HE21	1:B:260:GLN:C	2.13	0.48
1:C:59:MET:HE1	1:C:180:LEU:HD11	1.96	0.48
1:C:263:PRO:C	1:C:264:LEU:CG	2.82	0.48
1:D:104:TYR:O	1:D:104:TYR:CG	2.67	0.48
1:D:124:PHE:CE1	1:D:128:MET:CE	2.97	0.48
1:D:178:LEU:C	1:D:178:LEU:HD13	2.33	0.48
1:E:97:VAL:CA	1:E:104:TYR:OH	2.59	0.48
1:C:118:PHE:CE2	1:C:331:ILE:HG13	2.47	0.48
1:E:218:TYR:C	1:E:218:TYR:CD2	2.87	0.48
1:E:229:SER:HA	1:E:238:ILE:HA	1.95	0.48
1:E:293:PRO:O	1:E:295:PHE:HD2	1.96	0.48
1:D:62:LEU:HD12	1:D:128:MET:HE2	1.95	0.47
1:D:166:LEU:HD11	1:D:339:LYS:HB2	1.96	0.47
1:E:62:LEU:CG	1:E:128:MET:HE1	2.44	0.47
1:E:220:GLN:OE1	1:E:289:GLU:HG3	2.14	0.47
1:A:103:GLN:O	1:A:103:GLN:HG2	2.13	0.47
1:B:33:MET:HG2	1:B:306:VAL:CG1	2.44	0.47
1:B:59:MET:CE	1:B:180:LEU:HD13	2.22	0.47
1:B:230:ASP:OD1	1:B:230:ASP:N	2.47	0.47
1:E:90:LEU:HD23	1:E:93:PHE:CD1	2.49	0.47
1:E:256:VAL:HB	1:E:377:PHE:HB3	1.95	0.47
1:E:366:LEU:O	1:E:367:TYR:C	2.52	0.47
1:A:328:ASN:OD1	1:A:328:ASN:C	2.52	0.47
1:C:57:MET:HA	1:C:57:MET:CE	2.43	0.47
1:D:300:GLU:HB2	1:D:339:LYS:HG2	1.96	0.47
1:E:24:GLU:HG2	1:E:25:ALA:N	2.26	0.47
1:C:254:MET:O	1:C:378:PHE:HA	2.14	0.47
1:B:362:ARG:CG	1:C:367:TYR:CD1	2.93	0.47
1:C:38:ARG:NH2	1:C:261:GLU:HG2	2.30	0.47
1:E:251:ILE:HG22	1:E:252:SER:N	2.30	0.47
1:A:56:ALA:HA	1:A:110:ASN:HD21	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:VAL:HG13	1:B:325:LEU:HD12	1.97	0.47
1:C:62:LEU:HD23	1:C:87:PHE:CE2	2.47	0.47
1:C:176:THR:O	1:C:334:SER:HB2	2.15	0.47
1:C:193:GLN:CD	1:C:347:GLU:C	2.73	0.47
1:D:130:LYS:HD3	1:D:131:TYR:CZ	2.49	0.47
1:E:34:TYR:CE2	1:E:38:ARG:HD2	2.50	0.47
1:E:92:GLU:OE2	1:E:96:MET:CE	2.62	0.47
1:A:95:ASN:HA	1:A:98:THR:CG2	2.45	0.47
1:B:163:VAL:CG1	1:B:339:LYS:HG2	2.45	0.47
1:B:197:GLU:H	1:B:197:GLU:HG3	1.41	0.47
1:C:120:VAL:HG13	1:C:325:LEU:O	2.15	0.47
1:E:364:ALA:C	1:E:365:VAL:O	2.52	0.47
1:B:239:TYR:HH	1:B:279:TRP:HE1	1.61	0.47
1:D:23:GLU:HG3	1:D:89:PHE:CZ	2.50	0.47
1:D:59:MET:HE2	1:D:110:ASN:OD1	2.12	0.47
1:E:185:TYR:CE1	1:E:341:PHE:CD2	3.03	0.47
1:B:166:LEU:HD12	1:B:339:LYS:CB	2.43	0.47
1:B:229:SER:C	1:B:231:GLY:H	2.18	0.47
1:C:62:LEU:HD21	1:C:87:PHE:CE2	2.50	0.47
1:C:270:LEU:HD23	1:C:270:LEU:HA	1.60	0.46
1:D:315:ILE:CD1	1:D:316:PHE:CZ	2.97	0.46
1:E:178:LEU:CD1	1:E:333:LEU:HA	2.44	0.46
1:A:329:LYS:CA	1:A:330:GLU:HB2	2.46	0.46
1:C:360:ILE:HG21	1:C:362:ARG:NH1	2.30	0.46
1:C:118:PHE:CE2	1:C:328:ASN:ND2	2.83	0.46
1:D:93:PHE:HD2	1:D:93:PHE:N	2.12	0.46
1:E:23:GLU:HG3	1:E:89:PHE:CE2	2.50	0.46
1:A:178:LEU:CD1	1:A:333:LEU:HD12	2.45	0.46
1:A:363:MET:C	1:D:369:GLN:HB2	2.36	0.46
1:B:287:LYS:HD3	1:B:367:TYR:CZ	2.51	0.46
1:B:379:LEU:HD23	1:B:391:MET:CB	2.45	0.46
1:D:52:SER:CB	1:D:184:VAL:CG2	2.91	0.46
1:D:97:VAL:HA	1:D:104:TYR:OH	2.16	0.46
1:D:315:ILE:CD1	1:D:316:PHE:CE2	2.97	0.46
1:B:24:GLU:O	1:B:27:ALA:HB3	2.16	0.46
1:C:258:SER:OG	1:C:259:ARG:N	2.49	0.46
1:A:303:LEU:HB3	1:A:336:ALA:CB	2.45	0.46
1:B:47:LEU:HD13	1:B:378:PHE:HZ	1.80	0.46
1:B:365:VAL:HA	1:D:362:ARG:HB2	1.98	0.46
1:D:176:THR:O	1:D:334:SER:HB2	2.15	0.46
1:D:358:ILE:H	1:D:358:ILE:HG13	1.58	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:23:GLU:O	1:E:24:GLU:C	2.54	0.46
