Full wwPDB EM Validation Report ⓘ

Apr 28, 2024 – 06:17 am BST

PDB ID	:	5FJ7
EMDB ID	:	EMD-3187
Title	:	Structure of the P2 polymerase inside in vitro assembled bacteriophage phi6 polymerase complex, with P1 included
Authors	:	Ilca, S.; Kotecha, A.; Sun, X.; Poranen, M.P.; Stuart, D.I.; Huiskonen, J.T.
Deposited on	:	2015-10-06
Resolution	:	7.90 Å(reported)
Based on initial models	:	1HHS, 4K7H

This is a Full wwPDB EM 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/EMValidationReportHelp
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:

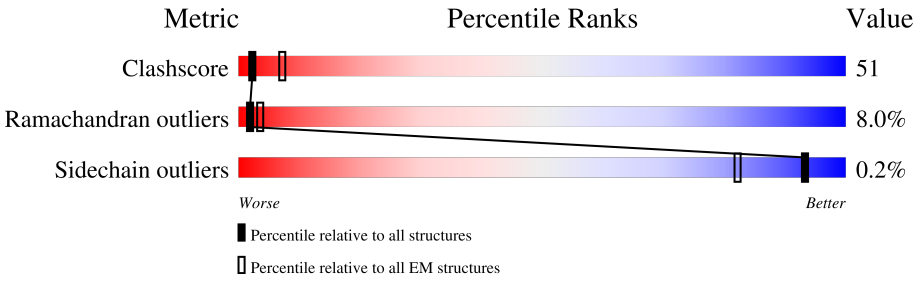
EMDB validation analysis	:	0.0.1.dev92
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 7.90 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)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	64% 33% 58% 7% .
1	B	761	66% 33% 59% 7% .
2	C	664	8% 23% 74% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17106 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 MAJOR INNER PROTEIN P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		
1	B	761	Total	C	N	O	S	0	0
			5920	3741	1048	1109	22		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P11126
B	1	GLY	-	expression tag	UNP P11126

- Molecule 2 is a protein called RNA-DIRECTED RNA POLYMERASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	664	Total	C	N	O	S	0	0
			5265	3342	914	977	32		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	456	MET	ILE	conflict	UNP P11124

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

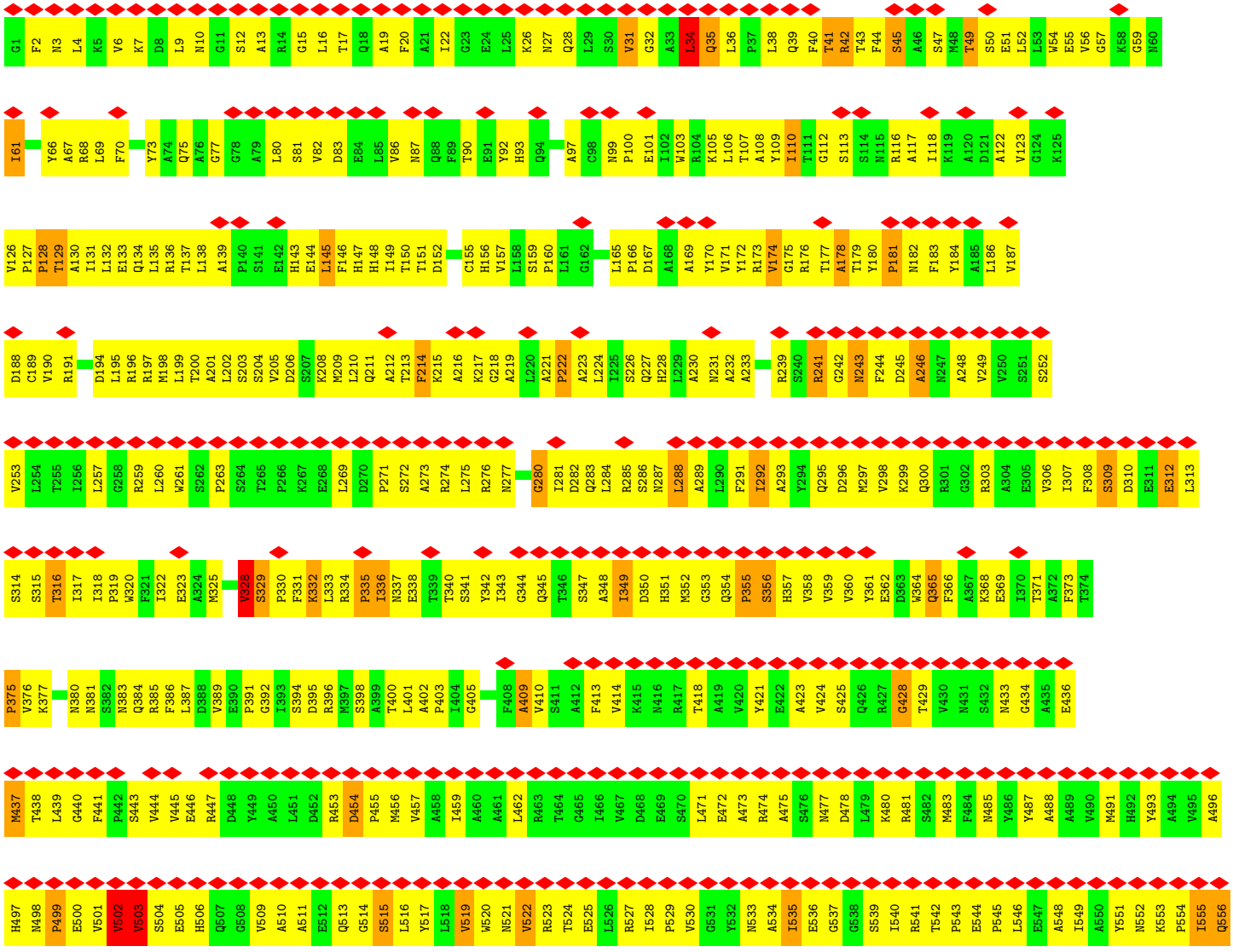
Mol	Chain	Residues	Atoms		AltConf
3	C	1	Total	Mn	0
			1	1	

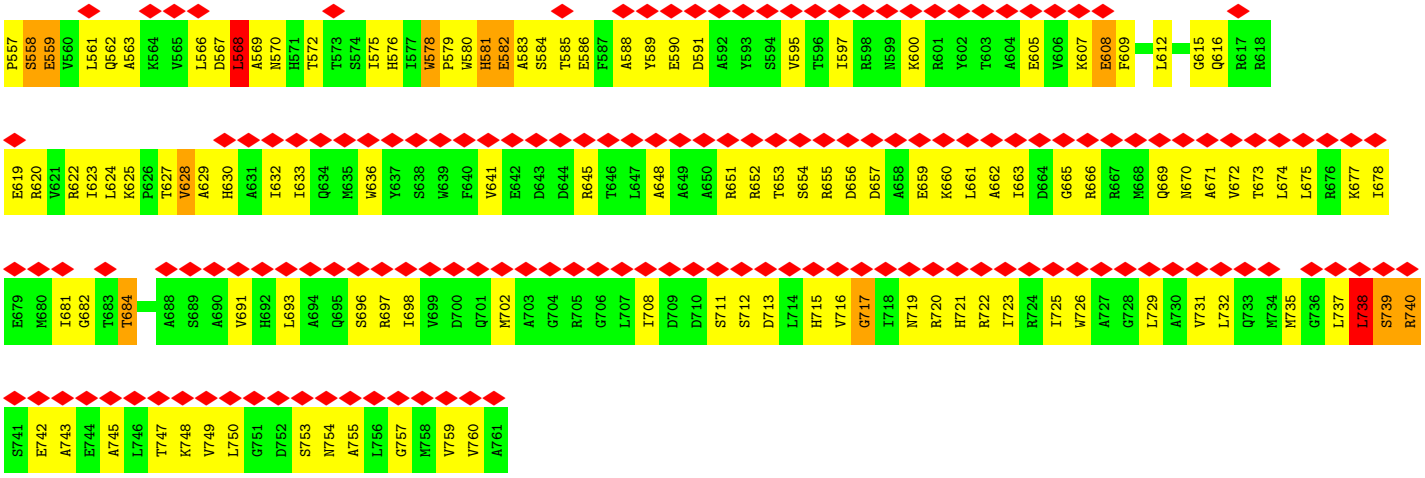
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: MAJOR INNER PROTEIN P1

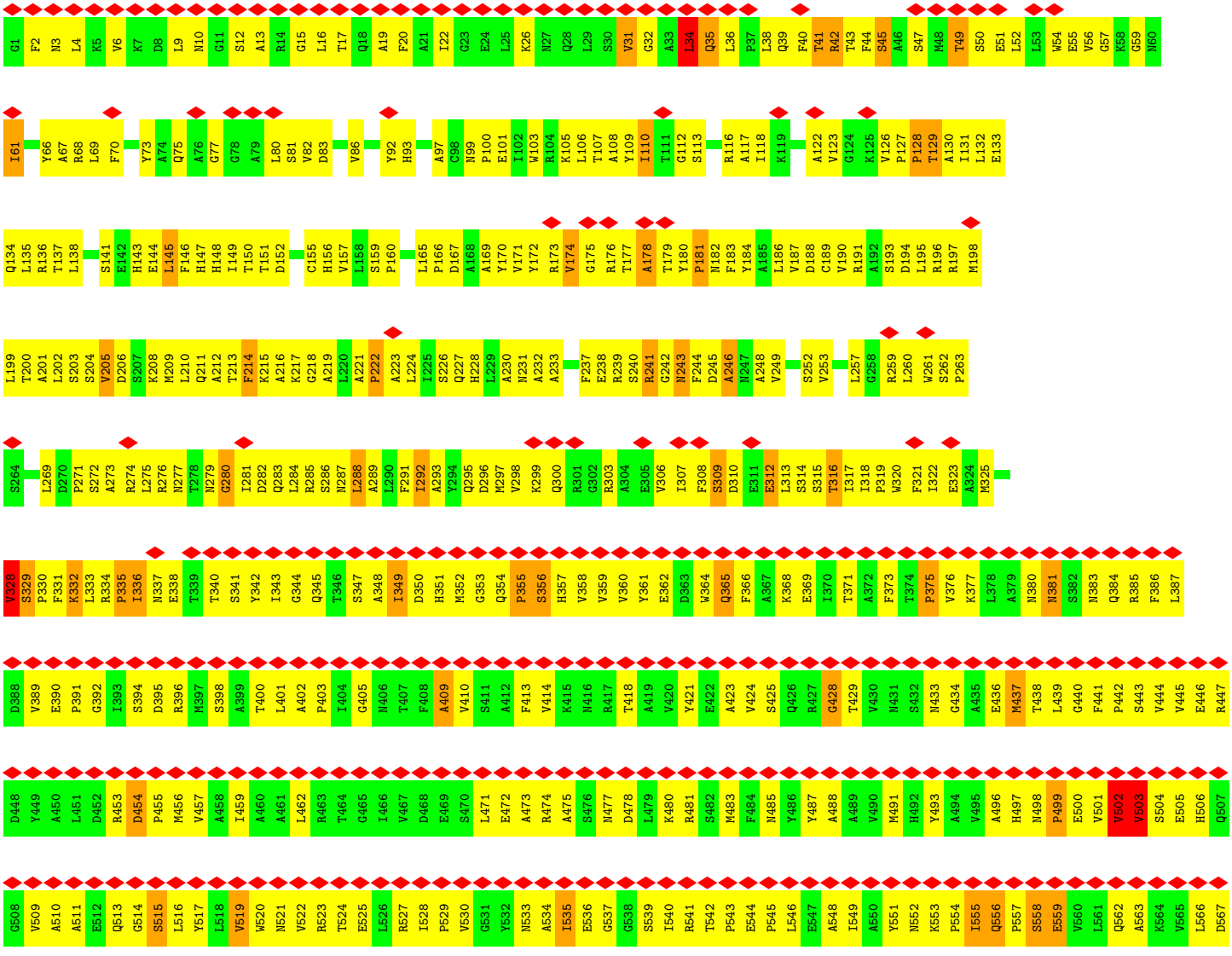
Chain A:





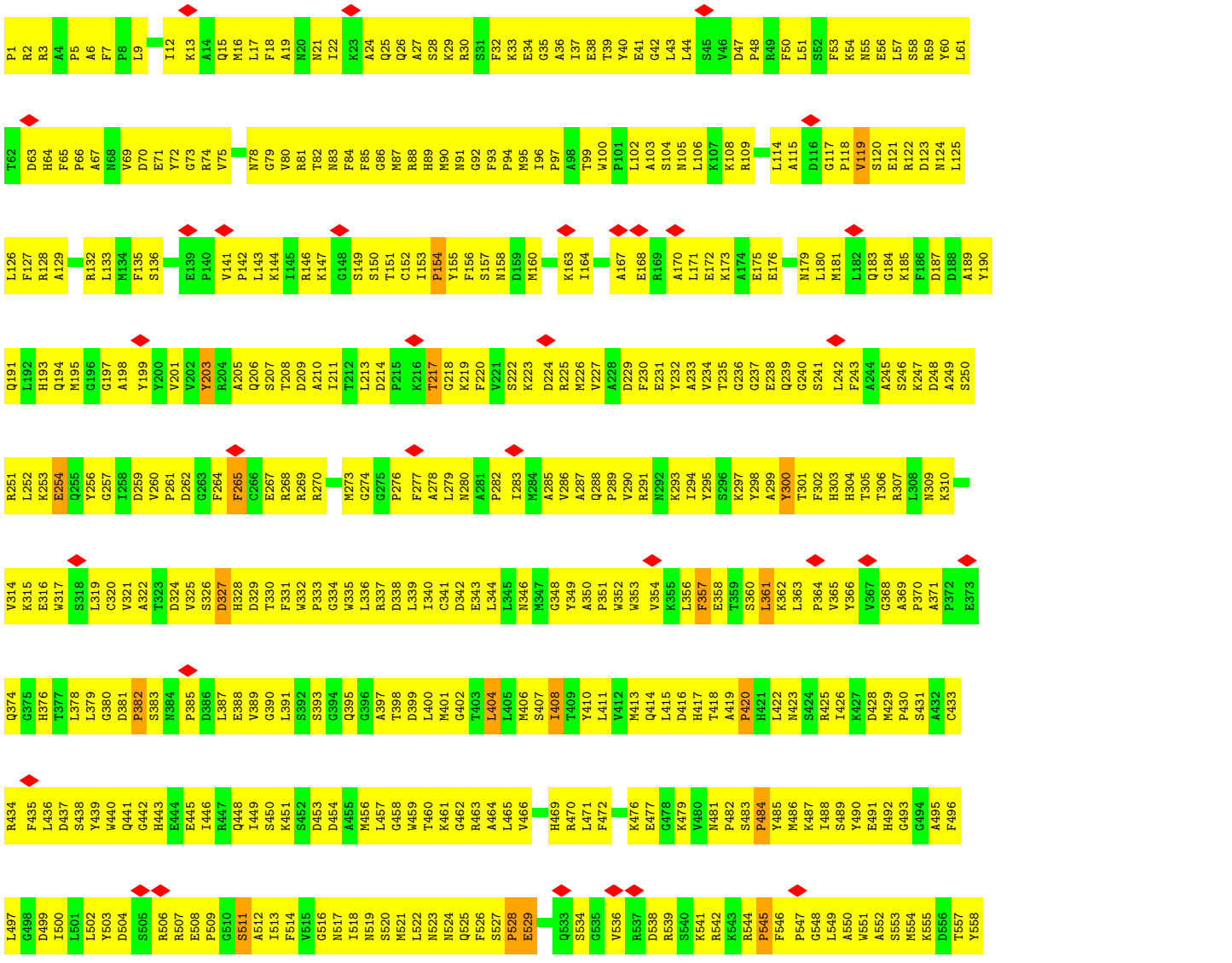
• Molecule 1: MAJOR INNER PROTEIN P1

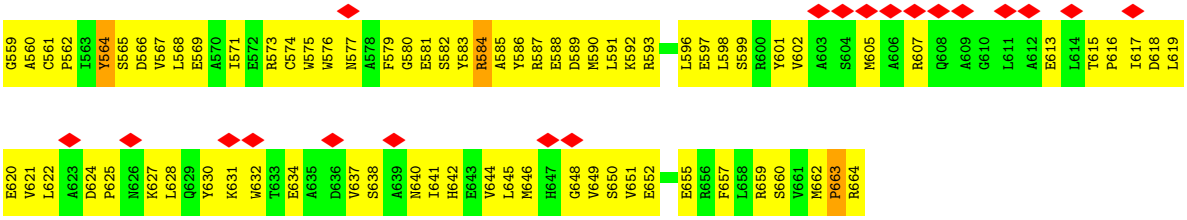
Chain B:



• Molecule 2: RNA-DIRECTED RNA POLYMERASE

Chain C:




G559 A560 C561 P562 I563 Y564 S565 D566 V567 L568 E569 A570 I571 E572 R573 C574 W575 W576 N577 A578 F579 G580 E581 S582 Y583 R584 A585 Y586 R587 E588 D589 M590 L591 K592 R593 L596 E597 L598 S599 R600 Y601 V602 A603 S604 M605 A606 R607 Q608 A609 G610 L611 A612 E613 L614 T615 P616 I617 D618 L619
E620 V621 L622 A623 D624 P625 M626 K627 L628 Q629 Y630 K631 W632 T633 E634 A635 D636 V637 S638 A639 N640 I641 H642 E643 V644 L645 M646 H647 G648 V649 S650 V651 E652 E655 R656 F657 L658 R659 S660 V661 M662 P663 R664

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	43216	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	0.16	Depositor
Minimum defocus (nm)	1100	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.074	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	135.0, 135.0, 135.0	wwPDB
Map dimensions	100, 100, 100	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.43	0/6040	0.70	7/8206 (0.1%)
1	B	0.43	0/6040	0.70	7/8206 (0.1%)
2	C	1.17	7/5396 (0.1%)	0.66	2/7297 (0.0%)
All	All	0.74	7/17476 (0.0%)	0.69	16/23709 (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	5
1	B	0	5
2	C	0	1
All	All	0	11

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	361	LEU	CG-CD1	52.88	3.47	1.51
2	C	357	PHE	CD1-CE1	26.88	1.93	1.39
2	C	357	PHE	CD2-CE2	26.52	1.92	1.39
2	C	357	PHE	CE2-CZ	25.99	1.86	1.37
2	C	357	PHE	CE1-CZ	25.62	1.86	1.37
2	C	357	PHE	CG-CD2	17.79	1.65	1.38
2	C	357	PHE	CG-CD1	17.00	1.64	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	361	LEU	CB-CG-CD1	11.31	130.23	111.00
1	B	128	PRO	CA-C-N	6.76	132.06	117.20
1	A	128	PRO	CA-C-N	6.75	132.05	117.20
1	A	128	PRO	C-N-CA	6.09	136.93	121.70
1	B	128	PRO	C-N-CA	6.09	136.93	121.70
2	C	361	LEU	CB-CG-CD2	-5.94	100.91	111.00
1	A	568	LEU	CA-CB-CG	5.92	128.92	115.30
1	B	568	LEU	CA-CB-CG	5.91	128.90	115.30
1	A	502	VAL	C-N-CA	5.79	136.19	121.70
1	B	502	VAL	C-N-CA	5.79	136.18	121.70
1	B	128	PRO	N-CA-C	5.33	125.96	112.10
1	A	128	PRO	N-CA-C	5.33	125.94	112.10
1	A	738	LEU	CA-CB-CG	5.22	127.30	115.30
1	B	738	LEU	CA-CB-CG	5.19	127.24	115.30
1	A	128	PRO	CA-C-O	-5.17	107.80	120.20
1	B	128	PRO	CA-C-O	-5.15	107.84	120.20

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	VAL	Peptide
1	A	34	LEU	Peptide
1	A	35	GLN	Peptide
1	A	365	GLN	Peptide
1	A	437	MET	Peptide
1	B	328	VAL	Peptide
1	B	34	LEU	Peptide
1	B	35	GLN	Peptide
1	B	365	GLN	Peptide
1	B	437	MET	Peptide
2	C	203	TYR	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	5920	0	5913	504	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5920	0	5907	641	0
2	C	5265	0	5154	718	0
3	C	1	0	0	0	0
All	All	17106	0	16974	1735	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 51.

