



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 04:50 AM UTC

PDB ID : 5G5L / pdb_00005g5l
EMDB ID : EMD-3439
Title : RNA polymerase I-Rrn3 complex at 4.8 Å resolution
Authors : Engel, C.; Plitzko, J.; Cramer, P.
Deposited on : 2016-05-26
Resolution : 4.80 Å (reported)
Based on initial model : 4C2M

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:

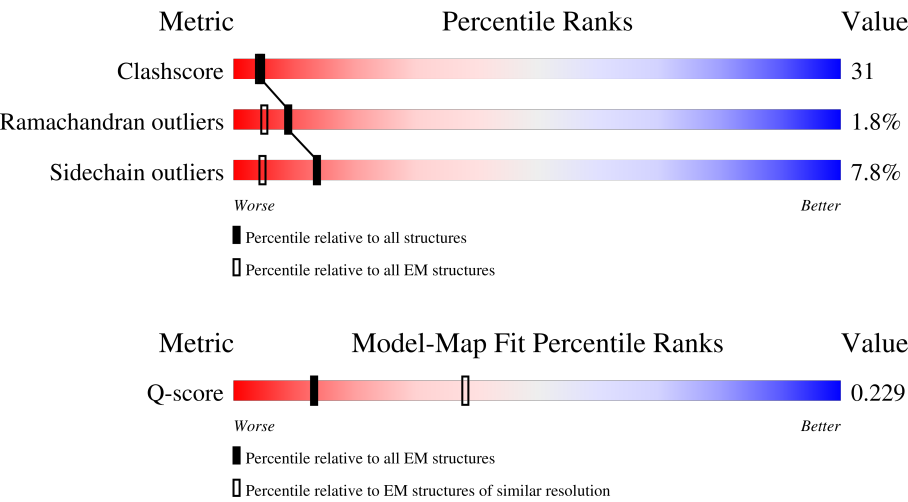
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.80 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.



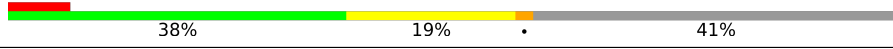
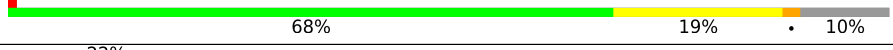
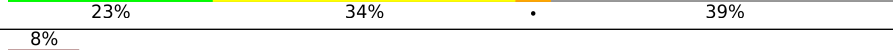
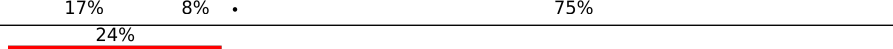
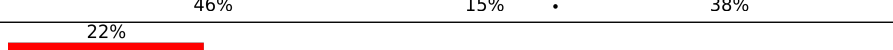
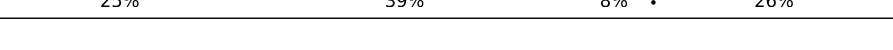
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1575 (4.30 - 5.30)

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 $\leq 5\%$. 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	1664	
2	B	1203	
3	C	335	
4	D	137	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	326	
8	H	146	
9	I	125	
10	J	70	
11	K	142	
12	L	70	
13	M	415	
14	N	233	
15	O	627	

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 37349 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 DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA190.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1480	Total	C	N	O	S	0	0
			11686	7384	2030	2211	61		

- Molecule 2 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA135.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1174	Total	C	N	O	S	0	0
			9327	5899	1635	1743	50		

- Molecule 3 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	305	Total	C	N	O	S	0	0
			2423	1539	416	460	8		

- Molecule 4 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	58	Total	C	N	O	0	0
			459	289	78	92		

- Molecule 5 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	212	Total	C	N	O	S	0	0
			1735	1102	306	316	11		

- Molecule 6 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	100	Total	C	N	O	S	0	0
			823	522	144	154	3		

- Molecule 7 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	193	Total	C	N	O	S	0	0
			1520	982	259	274	5		

- Molecule 8 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	131	Total	C	N	O	S	0	0
			1052	664	176	208	4		

- Molecule 9 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	107	Total	C	N	O	S	0	0
			820	511	138	162	9		

- Molecule 10 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	69	Total	C	N	O	S	0	0
			569	362	101	100	6		

- Molecule 11 is a protein called DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	101	Total	C	N	O	S	0	0
			793	496	130	162	5		

- Molecule 12 is a protein called DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	43	Total	C	N	O	S	0	0
			340	211	66	59	4		

- Molecule 13 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	105	Total	C	N	O	0	0
			833	528	138	167		

- Molecule 14 is a protein called DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34.

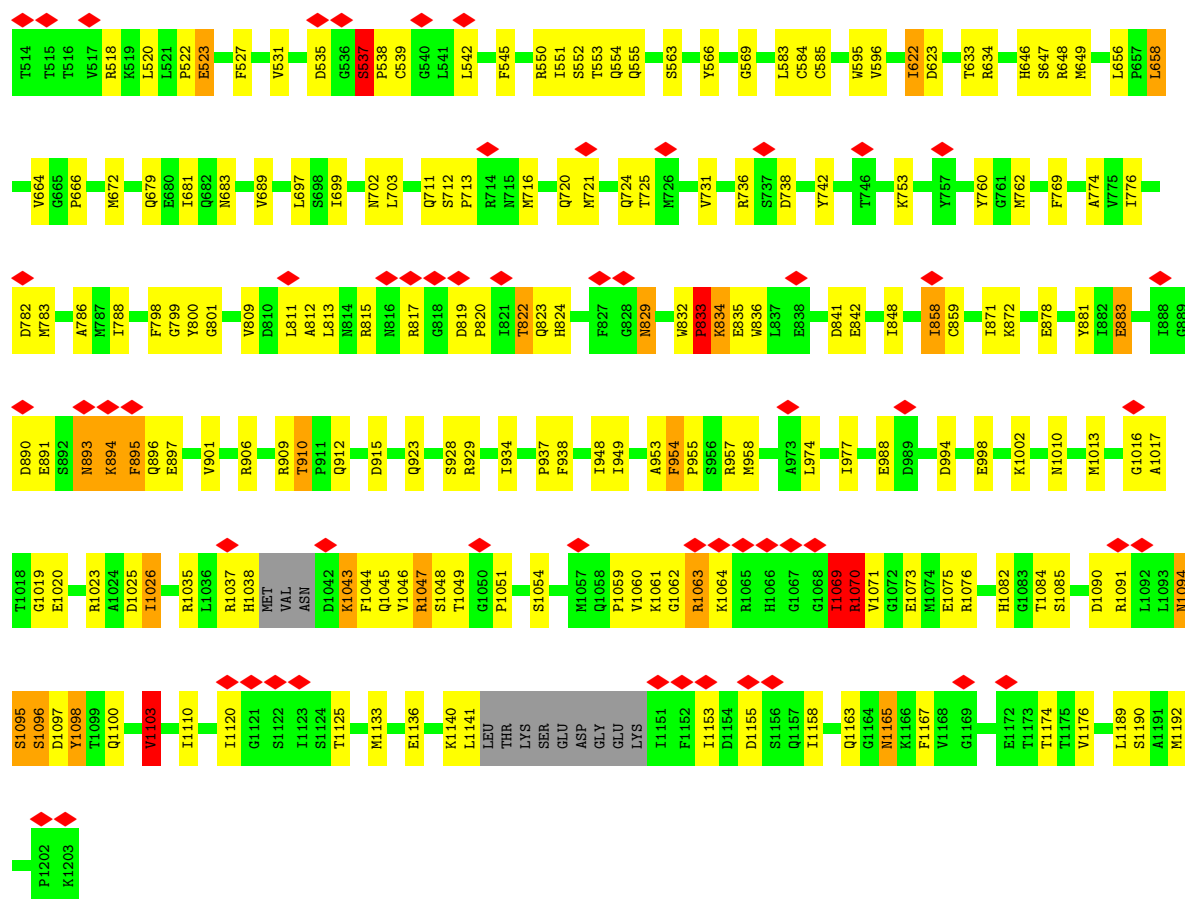
Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	145	Total	C	N	O	S	0	0
			1151	735	188	224	4		

- Molecule 15 is a protein called RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR RRN3.

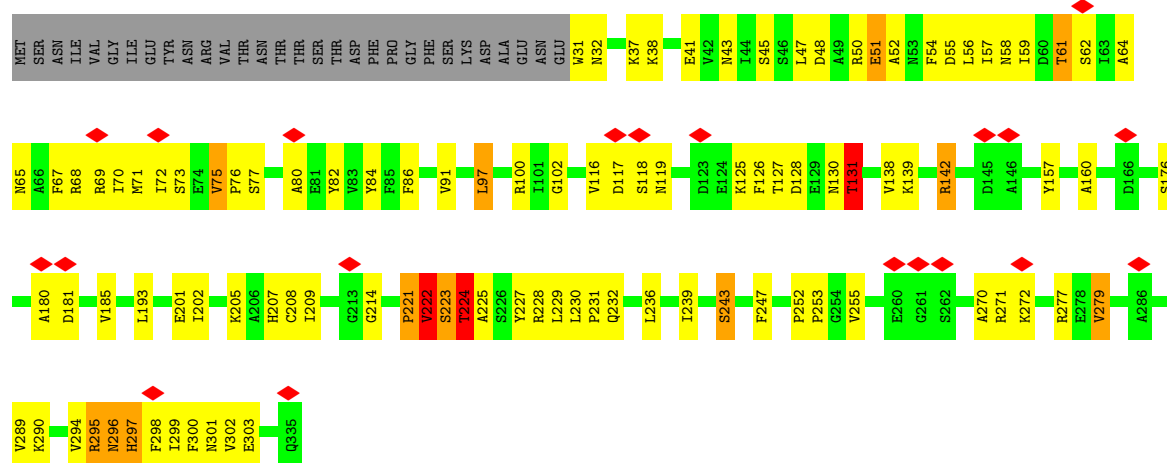
Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	463	Total	C	N	O	S	0	0
			3811	2473	623	694	21		

- Molecule 16 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
16	A	2	Total	Zn	0
			2	2	
16	B	1	Total	Zn	0
			1	1	
16	I	2	Total	Zn	0
			2	2	
16	J	1	Total	Zn	0
			1	1	
16	L	1	Total	Zn	0
			1	1	

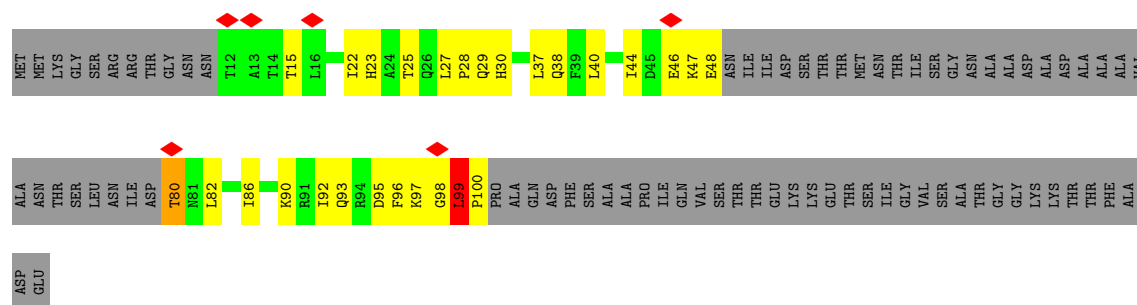


• Molecule 3: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC1

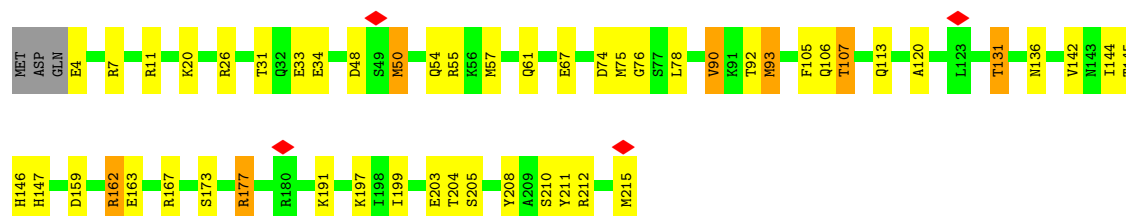
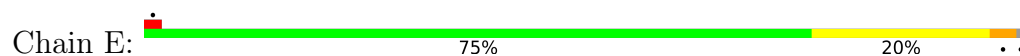


• Molecule 4: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA14

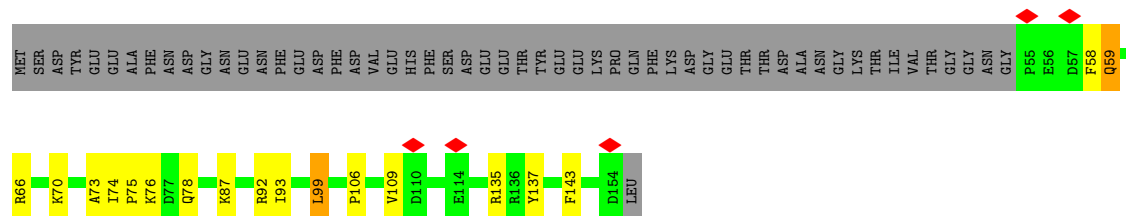




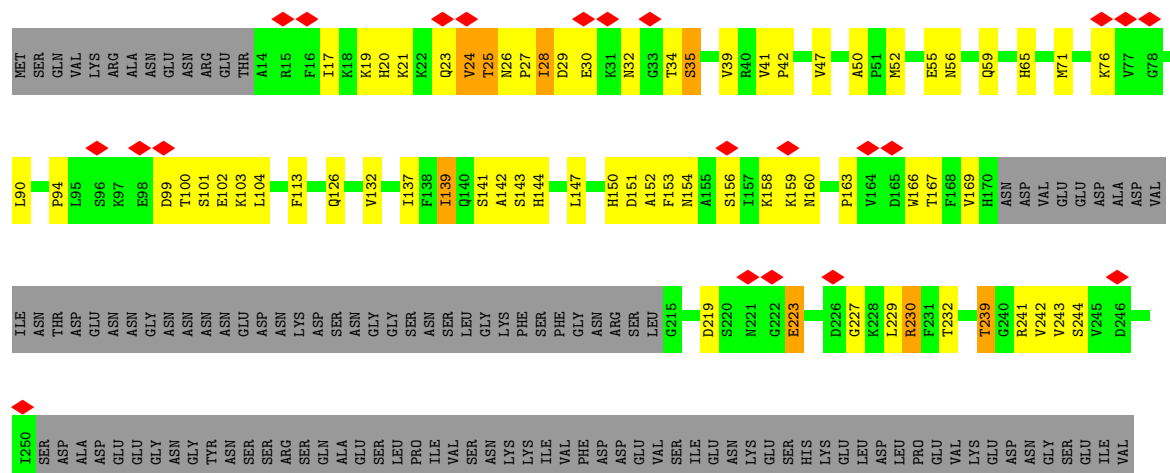
• Molecule 5: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 1



• Molecule 6: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 2



• Molecule 7: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA43



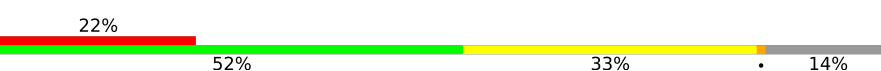
TYR
GLU
GLU
ASN
THR
GLU
SER
SER
ASP
ASP

• Molecule 8: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 3

Chain H:  68% 19% 10%

MET SER N3 D7 D8 I9 Y20 R25 I26 E27 L38 T39 L40 D41 D42 M43 V44 E45 L46 F47 P48 V57 N64 L65 ASP THR PRO ALA ASN ASP SER SER ALA THR ARG S78 A84 Y95 V96 E105 S108 L111 T112 A113 V114 Y115 F118
G119 G120 L121 L122 M123 Y129 Y141 I144 R145 R146

• Molecule 9: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA12

Chain I:  22% 52% 33% 14%

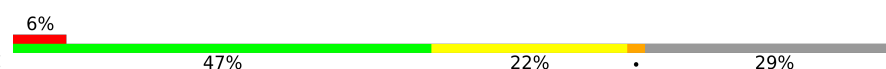
MET S2 V3 V4 G5 F9 C10 L11 G14 D15 P20 N21 A22 V23 L24 G25 S26 Q32 K39 S40 Q41 L45 V48 T49 D53 S59 L60 K63 V66 V67 K68 T69 S70 L71 K72 K73 N74 GLU LEU LYS ASP GLY ALA T81 I82 K83 E84 K85 C86
P87 Q88 C89 G90 N91 E92 E93 H94 H95 Y96 H97 T98 LEU GLN LEU SER ARG ALA GLN THR V110 F111 Y112 T115 S116 Y119 K120 F121 R122 T123 N124 M125

• Molecule 10: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 5

Chain J:  76% 19% 5%

M1 I2 V3 R6 S9 C10 G11 V14 E27 T34 A35 L36 R43 Y44 C45 C46 R47 R48 T57 N64 R69 ASP

• Molecule 11: DNA-DIRECTED RNA POLYMERASES I AND III SUBUNIT RPAC2

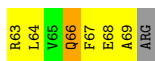
Chain K:  6% 47% 22% 29%

MET THR ASP ILE GLN LYS THR THR VAL THR PRO GLN PRO LYS HIS ILE GLN GLU GLU GLN GLN ASP VAL ASP MET THR GLY ASP ASP GLN GLU GLU GLU P42 P43 R44 E45 K48 L49 L50 T51 Q52 A53 T54 S55 E56 D57 S62 F63 Q64
I65 V66 E67 E68 T71 G72 G73 N74 Y78 Y79 I80 M81 K82 N83 I93 P94 H95 P96 N99 I103 R104 I105 E110 Q118 D123 V130 S133 K134 F135 I139 K140 S141 M142

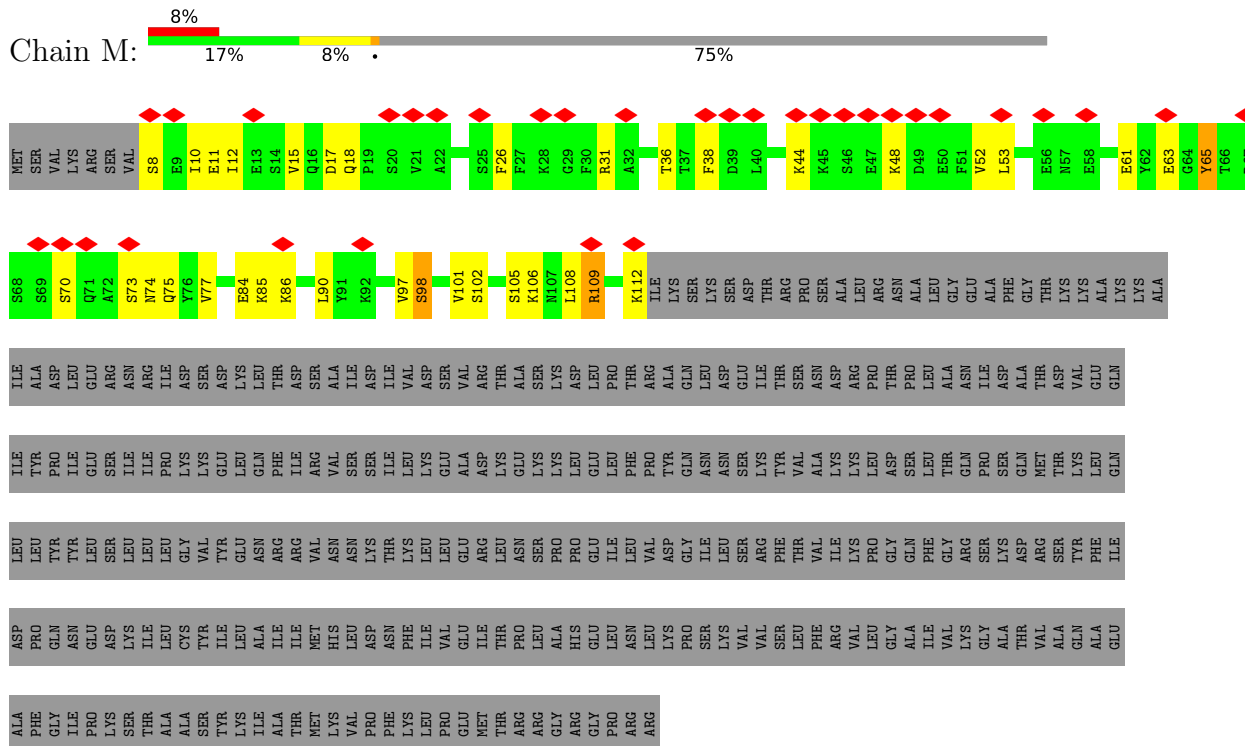
• Molecule 12: DNA-DIRECTED RNA POLYMERASES I, II, AND III SUBUNIT RPABC 4

Chain L:  6% 23% 34% 39%

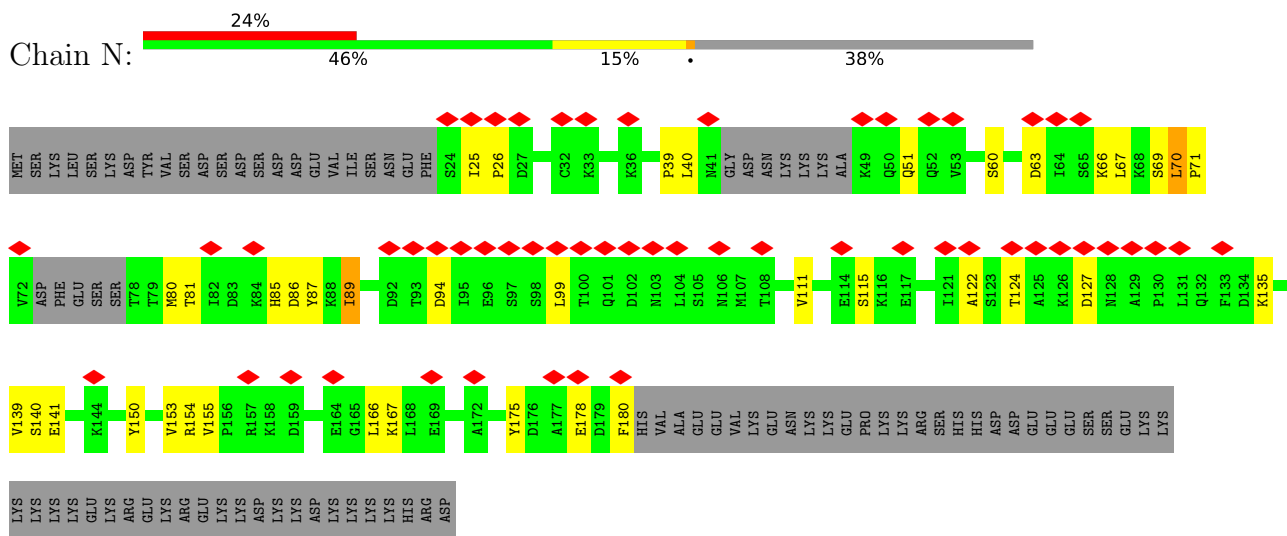
MET SER ARG GLU GLY PHE GLN ILE PRO THR ASN LEU ASP ALA ALA ALA GLY THR SER GLN ARG THR ALA THR L27 K28 Y29 I30 C31 A32 E33 C34 L38 S39 L40 S41 R42 T43 D44 A45 V46 R47 K49 D50 C51 G52 H53 R54 I55 I56 L57 K58 A59 R60 T61 K62



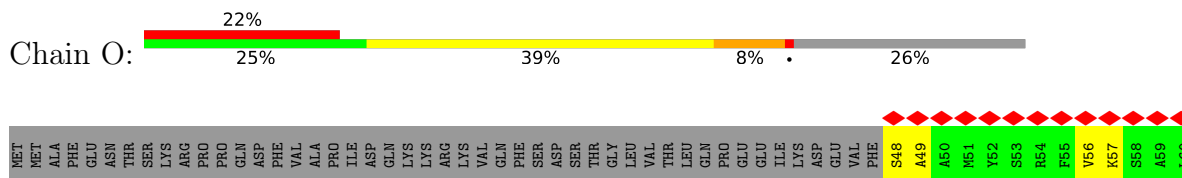
● Molecule 13: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA49



● Molecule 14: DNA-DIRECTED RNA POLYMERASE I SUBUNIT RPA34



● Molecule 15: RNA POLYMERASE I-SPECIFIC TRANSCRIPTION INITIATION FACTOR
RRN3





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	63445	Depositor
Resolution determination method	Not provided	
CTF correction method	RELION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	37037	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.079	Depositor
Minimum map value	-0.034	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size ($\text{\AA}$)	324.0, 324.0, 324.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	1/11900 (0.0%)	0.95	39/16073 (0.2%)
2	B	0.62	0/9533	0.95	32/12884 (0.2%)
3	C	0.54	0/2475	0.94	10/3354 (0.3%)
4	D	0.51	0/465	0.82	0/630
5	E	0.49	0/1771	0.88	4/2383 (0.2%)
6	F	0.56	0/838	0.85	0/1129
7	G	0.51	0/1558	0.90	4/2120 (0.2%)
8	H	0.52	0/1070	0.88	0/1449
9	I	0.51	0/831	0.85	0/1117
10	J	0.60	0/578	0.98	6/775 (0.8%)
11	K	0.54	0/804	0.93	6/1083 (0.6%)
12	L	0.44	0/342	0.84	2/454 (0.4%)
13	M	0.49	0/849	0.88	0/1140
14	N	0.47	0/1172	0.87	1/1580 (0.1%)
15	O	0.51	3/3897 (0.1%)	0.95	17/5268 (0.3%)
All	All	0.58	4/38083 (0.0%)	0.93	121/51439 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
15	O	0	5
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	198	PHE	C-N	-9.82	1.20	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1622	LEU	C-N	-6.24	1.25	1.33
15	O	212	THR	CA-CB	5.50	1.62	1.53
15	O	128	LEU	C-N	5.03	1.39	1.33