1:E:268:GLU:O	1:E:271:VAL:HG23	2.16	0.46
1:B:44:GLU:HA	1:B:45:ASN:HB2	1.98	0.46
1:B:365:VAL:HA	1:D:362:ARG:HB3	1.97	0.46
1:D:225:TYR:CG	1:D:226:GLY:N	2.84	0.46
1:E:33:MET:CE	1:E:53:ILE:CD1	2.94	0.46
1:E:259:ARG:CZ	1:E:260:GLN:H	2.28	0.46
1:A:33:MET:HE1	1:A:53:ILE:HD12	1.97	0.46
1:A:155:VAL:HG21	1:A:166:LEU:HD22	1.98	0.46
1:D:93:PHE:N	1:D:93:PHE:CD2	2.82	0.46
1:A:48:PHE:O	1:A:50:PRO:HD3	2.16	0.46
1:B:102:SER:O	1:B:103:GLN:HG3	2.16	0.46
1:E:87:PHE:N	1:E:87:PHE:CD1	2.70	0.46
1:A:56:ALA:HB1	1:A:180:LEU:HD21	1.98	0.46
1:A:92:GLU:O	1:A:96:MET:N	2.45	0.46
1:B:260:GLN:HE21	1:B:260:GLN:CA	2.28	0.46
1:C:93:PHE:C	1:C:95:ASN:H	2.18	0.46
1:C:100:LYS:O	1:C:101:GLU:C	2.55	0.46
1:D:243:GLU:OE2	1:D:383:ARG:HD3	2.16	0.46
1:E:162:LEU:HD13	1:E:185:TYR:CZ	2.51	0.46
1:E:185:TYR:CD1	1:E:341:PHE:CD2	3.04	0.46
1:E:317:ILE:HG22	1:E:318:LYS:N	2.31	0.46
1:A:173:ASP:C	1:A:175:ALA:N	2.70	0.45
1:B:167:VAL:HG12	1:B:337:ILE:CD1	2.28	0.45
1:B:403:SER:O	1:B:405:HIS:HB2	2.16	0.45
1:C:186:PHE:CD2	1:C:342:LEU:CD1	2.92	0.45
1:A:34:TYR:HB2	1:A:391:MET:HE3	1.97	0.45
1:A:93:PHE:C	1:A:95:ASN:N	2.69	0.45
1:A:118:PHE:HD2	1:A:328:ASN:CG	2.20	0.45
1:A:141:PHE:CG	1:A:176:THR:OG1	2.69	0.45
1:B:115:GLN:HA	1:B:139:VAL:O	2.16	0.45
1:C:268:GLU:OE1	1:C:272:LYS:NZ	2.45	0.45
1:C:274:GLN:NE2	1:C:388:ILE:HD11	2.31	0.45
1:D:62:LEU:HG	1:D:87:PHE:HE2	1.81	0.45
1:D:315:ILE:HD12	1:D:316:PHE:CG	2.51	0.45
1:D:353:ALA:C	1:D:354:VAL:HG23	2.36	0.45
1:A:42:GLU:O	1:A:42:GLU:HG2	2.16	0.45
1:A:112:LEU:HD13	1:A:180:LEU:HD13	1.98	0.45
1:A:223:PHE:O	1:A:285:LYS:HA	2.16	0.45
1:C:120:VAL:HA	1:C:325:LEU:O	2.16	0.45
1:D:33:MET:HE1	1:D:48:PHE:CD1	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:LYS:HG3	1:A:343:GLU:HB3	1.97	0.45
1:B:22:PRO:HB2	1:B:23:GLU:H	1.58	0.45
1:C:56:ALA:HA	1:C:110:ASN:HD21	1.81	0.45
1:D:167:VAL:HG12	1:D:337:ILE:HD12	1.99	0.45
1:D:297:VAL:CG2	1:D:394:VAL:HG22	2.42	0.45
1:E:56:ALA:HB1	1:E:180:LEU:HD21	1.99	0.45
1:E:61:GLU:O	1:E:62:LEU:C	2.53	0.45
1:E:120:VAL:CG2	1:E:325:LEU:CD1	2.88	0.45
1:A:321:ASN:OD1	1:A:323:THR:HG23	2.17	0.45
1:C:379:LEU:HD13	1:C:388:ILE:HD12	1.97	0.45
1:D:23:GLU:OE2	1:D:89:PHE:CZ	2.69	0.45
1:D:33:MET:HG3	1:D:310:LEU:HD11	1.97	0.45
1:E:191:LYS:HD2	1:E:245:PRO:HG2	1.97	0.45
1:A:262:VAL:HA	1:A:263:PRO:HD2	1.82	0.45
1:A:298:GLU:OE2	1:A:339:LYS:HE2	2.16	0.45
1:B:202:PHE:HB2	1:B:216:MET:HB2	1.98	0.45
1:C:51:LEU:HD21	1:C:93:PHE:HB3	1.99	0.45
1:C:277:GLU:C	1:C:279:TRP:H	2.20	0.45
1:D:92:GLU:HA	1:D:96:MET:HG2	1.99	0.45
1:A:41:GLY:O	1:A:42:GLU:C	2.55	0.45
1:B:34:TYR:O	1:B:38:ARG:HG3	2.16	0.45
1:C:315:ILE:HD11	1:C:316:PHE:CZ	2.52	0.45
1:A:263:PRO:O	1:A:266:THR:HB	2.17	0.45
1:B:401:ASN:C	1:B:402:THR:OG1	2.54	0.45
1:D:372:VAL:CG1	1:D:376:PHE:CD2	3.00	0.45
1:E:43:ASP:OD1	1:E:43:ASP:C	2.54	0.45
1:B:52:SER:CB	1:B:184:VAL:HG21	2.47	0.45
1:B:100:LYS:C	1:B:102:SER:N	2.69	0.45
1:E:108:ILE:HG22	1:E:184:VAL:HG22	1.99	0.45
1:E:374:HIS:HB2	1:E:375:PRO:CD	2.47	0.45
1:C:62:LEU:CD2	1:C:127:MET:HG2	2.47	0.45