All (1735) 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)
2:C:357:PHE:CE1	2:C:357:PHE:CZ	1.86	1.58
2:C:357:PHE:CD2	2:C:357:PHE:CE2	1.92	1.58
2:C:357:PHE:CZ	2:C:357:PHE:CE2	1.86	1.56
2:C:357:PHE:CE1	2:C:357:PHE:CD1	1.93	1.53
1:B:237:PHE:O	2:C:425:ARG:NH2	1.58	1.36
1:B:237:PHE:N	2:C:434:ARG:NH2	1.68	1.35
1:B:313:LEU:N	2:C:466:VAL:HG21	1.45	1.28
1:B:317:ILE:O	2:C:461:LYS:HD2	1.20	1.25
1:B:312:GLU:OE2	2:C:469:HIS:HB2	1.31	1.24
2:C:357:PHE:CD2	2:C:361:LEU:HG	1.75	1.22
1:B:312:GLU:CG	2:C:466:VAL:HG23	1.70	1.21
1:B:312:GLU:CG	2:C:466:VAL:CG2	2.20	1.20
2:C:357:PHE:CG	2:C:361:LEU:HG	1.76	1.20
1:B:237:PHE:N	2:C:434:ARG:HH22	0.93	1.19
1:B:316:THR:HG21	2:C:466:VAL:CA	1.72	1.18
1:B:312:GLU:HG2	2:C:466:VAL:CG2	1.73	1.16
1:B:312:GLU:OE1	2:C:470:ARG:HG3	1.44	1.15
1:B:316:THR:HG23	2:C:469:HIS:CD2	1.82	1.15
1:B:316:THR:O	2:C:465:LEU:HD23	1.48	1.14
1:B:319:PRO:C	2:C:461:LYS:NZ	2.00	1.14
1:B:316:THR:HG21	2:C:466:VAL:N	1.62	1.13
1:B:317:ILE:HD12	2:C:445:GLU:OE2	1.48	1.12
1:B:205:VAL:HG11	2:C:441:GLN:OE1	1.51	1.08
1:B:316:THR:HG23	2:C:469:HIS:NE2	1.68	1.08
1:B:205:VAL:HG13	2:C:441:GLN:CD	1.75	1.06
1:B:313:LEU:N	2:C:466:VAL:CG2	2.18	1.06
1:B:317:ILE:HB	2:C:465:LEU:HB3	1.37	1.04
1:B:316:THR:O	2:C:465:LEU:CD2	2.04	1.04
1:B:317:ILE:HG13	2:C:461:LYS:HA	1.39	1.04
2:C:357:PHE:CE2	2:C:361:LEU:CD1	2.41	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:LEU:H	2:C:466:VAL:CG2	1.71	1.03
1:B:205:VAL:CG1	2:C:441:GLN:CD	2.28	1.02
2:C:357:PHE:CE1	2:C:361:LEU:CD1	2.42	1.01
2:C:357:PHE:CD2	2:C:361:LEU:CD1	2.44	1.01
2:C:357:PHE:CD1	2:C:361:LEU:CD1	2.45	1.00
1:B:205:VAL:HG13	2:C:441:GLN:NE2	1.78	0.99
1:B:205:VAL:CG1	2:C:441:GLN:NE2	2.26	0.99
2:C:357:PHE:CZ	2:C:361:LEU:CD1	2.44	0.99
1:B:317:ILE:O	2:C:461:LYS:CD	2.12	0.96
1:B:317:ILE:CD1	2:C:445:GLU:OE2	2.13	0.96
1:B:237:PHE:H	2:C:434:ARG:NH2	1.45	0.95
1:B:117:ALA:H	1:B:221:ALA:H	1.10	0.95
1:B:237:PHE:C	2:C:425:ARG:NH2	2.12	0.95
1:B:312:GLU:CD	2:C:466:VAL:HG22	1.85	0.95
1:B:312:GLU:CG	2:C:466:VAL:HG22	1.97	0.94
2:C:555:LYS:HD2	2:C:559:GLY:HA3	1.50	0.94
2:C:357:PHE:CG	2:C:361:LEU:CD1	2.50	0.94
1:B:313:LEU:H	2:C:466:VAL:HG21	0.80	0.92
1:B:312:GLU:OE1	2:C:470:ARG:CG	2.18	0.91
1:B:312:GLU:OE2	2:C:469:HIS:CB	2.19	0.91
2:C:357:PHE:CE2	2:C:361:LEU:CG	2.54	0.91
1:B:312:GLU:HG2	2:C:466:VAL:HG23	0.92	0.91
1:B:312:GLU:CB	2:C:466:VAL:CG2	2.49	0.91
1:A:117:ALA:H	1:A:221:ALA:H	1.10	0.90
1:B:321:PHE:CB	2:C:461:LYS:HB3	2.00	0.90
2:C:357:PHE:CD2	2:C:361:LEU:CG	2.55	0.90
1:B:205:VAL:CG1	2:C:441:GLN:OE1	2.19	0.90
2:C:319:LEU:HB3	2:C:459:TRP:HB2	1.53	0.88
2:C:357:PHE:CZ	2:C:361:LEU:CG	2.57	0.88
1:B:316:THR:CG2	2:C:466:VAL:CA	2.54	0.86
2:C:18:PHE:HB3	2:C:24:ALA:HB1	1.57	0.86
2:C:357:PHE:CD1	2:C:361:LEU:CG	2.59	0.86
2:C:357:PHE:CE1	2:C:361:LEU:CG	2.59	0.86
1:B:321:PHE:CD1	2:C:461:LYS:HB3	2.11	0.85
1:B:322:ILE:H	2:C:461:LYS:HZ3	1.23	0.85
1:B:342:TYR:HA	1:B:559:GLU:HG3	1.57	0.85
2:C:60:TYR:O	2:C:64:HIS:ND1	2.08	0.84
1:A:342:TYR:HA	1:A:559:GLU:HG3	1.57	0.84
1:B:108:ALA:HA	1:B:112:GLY:HA3	1.59	0.84
2:C:332:TRP:HH2	2:C:337:ARG:HB2	1.43	0.84
1:B:322:ILE:N	2:C:461:LYS:NZ	2.22	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:PHE:H	2:C:434:ARG:HH22	0.85	0.83
1:A:108:ALA:HA	1:A:112:GLY:HA3	1.59	0.83
1:B:316:THR:CG2	2:C:466:VAL:N	2.41	0.83
1:A:4:LEU:HG	1:A:436:GLU:HB2	1.60	0.82
1:B:316:THR:HG21	2:C:466:VAL:HA	1.60	0.82
2:C:554:MET:HG2	2:C:564:TYR:HE1	1.44	0.82
1:A:527:ARG:HG3	1:A:529:PRO:HD3	1.61	0.82
1:B:239:ARG:C	2:C:425:ARG:NH1	2.33	0.82
1:B:527:ARG:HG3	1:B:529:PRO:HD3	1.61	0.82
1:A:502:VAL:HA	1:A:503:VAL:HG12	1.62	0.82
1:B:4:LEU:HG	1:B:436:GLU:HB2	1.60	0.82
1:B:317:ILE:HG13	2:C:461:LYS:CA	2.08	0.82
1:A:715:HIS:HD2	1:A:716:VAL:HG22	1.44	0.81
1:B:316:THR:CG2	2:C:466:VAL:HA	2.09	0.81
1:B:715:HIS:HD2	1:B:716:VAL:HG22	1.43	0.81
2:C:357:PHE:CG	2:C:361:LEU:CG	2.62	0.81
1:B:312:GLU:HB3	2:C:466:VAL:CG2	2.08	0.81
1:B:16:LEU:HA	1:B:487:TYR:HE1	1.46	0.80
1:A:582:GLU:O	1:A:625:LYS:NZ	2.15	0.80
1:B:502:VAL:HA	1:B:503:VAL:HG12	1.62	0.80
1:B:582:GLU:O	1:B:625:LYS:NZ	2.15	0.80
1:A:44:PHE:HA	1:A:333:LEU:HA	1.64	0.80
1:A:173:ARG:HB2	1:A:579:PRO:HG2	1.64	0.80
1:B:651:ARG:HB2	1:B:663:ILE:HD11	1.63	0.80
2:C:206:GLN:HB3	2:C:268:ARG:HB3	1.63	0.80
2:C:83:ASN:HB2	2:C:85:PHE:HD2	1.46	0.79
2:C:357:PHE:CD2	2:C:361:LEU:HD12	2.17	0.79
1:A:651:ARG:HB2	1:A:663:ILE:HD11	1.63	0.79
2:C:627:LYS:O	2:C:631:LYS:N	2.15	0.79
1:B:316:THR:CG2	2:C:465:LEU:HG	2.13	0.79
1:B:436:GLU:OE2	1:B:439:LEU:N	2.12	0.79
1:B:319:PRO:C	2:C:461:LYS:HZ3	1.84	0.79
2:C:146:ARG:NH1	2:C:645:LEU:O	2.16	0.79
1:A:16:LEU:HA	1:A:487:TYR:HE1	1.46	0.79
2:C:226:MET:HB3	2:C:242:LEU:HG	1.64	0.78
2:C:357:PHE:CZ	2:C:361:LEU:HD13	2.16	0.78
1:B:528:ILE:HG12	1:B:536:GLU:HB3	1.65	0.78
2:C:109:ARG:O	2:C:114:LEU:N	2.15	0.78
2:C:109:ARG:NH1	2:C:331:PHE:O	2.16	0.78
2:C:115:ALA:N	2:C:484:PRO:O	2.13	0.78
2:C:466:VAL:HA	2:C:469:HIS:CD2	2.18	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ILE:HG12	1:A:536:GLU:HB3	1.65	0.78
1:B:44:PHE:HA	1:B:333:LEU:HA	1.64	0.78
1:A:197:ARG:HA	1:A:200:THR:HG22	1.66	0.78
1:A:436:GLU:OE2	1:A:439:LEU:N	2.12	0.78
1:B:117:ALA:N	1:B:221:ALA:H	1.81	0.78
2:C:357:PHE:CD1	2:C:361:LEU:HD11	2.17	0.78
1:B:316:THR:C	2:C:465:LEU:HD23	2.02	0.77
1:B:195:LEU:HA	1:B:198:MET:HB3	1.67	0.77
1:B:317:ILE:HD11	2:C:462:GLY:N	1.99	0.77
1:B:173:ARG:HB2	1:B:579:PRO:HG2	1.64	0.77
2:C:203:TYR:OH	2:C:269:ARG:NH2	2.17	0.77
1:B:322:ILE:N	2:C:461:LYS:HZ3	1.81	0.77
1:B:321:PHE:HD1	2:C:461:LYS:HB3	1.49	0.77
1:B:197:ARG:HA	1:B:200:THR:HG22	1.66	0.77
1:B:320:TRP:N	2:C:461:LYS:NZ	2.32	0.77
1:B:189:CYS:HB3	1:B:323:GLU:HG3	1.67	0.77
1:B:410:VAL:HA	1:B:413:PHE:HB3	1.67	0.77
2:C:187:ASP:HA	2:C:190:TYR:HB3	1.67	0.77
1:A:588:ALA:HB1	1:A:589:TYR:HB2	1.67	0.76
1:B:316:THR:CG2	2:C:469:HIS:CD2	2.64	0.76
1:B:321:PHE:HB2	2:C:461:LYS:HB3	1.65	0.76
2:C:395:GLN:HE21	2:C:397:ALA:HB3	1.50	0.76
1:A:195:LEU:HA	1:A:198:MET:HB3	1.67	0.76
1:B:581:HIS:O	1:B:583:ALA:N	2.17	0.76
2:C:105:ASN:O	2:C:109:ARG:N	2.19	0.76
1:A:200:THR:HA	1:A:203:SER:HB3	1.67	0.76
1:A:387:LEU:HG	1:A:572:THR:HG21	1.66	0.76
1:A:410:VAL:HA	1:A:413:PHE:HB3	1.66	0.76
1:B:387:LEU:HG	1:B:572:THR:HG21	1.66	0.76
2:C:109:ARG:HG2	2:C:114:LEU:HD12	1.68	0.76
1:A:480:LYS:HA	1:A:483:MET:HG2	1.68	0.76
2:C:446:ILE:HG22	2:C:459:TRP:HE1	1.51	0.76
2:C:55:ASN:HA	2:C:88:ARG:HH12	1.49	0.76
2:C:575:TRP:CG	2:C:583:TYR:HB2	2.20	0.76
1:A:208:LYS:O	1:A:211:GLN:NE2	2.19	0.76
1:A:176:ARG:HH12	1:A:447:ARG:HA	1.49	0.75
1:B:208:LYS:O	1:B:211:GLN:NE2	2.19	0.75
1:B:176:ARG:HH12	1:B:447:ARG:HA	1.49	0.75
2:C:175:GLU:HA	2:C:352:TRP:CD2	2.22	0.75
2:C:395:GLN:HB3	2:C:398:THR:HG23	1.67	0.75
2:C:235:THR:HB	2:C:238:GLU:HB2	1.68	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LYS:HA	1:B:483:MET:HG2	1.68	0.75
1:B:633:ILE:HD13	1:B:738:LEU:HB3	1.69	0.75
2:C:206:GLN:HE21	2:C:208:THR:H	1.32	0.75
1:A:117:ALA:N	1:A:221:ALA:H	1.81	0.75
1:B:148:HIS:O	1:B:151:THR:OG1	2.04	0.75
1:A:189:CYS:HB3	1:A:323:GLU:HG3	1.67	0.74
1:A:134:GLN:O	1:A:137:THR:OG1	2.06	0.74
1:A:347:SER:HA	1:A:358:VAL:HG13	1.70	0.74
1:B:588:ALA:HB1	1:B:589:TYR:HB2	1.67	0.74
2:C:149:SER:OG	2:C:163:LYS:NZ	2.19	0.74
1:B:200:THR:HA	1:B:203:SER:HB3	1.67	0.74
1:B:317:ILE:HB	2:C:465:LEU:CB	2.17	0.74
2:C:90:MET:N	2:C:265:PHE:O	2.20	0.74
1:A:633:ILE:HD13	1:A:738:LEU:HB3	1.69	0.74
1:A:581:HIS:O	1:A:583:ALA:N	2.17	0.74
2:C:146:ARG:NH1	2:C:147:LYS:O	2.21	0.74
1:B:132:LEU:HD21	1:B:136:ARG:HH21	1.53	0.73
1:B:365:GLN:HA	1:B:562:GLN:HB2	1.70	0.73
1:A:359:VAL:HA	1:A:438:THR:HA	1.71	0.73
1:B:134:GLN:O	1:B:137:THR:OG1	2.05	0.73
1:B:316:THR:HG21	2:C:466:VAL:CB	2.18	0.73
1:B:717:GLY:O	1:B:721:HIS:N	2.16	0.73
2:C:88:ARG:NH2	2:C:262:ASP:O	2.21	0.73
2:C:269:ARG:NH2	2:C:370:PRO:O	2.20	0.73
1:A:365:GLN:HA	1:A:562:GLN:HB2	1.70	0.72
1:A:619:GLU:OE2	1:A:620:ARG:NH1	2.21	0.72
1:B:619:GLU:OE2	1:B:620:ARG:NH1	2.21	0.72
1:A:132:LEU:HD21	1:A:136:ARG:HH21	1.53	0.72
1:A:55:GLU:HG3	1:A:171:VAL:HG22	1.70	0.72
1:A:530:VAL:O	1:A:551:TYR:OH	2.07	0.72
2:C:17:LEU:HD21	2:C:197:GLY:HA3	1.71	0.72
1:B:347:SER:HA	1:B:358:VAL:HG13	1.70	0.72
1:B:359:VAL:HA	1:B:438:THR:HA	1.70	0.72
1:B:272:SER:HB2	1:B:275:LEU:HB3	1.72	0.72
1:B:533:ASN:HD22	1:B:543:PRO:HD2	1.55	0.72
1:B:55:GLU:HG3	1:B:171:VAL:HG22	1.70	0.72
1:A:148:HIS:O	1:A:151:THR:OG1	2.05	0.72
2:C:448:GLN:HA	2:C:457:LEU:HA	1.71	0.72
1:A:272:SER:HB2	1:A:275:LEU:HB3	1.72	0.71
1:A:334:ARG:HD3	1:A:338:GLU:HB2	1.72	0.71
1:A:630:HIS:HB2	1:A:737:LEU:HD22	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:MET:N	1:A:353:GLY:HA2	2.05	0.71
1:B:334:ARG:HD3	1:B:338:GLU:HB2	1.72	0.71
2:C:13:LYS:O	2:C:190:TYR:OH	2.08	0.71
2:C:252:LEU:O	2:C:257:GLY:N	2.22	0.71
1:B:630:HIS:HB2	1:B:737:LEU:HD22	1.72	0.71
2:C:250:SER:O	2:C:254:GLU:N	2.23	0.71
1:A:172:TYR:CD1	1:A:578:TRP:HB2	2.26	0.71
2:C:21:ASN:H	2:C:24:ALA:HB3	1.56	0.71
1:B:392:GLY:O	1:B:396:ARG:NH1	2.24	0.71
1:B:172:TYR:CD1	1:B:578:TRP:HB2	2.26	0.71
1:A:242:GLY:O	1:A:244:PHE:N	2.24	0.71
2:C:106:LEU:HD11	2:C:388:GLU:HG3	1.73	0.71
1:A:392:GLY:O	1:A:396:ARG:NH1	2.24	0.70
1:B:242:GLY:O	1:B:244:PHE:N	2.24	0.70
1:B:352:MET:N	1:B:353:GLY:HA2	2.05	0.70
2:C:180:LEU:O	2:C:185:LYS:N	2.23	0.70
1:B:40:PHE:HB2	1:B:288:LEU:HB3	1.73	0.70
1:B:316:THR:O	2:C:465:LEU:HD21	1.89	0.70
1:B:530:VAL:O	1:B:551:TYR:OH	2.07	0.70
1:B:655:ARG:N	1:B:656:ASP:HB2	2.07	0.70
2:C:357:PHE:CD1	2:C:361:LEU:HG	2.24	0.70
1:A:655:ARG:N	1:A:656:ASP:HB2	2.07	0.70
1:B:73:TYR:O	1:B:77:GLY:N	2.25	0.70
2:C:72:TYR:HA	2:C:476:LYS:HD2	1.73	0.70
2:C:315:LYS:NZ	2:C:511:SER:O	2.24	0.70
1:A:73:TYR:O	1:A:77:GLY:N	2.24	0.70
2:C:548:GLY:O	2:C:551:TRP:HB3	1.91	0.70
1:A:717:GLY:O	1:A:721:HIS:N	2.16	0.70
2:C:503:TYR:HB3	2:C:507:ARG:HA	1.74	0.70
1:A:533:ASN:HD22	1:A:543:PRO:HD2	1.55	0.70
1:B:40:PHE:HD2	1:B:289:ALA:HA	1.57	0.70
1:B:317:ILE:CG1	2:C:461:LYS:HA	2.18	0.70
2:C:368:GLY:O	2:C:376:HIS:N	2.24	0.70
2:C:589:ASP:HA	2:C:592:LYS:HD2	1.74	0.70
1:B:316:THR:HG23	2:C:465:LEU:HG	1.73	0.69
1:B:316:THR:HA	2:C:469:HIS:NE2	2.07	0.69
2:C:536:VAL:HG11	2:C:541:LYS:HD2	1.74	0.69
2:C:99:THR:HB	2:C:227:VAL:HB	1.74	0.69
1:A:453:ARG:NH2	1:A:474:ARG:O	2.26	0.69
1:A:712:SER:O	1:A:715:HIS:ND1	2.22	0.69
1:B:45:SER:OG	1:B:332:LYS:HB2	1.93	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:VAL:HG13	1:B:166:PRO:HD3	1.75	0.69
1:B:554:PRO:O	1:B:556:GLN:N	2.22	0.69
2:C:180:LEU:HB3	2:C:185:LYS:HB2	1.73	0.69
1:A:40:PHE:HD2	1:A:289:ALA:HA	1.57	0.69
1:A:534:ALA:O	1:A:536:GLU:N	2.26	0.69
1:B:321:PHE:HD1	2:C:461:LYS:CB	2.05	0.69
1:B:534:ALA:O	1:B:536:GLU:N	2.26	0.69
1:B:242:GLY:O	2:C:463:ARG:NH2	2.26	0.69
1:B:312:GLU:CD	2:C:466:VAL:CG2	2.53	0.69
2:C:387:LEU:HB3	2:C:389:VAL:HG13	1.75	0.69
2:C:454:ASP:OD2	2:C:497:LEU:N	2.24	0.69
1:A:126:VAL:HG13	1:A:166:PRO:HD3	1.75	0.69
1:A:385:ARG:HD2	1:A:580:TRP:HE1	1.57	0.69
1:B:316:THR:CG2	2:C:469:HIS:NE2	2.53	0.69
1:B:453:ARG:NH2	1:B:474:ARG:O	2.26	0.69
2:C:287:ALA:O	2:C:291:ARG:N	2.23	0.69
2:C:466:VAL:HA	2:C:469:HIS:HD2	1.57	0.69
2:C:615:THR:O	2:C:619:LEU:N	2.26	0.69
1:B:51:GLU:HA	1:B:174:VAL:HG21	1.75	0.69
1:B:312:GLU:OE1	2:C:466:VAL:HG22	1.93	0.69
1:A:296:ASP:O	1:A:300:GLN:N	2.19	0.69
2:C:81:ARG:NH1	2:C:493:GLY:O	2.25	0.69
2:C:231:GLU:O	2:C:235:THR:OG1	2.08	0.68
1:B:385:ARG:HD2	1:B:580:TRP:HE1	1.57	0.68
2:C:136:SER:OG	2:C:293:LYS:NZ	2.22	0.68
1:A:45:SER:OG	1:A:332:LYS:HB2	1.93	0.68
1:B:97:ALA:HA	1:B:103:TRP:HZ2	1.58	0.68
1:B:317:ILE:CB	2:C:465:LEU:HB3	2.19	0.68
1:A:40:PHE:HB2	1:A:288:LEU:HB3	1.73	0.68
1:A:112:GLY:HA2	1:A:116:ARG:HD3	1.76	0.68
1:B:321:PHE:CA	2:C:461:LYS:HB3	2.23	0.68
2:C:90:MET:HB3	2:C:93:PHE:HB2	1.74	0.68
1:B:712:SER:O	1:B:715:HIS:ND1	2.22	0.68
1:B:31:VAL:HG22	1:B:32:GLY:H	1.58	0.68
2:C:321:VAL:HB	2:C:457:LEU:HB2	1.76	0.68
1:B:112:GLY:HA2	1:B:116:ARG:HD3	1.76	0.67
1:B:283:GLN:O	1:B:286:SER:OG	2.09	0.67
2:C:414:GLN:O	2:C:418:THR:OG1	2.07	0.67
1:B:240:SER:N	2:C:425:ARG:NH1	2.41	0.67
1:A:97:ALA:HA	1:A:103:TRP:HZ2	1.58	0.67
1:B:238:GLU:HG3	2:C:434:ARG:NH1	2.09	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:293:LYS:O	2:C:297:LYS:N	2.22	0.67
1:A:51:GLU:HA	1:A:174:VAL:HG21	1.75	0.67
1:B:358:VAL:H	1:B:437:MET:HB3	1.60	0.67
2:C:70:ASP:O	2:C:492:HIS:NE2	2.28	0.67
1:A:368:LYS:HG2	1:A:402:ALA:HA	1.77	0.67
2:C:322:ALA:HA	2:C:456:MET:HG2	1.77	0.67
1:A:580:TRP:HA	1:A:581:HIS:O	1.95	0.67
1:B:312:GLU:HB3	2:C:466:VAL:HG22	1.74	0.67
1:A:691:VAL:HG12	1:A:723:ILE:HG12	1.77	0.67
1:B:691:VAL:HG12	1:B:723:ILE:HG12	1.77	0.67
2:C:66:PRO:O	2:C:78:ASN:ND2	2.28	0.67
1:B:456:MET:HA	1:B:459:ILE:HD12	1.78	0.66
1:B:580:TRP:HA	1:B:581:HIS:O	1.95	0.66
2:C:627:LYS:HB2	2:C:632:TRP:CZ3	2.29	0.66
1:B:505:GLU:HG2	1:B:515:SER:H	1.61	0.66
1:B:535:ILE:HD12	1:B:541:ARG:H	1.61	0.66
1:A:358:VAL:H	1:A:437:MET:HB3	1.60	0.66
1:B:521:ASN:O	1:B:539:SER:OG	2.10	0.66
2:C:30:ARG:O	2:C:376:HIS:NE2	2.28	0.66
1:A:456:MET:HA	1:A:459:ILE:HD12	1.78	0.66
1:B:239:ARG:HD2	2:C:438:SER:OG	1.96	0.66
1:B:368:LYS:HG2	1:B:402:ALA:HA	1.76	0.66
1:B:627:THR:O	1:B:629:ALA:N	2.29	0.66
2:C:248:ASP:OD2	2:C:251:ARG:N	2.27	0.66
1:A:31:VAL:HG22	1:A:32:GLY:H	1.58	0.66
1:A:315:SER:O	1:A:317:ILE:N	2.28	0.66
2:C:634:GLU:O	2:C:642:HIS:NE2	2.29	0.66
1:B:179:THR:N	1:B:180:TYR:HA	2.11	0.66
1:B:317:ILE:HD12	2:C:460:THR:O	1.96	0.66
2:C:341:CYS:HA	2:C:344:LEU:HD12	1.76	0.66
1:B:315:SER:O	1:B:317:ILE:N	2.28	0.66
1:B:92:TYR:HE2	1:B:150:THR:HG21	1.62	0.65
1:B:501:VAL:HG23	1:B:502:VAL:HG12	1.78	0.65
2:C:332:TRP:CH2	2:C:337:ARG:HB2	2.29	0.65
2:C:551:TRP:CZ2	2:C:584:ARG:HA	2.31	0.65
1:A:627:THR:O	1:A:629:ALA:N	2.29	0.65
2:C:381:ASP:O	2:C:383:SER:N	2.24	0.65
1:A:739:SER:OG	1:A:740:ARG:N	2.28	0.65
1:B:317:ILE:CD1	2:C:460:THR:O	2.44	0.65
1:B:655:ARG:H	1:B:656:ASP:HB2	1.61	0.65
2:C:545:PRO:HG2	2:C:625:PRO:HG2	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:GLN:NE2	1:A:286:SER:OG	2.30	0.65
1:A:395:ASP:OD1	1:A:396:ARG:N	2.30	0.65
1:A:535:ILE:HD12	1:A:541:ARG:H	1.60	0.65
1:B:283:GLN:NE2	1:B:286:SER:OG	2.30	0.65
1:B:312:GLU:CB	2:C:466:VAL:HG22	2.22	0.65
1:B:395:ASP:OD1	1:B:396:ARG:N	2.30	0.65
1:B:739:SER:OG	1:B:740:ARG:N	2.28	0.65
2:C:637:VAL:HB	2:C:642:HIS:CD2	2.31	0.65
1:A:505:GLU:HG2	1:A:515:SER:H	1.61	0.65
2:C:539:ARG:NH1	2:C:542:ARG:HH11	1.95	0.65
2:C:546:PHE:CE2	2:C:598:LEU:HB2	2.31	0.65
2:C:547:PRO:O	2:C:587:ARG:NH2	2.24	0.65
1:A:42:ARG:NH2	1:A:283:GLN:HE21	1.95	0.64
1:A:179:THR:N	1:A:180:TYR:HA	2.11	0.64
1:A:306:VAL:O	1:A:308:PHE:N	2.30	0.64
1:B:57:GLY:H	1:B:170:TYR:HB2	1.62	0.64
1:B:306:VAL:O	1:B:308:PHE:N	2.30	0.64
1:A:283:GLN:O	1:A:286:SER:OG	2.09	0.64
1:A:655:ARG:H	1:A:656:ASP:HB2	1.61	0.64
1:B:715:HIS:CD2	1:B:716:VAL:HG22	2.31	0.64
1:B:729:LEU:HD21	1:B:743:ALA:HB1	1.79	0.64
2:C:536:VAL:O	2:C:542:ARG:NH2	2.30	0.64
1:B:194:ASP:O	1:B:198:MET:N	2.25	0.64
2:C:235:THR:O	2:C:237:GLY:N	2.31	0.64
2:C:504:ASP:O	2:C:507:ARG:NH1	2.30	0.64
2:C:521:MET:HB2	2:C:558:TYR:HD2	1.63	0.64
1:A:144:GLU:HG2	1:A:145:LEU:H	1.63	0.64
2:C:94:PRO:HB2	2:C:269:ARG:HD2	1.78	0.64
2:C:277:PHE:O	2:C:280:ASN:N	2.31	0.64
2:C:534:SER:O	2:C:542:ARG:NH2	2.31	0.64
1:A:315:SER:OG	1:A:316:THR:N	2.30	0.64
1:B:358:VAL:N	1:B:437:MET:SD	2.71	0.64
2:C:299:ALA:HB1	2:C:303:HIS:HB2	1.80	0.64
2:C:587:ARG:NH1	2:C:590:MET:SD	2.71	0.64
1:B:42:ARG:NH2	1:B:283:GLN:HE21	1.96	0.64
1:B:375:PRO:HG3	1:B:622:ARG:HE	1.63	0.64
1:B:520:TRP:H	1:B:542:THR:H	1.46	0.64
2:C:459:TRP:HB3	2:C:465:LEU:HD13	1.79	0.64
1:A:580:TRP:CD2	1:A:581:HIS:HA	2.33	0.63
1:A:501:VAL:HG23	1:A:502:VAL:HG12	1.78	0.63
1:A:520:TRP:H	1:A:542:THR:H	1.46	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:554:PRO:O	1:A:556:GLN:N	2.22	0.63
1:A:729:LEU:HD21	1:A:743:ALA:HB1	1.79	0.63
1:B:77:GLY:O	1:B:474:ARG:NH1	2.28	0.63
1:B:144:GLU:HG2	1:B:145:LEU:H	1.63	0.63
2:C:417:HIS:HB2	2:C:471:LEU:HD22	1.80	0.63
1:A:178:ALA:O	1:A:332:LYS:NZ	2.31	0.63
1:A:502:VAL:HA	1:A:503:VAL:CG1	2.28	0.63
1:B:45:SER:HB3	1:B:334:ARG:HB2	1.80	0.63
1:B:178:ALA:O	1:B:332:LYS:NZ	2.31	0.63
2:C:40:TYR:HB2	2:C:43:LEU:HB3	1.80	0.63
1:A:360:VAL:HG22	1:A:438:THR:HG22	1.80	0.63
2:C:553:SER:O	2:C:557:THR:N	2.32	0.63
1:A:45:SER:HB3	1:A:334:ARG:HB2	1.80	0.63
1:A:92:TYR:HE2	1:A:150:THR:HG21	1.62	0.63
1:A:194:ASP:O	1:A:198:MET:N	2.25	0.63
1:B:580:TRP:CD2	1:B:581:HIS:HA	2.33	0.63
1:B:666:ARG:HD3	1:B:669:GLN:NE2	2.14	0.63
2:C:91:ASN:HA	2:C:267:GLU:HG3	1.79	0.63
1:A:607:LYS:O	1:A:609:PHE:N	2.32	0.63
1:B:360:VAL:HG22	1:B:438:THR:HG22	1.80	0.63
2:C:86:GLY:O	2:C:89:HIS:NE2	2.31	0.63
2:C:282:PRO:CG	2:C:353:TRP:HE1	2.12	0.63
1:A:375:PRO:HG3	1:A:622:ARG:HE	1.63	0.63
1:B:190:VAL:HG12	1:B:323:GLU:HB2	1.81	0.63
1:B:317:ILE:CG1	2:C:462:GLY:N	2.62	0.63
1:A:190:VAL:HG12	1:A:323:GLU:HB2	1.81	0.63
1:A:358:VAL:N	1:A:437:MET:SD	2.71	0.63
1:A:597:ILE:HD11	1:A:600:LYS:HE3	1.81	0.63
2:C:105:ASN:HD21	2:C:331:PHE:HA	1.63	0.63
2:C:369:ALA:HB2	2:C:376:HIS:CE1	2.34	0.63
2:C:108:LYS:HE3	2:C:331:PHE:HE1	1.62	0.63
2:C:337:ARG:HD2	2:C:358:GLU:HG3	1.81	0.63
2:C:449:ILE:HG12	2:C:456:MET:HB2	1.81	0.63
1:B:10:ASN:HA	1:B:17:THR:HG21	1.81	0.62
1:B:100:PRO:HA	1:B:103:TRP:HD1	1.63	0.62
1:B:607:LYS:O	1:B:609:PHE:N	2.32	0.62
1:A:10:ASN:HA	1:A:17:THR:HG21	1.81	0.62
1:A:40:PHE:CD2	1:A:289:ALA:HA	2.35	0.62
1:B:296:ASP:O	1:B:300:GLN:N	2.19	0.62
2:C:616:PRO:HA	2:C:619:LEU:HD12	1.81	0.62
1:A:61:ILE:HD11	1:A:199:LEU:HD21	1.80	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:PHE:HA	1:A:186:LEU:HD13	1.82	0.62
1:A:666:ARG:HD3	1:A:669:GLN:NE2	2.14	0.62
1:B:61:ILE:HD11	1:B:199:LEU:HD21	1.80	0.62
1:B:183:PHE:HA	1:B:186:LEU:HD13	1.82	0.62
2:C:227:VAL:H	2:C:243:PHE:H	1.48	0.62
2:C:576:TRP:O	2:C:580:GLY:HA2	1.98	0.62
1:B:4:LEU:H	1:B:436:GLU:HB2	1.64	0.62
1:B:498:ASN:HD22	1:B:500:GLU:HG2	1.64	0.62
2:C:333:PRO:HG2	2:C:336:LEU:HB2	1.82	0.62
2:C:369:ALA:HB2	2:C:376:HIS:HE1	1.64	0.62
1:B:296:ASP:HA	1:B:299:LYS:HB3	1.82	0.62
1:B:317:ILE:HG12	2:C:462:GLY:H	1.65	0.62
2:C:3:ARG:HE	2:C:234:VAL:HG21	1.65	0.62
2:C:118:PRO:HA	2:C:127:PHE:HE2	1.64	0.62
1:A:287:ASN:O	1:A:289:ALA:N	2.33	0.62
1:B:173:ARG:HD3	1:B:579:PRO:HG2	1.82	0.62
2:C:115:ALA:HB3	2:C:485:TYR:CE1	2.34	0.62
1:A:100:PRO:HA	1:A:103:TRP:HD1	1.63	0.62
1:B:205:VAL:CG1	2:C:441:GLN:HE22	2.08	0.62
1:B:287:ASN:O	1:B:289:ALA:N	2.33	0.62
2:C:151:THR:OG1	2:C:157:SER:N	2.32	0.62
2:C:38:GLU:HA	2:C:44:LEU:HD23	1.82	0.62
1:A:173:ARG:HD3	1:A:579:PRO:HG2	1.82	0.61
2:C:330:THR:HA	2:C:390:GLY:HA3	1.82	0.61
1:A:116:ARG:HB2	1:A:222:PRO:HA	1.83	0.61
1:A:498:ASN:HD22	1:A:500:GLU:HG2	1.64	0.61
1:B:42:ARG:HH21	1:B:286:SER:HG	1.48	0.61
1:B:666:ARG:HG3	1:B:670:ASN:HD21	1.65	0.61
2:C:261:PRO:HB2	2:C:264:PHE:CD2	2.35	0.61
1:A:4:LEU:H	1:A:436:GLU:HB2	1.64	0.61
1:A:349:ILE:HG13	1:A:350:ASP:H	1.66	0.61
1:B:597:ILE:HD11	1:B:600:LYS:HE3	1.81	0.61
2:C:327:ASP:HB3	2:C:331:PHE:CZ	2.36	0.61
1:A:57:GLY:H	1:A:170:TYR:HB2	1.62	0.61