All (121) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	460	GLU	N-CA-C	-17.73	90.91	112.89
15	O	598	PHE	N-CA-C	17.11	129.62	111.14
1	A	413	LEU	N-CA-C	-10.83	99.33	112.54
7	G	35	SER	CA-C-N	-8.63	111.30	122.77
7	G	35	SER	C-N-CA	-8.63	111.30	122.77
1	A	956	ARG	CA-C-O	8.62	122.94	117.94
1	A	1622	LEU	O-C-N	8.59	131.94	122.15
1	A	666	VAL	CB-CA-C	-8.42	102.40	110.65
2	B	211	ARG	N-CA-C	8.38	123.37	109.46
7	G	35	SER	O-C-N	7.89	132.17	123.10
2	B	537	SER	CA-C-N	-7.79	111.96	121.00
2	B	537	SER	C-N-CA	-7.79	111.96	121.00
1	A	1344	ILE	N-CA-C	7.78	117.85	110.53
15	O	599	LEU	N-CA-C	7.78	121.00	109.24
2	B	893	ASN	N-CA-C	7.43	120.31	111.02
3	C	279	VAL	CB-CA-C	-7.41	102.40	111.88
15	O	457	ARG	CA-C-N	-6.78	111.22	120.44
15	O	457	ARG	C-N-CA	-6.78	111.22	120.44
15	O	460	GLU	CA-C-N	-6.76	111.65	121.65
15	O	460	GLU	C-N-CA	-6.76	111.65	121.65
15	O	459	GLU	N-CA-C	-6.69	103.19	111.75
2	B	219	ARG	CA-C-N	6.58	128.06	119.84
2	B	219	ARG	C-N-CA	6.58	128.06	119.84
2	B	894	LYS	CB-CA-C	-6.54	108.33	117.23
1	A	1123	VAL	CB-CA-C	-6.54	103.48	112.04
2	B	1103	VAL	CB-CA-C	-6.52	100.78	110.82
2	B	1023	ARG	NE-CZ-NH2	-6.50	113.35	119.20
3	C	51	GLU	N-CA-C	6.44	119.68	109.50
2	B	261	ARG	CD-NE-CZ	6.34	133.28	124.40
1	A	397	ARG	CD-NE-CZ	6.33	133.25	124.40
1	A	412	SER	N-CA-C	6.30	118.75	109.24
10	J	64	ASN	CA-C-N	6.29	125.99	119.82
10	J	64	ASN	C-N-CA	6.29	125.99	119.82
2	B	622	ILE	CB-CA-C	-6.26	102.92	112.05
5	E	203	GLU	N-CA-C	-6.25	104.57	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	ARG	NE-CZ-NH2	-6.19	113.63	119.20
1	A	201	ARG	N-CA-C	6.08	120.76	113.23
1	A	329	ARG	NE-CZ-NH2	-6.07	113.74	119.20
1	A	59	ARG	CD-NE-CZ	6.04	132.86	124.40
3	C	75	VAL	CA-C-N	-6.00	113.58	119.76
3	C	75	VAL	C-N-CA	-6.00	113.58	119.76
2	B	448	ARG	NE-CZ-NH2	-5.99	113.81	119.20
2	B	452	ARG	CD-NE-CZ	5.98	132.77	124.40
15	O	436	ARG	N-CA-C	-5.95	104.79	111.28
2	B	832	TRP	CA-C-N	5.90	127.22	119.84
2	B	832	TRP	C-N-CA	5.90	127.22	119.84
2	B	72	VAL	N-CA-C	5.90	117.25	108.46
2	B	429	ARG	NE-CZ-NH2	-5.90	113.89	119.20
1	A	258	GLU	N-CA-C	5.88	118.17	111.11
15	O	128	LEU	CA-C-N	-5.88	114.32	120.38
15	O	128	LEU	C-N-CA	-5.88	114.32	120.38
2	B	658	LEU	N-CA-C	-5.88	100.96	109.31
1	A	59	ARG	NE-CZ-NH2	-5.88	113.91	119.20
2	B	448	ARG	CD-NE-CZ	5.80	132.52	124.40
1	A	956	ARG	CB-CA-C	-5.80	108.72	117.07
1	A	329	ARG	CD-NE-CZ	5.76	132.46	124.40
1	A	507	TYR	CA-C-N	-5.74	114.03	119.76
1	A	507	TYR	C-N-CA	-5.74	114.03	119.76
5	E	167	ARG	NE-CZ-NH2	-5.72	114.05	119.20
3	C	223	SER	N-CA-C	-5.68	104.95	112.34
1	A	416	ARG	NE-CZ-NH2	-5.67	114.09	119.20
11	K	44	ARG	CD-NE-CZ	5.67	132.34	124.40
11	K	95	HIS	CA-C-N	5.67	126.93	119.84
11	K	95	HIS	C-N-CA	5.67	126.93	119.84
1	A	659	THR	CA-C-N	-5.63	113.95	119.64
1	A	659	THR	C-N-CA	-5.63	113.95	119.64
2	B	634	ARG	CD-NE-CZ	5.63	132.28	124.40
1	A	1203	ASN	N-CA-C	5.61	117.60	109.07
11	K	44	ARG	NE-CZ-NH2	-5.61	114.15	119.20
1	A	416	ARG	CD-NE-CZ	5.61	132.25	124.40
15	O	369	LYS	N-CA-C	-5.60	105.08	111.07
1	A	422	ARG	CD-NE-CZ	5.60	132.23	124.40
1	A	827	THR	N-CA-C	5.57	115.46	108.45
2	B	634	ARG	NE-CZ-NH2	-5.56	114.19	119.20
2	B	429	ARG	CD-NE-CZ	5.56	132.18	124.40
15	O	458	GLU	O-C-N	5.56	128.09	122.09
1	A	498	PRO	CA-C-N	5.53	125.36	119.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	498	PRO	C-N-CA	5.53	125.36	119.28
1	A	549	MET	N-CA-C	5.52	119.10	110.32
15	O	198	PHE	O-C-N	-5.51	115.63	121.30
2	B	261	ARG	NE-CZ-NH2	-5.50	114.25	119.20
10	J	3	VAL	CA-C-N	-5.50	114.29	119.85
10	J	3	VAL	C-N-CA	-5.50	114.29	119.85
15	O	540	CYS	N-CA-C	5.50	122.52	110.80
2	B	910	THR	CA-C-N	-5.48	114.28	119.76
2	B	910	THR	C-N-CA	-5.48	114.28	119.76
12	L	28	LYS	N-CA-C	5.46	117.99	111.71
12	L	52	GLY	N-CA-C	-5.44	107.76	115.43
3	C	142	ARG	CD-NE-CZ	5.43	132.00	124.40
15	O	457	ARG	N-CA-C	5.41	122.32	110.80
1	A	397	ARG	NE-CZ-NH1	5.41	126.91	121.50
1	A	397	ARG	NE-CZ-NH2	-5.38	114.35	119.20
1	A	245	LYS	N-CA-C	5.37	118.03	109.65
5	E	167	ARG	CD-NE-CZ	5.36	131.90	124.40
14	N	127	ASP	N-CA-C	-5.34	106.25	114.16
15	O	456	GLU	N-CA-C	-5.32	107.33	112.97
1	A	1482	LYS	N-CA-C	5.28	117.89	110.23
1	A	329	ARG	NE-CZ-NH1	5.27	126.77	121.50
7	G	219	ASP	N-CA-C	5.27	116.79	109.31
3	C	185	VAL	CA-C-N	-5.23	114.53	119.76
3	C	185	VAL	C-N-CA	-5.23	114.53	119.76
1	A	59	ARG	NE-CZ-NH1	5.21	126.70	121.50
1	A	1543	SER	CA-C-N	5.20	127.68	120.29
1	A	1543	SER	C-N-CA	5.20	127.68	120.29
3	C	142	ARG	NE-CZ-NH2	-5.18	114.54	119.20
2	B	88	SER	N-CA-C	5.15	118.20	109.76
1	A	422	ARG	NE-CZ-NH2	-5.14	114.57	119.20
10	J	9	SER	CA-C-N	5.14	127.44	120.44
10	J	9	SER	C-N-CA	5.14	127.44	120.44
2	B	314	LYS	N-CA-C	-5.11	103.74	110.43
1	A	342	ARG	CD-NE-CZ	5.10	131.54	124.40
2	B	1054	SER	N-CA-C	5.08	117.48	111.33
1	A	342	ARG	NE-CZ-NH2	-5.08	114.62	119.20
1	A	1524	VAL	N-CA-C	5.07	115.41	108.12
5	E	167	ARG	NE-CZ-NH1	5.06	126.56	121.50
2	B	1110	ILE	CB-CA-C	-5.06	105.48	111.65
11	K	83	ASN	CA-C-N	5.04	124.70	119.56
11	K	83	ASN	C-N-CA	5.04	124.70	119.56
3	C	131	THR	N-CA-C	5.03	117.95	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	134	ARG	N-CA-C	5.02	117.02	109.23
2	B	511	GLN	N-CA-C	-5.02	107.21	113.38

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1343	ASP	Peptide
15	O	374	PRO	Peptide
15	O	375	THR	Peptide
15	O	411	ASN	Peptide
15	O	598	PHE	Peptide
15	O	599	LEU	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	11686	0	11770	706	0
2	B	9327	0	9214	496	0
3	C	2423	0	2409	290	0
4	D	459	0	461	104	0
5	E	1735	0	1764	42	0
6	F	823	0	840	64	0
7	G	1520	0	1529	167	0
8	H	1052	0	1021	18	0
9	I	820	0	805	71	0
10	J	569	0	585	6	0
11	K	793	0	790	42	0
12	L	340	0	361	46	0
13	M	833	0	826	32	0
14	N	1151	0	1169	45	0
15	O	3811	0	3800	773	0
16	A	2	0	0	0	0
16	B	1	0	0	0	0
16	I	2	0	0	0	0
16	J	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	L	1	0	0	0	0
All	All	37349	0	37344	2323	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 31.

All (2323) 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)
15:O:162:PHE:CB	15:O:214:ASN:CB	1.76	1.62
3:C:75:VAL:HG11	3:C:221:PRO:CG	1.33	1.52
1:A:478:TYR:HA	2:B:1048:SER:CA	1.42	1.50
1:A:436:ALA:CB	1:A:443:ALA:HB2	1.43	1.46
1:A:83:VAL:HG21	1:A:427:PHE:CZ	1.50	1.46
15:O:458:GLU:HA	15:O:461:VAL:CG2	1.26	1.44
15:O:458:GLU:CA	15:O:461:VAL:HG23	1.28	1.41
15:O:454:VAL:CB	15:O:514:PHE:HE2	1.30	1.41
1:A:478:TYR:CA	2:B:1048:SER:HA	1.53	1.38
1:A:436:ALA:HB2	1:A:443:ALA:CB	1.54	1.37
2:B:207:ILE:HG13	2:B:503:VAL:CG2	1.54	1.37
15:O:408:PHE:CZ	15:O:446:LEU:CD1	2.06	1.37
15:O:408:PHE:CZ	15:O:446:LEU:HD11	1.59	1.37
15:O:471:LYS:HB2	15:O:585:PHE:CE1	1.58	1.37
1:A:83:VAL:HG11	1:A:427:PHE:CE2	1.59	1.36
15:O:138:TYR:CE2	15:O:142:ILE:HD11	1.56	1.36
3:C:31:TRP:CB	11:K:82:LYS:HD2	1.54	1.35
15:O:454:VAL:HB	15:O:514:PHE:CE2	1.61	1.35
1:A:437:PHE:CZ	1:A:456:VAL:HG23	1.62	1.35
7:G:242:VAL:HG11	15:O:185:SER:OG	1.22	1.35
3:C:55:ASP:CG	3:C:299:ILE:HG12	1.51	1.34
1:A:437:PHE:CZ	1:A:456:VAL:CG2	2.11	1.34
2:B:42:VAL:CG1	2:B:46:ILE:HD11	1.57	1.33
3:C:75:VAL:HG11	3:C:221:PRO:CD	1.59	1.32
3:C:75:VAL:CG1	3:C:221:PRO:CG	2.07	1.31
3:C:54:PHE:CE2	3:C:300:PHE:HB2	1.66	1.30
1:A:477:ASN:OD1	2:B:1059:PRO:HG3	1.13	1.29
3:C:84:TYR:HE2	12:L:66:GLN:OE1	1.16	1.29
15:O:198:PHE:CD2	15:O:232:LEU:HG	1.65	1.29
4:D:30:HIS:NE2	7:G:26:ASN:OD1	1.66	1.27
15:O:432:LYS:HG2	15:O:608:GLU:O	1.23	1.27
4:D:25:THR:CG2	6:F:59:GLN:HE21	1.45	1.27

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:VAL:CG1	3:C:221:PRO:CD	2.14	1.26
3:C:84:TYR:CE2	12:L:66:GLN:OE1	1.87	1.26
1:A:478:TYR:N	2:B:1048:SER:O	1.66	1.25
1:A:1603:MET:HE2	1:A:1615:TYR:CD2	1.71	1.25
7:G:242:VAL:CG1	15:O:185:SER:OG	1.81	1.24
1:A:1008:ASP:OD2	1:A:1202:LEU:HD13	1.37	1.24
3:C:54:PHE:CE2	3:C:300:PHE:CB	2.20	1.24
15:O:431:ALA:CB	15:O:434:LEU:HD11	1.63	1.24
1:A:1348:VAL:HB	2:B:268:GLU:O	1.35	1.24
15:O:237:ILE:CB	15:O:381:ILE:HD12	1.68	1.24
7:G:158:LYS:CG	15:O:105:ASN:OD1	1.86	1.23
15:O:432:LYS:HB3	15:O:609:TYR:CA	1.69	1.23
1:A:756:LYS:HD3	9:I:85:LYS:NZ	1.51	1.23
2:B:769:PHE:CE1	2:B:798:PHE:CE1	2.26	1.22
4:D:30:HIS:CE1	7:G:26:ASN:OD1	1.92	1.22
15:O:432:LYS:CG	15:O:608:GLU:O	1.88	1.22
2:B:769:PHE:CE1	2:B:798:PHE:HE1	1.56	1.22
1:A:1605:THR:O	1:A:1606:SER:O	1.57	1.22
3:C:230:LEU:CD2	3:C:294:VAL:HG21	1.67	1.22
3:C:54:PHE:CZ	3:C:300:PHE:HB3	1.73	1.22
15:O:454:VAL:CB	15:O:514:PHE:CE2	2.17	1.22
3:C:131:THR:HG23	3:C:209:ILE:CG2	1.69	1.21
15:O:352:LEU:HD23	15:O:358:VAL:CG2	1.69	1.21
1:A:1011:VAL:HG11	1:A:1201:THR:C	1.63	1.21
15:O:373:LEU:HD11	15:O:416:LYS:CG	1.69	1.21
15:O:352:LEU:CD2	15:O:358:VAL:HG22	1.71	1.20
3:C:31:TRP:CD1	11:K:82:LYS:NZ	2.10	1.20
15:O:432:LYS:CB	15:O:609:TYR:HA	1.71	1.20
1:A:477:ASN:OD1	2:B:1059:PRO:CG	1.90	1.20
3:C:62:SER:HB2	11:K:74:ASN:ND2	1.51	1.20
15:O:426:SER:OG	15:O:594:TYR:HB2	1.42	1.19
1:A:1050:TYR:CE1	1:A:1185:VAL:HG11	1.76	1.19
15:O:247:GLU:OE1	15:O:325:ILE:HG12	1.42	1.19
15:O:390:GLN:O	15:O:609:TYR:CE1	1.94	1.19
3:C:55:ASP:HA	3:C:299:ILE:HA	1.20	1.18
3:C:54:PHE:O	3:C:300:PHE:N	1.76	1.18
15:O:237:ILE:CG2	15:O:381:ILE:HD12	1.73	1.18
1:A:1008:ASP:OD1	1:A:1202:LEU:HD22	1.43	1.18
7:G:141:SER:CB	15:O:138:TYR:OH	1.92	1.17
15:O:162:PHE:O	15:O:210:ASN:O	1.61	1.17
15:O:237:ILE:HB	15:O:381:ILE:HD12	1.22	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:PHE:CE1	1:A:456:VAL:HG23	1.78	1.17
2:B:207:ILE:CG1	2:B:503:VAL:CG2	2.22	1.17
1:A:1006:LEU:CD1	2:B:716:MET:SD	2.32	1.17
2:B:207:ILE:CG1	2:B:503:VAL:HG21	1.73	1.17
1:A:83:VAL:HG21	1:A:427:PHE:CE2	1.78	1.16
1:A:1006:LEU:HD11	2:B:716:MET:SD	1.85	1.16
7:G:158:LYS:CD	15:O:105:ASN:OD1	1.91	1.16
15:O:430:ARG:NH2	15:O:596:PRO:HD3	1.60	1.16
1:A:1048:PHE:CZ	5:E:211:TYR:HD1	1.64	1.16
1:A:756:LYS:CD	9:I:85:LYS:NZ	2.07	1.16
2:B:207:ILE:HG13	2:B:503:VAL:HG22	1.26	1.16
3:C:59:ILE:HG23	3:C:298:PHE:CE1	1.79	1.15
4:D:92:ILE:HG12	7:G:152:ALA:HB2	1.29	1.15
7:G:158:LYS:HG2	15:O:105:ASN:OD1	1.43	1.15
1:A:1344:ILE:HD12	2:B:329:TYR:HE2	1.10	1.14
1:A:556:ALA:HB2	15:O:246:ASN:ND2	1.63	1.14
15:O:219:ARG:NH2	15:O:360:VAL:HG21	1.63	1.14
15:O:408:PHE:CE2	15:O:446:LEU:HD11	1.83	1.14
15:O:408:PHE:CZ	15:O:446:LEU:HD13	1.81	1.13
7:G:143:SER:HB2	15:O:104:ILE:H	1.06	1.13
15:O:454:VAL:HA	15:O:514:PHE:CZ	1.83	1.12
2:B:42:VAL:HB	2:B:46:ILE:CD1	1.77	1.12
7:G:28:ILE:HG22	7:G:29:ASP:H	1.02	1.12
1:A:1348:VAL:CB	2:B:268:GLU:O	1.97	1.12
15:O:247:GLU:OE1	15:O:325:ILE:CG1	1.97	1.12
3:C:58:ASN:HA	3:C:296:ASN:CB	1.79	1.11
2:B:42:VAL:CG1	2:B:46:ILE:CD1	2.26	1.11
3:C:54:PHE:CD2	3:C:300:PHE:HB2	1.85	1.11
6:F:75:PRO:HG2	6:F:78:GLN:HB2	1.12	1.11
15:O:370:THR:O	15:O:374:PRO:HD3	1.51	1.11
15:O:598:PHE:HB3	15:O:599:LEU:HD13	1.12	1.11
15:O:156:MET:HG3	15:O:197:PHE:CE2	1.83	1.11
15:O:454:VAL:CG2	15:O:514:PHE:HE2	1.62	1.11
2:B:42:VAL:CB	2:B:46:ILE:CD1	2.29	1.10
7:G:158:LYS:HB3	15:O:105:ASN:ND2	1.65	1.10
13:M:101:VAL:CG1	13:M:106:LYS:HG3	1.81	1.10
1:A:1226:VAL:O	1:A:1598:PHE:HD2	1.34	1.10
15:O:129:PRO:HD2	15:O:132:THR:HB	1.32	1.10
15:O:156:MET:SD	15:O:197:PHE:CZ	2.45	1.10
15:O:446:LEU:O	15:O:449:TRP:HB3	1.51	1.10
1:A:83:VAL:CG1	1:A:427:PHE:CE2	2.34	1.10