1:D:155:VAL:HG21	1:D:166:LEU:HD22	1.99	0.45
1:D:379:LEU:HD23	1:D:391:MET:CB	2.47	0.45
1:E:329:LYS:HD2	1:E:329:LYS:HA	1.83	0.45
1:C:93:PHE:HA	1:C:96:MET:HB3	1.99	0.44
1:C:124:PHE:CE1	1:C:128:MET:CE	2.99	0.44
1:C:315:ILE:CD1	1:C:316:PHE:CD2	2.98	0.44
1:D:124:PHE:CE1	1:D:128:MET:HE3	2.52	0.44
1:A:62:LEU:HD23	1:A:87:PHE:CE2	2.50	0.44
1:D:78:TYR:O	1:D:79:ASP:HB3	2.17	0.44
1:B:108:ILE:HD12	1:B:108:ILE:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:SER:HA	1:B:238:ILE:HB	1.98	0.44
1:B:288:VAL:HG12	1:B:289:GLU:N	2.33	0.44
1:B:374:HIS:HB2	1:B:375:PRO:HD2	1.99	0.44
1:E:178:LEU:HD13	1:E:333:LEU:HD12	1.98	0.44
1:A:297:VAL:CG2	1:A:394:VAL:HG22	2.45	0.44
1:B:256:VAL:HG21	1:B:279:TRP:CH2	2.52	0.44
1:B:260:GLN:NE2	1:B:261:GLU:HB2	2.32	0.44
1:B:307:LEU:HD22	1:B:312:ILE:HD12	1.98	0.44
1:C:104:TYR:O	1:C:104:TYR:CG	2.71	0.44
1:C:166:LEU:HD23	1:C:181:ILE:HG13	1.97	0.44
1:D:316:PHE:CE1	1:D:333:LEU:HD23	2.52	0.44
1:E:23:GLU:CD	1:E:89:PHE:CZ	2.91	0.44
1:A:23:GLU:C	1:A:25:ALA:N	2.70	0.44
1:A:34:TYR:HE2	1:A:38:ARG:HD2	1.82	0.44
1:B:33:MET:HE2	1:B:33:MET:HB3	1.71	0.44
1:C:54:ALA:HA	1:C:76:MET:HE1	2.00	0.44
1:C:89:PHE:O	1:C:92:GLU:HB3	2.17	0.44
1:C:104:TYR:HA	1:C:188:GLY:HA2	1.99	0.44
1:E:167:VAL:HG11	1:E:337:ILE:HD13	1.99	0.44
1:A:268:GLU:N	1:A:269:PRO:CD	2.80	0.44
1:A:276:VAL:HG12	1:A:277:GLU:OE2	2.17	0.44
1:C:202:PHE:HB2	1:C:216:MET:HB2	2.00	0.44
1:D:115:GLN:HG3	1:D:116:ASN:N	2.33	0.44
1:B:354:VAL:HG12	1:B:357:MET:N	2.31	0.44
1:B:393:ARG:HG3	1:B:393:ARG:O	2.16	0.44
1:C:105:VAL:O	1:C:186:PHE:HA	2.18	0.44
1:C:115:GLN:NE2	1:C:140:ASP:HA	2.33	0.44
1:A:315:ILE:HD11	1:A:316:PHE:CZ	2.52	0.44
1:B:42:GLU:O	1:B:43:ASP:HB2	2.18	0.44
1:B:296:THR:HG22	1:B:400:MET:HE1	2.00	0.44
1:E:163:VAL:HG11	1:E:183:ALA:HB1	1.99	0.44
1:E:259:ARG:NE	1:E:260:GLN:H	2.15	0.44
1:A:316:PHE:CE1	1:A:333:LEU:HD23	2.53	0.44
1:B:115:GLN:CG	1:B:116:ASN:N	2.79	0.44
1:B:118:PHE:CE2	1:B:331:ILE:HG13	2.53	0.44
1:C:93:PHE:C	1:C:95:ASN:N	2.69	0.44
1:C:112:LEU:HD12	1:C:112:LEU:HA	1.82	0.44
1:E:33:MET:HE1	1:E:48:PHE:CD1	2.53	0.44
1:A:287:LYS:HZ1	1:A:353:ALA:HB2	1.79	0.43
1:C:193:GLN:CG	1:C:347:GLU:C	2.86	0.43
1:D:328:ASN:OD1	1:D:330:GLU:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:328:ASN:OD1	1:E:329:LYS:N	2.51	0.43
1:B:56:ALA:N	1:B:110:ASN:HD21	2.16	0.43
1:B:115:GLN:HB3	1:B:118:PHE:HD1	1.83	0.43
1:B:317:ILE:CG2	1:B:318:LYS:N	2.81	0.43
1:C:23:GLU:O	1:C:24:GLU:C	2.57	0.43
1:C:112:LEU:HD13	1:C:180:LEU:HD13	2.00	0.43
1:C:251:ILE:HG22	1:C:252:SER:N	2.33	0.43
1:A:56:ALA:CA	1:A:110:ASN:HD21	2.31	0.43
1:D:92:GLU:HG3	1:D:96:MET:HG2	1.99	0.43
1:E:268:GLU:O	1:E:269:PRO:C	2.57	0.43
1:A:287:LYS:NZ	1:A:353:ALA:HB2	2.26	0.43
1:B:41:GLY:O	1:B:42:GLU:C	2.57	0.43
1:B:259:ARG:HE	1:B:259:ARG:HB3	1.42	0.43
1:B:354:VAL:HG12	1:B:357:MET:H	1.84	0.43
1:C:49:SER:HB2	1:C:390:PHE:CD1	2.53	0.43
1:C:223:PHE:HD2	1:C:288:VAL:HB	1.84	0.43
1:D:294:ARG:HD3	1:D:346:GLU:OE1	2.19	0.43
1:A:173:ASP:C	1:A:175:ALA:H	2.21	0.43
1:A:222:GLU:HG2	1:A:287:LYS:CG	2.31	0.43
1:B:296:THR:CG2	1:B:400:MET:HE2	2.45	0.43