1:A:666:ARG:HA	1:A:669:GLN:HE22	1.65	0.61
1:A:715:HIS:CD2	1:A:716:VAL:HG22	2.31	0.61
1:B:172:TYR:HD1	1:B:578:TRP:HB2	1.65	0.61
1:B:205:VAL:HG11	2:C:441:GLN:CD	2.07	0.61
1:A:666:ARG:HG3	1:A:670:ASN:HD21	1.66	0.61
1:B:128:PRO:N	1:B:129:THR:HB	2.16	0.61
1:B:502:VAL:HA	1:B:503:VAL:CG1	2.28	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:TYR:CE2	1:A:549:ILE:HG12	2.36	0.61
1:B:321:PHE:CG	2:C:461:LYS:HB3	2.36	0.61
1:A:713:ASP:HA	1:A:715:HIS:CE1	2.36	0.61
1:A:754:ASN:N	1:A:755:ALA:HA	2.16	0.61
2:C:38:GLU:HA	2:C:44:LEU:HA	1.82	0.61
1:A:296:ASP:HA	1:A:299:LYS:HB3	1.82	0.61
1:B:40:PHE:CD2	1:B:289:ALA:HA	2.35	0.61
1:B:173:ARG:HE	1:B:566:LEU:HD21	1.65	0.61
1:B:666:ARG:HA	1:B:669:GLN:HE22	1.65	0.61
1:A:77:GLY:O	1:A:474:ARG:NH1	2.28	0.60
1:B:317:ILE:CD1	2:C:462:GLY:N	2.63	0.60
1:B:713:ASP:HA	1:B:715:HIS:CE1	2.36	0.60
2:C:597:GLU:OE2	2:C:601:TYR:OH	2.16	0.60
1:B:181:PRO:HD3	1:B:485:ASN:HD21	1.67	0.60
2:C:40:TYR:HD1	2:C:43:LEU:HD22	1.65	0.60
1:A:4:LEU:N	1:A:436:GLU:HB2	2.17	0.60
1:A:173:ARG:HE	1:A:566:LEU:HD21	1.65	0.60
1:A:176:ARG:NH2	1:A:447:ARG:HD2	2.17	0.60
1:B:176:ARG:NH2	1:B:447:ARG:HD2	2.16	0.60
1:B:319:PRO:CA	2:C:461:LYS:NZ	2.65	0.60
1:B:671:ALA:O	1:B:674:LEU:HG	2.01	0.60
2:C:84:PHE:O	2:C:87:MET:HE3	2.01	0.60
1:A:9:LEU:HA	1:A:12:SER:HB3	1.84	0.60
1:B:9:LEU:HA	1:B:12:SER:HB3	1.84	0.60
1:B:493:TYR:CE2	1:B:549:ILE:HG12	2.36	0.60
2:C:203:TYR:CE1	2:C:269:ARG:HB3	2.36	0.60
1:A:660:LYS:O	1:A:663:ILE:HG13	2.02	0.60
1:B:116:ARG:HB2	1:B:222:PRO:HA	1.83	0.60
1:B:242:GLY:C	2:C:463:ARG:NH2	2.55	0.60
1:B:316:THR:HG21	2:C:466:VAL:HB	1.84	0.60
2:C:152:CYS:HA	2:C:156:PHE:CD2	2.36	0.60
2:C:305:THR:H	2:C:309:ASN:HD22	1.50	0.60
2:C:307:ARG:NH2	2:C:514:PHE:O	2.35	0.60
1:A:505:GLU:HA	1:A:516:LEU:HB3	1.83	0.60
1:A:589:TYR:OH	1:A:740:ARG:NE	2.26	0.60
1:B:237:PHE:CA	2:C:434:ARG:HH22	2.02	0.60
1:B:754:ASN:N	1:B:755:ALA:HA	2.16	0.60
1:A:135:LEU:HD12	1:A:151:THR:HG22	1.84	0.60
1:B:4:LEU:N	1:B:436:GLU:HB2	2.17	0.60
1:B:739:SER:HG	1:B:742:GLU:CD	2.06	0.60
2:C:303:HIS:CG	2:C:309:ASN:HD21	2.20	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:PRO:HD3	1:A:485:ASN:HD21	1.67	0.60
1:A:343:ILE:N	1:A:559:GLU:OE2	2.34	0.60
2:C:246:SER:O	2:C:251:ARG:NH2	2.35	0.60
1:A:127:PRO:HG2	1:A:130:ALA:HB2	1.82	0.59
1:A:214:PHE:HA	1:A:215:LYS:O	2.02	0.59
1:B:127:PRO:HG2	1:B:130:ALA:HB2	1.83	0.59
1:B:135:LEU:HD12	1:B:151:THR:HG22	1.84	0.59
1:B:505:GLU:HA	1:B:516:LEU:HB3	1.83	0.59
2:C:189:ALA:O	2:C:194:GLN:N	2.34	0.59
2:C:279:LEU:HD13	2:C:356:LEU:HB3	1.84	0.59
1:A:42:ARG:HH21	1:A:286:SER:HG	1.48	0.59
1:B:214:PHE:HA	1:B:215:LYS:O	2.02	0.59
2:C:25:GLN:O	2:C:28:SER:OG	2.16	0.59
2:C:104:SER:HA	2:C:388:GLU:HB2	1.84	0.59
2:C:539:ARG:HG2	2:C:542:ARG:HD2	1.82	0.59
1:A:144:GLU:O	1:A:146:PHE:N	2.36	0.59
1:A:739:SER:HG	1:A:742:GLU:CD	2.06	0.59
2:C:6:ALA:HA	2:C:379:LEU:HD23	1.85	0.59
2:C:217:THR:HG23	2:C:219:LYS:HG2	1.85	0.59
2:C:360:SER:HA	2:C:363:LEU:HB2	1.83	0.59
1:A:306:VAL:HG12	1:A:309:SER:HA	1.85	0.59
1:A:395:ASP:O	1:A:398:SER:OG	2.14	0.59
1:A:715:HIS:CD2	1:A:716:VAL:H	2.21	0.59
1:B:13:ALA:HB1	1:B:16:LEU:HD12	1.83	0.59
1:B:61:ILE:HG13	1:B:66:TYR:HE2	1.68	0.59
1:B:349:ILE:HG13	1:B:350:ASP:H	1.65	0.59
1:B:360:VAL:HG13	1:B:438:THR:HG23	1.84	0.59
1:B:505:GLU:OE2	1:B:515:SER:OG	2.15	0.59
1:A:360:VAL:HG13	1:A:438:THR:HG23	1.84	0.59
1:A:472:GLU:HB3	1:A:475:ALA:HB3	1.83	0.59
1:A:671:ALA:O	1:A:674:LEU:HG	2.01	0.59
1:B:67:ALA:HA	1:B:70:PHE:HD2	1.68	0.59
1:B:660:LYS:O	1:B:663:ILE:HG13	2.02	0.59
2:C:16:MET:HG3	2:C:191:GLN:HE21	1.65	0.59
1:A:61:ILE:HG13	1:A:66:TYR:HE2	1.68	0.59
2:C:73:GLY:HA3	2:C:492:HIS:HA	1.85	0.59
1:A:128:PRO:N	1:A:129:THR:HB	2.16	0.59
1:A:172:TYR:HD1	1:A:578:TRP:HB2	1.65	0.59
1:B:321:PHE:HA	2:C:461:LYS:HB3	1.85	0.59
1:B:530:VAL:HG13	1:B:551:TYR:CZ	2.38	0.59
2:C:201:VAL:HA	2:C:273:MET:HG2	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:370:PRO:HG2	2:C:374:GLN:HB3	1.85	0.59
1:A:210:LEU:HD22	1:A:228:HIS:ND1	2.18	0.59
1:B:144:GLU:O	1:B:146:PHE:N	2.36	0.59
1:B:210:LEU:HD22	1:B:228:HIS:ND1	2.18	0.59
1:B:316:THR:HG22	2:C:465:LEU:HG	1.82	0.59
1:B:347:SER:H	1:B:554:PRO:HB3	1.68	0.59
1:B:315:SER:OG	1:B:316:THR:N	2.30	0.58
2:C:152:CYS:O	2:C:156:PHE:N	2.34	0.58
2:C:199:TYR:HB3	2:C:273:MET:HB3	1.84	0.58
2:C:227:VAL:HG22	2:C:243:PHE:O	2.03	0.58
2:C:573:ARG:NH2	2:C:574:CYS:SG	2.76	0.58
1:A:97:ALA:HA	1:A:103:TRP:CZ2	2.37	0.58
1:A:678:ILE:HG21	1:A:725:ILE:HG23	1.85	0.58
2:C:628:LEU:HD11	2:C:634:GLU:HA	1.85	0.58
1:A:47:SER:HB3	1:A:332:LYS:HD3	1.84	0.58
2:C:326:SER:HB2	2:C:487:LYS:HB2	1.85	0.58
2:C:605:MET:HG2	2:C:613:GLU:HG3	1.85	0.58
1:A:13:ALA:HB1	1:A:16:LEU:HD12	1.83	0.58
1:B:47:SER:HB3	1:B:332:LYS:HD3	1.84	0.58
1:B:589:TYR:OH	1:B:740:ARG:NE	2.26	0.58
2:C:597:GLU:HG3	2:C:601:TYR:CE2	2.39	0.58
1:A:702:MET:HG3	1:A:711:SER:HB3	1.86	0.58
1:B:445:VAL:HG13	1:B:455:PRO:HG3	1.85	0.58
1:B:472:GLU:HB3	1:B:475:ALA:HB3	1.83	0.58
1:A:180:TYR:CE1	1:A:331:PHE:HA	2.38	0.58
1:B:678:ILE:HG21	1:B:725:ILE:HG23	1.85	0.58
2:C:521:MET:HB2	2:C:558:TYR:CD2	2.39	0.58
1:A:200:THR:O	1:A:204:SER:N	2.37	0.58
1:B:715:HIS:CD2	1:B:716:VAL:H	2.21	0.58
2:C:555:LYS:NZ	2:C:559:GLY:O	2.34	0.58
1:A:347:SER:H	1:A:554:PRO:HB3	1.68	0.58
1:B:180:TYR:CE1	1:B:331:PHE:HA	2.38	0.58
1:B:200:THR:O	1:B:204:SER:N	2.37	0.58
1:B:238:GLU:H	2:C:434:ARG:CZ	2.17	0.58
1:B:316:THR:OG1	2:C:466:VAL:HG23	2.04	0.58
1:B:732:LEU:HG	1:B:738:LEU:HD11	1.86	0.58
2:C:72:TYR:HB2	2:C:74:ARG:HG2	1.86	0.58
1:A:530:VAL:HG13	1:A:551:TYR:CZ	2.38	0.58
1:A:568:LEU:HD12	1:A:569:ALA:N	2.19	0.58
1:B:568:LEU:HD12	1:B:569:ALA:N	2.19	0.58
1:B:740:ARG:N	1:B:742:GLU:OE1	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:59:ARG:NH2	2:C:262:ASP:OD2	2.36	0.58
1:B:173:ARG:HB2	1:B:579:PRO:CG	2.33	0.58
1:A:445:VAL:HG13	1:A:455:PRO:HG3	1.85	0.57
1:B:97:ALA:HA	1:B:103:TRP:CZ2	2.37	0.57
1:B:306:VAL:HG12	1:B:309:SER:HA	1.85	0.57
1:A:284:LEU:HG	1:A:287:ASN:ND2	2.19	0.57
1:A:358:VAL:H	1:A:437:MET:CB	2.17	0.57
1:A:375:PRO:HB2	1:A:385:ARG:HD3	1.86	0.57
2:C:124:ASN:HA	2:C:127:PHE:CD2	2.39	0.57
2:C:143:LEU:O	2:C:144:LYS:HD3	2.05	0.57
1:A:67:ALA:HA	1:A:70:PHE:HD2	1.68	0.57
1:B:4:LEU:O	1:B:436:GLU:N	2.37	0.57
1:B:433:ASN:HB3	1:B:434:GLY:CA	2.35	0.57
2:C:310:LYS:O	2:C:314:VAL:HG23	2.05	0.57
2:C:334:GLY:O	2:C:337:ARG:HB3	2.04	0.57
2:C:61:LEU:O	2:C:65:PHE:N	2.37	0.57
1:A:544:GLU:CD	1:A:546:LEU:H	2.08	0.57
1:A:669:GLN:HA	1:A:672:VAL:HB	1.85	0.57
1:B:702:MET:HG3	1:B:711:SER:HB3	1.86	0.57
2:C:105:ASN:HB2	2:C:108:LYS:HB3	1.86	0.57
2:C:151:THR:N	2:C:157:SER:O	2.30	0.57
2:C:657:PHE:O	2:C:660:SER:OG	2.15	0.57
1:B:400:THR:HG21	1:B:731:VAL:HG21	1.87	0.57
1:A:433:ASN:HB3	1:A:434:GLY:CA	2.34	0.57
2:C:176:GLU:O	2:C:180:LEU:HG	2.04	0.57
2:C:209:ASP:OD1	2:C:210:ALA:N	2.38	0.57
2:C:575:TRP:HD1	2:C:581:GLU:O	1.87	0.57
1:A:557:PRO:HB2	1:A:559:GLU:HB2	1.87	0.57
1:A:4:LEU:O	1:A:436:GLU:N	2.38	0.57
1:A:400:THR:HG21	1:A:731:VAL:HG21	1.87	0.57
1:A:505:GLU:OE2	1:A:515:SER:OG	2.15	0.57
1:A:732:LEU:HG	1:A:738:LEU:HD11	1.86	0.57
1:B:284:LEU:HG	1:B:287:ASN:ND2	2.19	0.56
1:B:375:PRO:HB2	1:B:385:ARG:HD3	1.86	0.56
2:C:280:ASN:HA	2:C:283:ILE:HD12	1.87	0.56
2:C:299:ALA:O	2:C:301:THR:N	2.38	0.56
1:B:52:LEU:O	1:B:174:VAL:HG13	2.05	0.56
1:B:669:GLN:HA	1:B:672:VAL:HB	1.85	0.56
2:C:3:ARG:HG3	2:C:234:VAL:HB	1.85	0.56
2:C:114:LEU:HD22	2:C:485:TYR:C	2.25	0.56
2:C:477:GLU:HB3	2:C:479:LYS:HE3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:591:ASP:OD2	1:A:726:TRP:NE1	2.38	0.56
1:B:337:ASN:ND2	1:B:496:ALA:HB2	2.21	0.56
1:B:342:TYR:O	1:B:362:GLU:HG2	2.05	0.56
2:C:180:LEU:HD12	2:C:189:ALA:HB2	1.86	0.56
2:C:621:VAL:HG11	2:C:637:VAL:HG22	1.87	0.56
1:A:337:ASN:ND2	1:A:496:ALA:HB2	2.21	0.56
1:A:661:LEU:O	1:A:665:GLY:N	2.35	0.56
1:B:358:VAL:H	1:B:437:MET:CB	2.17	0.56
1:B:558:SER:N	1:B:559:GLU:OE1	2.39	0.56
2:C:167:ALA:HB2	2:C:277:PHE:HE2	1.69	0.56
2:C:294:ILE:O	2:C:299:ALA:N	2.26	0.56
2:C:428:ASP:N	2:C:431:SER:OG	2.30	0.56
2:C:518:ILE:HG12	2:C:567:VAL:HG21	1.88	0.56
1:B:179:THR:HG21	1:B:488:ALA:HB1	1.87	0.56
1:B:312:GLU:CD	2:C:469:HIS:HB2	2.20	0.56
2:C:438:SER:O	2:C:442:GLY:N	2.38	0.56
1:A:568:LEU:HD12	1:A:569:ALA:H	1.71	0.56
1:A:342:TYR:O	1:A:362:GLU:HG2	2.05	0.56
1:B:473:ALA:O	1:B:477:ASN:ND2	2.39	0.56
2:C:32:PHE:CE2	2:C:34:GLU:HB3	2.41	0.56
2:C:481:ASN:ND2	2:C:486:MET:O	2.39	0.56
1:A:558:SER:N	1:A:559:GLU:OE1	2.39	0.56
2:C:30:ARG:HD2	2:C:33:LYS:HE2	1.88	0.56
1:A:16:LEU:HA	1:A:487:TYR:CE1	2.36	0.56
1:A:173:ARG:HB2	1:A:579:PRO:CG	2.33	0.56
1:B:319:PRO:O	2:C:461:LYS:NZ	2.28	0.56
1:A:349:ILE:HD13	1:A:357:HIS:H	1.71	0.56
1:B:274:ARG:HH12	1:B:312:GLU:HG3	1.71	0.56
1:B:349:ILE:HD13	1:B:357:HIS:H	1.71	0.56
1:B:544:GLU:CD	1:B:546:LEU:H	2.08	0.56
1:B:568:LEU:HD12	1:B:569:ALA:H	1.71	0.56
1:A:210:LEU:HG	1:A:213:THR:HA	1.88	0.55
1:B:354:GLN:NE2	1:B:525:GLU:OE1	2.38	0.55
1:B:557:PRO:HB2	1:B:559:GLU:HB2	1.87	0.55
2:C:60:TYR:O	2:C:63:ASP:HB3	2.07	0.55
2:C:69:VAL:HG11	2:C:493:GLY:H	1.70	0.55
2:C:209:ASP:CG	2:C:222:SER:HB2	2.26	0.55
2:C:499:ASP:HB3	2:C:514:PHE:CG	2.41	0.55
1:A:274:ARG:HH12	1:A:312:GLU:HG3	1.71	0.55
1:A:740:ARG:N	1:A:742:GLU:OE1	2.36	0.55
1:B:93:HIS:NE2	1:B:202:LEU:HD13	2.21	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:253:LYS:HB2	2:C:260:VAL:HG23	1.88	0.55
2:C:371:ALA:H	2:C:374:GLN:HB2	1.70	0.55
1:A:196:ARG:HH11	1:A:328:VAL:HG12	1.72	0.55
1:A:291:PHE:HZ	1:A:517:TYR:HA	1.71	0.55
1:B:291:PHE:HZ	1:B:517:TYR:HA	1.71	0.55
2:C:168:GLU:O	2:C:172:GLU:HG3	2.06	0.55
2:C:199:TYR:HB2	2:C:365:VAL:HG12	1.88	0.55
1:B:585:THR:N	1:B:586:GLU:HB2	2.22	0.55
2:C:47:ASP:O	2:C:51:LEU:HG	2.05	0.55
2:C:71:GLU:CD	2:C:71:GLU:H	2.07	0.55
2:C:173:LYS:HB2	2:C:193:HIS:CE1	2.41	0.55
1:A:179:THR:HG21	1:A:488:ALA:HB1	1.87	0.55
2:C:214:ASP:HB3	2:C:219:LYS:H	1.72	0.55
1:A:42:ARG:CZ	1:A:283:GLN:HE21	2.20	0.55
1:A:52:LEU:O	1:A:174:VAL:HG13	2.06	0.55
1:A:93:HIS:NE2	1:A:202:LEU:HD13	2.21	0.55
1:A:354:GLN:NE2	1:A:525:GLU:OE1	2.38	0.55
1:A:585:THR:N	1:A:586:GLU:HB2	2.22	0.55
1:B:34:LEU:HG	1:B:35:GLN:HG3	1.89	0.55
1:B:42:ARG:CZ	1:B:283:GLN:HE21	2.20	0.55
2:C:419:ALA:HB1	2:C:422:LEU:HB2	1.89	0.55
1:A:15:GLY:HA2	1:A:20:PHE:CG	2.42	0.55
1:A:473:ALA:O	1:A:477:ASN:ND2	2.39	0.55
1:B:22:ILE:HG21	1:B:515:SER:HB2	1.89	0.55
2:C:205:ALA:HB3	2:C:529:GLU:HG3	1.88	0.55
1:B:533:ASN:ND2	1:B:543:PRO:HD2	2.21	0.55
2:C:232:TYR:N	2:C:240:GLY:HA3	2.22	0.55
2:C:395:GLN:HG2	2:C:397:ALA:H	1.72	0.55
1:A:586:GLU:HB3	1:A:623:ILE:HG22	1.89	0.54
1:A:605:GLU:N	1:A:605:GLU:OE1	2.40	0.54
1:B:238:GLU:H	2:C:434:ARG:NH2	2.05	0.54
2:C:197:GLY:H	2:C:363:LEU:HD11	1.71	0.54
1:A:533:ASN:ND2	1:A:543:PRO:HD2	2.21	0.54
1:B:42:ARG:NH2	1:B:283:GLN:O	2.40	0.54
1:B:210:LEU:HG	1:B:213:THR:HA	1.88	0.54
1:B:558:SER:OG	1:B:559:GLU:N	2.40	0.54
1:B:591:ASP:OD2	1:B:726:TRP:NE1	2.38	0.54
2:C:69:VAL:HG22	2:C:75:VAL:HG22	1.89	0.54
1:A:22:ILE:HG21	1:A:515:SER:HB2	1.89	0.54
1:B:196:ARG:HH11	1:B:328:VAL:HG12	1.72	0.54
2:C:397:ALA:HB1	2:C:400:LEU:HD12	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:539:ARG:HE	2:C:545:PRO:HA	1.72	0.54
1:B:605:GLU:OE1	1:B:605:GLU:N	2.40	0.54
2:C:72:TYR:HD1	2:C:472:PHE:HZ	1.55	0.54
1:A:45:SER:HB2	1:A:334:ARG:CZ	2.38	0.54
1:A:214:PHE:HA	1:A:215:LYS:C	2.28	0.54
1:A:409:ALA:O	1:A:413:PHE:N	2.38	0.54
1:B:214:PHE:HA	1:B:215:LYS:C	2.28	0.54
2:C:94:PRO:HG2	2:C:96:ILE:HD11	1.88	0.54
2:C:143:LEU:HD12	2:C:285:ALA:HB2	1.89	0.54
2:C:329:ASP:HA	2:C:391:LEU:HD12	1.88	0.54
1:B:15:GLY:O	1:B:487:TYR:OH	2.21	0.54
1:B:45:SER:HB2	1:B:334:ARG:CZ	2.38	0.54
1:B:144:GLU:HB2	1:B:147:HIS:HB3	1.90	0.54
1:B:586:GLU:HB3	1:B:623:ILE:HG22	1.89	0.54
1:B:661:LEU:O	1:B:665:GLY:N	2.35	0.54
2:C:282:PRO:HG3	2:C:353:TRP:HE1	1.72	0.54
2:C:357:PHE:CE2	2:C:361:LEU:HG	2.42	0.54
1:B:446:GLU:HG3	1:B:627:THR:HB	1.90	0.54
2:C:55:ASN:HA	2:C:88:ARG:NH1	2.18	0.54
2:C:85:PHE:O	2:C:211:ILE:HD12	2.08	0.54
2:C:167:ALA:O	2:C:171:LEU:HG	2.08	0.54
1:A:38:LEU:H	1:A:501:VAL:HG21	1.73	0.54
1:A:42:ARG:NH2	1:A:283:GLN:O	2.40	0.54
1:A:165:LEU:N	1:A:166:PRO:HD2	2.23	0.54
1:A:350:ASP:O	1:A:352:MET:N	2.36	0.54
1:A:558:SER:OG	1:A:559:GLU:N	2.40	0.54
1:B:38:LEU:H	1:B:501:VAL:HG21	1.73	0.54
2:C:38:GLU:HG2	2:C:40:TYR:O	2.08	0.54
2:C:502:LEU:HB3	2:C:513:ILE:H	1.73	0.54
1:A:34:LEU:HG	1:A:35:GLN:HG3	1.89	0.54
1:A:366:PHE:HE1	1:A:629:ALA:HB2	1.73	0.54
1:A:693:LEU:O	1:A:697:ARG:HG2	2.08	0.54
1:B:317:ILE:HG13	2:C:460:THR:O	2.08	0.54
2:C:357:PHE:CE2	2:C:361:LEU:CB	2.91	0.54
2:C:528:PRO:HG2	2:C:544:ARG:NH1	2.22	0.54
1:A:344:GLY:N	1:A:361:TYR:O	2.27	0.53
1:B:343:ILE:N	1:B:559:GLU:OE2	2.34	0.53
1:B:641:VAL:O	1:B:645:ARG:HG2	2.08	0.53
2:C:190:TYR:O	2:C:194:GLN:HA	2.09	0.53
1:A:127:PRO:O	1:A:130:ALA:N	2.36	0.53
1:A:144:GLU:HB2	1:A:147:HIS:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ASN:ND2	1:A:184:TYR:HB2	2.23	0.53
2:C:317:TRP:O	2:C:509:PRO:HB2	2.08	0.53
1:A:99:ASN:ND2	1:A:101:GLU:OE2	2.41	0.53
1:B:15:GLY:HA2	1:B:20:PHE:CG	2.42	0.53
1:B:585:THR:HB	1:B:586:GLU:HA	1.90	0.53
1:B:693:LEU:O	1:B:697:ARG:HG2	2.08	0.53
2:C:446:ILE:HG22	2:C:459:TRP:NE1	2.20	0.53
2:C:481:ASN:ND2	2:C:483:SER:HB3	2.24	0.53
2:C:564:TYR:CE1	2:C:568:LEU:HD11	2.44	0.53
1:A:641:VAL:O	1:A:645:ARG:HG2	2.08	0.53
1:B:272:SER:HB2	1:B:275:LEU:CB	2.38	0.53
1:B:316:THR:HG22	2:C:465:LEU:CG	2.37	0.53
1:B:572:THR:HA	1:B:575:ILE:O	2.08	0.53
2:C:287:ALA:HB1	2:C:400:LEU:HD11	1.91	0.53
2:C:401:MET:O	2:C:404:LEU:HB3	2.09	0.53
2:C:516:GLY:H	2:C:560:ALA:HB3	1.74	0.53
1:A:446:GLU:HG3	1:A:627:THR:HB	1.90	0.53
1:B:196:ARG:HD3	1:B:328:VAL:HG12	1.89	0.53
2:C:268:ARG:HD3	2:C:270:ARG:HE	1.73	0.53
2:C:287:ALA:O	2:C:291:ARG:HG3	2.09	0.53
2:C:423:ASN:HA	2:C:426:ILE:HD12	1.90	0.53
1:A:42:ARG:H	1:A:336:ILE:HD13	1.73	0.53
1:A:170:TYR:HD1	1:A:576:HIS:CE1	2.27	0.53
1:A:196:ARG:HD3	1:A:328:VAL:HG12	1.89	0.53
1:B:26:LYS:HE3	1:B:509:VAL:HG22	1.91	0.53
1:B:44:PHE:HE1	1:B:180:TYR:H	1.56	0.53
1:B:527:ARG:HH11	1:B:528:ILE:H	1.56	0.53
2:C:56:GLU:OE2	2:C:577:ASN:ND2	2.37	0.53
2:C:141:VAL:HG22	2:C:289:PRO:HG3	1.90	0.53
2:C:179:ASN:OD1	2:C:352:TRP:HB3	2.09	0.53
2:C:616:PRO:O	2:C:620:GLU:HG2	2.08	0.53
2:C:641:ILE:HA	2:C:644:VAL:HB	1.91	0.53
1:A:143:HIS:CD2	1:A:146:PHE:HE2	2.26	0.53
1:A:159:SER:OG	1:A:160:PRO:HD3	2.09	0.53
1:B:170:TYR:HD1	1:B:576:HIS:CE1	2.27	0.53
2:C:12:ILE:O	2:C:16:MET:HG2	2.08	0.53
2:C:160:MET:O	2:C:164:ILE:HG12	2.08	0.53
2:C:399:ASP:OD1	2:C:400:LEU:N	2.41	0.53
1:A:572:THR:HA	1:A:575:ILE:O	2.08	0.53
1:B:2:PHE:H	1:B:439:LEU:HD11	1.74	0.53
1:B:99:ASN:ND2	1:B:101:GLU:OE2	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:HG12	2:C:462:GLY:N	2.20	0.53
1:B:345:GLN:HG2	1:B:555:ILE:HG12	1.91	0.53
2:C:650:SER:HB2	2:C:652:GLU:OE1	2.09	0.53
1:A:157:VAL:O	1:A:160:PRO:HD2	2.09	0.53
1:A:368:LYS:HE2	1:A:402:ALA:HA	1.91	0.53
1:B:182:ASN:ND2	1:B:184:TYR:HB2	2.23	0.53
1:B:365:GLN:OE1	1:B:563:ALA:HB3	2.09	0.53
1:B:713:ASP:HA	1:B:715:HIS:ND1	2.24	0.53
2:C:306:THR:OG1	2:C:309:ASN:N	2.42	0.53
1:A:26:LYS:HE3	1:A:509:VAL:HG22	1.91	0.53
1:A:285:ARG:O	1:A:288:LEU:HD13	2.09	0.53
1:A:713:ASP:HA	1:A:715:HIS:ND1	2.24	0.53
1:B:42:ARG:H	1:B:336:ILE:HD13	1.73	0.53
1:B:313:LEU:CA	2:C:466:VAL:HG21	2.34	0.53
1:B:366:PHE:HE1	1:B:629:ALA:HB2	1.73	0.53
1:B:368:LYS:HE2	1:B:402:ALA:HA	1.91	0.53
1:B:395:ASP:O	1:B:398:SER:OG	2.14	0.53
2:C:179:ASN:O	2:C:183:GLN:N	2.37	0.53
2:C:508:GLU:HB2	2:C:511:SER:HB3	1.90	0.53
1:B:702:MET:HB3	1:B:708:ILE:HA	1.91	0.52
2:C:273:MET:N	2:C:393:SER:OG	2.35	0.52
1:A:527:ARG:HH11	1:A:528:ILE:H	1.56	0.52
1:B:223:ALA:O	1:B:227:GLN:N	2.34	0.52
1:B:231:ASN:OD1	1:B:232:ALA:N	2.42	0.52
1:B:285:ARG:O	1:B:288:LEU:HD13	2.09	0.52
1:B:630:HIS:N	1:B:737:LEU:HD13	2.24	0.52
2:C:504:ASP:CG	2:C:511:SER:HB2	2.29	0.52
1:A:287:ASN:C	1:A:289:ALA:H	2.13	0.52
1:A:365:GLN:OE1	1:A:563:ALA:HB3	2.09	0.52
1:A:519:VAL:HG22	1:A:542:THR:N	2.25	0.52
1:A:720:ARG:HD2	1:A:760:VAL:HG21	1.91	0.52
1:B:105:LYS:HE2	1:B:138:LEU:HD11	1.91	0.52
1:B:165:LEU:N	1:B:166:PRO:HD2	2.23	0.52
2:C:48:PRO:HA	2:C:51:LEU:HD12	1.91	0.52
2:C:67:ALA:HA	2:C:80:VAL:HB	1.90	0.52
2:C:74:ARG:HB2	2:C:503:TYR:CD1	2.44	0.52
2:C:142:PRO:HB3	2:C:651:VAL:HB	1.91	0.52
2:C:575:TRP:CD2	2:C:583:TYR:HB2	2.44	0.52
2:C:627:LYS:HB3	2:C:631:LYS:HB3	1.92	0.52
1:A:44:PHE:HE1	1:A:180:TYR:H	1.56	0.52
1:B:16:LEU:HA	1:B:487:TYR:CE1	2.36	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:50:PHE:O	2:C:53:PHE:HB3	2.07	0.52
2:C:83:ASN:ND2	2:C:211:ILE:O	2.42	0.52
2:C:404:LEU:O	2:C:408:ILE:HG12	2.08	0.52
2:C:508:GLU:O	2:C:511:SER:OG	2.18	0.52
1:A:580:TRP:CH2	1:A:622:ARG:HD3	2.45	0.52
1:B:580:TRP:CH2	1:B:622:ARG:HD3	2.45	0.52
1:B:720:ARG:HD2	1:B:760:VAL:HG21	1.91	0.52
2:C:132:ARG:NH1	2:C:429:MET:HB3	2.24	0.52
2:C:180:LEU:HD22	2:C:185:LYS:HD2	1.90	0.52
2:C:206:GLN:HG3	2:C:208:THR:O	2.09	0.52
2:C:357:PHE:CE1	2:C:361:LEU:CD2	2.93	0.52
2:C:592:LYS:O	2:C:596:LEU:HG	2.09	0.52
1:A:231:ASN:OD1	1:A:232:ALA:N	2.42	0.52
1:A:702:MET:HB3	1:A:708:ILE:HA	1.91	0.52
1:A:732:LEU:HD21	1:A:738:LEU:HD21	1.91	0.52
1:B:732:LEU:HD21	1:B:738:LEU:HD21	1.92	0.52
2:C:117:GLY:HA2	2:C:335:TRP:CE3	2.44	0.52
2:C:628:LEU:HA	2:C:632:TRP:HB2	1.92	0.52
1:A:2:PHE:H	1:A:439:LEU:HD11	1.74	0.52
1:B:239:ARG:NH1	2:C:438:SER:OG	2.43	0.52
2:C:122:ARG:O	2:C:126:LEU:HG	2.09	0.52
2:C:213:LEU:HD13	2:C:220:PHE:CE1	2.45	0.52
1:A:106:LEU:O	1:A:110:ILE:HG12	2.10	0.52
1:B:313:LEU:N	2:C:466:VAL:HG23	2.20	0.52
1:B:472:GLU:HB3	1:B:475:ALA:CB	2.40	0.52
2:C:143:LEU:O	2:C:649:VAL:HB	2.10	0.52
1:A:15:GLY:O	1:A:487:TYR:OH	2.21	0.52
1:A:296:ASP:HB2	1:A:300:GLN:HG2	1.92	0.52
1:B:106:LEU:O	1:B:110:ILE:HG12	2.10	0.52
2:C:121:GLU:O	2:C:125:LEU:HG	2.10	0.52
2:C:438:SER:HA	2:C:441:GLN:HB2	1.90	0.52
1:A:17:THR:O	1:A:19:ALA:N	2.38	0.52
1:A:100:PRO:HA	1:A:103:TRP:CD1	2.45	0.52
1:A:252:SER:HB3	1:A:306:VAL:HG13	1.92	0.52
1:B:4:LEU:HG	1:B:436:GLU:CB	2.38	0.52
1:B:287:ASN:C	1:B:289:ALA:H	2.13	0.52
1:B:296:ASP:HB2	1:B:300:GLN:HG2	1.92	0.52
1:B:310:ASP:OD2	1:B:313:LEU:N	2.42	0.52
2:C:56:GLU:OE2	2:C:573:ARG:NH1	2.43	0.52
2:C:180:LEU:O	2:C:184:GLY:N	2.42	0.52
2:C:333:PRO:HG2	2:C:336:LEU:CB	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLY:H	1:A:541:ARG:HH21	1.59	0.51
1:B:143:HIS:CD2	1:B:146:PHE:HE2	2.26	0.51
1:B:159:SER:OG	1:B:160:PRO:HD3	2.09	0.51
1:B:276:ARG:HB2	1:B:281:ILE:HD11	1.92	0.51
1:B:409:ALA:O	1:B:413:PHE:N	2.38	0.51
2:C:9:LEU:HD13	2:C:366:TYR:CZ	2.44	0.51
2:C:83:ASN:HB2	2:C:85:PHE:CD2	2.35	0.51
2:C:642:HIS:O	2:C:646:MET:N	2.38	0.51
1:A:272:SER:HB2	1:A:275:LEU:CB	2.38	0.51
1:A:524:THR:HG21	1:A:540:ILE:HG12	1.92	0.51
1:B:196:ARG:O	1:B:197:ARG:NH1	2.40	0.51
2:C:343:GLU:HA	2:C:346:ASN:HB2	1.92	0.51
2:C:357:PHE:CE1	2:C:361:LEU:HD11	2.43	0.51
2:C:593:ARG:HA	2:C:596:LEU:HD12	1.93	0.51
1:A:472:GLU:HB3	1:A:475:ALA:CB	2.40	0.51
2:C:588:GLU:O	2:C:592:LYS:HG3	2.10	0.51
1:A:39:GLN:HA	1:A:501:VAL:HG11	1.92	0.51
1:A:105:LYS:HE2	1:A:138:LEU:HD11	1.91	0.51