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ALA:HB2	2:B:1046:VAL:HG23	1.23	1.10
7:G:154:ASN:HD21	15:O:182:MET:HE3	1.10	1.10
15:O:240:ILE:HG21	15:O:332:LEU:HB2	1.24	1.10
1:A:1011:VAL:HG11	1:A:1201:THR:O	1.51	1.10
3:C:31:TRP:CE3	11:K:82:LYS:HG3	1.86	1.10
3:C:58:ASN:CA	3:C:296:ASN:HB2	1.81	1.10
4:D:25:THR:HG22	6:F:59:GLN:HE21	1.07	1.10
7:G:158:LYS:CB	15:O:105:ASN:ND2	2.15	1.10
1:A:475:ARG:HD2	2:B:1059:PRO:O	1.51	1.09
3:C:59:ILE:CG2	3:C:298:PHE:CD1	2.35	1.09
15:O:425:GLY:HA2	15:O:483:ILE:HD11	1.34	1.09
3:C:55:ASP:OD1	3:C:299:ILE:HG12	1.53	1.09
7:G:158:LYS:HA	15:O:105:ASN:HD21	1.08	1.09
15:O:447:THR:O	15:O:450:LEU:HB2	1.50	1.09
3:C:31:TRP:HB3	11:K:82:LYS:HD2	1.17	1.09
3:C:56:LEU:HB2	3:C:298:PHE:HB2	1.35	1.09
3:C:230:LEU:HD23	3:C:294:VAL:CG2	1.83	1.09
1:A:436:ALA:CB	1:A:443:ALA:CB	2.21	1.08
1:A:475:ARG:CD	2:B:1059:PRO:O	2.00	1.08
3:C:230:LEU:HD12	3:C:231:PRO:CD	1.84	1.08
4:D:28:PRO:HG2	7:G:24:VAL:HG11	1.28	1.08
15:O:138:TYR:CE2	15:O:142:ILE:CD1	2.35	1.08
15:O:201:LYS:HD2	15:O:239:SER:OG	1.54	1.08
1:A:478:TYR:CZ	2:B:1049:THR:HG23	1.88	1.08
1:A:1011:VAL:CG1	1:A:1201:THR:O	2.00	1.08
1:A:1055:ILE:CD1	1:A:1063:MET:HE1	1.84	1.08
2:B:42:VAL:CB	2:B:46:ILE:HD11	1.84	1.08
4:D:25:THR:HA	6:F:59:GLN:HG2	1.32	1.08
15:O:129:PRO:CD	15:O:132:THR:HB	1.83	1.08
3:C:75:VAL:HB	3:C:221:PRO:HD3	1.36	1.07
3:C:57:ILE:HA	3:C:297:HIS:HA	1.14	1.07
15:O:156:MET:SD	15:O:197:PHE:HZ	1.78	1.07
1:A:478:TYR:CZ	2:B:1049:THR:CG2	2.38	1.07
1:A:1055:ILE:HD12	1:A:1063:MET:HE1	1.31	1.07
3:C:230:LEU:HD12	3:C:231:PRO:HD3	1.36	1.07
15:O:138:TYR:CZ	15:O:142:ILE:HD11	1.89	1.07
1:A:475:ARG:NH2	2:B:1061:LYS:HB2	1.70	1.06
1:A:1008:ASP:O	1:A:1011:VAL:HG23	1.53	1.06
13:M:101:VAL:HG11	13:M:106:LYS:HG3	1.27	1.06
15:O:245:GLN:HG3	15:O:378:THR:HA	1.15	1.06
2:B:42:VAL:HG12	2:B:46:ILE:CD1	1.84	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:431:ALA:HB3	15:O:434:LEU:HD11	1.37	1.06
3:C:41:GLU:HB3	3:C:57:ILE:CG2	1.83	1.06
7:G:158:LYS:HB3	15:O:105:ASN:CG	1.79	1.06
15:O:198:PHE:CD1	15:O:236:LYS:HE3	1.90	1.06
15:O:240:ILE:HG22	15:O:332:LEU:HD22	1.08	1.06
1:A:1053:ASP:OD2	1:A:1580:ARG:NH2	1.88	1.06
3:C:75:VAL:HG11	3:C:221:PRO:HG2	1.06	1.05
15:O:162:PHE:CA	15:O:214:ASN:CB	2.33	1.05
1:A:408:LYS:HA	1:A:411:VAL:CG1	1.85	1.05
2:B:42:VAL:C	2:B:46:ILE:HD12	1.82	1.05
15:O:152:GLN:HG2	15:O:193:TYR:OH	1.52	1.05
15:O:431:ALA:HB1	15:O:434:LEU:HD11	1.34	1.05
1:A:1179:ILE:HD11	1:A:1183:GLU:HG3	1.33	1.05
15:O:240:ILE:CG2	15:O:332:LEU:HD22	1.87	1.05
1:A:1048:PHE:CZ	5:E:211:TYR:CD1	2.44	1.05
15:O:198:PHE:CZ	15:O:236:LYS:HG3	1.92	1.05
3:C:75:VAL:CB	3:C:221:PRO:CD	2.35	1.04
15:O:488:HIS:CG	15:O:489:ASN:H	1.74	1.04
15:O:390:GLN:NE2	15:O:432:LYS:H	1.54	1.04
3:C:131:THR:HG23	3:C:209:ILE:HG22	1.08	1.04
7:G:241:ARG:CB	15:O:189:PHE:CE2	2.39	1.04
15:O:152:GLN:CG	15:O:193:TYR:OH	2.04	1.04
1:A:83:VAL:HG11	1:A:427:PHE:CD2	1.90	1.04
1:A:502:ALA:HB1	1:A:581:ILE:CG2	1.87	1.04
7:G:141:SER:HB2	15:O:138:TYR:OH	1.53	1.04
15:O:174:ASP:HA	15:O:177:LYS:HE2	1.40	1.03
15:O:435:SER:HB3	15:O:438:GLN:HG3	1.37	1.03
4:D:25:THR:CG2	6:F:59:GLN:NE2	2.21	1.03
15:O:237:ILE:HB	15:O:381:ILE:CD1	1.88	1.03
1:A:1003:ARG:NE	2:B:520:LEU:HB2	1.74	1.03
12:L:68:GLU:HG2	12:L:69:ALA:H	1.23	1.03
1:A:1050:TYR:CE1	1:A:1185:VAL:CG1	2.42	1.02
4:D:80:THR:OG1	15:O:227:PHE:CG	2.08	1.02
1:A:782:ASP:OD2	1:A:931:SER:O	1.78	1.02
2:B:472:SER:CB	2:B:476:LEU:HD12	1.88	1.02
2:B:1155:ASP:OD2	7:G:239:THR:OG1	1.76	1.02
3:C:59:ILE:CG2	3:C:298:PHE:CE1	2.43	1.02
1:A:413:LEU:HB3	1:A:417:ARG:NH2	1.75	1.02
15:O:241:ASP:OD1	15:O:378:THR:HG22	1.58	1.02
1:A:909:SER:OG	9:I:83:LYS:CE	2.08	1.01
3:C:51:GLU:HB3	3:C:303:GLU:HG2	1.42	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:369:LYS:O	15:O:373:LEU:N	1.91	1.01
1:A:392:THR:CG2	1:A:430:ILE:HB	1.88	1.01
1:A:480:ALA:CB	2:B:1046:VAL:HG23	1.90	1.01
3:C:56:LEU:CD1	3:C:300:PHE:CE1	2.44	1.01
15:O:201:LYS:CD	15:O:239:SER:OG	2.09	1.01
15:O:428:ILE:HG23	15:O:439:ILE:HG21	1.38	1.00
3:C:45:SER:HB2	3:C:271:ARG:NH2	1.76	1.00
7:G:158:LYS:CA	15:O:105:ASN:HD21	1.75	1.00
1:A:408:LYS:HA	1:A:411:VAL:HG12	1.40	1.00
1:A:799:GLU:HG3	1:A:1062:HIS:CG	1.95	1.00
7:G:158:LYS:HZ3	15:O:108:GLU:CG	1.27	1.00
15:O:348:THR:HG22	15:O:351:SER:HB3	1.42	1.00
3:C:71:MET:HE1	3:C:302:VAL:HG22	1.41	1.00
15:O:352:LEU:HA	15:O:358:VAL:HG23	1.44	1.00
3:C:31:TRP:CD1	11:K:82:LYS:HZ3	1.72	1.00
1:A:756:LYS:CD	9:I:85:LYS:HZ2	1.70	1.00
1:A:782:ASP:OD1	1:A:783:LYS:N	1.93	1.00
15:O:240:ILE:HG21	15:O:332:LEU:CB	1.92	1.00
15:O:352:LEU:HD23	15:O:358:VAL:HG22	1.00	1.00
15:O:428:ILE:HD12	15:O:439:ILE:HG23	1.44	1.00
15:O:471:LYS:CB	15:O:585:PHE:CE1	2.45	0.99
2:B:75:ASP:HB3	2:B:440:PHE:CE2	1.97	0.99
15:O:454:VAL:CG2	15:O:514:PHE:CE2	2.44	0.99
7:G:143:SER:CB	15:O:104:ILE:H	1.75	0.99
15:O:158:LEU:HD23	15:O:172:HIS:HD2	1.25	0.99
1:A:1006:LEU:HD12	2:B:716:MET:SD	2.01	0.99
1:A:1055:ILE:HD12	1:A:1063:MET:CE	1.91	0.99
7:G:158:LYS:CA	15:O:105:ASN:ND2	2.25	0.99
1:A:1344:ILE:HD12	2:B:329:TYR:CE2	1.97	0.98
2:B:70:GLU:CB	2:B:98:SER:HB3	1.93	0.98
2:B:1019:GLY:HA3	3:C:65:ASN:HB2	1.45	0.98
3:C:54:PHE:CZ	3:C:300:PHE:CB	2.41	0.98
3:C:84:TYR:CD2	12:L:66:GLN:HB2	1.99	0.98
7:G:158:LYS:HD3	15:O:105:ASN:CG	1.88	0.98
2:B:70:GLU:HB3	2:B:98:SER:HB3	0.99	0.98
15:O:240:ILE:CG2	15:O:332:LEU:HD13	1.93	0.98
15:O:373:LEU:HD11	15:O:416:LYS:HG3	1.43	0.98
7:G:241:ARG:CB	15:O:189:PHE:HE2	1.76	0.98
15:O:598:PHE:CB	15:O:599:LEU:HD13	1.92	0.98
15:O:241:ASP:CG	15:O:378:THR:HG22	1.88	0.98
1:A:392:THR:HG21	1:A:430:ILE:CB	1.94	0.98