1:B:355:SER:O	1:B:357:MET:HG2	2.18	0.43
1:C:162:LEU:HD13	1:C:185:TYR:CE1	2.54	0.43
1:D:218:TYR:CG	1:D:219:GLN:N	2.86	0.43
1:E:216:MET:HE3	1:E:373:ASP:HB3	2.01	0.43
1:A:178:LEU:HD13	1:A:178:LEU:C	2.39	0.43
1:A:247:GLU:HG2	1:A:349:SER:OG	2.19	0.43
1:B:72:ILE:O	1:B:76:MET:HG2	2.17	0.43
1:B:257:LEU:HD11	1:B:374:HIS:CE1	2.54	0.43
1:B:260:GLN:HG2	1:B:261:GLU:N	2.33	0.43
1:C:97:VAL:CA	1:C:104:TYR:OH	2.63	0.43
1:C:126:GLN:HE21	1:C:126:GLN:HB3	1.54	0.43
1:D:23:GLU:HG3	1:D:89:PHE:CE2	2.54	0.43
1:D:24:GLU:O	1:D:27:ALA:CB	2.56	0.43
1:D:178:LEU:HD12	1:D:332:PHE:O	2.18	0.43
1:D:322:LEU:HD12	1:D:331:ILE:HG22	1.98	0.43
1:E:23:GLU:C	1:E:25:ALA:N	2.71	0.43
1:A:118:PHE:CG	1:A:331:ILE:HD11	2.53	0.43
1:C:89:PHE:O	1:C:92:GLU:CB	2.67	0.43
1:C:103:GLN:CG	1:C:104:TYR:N	2.58	0.43
1:C:173:ASP:C	1:C:175:ALA:N	2.66	0.43
1:D:46:ILE:O	1:D:392:GLY:HA3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:LYS:HZ1	1:D:357:MET:N	2.17	0.43
1:A:95:ASN:CA	1:A:98:THR:CG2	2.97	0.43
1:B:162:LEU:HB3	1:B:185:TYR:CD1	2.52	0.43
1:B:328:ASN:OD1	1:B:328:ASN:C	2.56	0.43
1:C:49:SER:HA	1:C:50:PRO:HD2	1.88	0.43
1:E:36:ARG:HH21	1:E:305:ASP:CG	2.22	0.43
1:E:297:VAL:HG21	1:E:394:VAL:HG22	1.99	0.43
1:E:365:VAL:O	1:E:367:TYR:CB	2.65	0.43
1:A:31:VAL:CA	1:A:391:MET:HE1	2.42	0.43
1:A:175:ALA:HB3	1:A:176:THR:CA	2.49	0.43
1:B:55:LEU:HD23	1:B:90:LEU:HB3	2.01	0.43
1:B:118:PHE:O	1:B:138:HIS:HE1	2.01	0.43
1:B:268:GLU:N	1:B:269:PRO:HD2	2.34	0.43
1:B:315:ILE:HD11	1:B:316:PHE:CZ	2.53	0.43
1:C:33:MET:HE2	1:C:33:MET:HB3	1.87	0.43
1:C:268:GLU:N	1:C:269:PRO:HD2	2.34	0.43
1:E:287:LYS:CD	1:E:367:TYR:CZ	2.93	0.43
1:A:251:ILE:CG2	1:A:252:SER:N	2.81	0.43
1:B:362:ARG:CB	1:C:367:TYR:HD1	2.29	0.43
1:B:402:THR:O	1:B:403:SER:HB2	2.19	0.43
1:C:90:LEU:C	1:C:92:GLU:N	2.70	0.43
1:C:300:GLU:HA	1:C:338:HIS:O	2.19	0.43
1:B:100:LYS:O	1:B:102:SER:N	2.51	0.42
1:C:178:LEU:HD12	1:C:178:LEU:H	1.84	0.42
1:C:195:ARG:NH2	1:C:358:ILE:H	2.17	0.42
1:D:52:SER:HB2	1:D:184:VAL:CG2	2.49	0.42
1:E:304:LYS:HD3	1:E:308:LYS:NZ	2.33	0.42
1:E:329:LYS:N	1:E:330:GLU:HB2	2.34	0.42
1:A:84:GLY:CA	1:A:85:GLU:CB	2.46	0.42
1:B:33:MET:HE1	1:B:48:PHE:CD1	2.54	0.42
1:B:65:GLN:O	1:B:66:GLY:C	2.57	0.42
1:B:218:TYR:CG	1:B:219:GLN:N	2.87	0.42
1:B:296:THR:HG21	1:B:400:MET:CE	2.48	0.42
1:B:354:VAL:HA	1:B:356:GLY:CA	2.49	0.42
1:C:165:ASP:OD1	1:C:165:ASP:O	2.37	0.42
1:C:166:LEU:CD1	1:C:339:LYS:HB2	2.50	0.42
1:E:112:LEU:HD12	1:E:112:LEU:HA	1.77	0.42
1:B:232:SER:O	1:B:234:GLU:N	2.52	0.42
1:B:303:LEU:HB3	1:B:336:ALA:HB1	2.01	0.42
1:C:31:VAL:HG11	1:C:268:GLU:HG2	2.01	0.42
1:C:115:GLN:HB3	1:C:118:PHE:CD1	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:GLY:O	1:D:42:GLU:C	2.57	0.42
1:D:363:MET:O	1:D:363:MET:CG	2.45	0.42
1:E:118:PHE:CD2	1:E:328:ASN:CG	2.93	0.42
1:A:222:GLU:HG3	1:A:287:LYS:CG	2.35	0.42
1:B:162:LEU:HD13	1:B:185:TYR:CD2	2.54	0.42
1:B:193:GLN:HB3	1:B:348:GLY:N	2.34	0.42
1:B:260:GLN:HE21	1:B:260:GLN:N	2.17	0.42
1:C:225:TYR:HA	1:C:241:VAL:O	2.18	0.42
1:D:166:LEU:HD21	1:D:181:ILE:HG23	2.01	0.42
1:E:118:PHE:CD2	1:E:331:ILE:HD11	2.54	0.42