1:B:39:GLN:HA	1:B:501:VAL:HG11	1.92	0.51
1:B:42:ARG:NH2	1:B:286:SER:OG	2.40	0.51
1:B:310:ASP:OD2	2:C:466:VAL:HG21	2.11	0.51
1:B:387:LEU:H	1:B:572:THR:HG22	1.76	0.51
1:B:519:VAL:HG22	1:B:542:THR:N	2.25	0.51
1:A:630:HIS:N	1:A:737:LEU:HD13	2.24	0.51
1:B:252:SER:HB3	1:B:306:VAL:HG13	1.93	0.51
2:C:36:ALA:HA	2:C:92:GLY:HA3	1.92	0.51
2:C:50:PHE:HB2	2:C:579:PHE:CZ	2.45	0.51
2:C:251:ARG:O	2:C:254:GLU:HB3	2.10	0.51
2:C:395:GLN:HG2	2:C:397:ALA:N	2.25	0.51
2:C:552:ALA:HB2	2:C:591:LEU:HD22	1.93	0.51
1:A:345:GLN:HG2	1:A:555:ILE:HG12	1.91	0.51
1:B:157:VAL:O	1:B:160:PRO:HD2	2.09	0.51
1:B:698:ILE:O	1:B:702:MET:HE2	2.09	0.51
2:C:539:ARG:HH21	2:C:545:PRO:HA	1.75	0.51
2:C:638:SER:O	2:C:642:HIS:HB2	2.11	0.51
1:B:54:TRP:CZ3	1:B:174:VAL:HG12	2.46	0.51
1:B:350:ASP:O	1:B:352:MET:N	2.36	0.51
2:C:96:ILE:HB	2:C:251:ARG:HH12	1.75	0.51
2:C:207:SER:HB3	2:C:528:PRO:O	2.10	0.51
2:C:337:ARG:HA	2:C:340:ILE:HD12	1.93	0.51
2:C:366:TYR:OH	2:C:376:HIS:HA	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:420:PRO:HA	2:C:423:ASN:ND2	2.26	0.51
2:C:539:ARG:NH2	2:C:544:ARG:O	2.43	0.51
1:A:245:ASP:HB2	1:A:248:ALA:HB3	1.93	0.51
1:A:352:MET:SD	1:A:355:PRO:HD2	2.51	0.51
1:A:585:THR:HB	1:A:586:GLU:HA	1.91	0.51
1:B:312:GLU:HB3	2:C:466:VAL:HG21	1.90	0.51
2:C:353:TRP:HA	2:C:356:LEU:HD12	1.92	0.51
2:C:662:MET:O	2:C:664:ARG:N	2.44	0.51
1:A:54:TRP:CZ3	1:A:174:VAL:HG12	2.46	0.51
1:B:320:TRP:CH2	2:C:460:THR:HB	2.46	0.51
1:B:344:GLY:N	1:B:361:TYR:O	2.27	0.51
1:A:443:SER:O	1:A:447:ARG:HG2	2.12	0.50
2:C:16:MET:HB2	2:C:190:TYR:CZ	2.45	0.50
2:C:411:LEU:HD21	2:C:435:PHE:CZ	2.46	0.50
1:A:387:LEU:H	1:A:572:THR:HG22	1.76	0.50
1:B:334:ARG:HD3	1:B:338:GLU:CB	2.41	0.50
1:B:352:MET:SD	1:B:355:PRO:HD2	2.51	0.50
2:C:288:GLN:HA	2:C:291:ARG:HD2	1.93	0.50
2:C:298:TYR:HE1	2:C:437:ASP:OD1	1.95	0.50
1:A:261:TRP:CE2	1:A:288:LEU:HG	2.46	0.50
1:B:524:THR:HG21	1:B:540:ILE:HG12	1.91	0.50
2:C:99:THR:CB	2:C:227:VAL:HB	2.41	0.50
2:C:333:PRO:O	2:C:336:LEU:HB3	2.11	0.50
1:A:284:LEU:C	1:A:287:ASN:H	2.14	0.50
1:A:366:PHE:HD2	1:A:405:GLY:HA2	1.77	0.50
1:A:698:ILE:O	1:A:702:MET:HE2	2.11	0.50
1:B:16:LEU:HD11	1:B:462:LEU:HB3	1.94	0.50
1:B:81:SER:HB2	1:B:188:ASP:OD2	2.12	0.50
1:B:100:PRO:HA	1:B:103:TRP:CD1	2.45	0.50
1:B:261:TRP:CE2	1:B:288:LEU:HG	2.46	0.50
1:B:502:VAL:HA	1:B:503:VAL:CB	2.42	0.50
2:C:100:TRP:HB2	2:C:229:ASP:C	2.32	0.50
2:C:320:CYS:HA	2:C:457:LEU:O	2.12	0.50
2:C:350:ALA:HB1	2:C:352:TRP:CE2	2.46	0.50
1:A:103:TRP:O	1:A:226:SER:OG	2.26	0.50
1:A:276:ARG:HB2	1:A:281:ILE:HD11	1.92	0.50
1:A:391:PRO:HA	1:A:394:SER:HB2	1.93	0.50
1:B:245:ASP:HB2	1:B:248:ALA:HB3	1.92	0.50
1:B:321:PHE:HB2	2:C:461:LYS:CB	2.38	0.50
1:B:321:PHE:HA	2:C:461:LYS:CB	2.40	0.50
2:C:273:MET:O	2:C:393:SER:OG	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:279:LEU:O	2:C:282:PRO:HG2	2.11	0.50
1:A:347:SER:O	1:A:358:VAL:HG22	2.11	0.50
2:C:15:GLN:HE22	2:C:25:GLN:NE2	2.10	0.50
2:C:557:THR:OG1	2:C:620:GLU:OE2	2.24	0.50
2:C:627:LYS:HG2	2:C:630:TYR:CZ	2.47	0.50
1:B:391:PRO:HA	1:B:394:SER:HB2	1.93	0.50
1:B:443:SER:O	1:B:447:ARG:HG2	2.12	0.50
2:C:38:GLU:OE2	2:C:42:GLY:N	2.28	0.50
2:C:40:TYR:O	2:C:43:LEU:N	2.45	0.50
2:C:124:ASN:ND2	2:C:128:ARG:HE	2.10	0.50
2:C:554:MET:HG2	2:C:564:TYR:CE1	2.35	0.50
2:C:617:ILE:O	2:C:621:VAL:HG23	2.11	0.50
1:A:196:ARG:O	1:A:197:ARG:NH1	2.40	0.50
1:A:334:ARG:HD3	1:A:338:GLU:CB	2.41	0.50
1:B:42:ARG:H	1:B:336:ILE:CD1	2.25	0.50
1:B:61:ILE:HG13	1:B:66:TYR:CE2	2.47	0.50
2:C:413:MET:HG2	2:C:471:LEU:HD21	1.92	0.50
1:A:144:GLU:HG2	1:A:145:LEU:N	2.26	0.49
1:A:477:ASN:OD1	1:A:478:ASP:N	2.45	0.49
1:A:502:VAL:HA	1:A:503:VAL:CB	2.42	0.49
1:B:284:LEU:C	1:B:287:ASN:H	2.14	0.49
1:B:366:PHE:HD2	1:B:405:GLY:HA2	1.77	0.49
2:C:50:PHE:HB2	2:C:579:PHE:HZ	1.76	0.49
2:C:250:SER:HA	2:C:253:LYS:HB3	1.94	0.49
2:C:282:PRO:HB3	2:C:657:PHE:CE2	2.46	0.49
2:C:287:ALA:HA	2:C:290:VAL:HB	1.94	0.49
2:C:295:TYR:O	2:C:299:ALA:HB2	2.12	0.49
2:C:58:SER:HA	2:C:84:PHE:HB2	1.94	0.49
2:C:348:GLY:HA3	2:C:663:PRO:HB3	1.92	0.49
2:C:582:SER:OG	2:C:584:ARG:HB3	2.11	0.49
1:A:42:ARG:H	1:A:336:ILE:CD1	2.25	0.49
1:A:155:CYS:O	1:A:159:SER:N	2.45	0.49
1:B:32:GLY:H	1:B:541:ARG:HH21	1.59	0.49
1:B:127:PRO:C	1:B:129:THR:HB	2.33	0.49
1:B:340:THR:O	1:B:343:ILE:HG22	2.12	0.49
1:B:369:GLU:HA	1:B:398:SER:HB2	1.94	0.49
1:B:715:HIS:CG	1:B:716:VAL:H	2.29	0.49
2:C:328:HIS:ND1	2:C:453:ASP:HB3	2.27	0.49
2:C:363:LEU:HD12	2:C:364:PRO:HD2	1.94	0.49
2:C:521:MET:O	2:C:525:GLN:HG3	2.12	0.49
1:A:16:LEU:HD11	1:A:462:LEU:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:SER:HB2	1:A:188:ASP:OD2	2.12	0.49
1:A:128:PRO:HG2	1:A:129:THR:OG1	2.12	0.49
1:A:585:THR:O	1:A:622:ARG:HG2	2.12	0.49
1:B:17:THR:O	1:B:19:ALA:N	2.38	0.49
1:B:347:SER:O	1:B:358:VAL:HG22	2.11	0.49
1:B:433:ASN:HB3	1:B:434:GLY:C	2.33	0.49
1:B:567:ASP:O	1:B:569:ALA:N	2.45	0.49
2:C:117:GLY:O	2:C:485:TYR:OH	2.13	0.49
2:C:324:ASP:HB2	2:C:491:GLU:N	2.27	0.49
2:C:357:PHE:CD1	2:C:361:LEU:HD21	2.48	0.49
2:C:602:VAL:HG11	2:C:605:MET:HB2	1.95	0.49
1:A:196:ARG:HB3	1:A:197:ARG:NH1	2.27	0.49
1:B:144:GLU:HG2	1:B:145:LEU:N	2.26	0.49
1:B:317:ILE:HB	2:C:465:LEU:HD23	1.94	0.49
1:B:317:ILE:HD11	2:C:461:LYS:C	2.32	0.49
1:B:477:ASN:OD1	1:B:478:ASP:N	2.45	0.49
1:B:585:THR:O	1:B:622:ARG:HG2	2.12	0.49
2:C:352:TRP:O	2:C:356:LEU:HG	2.11	0.49
2:C:438:SER:OG	2:C:443:HIS:HB2	2.12	0.49
2:C:551:TRP:CH2	2:C:584:ARG:HA	2.47	0.49
1:A:310:ASP:OD2	1:A:313:LEU:N	2.42	0.49
1:A:516:LEU:HD12	1:A:516:LEU:O	2.13	0.49
1:A:745:ALA:O	1:A:749:VAL:HG23	2.12	0.49
1:B:312:GLU:CD	2:C:470:ARG:HG3	2.27	0.49
1:B:396:ARG:HE	1:B:612:LEU:HB3	1.77	0.49
2:C:336:LEU:O	2:C:340:ILE:HG13	2.12	0.49
1:A:61:ILE:HG13	1:A:66:TYR:CE2	2.47	0.49
1:A:340:THR:O	1:A:343:ILE:HG22	2.12	0.49
1:B:383:ASN:O	1:B:385:ARG:N	2.38	0.49
2:C:27:ALA:HA	2:C:30:ARG:HB2	1.94	0.49
2:C:316:GLU:HB2	2:C:317:TRP:CD1	2.48	0.49
1:B:239:ARG:CZ	2:C:438:SER:OG	2.61	0.49
1:B:516:LEU:O	1:B:516:LEU:HD12	2.13	0.49
1:B:103:TRP:O	1:B:226:SER:OG	2.26	0.49
1:B:196:ARG:HB3	1:B:197:ARG:NH1	2.27	0.49
1:B:257:LEU:HB3	1:B:261:TRP:CZ2	2.48	0.49
1:B:375:PRO:CG	1:B:622:ARG:HE	2.26	0.49
2:C:95:MET:HG2	2:C:268:ARG:HA	1.95	0.49
2:C:310:LYS:HB2	2:C:514:PHE:HE2	1.78	0.49
2:C:395:GLN:HE21	2:C:397:ALA:CB	2.25	0.49
2:C:517:ASN:OD1	2:C:519:ASN:N	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:618:ASP:O	2:C:622:LEU:HG	2.12	0.49
1:A:410:VAL:CA	1:A:413:PHE:HB3	2.41	0.49
1:A:567:ASP:O	1:A:569:ALA:N	2.45	0.49
2:C:199:TYR:CE2	2:C:363:LEU:HB3	2.48	0.49
1:A:375:PRO:CG	1:A:622:ARG:HE	2.26	0.48
1:A:418:THR:O	1:A:421:TYR:CD1	2.66	0.48
1:B:127:PRO:O	1:B:130:ALA:N	2.36	0.48
2:C:288:GLN:HB3	2:C:289:PRO:HD3	1.95	0.48
2:C:416:ASP:HB2	2:C:417:HIS:CD2	2.48	0.48
2:C:625:PRO:O	2:C:628:LEU:HB3	2.13	0.48
1:A:42:ARG:NH2	1:A:286:SER:OG	2.40	0.48
1:A:369:GLU:HA	1:A:398:SER:HB2	1.93	0.48
1:B:556:GLN:OE1	1:B:557:PRO:HD2	2.13	0.48
2:C:119:VAL:HB	2:C:123:ASP:OD2	2.12	0.48
2:C:123:ASP:HA	2:C:126:LEU:HD12	1.95	0.48
2:C:249:ALA:HB3	2:C:260:VAL:HG13	1.95	0.48
2:C:350:ALA:O	2:C:354:VAL:HG23	2.13	0.48
2:C:429:MET:HB2	2:C:430:PRO:HD3	1.95	0.48
2:C:583:TYR:HA	2:C:586:TYR:HB3	1.94	0.48
1:A:4:LEU:HG	1:A:436:GLU:CB	2.37	0.48
2:C:39:THR:N	2:C:43:LEU:O	2.46	0.48
2:C:406:MET:HB3	2:C:410:TYR:CZ	2.48	0.48
1:A:433:ASN:HB3	1:A:434:GLY:C	2.33	0.48
1:A:715:HIS:CG	1:A:716:VAL:H	2.30	0.48
1:B:128:PRO:HG2	1:B:129:THR:OG1	2.12	0.48
2:C:118:PRO:HA	2:C:127:PHE:CE2	2.46	0.48
2:C:277:PHE:CD1	2:C:280:ASN:HB2	2.48	0.48
2:C:547:PRO:HB2	2:C:587:ARG:HH12	1.78	0.48
1:A:127:PRO:C	1:A:129:THR:HB	2.33	0.48
1:A:257:LEU:HB3	1:A:261:TRP:CZ2	2.48	0.48
1:A:433:ASN:HB3	1:A:434:GLY:HA3	1.95	0.48
1:A:719:ASN:OD1	1:A:720:ARG:N	2.46	0.48
1:A:747:THR:HA	1:A:750:LEU:HG	1.96	0.48
1:B:155:CYS:O	1:B:159:SER:N	2.45	0.48
1:B:745:ALA:O	1:B:749:VAL:HG23	2.12	0.48
2:C:339:LEU:O	2:C:342:ASP:HB3	2.14	0.48
1:A:49:THR:OG1	1:A:50:SER:N	2.44	0.48
1:A:556:GLN:OE1	1:A:557:PRO:HD2	2.13	0.48
1:A:729:LEU:O	1:A:732:LEU:HB3	2.14	0.48
1:B:335:PRO:HB2	1:B:338:GLU:OE2	2.14	0.48
2:C:19:ALA:HB2	2:C:155:TYR:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:411:LEU:O	2:C:415:LEU:HG	2.13	0.48
2:C:555:LYS:HB2	2:C:564:TYR:CZ	2.49	0.48
1:A:83:ASP:OD1	1:A:191:ARG:NE	2.47	0.48
1:A:396:ARG:HE	1:A:612:LEU:HB3	1.77	0.48
1:B:418:THR:O	1:B:421:TYR:CD1	2.66	0.48
2:C:190:TYR:C	2:C:194:GLN:HA	2.34	0.48
2:C:199:TYR:HE2	2:C:363:LEU:HB3	1.79	0.48
2:C:428:ASP:CG	2:C:430:PRO:HD2	2.33	0.48
1:A:51:GLU:CA	1:A:174:VAL:HG21	2.44	0.48
1:A:253:VAL:HG11	1:A:322:ILE:HD13	1.95	0.48
1:A:362:GLU:HB2	1:A:364:TRP:HE1	1.79	0.48
1:A:493:TYR:CZ	1:A:549:ILE:HG12	2.49	0.48
1:A:672:VAL:HA	1:A:675:LEU:HD12	1.96	0.48
1:B:477:ASN:O	1:B:481:ARG:N	2.47	0.48
1:B:669:GLN:O	1:B:673:THR:N	2.39	0.48
2:C:436:LEU:HD21	2:C:440:TRP:CE2	2.48	0.48
1:A:16:LEU:HD21	1:A:462:LEU:HD13	1.96	0.48
1:B:243:ASN:HD21	2:C:422:LEU:HD22	1.78	0.48
2:C:170:ALA:HB2	2:C:278:ALA:HB1	1.96	0.48
2:C:476:LYS:HA	2:C:490:TYR:CD1	2.49	0.48
2:C:477:GLU:HB3	2:C:479:LYS:HG3	1.96	0.48
1:A:423:ALA:HA	1:A:424:VAL:HA	1.48	0.48
1:B:109:TYR:OH	1:B:130:ALA:HB1	2.14	0.48
1:B:317:ILE:CG1	2:C:460:THR:O	2.61	0.48
1:B:433:ASN:HB3	1:B:434:GLY:HA3	1.95	0.48
1:A:376:VAL:O	1:A:386:PHE:N	2.47	0.47
1:A:441:PHE:HB2	1:A:444:VAL:HG22	1.96	0.47
1:A:739:SER:OG	1:A:742:GLU:OE1	2.32	0.47
1:B:719:ASN:OD1	1:B:720:ARG:N	2.46	0.47
1:B:747:THR:HA	1:B:750:LEU:HG	1.96	0.47
2:C:250:SER:HA	2:C:260:VAL:HG21	1.96	0.47
2:C:511:SER:OG	2:C:512:ALA:N	2.46	0.47
1:A:335:PRO:HB2	1:A:338:GLU:OE2	2.14	0.47
1:B:16:LEU:HD21	1:B:462:LEU:HD13	1.96	0.47
1:B:83:ASP:OD1	1:B:191:ARG:NE	2.47	0.47
1:B:253:VAL:HG11	1:B:322:ILE:HD13	1.95	0.47
1:B:349:ILE:HD11	1:B:356:SER:HB2	1.96	0.47
1:B:362:GLU:HB2	1:B:364:TRP:HE1	1.79	0.47
1:B:533:ASN:ND2	1:B:542:THR:OG1	2.47	0.47
1:B:757:GLY:HA3	1:B:759:VAL:H	1.79	0.47
2:C:89:HIS:HE2	2:C:208:THR:HA	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:PRO:HB2	2:C:264:PHE:HD2	1.79	0.47
2:C:641:ILE:O	2:C:645:LEU:N	2.41	0.47
1:B:66:TYR:HA	1:B:69:LEU:HD12	1.95	0.47
1:B:729:LEU:O	1:B:732:LEU:HB3	2.14	0.47
2:C:451:LYS:HD3	2:C:497:LEU:HD21	1.96	0.47
1:A:80:LEU:HD21	1:A:477:ASN:HD21	1.79	0.47
1:A:146:PHE:HA	1:A:149:ILE:HB	1.97	0.47
1:A:349:ILE:HD11	1:A:356:SER:HB2	1.97	0.47
1:A:533:ASN:ND2	1:A:542:THR:OG1	2.47	0.47
1:A:535:ILE:HG13	1:A:540:ILE:HG23	1.96	0.47
1:A:580:TRP:CE3	1:A:581:HIS:HA	2.49	0.47
1:A:696:SER:OG	1:A:697:ARG:NH1	2.47	0.47
1:A:757:GLY:HA3	1:A:759:VAL:H	1.79	0.47
1:B:80:LEU:HD21	1:B:477:ASN:HD21	1.79	0.47
1:B:410:VAL:CA	1:B:413:PHE:HB3	2.41	0.47
2:C:499:ASP:HB3	2:C:514:PHE:CD2	2.49	0.47
1:A:109:TYR:OH	1:A:130:ALA:HB1	2.14	0.47
1:A:371:THR:HB	1:A:389:VAL:HG23	1.96	0.47
1:A:648:ALA:O	1:A:652:ARG:HG3	2.14	0.47
1:B:189:CYS:O	1:B:193:SER:OG	2.22	0.47
1:B:243:ASN:ND2	2:C:422:LEU:CD2	2.77	0.47
1:B:696:SER:OG	1:B:697:ARG:NH1	2.47	0.47
2:C:17:LEU:HB3	2:C:154:PRO:HA	1.96	0.47
1:A:282:ASP:OD1	1:A:282:ASP:N	2.48	0.47
1:A:282:ASP:O	1:A:285:ARG:HB3	2.14	0.47
1:B:6:VAL:HG11	1:B:530:VAL:HG23	1.96	0.47
1:B:376:VAL:O	1:B:386:PHE:N	2.47	0.47
1:B:441:PHE:HB2	1:B:444:VAL:HG22	1.96	0.47
1:B:535:ILE:HG13	1:B:540:ILE:HG23	1.96	0.47
1:B:648:ALA:O	1:B:652:ARG:HG3	2.14	0.47
2:C:1:PRO:HA	2:C:238:GLU:HG3	1.97	0.47
2:C:382:PRO:HA	2:C:385:PRO:HG3	1.95	0.47
2:C:503:TYR:HD2	2:C:508:GLU:N	2.13	0.47
2:C:555:LYS:HB2	2:C:564:TYR:OH	2.14	0.47
1:A:344:GLY:HA2	1:A:557:PRO:HB3	1.96	0.47
1:B:49:THR:OG1	1:B:50:SER:N	2.44	0.47
1:B:146:PHE:HA	1:B:149:ILE:HB	1.97	0.47
1:B:344:GLY:HA2	1:B:557:PRO:HB3	1.96	0.47
1:B:708:ILE:O	1:B:711:SER:OG	2.22	0.47
2:C:299:ALA:O	2:C:302:PHE:N	2.46	0.47
2:C:564:TYR:O	2:C:568:LEU:HD13	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:565:SER:O	2:C:568:LEU:HB2	2.15	0.47
1:B:51:GLU:CA	1:B:174:VAL:HG21	2.43	0.47
1:B:493:TYR:CZ	1:B:549:ILE:HG12	2.49	0.47
1:B:745:ALA:O	1:B:748:LYS:HB3	2.15	0.47
2:C:74:ARG:HD2	2:C:507:ARG:HB3	1.96	0.47
2:C:454:ASP:OD2	2:C:497:LEU:HD12	2.15	0.47
1:A:6:VAL:HG11	1:A:530:VAL:HG23	1.96	0.47
1:A:303:ARG:HB2	1:A:513:GLN:OE1	2.15	0.47
1:A:337:ASN:HD21	1:A:496:ALA:HB2	1.80	0.47
2:C:28:SER:OG	2:C:29:LYS:HG3	2.15	0.47
2:C:78:ASN:OD1	2:C:79:GLY:N	2.48	0.47
2:C:121:GLU:O	2:C:124:ASN:HB3	2.15	0.47
1:A:66:TYR:HA	1:A:69:LEU:HD12	1.95	0.47
1:A:69:LEU:HD22	1:A:172:TYR:HD2	1.80	0.47
1:A:117:ALA:H	1:A:221:ALA:N	1.94	0.47
1:A:308:PHE:HE2	1:A:318:ILE:HG13	1.80	0.47
1:B:263:PRO:HG3	1:B:504:SER:HA	1.97	0.47
1:B:502:VAL:HG23	1:B:503:VAL:HG12	1.97	0.47
1:B:580:TRP:CE3	1:B:581:HIS:HA	2.49	0.47
2:C:319:LEU:O	2:C:458:GLY:HA2	2.15	0.47
2:C:364:PRO:HG2	2:C:382:PRO:HG3	1.97	0.47
1:A:149:ILE:HA	1:A:152:ASP:OD2	2.15	0.46
1:A:280:GLY:N	1:A:282:ASP:OD1	2.48	0.46
1:A:328:VAL:HG23	1:A:329:SER:HB2	1.97	0.46
1:B:316:THR:CA	2:C:469:HIS:NE2	2.78	0.46
1:B:328:VAL:HG23	1:B:329:SER:HB2	1.97	0.46
1:B:672:VAL:HA	1:B:675:LEU:HD12	1.96	0.46
2:C:100:TRP:HD1	2:C:229:ASP:HA	1.80	0.46
1:A:418:THR:O	1:A:421:TYR:HD1	1.99	0.46
1:A:498:ASN:OD1	1:A:499:PRO:HD2	2.15	0.46
1:A:502:VAL:HG23	1:A:503:VAL:HG12	1.97	0.46
1:A:503:VAL:HG21	1:A:517:TYR:C	2.36	0.46
1:A:745:ALA:O	1:A:748:LYS:HB3	2.15	0.46
1:B:371:THR:HB	1:B:389:VAL:HG23	1.96	0.46
2:C:252:LEU:HD22	2:C:256:TYR:CD2	2.50	0.46
1:A:329:SER:HB3	1:A:331:PHE:HB3	1.98	0.46
1:B:181:PRO:HB2	1:B:182:ASN:H	1.43	0.46
1:B:320:TRP:HA	1:B:325:MET:HE1	1.97	0.46
1:B:385:ARG:HD2	1:B:580:TRP:NE1	2.29	0.46
1:B:503:VAL:HG21	1:B:517:TYR:C	2.36	0.46
2:C:72:TYR:CD1	2:C:472:PHE:HZ	2.32	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:129:ALA:O	2:C:133:LEU:HG	2.15	0.46
2:C:366:TYR:HD1	2:C:378:LEU:HA	1.79	0.46
1:A:57:GLY:N	1:A:170:TYR:HB2	2.30	0.46
1:B:282:ASP:O	1:B:285:ARG:HB3	2.14	0.46
1:B:308:PHE:HE2	1:B:318:ILE:HG13	1.80	0.46
2:C:146:ARG:O	2:C:163:LYS:NZ	2.48	0.46
2:C:539:ARG:HH11	2:C:542:ARG:HH11	1.63	0.46
1:A:212:ALA:HB3	1:A:219:ALA:HB3	1.97	0.46
1:B:36:LEU:C	1:B:502:VAL:HG11	2.35	0.46
1:B:69:LEU:HD22	1:B:172:TYR:HD2	1.80	0.46
1:B:149:ILE:HA	1:B:152:ASP:OD2	2.15	0.46
1:B:280:GLY:N	1:B:282:ASP:OD1	2.48	0.46
1:B:321:PHE:CD1	2:C:461:LYS:C	2.89	0.46
1:B:678:ILE:HA	1:B:681:ILE:HG12	1.97	0.46
1:A:56:VAL:HG13	1:A:66:TYR:CE1	2.50	0.46
1:B:279:ASN:OD1	2:C:506:ARG:HG2	2.16	0.46
2:C:15:GLN:HE22	2:C:25:GLN:HE22	1.62	0.46
2:C:95:MET:HA	2:C:251:ARG:HH22	1.79	0.46
2:C:286:VAL:O	2:C:290:VAL:HG23	2.15	0.46
2:C:306:THR:O	2:C:309:ASN:HB3	2.15	0.46
2:C:357:PHE:CD1	2:C:361:LEU:CD2	2.99	0.46
2:C:362:LYS:HE3	2:C:388:GLU:OE2	2.16	0.46
1:A:281:ILE:HG22	1:A:319:PRO:HB2	1.98	0.46
1:A:580:TRP:HA	1:A:581:HIS:C	2.36	0.46
1:B:176:ARG:C	1:B:447:ARG:HH12	2.19	0.46
1:B:209:MET:O	1:B:210:LEU:HB2	2.16	0.46
1:B:210:LEU:HB3	1:B:212:ALA:O	2.16	0.46
1:B:303:ARG:HB2	1:B:513:GLN:OE1	2.15	0.46
1:B:498:ASN:OD1	1:B:499:PRO:HD2	2.15	0.46
1:B:566:LEU:HD12	1:B:568:LEU:HD23	1.98	0.46
1:B:739:SER:OG	1:B:742:GLU:OE1	2.32	0.46
2:C:73:GLY:CA	2:C:492:HIS:HA	2.45	0.46
2:C:525:GLN:HE22	2:C:571:ILE:HD13	1.81	0.46
1:A:365:GLN:CA	1:A:562:GLN:HB2	2.41	0.46
1:A:559:GLU:OE1	1:A:559:GLU:N	2.49	0.46
1:A:566:LEU:HD12	1:A:568:LEU:HD23	1.98	0.46
1:B:56:VAL:HG13	1:B:66:TYR:CE1	2.50	0.46
1:B:316:THR:CG2	2:C:465:LEU:C	2.84	0.46
1:B:349:ILE:HD12	1:B:349:ILE:HA	1.78	0.46
1:B:685:GLY:HA2	1:B:686:ILE:HA	1.53	0.46
2:C:17:LEU:HD22	2:C:153:ILE:HG23	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:105:ASN:ND2	2:C:330:THR:O	2.48	0.46
2:C:114:LEU:HD22	2:C:486:MET:N	2.30	0.46
2:C:226:MET:HB3	2:C:242:LEU:CG	2.41	0.46
2:C:495:ALA:HB2	2:C:500:ILE:HG12	1.98	0.46
2:C:496:PHE:CE2	2:C:497:LEU:HD13	2.51	0.46
1:A:75:GLN:HE22	1:A:447:ARG:NH2	2.14	0.46
1:A:678:ILE:HA	1:A:681:ILE:HG12	1.97	0.46
1:B:75:GLN:HE22	1:B:447:ARG:NH2	2.14	0.46
1:B:410:VAL:O	1:B:414:VAL:HG23	2.16	0.46
1:B:503:VAL:HG22	1:B:504:SER:H	1.81	0.46
2:C:290:VAL:O	2:C:293:LYS:HB3	2.16	0.46
1:A:317:ILE:O	1:A:320:TRP:HB3	2.16	0.46
1:B:261:TRP:HE1	1:B:288:LEU:HD11	1.81	0.46
1:B:365:GLN:CA	1:B:562:GLN:HB2	2.41	0.46
1:B:666:ARG:HA	1:B:669:GLN:NE2	2.31	0.46
1:B:666:ARG:O	1:B:670:ASN:ND2	2.49	0.46
1:B:712:SER:C	1:B:715:HIS:HD1	2.16	0.46
2:C:88:ARG:HG2	2:C:264:PHE:HE1	1.81	0.46
2:C:175:GLU:HG3	2:C:352:TRP:CD1	2.51	0.46
2:C:224:ASP:OD1	2:C:247:LYS:NZ	2.39	0.46
2:C:326:SER:O	2:C:486:MET:HE1	2.16	0.46
2:C:407:SER:HA	2:C:410:TYR:CD2	2.50	0.46
2:C:411:LEU:O	2:C:414:GLN:HB2	2.16	0.46
1:A:36:LEU:C	1:A:502:VAL:HG11	2.36	0.45
1:A:454:ASP:HA	1:A:455:PRO:HD2	1.82	0.45
1:A:477:ASN:O	1:A:481:ARG:N	2.47	0.45
1:B:281:ILE:HG22	1:B:319:PRO:HB2	1.98	0.45
2:C:3:ARG:NH2	2:C:231:GLU:OE2	2.49	0.45
2:C:115:ALA:HB3	2:C:485:TYR:CZ	2.51	0.45
2:C:302:PHE:O	2:C:304:HIS:CD2	2.69	0.45
2:C:315:LYS:HA	2:C:509:PRO:O	2.15	0.45
2:C:335:TRP:HA	2:C:338:ASP:OD2	2.16	0.45
2:C:402:GLY:O	2:C:406:MET:HG2	2.16	0.45
2:C:481:ASN:HD21	2:C:483:SER:HB3	1.81	0.45
2:C:518:ILE:O	2:C:522:LEU:HG	2.16	0.45
1:A:156:HIS:O	1:A:159:SER:OG	2.30	0.45
1:A:209:MET:O	1:A:210:LEU:HB2	2.16	0.45
1:A:315:SER:O	1:A:319:PRO:HD2	2.16	0.45
1:A:350:ASP:N	1:A:350:ASP:OD1	2.49	0.45
1:A:666:ARG:O	1:A:670:ASN:ND2	2.49	0.45
1:B:101:GLU:OE1	1:B:101:GLU:N	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:503:VAL:HG11	1:B:517:TYR:O	2.16	0.45
1:B:559:GLU:OE1	1:B:559:GLU:N	2.49	0.45
1:A:263:PRO:HG3	1:A:504:SER:HA	1.97	0.45
1:B:45:SER:C	1:B:332:LYS:HD2	2.37	0.45
1:B:117:ALA:H	1:B:221:ALA:N	1.94	0.45
1:B:316:THR:HG23	2:C:466:VAL:HA	1.92	0.45
1:B:317:ILE:O	1:B:320:TRP:HB3	2.16	0.45
1:B:371:THR:O	1:B:623:ILE:HD12	2.16	0.45
2:C:69:VAL:HA	2:C:75:VAL:HA	1.97	0.45
2:C:199:TYR:HA	2:C:274:GLY:O	2.17	0.45
2:C:518:ILE:O	2:C:521:MET:HB3	2.16	0.45
1:A:261:TRP:HE1	1:A:288:LEU:HD11	1.81	0.45
1:A:298:VAL:HG21	1:A:514:GLY:O	2.17	0.45
1:B:159:SER:HG	1:B:160:PRO:HD3	1.81	0.45
1:B:201:ALA:HB1	1:B:239:ARG:HD3	1.98	0.45
1:B:282:ASP:OD1	1:B:282:ASP:N	2.48	0.45
1:B:595:VAL:HG12	1:B:597:ILE:HG23	1.99	0.45
2:C:69:VAL:HG22	2:C:75:VAL:HG13	1.98	0.45
2:C:144:LYS:HD2	2:C:648:GLY:HA2	1.99	0.45
2:C:344:LEU:HD13	2:C:354:VAL:HG22	1.98	0.45
1:A:45:SER:C	1:A:332:LYS:HD2	2.37	0.45
1:A:176:ARG:C	1:A:447:ARG:HH12	2.19	0.45
1:A:210:LEU:HB3	1:A:212:ALA:O	2.16	0.45
1:A:615:GLY:HA2	1:A:616:GLN:HA	1.64	0.45
1:A:652:ARG:O	1:A:653:THR:OG1	2.30	0.45
1:B:156:HIS:O	1:B:159:SER:OG	2.30	0.45
1:B:315:SER:O	1:B:319:PRO:HD2	2.16	0.45
1:B:328:VAL:HG23	1:B:329:SER:CB	2.46	0.45
2:C:521:MET:SD	2:C:554:MET:HG3	2.56	0.45
1:A:16:LEU:HD21	1:A:462:LEU:HB3	1.99	0.45
1:A:101:GLU:OE1	1:A:101:GLU:N	2.49	0.45
1:A:313:LEU:HB3	1:A:314:SER:HB3	1.99	0.45
1:A:567:ASP:OD2	1:A:570:ASN:ND2	2.31	0.45
1:A:669:GLN:O	1:A:673:THR:N	2.39	0.45
1:B:212:ALA:HB3	1:B:219:ALA:HB3	1.97	0.45
1:B:313:LEU:HB3	1:B:314:SER:HB3	1.99	0.45
2:C:53:PHE:O	2:C:57:LEU:HB2	2.17	0.45
1:A:595:VAL:HG12	1:A:597:ILE:HG23	1.99	0.45
1:B:337:ASN:O	1:B:341:SER:N	2.50	0.45
1:B:510:ALA:HA	1:B:511:ALA:HA	1.72	0.45
1:B:567:ASP:OD2	1:B:570:ASN:ND2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:100:TRP:CD1	2:C:229:ASP:HA	2.52	0.45