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:75:PRO:HG2	6:F:78:GLN:CB	1.92	0.98
1:A:909:SER:OG	9:I:83:LYS:HE2	1.62	0.97
7:G:158:LYS:CB	15:O:105:ASN:CG	2.35	0.97
1:A:83:VAL:CG2	1:A:427:PHE:CZ	2.47	0.97
4:D:96:PHE:HE1	7:G:150:HIS:HB3	1.28	0.97
7:G:158:LYS:CG	15:O:105:ASN:CG	2.37	0.97
15:O:423:TYR:HD1	15:O:594:TYR:CE2	1.82	0.97
13:M:105:SER:HA	13:M:108:LEU:HG	1.46	0.97
1:A:392:THR:HG21	1:A:430:ILE:HB	0.98	0.97
1:A:509:GLU:OE2	1:A:579:ARG:NE	1.97	0.97
1:A:953:GLU:HG2	1:A:1205:PHE:CE2	2.00	0.97
2:B:70:GLU:HB3	2:B:98:SER:CB	1.93	0.97
15:O:454:VAL:HB	15:O:514:PHE:HE2	0.99	0.96
1:A:476:VAL:HG11	2:B:1071:VAL:HG23	1.47	0.96
1:A:480:ALA:HB2	2:B:1046:VAL:CG2	1.95	0.96
1:A:1660:VAL:O	7:G:102:GLU:HA	1.65	0.96
3:C:59:ILE:HG22	3:C:298:PHE:CD1	1.98	0.96
7:G:158:LYS:NZ	15:O:108:GLU:CG	1.78	0.96
1:A:83:VAL:CG2	1:A:427:PHE:CE2	2.48	0.96
1:A:966:LEU:HD22	1:A:997:PHE:CZ	2.00	0.96
2:B:769:PHE:CD1	2:B:798:PHE:HE1	1.83	0.96
14:N:85:HIS:HE1	14:N:141:GLU:CD	1.72	0.96
15:O:156:MET:CG	15:O:197:PHE:CE2	2.48	0.96
1:A:1055:ILE:HG21	1:A:1060:GLU:HG3	1.47	0.95
1:A:1:MET:HG2	2:B:1098:TYR:CZ	2.01	0.95
1:A:502:ALA:HB1	1:A:581:ILE:HG21	1.46	0.95
7:G:158:LYS:HD3	15:O:105:ASN:OD1	1.66	0.95
1:A:478:TYR:C	2:B:1047:ARG:O	2.08	0.95
1:A:516:ILE:HG12	15:O:376:TYR:CE2	2.01	0.95
15:O:440:ILE:HG23	15:O:491:PHE:HE1	1.27	0.95
3:C:31:TRP:CD1	11:K:82:LYS:HZ2	1.78	0.95
15:O:408:PHE:HZ	15:O:446:LEU:HD11	1.25	0.95
1:A:502:ALA:CB	1:A:581:ILE:HG21	1.97	0.95
2:B:1090:ASP:OD1	2:B:1095:SER:OG	1.85	0.95
15:O:454:VAL:HG23	15:O:514:PHE:CE2	2.01	0.95
1:A:1344:ILE:CD1	2:B:329:TYR:HE2	1.78	0.94
2:B:77:LYS:NZ	2:B:438:ILE:O	1.99	0.94
3:C:71:MET:HE1	3:C:302:VAL:CG2	1.96	0.94
15:O:63:LEU:HD12	15:O:71:ILE:HG13	1.47	0.94
15:O:432:LYS:HB2	15:O:609:TYR:C	1.93	0.94
15:O:374:PRO:O	15:O:419:LYS:NZ	2.01	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:ASP:OD2	1:A:405:LYS:HE3	1.67	0.94
15:O:234:ILE:CG2	15:O:371:HIS:HD2	1.81	0.94
3:C:75:VAL:HB	3:C:221:PRO:CD	1.94	0.94
1:A:799:GLU:HG3	1:A:1062:HIS:ND1	1.83	0.93
1:A:990:ILE:HA	1:A:994:GLU:OE1	1.69	0.93
2:B:894:LYS:H	12:L:54:ARG:NH2	1.66	0.93
15:O:342:HIS:CD2	15:O:346:GLN:HE21	1.85	0.93
15:O:417:LYS:HD2	15:O:472:HIS:CE1	2.02	0.93
1:A:878:ARG:HG2	9:I:67:VAL:HG11	1.48	0.93
2:B:209:GLN:HG2	2:B:210:ARG:H	1.31	0.93
2:B:211:ARG:HG2	2:B:401:GLU:OE1	1.68	0.93
3:C:57:ILE:HD12	3:C:297:HIS:ND1	1.82	0.93
15:O:198:PHE:HD2	15:O:232:LEU:HG	1.05	0.93
3:C:62:SER:CB	11:K:74:ASN:ND2	2.32	0.93
15:O:342:HIS:O	15:O:346:GLN:HG2	1.68	0.93
3:C:75:VAL:CG1	3:C:221:PRO:HG2	1.89	0.93
4:D:80:THR:OG1	15:O:227:PHE:CD2	2.20	0.93
15:O:358:VAL:O	15:O:362:ASN:ND2	2.00	0.93
1:A:413:LEU:HB3	1:A:417:ARG:HH21	1.29	0.93
3:C:58:ASN:H	3:C:296:ASN:C	1.75	0.93
4:D:92:ILE:HG22	4:D:96:PHE:CZ	2.03	0.93
3:C:75:VAL:CB	3:C:221:PRO:HD2	1.97	0.92
15:O:598:PHE:HB3	15:O:599:LEU:CD1	1.99	0.92
3:C:131:THR:CG2	3:C:209:ILE:HG22	1.98	0.92
7:G:154:ASN:HD21	15:O:182:MET:CE	1.82	0.92
1:A:83:VAL:HG21	1:A:427:PHE:HZ	1.13	0.92
15:O:224:GLU:OE1	15:O:224:GLU:N	2.02	0.92
1:A:756:LYS:HD3	9:I:85:LYS:HZ1	1.19	0.92
3:C:71:MET:SD	3:C:225:ALA:HB1	2.10	0.92
15:O:147:ILE:O	15:O:149:LYS:N	2.03	0.92
15:O:386:PHE:HD2	15:O:606:MET:CE	1.83	0.92
15:O:390:GLN:O	15:O:609:TYR:HE1	1.52	0.92
15:O:435:SER:CB	15:O:438:GLN:HG3	1.98	0.92
1:A:1658:ALA:O	7:G:104:LEU:HA	1.70	0.91
15:O:240:ILE:HG22	15:O:332:LEU:CD2	1.98	0.91
6:F:74:ILE:HG23	6:F:75:PRO:HD2	1.51	0.91
7:G:28:ILE:HG22	7:G:29:ASP:N	1.81	0.91
1:A:1348:VAL:HB	2:B:268:GLU:C	1.95	0.91
2:B:894:LYS:H	12:L:54:ARG:HH21	0.92	0.91
15:O:219:ARG:NH2	15:O:360:VAL:CG2	2.32	0.91
15:O:408:PHE:HZ	15:O:446:LEU:CD1	1.74	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:ALA:O	3:C:301:ASN:HA	1.69	0.91
3:C:253:PRO:HB2	14:N:180:PHE:CD1	2.06	0.91
15:O:390:GLN:NE2	15:O:609:TYR:HB3	1.86	0.91
15:O:240:ILE:HG21	15:O:332:LEU:HD13	1.51	0.91
1:A:1036:ASN:O	1:A:1049:MET:HA	1.71	0.91
15:O:478:GLN:HE21	15:O:592:PHE:HZ	1.19	0.91
1:A:412:SER:O	1:A:416:ARG:N	2.03	0.90
2:B:42:VAL:HG11	2:B:46:ILE:HD11	1.52	0.90
2:B:894:LYS:N	12:L:54:ARG:HH21	1.69	0.90
2:B:472:SER:OG	2:B:476:LEU:HD12	1.71	0.90
3:C:230:LEU:HD23	3:C:294:VAL:HG21	0.91	0.90
15:O:342:HIS:CE1	15:O:346:GLN:HG3	2.05	0.90
15:O:426:SER:OG	15:O:594:TYR:CB	2.18	0.90
7:G:242:VAL:HG11	15:O:185:SER:HG	1.25	0.90
1:A:1055:ILE:HD11	1:A:1174:TYR:CE2	2.06	0.90
15:O:240:ILE:CG2	15:O:332:LEU:HB2	2.01	0.90
4:D:25:THR:HA	6:F:59:GLN:CG	1.99	0.90
15:O:454:VAL:HA	15:O:514:PHE:HZ	1.34	0.90
1:A:756:LYS:CD	9:I:85:LYS:HZ1	1.76	0.90
1:A:1048:PHE:HE2	5:E:211:TYR:H	1.11	0.90
15:O:471:LYS:HB2	15:O:585:PHE:HE1	1.00	0.90
1:A:516:ILE:HG21	15:O:376:TYR:OH	1.72	0.90
3:C:41:GLU:HB3	3:C:57:ILE:HG21	1.53	0.90
4:D:28:PRO:HG2	7:G:24:VAL:CG1	2.01	0.90
1:A:413:LEU:O	1:A:417:ARG:NE	2.05	0.90
3:C:75:VAL:HG11	3:C:221:PRO:HD2	1.54	0.90
15:O:158:LEU:HD23	15:O:172:HIS:CD2	2.07	0.90
15:O:426:SER:CB	15:O:594:TYR:HB2	2.01	0.90
1:A:1661:PRO:C	7:G:101:SER:O	2.13	0.89
3:C:31:TRP:CG	11:K:82:LYS:HD2	2.06	0.89
3:C:86:PHE:CE1	12:L:64:LEU:HD13	2.07	0.89
15:O:198:PHE:CG	15:O:236:LYS:HE3	2.06	0.89
1:A:1226:VAL:O	1:A:1598:PHE:CD2	2.24	0.89
3:C:64:ALA:C	3:C:227:TYR:HE2	1.80	0.89
7:G:158:LYS:HA	15:O:105:ASN:ND2	1.85	0.89
15:O:194:LEU:O	15:O:232:LEU:HD21	1.72	0.89
15:O:421:LEU:HD13	15:O:476:ALA:HB2	1.54	0.89
2:B:478:LEU:HD13	2:B:484:TYR:CE1	2.06	0.89
4:D:96:PHE:CE1	7:G:150:HIS:HB3	2.07	0.89
1:A:1050:TYR:HE1	1:A:1185:VAL:CG1	1.83	0.89
1:A:1179:ILE:HD11	1:A:1183:GLU:CG	2.01	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:THR:HG21	15:O:227:PHE:HB3	1.53	0.89
15:O:129:PRO:CG	15:O:132:THR:HB	2.01	0.89
3:C:37:LYS:HD2	11:K:130:VAL:HG22	1.54	0.89
2:B:42:VAL:CB	2:B:46:ILE:HD12	2.00	0.89
15:O:432:LYS:CB	15:O:609:TYR:CA	2.41	0.89
15:O:457:ARG:HA	15:O:460:GLU:HB2	1.54	0.89
1:A:413:LEU:C	1:A:417:ARG:HH21	1.81	0.89
15:O:219:ARG:HH21	15:O:360:VAL:CG2	1.85	0.89
1:A:891:ILE:CD1	9:I:71:LEU:HB2	2.03	0.89
13:M:102:SER:O	13:M:106:LYS:HB2	1.73	0.89
1:A:406:LEU:CD1	1:A:411:VAL:HB	2.03	0.88
6:F:66:ARG:CZ	7:G:90:LEU:HD13	2.02	0.88
2:B:894:LYS:HG2	12:L:47:ARG:CD	2.04	0.88
1:A:401:ASP:O	1:A:405:LYS:HB2	1.74	0.88
1:A:1008:ASP:CG	1:A:1202:LEU:HD13	1.98	0.88
3:C:56:LEU:HD11	3:C:300:PHE:CE1	2.08	0.88
4:D:28:PRO:CG	7:G:24:VAL:HG11	2.03	0.88
1:A:83:VAL:CG1	1:A:427:PHE:HE2	1.80	0.88
1:A:1348:VAL:CG2	2:B:268:GLU:O	2.21	0.88
1:A:1038:ILE:HG12	1:A:1049:MET:O	1.74	0.88
15:O:521:ASN:HD22	15:O:524:VAL:H	1.22	0.88
3:C:230:LEU:CD1	3:C:231:PRO:CD	2.52	0.88
1:A:556:ALA:HB2	15:O:246:ASN:HD22	1.38	0.88
2:B:769:PHE:CE1	2:B:798:PHE:CZ	2.61	0.88
15:O:488:HIS:ND1	15:O:489:ASN:N	2.21	0.88
15:O:488:HIS:O	15:O:490:ILE:N	2.06	0.88
15:O:459:GLU:O	15:O:463:GLN:HG3	1.73	0.87
3:C:75:VAL:CB	3:C:221:PRO:HD3	2.01	0.87
1:A:1662:ASN:HA	7:G:101:SER:HB2	1.57	0.87
3:C:230:LEU:CD1	3:C:231:PRO:HD2	2.04	0.87
15:O:417:LYS:CD	15:O:472:HIS:CE1	2.57	0.87
1:A:756:LYS:HD2	9:I:85:LYS:NZ	1.86	0.87
15:O:198:PHE:HD2	15:O:232:LEU:CG	1.86	0.87
3:C:131:THR:CG2	3:C:209:ILE:CG2	2.51	0.87
1:A:475:ARG:HD3	2:B:1059:PRO:O	1.73	0.87
1:A:1055:ILE:HD12	1:A:1063:MET:SD	2.14	0.87
7:G:158:LYS:HZ3	15:O:108:GLU:HG2	1.39	0.87
1:A:1:MET:HA	2:B:1098:TYR:CD1	2.10	0.87
1:A:862:THR:O	9:I:67:VAL:HG12	1.73	0.87
3:C:70:ILE:HD11	11:K:71:THR:CG2	2.04	0.87
3:C:75:VAL:CG1	3:C:221:PRO:HG3	2.03	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1660:VAL:HG22	7:G:103:LYS:O	1.75	0.86
4:D:25:THR:O	6:F:59:GLN:HG3	1.75	0.86
1:A:636:HIS:ND1	2:B:1091:ARG:NH2	2.22	0.86
1:A:1600:ARG:CD	1:A:1616:GLU:OE1	2.24	0.86
11:K:66:VAL:HG12	11:K:67:GLU:HG2	1.57	0.86
3:C:56:LEU:HG	3:C:300:PHE:CD1	2.10	0.86
4:D:80:THR:CB	15:O:227:PHE:CD2	2.58	0.86
1:A:408:LYS:CA	1:A:411:VAL:HG12	2.04	0.86
3:C:31:TRP:CD2	11:K:82:LYS:HG3	2.10	0.86
7:G:143:SER:HB2	15:O:104:ILE:N	1.89	0.86
1:A:475:ARG:HH22	2:B:1061:LYS:HB2	1.36	0.86
3:C:59:ILE:HG22	3:C:298:PHE:HD1	1.38	0.86
4:D:25:THR:HB	6:F:59:GLN:CD	2.00	0.86
1:A:996:TYR:HE1	1:A:1000:MET:HE3	1.39	0.86
15:O:457:ARG:C	15:O:460:GLU:HB2	2.01	0.86
1:A:878:ARG:HE	9:I:67:VAL:CG1	1.87	0.86
1:A:996:TYR:CE1	1:A:1000:MET:HE3	2.10	0.86
1:A:1003:ARG:CZ	2:B:520:LEU:HB2	2.04	0.86
3:C:31:TRP:HB3	11:K:82:LYS:CD	2.03	0.86
15:O:366:THR:O	15:O:370:THR:HG23	1.75	0.86
15:O:417:LYS:HB3	15:O:472:HIS:NE2	1.91	0.86
1:A:620:ASN:OD1	1:A:667:ARG:NH2	2.07	0.86
4:D:80:THR:CG2	15:O:227:PHE:HB3	2.06	0.86
1:A:468:ARG:NE	1:A:1021:ARG:NH1	2.23	0.86
7:G:141:SER:CA	15:O:138:TYR:OH	2.24	0.86
15:O:521:ASN:ND2	15:O:523:ASN:H	1.74	0.86
1:A:782:ASP:CG	1:A:931:SER:O	2.18	0.85
15:O:457:ARG:O	15:O:460:GLU:HB2	1.76	0.85
15:O:458:GLU:CA	15:O:461:VAL:CG2	2.08	0.85
1:A:1008:ASP:OD1	1:A:1202:LEU:CD2	2.24	0.85
3:C:31:TRP:CG	11:K:82:LYS:NZ	2.44	0.85
15:O:181:ARG:CB	15:O:181:ARG:HH11	1.89	0.85
15:O:163:ILE:HG22	15:O:211:TYR:HB2	1.58	0.85
7:G:154:ASN:ND2	15:O:182:MET:HE3	1.92	0.85
15:O:396:MET:HE1	15:O:434:LEU:HD12	1.58	0.85
15:O:408:PHE:CE2	15:O:446:LEU:CD1	2.50	0.85
1:A:1060:GLU:HA	1:A:1063:MET:HG3	1.55	0.84
7:G:158:LYS:CD	15:O:105:ASN:CG	2.48	0.84
15:O:369:LYS:HB3	15:O:369:LYS:HZ3	1.37	0.84
1:A:392:THR:HB	1:A:430:ILE:HD13	1.59	0.84
2:B:472:SER:HB3	2:B:476:LEU:HD12	1.57	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:25:THR:HG22	7:G:26:ASN:H	1.40	0.84
15:O:181:ARG:HH11	15:O:181:ARG:HB2	1.41	0.84
15:O:237:ILE:HG22	15:O:381:ILE:HD12	1.60	0.84
15:O:361:PHE:O	15:O:365:THR:HG23	1.78	0.84
1:A:1055:ILE:HG23	1:A:1063:MET:SD	2.17	0.84
3:C:253:PRO:HB2	14:N:180:PHE:HD1	1.41	0.84
15:O:243:GLU:HA	15:O:246:ASN:ND2	1.90	0.84
15:O:447:THR:HG22	15:O:480:LEU:HD22	1.58	0.84
1:A:436:ALA:HB2	1:A:443:ALA:HB2	0.86	0.84
1:A:1019:LEU:HD12	1:A:1227:MET:HG3	1.58	0.84
1:A:1600:ARG:HD2	1:A:1616:GLU:OE1	1.77	0.84
2:B:472:SER:CB	2:B:476:LEU:CD1	2.54	0.84
15:O:240:ILE:CB	15:O:332:LEU:HD13	2.07	0.84
2:B:37:LEU:HD13	2:B:760:TYR:CZ	2.12	0.84
2:B:42:VAL:O	2:B:46:ILE:HD12	1.76	0.84
4:D:96:PHE:HE1	7:G:150:HIS:CB	1.91	0.84
6:F:74:ILE:CG2	6:F:75:PRO:HD2	2.08	0.84
15:O:422:GLN:NE2	15:O:592:PHE:CE2	2.45	0.84
7:G:242:VAL:HG12	15:O:185:SER:OG	1.77	0.83
2:B:894:LYS:O	2:B:896:GLN:N	2.11	0.83
15:O:398:SER:O	15:O:401:VAL:HG12	1.79	0.83
15:O:467:MET:HG3	15:O:519:PHE:CZ	2.13	0.83
1:A:436:ALA:CA	1:A:443:ALA:HB2	2.09	0.83
1:A:863:ASN:ND2	9:I:68:LYS:N	2.25	0.83
3:C:86:PHE:HE1	12:L:64:LEU:HD13	1.42	0.83
15:O:359:GLY:HA2	15:O:362:ASN:HD22	1.43	0.83
1:A:990:ILE:HB	1:A:994:GLU:HB2	1.61	0.83
1:A:990:ILE:CA	1:A:994:GLU:OE1	2.26	0.83
3:C:51:GLU:HB3	3:C:303:GLU:CG	2.08	0.83
15:O:240:ILE:HG21	15:O:332:LEU:CD1	2.08	0.83
15:O:156:MET:CG	15:O:197:PHE:CZ	2.61	0.83
15:O:370:THR:O	15:O:374:PRO:CD	2.25	0.83
2:B:207:ILE:HG12	2:B:503:VAL:HG21	1.59	0.83
15:O:242:VAL:HA	15:O:378:THR:HG21	1.60	0.83
15:O:390:GLN:NE2	15:O:432:LYS:N	2.25	0.83
1:A:1026:GLN:OE1	1:A:1603:MET:HB2	1.78	0.83
4:D:25:THR:CA	6:F:59:GLN:HG2	2.07	0.83
15:O:428:ILE:CG2	15:O:439:ILE:HG21	2.09	0.83
15:O:457:ARG:CA	15:O:460:GLU:HB2	2.09	0.83
1:A:1:MET:HA	2:B:1098:TYR:CE1	2.13	0.83
1:A:556:ALA:CB	15:O:246:ASN:HD22	1.90	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:372:VAL:C	15:O:374:PRO:HD2	2.04	0.83
15:O:454:VAL:CA	15:O:514:PHE:CE2	2.62	0.83
1:A:1654:PHE:CZ	6:F:92:ARG:HD3	2.14	0.83
3:C:253:PRO:HG2	14:N:180:PHE:HB3	1.61	0.83
1:A:1179:ILE:CD1	1:A:1183:GLU:HG3	2.09	0.83
15:O:352:LEU:O	15:O:358:VAL:HG21	1.77	0.83
15:O:488:HIS:CG	15:O:489:ASN:N	2.40	0.83
1:A:1575:ILE:CG1	9:I:122:ARG:HH12	1.92	0.82
15:O:242:VAL:N	15:O:378:THR:HG21	1.94	0.82
15:O:440:ILE:HG23	15:O:491:PHE:CE1	2.13	0.82
1:A:406:LEU:HD13	1:A:411:VAL:HB	1.60	0.82
15:O:246:ASN:OD1	15:O:247:GLU:N	2.11	0.82
3:C:55:ASP:HA	3:C:299:ILE:CA	2.07	0.82
1:A:437:PHE:CZ	1:A:456:VAL:HG21	2.14	0.82
4:D:25:THR:HB	6:F:59:GLN:NE2	1.94	0.82
3:C:55:ASP:CA	3:C:299:ILE:HA	2.08	0.82
7:G:158:LYS:HD3	15:O:105:ASN:CB	2.09	0.82
1:A:1:MET:HG2	2:B:1098:TYR:CE2	2.12	0.82
1:A:556:ALA:CB	15:O:246:ASN:ND2	2.41	0.82
4:D:95:ASP:OD2	7:G:150:HIS:HA	1.80	0.82
15:O:245:GLN:HG3	15:O:378:THR:CA	2.05	0.82
4:D:25:THR:CA	6:F:59:GLN:CG	2.57	0.82
7:G:158:LYS:NZ	15:O:108:GLU:HG2	1.95	0.82
1:A:863:ASN:HD22	9:I:67:VAL:HA	1.45	0.81
15:O:386:PHE:CD2	15:O:606:MET:CE	2.62	0.81
2:B:472:SER:HB3	2:B:476:LEU:CD1	2.11	0.81
2:B:776:ILE:HB	2:B:1026:ILE:HD13	1.60	0.81
15:O:162:PHE:HA	15:O:214:ASN:CB	2.09	0.81
15:O:383:TYR:CD2	15:O:597:LEU:HD22	2.15	0.81
1:A:50:TYR:HE1	1:A:368:ARG:O	1.64	0.81
15:O:237:ILE:CG2	15:O:381:ILE:CD1	2.57	0.81
3:C:71:MET:HE2	3:C:225:ALA:HB2	1.60	0.81
15:O:454:VAL:HA	15:O:514:PHE:CE2	2.15	0.81
1:A:1011:VAL:HG13	1:A:1201:THR:O	1.80	0.81
1:A:1316:VAL:HG21	1:A:1498:ILE:HA	1.63	0.81
3:C:253:PRO:O	14:N:180:PHE:CD1	2.34	0.81
4:D:80:THR:HG21	15:O:227:PHE:CD2	2.16	0.81
15:O:369:LYS:HE2	15:O:370:THR:CG2	2.10	0.81
3:C:31:TRP:CG	11:K:82:LYS:HZ2	1.99	0.81
3:C:75:VAL:HG12	3:C:221:PRO:CG	2.11	0.81
15:O:458:GLU:HA	15:O:461:VAL:HG21	1.59	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:PRO:HG2	15:O:371:HIS:ND1	1.97	0.80
15:O:243:GLU:HA	15:O:246:ASN:HD21	1.46	0.80
1:A:966:LEU:HD22	1:A:997:PHE:HZ	1.44	0.80
12:L:34:CYS:HB3	12:L:51:CYS:SG	2.21	0.80
14:N:85:HIS:CE1	14:N:141:GLU:CD	2.60	0.80
15:O:387:HIS:HB2	15:O:606:MET:SD	2.21	0.80
1:A:1004:GLU:HA	1:A:1007:ILE:HD12	1.64	0.80
2:B:208:VAL:HG23	2:B:401:GLU:HG2	1.64	0.80
3:C:57:ILE:HA	3:C:297:HIS:CA	2.05	0.80
4:D:92:ILE:CG2	4:D:96:PHE:CZ	2.63	0.80
15:O:371:HIS:C	15:O:374:PRO:HD2	2.06	0.80
1:A:1000:MET:HG2	2:B:520:LEU:HD23	1.62	0.80
3:C:37:LYS:HD2	11:K:130:VAL:CG2	2.11	0.80
3:C:56:LEU:HD12	3:C:300:PHE:HE1	1.46	0.80
4:D:28:PRO:HD2	7:G:24:VAL:HG13	1.62	0.80
15:O:240:ILE:HG21	15:O:332:LEU:CG	2.11	0.80
15:O:432:LYS:CB	15:O:609:TYR:C	2.54	0.80
7:G:141:SER:HA	15:O:138:TYR:OH	1.82	0.80
3:C:75:VAL:HG21	3:C:221:PRO:HD2	1.64	0.80
15:O:166:ILE:CD1	15:O:213:SER:OG	2.30	0.80
6:F:75:PRO:CG	6:F:78:GLN:HB2	2.05	0.79
1:A:478:TYR:CE1	2:B:1049:THR:HG23	2.16	0.79
1:A:996:TYR:O	1:A:1000:MET:HG3	1.83	0.79
1:A:1655:ASP:HB2	6:F:135:ARG:HB3	1.65	0.79
3:C:31:TRP:HB2	11:K:82:LYS:HD2	1.59	0.79
1:A:403:LEU:CD1	1:A:419:ILE:HG21	2.12	0.79
15:O:234:ILE:HG21	15:O:371:HIS:CD2	2.18	0.79
4:D:25:THR:CB	6:F:59:GLN:NE2	2.46	0.79
15:O:436:ARG:O	15:O:440:ILE:HG13	1.82	0.79
1:A:401:ASP:OD2	1:A:405:LYS:CE	2.31	0.79
1:A:401:ASP:O	1:A:405:LYS:CB	2.31	0.79
15:O:129:PRO:HG2	15:O:132:THR:HB	1.63	0.79
2:B:480:GLN:OE1	2:B:480:GLN:N	2.14	0.78
15:O:584:GLN:OE1	15:O:584:GLN:N	2.11	0.78
1:A:638:PRO:HA	2:B:1090:ASP:OD2	1.82	0.78
1:A:953:GLU:HA	1:A:1205:PHE:CD2	2.18	0.78
2:B:42:VAL:HG12	2:B:46:ILE:CG1	2.14	0.78
2:B:566:TYR:HD2	13:M:73:SER:OG	1.66	0.78
3:C:253:PRO:CB	14:N:180:PHE:HD1	1.95	0.78
15:O:243:GLU:O	15:O:246:ASN:OD1	1.99	0.78
15:O:478:GLN:NE2	15:O:592:PHE:HZ	1.81	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:OG1	1:A:435:ASN:ND2	2.16	0.78
2:B:75:ASP:HB3	2:B:440:PHE:CZ	2.17	0.78
15:O:432:LYS:HG2	15:O:608:GLU:C	2.07	0.78
1:A:1348:VAL:HG11	2:B:268:GLU:HB2	1.66	0.78
3:C:64:ALA:C	3:C:227:TYR:CE2	2.60	0.78
15:O:174:ASP:CA	15:O:177:LYS:HE2	2.12	0.78
3:C:50:ARG:O	3:C:303:GLU:HA	1.84	0.78
1:A:1344:ILE:HG22	2:B:333:LYS:HB3	1.66	0.78
3:C:75:VAL:CG2	3:C:221:PRO:HD2	2.14	0.78
4:D:23:HIS:CD2	6:F:58:PHE:CE2	2.71	0.78
15:O:241:ASP:C	15:O:378:THR:HG21	2.08	0.78
15:O:242:VAL:CA	15:O:378:THR:HG21	2.14	0.78
15:O:373:LEU:CD1	15:O:416:LYS:HG3	2.13	0.78
1:A:1604:GLU:O	1:A:1612:LYS:HE2	1.83	0.78
2:B:934:ILE:HG22	3:C:72:ILE:HB	1.66	0.78
15:O:129:PRO:HG2	15:O:132:THR:CB	2.14	0.78
15:O:430:ARG:NH2	15:O:596:PRO:CD	2.44	0.78
4:D:28:PRO:CG	7:G:24:VAL:CG1	2.62	0.77