1:A:187:LYS:CG	1:A:343:GLU:HB3	2.49	0.42
1:C:182:ASN:O	1:C:338:HIS:HA	2.19	0.42
1:C:315:ILE:HD12	1:C:316:PHE:CG	2.54	0.42
1:D:33:MET:HB3	1:D:33:MET:HE2	1.92	0.42
1:D:193:GLN:HE21	1:D:350:GLU:HA	1.84	0.42
1:A:89:PHE:CE2	1:A:93:PHE:HZ	2.37	0.42
1:A:109:ALA:HB1	1:A:154:TRP:HZ3	1.77	0.42
1:A:190:TRP:HA	1:A:190:TRP:CE3	2.54	0.42
1:A:211:GLU:HB2	1:B:200:ARG:CZ	2.50	0.42
1:C:178:LEU:CD1	1:C:178:LEU:O	2.68	0.42
1:D:34:TYR:O	1:D:38:ARG:HG3	2.20	0.42
1:A:173:ASP:OD1	1:A:175:ALA:CB	2.68	0.42
1:A:175:ALA:CB	1:A:176:THR:CA	2.97	0.42
1:B:94:SER:O	1:B:98:THR:HG21	2.20	0.42
1:B:308:LYS:HA	1:B:312:ILE:O	2.20	0.42
1:A:95:ASN:HA	1:A:98:THR:HG23	2.02	0.42
1:A:165:ASP:CG	1:A:165:ASP:O	2.58	0.42
1:A:168:SER:HB2	1:A:169:PRO:CD	2.49	0.42
1:A:173:ASP:OD1	1:A:175:ALA:HB3	2.20	0.42
1:B:377:PHE:HZ	1:B:391:MET:HE3	1.85	0.42
1:D:98:THR:HG23	1:D:99:ALA:N	2.35	0.42
1:E:33:MET:HB3	1:E:33:MET:HE2	1.87	0.42
1:E:191:LYS:HZ1	1:E:383:ARG:NH1	2.17	0.42
1:E:214:ILE:HD11	1:E:216:MET:CE	2.50	0.42
1:C:65:GLN:HG3	1:C:323:THR:OG1	2.20	0.42
1:C:264:LEU:O	1:C:267:LEU:CA	2.67	0.42
1:E:55:LEU:HD21	1:E:93:PHE:HB2	2.01	0.42
1:E:61:GLU:CD	1:E:73:ARG:HE	2.23	0.42
1:B:33:MET:HE3	1:B:53:ILE:CD1	2.50	0.42
1:C:163:VAL:HG13	1:C:339:LYS:CD	2.26	0.42
1:C:252:SER:HB3	1:C:383:ARG:HD2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:PRO:HD2	1:C:398:GLU:OE1	2.20	0.42
1:D:113:PHE:CE2	1:D:151:ILE:HG12	2.55	0.42
1:D:115:GLN:HB3	1:D:118:PHE:HD1	1.81	0.42
1:E:34:TYR:CE2	1:E:38:ARG:CD	3.03	0.42
1:E:118:PHE:CG	1:E:331:ILE:HD11	2.54	0.42
1:E:184:VAL:HG11	1:E:390:PHE:CZ	2.55	0.42
1:B:298:GLU:HG2	1:B:341:PHE:CD1	2.55	0.41
1:B:298:GLU:CG	1:B:341:PHE:HD1	2.32	0.41
1:C:98:THR:C	1:C:100:LYS:H	2.23	0.41
1:C:104:TYR:HA	1:C:188:GLY:HA3	2.01	0.41
1:C:298:GLU:OE2	1:C:339:LYS:CE	2.68	0.41
1:D:230:ASP:OD2	1:D:230:ASP:N	2.49	0.41
1:D:363:MET:O	1:D:364:ALA:CB	2.68	0.41
1:A:120:VAL:HG13	1:A:325:LEU:O	2.19	0.41
1:A:178:LEU:HD12	1:A:332:PHE:O	2.20	0.41
1:A:304:LYS:HD3	1:A:308:LYS:HE3	2.02	0.41
1:C:223:PHE:O	1:C:285:LYS:HA	2.20	0.41
1:C:260:GLN:HG3	1:C:261:GLU:H	1.85	0.41
1:E:162:LEU:HD13	1:E:185:TYR:CE1	2.55	0.41
1:E:228:PHE:O	1:E:238:ILE:HA	2.20	0.41
1:A:168:SER:CB	1:A:169:PRO:CD	2.99	0.41
1:A:299:GLN:OE1	1:A:300:GLU:N	2.51	0.41
1:B:296:THR:CG2	1:B:400:MET:CE	2.97	0.41
1:B:356:GLY:CA	1:B:360:ILE:HB	2.51	0.41
1:C:197:GLU:OE1	1:C:358:ILE:CG2	2.68	0.41
1:D:112:LEU:HD12	1:D:112:LEU:HA	1.76	0.41
1:E:97:VAL:HA	1:E:104:TYR:HH	1.83	0.41
1:E:186:PHE:CD2	1:E:186:PHE:C	2.93	0.41
1:A:276:VAL:HA	1:A:279:TRP:CE3	2.55	0.41
1:B:34:TYR:OH	1:B:268:GLU:OE2	2.27	0.41
1:B:62:LEU:CD2	1:B:87:PHE:HE2	2.33	0.41
1:B:91:LYS:HE2	1:B:95:ASN:HD22	1.86	0.41
1:B:332:PHE:N	1:B:332:PHE:CD2	2.89	0.41
1:C:90:LEU:HD13	1:C:132:PHE:HE1	1.85	0.41
1:C:322:LEU:C	1:C:324:GLY:H	2.24	0.41
1:D:93:PHE:C	1:D:95:ASN:H	2.23	0.41
1:D:99:ALA:O	1:D:100:LYS:C	2.58	0.41
1:D:175:ALA:O	1:D:176:THR:C	2.58	0.41
1:A:49:SER:HB2	1:A:390:PHE:CE1	2.55	0.41
1:B:298:GLU:CG	1:B:341:PHE:CD1	3.03	0.41
1:C:124:PHE:CE1	1:C:128:MET:HE3	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:197:GLU:O	1:E:200:ARG:HD3	2.20	0.41