2:C:144:LYS:CD	2:C:648:GLY:HA2	2.47	0.45
2:C:253:LYS:HD3	2:C:259:ASP:HA	1.97	0.45
2:C:307:ARG:HH22	2:C:513:ILE:HD12	1.82	0.45
2:C:332:TRP:NE1	2:C:336:LEU:HD23	2.31	0.45
1:A:224:LEU:HA	1:A:227:GLN:HB3	1.99	0.45
1:A:410:VAL:O	1:A:414:VAL:HG23	2.17	0.45
1:A:428:GLY:HA3	1:A:429:THR:HA	1.59	0.45
1:B:580:TRP:HA	1:B:581:HIS:C	2.36	0.45
2:C:69:VAL:HG11	2:C:493:GLY:N	2.32	0.45
2:C:120:SER:OG	2:C:122:ARG:HB3	2.16	0.45
1:A:260:LEU:HD11	1:A:285:ARG:HH12	1.82	0.45
1:A:349:ILE:HD12	1:A:349:ILE:HA	1.79	0.45
1:A:371:THR:O	1:A:623:ILE:HD12	2.16	0.45
1:A:383:ASN:O	1:A:385:ARG:N	2.38	0.45
1:A:503:VAL:HG22	1:A:504:SER:H	1.81	0.45
1:A:666:ARG:HA	1:A:669:GLN:NE2	2.31	0.45
1:B:350:ASP:OD1	1:B:350:ASP:N	2.49	0.45
1:B:652:ARG:O	1:B:653:THR:OG1	2.30	0.45
1:A:55:GLU:OE1	1:A:55:GLU:N	2.50	0.45
1:A:337:ASN:O	1:A:341:SER:N	2.50	0.45
1:B:298:VAL:HG21	1:B:514:GLY:O	2.17	0.45
1:B:329:SER:HB3	1:B:331:PHE:HB3	1.98	0.45
1:B:366:PHE:O	1:B:368:LYS:HD2	2.17	0.45
1:B:418:THR:O	1:B:421:TYR:HD1	1.99	0.45
1:B:674:LEU:HA	1:B:677:LYS:HG2	1.99	0.45
2:C:102:LEU:O	2:C:389:VAL:HG12	2.17	0.45
2:C:317:TRP:HH2	2:C:449:ILE:HG23	1.81	0.45
1:A:223:ALA:O	1:A:227:GLN:N	2.34	0.44
1:A:328:VAL:HG23	1:A:329:SER:CB	2.46	0.44
1:A:674:LEU:HA	1:A:677:LYS:NZ	2.32	0.44
1:B:116:ARG:HA	1:B:118:ILE:H	1.82	0.44
1:B:174:VAL:HB	1:B:175:GLY:H	1.57	0.44
1:B:211:GLN:O	1:B:218:GLY:HA3	2.18	0.44
1:B:271:PRO:HA	1:B:276:ARG:HD3	2.00	0.44
1:B:425:SER:OG	1:B:659:GLU:OE2	2.26	0.44
2:C:82:THR:HG22	2:C:83:ASN:O	2.17	0.44
1:A:385:ARG:HD2	1:A:580:TRP:NE1	2.29	0.44
1:A:674:LEU:HA	1:A:677:LYS:HG2	2.00	0.44
1:B:337:ASN:HD21	1:B:496:ALA:HB2	1.80	0.44
1:B:366:PHE:CD2	1:B:405:GLY:HA2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:504:ASP:OD2	2:C:506:ARG:NH2	2.50	0.44
1:A:320:TRP:HA	1:A:325:MET:HE1	1.98	0.44
1:A:500:GLU:HB3	1:A:521:ASN:H	1.83	0.44
2:C:135:PHE:HB3	2:C:349:TYR:CE1	2.52	0.44
2:C:146:ARG:HB3	2:C:149:SER:HB3	1.98	0.44
2:C:253:LYS:HB2	2:C:260:VAL:CG2	2.47	0.44
2:C:526:PHE:C	2:C:528:PRO:HD3	2.37	0.44
1:A:216:ALA:HA	1:A:217:LYS:HA	1.72	0.44
1:B:737:LEU:O	1:B:738:LEU:HG	2.18	0.44
2:C:222:SER:O	2:C:247:LYS:NZ	2.50	0.44
2:C:253:LYS:O	2:C:257:GLY:HA2	2.16	0.44
2:C:363:LEU:O	2:C:387:LEU:HD12	2.17	0.44
2:C:453:ASP:OD1	2:C:454:ASP:N	2.51	0.44
2:C:554:MET:HB3	2:C:554:MET:HE2	1.83	0.44
2:C:598:LEU:HA	2:C:601:TYR:CD2	2.53	0.44
1:A:201:ALA:HB1	1:A:239:ARG:HD3	1.98	0.44
1:B:16:LEU:HD21	1:B:462:LEU:HB3	1.99	0.44
1:B:362:GLU:OE1	1:B:443:SER:OG	2.35	0.44
2:C:628:LEU:HD12	2:C:632:TRP:O	2.16	0.44
1:A:497:HIS:HE2	1:A:548:ALA:C	2.20	0.44
1:B:107:THR:OG1	1:B:226:SER:OG	2.18	0.44
1:B:260:LEU:HD11	1:B:285:ARG:HH12	1.82	0.44
1:B:389:VAL:HG13	1:B:391:PRO:HD3	1.99	0.44
1:B:674:LEU:HA	1:B:677:LYS:NZ	2.32	0.44
2:C:38:GLU:CD	2:C:41:GLU:HA	2.37	0.44
2:C:288:GLN:CA	2:C:291:ARG:HH11	2.30	0.44
2:C:550:ALA:HA	2:C:553:SER:OG	2.17	0.44
2:C:637:VAL:HB	2:C:642:HIS:HD2	1.82	0.44
1:A:116:ARG:HA	1:A:118:ILE:H	1.82	0.44
1:A:358:VAL:N	1:A:437:MET:HB3	2.31	0.44
1:A:424:VAL:HG12	1:A:425:SER:O	2.18	0.44
1:A:454:ASP:O	1:A:457:VAL:HG12	2.18	0.44
1:A:503:VAL:HG11	1:A:517:TYR:O	2.16	0.44
1:B:3:ASN:HA	1:B:436:GLU:HB3	1.98	0.44
1:B:55:GLU:OE1	1:B:55:GLU:N	2.51	0.44
2:C:153:ILE:HG21	2:C:198:ALA:O	2.18	0.44
2:C:213:LEU:HD11	2:C:218:GLY:HA2	2.00	0.44
2:C:466:VAL:HG13	2:C:470:ARG:HH12	1.82	0.44
2:C:659:ARG:HA	2:C:664:ARG:O	2.18	0.44
1:A:3:ASN:HA	1:A:436:GLU:HB3	1.98	0.44
1:A:362:GLU:OE1	1:A:443:SER:OG	2.35	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:590:GLU:OE1	1:A:607:LYS:HD3	2.18	0.44
1:A:732:LEU:O	1:A:735:MET:HB3	2.18	0.44
2:C:198:ALA:HA	2:C:364:PRO:O	2.18	0.44
2:C:565:SER:HA	2:C:568:LEU:HD13	1.99	0.44
1:A:59:GLY:HA3	1:A:155:CYS:HB3	2.00	0.44
1:A:737:LEU:O	1:A:738:LEU:HG	2.18	0.44
1:B:368:LYS:HE2	1:B:402:ALA:O	2.18	0.44
1:B:500:GLU:HB3	1:B:521:ASN:H	1.83	0.44
2:C:337:ARG:CZ	2:C:362:LYS:HD2	2.48	0.44
2:C:521:MET:HA	2:C:524:ASN:OD1	2.17	0.44
2:C:528:PRO:HG2	2:C:544:ARG:HH12	1.83	0.44
2:C:555:LYS:HD3	2:C:564:TYR:CE2	2.53	0.44
2:C:584:ARG:O	2:C:588:GLU:HG3	2.18	0.44
1:A:211:GLN:O	1:A:218:GLY:HA3	2.18	0.43
1:A:368:LYS:HE2	1:A:402:ALA:O	2.18	0.43
1:A:630:HIS:HD2	1:A:633:ILE:HD11	1.83	0.43
1:B:66:TYR:HD1	1:B:69:LEU:HD12	1.83	0.43
1:B:177:THR:HA	1:B:447:ARG:HH22	1.83	0.43
1:B:199:LEU:HD23	1:B:203:SER:HB2	1.99	0.43
1:B:719:ASN:O	1:B:722:ARG:HB3	2.18	0.43
1:B:732:LEU:O	1:B:735:MET:HB3	2.18	0.43
2:C:75:VAL:O	2:C:503:TYR:N	2.43	0.43
2:C:105:ASN:HB2	2:C:108:LYS:HD3	2.00	0.43
2:C:152:CYS:N	2:C:156:PHE:HA	2.32	0.43
2:C:517:ASN:OD1	2:C:518:ILE:N	2.51	0.43
1:A:271:PRO:HA	1:A:276:ARG:HD3	2.00	0.43
1:A:366:PHE:CD2	1:A:405:GLY:HA2	2.52	0.43
1:A:521:ASN:O	1:A:539:SER:OG	2.10	0.43
1:B:57:GLY:N	1:B:170:TYR:HB2	2.30	0.43
1:B:216:ALA:HA	1:B:217:LYS:HA	1.72	0.43
1:B:549:ILE:HA	1:B:552:ASN:HB2	2.00	0.43
1:B:754:ASN:HB3	1:B:755:ALA:C	2.39	0.43
2:C:128:ARG:HA	2:C:339:LEU:HD21	2.00	0.43
2:C:300:TYR:CZ	2:C:442:GLY:HA3	2.53	0.43
2:C:411:LEU:HD21	2:C:435:PHE:CE2	2.53	0.43
1:A:138:LEU:HB3	1:A:139:ALA:H	1.69	0.43
1:A:176:ARG:NH1	1:A:447:ARG:HA	2.26	0.43
1:A:366:PHE:O	1:A:368:LYS:HD2	2.17	0.43
1:A:715:HIS:HB2	1:A:716:VAL:HG13	2.01	0.43
1:B:41:THR:OG1	1:B:42:ARG:N	2.51	0.43
1:B:68:ARG:CZ	1:B:330:PRO:HG3	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:HIS:HE2	1:B:548:ALA:C	2.20	0.43
1:B:590:GLU:OE1	1:B:607:LYS:HD3	2.18	0.43
2:C:40:TYR:CD1	2:C:43:LEU:HD22	2.49	0.43
2:C:151:THR:HG23	2:C:157:SER:O	2.19	0.43
2:C:251:ARG:C	2:C:254:GLU:HB3	2.38	0.43
2:C:328:HIS:CG	2:C:453:ASP:HB3	2.53	0.43
2:C:344:LEU:HB3	2:C:349:TYR:HB2	2.00	0.43
2:C:585:ALA:HA	2:C:588:GLU:OE1	2.18	0.43
2:C:652:GLU:O	2:C:655:GLU:HB3	2.18	0.43
1:A:199:LEU:HD23	1:A:203:SER:HB2	1.99	0.43
1:A:345:GLN:HE22	1:A:549:ILE:HG23	1.83	0.43
1:A:682:GLY:O	1:A:684:THR:N	2.51	0.43
1:A:754:ASN:H	1:A:755:ALA:HA	1.83	0.43
1:B:204:SER:O	1:B:206:ASP:N	2.52	0.43
1:B:221:ALA:HB1	1:B:224:LEU:HB3	1.99	0.43
1:B:369:GLU:HA	1:B:398:SER:CB	2.49	0.43
1:B:590:GLU:OE2	1:B:607:LYS:HA	2.18	0.43
2:C:96:ILE:O	2:C:246:SER:N	2.51	0.43
2:C:135:PHE:HB3	2:C:349:TYR:CZ	2.52	0.43
2:C:150:SER:HA	2:C:158:ASN:HA	2.00	0.43
1:A:56:VAL:HB	1:A:170:TYR:HB2	2.00	0.43
1:A:66:TYR:HD1	1:A:69:LEU:HD12	1.83	0.43
1:A:87:ASN:O	1:A:90:THR:OG1	2.28	0.43
1:A:293:ALA:O	1:A:297:MET:HB2	2.19	0.43
1:B:345:GLN:HE22	1:B:549:ILE:HG23	1.83	0.43
1:B:358:VAL:N	1:B:437:MET:HB3	2.31	0.43
1:B:441:PHE:HA	1:B:442:PRO:HD2	1.73	0.43
2:C:154:PRO:HD3	2:C:276:PRO:HA	2.00	0.43
2:C:406:MET:HE1	2:C:488:ILE:CD1	2.49	0.43
2:C:615:THR:O	2:C:619:LEU:HG	2.18	0.43
1:A:359:VAL:HG22	1:A:437:MET:O	2.19	0.43
1:A:628:VAL:O	1:A:632:ILE:HD12	2.19	0.43
1:B:54:TRP:CH2	1:B:174:VAL:HG12	2.54	0.43
1:B:322:ILE:H	2:C:461:LYS:NZ	1.79	0.43
1:B:424:VAL:HG12	1:B:425:SER:O	2.18	0.43
2:C:3:ARG:HH21	2:C:234:VAL:HG21	1.83	0.43
2:C:51:LEU:HB3	2:C:264:PHE:CE2	2.53	0.43
2:C:120:SER:O	2:C:123:ASP:HB2	2.18	0.43
2:C:223:LYS:HD3	2:C:225:ARG:NH1	2.34	0.43
2:C:279:LEU:HD23	2:C:360:SER:HB3	2.00	0.43
1:A:54:TRP:CH2	1:A:174:VAL:HG12	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:LEU:HD23	1:B:39:GLN:O	2.19	0.43
1:B:56:VAL:HB	1:B:170:TYR:HB2	2.00	0.43
1:B:348:ALA:O	1:B:349:ILE:HG22	2.18	0.43
1:B:566:LEU:CD1	1:B:568:LEU:HB3	2.49	0.43
2:C:171:LEU:HA	2:C:657:PHE:CD1	2.54	0.43
2:C:232:TYR:HB2	2:C:241:SER:N	2.34	0.43
1:A:177:THR:HA	1:A:447:ARG:HH22	1.83	0.43
1:A:259:ARG:HG3	1:A:269:LEU:HD13	2.01	0.43
1:A:291:PHE:O	1:A:292:ILE:HB	2.19	0.43
1:A:389:VAL:HG13	1:A:391:PRO:HD3	1.99	0.43
1:A:566:LEU:CD1	1:A:568:LEU:HB3	2.49	0.43
1:B:259:ARG:O	1:B:262:SER:OG	2.23	0.43
1:B:402:ALA:HB3	1:B:403:PRO:HD3	2.01	0.43
1:B:454:ASP:O	1:B:457:VAL:HG12	2.18	0.43
1:B:544:GLU:HG2	1:B:545:PRO:HD2	2.01	0.43
1:B:630:HIS:HD2	1:B:633:ILE:HD11	1.83	0.43
2:C:146:ARG:HD2	2:C:645:LEU:O	2.19	0.43
2:C:448:GLN:HB3	2:C:457:LEU:HD23	1.99	0.43
1:A:41:THR:OG1	1:A:42:ARG:N	2.51	0.43
1:A:241:ARG:HG3	1:A:243:ASN:H	1.84	0.43
1:A:369:GLU:HA	1:A:398:SER:CB	2.49	0.43
1:A:754:ASN:HB3	1:A:755:ALA:C	2.39	0.43
1:B:182:ASN:HD21	1:B:184:TYR:HD2	1.67	0.43
1:B:224:LEU:HA	1:B:227:GLN:HB3	1.99	0.43
1:B:523:ARG:HA	1:B:539:SER:HB2	2.01	0.43
2:C:54:LYS:NZ	2:C:91:ASN:HD22	2.17	0.43
2:C:413:MET:CE	2:C:482:PRO:HG2	2.49	0.43
2:C:596:LEU:O	2:C:599:SER:OG	2.20	0.43
1:A:107:THR:OG1	1:A:226:SER:OG	2.18	0.43
1:A:204:SER:O	1:A:206:ASP:N	2.52	0.43
1:A:377:LYS:HD2	1:A:380:ASN:HA	2.01	0.43
1:A:549:ILE:HA	1:A:552:ASN:HB2	2.00	0.43
1:B:82:VAL:O	1:B:86:VAL:HG23	2.19	0.43
1:B:520:TRP:CH2	1:B:545:PRO:HG3	2.54	0.43
2:C:171:LEU:HD22	2:C:657:PHE:CG	2.54	0.43
2:C:210:ALA:HB3	2:C:223:LYS:HB2	2.00	0.43
2:C:232:TYR:CE2	2:C:237:GLY:HA2	2.54	0.43
2:C:232:TYR:HA	2:C:239:GLN:O	2.18	0.43
2:C:302:PHE:HZ	2:C:440:TRP:CD2	2.36	0.43
2:C:520:SER:HA	2:C:523:ASN:ND2	2.34	0.43
2:C:627:LYS:HB2	2:C:632:TRP:HZ3	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ALA:HB1	1:A:224:LEU:HB3	2.00	0.42
1:B:291:PHE:O	1:B:292:ILE:HB	2.19	0.42
1:B:293:ALA:O	1:B:297:MET:HB2	2.19	0.42
1:B:377:LYS:HD2	1:B:380:ASN:HA	2.01	0.42
2:C:86:GLY:O	2:C:208:THR:HA	2.18	0.42
2:C:124:ASN:HD21	2:C:128:ARG:HE	1.66	0.42
2:C:523:ASN:O	2:C:527:SER:N	2.51	0.42
2:C:627:LYS:HA	2:C:630:TYR:CE1	2.54	0.42
1:A:38:LEU:HD23	1:A:39:GLN:O	2.19	0.42
1:A:68:ARG:CZ	1:A:330:PRO:HG3	2.49	0.42
1:A:413:PHE:CZ	1:A:636:TRP:HA	2.54	0.42
1:A:520:TRP:CH2	1:A:545:PRO:HG3	2.54	0.42
1:B:59:GLY:HA3	1:B:155:CYS:HB3	2.00	0.42
1:B:259:ARG:HG3	1:B:269:LEU:HD13	2.01	0.42
1:B:655:ARG:H	1:B:656:ASP:CB	2.30	0.42
2:C:181:MET:C	2:C:184:GLY:H	2.23	0.42
2:C:235:THR:O	2:C:238:GLU:N	2.36	0.42
2:C:298:TYR:CD2	2:C:440:TRP:HE3	2.38	0.42
1:A:182:ASN:HD21	1:A:184:TYR:HD2	1.67	0.42
1:A:331:PHE:O	1:A:332:LYS:HG2	2.19	0.42
1:A:373:PHE:CE1	1:A:387:LEU:HD22	2.54	0.42
2:C:17:LEU:O	2:C:154:PRO:HB2	2.19	0.42
2:C:81:ARG:HG3	2:C:82:THR:OG1	2.19	0.42
2:C:201:VAL:HG23	2:C:366:TYR:O	2.19	0.42
2:C:566:ASP:HA	2:C:569:GLU:CD	2.39	0.42
1:A:82:VAL:O	1:A:86:VAL:HG23	2.19	0.42
1:A:355:PRO:O	1:A:356:SER:OG	2.28	0.42
1:A:510:ALA:HA	1:A:511:ALA:HA	1.72	0.42
1:A:523:ARG:HA	1:A:539:SER:HB2	2.01	0.42
1:A:655:ARG:H	1:A:656:ASP:CB	2.30	0.42
1:A:719:ASN:O	1:A:722:ARG:HB3	2.18	0.42
1:B:44:PHE:HE1	1:B:180:TYR:N	2.18	0.42
1:B:357:HIS:HA	1:B:437:MET:HG2	2.02	0.42
1:B:368:LYS:HA	1:B:401:LEU:HD23	2.01	0.42
1:B:628:VAL:O	1:B:632:ILE:HD12	2.19	0.42
1:B:682:GLY:O	1:B:684:THR:N	2.51	0.42
1:B:715:HIS:HB2	1:B:716:VAL:HG13	2.01	0.42
2:C:102:LEU:HD12	2:C:233:ALA:HA	2.00	0.42
2:C:250:SER:HA	2:C:253:LYS:CB	2.50	0.42
2:C:413:MET:CG	2:C:417:HIS:HD2	2.33	0.42
1:A:357:HIS:HA	1:A:437:MET:HG2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:80:LEU:HA	1:B:81:SER:HA	1.78	0.42
1:B:241:ARG:HG3	1:B:243:ASN:H	1.84	0.42
1:B:331:PHE:O	1:B:332:LYS:HG2	2.19	0.42
2:C:5:PRO:HB2	2:C:7:PHE:CE1	2.55	0.42
2:C:151:THR:HG22	2:C:163:LYS:CG	2.49	0.42
1:A:289:ALA:C	1:A:291:PHE:H	2.22	0.42
1:A:348:ALA:O	1:A:349:ILE:HG22	2.18	0.42
1:A:590:GLU:OE2	1:A:607:LYS:HA	2.18	0.42
1:B:133:GLU:O	1:B:137:THR:HG23	2.20	0.42
1:B:359:VAL:HG22	1:B:437:MET:O	2.19	0.42
1:B:413:PHE:CZ	1:B:636:TRP:HA	2.54	0.42
1:B:553:LYS:O	1:B:555:ILE:HG23	2.20	0.42
2:C:193:HIS:HB3	2:C:195:MET:HG3	2.00	0.42
2:C:230:PHE:O	2:C:234:VAL:HG22	2.20	0.42
2:C:353:TRP:O	2:C:356:LEU:HB2	2.20	0.42
1:A:43:THR:HA	1:A:289:ALA:CB	2.50	0.42
1:A:212:ALA:H	1:A:218:GLY:C	2.23	0.42
1:A:246:ALA:O	1:A:249:VAL:HG22	2.19	0.42
1:A:553:LYS:O	1:A:555:ILE:HG23	2.20	0.42
2:C:26:GLN:O	2:C:30:ARG:N	2.53	0.42
2:C:283:ILE:HG23	2:C:397:ALA:HB2	2.01	0.42
1:A:2:PHE:HE2	1:A:4:LEU:HD23	1.85	0.42
1:A:608:GLU:HG3	1:A:609:PHE:N	2.35	0.42
1:B:212:ALA:H	1:B:218:GLY:C	2.23	0.42
1:B:289:ALA:C	1:B:291:PHE:H	2.22	0.42
1:B:383:ASN:C	1:B:385:ARG:H	2.22	0.42
2:C:430:PRO:O	2:C:433:CYS:HB2	2.20	0.42
2:C:484:PRO:HG2	2:C:485:TYR:CE2	2.55	0.42
2:C:549:LEU:HA	2:C:591:LEU:HD13	2.01	0.42
1:A:41:THR:HG23	1:A:286:SER:O	2.20	0.42
1:B:2:PHE:HE2	1:B:4:LEU:HD23	1.85	0.42
1:B:243:ASN:ND2	2:C:422:LEU:HD21	2.35	0.42
1:B:246:ALA:O	1:B:249:VAL:HG22	2.19	0.42
1:B:657:ASP:O	1:B:660:LYS:HG2	2.20	0.42
2:C:350:ALA:HA	2:C:351:PRO:HD3	1.71	0.42
2:C:381:ASP:C	2:C:383:SER:H	2.18	0.42
1:A:331:PHE:C	1:A:332:LYS:HG2	2.41	0.42
1:A:368:LYS:HA	1:A:401:LEU:HD23	2.01	0.42
2:C:55:ASN:OD1	2:C:59:ARG:NE	2.43	0.42
2:C:96:ILE:H	2:C:251:ARG:HH22	1.68	0.42
2:C:96:ILE:HG12	2:C:269:ARG:NH1	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:414:GLN:NE2	2:C:457:LEU:HD22	2.35	0.42
1:B:43:THR:HA	1:B:289:ALA:CB	2.50	0.41
1:B:377:LYS:HE3	1:B:377:LYS:HB3	1.86	0.41
1:B:754:ASN:H	1:B:755:ALA:HA	1.83	0.41
2:C:209:ASP:OD2	2:C:222:SER:HB2	2.20	0.41
2:C:559:GLY:HA2	2:C:564:TYR:CD1	2.55	0.41
1:A:133:GLU:O	1:A:137:THR:HG23	2.20	0.41
1:A:366:PHE:HD1	1:A:366:PHE:HA	1.75	0.41
1:B:314:SER:HA	1:B:315:SER:C	2.40	0.41
1:B:498:ASN:C	1:B:500:GLU:H	2.24	0.41
1:B:536:GLU:N	1:B:536:GLU:OE1	2.40	0.41
1:B:610:GLU:OE1	1:B:610:GLU:N	2.48	0.41
1:B:659:GLU:O	1:B:662:ALA:HB3	2.20	0.41
2:C:324:ASP:HB3	2:C:489:SER:O	2.20	0.41
2:C:325:VAL:HA	2:C:488:ILE:CD1	2.51	0.41
2:C:551:TRP:HB2	2:C:587:ARG:NH2	2.35	0.41
1:A:402:ALA:HB3	1:A:403:PRO:HD3	2.01	0.41
1:B:243:ASN:ND2	2:C:422:LEU:HD22	2.35	0.41
1:B:313:LEU:HA	1:B:314:SER:HA	1.83	0.41
1:B:373:PHE:CE1	1:B:387:LEU:HD22	2.55	0.41
1:B:608:GLU:HG3	1:B:609:PHE:N	2.35	0.41
1:A:366:PHE:CE1	1:A:629:ALA:HB2	2.54	0.41
1:A:383:ASN:C	1:A:385:ARG:H	2.22	0.41
1:A:544:GLU:HG2	1:A:545:PRO:HD2	2.01	0.41
1:B:3:ASN:HA	1:B:436:GLU:CB	2.50	0.41
1:B:41:THR:HG23	1:B:286:SER:O	2.20	0.41
1:B:141:SER:HB3	1:B:144:GLU:HA	2.03	0.41
2:C:35:GLY:HA2	2:C:93:PHE:HE1	1.85	0.41
2:C:173:LYS:HB3	2:C:176:GLU:HB3	2.02	0.41
2:C:214:ASP:O	2:C:218:GLY:N	2.43	0.41
2:C:414:GLN:O	2:C:419:ALA:N	2.45	0.41
1:B:169:ALA:HB3	1:B:575:ILE:HG13	2.03	0.41
1:B:239:ARG:CD	2:C:438:SER:OG	2.67	0.41
1:B:292:ILE:HA	1:B:295:GLN:CG	2.50	0.41
1:B:349:ILE:HG21	1:B:354:GLN:O	2.20	0.41
2:C:3:ARG:CZ	2:C:230:PHE:HE2	2.33	0.41
2:C:96:ILE:C	2:C:245:ALA:HB1	2.41	0.41
2:C:326:SER:OG	2:C:331:PHE:HE2	2.03	0.41
2:C:411:LEU:HD13	2:C:439:TYR:CZ	2.55	0.41
2:C:465:LEU:HG	2:C:469:HIS:NE2	2.35	0.41
2:C:536:VAL:HG12	2:C:538:ASP:H	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LEU:O	1:A:190:VAL:HG13	2.21	0.41
1:A:498:ASN:C	1:A:500:GLU:H	2.24	0.41
1:A:657:ASP:O	1:A:660:LYS:HG2	2.20	0.41
1:B:128:PRO:O	1:B:131:ILE:HB	2.21	0.41
1:B:183:PHE:O	1:B:187:VAL:HG23	2.21	0.41
1:B:292:ILE:HD11	1:B:491:MET:HG3	2.02	0.41
1:B:428:GLY:HA3	1:B:429:THR:HA	1.59	0.41
1:B:521:ASN:HA	1:B:540:ILE:O	2.21	0.41
2:C:103:ALA:HA	2:C:389:VAL:HG12	2.03	0.41
2:C:160:MET:HA	2:C:163:LYS:HE2	2.03	0.41
2:C:301:THR:HG22	2:C:450:SER:OG	2.21	0.41
2:C:496:PHE:O	2:C:499:ASP:HB2	2.20	0.41
1:A:44:PHE:HE1	1:A:180:TYR:N	2.18	0.41
1:A:174:VAL:HB	1:A:175:GLY:H	1.57	0.41
1:A:349:ILE:HG21	1:A:354:GLN:O	2.20	0.41
1:A:436:GLU:CD	1:A:438:THR:H	2.23	0.41
1:B:381:ASN:N	1:B:381:ASN:OD1	2.54	0.41
1:B:454:ASP:HA	1:B:455:PRO:HD2	1.82	0.41
2:C:288:GLN:HA	2:C:291:ARG:HH11	1.85	0.41
2:C:539:ARG:HH21	2:C:545:PRO:CA	2.34	0.41
1:A:7:LYS:N	1:A:433:ASN:OD1	2.25	0.41
1:A:128:PRO:O	1:A:131:ILE:HB	2.21	0.41
1:A:128:PRO:HD3	1:A:166:PRO:HB2	2.03	0.41
1:A:183:PHE:O	1:A:187:VAL:HG23	2.21	0.41
1:A:281:ILE:O	1:A:284:LEU:HB2	2.21	0.41
1:A:292:ILE:HA	1:A:295:GLN:CG	2.50	0.41
1:A:292:ILE:HD11	1:A:491:MET:HG3	2.02	0.41
1:B:257:LEU:O	1:B:260:LEU:HB3	2.21	0.41
1:B:284:LEU:HA	1:B:287:ASN:CG	2.41	0.41
1:B:313:LEU:HB2	2:C:466:VAL:HG11	1.96	0.41
2:C:13:LYS:NZ	2:C:187:ASP:OD2	2.46	0.41
2:C:105:ASN:ND2	2:C:331:PHE:HA	2.34	0.41
2:C:294:ILE:O	2:C:298:TYR:HB2	2.21	0.41
2:C:357:PHE:CE2	2:C:361:LEU:HD13	2.47	0.41
2:C:361:LEU:N	2:C:361:LEU:HD23	2.35	0.41
1:A:230:ALA:HA	1:A:233:ALA:HB3	2.03	0.41
1:A:257:LEU:O	1:A:260:LEU:HB3	2.21	0.41
1:A:284:LEU:HA	1:A:287:ASN:CG	2.41	0.41
1:A:349:ILE:CD1	1:A:356:SER:HB2	2.51	0.41
1:B:186:LEU:O	1:B:190:VAL:HG13	2.21	0.41
1:B:331:PHE:C	1:B:332:LYS:HG2	2.40	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ARG:HG3	1:B:335:PRO:HD2	2.03	0.41
1:B:423:ALA:HA	1:B:424:VAL:HA	1.48	0.41
1:B:436:GLU:CD	1:B:438:THR:H	2.23	0.41
1:B:506:HIS:CD2	1:B:517:TYR:CE2	3.09	0.41
1:B:629:ALA:HA	1:B:632:ILE:HD13	2.02	0.41
2:C:96:ILE:H	2:C:251:ARG:NH2	2.19	0.41
2:C:335:TRP:O	2:C:338:ASP:HB2	2.20	0.41
1:A:4:LEU:H	1:A:436:GLU:CB	2.34	0.41
1:A:334:ARG:HG3	1:A:335:PRO:HD2	2.03	0.41
1:A:753:SER:HA	1:A:754:ASN:HA	1.86	0.41
1:B:313:LEU:HD11	2:C:466:VAL:H	1.80	0.41
1:B:349:ILE:HG13	1:B:353:GLY:O	2.21	0.41
1:B:361:TYR:CG	1:B:414:VAL:HG21	2.56	0.41
2:C:299:ALA:HA	2:C:302:PHE:HB2	2.02	0.41
2:C:561:CYS:HA	2:C:562:PRO:HD3	1.89	0.41
2:C:565:SER:HA	2:C:568:LEU:HD22	2.03	0.41
1:B:674:LEU:HA	1:B:677:LYS:HZ2	1.85	0.40
2:C:327:ASP:HB3	2:C:331:PHE:CE2	2.55	0.40
2:C:435:PHE:CE1	2:C:439:TYR:HB2	2.56	0.40
1:A:261:TRP:CZ3	1:A:291:PHE:HD1	2.39	0.40
1:A:313:LEU:HA	1:A:314:SER:HA	1.83	0.40
1:A:506:HIS:CD2	1:A:517:TYR:CE2	3.09	0.40
1:A:657:ASP:HA	1:A:660:LYS:HE3	2.03	0.40
1:B:349:ILE:CD1	1:B:356:SER:HB2	2.51	0.40
1:B:368:LYS:HG2	1:B:402:ALA:CA	2.49	0.40
1:B:657:ASP:HA	1:B:660:LYS:HE3	2.03	0.40
1:B:657:ASP:HA	1:B:660:LYS:HG2	2.04	0.40
1:B:720:ARG:HA	1:B:723:ILE:HG22	2.04	0.40
2:C:37:ILE:HG21	2:C:529:GLU:O	2.21	0.40
2:C:74:ARG:HB2	2:C:503:TYR:CE1	2.55	0.40
2:C:298:TYR:OH	2:C:437:ASP:HA	2.21	0.40
2:C:469:HIS:O	2:C:472:PHE:HB3	2.20	0.40
2:C:546:PHE:HE2	2:C:598:LEU:HD13	1.86	0.40
2:C:575:TRP:CD1	2:C:583:TYR:HB2	2.56	0.40
2:C:663:PRO:O	2:C:664:ARG:HB2	2.22	0.40
1:A:27:ASN:OD1	1:A:28:GLN:N	2.54	0.40
1:A:144:GLU:O	1:A:147:HIS:N	2.27	0.40
1:A:386:PHE:HE1	1:A:576:HIS:H	1.68	0.40
1:A:436:GLU:O	1:A:438:THR:N	2.54	0.40
1:A:659:GLU:O	1:A:662:ALA:HB3	2.20	0.40
1:B:230:ALA:HA	1:B:233:ALA:HB3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASN:C	1:B:289:ALA:N	2.75	0.40
1:B:386:PHE:HE1	1:B:576:HIS:H	1.68	0.40
2:C:539:ARG:HG3	2:C:601:TYR:OH	2.21	0.40
2:C:586:TYR:HD2	2:C:587:ARG:HG2	1.85	0.40
1:A:169:ALA:HB3	1:A:575:ILE:HG13	2.03	0.40
1:A:314:SER:HA	1:A:315:SER:C	2.41	0.40
1:A:500:GLU:HG3	1:A:522:VAL:N	2.36	0.40
1:A:521:ASN:HA	1:A:540:ILE:O	2.21	0.40
1:A:720:ARG:HA	1:A:723:ILE:HG22	2.04	0.40
1:B:281:ILE:O	1:B:284:LEU:HB2	2.21	0.40
1:B:313:LEU:CB	2:C:466:VAL:HG21	2.51	0.40
2:C:175:GLU:HA	2:C:352:TRP:CG	2.55	0.40
2:C:332:TRP:HA	2:C:333:PRO:HD2	1.94	0.40
2:C:472:PHE:CZ	2:C:476:LYS:HD3	2.57	0.40
1:A:342:TYR:CD2	1:A:561:LEU:HD22	2.57	0.40
1:A:349:ILE:HG13	1:A:353:GLY:O	2.21	0.40
1:B:128:PRO:HD3	1:B:166:PRO:HB2	2.03	0.40
1:B:173:ARG:HH11	1:B:579:PRO:HG2	1.86	0.40
1:B:313:LEU:HD21	2:C:466:VAL:HG12	1.49	0.40
1:B:328:VAL:O	1:B:331:PHE:HD1	2.05	0.40
1:B:389:VAL:HG22	1:B:390:GLU:N	2.37	0.40
2:C:364:PRO:HB3	2:C:380:GLY:HA3	2.04	0.40
2:C:573:ARG:HG2	2:C:577:ASN:HD21	1.86	0.40
2:C:620:GLU:O	2:C:624:ASP:HB3	2.21	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 PDB entries followed by that with respect to all EM entries.