2:B:68:ILE:HD11	2:B:414:LYS:HG3	1.66	0.77
2:B:1043:LYS:HD3	2:B:1063:ARG:NH2	1.97	0.77
1:A:1344:ILE:HG22	2:B:333:LYS:CB	2.15	0.77
15:O:162:PHE:O	15:O:210:ASN:C	2.27	0.77
1:A:509:GLU:CD	1:A:579:ARG:HE	1.92	0.77
1:A:1:MET:HB2	2:B:1098:TYR:CG	2.19	0.77
1:A:475:ARG:CZ	2:B:1061:LYS:HB2	2.14	0.77
2:B:467:THR:HB	2:B:469:ASN:ND2	2.00	0.77
15:O:186:SER:O	15:O:190:ILE:HG22	1.84	0.77
15:O:414:ALA:O	15:O:418:ILE:HD12	1.85	0.77
15:O:234:ILE:CG2	15:O:371:HIS:CD2	2.66	0.77
1:A:1662:ASN:CA	7:G:101:SER:HB2	2.13	0.76
3:C:75:VAL:HG12	3:C:221:PRO:HG3	1.63	0.76
9:I:60:LEU:HA	9:I:63:LYS:HG3	1.65	0.76
15:O:359:GLY:O	15:O:363:THR:HG22	1.85	0.76
15:O:425:GLY:HA2	15:O:483:ILE:CD1	2.13	0.76
2:B:878:GLU:OE2	2:B:909:ARG:NH1	2.17	0.76
15:O:174:ASP:O	15:O:177:LYS:HG2	1.85	0.76
15:O:240:ILE:HB	15:O:332:LEU:HD13	1.66	0.76
1:A:437:PHE:HZ	1:A:456:VAL:CG2	1.98	0.76
3:C:56:LEU:CD1	3:C:300:PHE:HE1	1.95	0.76
15:O:360:VAL:O	15:O:364:LEU:HG	1.83	0.76
2:B:328:GLN:HE22	13:M:109:ARG:HH21	1.31	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:75:VAL:CG1	3:C:221:PRO:HD3	2.10	0.76
15:O:62:ASP:HB3	15:O:67:ASP:OD2	1.86	0.76
1:A:438:ILE:HG23	2:B:1192:MET:HG2	1.68	0.76
3:C:55:ASP:OD1	3:C:299:ILE:CG1	2.34	0.76
15:O:484:PHE:CE1	15:O:502:LEU:CD1	2.69	0.76
1:A:502:ALA:HB1	1:A:581:ILE:HG22	1.64	0.76
1:A:641:GLU:HB2	6:F:99:LEU:HD13	1.68	0.76
2:B:1069:ILE:HG22	2:B:1070:ARG:H	1.50	0.76
15:O:158:LEU:CD2	15:O:172:HIS:CD2	2.67	0.76
15:O:386:PHE:HD2	15:O:606:MET:HE1	1.48	0.76
1:A:478:TYR:CE2	2:B:1049:THR:CG2	2.68	0.76
15:O:454:VAL:CA	15:O:514:PHE:CZ	2.67	0.76
1:A:1028:GLU:HG3	1:A:1029:GLY:N	2.00	0.76
3:C:131:THR:HG23	3:C:209:ILE:HG23	1.68	0.76
7:G:159:LYS:H	15:O:105:ASN:HD22	1.32	0.76
1:A:1055:ILE:CG2	1:A:1060:GLU:HG3	2.16	0.76
3:C:70:ILE:HD11	11:K:71:THR:HG21	1.67	0.76
7:G:154:ASN:OD1	15:O:183:ILE:HG12	1.85	0.76
1:A:1052:GLY:O	5:E:205:SER:HB2	1.85	0.76
3:C:62:SER:HB2	11:K:74:ASN:CG	2.10	0.76
1:A:878:ARG:NE	9:I:67:VAL:CG1	2.48	0.75
1:A:1050:TYR:CD1	1:A:1185:VAL:HG11	2.20	0.75
2:B:769:PHE:HE1	2:B:798:PHE:CZ	2.03	0.75
15:O:219:ARG:HH22	15:O:360:VAL:HG21	1.47	0.75
6:F:66:ARG:NH2	7:G:90:LEU:HD13	2.01	0.75
15:O:359:GLY:HA2	15:O:362:ASN:ND2	2.01	0.75
1:A:1019:LEU:CD1	1:A:1227:MET:HG3	2.17	0.75
15:O:166:ILE:HD13	15:O:213:SER:OG	1.86	0.75
15:O:461:VAL:HG13	15:O:467:MET:HE1	1.65	0.75
1:A:891:ILE:HD13	9:I:71:LEU:HB2	1.68	0.75
1:A:1048:PHE:HE2	5:E:211:TYR:N	1.83	0.75
15:O:428:ILE:HD12	15:O:439:ILE:CG2	2.16	0.75
1:A:1048:PHE:CE2	5:E:211:TYR:N	2.53	0.75
2:B:42:VAL:HB	2:B:46:ILE:HD11	1.51	0.75
2:B:207:ILE:CG1	2:B:503:VAL:HG22	2.04	0.75
3:C:131:THR:HG22	3:C:208:CYS:O	1.86	0.75
4:D:44:ILE:HG21	4:D:90:LYS:HE3	1.69	0.75
15:O:230:TRP:CE2	15:O:364:LEU:HD21	2.20	0.75
15:O:198:PHE:CE2	15:O:232:LEU:HG	2.22	0.75
15:O:342:HIS:NE2	15:O:346:GLN:NE2	2.34	0.75
3:C:31:TRP:CB	11:K:82:LYS:CD	2.51	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:PHE:CE1	1:A:456:VAL:CG2	2.58	0.74
15:O:101:SER:HB3	15:O:142:ILE:HD12	1.69	0.74
15:O:440:ILE:CG2	15:O:491:PHE:HE1	2.01	0.74
15:O:484:PHE:CE1	15:O:502:LEU:HD12	2.21	0.74
1:A:1348:VAL:CG1	2:B:268:GLU:HB2	2.18	0.74
3:C:45:SER:CB	3:C:271:ARG:NH2	2.49	0.74
4:D:96:PHE:HE1	7:G:150:HIS:CG	2.04	0.74
1:A:556:ALA:HB1	15:O:243:GLU:OE2	1.88	0.74
1:A:1575:ILE:HG12	9:I:122:ARG:HH12	1.52	0.74
15:O:241:ASP:OD1	15:O:378:THR:CG2	2.33	0.74
3:C:64:ALA:O	3:C:227:TYR:HE2	1.69	0.74
15:O:369:LYS:HE2	15:O:370:THR:HG23	1.67	0.74
4:D:25:THR:HG22	6:F:59:GLN:NE2	1.93	0.74
15:O:143:LEU:HD11	15:O:150:TRP:CD1	2.22	0.74
15:O:374:PRO:HG2	15:O:375:THR:HG23	1.69	0.74
15:O:484:PHE:HE1	15:O:502:LEU:HD12	1.52	0.74
3:C:82:TYR:CD1	12:L:68:GLU:HG3	2.22	0.74
15:O:238:ILE:HD11	15:O:371:HIS:HB3	1.70	0.74
15:O:390:GLN:HE22	15:O:432:LYS:N	1.86	0.74
15:O:421:LEU:CD1	15:O:476:ALA:HB2	2.18	0.74
2:B:401:GLU:HG3	2:B:402:VAL:N	2.03	0.74
15:O:407:SER:HB2	15:O:408:PHE:CD1	2.22	0.74
1:A:411:VAL:HG22	1:A:412:SER:H	1.52	0.73
2:B:42:VAL:HB	2:B:46:ILE:HD12	1.59	0.73
2:B:518:ARG:NH2	2:B:537:SER:O	2.21	0.73
15:O:371:HIS:O	15:O:374:PRO:HD2	1.88	0.73
1:A:1048:PHE:HB2	5:E:208:TYR:OH	1.89	0.73
4:D:37:LEU:HD22	4:D:97:LYS:HE3	1.70	0.73
15:O:245:GLN:HA	15:O:245:GLN:HE21	1.51	0.73
15:O:423:TYR:CD1	15:O:594:TYR:CE2	2.72	0.73
1:A:527:PRO:O	1:A:580:HIS:CE1	2.41	0.73
4:D:25:THR:HB	6:F:59:GLN:CG	2.19	0.73
1:A:1603:MET:HE2	1:A:1615:TYR:HD2	1.46	0.73
2:B:478:LEU:HD13	2:B:484:TYR:HE1	1.50	0.73
3:C:55:ASP:OD1	3:C:299:ILE:HG23	1.88	0.73
2:B:1020:GLU:HG2	3:C:61:THR:HG21	1.70	0.73
3:C:253:PRO:O	14:N:180:PHE:CE1	2.41	0.73
7:G:143:SER:OG	15:O:101:SER:O	2.06	0.73
7:G:144:HIS:NE2	15:O:145:SER:CB	2.51	0.73
15:O:120:ILE:CD1	15:O:150:TRP:CE3	2.71	0.73
15:O:194:LEU:CD2	15:O:225:LEU:HD11	2.19	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:28:ILE:CG2	7:G:29:ASP:H	1.89	0.73
15:O:201:LYS:HD3	15:O:239:SER:OG	1.88	0.73
3:C:52:ALA:O	3:C:301:ASN:CG	2.31	0.73
15:O:373:LEU:HD11	15:O:416:LYS:HG2	1.65	0.73
3:C:71:MET:HE2	3:C:225:ALA:CB	2.18	0.73
15:O:237:ILE:HG22	15:O:381:ILE:HB	1.71	0.73
15:O:356:GLU:O	15:O:360:VAL:HG23	1.88	0.73
3:C:56:LEU:HG	3:C:300:PHE:HD1	1.53	0.73
4:D:92:ILE:HG12	7:G:152:ALA:CB	2.16	0.73
1:A:1305:GLU:OE2	9:I:63:LYS:NZ	2.16	0.72
2:B:552:SER:O	2:B:647:SER:N	2.21	0.72
15:O:152:GLN:HG3	15:O:193:TYR:OH	1.89	0.72
15:O:156:MET:SD	15:O:197:PHE:CE2	2.82	0.72
15:O:241:ASP:CG	15:O:380:SER:HB2	2.14	0.72
15:O:348:THR:CG2	15:O:351:SER:HB3	2.19	0.72
1:A:50:TYR:CE1	1:A:368:ARG:O	2.42	0.72
1:A:497:VAL:HG22	1:A:635:MET:HE1	1.70	0.72
15:O:386:PHE:HD2	15:O:606:MET:HE2	1.54	0.72
3:C:54:PHE:O	3:C:299:ILE:C	2.32	0.72
15:O:234:ILE:HG22	15:O:371:HIS:HD2	1.53	0.72
15:O:447:THR:O	15:O:450:LEU:CB	2.33	0.72
15:O:390:GLN:HE21	15:O:432:LYS:H	1.38	0.72
2:B:207:ILE:CD1	2:B:503:VAL:CG2	2.68	0.72
15:O:352:LEU:CA	15:O:358:VAL:HG23	2.19	0.72
4:D:23:HIS:CD2	6:F:58:PHE:CZ	2.78	0.72
1:A:1011:VAL:C	1:A:1201:THR:HG21	2.15	0.72
1:A:413:LEU:CB	1:A:417:ARG:HH21	2.03	0.72
1:A:438:ILE:CG2	2:B:1192:MET:HE2	2.20	0.72
15:O:488:HIS:CD2	15:O:489:ASN:OD1	2.42	0.72
1:A:878:ARG:HE	9:I:67:VAL:HG12	1.53	0.72
1:A:1056:ASP:OD1	1:A:1179:ILE:HD13	1.90	0.72
2:B:938:PHE:CE1	3:C:68:ARG:CZ	2.73	0.72
2:B:938:PHE:CZ	3:C:68:ARG:HD2	2.24	0.72
2:B:207:ILE:CD1	2:B:503:VAL:HG21	2.20	0.72
3:C:56:LEU:CB	3:C:298:PHE:HB2	2.17	0.72
4:D:23:HIS:HD2	6:F:58:PHE:CZ	2.07	0.72
8:H:40:LEU:HD13	8:H:123:MET:HE3	1.72	0.72
15:O:225:LEU:O	15:O:225:LEU:HD13	1.89	0.72
1:A:478:TYR:CA	2:B:1048:SER:CA	2.34	0.71
3:C:45:SER:CB	3:C:271:ARG:HH22	2.03	0.71
15:O:432:LYS:HB3	15:O:609:TYR:HA	0.81	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:152:LEU:HD13	2:B:443:LYS:HG3	1.71	0.71
3:C:54:PHE:O	3:C:299:ILE:HA	1.90	0.71
15:O:158:LEU:HD22	15:O:172:HIS:HA	1.71	0.71
15:O:241:ASP:C	15:O:378:THR:CG2	2.63	0.71
1:A:411:VAL:HG22	1:A:412:SER:N	2.05	0.71
1:A:527:PRO:O	1:A:580:HIS:HE1	1.73	0.71
1:A:1003:ARG:HD2	2:B:520:LEU:H	1.56	0.71
2:B:281:CYS:HA	2:B:323:ARG:HD2	1.72	0.71
2:B:1069:ILE:HD12	2:B:1069:ILE:N	2.05	0.71
15:O:361:PHE:CE1	15:O:365:THR:HG21	2.24	0.71
1:A:524:ILE:O	1:A:554:ARG:NH1	2.23	0.71
2:B:1069:ILE:HG22	2:B:1070:ARG:N	2.03	0.71
3:C:52:ALA:O	3:C:301:ASN:OD1	2.07	0.71
1:A:356:PHE:C	1:A:357:MET:HG3	2.14	0.71
15:O:390:GLN:CD	15:O:609:TYR:HB3	2.15	0.71
1:A:478:TYR:CD1	2:B:1048:SER:HB2	2.25	0.71
1:A:1048:PHE:CD2	5:E:210:SER:HA	2.26	0.71
4:D:92:ILE:CG1	7:G:152:ALA:HB2	2.16	0.71
15:O:128:LEU:HB3	15:O:129:PRO:CD	2.21	0.71
1:A:468:ARG:NE	1:A:1021:ARG:HH12	1.89	0.71
1:A:1038:ILE:HD11	1:A:1050:TYR:HA	1.71	0.71
1:A:83:VAL:CG2	1:A:427:PHE:HE2	2.03	0.71
2:B:211:ARG:NH2	2:B:239:VAL:HG21	2.06	0.71
3:C:31:TRP:CE3	11:K:82:LYS:CG	2.69	0.71
3:C:70:ILE:HD11	11:K:71:THR:HG23	1.71	0.71
6:F:106:PRO:HG2	7:G:55:GLU:HG3	1.73	0.71
15:O:352:LEU:O	15:O:358:VAL:CG2	2.39	0.71
1:A:990:ILE:HB	1:A:994:GLU:CB	2.21	0.70
2:B:470:LEU:HB2	2:B:484:TYR:CE2	2.26	0.70
2:B:1165:ASN:OD1	2:B:1165:ASN:N	2.24	0.70
3:C:54:PHE:CE2	3:C:300:PHE:CG	2.78	0.70
15:O:198:PHE:CE1	15:O:236:LYS:HG3	2.25	0.70
1:A:572:THR:HA	7:G:52:MET:HE3	1.73	0.70
15:O:386:PHE:CD2	15:O:606:MET:HE1	2.25	0.70
15:O:459:GLU:O	15:O:463:GLN:CG	2.37	0.70
3:C:64:ALA:CB	3:C:298:PHE:CE2	2.73	0.70
9:I:2:SER:HB2	9:I:11:LEU:HD21	1.72	0.70
15:O:373:LEU:N	15:O:374:PRO:CD	2.54	0.70
15:O:447:THR:CG2	15:O:480:LEU:HD22	2.21	0.70
1:A:891:ILE:HD12	9:I:71:LEU:HB2	1.71	0.70
7:G:158:LYS:HD3	15:O:105:ASN:HB3	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:894:LYS:N	12:L:54:ARG:NH2	2.34	0.70
7:G:159:LYS:H	15:O:105:ASN:ND2	1.89	0.70
4:D:80:THR:HG21	15:O:227:PHE:HD2	1.56	0.70
15:O:225:LEU:O	15:O:227:PHE:N	2.24	0.70
15:O:428:ILE:O	15:O:487:ARG:NE	2.24	0.70
1:A:1246:VAL:O	1:A:1517:ARG:NH2	2.25	0.70
3:C:55:ASP:CG	3:C:299:ILE:CG1	2.47	0.70
15:O:373:LEU:HD12	15:O:373:LEU:O	1.91	0.70
1:A:436:ALA:HB1	1:A:443:ALA:CB	2.19	0.70
1:A:478:TYR:CE2	2:B:1049:THR:HG22	2.27	0.70
15:O:426:SER:HG	15:O:594:TYR:HB2	1.54	0.70
3:C:223:SER:O	3:C:224:THR:HB	1.92	0.70
2:B:291:GLY:HA3	2:B:375:LEU:HD13	1.74	0.70
1:A:436:ALA:O	1:A:440:SER:HA	1.91	0.69
2:B:64:GLY:O	2:B:68:ILE:HG13	1.92	0.69
3:C:54:PHE:N	3:C:300:PHE:O	2.21	0.69
13:M:38:PHE:HB3	13:M:53:LEU:HD11	1.73	0.69
15:O:369:LYS:HB3	15:O:369:LYS:NZ	2.04	0.69
1:A:406:LEU:CD1	1:A:411:VAL:CB	2.71	0.69
1:A:438:ILE:CG2	2:B:1192:MET:HG2	2.23	0.69
1:A:782:ASP:OD1	1:A:931:SER:O	2.10	0.69
1:A:782:ASP:CG	1:A:783:LYS:N	2.50	0.69
1:A:1348:VAL:HG23	2:B:268:GLU:O	1.91	0.69
1:A:1049:MET:HG2	1:A:1050:TYR:H	1.55	0.69
2:B:42:VAL:HG12	2:B:46:ILE:HG13	1.73	0.69
2:B:211:ARG:CG	2:B:401:GLU:OE1	2.39	0.69
3:C:222:VAL:C	3:C:224:THR:N	2.49	0.69
1:A:99:ARG:O	1:A:109:ARG:NH2	2.24	0.69
1:A:953:GLU:C	1:A:1205:PHE:CB	2.66	0.69
2:B:300:SER:OG	9:I:49:THR:HG22	1.92	0.69
7:G:156:SER:CB	15:O:146:SER:HA	2.22	0.69
15:O:220:GLY:O	15:O:221:TYR:CD1	2.46	0.69
1:A:1:MET:CA	2:B:1098:TYR:CD1	2.75	0.69
4:D:99:LEU:HB3	4:D:100:PRO:CD	2.22	0.69
15:O:369:LYS:O	15:O:373:LEU:CB	2.41	0.69
1:A:478:TYR:CA	2:B:1047:ARG:O	2.41	0.69
3:C:31:TRP:CG	11:K:82:LYS:CD	2.76	0.69
3:C:41:GLU:HB3	3:C:57:ILE:HG22	1.74	0.69
3:C:253:PRO:HB2	14:N:180:PHE:CB	2.22	0.69
15:O:156:MET:HE2	15:O:193:TYR:CE1	2.28	0.69
1:A:982:VAL:HG13	1:A:994:GLU:OE2	1.92	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1573:TYR:O	9:I:122:ARG:NH2	2.26	0.69
15:O:417:LYS:HD3	15:O:472:HIS:HE1	1.57	0.69
1:A:1348:VAL:HG23	2:B:269:TYR:HA	1.75	0.68
4:D:48:GLU:CG	4:D:86:ILE:CD1	2.71	0.68
1:A:953:GLU:C	1:A:1205:PHE:HB3	2.18	0.68
2:B:769:PHE:CD1	2:B:798:PHE:CE1	2.68	0.68
2:B:1002:LYS:HD2	14:N:166:LEU:HB2	1.74	0.68
4:D:25:THR:CB	6:F:59:GLN:CG	2.71	0.68
15:O:174:ASP:HA	15:O:177:LYS:CE	2.22	0.68
2:B:566:TYR:HB3	13:M:74:ASN:OD1	1.94	0.68
15:O:390:GLN:CB	15:O:609:TYR:CD1	2.76	0.68
1:A:432:ASN:HD21	1:A:444:GLN:H	1.38	0.68
1:A:478:TYR:HA	2:B:1048:SER:C	2.18	0.68
3:C:64:ALA:HB1	3:C:227:TYR:CE2	2.29	0.68
3:C:71:MET:CE	3:C:225:ALA:CB	2.71	0.68
15:O:430:ARG:HH21	15:O:596:PRO:HD3	1.55	0.68
1:A:478:TYR:N	2:B:1048:SER:C	2.52	0.68
2:B:934:ILE:CG2	3:C:73:SER:HB3	2.24	0.68
3:C:55:ASP:HB3	3:C:297:HIS:CD2	2.28	0.68
2:B:1043:LYS:HG3	2:B:1063:ARG:NE	2.09	0.68
4:D:80:THR:CG2	15:O:227:PHE:CD2	2.76	0.68
15:O:430:ARG:HH22	15:O:596:PRO:HD3	1.58	0.68
1:A:35:PRO:HA	1:A:390:LEU:CD1	2.24	0.68
1:A:209:THR:HG21	5:E:173:SER:OG	1.93	0.68
15:O:343:VAL:CG1	15:O:388:VAL:CG2	2.71	0.68
2:B:207:ILE:HD11	2:B:503:VAL:CG1	2.25	0.68
15:O:237:ILE:CB	15:O:381:ILE:CD1	2.57	0.68
1:A:572:THR:HA	7:G:52:MET:CE	2.23	0.67
2:B:938:PHE:CE1	3:C:68:ARG:NE	2.61	0.67
15:O:368:PHE:O	15:O:372:VAL:HG23	1.94	0.67
3:C:57:ILE:HD12	3:C:297:HIS:CE1	2.29	0.67
15:O:474:TYR:HB3	15:O:520:CYS:SG	2.33	0.67
2:B:566:TYR:CE2	13:M:70:SER:HA	2.30	0.67
3:C:57:ILE:CD1	3:C:297:HIS:ND1	2.56	0.67
5:E:76:GLY:HA3	5:E:106:GLN:HB2	1.76	0.67
15:O:458:GLU:HG3	15:O:514:PHE:CZ	2.28	0.67
15:O:66:ASN:HD22	15:O:66:ASN:N	1.89	0.67
1:A:381:SER:HB2	1:A:453:ILE:CG2	2.24	0.67
1:A:436:ALA:HB2	1:A:443:ALA:HB1	1.66	0.67
2:B:1043:LYS:CG	2:B:1063:ARG:CZ	2.68	0.67
15:O:431:ALA:HB1	15:O:434:LEU:CD1	2.20	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HB2	1:A:358:ASP:O	1.94	0.67
4:D:48:GLU:HG2	4:D:86:ILE:HD11	1.76	0.67
1:A:1006:LEU:HB3	2:B:539:CYS:SG	2.34	0.67
7:G:142:ALA:C	15:O:102:SER:O	2.38	0.67
15:O:225:LEU:HD13	15:O:225:LEU:C	2.19	0.67
15:O:471:LYS:HB2	15:O:585:PHE:CZ	2.25	0.67
1:A:1011:VAL:C	1:A:1201:THR:CG2	2.68	0.67
1:A:1344:ILE:HG21	2:B:333:LYS:HG3	1.76	0.67
1:A:1556:GLU:OE2	5:E:212:ARG:NH1	2.28	0.67
3:C:71:MET:O	3:C:222:VAL:HG21	1.94	0.67
15:O:371:HIS:O	15:O:374:PRO:HG2	1.95	0.67
1:A:406:LEU:HD12	1:A:406:LEU:O	1.94	0.67
3:C:84:TYR:HD2	12:L:66:GLN:HB2	1.59	0.67
15:O:108:GLU:HB2	15:O:147:ILE:HD11	1.76	0.67
1:A:1027:LEU:O	1:A:1028:GLU:HG2	1.95	0.66
1:A:1603:MET:HG2	1:A:1611:MET:HE1	1.77	0.66
2:B:470:LEU:HD22	2:B:484:TYR:OH	1.95	0.66
3:C:86:PHE:HE1	12:L:64:LEU:CD1	2.08	0.66
3:C:253:PRO:CG	14:N:180:PHE:HB3	2.25	0.66
15:O:371:HIS:O	15:O:374:PRO:CG	2.43	0.66
2:B:207:ILE:HD11	2:B:503:VAL:HG11	1.76	0.66
3:C:222:VAL:C	3:C:224:THR:H	2.03	0.66
15:O:240:ILE:CG2	15:O:332:LEU:CD1	2.67	0.66
1:A:1050:TYR:CE1	1:A:1185:VAL:HG12	2.29	0.66
3:C:131:THR:CG2	3:C:209:ILE:HG23	2.25	0.66
4:D:25:THR:CA	6:F:59:GLN:HG3	2.24	0.66
13:M:101:VAL:HG12	13:M:106:LYS:HG3	1.72	0.66
15:O:390:GLN:HB3	15:O:609:TYR:CD1	2.30	0.66
1:A:113:VAL:HG21	1:A:178:LEU:HD13	1.77	0.66
3:C:223:SER:HB2	3:C:303:GLU:HB3	1.76	0.66
1:A:863:ASN:HD22	9:I:67:VAL:CA	2.07	0.66
4:D:96:PHE:CE1	7:G:150:HIS:CG	2.83	0.66
15:O:240:ILE:CG2	15:O:332:LEU:CD2	2.63	0.66
1:A:437:PHE:O	1:A:455:GLY:HA3	1.96	0.66
7:G:242:VAL:HG21	15:O:183:ILE:CG2	2.26	0.66
15:O:434:LEU:HD12	15:O:434:LEU:N	2.10	0.66
1:A:403:LEU:HD12	1:A:419:ILE:HG21	1.77	0.66
15:O:428:ILE:HG23	15:O:439:ILE:CG2	2.23	0.66
1:A:478:TYR:H	2:B:1048:SER:C	2.03	0.66
1:A:1000:MET:CG	2:B:520:LEU:HD23	2.26	0.66
1:A:1344:ILE:CG2	2:B:333:LYS:HG3	2.26	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:31:TRP:NE1	11:K:82:LYS:HZ2	1.93	0.66
15:O:386:PHE:CD2	15:O:606:MET:HE2	2.28	0.66
1:A:109:ARG:NH1	1:A:230:ARG:O	2.29	0.66
1:A:1055:ILE:HD11	1:A:1063:MET:HE1	1.78	0.66
15:O:454:VAL:HG23	15:O:458:GLU:HG3	1.77	0.66
1:A:403:LEU:CD1	1:A:419:ILE:CG2	2.74	0.66
15:O:247:GLU:OE1	15:O:325:ILE:HG13	1.95	0.66
2:B:209:GLN:HG2	2:B:210:ARG:N	2.07	0.65
2:B:209:GLN:O	2:B:401:GLU:N	2.27	0.65
15:O:454:VAL:HG23	15:O:458:GLU:CD	2.20	0.65
1:A:1000:MET:HG2	2:B:520:LEU:CD2	2.25	0.65
3:C:52:ALA:O	3:C:301:ASN:CA	2.42	0.65
15:O:422:GLN:NE2	15:O:592:PHE:CD2	2.65	0.65
1:A:478:TYR:CA	2:B:1048:SER:O	2.44	0.65
1:A:756:LYS:HD3	9:I:85:LYS:HZ2	1.32	0.65
2:B:300:SER:OG	9:I:49:THR:CG2	2.44	0.65
2:B:711:GLN:HG2	2:B:713:PRO:HD2	1.78	0.65
3:C:230:LEU:CG	3:C:294:VAL:HG21	2.26	0.65
15:O:146:SER:O	15:O:148:PRO:HD3	1.95	0.65
15:O:219:ARG:HH21	15:O:360:VAL:HG22	1.60	0.65
2:B:891:GLU:HA	12:L:54:ARG:NE	2.12	0.65
3:C:272:LYS:HG2	14:N:175:TYR:CD1	2.32	0.65
4:D:48:GLU:HG3	4:D:86:ILE:HD12	1.78	0.65
15:O:458:GLU:CG	15:O:514:PHE:CZ	2.79	0.65
1:A:799:GLU:HG3	1:A:1062:HIS:CE1	2.32	0.65
1:A:1034:TYR:CD1	1:A:1181:PRO:HG2	2.32	0.65
2:B:566:TYR:CD2	13:M:73:SER:OG	2.48	0.65
2:B:938:PHE:CZ	3:C:68:ARG:CD	2.80	0.65
4:D:99:LEU:HB3	4:D:100:PRO:HD3	1.78	0.65
15:O:343:VAL:CG1	15:O:388:VAL:HG23	2.27	0.65
1:A:406:LEU:CD1	1:A:411:VAL:CG2	2.74	0.65
1:A:1261:VAL:HG13	1:A:1265:GLU:CD	2.22	0.65
2:B:341:SER:OG	2:B:343:ASP:OD1	2.13	0.65
4:D:25:THR:HG21	6:F:59:GLN:NE2	2.12	0.65
15:O:241:ASP:OD1	15:O:379:ARG:C	2.39	0.65
1:A:502:ALA:CB	1:A:581:ILE:CG2	2.63	0.65