1:C:229:SER:HB3	1:D:361:SER:HA	2.02	0.41
1:D:166:LEU:HD12	1:D:339:LYS:HB2	2.03	0.41
1:E:315:ILE:HD13	1:E:333:LEU:HD23	2.03	0.41
1:A:115:GLN:HB3	1:A:118:PHE:CE1	2.55	0.41
1:A:274:GLN:NE2	1:A:274:GLN:C	2.73	0.41
1:B:298:GLU:HA	1:B:340:SER:O	2.21	0.41
1:C:185:TYR:CE1	1:C:341:PHE:CD2	3.08	0.41
1:E:181:ILE:HD12	1:E:337:ILE:HD12	1.99	0.41
1:E:377:PHE:HZ	1:E:391:MET:HE3	1.85	0.41
1:A:193:GLN:HB3	1:A:348:GLY:CA	2.50	0.41
1:B:331:ILE:CG2	1:B:332:PHE:N	2.84	0.41
1:C:178:LEU:HD13	1:C:178:LEU:O	2.21	0.41
1:C:185:TYR:HE1	1:C:341:PHE:CE2	2.38	0.41
1:C:317:ILE:CG2	1:C:318:LYS:N	2.84	0.41
1:E:128:MET:HE2	1:E:128:MET:HB2	1.89	0.41
1:A:166:LEU:CD2	1:A:181:ILE:HG13	2.50	0.41
1:C:64:ALA:C	1:C:65:GLN:HG2	2.39	0.41
1:C:269:PRO:O	1:C:270:LEU:C	2.58	0.41
1:D:33:MET:HE1	1:D:53:ILE:HD12	2.02	0.41
1:D:120:VAL:HA	1:D:325:LEU:O	2.20	0.41
1:D:242:LEU:HD23	1:D:255:LEU:HD12	2.02	0.41
1:E:190:TRP:HA	1:E:190:TRP:CE3	2.56	0.41
1:A:369:GLN:HG2	1:D:364:ALA:H	1.85	0.41
1:B:115:GLN:HG3	1:B:116:ASN:H	1.85	0.41
1:C:95:ASN:HA	1:C:98:THR:CG2	2.49	0.41
1:C:153:LYS:HD2	1:C:153:LYS:HA	1.80	0.41
1:C:165:ASP:O	1:C:165:ASP:CG	2.59	0.41
1:D:23:GLU:O	1:D:26:ILE:N	2.54	0.41
1:D:23:GLU:CG	1:D:89:PHE:CZ	3.04	0.41
1:D:62:LEU:CG	1:D:87:PHE:HE2	2.34	0.41
1:D:106:MET:HG2	1:D:186:PHE:HD1	1.86	0.41
1:D:293:PRO:HD3	1:D:372:VAL:HB	2.02	0.41
1:E:108:ILE:HD12	1:E:108:ILE:O	2.20	0.41
1:E:118:PHE:CD2	1:E:331:ILE:CG1	3.03	0.41
1:E:118:PHE:CB	1:E:331:ILE:HD11	2.51	0.41
1:E:228:PHE:N	1:E:228:PHE:CD2	2.88	0.41
1:B:95:ASN:CA	1:B:98:THR:HG22	2.50	0.41
1:B:260:GLN:CD	1:B:261:GLU:N	2.70	0.41
1:D:194:PHE:CE1	1:D:219:GLN:HG2	2.56	0.41
1:A:107:LYS:HB2	1:A:185:TYR:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:ILE:HB	1:A:361:SER:H	1.42	0.40
1:B:193:GLN:CG	1:B:349:SER:C	2.87	0.40
1:C:263:PRO:O	1:C:264:LEU:CG	2.68	0.40
1:D:176:THR:HA	1:D:334:SER:OG	2.21	0.40
1:E:123:GLU:O	1:E:124:PHE:C	2.59	0.40
1:E:178:LEU:HD11	1:E:333:LEU:HA	2.04	0.40
1:E:259:ARG:HD3	1:E:259:ARG:C	2.36	0.40
1:A:304:LYS:O	1:A:305:ASP:C	2.60	0.40
1:B:57:MET:CE	1:B:57:MET:CA	2.95	0.40
1:B:62:LEU:HD23	1:B:62:LEU:HA	1.82	0.40
1:B:115:GLN:HB3	1:B:118:PHE:CE1	2.57	0.40
1:B:229:SER:C	1:B:231:GLY:N	2.75	0.40
1:B:357:MET:HE3	1:C:259:ARG:NE	2.36	0.40
1:D:193:GLN:HB3	1:D:348:GLY:C	2.41	0.40
1:D:327:ASP:OD1	1:D:328:ASN:N	2.54	0.40
1:E:124:PHE:HZ	1:E:128:MET:HE3	1.75	0.40
1:A:33:MET:HE1	1:A:53:ILE:CD1	2.51	0.40
1:A:369:GLN:H	1:D:364:ALA:H	1.69	0.40
1:B:168:SER:CB	1:B:169:PRO:CD	3.00	0.40
1:C:64:ALA:O	1:C:65:GLN:HG2	2.21	0.40
1:C:166:LEU:HD12	1:C:339:LYS:HB2	2.04	0.40
1:D:43:ASP:O	1:D:43:ASP:OD1	2.39	0.40
1:D:56:ALA:N	1:D:110:ASN:HD21	2.18	0.40
1:E:199:THR:O	1:E:200:ARG:HG3	2.22	0.40
1:A:49:SER:HB3	1:A:52:SER:HB3	2.03	0.40
1:A:295:PHE:CE1	1:A:297:VAL:HG23	2.57	0.40
1:A:315:ILE:HG22	1:A:322:LEU:HD21	2.03	0.40
1:A:322:LEU:C	1:A:324:GLY:H	2.24	0.40
1:C:43:ASP:O	1:C:43:ASP:OD2	2.38	0.40
1:C:294:ARG:NH1	1:C:346:GLU:OE2	2.53	0.40
1:C:365:VAL:H	1:C:365:VAL:HG23	1.57	0.40
1:D:23:GLU:CG	1:D:89:PHE:HZ	2.34	0.40