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	759/761 (100%)	594 (78%)	91 (12%)	74 (10%)	0 10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	759/761 (100%)	594 (78%)	91 (12%)	74 (10%)	0 10
2	C	662/664 (100%)	575 (87%)	61 (9%)	26 (4%)	3 23
All	All	2180/2186 (100%)	1763 (81%)	243 (11%)	174 (8%)	2 12

All (174) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	VAL
1	A	41	THR
1	A	129	THR
1	A	145	LEU
1	A	174	VAL
1	A	222	PRO
1	A	243	ASN
1	A	288	LEU
1	A	292	ILE
1	A	307	ILE
1	A	349	ILE
1	A	503	VAL
1	A	535	ILE
1	A	568	LEU
1	A	581	HIS
1	A	582	GLU
1	A	608	GLU
1	A	684	THR
1	A	738	LEU
1	B	31	VAL
1	B	41	THR
1	B	129	THR
1	B	145	LEU
1	B	174	VAL
1	B	222	PRO
1	B	243	ASN
1	B	288	LEU
1	B	292	ILE
1	B	307	ILE
1	B	332	LYS
1	B	349	ILE
1	B	503	VAL
1	B	535	ILE
1	B	568	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	581	HIS
1	B	582	GLU
1	B	608	GLU
1	B	684	THR
1	B	738	LEU
2	C	22	ILE
2	C	154	PRO
2	C	236	GLY
2	C	528	PRO
2	C	564	TYR
1	A	45	SER
1	A	61	ILE
1	A	110	ILE
1	A	122	ALA
1	A	181	PRO
1	A	241	ARG
1	A	277	ASN
1	A	309	SER
1	A	316	THR
1	A	332	LYS
1	A	355	PRO
1	A	356	SER
1	A	381	ASN
1	A	502	VAL
1	A	522	VAL
1	A	537	GLY
1	A	555	ILE
1	A	558	SER
1	A	559	GLU
1	A	717	GLY
1	A	740	ARG
1	B	45	SER
1	B	61	ILE
1	B	110	ILE
1	B	122	ALA
1	B	181	PRO
1	B	241	ARG
1	B	277	ASN
1	B	309	SER
1	B	316	THR
1	B	355	PRO
1	B	356	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	381	ASN
1	B	502	VAL
1	B	522	VAL
1	B	537	GLY
1	B	555	ILE
1	B	558	SER
1	B	559	GLU
1	B	717	GLY
1	B	740	ARG
2	C	265	PHE
2	C	300	TYR
2	C	327	ASP
2	C	404	LEU
2	C	511	SER
2	C	545	PRO
1	A	34	LEU
1	A	167	ASP
1	A	205	VAL
1	A	214	PHE
1	A	335	PRO
1	A	351	HIS
1	A	384	GLN
1	A	409	ALA
1	A	584	SER
1	A	654	SER
1	A	739	SER
1	B	34	LEU
1	B	167	ASP
1	B	205	VAL
1	B	214	PHE
1	B	335	PRO
1	B	351	HIS
1	B	384	GLN
1	B	409	ALA
1	B	584	SER
1	B	654	SER
1	B	739	SER
2	C	2	ARG
2	C	382	PRO
2	C	529	GLU
2	C	584	ARG
1	A	113	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	178	ALA
1	A	273	ALA
1	A	312	GLU
1	A	375	PRO
1	A	556	GLN
1	B	49	THR
1	B	113	SER
1	B	178	ALA
1	B	273	ALA
1	B	312	GLU
1	B	375	PRO
1	B	556	GLN
2	C	119	VAL
2	C	254	GLU
2	C	464	ALA
1	A	42	ARG
1	A	49	THR
1	A	123	VAL
1	A	328	VAL
1	A	454	ASP
1	A	499	PRO
1	A	515	SER
1	A	624	LEU
1	A	628	VAL
1	B	42	ARG
1	B	123	VAL
1	B	328	VAL
1	B	454	ASP
1	B	499	PRO
1	B	515	SER
1	B	624	LEU
1	B	628	VAL
2	C	217	THR
2	C	484	PRO
2	C	607	ARG
1	A	246	ALA
1	A	329	SER
1	A	471	LEU
1	A	578	TRP
1	B	246	ALA
1	B	329	SER
1	B	471	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	578	TRP
2	C	640	ASN
1	A	336	ILE
1	A	440	GLY
1	B	336	ILE
1	B	440	GLY
2	C	408	ILE
2	C	420	PRO
1	A	428	GLY
1	B	428	GLY
1	A	280	GLY
1	B	280	GLY
2	C	663	PRO
2	C	97	PRO