15:O:241:ASP:CB	15:O:380:SER:HB2	2.26	0.65
15:O:488:HIS:NE2	15:O:489:ASN:OD1	2.29	0.65
1:A:1651:THR:OG1	2:B:1085:SER:OG	2.14	0.65
3:C:59:ILE:HG23	3:C:298:PHE:HE1	1.54	0.65
7:G:144:HIS:NE2	15:O:145:SER:HB2	2.12	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:241:ASP:HA	15:O:380:SER:HB2	1.78	0.65
1:A:406:LEU:HD11	1:A:411:VAL:HG21	1.78	0.65
1:A:438:ILE:HG23	2:B:1192:MET:CE	2.26	0.65
2:B:915:ASP:OD1	2:B:1038:HIS:HD2	1.78	0.65
2:B:923:GLN:NE2	2:B:953:ALA:O	2.30	0.65
15:O:343:VAL:HG11	15:O:388:VAL:CG2	2.27	0.65
7:G:156:SER:HB2	15:O:146:SER:HA	1.78	0.64
15:O:417:LYS:CD	15:O:472:HIS:HE1	2.10	0.64
15:O:428:ILE:HD12	15:O:439:ILE:HD12	1.79	0.64
1:A:1575:ILE:HG13	9:I:122:ARG:HH12	1.60	0.64
2:B:373:MET:HG3	2:B:377:MET:HE3	1.79	0.64
15:O:374:PRO:CG	15:O:375:THR:HG23	2.27	0.64
1:A:834:ARG:NH2	2:B:994:ASP:OD1	2.30	0.64
1:A:1053:ASP:O	1:A:1054:ALA:HB3	1.97	0.64
1:A:1262:LEU:CD2	1:A:1497:ILE:HG12	2.28	0.64
2:B:1120:ILE:HD12	15:O:117:GLN:HE22	1.63	0.64
3:C:54:PHE:CE1	3:C:300:PHE:HB3	2.31	0.64
7:G:159:LYS:HB3	15:O:103:ASN:OD1	1.98	0.64
15:O:510:VAL:HG13	15:O:517:LEU:HD11	1.79	0.64
2:B:623:ASP:O	2:B:648:ARG:NH1	2.25	0.64
1:A:1023:LEU:HD23	1:A:1598:PHE:CD1	2.32	0.64
1:A:1344:ILE:CD1	2:B:329:TYR:CE2	2.71	0.64
2:B:469:ASN:HA	2:B:481:VAL:O	1.97	0.64
3:C:86:PHE:CE1	12:L:64:LEU:CD1	2.79	0.64
1:A:83:VAL:CB	1:A:427:PHE:CE2	2.81	0.64
1:A:413:LEU:O	1:A:417:ARG:NH2	2.30	0.64
1:A:480:ALA:CB	2:B:1046:VAL:CG2	2.63	0.64
1:A:1036:ASN:HB3	1:A:1049:MET:HG3	1.78	0.64
3:C:82:TYR:HE1	12:L:68:GLU:OE1	1.80	0.64
7:G:144:HIS:NE2	15:O:145:SER:HB3	2.13	0.64
1:A:1038:ILE:CG1	1:A:1049:MET:O	2.44	0.64
1:A:1273:THR:HG23	9:I:48:VAL:HG22	1.79	0.64
2:B:699:ILE:HD13	2:B:760:TYR:CE1	2.32	0.64
15:O:108:GLU:HG3	15:O:108:GLU:O	1.96	0.64
15:O:240:ILE:CG2	15:O:332:LEU:CG	2.76	0.64
1:A:995:TYR:O	1:A:999:CYS:HB2	1.98	0.64
1:A:1055:ILE:CG2	1:A:1063:MET:SD	2.85	0.64
3:C:73:SER:O	3:C:214:GLY:N	2.31	0.64
5:E:20:LYS:HE2	5:E:34:GLU:HG2	1.80	0.64
15:O:170:VAL:HG13	15:O:171:CYS:N	2.12	0.64
1:A:478:TYR:OH	2:B:1049:THR:HG21	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:PHE:O	3:C:299:ILE:CA	2.45	0.64
1:A:399:LEU:CD2	1:A:423:LEU:HA	2.28	0.64
1:A:1021:ARG:HD3	2:B:1073:GLU:OE1	1.98	0.64
15:O:368:PHE:CE2	15:O:382:GLN:HA	2.33	0.64
15:O:383:TYR:CE2	15:O:597:LEU:HD22	2.33	0.64
4:D:25:THR:CB	6:F:59:GLN:HE21	2.06	0.63
12:L:68:GLU:HG2	12:L:69:ALA:N	2.01	0.63
1:A:1322:ILE:HD12	1:A:1457:ILE:HD11	1.79	0.63
8:H:44:VAL:HG22	8:H:48:PRO:HA	1.81	0.63
15:O:454:VAL:HG23	15:O:458:GLU:CG	2.28	0.63
1:A:476:VAL:HG11	2:B:1071:VAL:CG2	2.25	0.63
1:A:1654:PHE:CE2	6:F:92:ARG:HD3	2.33	0.63
3:C:41:GLU:CB	3:C:57:ILE:CG2	2.70	0.63
15:O:392:GLN:HB2	15:O:395:LEU:HD22	1.79	0.63
15:O:426:SER:OG	15:O:594:TYR:CA	2.46	0.63
1:A:1026:GLN:HE22	1:A:1603:MET:HA	1.61	0.63
15:O:454:VAL:HG23	15:O:458:GLU:OE2	1.98	0.63
1:A:413:LEU:C	1:A:417:ARG:NH2	2.56	0.63
2:B:281:CYS:HA	2:B:323:ARG:CD	2.29	0.63
3:C:75:VAL:CG1	3:C:221:PRO:HD2	2.06	0.63
7:G:141:SER:CB	15:O:138:TYR:CZ	2.81	0.63
1:A:888:LYS:HE2	9:I:69:THR:HG22	1.79	0.63
1:A:1600:ARG:NE	1:A:1616:GLU:OE1	2.30	0.63
2:B:475:GLY:O	2:B:476:LEU:HB2	1.98	0.63
15:O:155:SER:HA	15:O:158:LEU:HD12	1.81	0.63
15:O:379:ARG:CB	15:O:382:GLN:HE22	2.12	0.63
1:A:401:ASP:OD2	1:A:405:LYS:NZ	2.32	0.63
1:A:402:ASP:O	1:A:406:LEU:HD23	1.99	0.63
1:A:408:LYS:HA	1:A:411:VAL:HG11	1.79	0.63
1:A:1655:ASP:N	6:F:135:ARG:O	2.28	0.63
4:D:80:THR:CG2	15:O:227:PHE:CB	2.75	0.63
6:F:70:LYS:HG3	7:G:94:PRO:HB2	1.80	0.63
15:O:373:LEU:N	15:O:374:PRO:HD2	2.14	0.63
1:A:1060:GLU:O	1:A:1060:GLU:HG2	1.98	0.63
4:D:23:HIS:HD2	6:F:58:PHE:CE2	2.16	0.63
7:G:158:LYS:CE	15:O:105:ASN:OD1	2.47	0.63
15:O:245:GLN:HA	15:O:245:GLN:NE2	2.14	0.63
15:O:471:LYS:HG3	15:O:472:HIS:N	2.14	0.63
1:A:436:ALA:O	1:A:440:SER:CA	2.46	0.62
1:A:509:GLU:HG2	1:A:579:ARG:HG2	1.81	0.62
3:C:75:VAL:HG12	3:C:76:PRO:O	1.98	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:142:ALA:O	15:O:102:SER:O	2.16	0.62
12:L:68:GLU:CG	12:L:69:ALA:H	2.05	0.62
1:A:83:VAL:CG2	1:A:427:PHE:HZ	2.01	0.62
1:A:991:LYS:N	1:A:994:GLU:OE1	2.31	0.62
15:O:181:ARG:HH11	15:O:181:ARG:CG	2.12	0.62
1:A:438:ILE:HG23	2:B:1192:MET:HE2	1.81	0.62
1:A:1050:TYR:HB2	1:A:1179:ILE:HG21	1.81	0.62
2:B:42:VAL:CA	2:B:46:ILE:HD12	2.29	0.62
4:D:25:THR:C	6:F:59:GLN:HG3	2.24	0.62
15:O:151:TRP:CZ2	15:O:176:LEU:HD23	2.35	0.62
3:C:41:GLU:O	3:C:57:ILE:HG22	1.99	0.62
15:O:98:ASP:OD2	15:O:135:LYS:HD3	1.99	0.62
15:O:457:ARG:HA	15:O:460:GLU:CB	2.30	0.62
2:B:40:GLU:OE1	2:B:550:ARG:NH2	2.32	0.62
15:O:447:THR:HA	15:O:450:LEU:HD12	1.80	0.62
1:A:406:LEU:HD12	1:A:411:VAL:HB	1.82	0.62
2:B:467:THR:C	2:B:469:ASN:H	2.07	0.62
5:E:197:LYS:HD3	5:E:199:ILE:HD11	1.79	0.62
1:A:1028:GLU:CG	1:A:1029:GLY:N	2.62	0.62
1:A:1657:LEU:HD21	6:F:135:ARG:CZ	2.30	0.62
2:B:554:GLN:HA	2:B:646:HIS:CD2	2.34	0.62
2:B:1043:LYS:HG3	2:B:1063:ARG:CD	2.29	0.62
3:C:58:ASN:N	3:C:296:ASN:O	2.30	0.62
15:O:460:GLU:O	15:O:469:ARG:NH1	2.32	0.62
1:A:891:ILE:CD1	9:I:71:LEU:CB	2.77	0.62
3:C:59:ILE:O	3:C:298:PHE:HE1	1.83	0.62
15:O:343:VAL:HG12	15:O:388:VAL:HG23	1.82	0.62
15:O:435:SER:HB3	15:O:438:GLN:CG	2.23	0.62
1:A:1348:VAL:CG2	2:B:268:GLU:C	2.72	0.62
3:C:62:SER:CB	11:K:74:ASN:HD21	2.12	0.62
15:O:368:PHE:CE2	15:O:385:MET:HB2	2.34	0.62
15:O:581:THR:HA	15:O:584:GLN:NE2	2.15	0.62
2:B:934:ILE:HG23	3:C:73:SER:HB3	1.82	0.61
3:C:55:ASP:OD2	3:C:299:ILE:HG12	1.97	0.61
4:D:47:LYS:HD2	4:D:82:LEU:HD21	1.82	0.61
15:O:100:LEU:HD22	15:O:107:ILE:HD11	1.82	0.61
15:O:144:CYS:O	15:O:148:PRO:HG3	2.00	0.61
12:L:30:ILE:CD1	12:L:59:ALA:HB2	2.29	0.61
15:O:431:ALA:HB3	15:O:434:LEU:CD1	2.23	0.61
15:O:447:THR:CG2	15:O:480:LEU:CD2	2.79	0.61
15:O:450:LEU:O	15:O:454:VAL:HG12	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:THR:CG2	3:C:208:CYS:O	2.48	0.61
15:O:158:LEU:HB3	15:O:172:HIS:HB3	1.82	0.61
1:A:406:LEU:HD13	1:A:411:VAL:CB	2.27	0.61
1:A:1025:LYS:HZ2	2:B:1076:ARG:NH1	1.98	0.61
5:E:145:THR:C	5:E:147:HIS:H	2.08	0.61
1:A:799:GLU:CD	1:A:1062:HIS:HB2	2.25	0.61
1:A:1662:ASN:N	7:G:101:SER:O	2.32	0.61
2:B:769:PHE:HE1	2:B:798:PHE:HZ	1.48	0.61
7:G:141:SER:HB3	15:O:138:TYR:OH	1.95	0.61
15:O:447:THR:HG22	15:O:480:LEU:CD2	2.28	0.61
1:A:413:LEU:O	1:A:417:ARG:CZ	2.47	0.61
2:B:1069:ILE:O	2:B:1070:ARG:HB2	2.00	0.61
6:F:73:ALA:HB2	6:F:143:PHE:CZ	2.36	0.61
15:O:181:ARG:HB2	15:O:181:ARG:NH1	2.12	0.61
15:O:369:LYS:HG3	15:O:406:ILE:HD11	1.83	0.61
15:O:396:MET:SD	15:O:434:LEU:HA	2.41	0.61
1:A:1050:TYR:CB	1:A:1179:ILE:HG21	2.31	0.61
2:B:923:GLN:NE2	2:B:957:ARG:HD2	2.16	0.61
3:C:71:MET:CE	3:C:225:ALA:HB1	2.30	0.61
12:L:30:ILE:HD11	12:L:59:ALA:HB2	1.82	0.61
15:O:67:ASP:OD1	15:O:69:THR:HB	2.00	0.61
1:A:509:GLU:HG3	1:A:579:ARG:HD3	1.81	0.61
1:A:1660:VAL:CG2	7:G:103:LYS:HB2	2.30	0.61
3:C:71:MET:SD	3:C:225:ALA:CB	2.88	0.61
4:D:44:ILE:HD13	4:D:90:LYS:HG3	1.82	0.61
15:O:98:ASP:CG	15:O:135:LYS:HD3	2.26	0.61
15:O:408:PHE:CE1	15:O:446:LEU:HD13	2.35	0.61
1:A:564:PRO:HB2	15:O:371:HIS:CE1	2.36	0.61
15:O:56:VAL:HG21	15:O:99:ILE:HD12	1.82	0.61
15:O:371:HIS:O	15:O:374:PRO:CD	2.49	0.61
1:A:479:ALA:HB2	2:B:1091:ARG:HH22	1.65	0.60
2:B:552:SER:OG	2:B:647:SER:N	2.35	0.60
8:H:25:ARG:NH1	8:H:27:GLU:OE2	2.34	0.60
15:O:457:ARG:O	15:O:460:GLU:CB	2.47	0.60
15:O:467:MET:HG3	15:O:519:PHE:CE2	2.36	0.60
15:O:582:ARG:O	15:O:586:ILE:HG13	2.01	0.60
1:A:932:GLY:O	9:I:125:ASN:ND2	2.34	0.60
1:A:1344:ILE:HG22	2:B:333:LYS:CG	2.31	0.60
1:A:1651:THR:OG1	2:B:1085:SER:CB	2.49	0.60
1:A:1052:GLY:O	5:E:205:SER:CB	2.48	0.60
1:A:1655:ASP:CG	6:F:137:TYR:CE2	2.76	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:93:MET:HG3	5:E:120:ALA:HB1	1.82	0.60
15:O:447:THR:C	15:O:450:LEU:H	2.09	0.60
15:O:487:ARG:HH11	15:O:487:ARG:CG	2.14	0.60
1:A:799:GLU:OE2	1:A:1062:HIS:HB2	2.01	0.60
1:A:1482:LYS:HE2	2:B:304:ASP:CG	2.26	0.60
2:B:938:PHE:CD1	3:C:68:ARG:CZ	2.83	0.60
1:A:1261:VAL:HG13	1:A:1265:GLU:OE1	2.01	0.60
2:B:1020:GLU:CG	3:C:61:THR:HG21	2.32	0.60
3:C:272:LYS:CG	14:N:175:TYR:CE1	2.83	0.60
4:D:80:THR:HG21	15:O:227:PHE:CB	2.28	0.60
7:G:143:SER:CB	15:O:101:SER:O	2.48	0.60
1:A:1034:TYR:HA	1:A:1181:PRO:CG	2.32	0.60
2:B:1090:ASP:O	2:B:1095:SER:N	2.34	0.60
1:A:246:ASP:HB3	1:A:248:PHE:H	1.66	0.60
1:A:1226:VAL:HG12	1:A:1227:MET:HG2	1.83	0.60
1:A:449:GLY:O	1:A:451:VAL:N	2.34	0.60
1:A:1038:ILE:HG12	1:A:1049:MET:C	2.27	0.60
1:A:1049:MET:C	1:A:1051:GLY:H	2.09	0.60
2:B:228:SER:HB2	2:B:253:LEU:HD23	1.84	0.60
3:C:84:TYR:CE2	12:L:66:GLN:CD	2.77	0.60
1:A:84:PRO:HG2	1:A:318:THR:HG22	1.84	0.60
1:A:477:ASN:O	1:A:478:TYR:HB2	2.01	0.60
2:B:699:ILE:CD1	2:B:760:TYR:CE1	2.85	0.60
1:A:87:ASN:HB2	1:A:357:MET:SD	2.42	0.60
15:O:98:ASP:OD2	15:O:135:LYS:NZ	2.35	0.60
15:O:369:LYS:HD2	15:O:369:LYS:C	2.27	0.60
1:A:1026:GLN:OE1	1:A:1603:MET:CB	2.48	0.59
3:C:55:ASP:HB3	3:C:297:HIS:NE2	2.17	0.59
1:A:1008:ASP:O	1:A:1011:VAL:CG2	2.41	0.59
1:A:1034:TYR:HA	1:A:1181:PRO:HG3	1.84	0.59
1:A:1054:ALA:O	1:A:1178:LEU:HD23	2.02	0.59
2:B:1019:GLY:HA3	3:C:65:ASN:CB	2.27	0.59
15:O:198:PHE:CD1	15:O:236:LYS:CE	2.78	0.59
1:A:406:LEU:HD13	1:A:411:VAL:CG2	2.31	0.59
6:F:106:PRO:HG2	7:G:55:GLU:CG	2.30	0.59
1:A:699:CYS:O	1:A:815:ARG:NH1	2.35	0.59
2:B:207:ILE:O	2:B:207:ILE:HG22	2.02	0.59
2:B:481:VAL:O	2:B:481:VAL:HG12	2.01	0.59
1:A:35:PRO:HA	1:A:390:LEU:HD12	1.84	0.59
1:A:1027:LEU:HD21	1:A:1588:MET:HG2	1.84	0.59
1:A:1608:SER:OG	1:A:1632:GLU:OE2	2.20	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:878:ARG:HG2	9:I:67:VAL:CG1	2.29	0.59
2:B:211:ARG:HB3	2:B:239:VAL:CG1	2.32	0.59
2:B:551:ILE:HA	2:B:648:ARG:O	2.02	0.59
2:B:566:TYR:HB2	13:M:73:SER:OG	2.03	0.59
1:A:720:PHE:CE2	8:H:141:TYR:HE2	2.21	0.59
1:A:977:MET:HE1	1:A:991:LYS:HD2	1.83	0.59
5:E:55:ARG:NH2	5:E:113:GLN:OE1	2.36	0.59
15:O:374:PRO:HB2	15:O:375:THR:HG23	1.85	0.59
15:O:390:GLN:HB2	15:O:609:TYR:CD1	2.37	0.59
1:A:509:GLU:O	1:A:576:LYS:HA	2.03	0.59
1:A:863:ASN:ND2	9:I:68:LYS:H	2.01	0.59
1:A:996:TYR:HE1	1:A:1000:MET:CE	2.14	0.59
15:O:101:SER:HB3	15:O:142:ILE:CD1	2.33	0.59
15:O:377:TYR:O	15:O:378:THR:OG1	2.20	0.59
15:O:488:HIS:C	15:O:490:ILE:H	2.10	0.59
1:A:516:ILE:HG21	15:O:376:TYR:CZ	2.38	0.59
1:A:581:ILE:HG13	1:A:582:LYS:H	1.68	0.59
2:B:328:GLN:NE2	13:M:109:ARG:HH21	1.99	0.59
2:B:829:ASN:OD1	2:B:829:ASN:N	2.36	0.59
15:O:372:VAL:C	15:O:374:PRO:CD	2.76	0.59
1:A:478:TYR:CA	2:B:1048:SER:C	2.74	0.59
2:B:110:ASN:O	2:B:112:GLY:N	2.35	0.59
2:B:209:GLN:O	2:B:401:GLU:HG2	2.03	0.59
2:B:563:SER:CB	13:M:73:SER:HB3	2.33	0.59
3:C:231:PRO:HG2	3:C:270:ALA:HB1	1.83	0.59
3:C:272:LYS:HG2	14:N:175:TYR:CE1	2.38	0.59
15:O:369:LYS:HD3	15:O:373:LEU:HD22	1.85	0.59
15:O:428:ILE:CD1	15:O:439:ILE:HD12	2.33	0.59
1:A:990:ILE:CB	1:A:994:GLU:OE1	2.51	0.58
2:B:538:PRO:HB2	2:B:542:LEU:HG	1.84	0.58
15:O:241:ASP:O	15:O:378:THR:CG2	2.51	0.58
15:O:348:THR:HG23	15:O:351:SER:H	1.67	0.58
15:O:607:LYS:HG3	15:O:608:GLU:N	2.17	0.58
1:A:412:SER:C	1:A:414:GLU:N	2.56	0.58
1:A:1048:PHE:HZ	5:E:211:TYR:CD1	2.18	0.58
3:C:253:PRO:CB	14:N:180:PHE:HB3	2.33	0.58
7:G:159:LYS:N	15:O:105:ASN:HD22	2.01	0.58
1:A:598:ALA:HB1	1:A:601:MET:HE3	1.85	0.58
7:G:30:GLU:HA	7:G:32:ASN:N	2.18	0.58
15:O:129:PRO:CG	15:O:132:THR:CB	2.74	0.58
15:O:164:LEU:O	15:O:165:PRO:O	2.20	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:369:LYS:CE	15:O:370:THR:HG22	2.33	0.58
1:A:415:ASP:HA	1:A:418:VAL:HG12	1.84	0.58
1:A:1055:ILE:HD11	1:A:1174:TYR:CD2	2.39	0.58
1:A:1074:TYR:HE2	1:A:1159:ASP:HB3	1.68	0.58
1:A:1660:VAL:HG23	7:G:103:LYS:HB2	1.85	0.58
2:B:328:GLN:HE22	13:M:109:ARG:NH2	1.99	0.58
2:B:415:GLU:OE2	2:B:474:SER:OG	2.21	0.58
1:A:437:PHE:CZ	1:A:456:VAL:HG22	2.28	0.58
1:A:1603:MET:HE2	1:A:1615:TYR:CG	2.35	0.58
4:D:48:GLU:HG3	4:D:86:ILE:CD1	2.32	0.58
11:K:68:GLU:HG2	11:K:72:LEU:HD23	1.86	0.58
15:O:454:VAL:CG2	15:O:458:GLU:OE2	2.51	0.58
1:A:468:ARG:HE	1:A:1021:ARG:NH1	2.00	0.58
2:B:1019:GLY:CA	3:C:65:ASN:HB2	2.28	0.58
3:C:221:PRO:O	3:C:222:VAL:HG13	2.04	0.58
4:D:25:THR:HG21	6:F:59:GLN:HE21	1.57	0.58
4:D:27:LEU:HD22	7:G:23:GLN:O	2.03	0.58
1:A:1660:VAL:HG22	7:G:103:LYS:C	2.28	0.58
3:C:253:PRO:HB2	14:N:180:PHE:HB3	1.85	0.58
15:O:484:PHE:CD1	15:O:502:LEU:HD13	2.38	0.58
7:G:159:LYS:N	15:O:105:ASN:ND2	2.51	0.58
15:O:488:HIS:C	15:O:490:ILE:N	2.59	0.58
2:B:33:SER:C	2:B:35:PHE:H	2.12	0.58
2:B:923:GLN:HG2	2:B:949:ILE:HD11	1.84	0.58
2:B:1016:GLY:O	3:C:69:ARG:HD2	2.04	0.58
13:M:10:ILE:HB	14:N:70:LEU:HB3	1.86	0.58
1:A:406:LEU:CD1	1:A:411:VAL:HG21	2.34	0.58
2:B:117:VAL:HG13	2:B:117:VAL:O	2.03	0.58
4:D:48:GLU:OE1	4:D:90:LYS:NZ	2.37	0.58
12:L:38:LEU:HD12	12:L:49:LYS:HG3	1.85	0.58
15:O:421:LEU:HD13	15:O:476:ALA:CB	2.31	0.58
15:O:423:TYR:HD1	15:O:594:TYR:CZ	2.20	0.58
12:L:33:GLU:HG3	12:L:53:HIS:CE1	2.39	0.57
15:O:174:ASP:O	15:O:177:LYS:CG	2.52	0.57
1:A:407:GLN:O	1:A:411:VAL:HG12	2.04	0.57
1:A:581:ILE:HG13	1:A:582:LYS:N	2.19	0.57
14:N:89:ILE:HG12	14:N:139:VAL:HG22	1.85	0.57
1:A:408:LYS:C	1:A:411:VAL:HG12	2.29	0.57
3:C:56:LEU:CG	3:C:300:PHE:CD1	2.86	0.57
15:O:369:LYS:O	15:O:373:LEU:HB3	2.04	0.57
1:A:476:VAL:CG1	2:B:1071:VAL:HG23	2.30	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:ILE:HG22	1:A:1060:GLU:HB2	1.87	0.57
15:O:247:GLU:HB3	15:O:325:ILE:HD11	1.86	0.57
15:O:471:LYS:CB	15:O:585:PHE:HE1	1.94	0.57
2:B:848:ILE:HB	12:L:60:ARG:HG3	1.86	0.57
3:C:51:GLU:CB	3:C:303:GLU:CG	2.80	0.57
15:O:390:GLN:C	15:O:609:TYR:CE1	2.81	0.57
15:O:487:ARG:O	15:O:490:ILE:HB	2.03	0.57
1:A:493:ASN:HB3	1:A:654:ASP:OD1	2.04	0.57
1:A:782:ASP:O	1:A:784:SER:N	2.38	0.57
1:A:953:GLU:HA	1:A:1205:PHE:CG	2.40	0.57
2:B:207:ILE:HD11	2:B:503:VAL:CG2	2.34	0.57
2:B:893:ASN:HA	12:L:54:ARG:NH2	2.20	0.57
6:F:66:ARG:CZ	7:G:90:LEU:CD1	2.80	0.57
7:G:143:SER:HB3	15:O:103:ASN:N	2.20	0.57
15:O:173:HIS:CD2	15:O:217:LYS:HG2	2.39	0.57
15:O:391:GLN:OE1	15:O:609:TYR:OH	2.23	0.57
1:A:1003:ARG:NE	2:B:520:LEU:CB	2.61	0.57
15:O:128:LEU:HD22	15:O:129:PRO:HD3	1.86	0.57
15:O:190:ILE:HA	15:O:193:TYR:CD2	2.39	0.57
15:O:417:LYS:HB3	15:O:472:HIS:CE1	2.39	0.57
15:O:484:PHE:CE1	15:O:502:LEU:HD13	2.39	0.57
1:A:468:ARG:NE	1:A:1021:ARG:CZ	2.63	0.57
1:A:1235:THR:O	1:A:1544:ASN:ND2	2.38	0.57
2:B:833:PRO:HG2	2:B:836:TRP:CE2	2.40	0.57
15:O:230:TRP:CZ2	15:O:364:LEU:HD11	2.39	0.57
15:O:422:GLN:NE2	15:O:592:PHE:CZ	2.69	0.57
1:A:18:ILE:HD12	1:A:354:SER:HB3	1.85	0.57
1:A:727:THR:HG21	8:H:119:GLY:O	2.05	0.57
1:A:988:SER:HB2	2:B:988:GLU:HG2	1.87	0.57
1:A:1606:SER:HB3	1:A:1611:MET:HE3	1.87	0.57
2:B:1043:LYS:HG3	2:B:1063:ARG:HD2	1.85	0.57
1:A:1048:PHE:O	1:A:1049:MET:HB2	2.04	0.57
3:C:56:LEU:CG	3:C:300:PHE:CE1	2.88	0.57
4:D:48:GLU:CG	4:D:86:ILE:HD11	2.35	0.57
15:O:158:LEU:HD22	15:O:172:HIS:CB	2.35	0.57
1:A:563:THR:HA	15:O:375:THR:HG21	1.87	0.56
2:B:894:LYS:HG2	12:L:47:ARG:HD2	1.86	0.56
2:B:894:LYS:HG2	12:L:47:ARG:NE	2.19	0.56
2:B:1020:GLU:CG	3:C:61:THR:OG1	2.53	0.56
15:O:154:VAL:O	15:O:158:LEU:HG	2.04	0.56
1:A:412:SER:HB3	1:A:414:GLU:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:207:ILE:HD11	2:B:503:VAL:HG21	1.87	0.56
2:B:800:TYR:CD1	2:B:801:GLY:N	2.73	0.56
3:C:82:TYR:CE1	12:L:68:GLU:OE1	2.58	0.56
4:D:28:PRO:HD2	7:G:24:VAL:CG1	2.35	0.56
6:F:75:PRO:HG2	6:F:78:GLN:CG	2.34	0.56
7:G:20:HIS:O	7:G:20:HIS:ND1	2.38	0.56
1:A:1050:TYR:CG	1:A:1179:ILE:HG21	2.40	0.56
2:B:338:PHE:HZ	2:B:357:ILE:HD12	1.70	0.56
2:B:890:ASP:O	12:L:54:ARG:NE	2.38	0.56
2:B:1013:MET:SD	2:B:1026:ILE:HG12	2.45	0.56
3:C:223:SER:HB2	3:C:303:GLU:CB	2.35	0.56
5:E:90:VAL:HG13	5:E:120:ALA:HA	1.88	0.56
7:G:56:ASN:HB3	7:G:59:GLN:HB3	1.86	0.56
7:G:143:SER:CB	15:O:104:ILE:N	2.57	0.56