1:D:71:GLU:CD	1:D:314:GLU:CG	2.90	0.40
1:B:49:SER:HB2	1:B:390:PHE:CE1	2.56	0.40
1:C:184:VAL:HG11	1:C:390:PHE:CZ	2.56	0.40
1:D:335:LYS:HD3	1:D:335:LYS:HA	1.94	0.40
1:E:61:GLU:CD	1:E:87:PHE:HZ	2.24	0.40
1:E:239:TYR:CB	1:E:267:LEU:HD11	2.52	0.40
1:E:294:ARG:NH1	1:E:346:GLU:OE2	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	354/407 (87%)	316 (89%)	26 (7%)	12 (3%)	3 21
1	B	370/407 (91%)	299 (81%)	45 (12%)	26 (7%)	1 7
1	C	350/407 (86%)	290 (83%)	45 (13%)	15 (4%)	2 17
1	D	353/407 (87%)	310 (88%)	32 (9%)	11 (3%)	4 23
1	E	328/407 (81%)	280 (85%)	37 (11%)	11 (3%)	3 21
All	All	1755/2035 (86%)	1495 (85%)	185 (10%)	75 (4%)	2 17

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	TYR
1	B	103	GLN
1	B	104	TYR
1	B	330	GLU
1	B	352	ALA
1	B	353	ALA
1	B	354	VAL
1	B	356	GLY
1	B	358	ILE
1	B	360	ILE
1	B	361	SER
1	B	364	ALA
1	B	399	THR
1	B	404	GLY
1	B	406	ASP
1	C	232	SER
1	C	262	VAL
1	C	263	PRO
1	C	358	ILE
1	C	360	ILE
1	C	361	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	363	MET
1	C	366	LEU
1	D	42	GLU
1	D	176	THR
1	D	360	ILE
1	D	361	SER
1	D	363	MET
1	E	87	PHE
1	E	330	GLU
1	E	363	MET
1	E	365	VAL
1	E	367	TYR
1	E	368	PRO
1	A	86	GLU
1	A	98	THR
1	A	104	TYR
1	A	330	GLU
1	A	398	GLU
1	B	99	ALA
1	B	233	ASN
1	B	234	GLU
1	B	239	TYR
1	C	174	ALA
1	C	278	GLU
1	D	43	ASP
1	D	102	SER
1	D	359	ALA
1	D	364	ALA
1	E	98	THR
1	E	125	LEU
1	A	87	PHE
1	A	174	ALA
1	B	24	GLU
1	B	32	ASN
1	B	355	SER
1	B	402	THR
1	C	99	ALA
1	E	24	GLU
1	A	24	GLU
1	A	85	GLU
1	A	94	SER
1	C	98	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	352	ALA
1	B	98	THR
1	D	66	GLY
1	E	42	GLU
1	A	102	SER
1	B	383	ARG
1	C	367	TYR
1	E	369	GLN
1	C	41	GLY
1	B	66	GLY
1	B	41	GLY
1	C	276	VAL

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	319/355 (90%)	290 (91%)	29 (9%)	9	32
1	B	330/355 (93%)	291 (88%)	39 (12%)	5	21
1	C	318/355 (90%)	281 (88%)	37 (12%)	5	22
1	D	320/355 (90%)	297 (93%)	23 (7%)	14	43
1	E	304/355 (86%)	279 (92%)	25 (8%)	11	38
All	All	1591/1775 (90%)	1438 (90%)	153 (10%)	8	29

All (153) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	30	SER
1	A	44	GLU
1	A	92	GLU
1	A	101	GLU
1	A	104	TYR
1	A	119	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	178	LEU
1	A	197	GLU
1	A	199	THR
1	A	200	ARG
1	A	203	SER
1	A	213	GLN
1	A	247	GLU
1	A	261	GLU
1	A	266	THR
1	A	274	GLN
1	A	277	GLU
1	A	287	LYS
1	A	296	THR
1	A	299	GLN
1	A	303	LEU
1	A	318	LYS
1	A	325	LEU
1	A	337	ILE
1	A	362	ARG
1	A	384	ARG
1	A	391	MET
1	A	398	GLU
1	B	92	GLU
1	B	97	VAL
1	B	101	GLU
1	B	104	TYR
1	B	106	MET
1	B	161	ASN
1	B	178	LEU
1	B	191	LYS
1	B	193	GLN
1	B	197	GLU
1	B	200	ARG
1	B	208	ASP
1	B	229	SER
1	B	230	ASP
1	B	238	ILE
1	B	239	TYR
1	B	259	ARG
1	B	260	GLN
1	B	261	GLU
1	B	296	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	299	GLN
1	B	325	LEU
1	B	326	SER
1	B	329	LYS
1	B	330	GLU
1	B	332	PHE
1	B	354	VAL
1	B	355	SER
1	B	357	MET
1	B	358	ILE
1	B	361	SER
1	B	362	ARG
1	B	363	MET
1	B	366	LEU
1	B	384	ARG
1	B	387	THR
1	B	400	MET
1	B	402	THR
1	B	407	PHE
1	C	30	SER
1	C	43	ASP
1	C	59	MET
1	C	87	PHE