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 PDB entries followed by that with respect to all EM entries.

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	629/629 (100%)	627 (100%)	2 (0%)	92 95
1	B	629/629 (100%)	627 (100%)	2 (0%)	92 95
2	C	557/557 (100%)	557 (100%)	0	100 100
All	All	1815/1815 (100%)	1811 (100%)	4 (0%)	93 96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	503	VAL
1	A	519	VAL
1	B	503	VAL
1	B	519	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	283	GLN
1	A	337	ASN
1	A	345	GLN
1	A	380	ASN
1	A	485	ASN
1	A	492	HIS
1	A	506	HIS
1	A	670	ASN
1	A	695	GLN
1	B	156	HIS
1	B	243	ASN
1	B	283	GLN
1	B	337	ASN
1	B	345	GLN
1	B	485	ASN
1	B	492	HIS
1	B	506	HIS
1	B	670	ASN
1	B	695	GLN
2	C	15	GLN
2	C	91	ASN
2	C	105	ASN
2	C	158	ASN
2	C	191	GLN
2	C	193	HIS
2	C	304	HIS
2	C	309	ASN
2	C	395	GLN
2	C	417	HIS
2	C	448	GLN
2	C	469	HIS
2	C	481	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

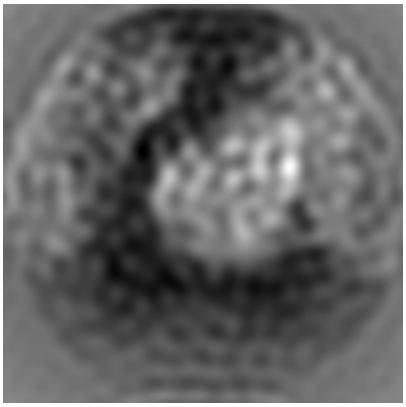
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3187. These allow visual inspection of the internal detail of the map and identification of artifacts.

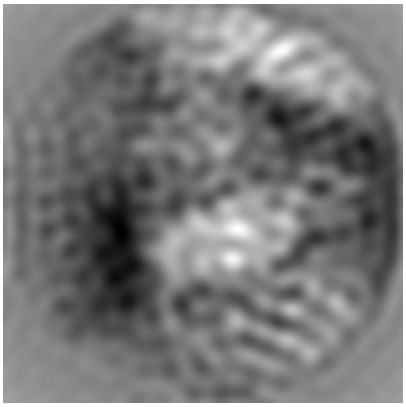
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

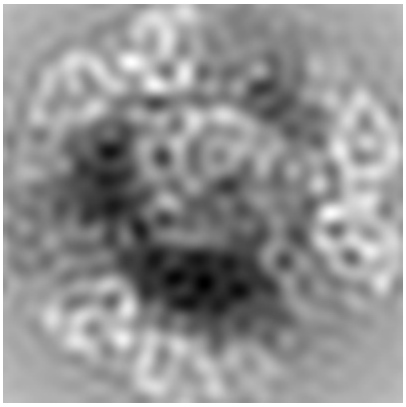
6.1.1 Primary map



X



Y

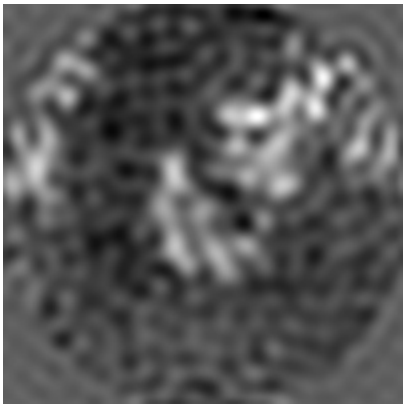


Z

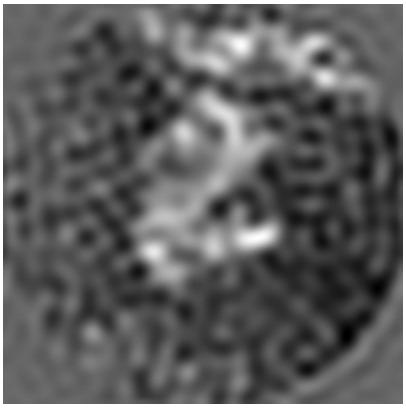
The images above show the map projected in three orthogonal directions.