15:O:109:SER:OG	15:O:111:ARG:HG3	2.05	0.56
1:A:966:LEU:CD2	1:A:997:PHE:CZ	2.83	0.56
3:C:56:LEU:HD12	3:C:300:PHE:CE1	2.23	0.56
11:K:49:LEU:HD23	11:K:51:THR:HG23	1.86	0.56
15:O:458:GLU:HG2	15:O:514:PHE:CZ	2.40	0.56
2:B:1020:GLU:HG2	3:C:61:THR:OG1	2.06	0.56
3:C:86:PHE:HE2	3:C:205:LYS:HG3	1.69	0.56
12:L:63:ARG:HG3	12:L:64:LEU:H	1.69	0.56
1:A:477:ASN:OD1	2:B:1047:ARG:NH1	2.39	0.56
2:B:208:VAL:HG23	2:B:401:GLU:CG	2.35	0.56
2:B:554:GLN:CA	2:B:646:HIS:CD2	2.89	0.56
7:G:141:SER:HB3	15:O:138:TYR:CZ	2.41	0.56
14:N:69:SER:OG	14:N:70:LEU:N	2.37	0.56
15:O:432:LYS:HG3	15:O:608:GLU:O	1.96	0.56
15:O:447:THR:HA	15:O:450:LEU:CG	2.35	0.56
1:A:990:ILE:HB	1:A:994:GLU:OE1	2.06	0.56
15:O:191:ASP:O	15:O:194:LEU:HB2	2.06	0.56
15:O:205:ARG:O	15:O:209:VAL:HG12	2.05	0.56
2:B:480:GLN:HB3	2:B:507:SER:OG	2.05	0.56
13:M:15:VAL:HG22	13:M:90:LEU:HB2	1.88	0.56
15:O:63:LEU:HD23	15:O:111:ARG:HD2	1.87	0.56
1:A:35:PRO:HA	1:A:390:LEU:HD13	1.88	0.56
1:A:797:LEU:HD13	1:A:809:VAL:HG21	1.87	0.56
2:B:472:SER:O	2:B:473:GLN:C	2.48	0.56
15:O:129:PRO:HG2	15:O:132:THR:OG1	2.06	0.56
15:O:440:ILE:CG2	15:O:491:PHE:CE1	2.82	0.56
15:O:458:GLU:CB	15:O:461:VAL:CG2	2.80	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:484:PHE:CD1	15:O:502:LEU:CD1	2.89	0.56
1:A:468:ARG:CZ	1:A:1021:ARG:NH1	2.65	0.56
1:A:1655:ASP:CB	6:F:135:ARG:HB3	2.36	0.56
2:B:470:LEU:HB3	2:B:481:VAL:HG13	1.87	0.56
3:C:64:ALA:CB	3:C:298:PHE:CD2	2.89	0.56
1:A:87:ASN:CB	1:A:357:MET:SD	2.94	0.55
1:A:478:TYR:OH	2:B:1049:THR:CG2	2.51	0.55
1:A:1655:ASP:CG	6:F:137:TYR:HE2	2.14	0.55
2:B:1020:GLU:HG2	3:C:61:THR:CG2	2.34	0.55
1:A:1:MET:CG	2:B:1098:TYR:CE2	2.88	0.55
1:A:527:PRO:C	1:A:580:HIS:HE1	2.14	0.55
2:B:470:LEU:HB2	2:B:484:TYR:HE2	1.66	0.55
2:B:819:ASP:CG	2:B:820:PRO:HD2	2.31	0.55
15:O:166:ILE:HD11	15:O:213:SER:OG	2.06	0.55
15:O:343:VAL:CG1	15:O:388:VAL:HG21	2.36	0.55
15:O:369:LYS:HE2	15:O:370:THR:HG22	1.87	0.55
1:A:863:ASN:HD22	9:I:67:VAL:C	2.15	0.55
1:A:1162:ASN:HD21	1:A:1164:LYS:HB2	1.71	0.55
1:A:916:THR:O	1:A:919:LYS:NZ	2.40	0.55
1:A:1575:ILE:HG13	9:I:122:ARG:HH22	1.71	0.55
2:B:934:ILE:CG2	3:C:72:ILE:HB	2.35	0.55
15:O:359:GLY:CA	15:O:362:ASN:HD22	2.16	0.55
15:O:447:THR:O	15:O:450:LEU:N	2.39	0.55
15:O:447:THR:HA	15:O:450:LEU:HG	1.88	0.55
1:A:389:VAL:HA	1:A:430:ILE:HD11	1.88	0.55
1:A:1050:TYR:CD2	1:A:1179:ILE:HG21	2.41	0.55
1:A:1348:VAL:N	2:B:268:GLU:O	2.37	0.55
2:B:859:CYS:HB3	2:B:872:LYS:HB2	1.88	0.55
10:J:10:CYS:HB3	10:J:43:ARG:NH1	2.21	0.55
13:M:11:GLU:N	13:M:86:LYS:O	2.36	0.55
15:O:432:LYS:HB2	15:O:610:TYR:N	2.20	0.55
1:A:437:PHE:CE2	1:A:456:VAL:CG2	2.85	0.55
1:A:1657:LEU:HD22	7:G:104:LEU:HD13	1.89	0.55
3:C:139:LYS:HG2	3:C:201:GLU:HB3	1.89	0.55
5:E:144:ILE:O	5:E:147:HIS:HB2	2.07	0.55
15:O:343:VAL:HG11	15:O:388:VAL:HG21	1.89	0.55
15:O:396:MET:HE1	15:O:434:LEU:CD1	2.33	0.55
15:O:447:THR:HA	15:O:450:LEU:CD1	2.36	0.55
15:O:517:LEU:HD12	15:O:543:ILE:HG21	1.88	0.55
1:A:405:LYS:HG2	1:A:405:LYS:O	2.07	0.55
5:E:159:ASP:OD1	5:E:162:ARG:NH1	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:143:SER:HB3	15:O:101:SER:O	2.06	0.55
1:A:1024:THR:O	1:A:1028:GLU:HB3	2.07	0.55
1:A:1162:ASN:HD22	1:A:1165:LYS:HG3	1.71	0.55
2:B:322:ASN:HB3	2:B:325:GLN:H	1.71	0.55
3:C:56:LEU:HG	3:C:300:PHE:CE1	2.41	0.55
15:O:164:LEU:HB3	15:O:165:PRO:HD2	1.89	0.55
15:O:432:LYS:CB	15:O:608:GLU:O	2.55	0.55
2:B:1133:MET:HE3	7:G:17:ILE:HD13	1.88	0.55
4:D:80:THR:OG1	15:O:227:PHE:CD1	2.55	0.55
7:G:25:THR:HG22	7:G:26:ASN:N	2.17	0.55
7:G:28:ILE:CG2	7:G:29:ASP:N	2.56	0.55
15:O:371:HIS:C	15:O:374:PRO:CD	2.78	0.55
1:A:1596:LEU:HD22	1:A:1602:GLY:HA2	1.89	0.55
2:B:373:MET:O	2:B:377:MET:HG3	2.08	0.55
3:C:45:SER:HB2	3:C:271:ARG:CZ	2.35	0.55
3:C:57:ILE:CG1	3:C:297:HIS:ND1	2.70	0.55
15:O:158:LEU:HD22	15:O:172:HIS:CA	2.36	0.55
1:A:863:ASN:HD21	9:I:68:LYS:N	2.05	0.54
15:O:147:ILE:O	15:O:147:ILE:HG22	2.07	0.54
2:B:42:VAL:HG21	2:B:190:ILE:HB	1.89	0.54
7:G:143:SER:HA	15:O:103:ASN:HA	1.90	0.54
15:O:396:MET:HE1	15:O:433:LYS:C	2.33	0.54
1:A:479:ALA:HB2	2:B:1091:ARG:NH2	2.22	0.54
1:A:800:VAL:HG23	1:A:1068:PHE:CZ	2.41	0.54
1:A:827:THR:OG1	1:A:828:CYS:N	2.36	0.54
3:C:253:PRO:HB2	14:N:180:PHE:CG	2.42	0.54
15:O:368:PHE:C	15:O:368:PHE:CD1	2.85	0.54
15:O:158:LEU:CD2	15:O:172:HIS:HD2	2.01	0.54
15:O:487:ARG:NH2	15:O:611:ILE:HD12	2.22	0.54
1:A:399:LEU:HD11	1:A:423:LEU:HG	1.89	0.54
1:A:402:ASP:HA	1:A:405:LYS:HB3	1.88	0.54
2:B:401:GLU:HG3	2:B:402:VAL:H	1.69	0.54
2:B:799:GLY:O	2:B:1035:ARG:NH1	2.39	0.54
2:B:1019:GLY:CA	3:C:65:ASN:CG	2.81	0.54
4:D:48:GLU:HG2	4:D:86:ILE:CD1	2.36	0.54
5:E:145:THR:C	5:E:147:HIS:N	2.65	0.54
7:G:229:LEU:HD12	7:G:230:ARG:H	1.72	0.54
15:O:241:ASP:CA	15:O:380:SER:HB2	2.38	0.54
15:O:360:VAL:O	15:O:363:THR:HG23	2.06	0.54
1:A:1008:ASP:OD1	1:A:1202:LEU:HB3	2.07	0.54
1:A:1446:ARG:O	1:A:1450:ILE:HG13	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:284:SER:OG	2:B:287:GLU:HG3	2.07	0.54
3:C:58:ASN:HA	3:C:296:ASN:HB2	0.84	0.54
3:C:253:PRO:CA	14:N:180:PHE:HD1	2.20	0.54
4:D:30:HIS:HE2	7:G:26:ASN:CG	2.11	0.54
1:A:878:ARG:CZ	9:I:66:VAL:HG23	2.38	0.54
1:A:1347:ALA:HA	2:B:269:TYR:CE1	2.43	0.54
3:C:59:ILE:HG22	3:C:298:PHE:CE1	2.31	0.54
15:O:169:THR:HA	15:O:172:HIS:ND1	2.22	0.54
15:O:426:SER:HB3	15:O:594:TYR:HD2	1.72	0.54
1:A:1344:ILE:CG2	2:B:333:LYS:CG	2.86	0.54
9:I:71:LEU:HG	9:I:72:LYS:O	2.08	0.54
1:A:1605:THR:O	1:A:1606:SER:C	2.40	0.54
1:A:1651:THR:OG1	2:B:1085:SER:HB2	2.07	0.54
3:C:253:PRO:CB	14:N:180:PHE:CD1	2.79	0.54
15:O:100:LEU:HD22	15:O:107:ILE:CD1	2.38	0.54
15:O:423:TYR:CD1	15:O:594:TYR:CZ	2.95	0.54
1:A:556:ALA:CA	15:O:246:ASN:HD22	2.20	0.54
2:B:21:ARG:NH1	2:B:22:GLU:OE1	2.40	0.54
2:B:1043:LYS:CG	2:B:1063:ARG:NE	2.70	0.54
7:G:132:VAL:HG22	7:G:232:THR:HG22	1.90	0.54
15:O:361:PHE:CD1	15:O:361:PHE:C	2.86	0.54
15:O:391:GLN:NE2	15:O:609:TYR:CE2	2.76	0.54
1:A:982:VAL:HG13	1:A:994:GLU:CD	2.33	0.53
2:B:788:ILE:HB	2:B:948:ILE:HB	1.89	0.53
1:A:389:VAL:HA	1:A:430:ILE:CD1	2.38	0.53
1:A:1136:VAL:HG22	1:A:1174:TYR:CG	2.44	0.53
3:C:55:ASP:CB	3:C:297:HIS:HE2	2.21	0.53
3:C:71:MET:CE	3:C:225:ALA:HB2	2.33	0.53
3:C:97:LEU:HD11	3:C:202:ILE:HD13	1.90	0.53
15:O:368:PHE:CZ	15:O:385:MET:HB2	2.43	0.53
15:O:468:GLU:C	15:O:470:PHE:H	2.15	0.53
1:A:641:GLU:HB2	6:F:99:LEU:CD1	2.36	0.53
3:C:55:ASP:OD1	3:C:299:ILE:CG2	2.56	0.53
9:I:96:TYR:HA	9:I:111:PHE:O	2.09	0.53
15:O:69:THR:O	15:O:73:ILE:HG13	2.07	0.53
1:A:440:SER:C	1:A:442:LYS:H	2.17	0.53
2:B:398:GLN:HG2	2:B:398:GLN:O	2.06	0.53
15:O:147:ILE:HG22	15:O:149:LYS:HB3	1.90	0.53
1:A:91:PHE:CD2	1:A:249:THR:HG22	2.43	0.53
1:A:1655:ASP:HB2	6:F:135:ARG:CB	2.38	0.53
2:B:566:TYR:HD2	13:M:73:SER:HG	1.56	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:762:MET:HE2	2:B:762:MET:HA	1.91	0.53
7:G:158:LYS:HG2	15:O:105:ASN:CG	2.19	0.53
1:A:1482:LYS:HE2	2:B:304:ASP:OD2	2.08	0.53
2:B:470:LEU:O	2:B:481:VAL:CG1	2.56	0.53
4:D:37:LEU:CD2	4:D:97:LYS:HE3	2.38	0.53
13:M:75:GLN:HB2	14:N:60:SER:HA	1.91	0.53
15:O:63:LEU:CD2	15:O:111:ARG:HD2	2.38	0.53
15:O:342:HIS:O	15:O:346:GLN:CG	2.51	0.53
1:A:1008:ASP:OD1	1:A:1202:LEU:CG	2.56	0.53
2:B:563:SER:HA	13:M:73:SER:OG	2.08	0.53
2:B:934:ILE:HG21	3:C:73:SER:HB3	1.91	0.53
3:C:67:PHE:O	3:C:71:MET:HG3	2.08	0.53
15:O:218:LEU:HD23	15:O:229:ILE:HD11	1.90	0.53
15:O:238:ILE:CD1	15:O:371:HIS:HB3	2.37	0.53
15:O:390:GLN:HB2	15:O:609:TYR:CG	2.43	0.53
1:A:248:PHE:CD1	1:A:442:LYS:O	2.62	0.53
1:A:932:GLY:C	9:I:125:ASN:HD21	2.16	0.53
1:A:1289:SER:HB3	1:A:1475:GLU:HG2	1.91	0.53
1:A:1344:ILE:CG2	2:B:333:LYS:CB	2.86	0.53
2:B:317:TYR:HB3	2:B:320:LEU:HD12	1.89	0.53
4:D:28:PRO:CD	7:G:24:VAL:HG13	2.35	0.53
4:D:92:ILE:HG22	4:D:96:PHE:CE2	2.41	0.53
11:K:48:LYS:HE2	11:K:64:GLN:NE2	2.23	0.53
15:O:374:PRO:CB	15:O:375:THR:HG23	2.39	0.53
2:B:472:SER:O	2:B:474:SER:N	2.41	0.53
3:C:131:THR:HG21	3:C:207:HIS:HB3	1.91	0.53
4:D:23:HIS:CD2	6:F:58:PHE:CD2	2.97	0.53
4:D:48:GLU:CD	4:D:90:LYS:NZ	2.66	0.53
7:G:30:GLU:HA	7:G:32:ASN:H	1.74	0.53
13:M:12:ILE:HD12	14:N:67:LEU:HB2	1.90	0.53
15:O:189:PHE:CD1	15:O:190:ILE:N	2.76	0.53
15:O:520:CYS:O	15:O:521:ASN:O	2.27	0.53
1:A:1317:ILE:HA	1:A:1321:PHE:HB3	1.90	0.53
2:B:207:ILE:CD1	2:B:503:VAL:HG22	2.36	0.53
2:B:211:ARG:NH2	2:B:243:GLN:OE1	2.42	0.53
3:C:272:LYS:HG3	14:N:175:TYR:CE1	2.44	0.53
7:G:158:LYS:HZ2	15:O:108:GLU:CG	2.03	0.53
15:O:468:GLU:C	15:O:470:PHE:N	2.65	0.53
2:B:555:GLN:HB2	2:B:646:HIS:CE1	2.44	0.52
15:O:446:LEU:C	15:O:449:TRP:HB3	2.31	0.52
1:A:477:ASN:OD1	2:B:1059:PRO:HG2	1.99	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:VAL:HG23	1:A:1068:PHE:HZ	1.73	0.52
1:A:1605:THR:C	1:A:1606:SER:O	2.37	0.52
2:B:664:VAL:HG22	2:B:672:MET:HE1	1.91	0.52
2:B:800:TYR:CD1	2:B:800:TYR:C	2.87	0.52
2:B:894:LYS:HG2	12:L:47:ARG:HD3	1.89	0.52
3:C:64:ALA:CB	3:C:227:TYR:CE2	2.92	0.52
15:O:146:SER:C	15:O:148:PRO:HD3	2.34	0.52
15:O:467:MET:HA	15:O:467:MET:HE2	1.91	0.52
3:C:64:ALA:HB3	3:C:298:PHE:CE2	2.44	0.52
15:O:66:ASN:N	15:O:66:ASN:ND2	2.53	0.52
15:O:499:GLU:O	15:O:502:LEU:HG	2.09	0.52
3:C:127:THR:H	3:C:130:ASN:HB2	1.74	0.52
7:G:142:ALA:HB3	15:O:102:SER:HA	1.91	0.52
9:I:59:SER:O	9:I:63:LYS:HG3	2.09	0.52
15:O:337:THR:O	15:O:341:THR:OG1	2.27	0.52
2:B:22:GLU:O	2:B:26:ILE:HG13	2.10	0.52
2:B:552:SER:C	2:B:647:SER:H	2.16	0.52
7:G:242:VAL:HG21	15:O:183:ILE:HG21	1.91	0.52
9:I:59:SER:O	9:I:63:LYS:CG	2.57	0.52
1:A:509:GLU:HG3	1:A:579:ARG:CD	2.39	0.52
1:A:969:PHE:CE2	1:A:978:ALA:HA	2.44	0.52
2:B:527:PHE:CE1	2:B:666:PRO:HG3	2.45	0.52
2:B:915:ASP:OD1	2:B:1038:HIS:CD2	2.61	0.52
15:O:348:THR:HG22	15:O:351:SER:CB	2.26	0.52
2:B:833:PRO:O	2:B:834:LYS:HB3	2.10	0.52
3:C:82:TYR:CE1	12:L:68:GLU:HG3	2.44	0.52
15:O:155:SER:HB2	15:O:176:LEU:HD21	1.91	0.52
15:O:156:MET:HG3	15:O:197:PHE:HE2	1.60	0.52
15:O:373:LEU:CD1	15:O:416:LYS:CG	2.62	0.52
1:A:441:THR:HG22	1:A:441:THR:O	2.10	0.52
2:B:42:VAL:O	2:B:46:ILE:CD1	2.52	0.52
2:B:134:ARG:HD2	2:B:160:GLY:HA3	1.91	0.52
4:D:37:LEU:HD22	4:D:97:LYS:CE	2.39	0.52
13:M:105:SER:HA	13:M:108:LEU:CG	2.29	0.52
15:O:206:ARG:HA	15:O:209:VAL:HG12	1.90	0.52
15:O:402:THR:O	15:O:406:ILE:HG13	2.10	0.52
15:O:458:GLU:CG	15:O:514:PHE:CE2	2.92	0.52
3:C:51:GLU:CB	3:C:303:GLU:HG3	2.40	0.52
7:G:26:ASN:HD21	7:G:126:GLN:HE21	1.56	0.52
15:O:459:GLU:HG3	15:O:460:GLU:N	2.25	0.52
1:A:438:ILE:HG22	2:B:1192:MET:HE2	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:497:VAL:HG21	1:A:605:VAL:HG13	1.92	0.51
1:A:722:PRO:HG2	8:H:46:LEU:HD13	1.90	0.51
2:B:37:LEU:CD1	2:B:760:TYR:CZ	2.90	0.51
15:O:415:GLU:O	15:O:419:LYS:HG3	2.10	0.51
15:O:518:LYS:HD3	15:O:519:PHE:CZ	2.45	0.51
1:A:636:HIS:CE1	2:B:1091:ARG:HH21	2.28	0.51
1:A:986:PHE:CD2	2:B:958:MET:HE2	2.46	0.51
2:B:307:GLU:OE2	2:B:311:ARG:NH1	2.43	0.51
2:B:938:PHE:CD1	3:C:68:ARG:NE	2.78	0.51
2:B:1069:ILE:N	2:B:1069:ILE:CD1	2.73	0.51
2:B:1120:ILE:CD1	15:O:117:GLN:HE22	2.23	0.51
3:C:47:LEU:HD23	3:C:48:ASP:N	2.25	0.51
15:O:241:ASP:O	15:O:378:THR:HG23	2.10	0.51
15:O:426:SER:HB3	15:O:594:TYR:HB2	1.88	0.51
15:O:478:GLN:OE1	15:O:521:ASN:HB2	2.10	0.51
1:A:87:ASN:HA	1:A:357:MET:SD	2.50	0.51
1:A:1011:VAL:CG1	1:A:1201:THR:C	2.43	0.51
15:O:98:ASP:OD2	15:O:135:LYS:CE	2.58	0.51
15:O:457:ARG:O	15:O:461:VAL:HG23	2.10	0.51
15:O:488:HIS:O	15:O:489:ASN:C	2.54	0.51
1:A:1003:ARG:CD	2:B:520:LEU:N	2.73	0.51
1:A:1657:LEU:HB3	7:G:104:LEU:HB3	1.93	0.51
2:B:1047:ARG:NH2	2:B:1051:PRO:O	2.43	0.51
3:C:64:ALA:O	3:C:227:TYR:CE2	2.58	0.51
3:C:71:MET:HE1	3:C:302:VAL:HG21	1.89	0.51
15:O:158:LEU:HD22	15:O:172:HIS:CD2	2.46	0.51
15:O:383:TYR:CZ	15:O:597:LEU:HB2	2.46	0.51
1:A:392:THR:CB	1:A:430:ILE:HD13	2.37	0.51
2:B:527:PHE:CD1	2:B:666:PRO:HG3	2.46	0.51
4:D:95:ASP:OD2	7:G:150:HIS:CA	2.56	0.51
7:G:143:SER:HB3	15:O:102:SER:C	2.35	0.51
8:H:38:LEU:HD11	8:H:123:MET:HE2	1.93	0.51
11:K:55:SER:OG	11:K:57:ASP:OD1	2.28	0.51
15:O:151:TRP:HZ2	15:O:176:LEU:HA	1.76	0.51
15:O:379:ARG:CB	15:O:382:GLN:NE2	2.74	0.51
15:O:487:ARG:CG	15:O:487:ARG:NH1	2.73	0.51
1:A:401:ASP:O	1:A:405:LYS:HB3	2.09	0.51
1:A:1028:GLU:CG	1:A:1029:GLY:H	2.24	0.51
1:A:1056:ASP:OD2	1:A:1179:ILE:HA	2.11	0.51
1:A:1089:LEU:HD11	1:A:1175:MET:HE1	1.92	0.51
3:C:31:TRP:CD2	11:K:82:LYS:CG	2.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:247:GLU:OE1	15:O:325:ILE:CD1	2.57	0.51
1:A:954:GLY:N	1:A:1205:PHE:HB3	2.25	0.51
2:B:300:SER:CB	9:I:49:THR:HG22	2.41	0.51
3:C:229:LEU:HD22	3:C:295:ARG:O	2.11	0.51
15:O:369:LYS:CE	15:O:370:THR:CG2	2.86	0.51
1:A:412:SER:C	1:A:414:GLU:H	2.17	0.51
1:A:475:ARG:HB3	2:B:1059:PRO:HB2	1.90	0.51
1:A:840:ASN:O	1:A:844:THR:HG23	2.11	0.51
2:B:769:PHE:CZ	2:B:798:PHE:CE1	2.91	0.51
3:C:131:THR:HG22	3:C:208:CYS:N	2.26	0.51
7:G:244:SER:HB2	15:O:148:PRO:HD2	1.91	0.51
15:O:163:ILE:HA	15:O:211:TYR:N	1.97	0.51
15:O:198:PHE:CD2	15:O:232:LEU:CG	2.60	0.51
1:A:1003:ARG:CD	2:B:520:LEU:H	2.23	0.51
1:A:1450:ILE:HD12	1:A:1460:TYR:CD2	2.46	0.51
2:B:934:ILE:HG21	3:C:69:ARG:O	2.10	0.51
15:O:248:LEU:HD23	15:O:248:LEU:O	2.10	0.51
1:A:509:GLU:OE2	1:A:579:ARG:CZ	2.58	0.50
1:A:601:MET:HE2	1:A:656:GLN:HB2	1.92	0.50
1:A:880:GLN:OE1	2:B:633:THR:O	2.27	0.50
1:A:991:LYS:HB3	1:A:993:GLN:OE1	2.11	0.50
1:A:1048:PHE:CE2	5:E:211:TYR:HD1	2.21	0.50
1:A:1660:VAL:O	7:G:103:LYS:N	2.39	0.50
2:B:721:MET:HE2	2:B:721:MET:HA	1.92	0.50
2:B:934:ILE:HG21	3:C:73:SER:CB	2.41	0.50
3:C:131:THR:HG22	3:C:208:CYS:C	2.35	0.50
3:C:296:ASN:O	3:C:297:HIS:HB2	2.11	0.50
4:D:28:PRO:CD	7:G:24:VAL:CG1	2.89	0.50
15:O:446:LEU:O	15:O:449:TRP:CB	2.42	0.50
1:A:478:TYR:HD1	2:B:1048:SER:HB2	1.76	0.50
1:A:564:PRO:HB2	15:O:371:HIS:HE1	1.76	0.50
1:A:1660:VAL:N	7:G:103:LYS:O	2.41	0.50
4:D:80:THR:HG23	15:O:227:PHE:HB3	1.88	0.50
10:J:1:MET:HG2	10:J:57:ILE:HB	1.93	0.50
1:A:1326:GLU:OE2	1:A:1454:HIS:HB3	2.11	0.50
2:B:554:GLN:C	2:B:646:HIS:CD2	2.90	0.50
2:B:894:LYS:HD3	12:L:47:ARG:NH1	2.26	0.50
2:B:1010:ASN:HB3	2:B:1025:ASP:HB3	1.93	0.50
15:O:591:TYR:CE2	15:O:593:PRO:HG3	2.46	0.50
1:A:970:LYS:HG2	1:A:973:GLU:HG2	1.92	0.50
2:B:469:ASN:CA	2:B:481:VAL:O	2.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1002:LYS:CD	14:N:166:LEU:HB2	2.40	0.50
3:C:71:MET:CE	3:C:302:VAL:HG22	2.29	0.50
6:F:74:ILE:CG2	6:F:75:PRO:CD	2.87	0.50
1:A:437:PHE:CE2	1:A:456:VAL:HG23	2.36	0.50
1:A:1003:ARG:CD	2:B:520:LEU:HB2	2.41	0.50
2:B:68:ILE:HD11	2:B:414:LYS:CG	2.39	0.50
2:B:293:ILE:HG12	2:B:306:LEU:HD13	1.94	0.50
2:B:472:SER:HB3	2:B:476:LEU:HD11	1.92	0.50
8:H:26:ILE:HD12	8:H:42:ILE:HD12	1.93	0.50
15:O:190:ILE:HD13	15:O:190:ILE:C	2.37	0.50
15:O:242:VAL:HA	15:O:378:THR:CG2	2.37	0.50
15:O:352:LEU:HD22	15:O:358:VAL:HG22	1.81	0.50
2:B:203:ILE:HG21	2:B:405:GLY:HA2	1.93	0.50
2:B:284:SER:HB2	9:I:14:GLY:HA3	1.93	0.50
3:C:230:LEU:HD11	3:C:231:PRO:HD2	1.92	0.50
4:D:44:ILE:CG2	4:D:90:LYS:HE3	2.40	0.50
14:N:87:TYR:CE1	14:N:141:GLU:OE1	2.64	0.50
15:O:359:GLY:CA	15:O:362:ASN:ND2	2.73	0.50
15:O:488:HIS:O	15:O:491:PHE:N	2.37	0.50
1:A:505:LEU:HD12	1:A:581:ILE:HD13	1.93	0.50
3:C:100:ARG:NH2	10:J:3:VAL:O	2.44	0.50
15:O:169:THR:O	15:O:170:VAL:C	2.54	0.50
15:O:208:LEU:O	15:O:212:THR:HG23	2.12	0.50
1:A:863:ASN:ND2	9:I:67:VAL:C	2.70	0.50
1:A:953:GLU:CA	1:A:1205:PHE:CG	2.95	0.50
2:B:328:GLN:NE2	13:M:109:ARG:NH2	2.59	0.50
3:C:47:LEU:HD23	3:C:48:ASP:H	1.77	0.50
3:C:222:VAL:O	3:C:224:THR:N	2.44	0.50
3:C:231:PRO:HG2	3:C:270:ALA:CB	2.42	0.50
1:A:1025:LYS:NZ	2:B:1076:ARG:NH1	2.59	0.50
1:A:1048:PHE:CE2	5:E:210:SER:HA	2.46	0.50
1:A:1056:ASP:HB2	1:A:1177:SER:O	2.11	0.50
2:B:858:ILE:HD13	2:B:872:LYS:O	2.11	0.50
15:O:352:LEU:CA	15:O:358:VAL:CG2	2.90	0.50
1:A:1003:ARG:HD2	2:B:520:LEU:N	2.23	0.49