1	C	89	PHE
1	C	97	VAL
1	C	98	THR
1	C	104	TYR
1	C	106	MET
1	C	126	GLN
1	C	176	THR
1	C	178	LEU
1	C	195	ARG
1	C	202	PHE
1	C	222	GLU
1	C	238	ILE
1	C	239	TYR
1	C	247	GLU
1	C	250	GLU
1	C	261	GLU
1	C	267	LEU
1	C	271	VAL
1	C	272	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	276	VAL
1	C	282	SER
1	C	284	LYS
1	C	296	THR
1	C	299	GLN
1	C	325	LEU
1	C	326	SER
1	C	331	ILE
1	C	337	ILE
1	C	357	MET
1	C	358	ILE
1	C	360	ILE
1	C	365	VAL
1	C	367	TYR
1	D	24	GLU
1	D	26	ILE
1	D	52	SER
1	D	86	GLU
1	D	92	GLU
1	D	103	GLN
1	D	104	TYR
1	D	112	LEU
1	D	123	GLU
1	D	126	GLN
1	D	138	HIS
1	D	168	SER
1	D	178	LEU
1	D	209	GLU
1	D	230	ASP
1	D	296	THR
1	D	299	GLN
1	D	325	LEU
1	D	339	LYS
1	D	350	GLU
1	D	363	MET
1	D	366	LEU
1	D	384	ARG
1	E	24	GLU
1	E	43	ASP
1	E	62	LEU
1	E	86	GLU
1	E	87	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	103	GLN
1	E	104	TYR
1	E	112	LEU
1	E	123	GLU
1	E	125	LEU
1	E	142	SER
1	E	168	SER
1	E	176	THR
1	E	178	LEU
1	E	193	GLN
1	E	197	GLU
1	E	209	GLU
1	E	230	ASP
1	E	259	ARG
1	E	296	THR
1	E	299	GLN
1	E	329	LYS
1	E	330	GLU
1	E	362	ARG
1	E	365	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	126	GLN
1	A	143	GLN
1	A	193	GLN
1	A	240	GLN
1	A	274	GLN
1	A	369	GLN
1	A	396	HIS
1	B	126	GLN
1	B	138	HIS
1	B	158	ASN
1	B	182	ASN
1	B	193	GLN
1	B	198	ASN
1	B	220	GLN
1	B	260	GLN
1	B	299	GLN
1	B	396	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	405	HIS
1	C	126	GLN
1	C	138	HIS
1	C	220	GLN
1	C	396	HIS
1	D	103	GLN
1	D	126	GLN
1	D	161	ASN
1	D	193	GLN
1	D	220	GLN
1	D	396	HIS
1	E	103	GLN
1	E	110	ASN
1	E	126	GLN
1	E	161	ASN
1	E	213	GLN
1	E	396	HIS

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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	364/407 (89%)	-0.06	6 (1%)	72	59	68, 82, 116, 133	0
1	B	376/407 (92%)	0.01	13 (3%)	44	27	28, 83, 116, 132	0
1	C	358/407 (87%)	-0.02	2 (0%)	89	84	63, 83, 108, 135	0
1	D	363/407 (89%)	-0.04	12 (3%)	46	29	54, 82, 116, 132	0
1	E	340/407 (83%)	0.12	16 (4%)	31	17	68, 82, 114, 132	0
All	All	1801/2035 (88%)	0.00	49 (2%)	54	38	28, 83, 116, 135	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	96	MET	5.3
1	D	96	MET	4.4
1	B	327	ASP	4.4
1	B	233	ASN	4.3
1	B	401	ASN	4.3
1	B	131	TYR	3.8
1	E	131	TYR	3.7
1	E	96	MET	3.6
1	B	400	MET	3.1
1	D	78	TYR	3.0
1	E	327	ASP	3.0
1	E	61	GLU	2.9
1	B	402	THR	2.9
1	A	126	GLN	2.8
1	D	319	ASP	2.7
1	E	274	GLN	2.7
1	E	222	GLU	2.6
1	B	406	ASP	2.5
1	B	123	GLU	2.5
1	A	96	MET	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	73	ARG	2.5
1	E	323	THR	2.5
1	A	329	LYS	2.5
1	B	70	LYS	2.5
1	C	327	ASP	2.4
1	B	329	LYS	2.4
1	B	403	SER	2.4
1	E	130	LYS	2.4
1	A	70	LYS	2.3
1	E	123	GLU	2.3
1	D	70	LYS	2.3
1	D	318	LYS	2.3
1	D	327	ASP	2.3
1	D	131	TYR	2.3
1	A	78	TYR	2.3
1	D	261	GLU	2.2
1	D	138	HIS	2.2
1	E	329	LYS	2.2
1	E	249	ASP	2.2
1	D	79	ASP	2.2
1	D	100	LYS	2.2
1	E	318	LYS	2.1
1	E	261	GLU	2.1
1	E	284	LYS	2.0
1	D	231	GLY	2.0
1	E	317	ILE	2.0
1	A	73	ARG	2.0
1	B	103	GLN	2.0
1	C	131	TYR	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 monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.