6.2 Central slices

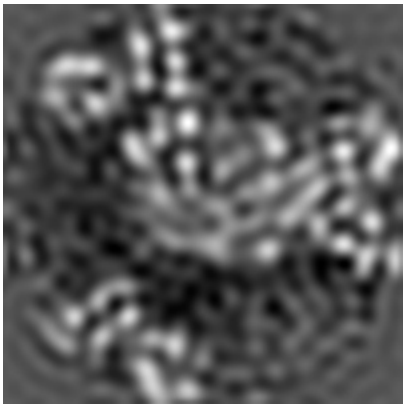
6.2.1 Primary map



X Index: 50



Y Index: 50

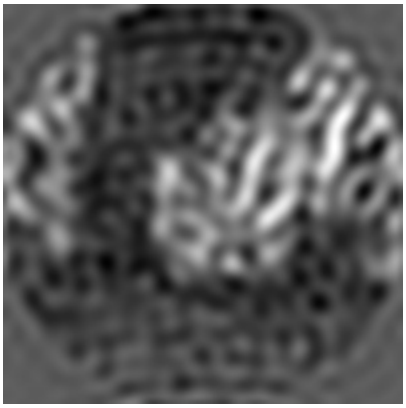


Z Index: 50

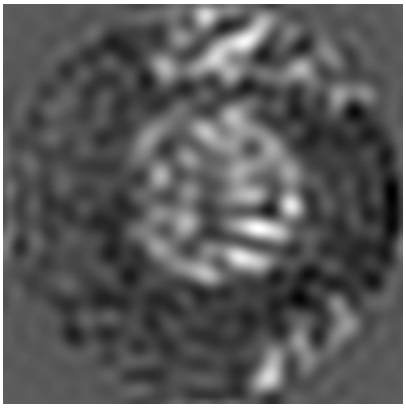
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

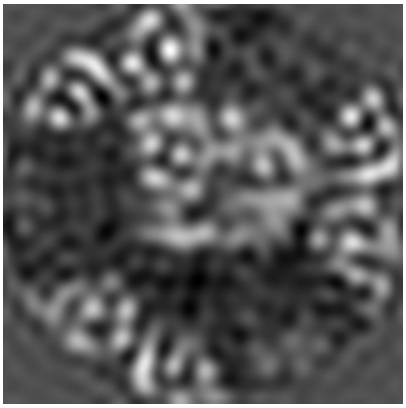
6.3.1 Primary map



X Index: 45



Y Index: 64

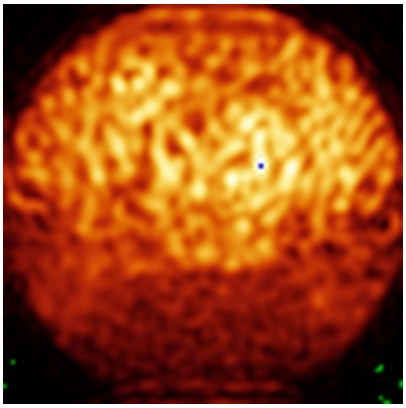


Z Index: 57

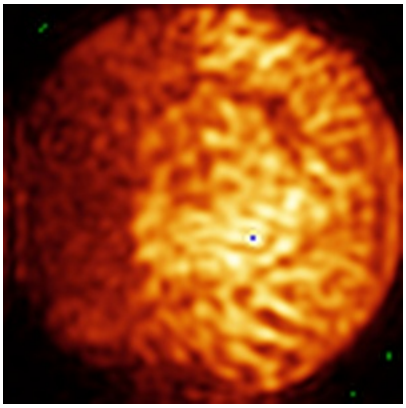
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

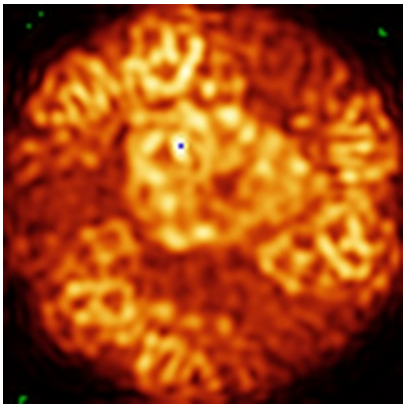
6.4.1 Primary map



X



Y

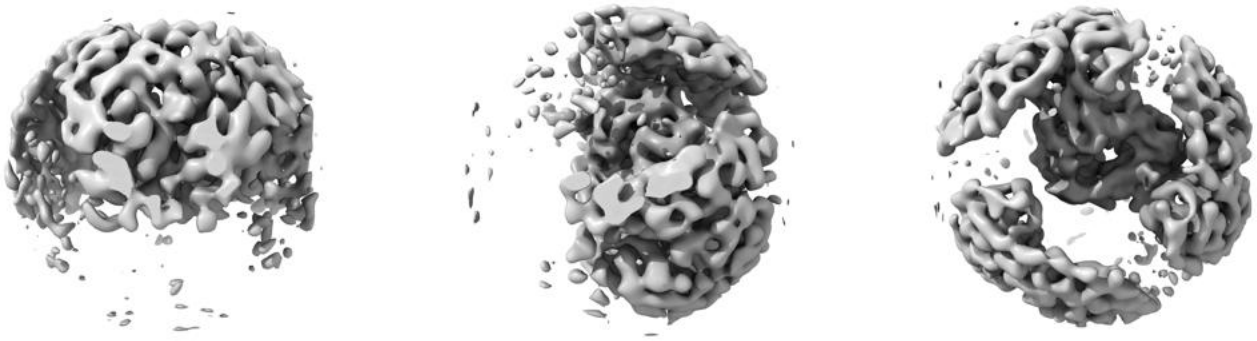


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

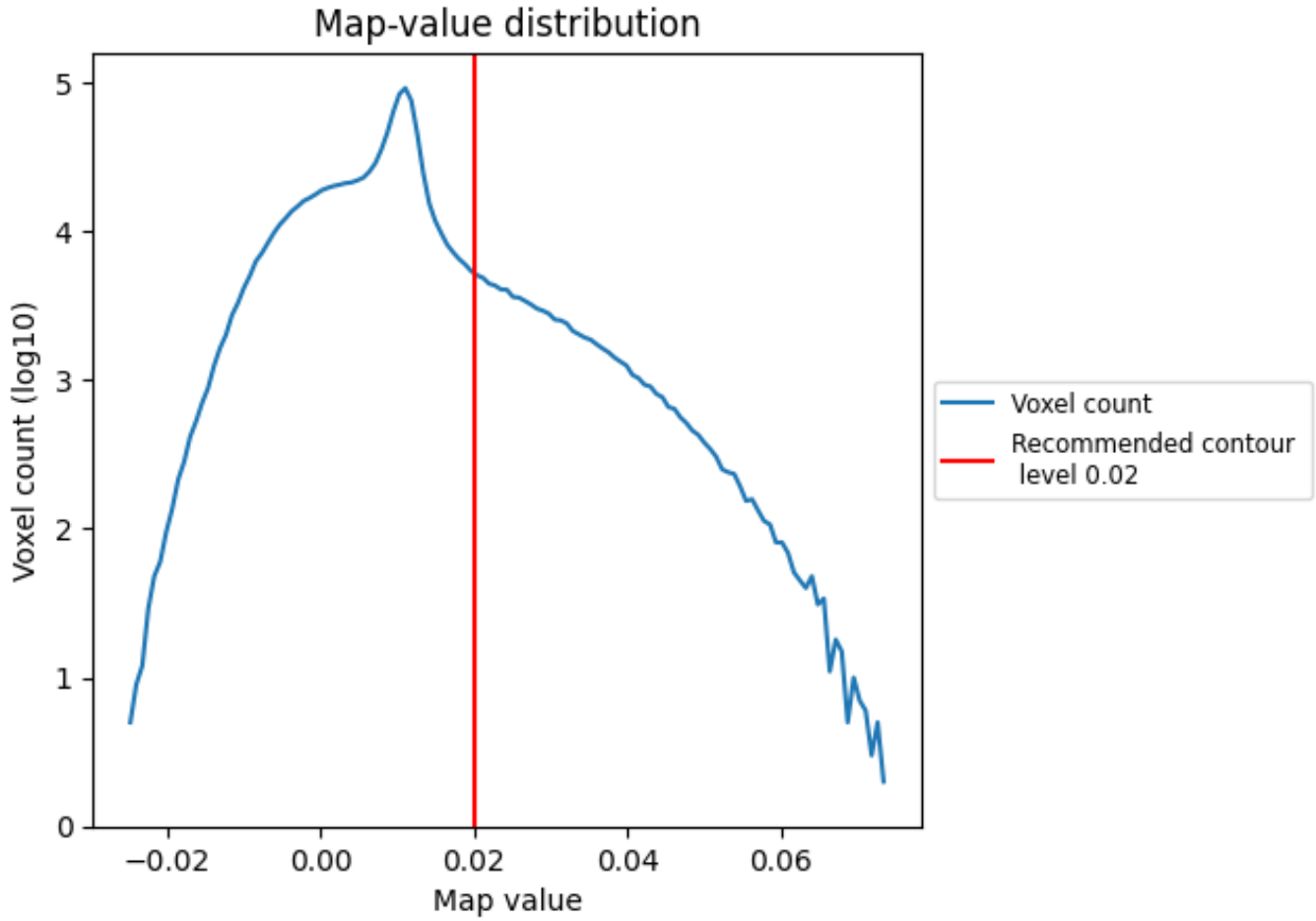
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

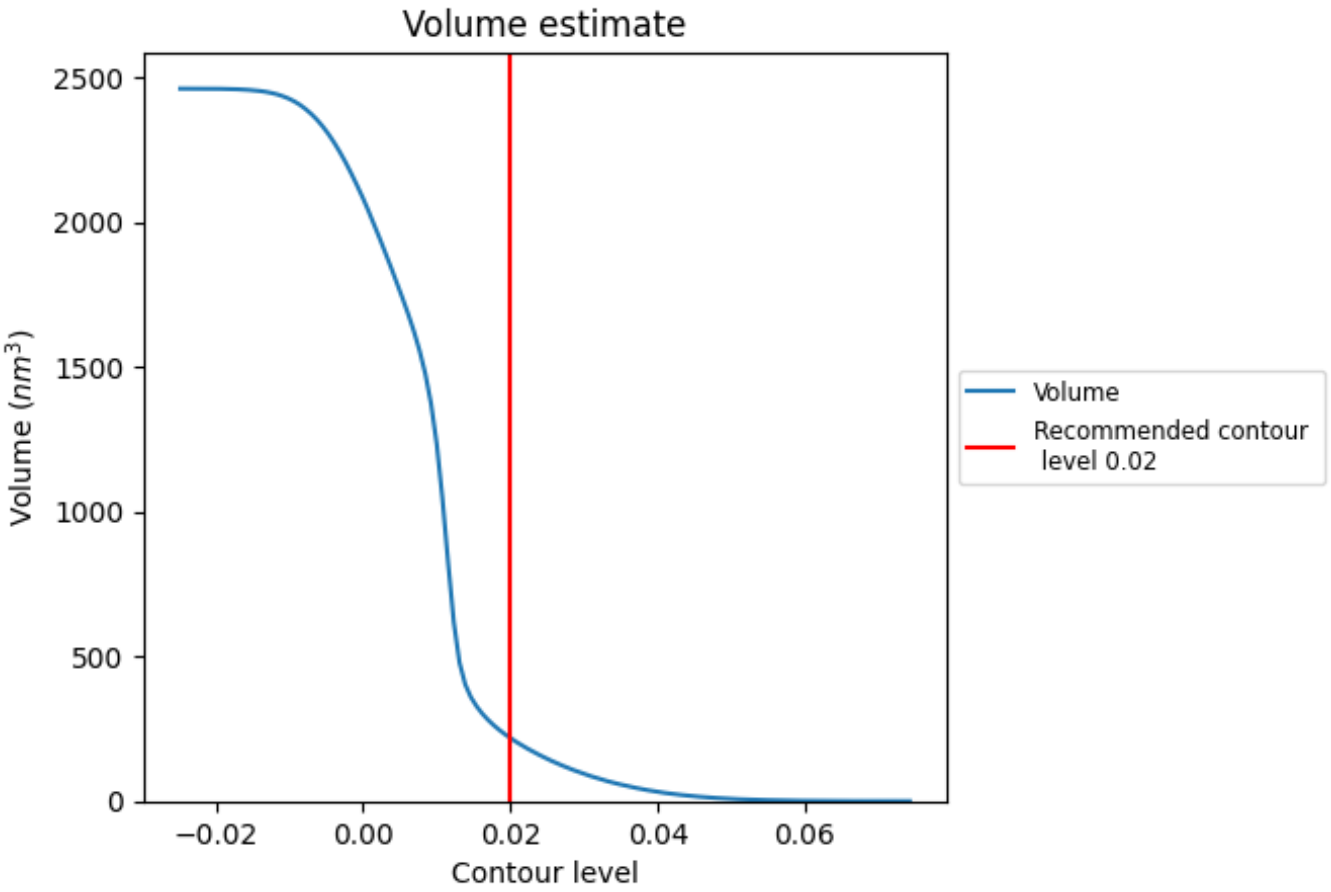
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

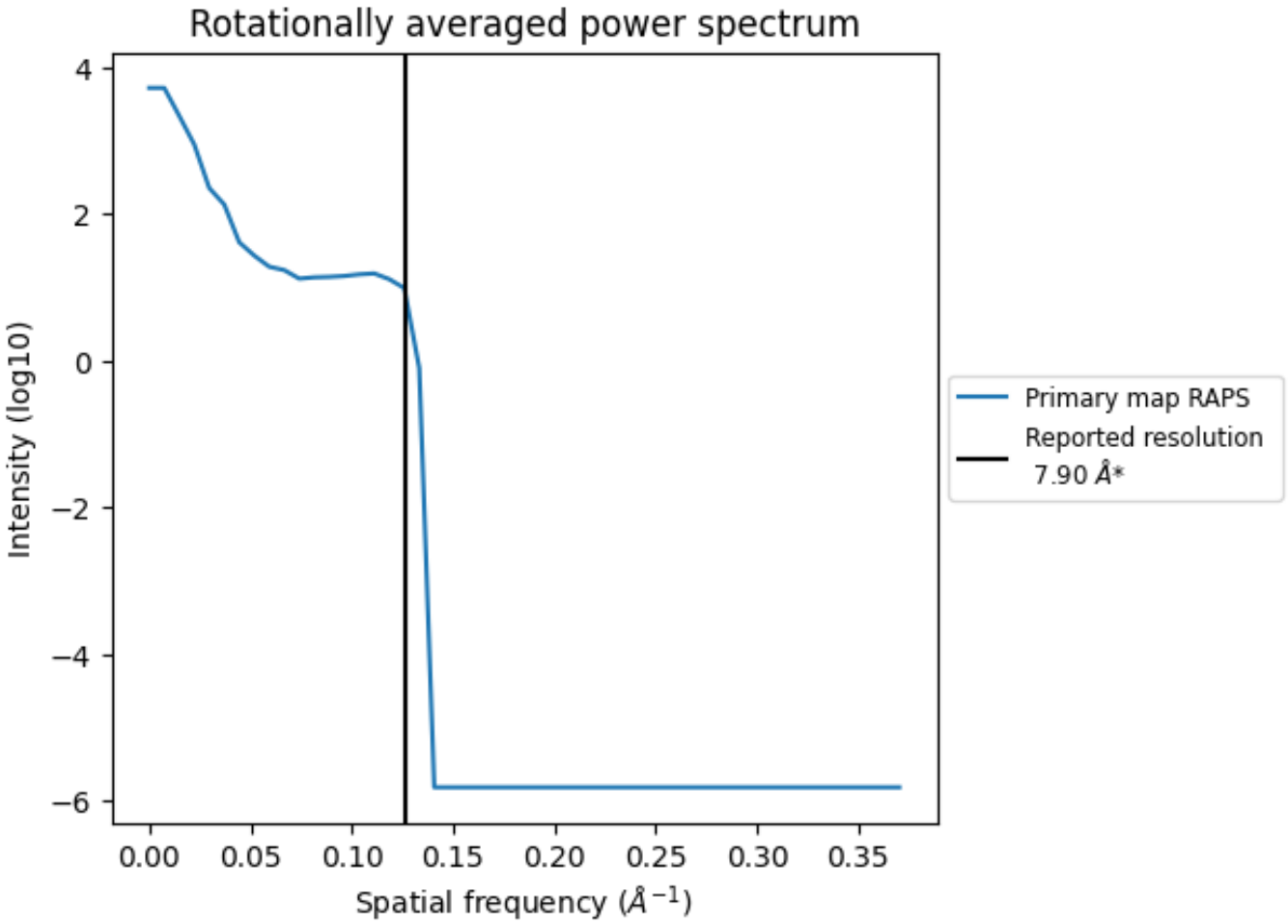
7.2 Volume estimate



The volume at the recommended contour level is 218 nm^3; this corresponds to an approximate mass of 197 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.127 Å^{-1}

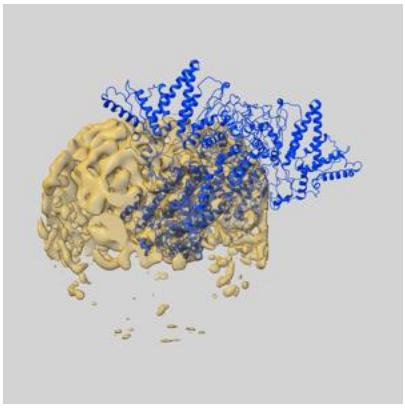
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

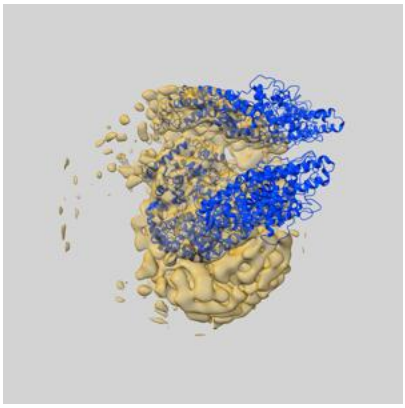
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3187 and PDB model 5FJ7. Per-residue inclusion information can be found in section 3 on page 4.

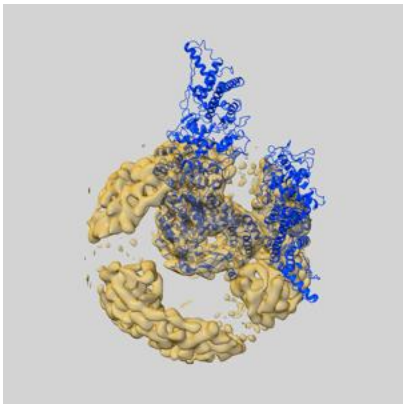
9.1 Map-model overlay



X



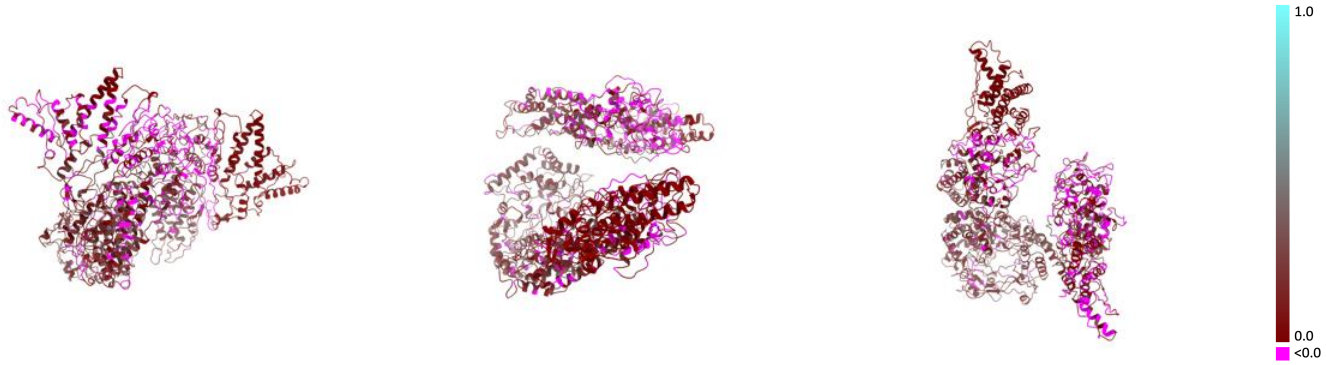
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

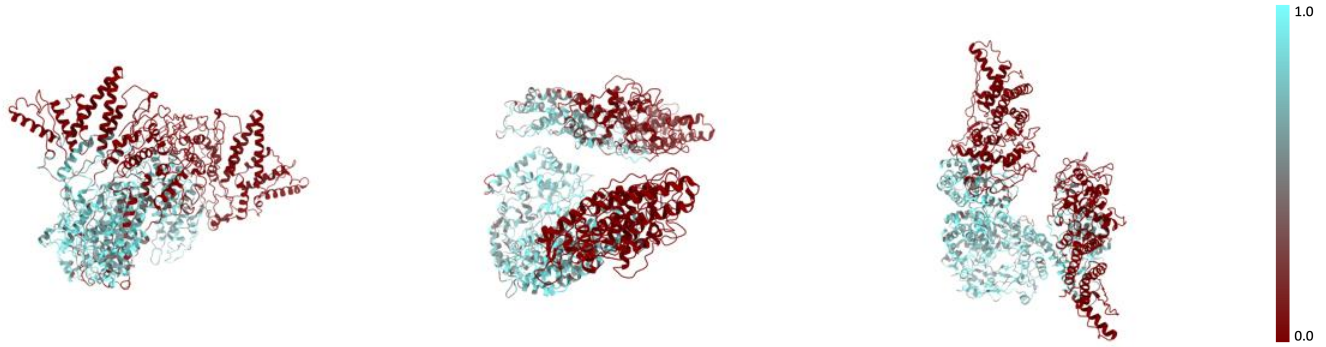
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

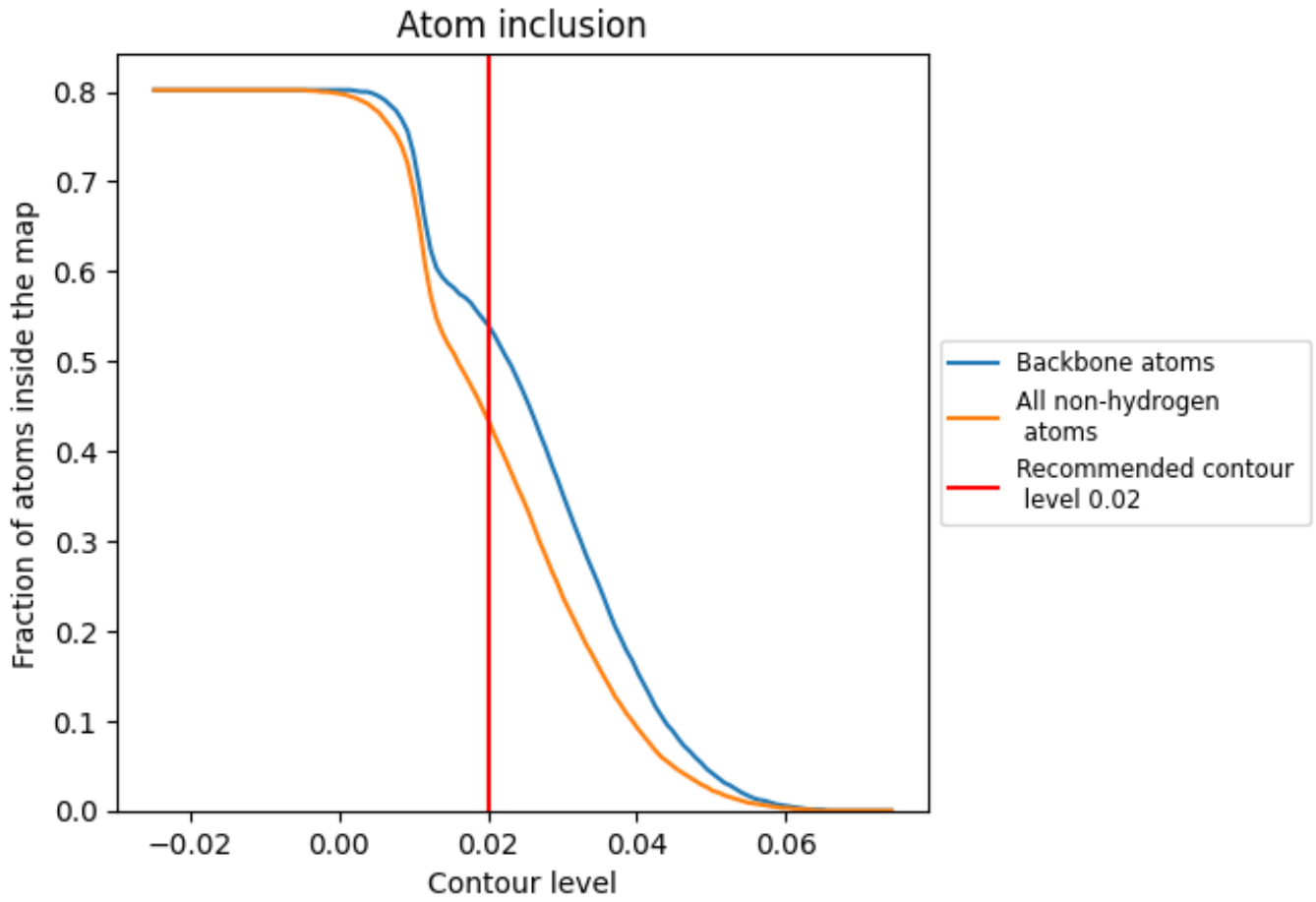
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 54% of all backbone atoms, 44% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4350	0.0980
A	0.2920	0.0640
B	0.2760	0.0630
C	0.7760	0.1760