6:F:75:PRO:HG3	6:F:78:GLN:CD	2.37	0.49
7:G:47:VAL:HB	7:G:65:HIS:CD2	2.47	0.49
14:N:85:HIS:CE1	14:N:141:GLU:OE1	2.64	0.49
15:O:453:TYR:CE1	15:O:473:PHE:HB2	2.47	0.49
1:A:1006:LEU:HD21	2:B:535:ASP:CB	2.42	0.49
7:G:143:SER:HB3	15:O:103:ASN:CA	2.42	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:324:GLY:O	15:O:326:LYS:N	2.44	0.49
15:O:368:PHE:CD2	15:O:385:MET:HG2	2.47	0.49
1:A:381:SER:HB2	1:A:453:ILE:HG21	1.93	0.49
2:B:338:PHE:CE1	2:B:353:VAL:HG22	2.47	0.49
4:D:23:HIS:CG	6:F:58:PHE:CD2	3.00	0.49
7:G:242:VAL:HG21	15:O:183:ILE:HG23	1.93	0.49
9:I:91:ASN:OD1	9:I:92:GLU:N	2.45	0.49
1:A:412:SER:H	1:A:415:ASP:HB2	1.76	0.49
1:A:507:TYR:HB2	1:A:637:PHE:CE2	2.47	0.49
1:A:1053:ASP:HB2	5:E:204:THR:CG2	2.43	0.49
1:A:1622:LEU:HD21	2:B:1189:LEU:HD22	1.94	0.49
2:B:1043:LYS:HE2	2:B:1063:ARG:CD	2.42	0.49
2:B:1120:ILE:HD12	15:O:117:GLN:NE2	2.27	0.49
15:O:430:ARG:O	15:O:431:ALA:O	2.31	0.49
15:O:581:THR:HA	15:O:584:GLN:CD	2.37	0.49
1:A:995:TYR:O	1:A:999:CYS:N	2.35	0.49
1:A:1148:LEU:HD22	1:A:1163:GLU:HG3	1.92	0.49
2:B:211:ARG:HG2	2:B:211:ARG:HH11	1.77	0.49
3:C:231:PRO:HG2	3:C:270:ALA:C	2.37	0.49
12:L:45:ALA:O	12:L:47:ARG:N	2.46	0.49
15:O:173:HIS:CE1	15:O:217:LYS:HB3	2.47	0.49
15:O:426:SER:OG	15:O:594:TYR:C	2.54	0.49
1:A:1034:TYR:HA	1:A:1181:PRO:HB3	1.95	0.49
1:A:1500:GLN:HG2	1:A:1501:ILE:N	2.28	0.49
15:O:173:HIS:CD2	15:O:217:LYS:CG	2.95	0.49
15:O:488:HIS:CE1	15:O:489:ASN:H	2.27	0.49
1:A:1026:GLN:NE2	1:A:1603:MET:HA	2.26	0.49
15:O:177:LYS:HG3	15:O:178:TYR:N	2.26	0.49
15:O:443:ALA:O	15:O:447:THR:HG23	2.12	0.49
2:B:211:ARG:HG2	2:B:211:ARG:NH1	2.28	0.49
6:F:75:PRO:HG3	6:F:78:GLN:NE2	2.27	0.49
15:O:174:ASP:C	15:O:177:LYS:HG2	2.36	0.49
15:O:507:GLN:O	15:O:511:ILE:HG23	2.12	0.49
1:A:476:VAL:O	2:B:1059:PRO:HG2	2.13	0.49
1:A:795:HIS:NE2	1:A:1062:HIS:HE1	2.11	0.49
1:A:1661:PRO:CA	7:G:101:SER:O	2.61	0.49
2:B:252:TYR:OH	2:B:305:ARG:NH1	2.44	0.49
2:B:262:PHE:CD1	2:B:357:ILE:HD13	2.48	0.49
2:B:399:HIS:C	2:B:400:GLN:CG	2.86	0.49
13:M:65:TYR:CE1	13:M:97:VAL:HB	2.48	0.49
15:O:234:ILE:O	15:O:238:ILE:HG13	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PHE:CZ	1:A:249:THR:HA	2.46	0.49
1:A:582:LYS:O	1:A:585:ASP:HB2	2.12	0.49
1:A:1662:ASN:N	7:G:101:SER:HB2	2.28	0.49
3:C:31:TRP:NE1	11:K:78:TYR:OH	2.46	0.49
3:C:57:ILE:O	3:C:58:ASN:HB2	2.12	0.49
15:O:163:ILE:HG22	15:O:207:LYS:O	2.12	0.49
15:O:391:GLN:CD	15:O:609:TYR:OH	2.55	0.49
15:O:434:LEU:CD1	15:O:434:LEU:N	2.75	0.49
1:A:1053:ASP:HB2	5:E:204:THR:HG22	1.95	0.48
2:B:281:CYS:HA	2:B:323:ARG:NE	2.28	0.48
15:O:459:GLU:C	15:O:461:VAL:N	2.61	0.48
1:A:475:ARG:NH1	2:B:1061:LYS:HB2	2.28	0.48
1:A:782:ASP:O	1:A:783:LYS:C	2.56	0.48
1:A:1200:MET:HE1	1:A:1569:VAL:HG12	1.95	0.48
2:B:225:ARG:NH2	2:B:261:ARG:HD3	2.27	0.48
4:D:95:ASP:OD1	7:G:151:ASP:HB2	2.12	0.48
7:G:137:ILE:HG13	7:G:227:GLY:O	2.13	0.48
8:H:112:ILE:HD12	8:H:129:TYR:HB2	1.93	0.48
15:O:591:TYR:HE2	15:O:593:PRO:HG3	1.77	0.48
1:A:34:ASN:C	1:A:390:LEU:HD13	2.38	0.48
1:A:1050:TYR:HE1	1:A:1185:VAL:HG12	1.67	0.48
1:A:1055:ILE:CG2	1:A:1060:GLU:HB2	2.43	0.48
1:A:1260:LYS:HE2	1:A:1262:LEU:HD11	1.95	0.48
2:B:209:GLN:CG	2:B:210:ARG:H	2.08	0.48
2:B:1043:LYS:HG3	2:B:1063:ARG:CZ	2.43	0.48
15:O:391:GLN:HE22	15:O:609:TYR:HE2	1.61	0.48
1:A:50:TYR:CD1	1:A:365:THR:HG23	2.47	0.48
5:E:145:THR:O	5:E:147:HIS:N	2.46	0.48
6:F:75:PRO:CG	6:F:78:GLN:CD	2.87	0.48
15:O:91:LYS:HG3	15:O:92:ASN:N	2.28	0.48
15:O:383:TYR:CG	15:O:597:LEU:HD22	2.47	0.48
15:O:597:LEU:HD12	15:O:598:PHE:H	1.77	0.48
2:B:471:VAL:O	2:B:471:VAL:HG12	2.13	0.48
2:B:929:ARG:HH22	11:K:96:PRO:HB2	1.77	0.48
5:E:54:GLN:HB2	5:E:57:MET:HE2	1.96	0.48
15:O:199:PRO:HB2	15:O:208:LEU:HD23	1.95	0.48
15:O:369:LYS:C	15:O:369:LYS:CD	2.86	0.48
1:A:365:THR:O	1:A:368:ARG:N	2.37	0.48
1:A:413:LEU:CA	1:A:417:ARG:HH21	2.27	0.48
1:A:721:LYS:HB3	8:H:96:VAL:HB	1.95	0.48
2:B:550:ARG:O	2:B:649:MET:HA	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:111:VAL:HG13	14:N:122:ALA:HB2	1.96	0.48
15:O:241:ASP:OD1	15:O:380:SER:HB2	2.13	0.48
15:O:408:PHE:CD2	15:O:449:TRP:CE2	3.02	0.48
15:O:440:ILE:HD13	15:O:491:PHE:CD1	2.48	0.48
15:O:484:PHE:O	15:O:488:HIS:HB3	2.14	0.48
1:A:399:LEU:HD22	1:A:423:LEU:HA	1.95	0.48
1:A:597:LYS:HB2	2:B:1082:HIS:CE1	2.48	0.48
1:A:782:ASP:C	1:A:784:SER:N	2.71	0.48
1:A:1003:ARG:HD2	2:B:520:LEU:CB	2.43	0.48
6:F:76:LYS:C	6:F:78:GLN:H	2.22	0.48
1:A:40:ASN:N	1:A:40:ASN:OD1	2.44	0.48
1:A:480:ALA:CA	2:B:1046:VAL:HG23	2.42	0.48
1:A:684:ASP:OD1	8:H:20:TYR:HB3	2.13	0.48
1:A:747:ILE:HD13	1:A:748:ASN:H	1.77	0.48
2:B:480:GLN:O	2:B:484:TYR:OH	2.30	0.48
3:C:157:TYR:HB2	3:C:160:ALA:HB2	1.94	0.48
4:D:92:ILE:CD1	7:G:152:ALA:CB	2.92	0.48
5:E:61:GLN:HE21	5:E:105:PHE:HE1	1.61	0.48
15:O:369:LYS:HE2	15:O:370:THR:N	2.28	0.48
15:O:477:PHE:CE2	15:O:481:CYS:SG	3.07	0.48
1:A:869:PRO:HG2	1:A:872:ASP:HB2	1.96	0.48
1:A:1006:LEU:CD2	2:B:535:ASP:HB2	2.43	0.48
1:A:1023:LEU:CD2	1:A:1598:PHE:CD1	2.97	0.48
1:A:1162:ASN:ND2	1:A:1165:LYS:HG3	2.29	0.48
2:B:552:SER:O	2:B:647:SER:CA	2.61	0.48
2:B:1133:MET:CE	7:G:17:ILE:HD13	2.44	0.48
15:O:66:ASN:CG	15:O:111:ARG:NH1	2.72	0.48
15:O:369:LYS:HD2	15:O:370:THR:HA	1.95	0.48
1:A:1055:ILE:CG2	1:A:1060:GLU:CG	2.90	0.48
1:A:1312:GLU:O	1:A:1316:VAL:HG23	2.13	0.48
2:B:70:GLU:CB	2:B:97:VAL:O	2.62	0.48
2:B:894:LYS:HD3	12:L:47:ARG:CZ	2.44	0.48
2:B:1045:GLN:HB3	2:B:1063:ARG:HG3	1.95	0.48
1:A:747:ILE:HD13	1:A:748:ASN:N	2.29	0.47
4:D:92:ILE:HD11	7:G:152:ALA:HB1	1.95	0.47
7:G:158:LYS:HE2	15:O:105:ASN:OD1	2.14	0.47
15:O:151:TRP:CZ2	15:O:176:LEU:HA	2.49	0.47
15:O:225:LEU:HD12	15:O:229:ILE:HG13	1.96	0.47
15:O:412:GLU:O	15:O:413:ALA:C	2.57	0.47
1:A:959:VAL:HG22	1:A:965:THR:HG22	1.95	0.47
1:A:960:MET:SD	2:B:522:PRO:HB2	2.54	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1305:GLU:CD	9:I:63:LYS:HE3	2.39	0.47
2:B:73:ILE:HB	2:B:425:ILE:HD12	1.96	0.47
2:B:1017:ALA:C	3:C:65:ASN:ND2	2.72	0.47
4:D:80:THR:HG21	15:O:227:PHE:CG	2.48	0.47
15:O:369:LYS:O	15:O:373:LEU:CA	2.60	0.47
15:O:478:GLN:NE2	15:O:592:PHE:CZ	2.69	0.47
2:B:73:ILE:HD12	2:B:425:ILE:HG23	1.95	0.47
2:B:208:VAL:CG2	2:B:401:GLU:CG	2.92	0.47
3:C:230:LEU:CG	3:C:294:VAL:CG2	2.92	0.47
15:O:120:ILE:HD13	15:O:150:TRP:CE3	2.49	0.47
1:A:1348:VAL:HB	2:B:268:GLU:CA	2.43	0.47
1:A:1348:VAL:CB	2:B:268:GLU:C	2.70	0.47
2:B:552:SER:O	2:B:647:SER:HA	2.14	0.47
2:B:584:CYS:HB3	2:B:596:VAL:HG23	1.95	0.47
10:J:6:ARG:HD2	10:J:11:GLY:O	2.13	0.47
15:O:225:LEU:C	15:O:225:LEU:CD1	2.86	0.47
1:A:1048:PHE:CE1	5:E:211:TYR:CD1	3.01	0.47
1:A:1261:VAL:HG12	1:A:1262:LEU:N	2.28	0.47
1:A:1482:LYS:HE2	2:B:304:ASP:OD1	2.15	0.47
5:E:48:ASP:OD1	5:E:50:MET:HB3	2.13	0.47
1:A:258:GLU:HA	1:A:261:ILE:HD12	1.97	0.47
2:B:338:PHE:CZ	2:B:357:ILE:HD12	2.49	0.47
2:B:470:LEU:O	2:B:481:VAL:HG13	2.15	0.47
15:O:107:ILE:O	15:O:109:SER:N	2.46	0.47
1:A:439:ASP:HB3	1:A:442:LYS:HD2	1.96	0.47
1:A:741:PRO:HA	1:A:742:PRO:HD3	1.68	0.47
1:A:1573:TYR:HB3	9:I:122:ARG:NH2	2.30	0.47
2:B:812:ALA:HA	2:B:815:ARG:HD3	1.95	0.47
2:B:1020:GLU:HG2	3:C:61:THR:CB	2.44	0.47
3:C:126:PHE:HD1	3:C:131:THR:HG1	1.62	0.47
15:O:237:ILE:CG2	15:O:381:ILE:CG1	2.93	0.47
15:O:460:GLU:O	15:O:469:ARG:NH2	2.47	0.47
15:O:471:LYS:CG	15:O:472:HIS:N	2.75	0.47
15:O:521:ASN:ND2	15:O:523:ASN:N	2.54	0.47
1:A:19:LEU:HD11	2:B:1190:SER:HB2	1.96	0.47
2:B:396:ALA:HB1	2:B:523:GLU:HG3	1.96	0.47
2:B:399:HIS:C	2:B:400:GLN:HG3	2.40	0.47
3:C:247:PHE:HE1	3:C:289:VAL:HG21	1.80	0.47
1:A:479:ALA:HB2	1:A:636:HIS:ND1	2.29	0.47
3:C:31:TRP:NE1	11:K:82:LYS:NZ	2.54	0.47
3:C:86:PHE:CD1	12:L:64:LEU:HD13	2.46	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:109:ARG:HH22	13:M:112:LYS:HG3	1.79	0.47
15:O:170:VAL:CG1	15:O:171:CYS:N	2.78	0.47
15:O:176:LEU:HD13	15:O:218:LEU:HD13	1.96	0.47
1:A:55:GLY:HA2	1:A:62:CYS:SG	2.56	0.47
1:A:1070:LEU:C	1:A:1072:ASN:H	2.21	0.47
2:B:413:LEU:O	2:B:417:ILE:HG13	2.14	0.47
15:O:129:PRO:O	15:O:133:LEU:CB	2.62	0.47
15:O:602:TYR:O	15:O:606:MET:HG2	2.15	0.47
2:B:203:ILE:CG2	2:B:405:GLY:HA2	2.45	0.46
2:B:448:ARG:HA	2:B:451:MET:HE3	1.97	0.46
2:B:470:LEU:N	2:B:481:VAL:O	2.47	0.46
2:B:569:GLY:HA2	14:N:140:SER:OG	2.15	0.46
2:B:1103:VAL:HG22	2:B:1176:VAL:HG22	1.97	0.46
3:C:231:PRO:CG	3:C:270:ALA:O	2.62	0.46
3:C:239:ILE:HG23	3:C:243:SER:HB3	1.96	0.46
15:O:138:TYR:CD2	15:O:142:ILE:CD1	2.92	0.46
1:A:364:PRO:HB2	1:A:367:PHE:CD2	2.51	0.46
1:A:403:LEU:CD2	1:A:423:LEU:HD11	2.45	0.46
1:A:953:GLU:C	1:A:1205:PHE:CG	2.94	0.46
1:A:1320:GLN:HE21	1:A:1320:GLN:HB2	1.56	0.46
2:B:681:ILE:O	14:N:154:ARG:NE	2.36	0.46
2:B:736:ARG:HD3	2:B:738:ASP:OD2	2.15	0.46
4:D:46:GLU:OE1	4:D:47:LYS:HE2	2.15	0.46
4:D:95:ASP:HB2	7:G:151:ASP:HB3	1.97	0.46
15:O:170:VAL:HG13	15:O:171:CYS:H	1.79	0.46
15:O:206:ARG:HA	15:O:209:VAL:CG1	2.44	0.46
15:O:388:VAL:HG13	15:O:389:SER:N	2.31	0.46
1:A:492:THR:HG23	1:A:811:SER:OG	2.14	0.46
1:A:1053:ASP:O	1:A:1054:ALA:CB	2.62	0.46
1:A:1060:GLU:HA	1:A:1063:MET:CG	2.37	0.46
1:A:1258:ILE:HB	1:A:1501:ILE:HD12	1.97	0.46
1:A:1440:ASN:HA	1:A:1443:GLN:HB2	1.96	0.46
3:C:231:PRO:HG3	3:C:270:ALA:O	2.16	0.46
15:O:181:ARG:CG	15:O:181:ARG:NH1	2.77	0.46
2:B:679:GLN:HG3	14:N:155:VAL:O	2.14	0.46
9:I:23:VAL:O	9:I:39:LYS:NZ	2.48	0.46
11:K:93:ILE:HA	11:K:94:PRO:HD2	1.75	0.46
15:O:74:ILE:O	15:O:78:VAL:HG13	2.16	0.46
15:O:148:PRO:HB3	15:O:183:ILE:HD13	1.98	0.46
15:O:433:LYS:HG3	15:O:433:LYS:O	2.16	0.46
1:A:211:THR:HG23	5:E:177:ARG:CZ	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:LEU:HD13	2:B:371:PHE:N	2.30	0.46
4:D:95:ASP:HB2	7:G:151:ASP:CB	2.46	0.46
7:G:159:LYS:HD2	15:O:103:ASN:CG	2.39	0.46
15:O:506:PHE:HD2	15:O:537:VAL:CG1	2.28	0.46
1:A:411:VAL:CG2	1:A:412:SER:N	2.76	0.46
1:A:507:TYR:HB2	1:A:637:PHE:CZ	2.51	0.46
2:B:401:GLU:C	2:B:402:VAL:HG23	2.41	0.46
2:B:467:THR:O	2:B:469:ASN:N	2.49	0.46
2:B:553:THR:C	2:B:646:HIS:HD2	2.23	0.46
7:G:141:SER:HB2	15:O:138:TYR:CZ	2.43	0.46
15:O:352:LEU:HA	15:O:358:VAL:CG2	2.31	0.46
1:A:94:LEU:HD11	1:A:356:PHE:CZ	2.51	0.46
1:A:1003:ARG:CD	2:B:520:LEU:CB	2.93	0.46
1:A:1028:GLU:HG3	1:A:1637:PRO:HG2	1.97	0.46
2:B:265:ARG:NH2	2:B:339:GLN:OE1	2.48	0.46
2:B:822:THR:HB	2:B:823:GLN:HG3	1.98	0.46
3:C:41:GLU:C	3:C:57:ILE:HG22	2.41	0.46
4:D:48:GLU:CG	4:D:86:ILE:HD12	2.39	0.46
15:O:413:ALA:C	15:O:415:GLU:N	2.72	0.46
15:O:444:SER:O	15:O:447:THR:OG1	2.23	0.46
1:A:589:MET:HE1	1:A:614:LEU:HD13	1.98	0.46
1:A:1049:MET:C	1:A:1051:GLY:N	2.74	0.46
2:B:202:LEU:HD13	2:B:500:PHE:CE1	2.51	0.46
2:B:1020:GLU:CD	3:C:61:THR:HG21	2.40	0.46
3:C:50:ARG:O	3:C:303:GLU:CA	2.58	0.46
3:C:57:ILE:CA	3:C:297:HIS:HA	2.09	0.46
4:D:25:THR:CB	6:F:59:GLN:HG2	2.39	0.46
5:E:67:GLU:CD	5:E:67:GLU:H	2.23	0.46
15:O:358:VAL:C	15:O:362:ASN:ND2	2.73	0.46
15:O:447:THR:HB	15:O:505:PHE:CE2	2.51	0.46
15:O:459:GLU:O	15:O:463:GLN:CB	2.63	0.46
1:A:5:LYS:HB3	1:A:5:LYS:HE2	1.68	0.46
1:A:184:LYS:HA	1:A:187:GLU:HG2	1.98	0.46
1:A:1575:ILE:HG13	9:I:122:ARG:NH1	2.29	0.46
2:B:774:ALA:HB1	2:B:1026:ILE:HD11	1.97	0.46
2:B:890:ASP:HB3	2:B:896:GLN:OE1	2.15	0.46
2:B:1120:ILE:CD1	15:O:117:GLN:NE2	2.79	0.46
5:E:131:THR:HG21	5:E:191:LYS:CE	2.45	0.46
15:O:239:SER:O	15:O:243:GLU:HG2	2.16	0.46
1:A:412:SER:HB3	1:A:414:GLU:HB3	1.96	0.46
1:A:618:TYR:CE1	2:B:783:MET:HB2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:ILE:HD11	1:A:1183:GLU:CD	2.40	0.46
2:B:293:ILE:CD1	2:B:302:LEU:HB3	2.46	0.46
4:D:92:ILE:CD1	7:G:152:ALA:HB1	2.45	0.46
1:A:356:PHE:C	1:A:357:MET:CG	2.86	0.45
1:A:1019:LEU:CD1	1:A:1227:MET:CG	2.91	0.45
2:B:292:ILE:HB	2:B:306:LEU:HD11	1.98	0.45
2:B:427:GLN:HA	2:B:430:MET:HE3	1.98	0.45
2:B:724:GLN:O	2:B:1037:ARG:HG3	2.17	0.45
3:C:58:ASN:N	3:C:296:ASN:C	2.59	0.45
4:D:28:PRO:CB	7:G:24:VAL:HG11	2.46	0.45
13:M:26:PHE:CE1	13:M:98:SER:HB2	2.51	0.45
15:O:48:SER:O	15:O:49:ALA:C	2.57	0.45
15:O:428:ILE:CG2	15:O:439:ILE:CG2	2.86	0.45
15:O:506:PHE:CG	15:O:528:PHE:HZ	2.34	0.45
1:A:436:ALA:O	1:A:440:SER:N	2.49	0.45
1:A:437:PHE:C	1:A:439:ASP:H	2.22	0.45
1:A:954:GLY:N	1:A:1205:PHE:CB	2.79	0.45
2:B:1094:ASN:C	2:B:1096:SER:H	2.24	0.45
4:D:40:LEU:HD13	4:D:93:GLN:HB2	1.98	0.45
9:I:89:CYS:SG	9:I:91:ASN:HB2	2.56	0.45
11:K:80:ILE:HD13	11:K:105:ILE:HD11	1.98	0.45
15:O:458:GLU:HG3	15:O:514:PHE:CE2	2.51	0.45
15:O:485:CYS:SG	15:O:531:ILE:HD12	2.56	0.45
1:A:440:SER:C	1:A:442:LYS:N	2.74	0.45
2:B:68:ILE:CD1	2:B:414:LYS:HG3	2.41	0.45
2:B:480:GLN:CB	2:B:507:SER:OG	2.64	0.45
3:C:54:PHE:CD1	3:C:300:PHE:O	2.69	0.45
3:C:228:ARG:HG3	3:C:299:ILE:HB	1.98	0.45
15:O:69:THR:HG22	15:O:70:GLN:N	2.31	0.45
15:O:245:GLN:O	15:O:248:LEU:N	2.39	0.45
15:O:370:THR:O	15:O:374:PRO:CG	2.63	0.45
15:O:459:GLU:O	15:O:463:GLN:N	2.50	0.45
1:A:996:TYR:CE1	1:A:1000:MET:CE	2.90	0.45
1:A:1237:GLN:H	1:A:1544:ASN:HB2	1.81	0.45
2:B:841:ASP:OD1	2:B:842:GLU:N	2.40	0.45
2:B:1020:GLU:HG3	3:C:61:THR:OG1	2.17	0.45
3:C:294:VAL:O	3:C:294:VAL:HG12	2.15	0.45
3:C:295:ARG:HD3	3:C:295:ARG:HA	1.66	0.45
7:G:143:SER:CB	15:O:103:ASN:HA	2.46	0.45
15:O:156:MET:HE2	15:O:193:TYR:CD1	2.52	0.45
1:A:782:ASP:O	1:A:785:GLN:N	2.27	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:GLU:HG2	1:A:1205:PHE:CD2	2.50	0.45
1:A:1006:LEU:HD21	2:B:535:ASP:HB2	1.98	0.45
1:A:1048:PHE:HZ	5:E:211:TYR:HB2	1.81	0.45
1:A:1657:LEU:HD22	7:G:104:LEU:CD1	2.45	0.45
2:B:61:LEU:HA	2:B:61:LEU:HD23	1.76	0.45
2:B:646:HIS:O	2:B:647:SER:HB2	2.16	0.45
7:G:242:VAL:HG12	15:O:185:SER:CB	2.46	0.45
15:O:372:VAL:CG1	15:O:423:TYR:OH	2.64	0.45
1:A:891:ILE:CD1	9:I:71:LEU:N	2.80	0.45
1:A:1348:VAL:CA	2:B:268:GLU:O	2.63	0.45
2:B:585:CYS:HB2	2:B:595:TRP:CZ3	2.51	0.45
4:D:80:THR:CG2	15:O:227:PHE:CG	2.99	0.45
15:O:148:PRO:HB3	15:O:183:ILE:CD1	2.46	0.45
15:O:407:SER:CB	15:O:408:PHE:CD1	2.95	0.45
15:O:521:ASN:HD22	15:O:523:ASN:H	1.59	0.45
1:A:799:GLU:CG	1:A:1062:HIS:CG	2.85	0.45
1:A:799:GLU:CG	1:A:1062:HIS:ND1	2.69	0.45
1:A:1154:LEU:O	1:A:1158:SER:HB2	2.17	0.45
1:A:1291:VAL:HG22	1:A:1473:LYS:HG3	1.99	0.45
1:A:1657:LEU:HD11	6:F:135:ARG:HB2	1.98	0.45
3:C:117:ASP:OD1	3:C:119:ASN:ND2	2.44	0.45
3:C:176:SER:O	3:C:180:ALA:HB2	2.16	0.45
13:M:65:TYR:HE1	13:M:97:VAL:HB	1.81	0.45
15:O:369:LYS:HE3	15:O:370:THR:HG22	1.99	0.45
15:O:384:ILE:HA	15:O:602:TYR:OH	2.16	0.45
15:O:408:PHE:HZ	15:O:446:LEU:CD2	2.30	0.45
15:O:468:GLU:O	15:O:470:PHE:N	2.49	0.45
1:A:365:THR:C	1:A:367:PHE:N	2.73	0.45
1:A:878:ARG:NE	9:I:67:VAL:HG13	2.30	0.45
2:B:1158:ILE:HA	2:B:1167:PHE:O	2.17	0.45
5:E:7:ARG:O	5:E:11:ARG:HG3	2.17	0.45
15:O:98:ASP:OD2	15:O:135:LYS:CD	2.64	0.45
15:O:237:ILE:HG22	15:O:381:ILE:CB	2.44	0.45
1:A:1463:ASP:HB2	1:A:1469:TRP:CE2	2.52	0.45
3:C:57:ILE:HG13	3:C:296:ASN:O	2.17	0.45
11:K:49:LEU:HG	11:K:54:THR:HG21	1.98	0.45
1:A:598:ALA:CB	1:A:601:MET:HE3	2.47	0.45
3:C:71:MET:CB	3:C:225:ALA:HB3	2.47	0.45
4:D:22:ILE:O	7:G:76:LYS:HG2	2.17	0.45
5:E:144:ILE:HG13	5:E:145:THR:N	2.32	0.45
13:M:61:GLU:OE2	13:M:106:LYS:NZ	2.43	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:THR:HG1	1:A:435:ASN:HD21	1.58	0.44
1:A:878:ARG:NH2	9:I:66:VAL:HG23	2.32	0.44
1:A:1054:ALA:HB1	1:A:1178:LEU:HD22	1.98	0.44
7:G:17:ILE:C	7:G:19:LYS:H	2.25	0.44
7:G:163:PRO:HG2	7:G:166:TRP:CD1	2.53	0.44
15:O:426:SER:HB3	15:O:594:TYR:CD2	2.50	0.44
1:A:54:LEU:HD13	1:A:368:ARG:NH2	2.33	0.44
1:A:401:ASP:CG	1:A:405:LYS:HE3	2.40	0.44
1:A:799:GLU:HG3	1:A:1062:HIS:CD2	2.49	0.44
2:B:470:LEU:HD22	2:B:478:LEU:HD12	1.99	0.44
2:B:683:ASN:HA	14:N:150:TYR:CZ	2.53	0.44
15:O:143:LEU:HD11	15:O:150:TRP:HD1	1.77	0.44
1:A:437:PHE:CE2	1:A:456:VAL:HG21	2.52	0.44
1:A:480:ALA:HA	2:B:1046:VAL:HA	1.97	0.44
1:A:1063:MET:HB3	1:A:1063:MET:HE2	1.66	0.44
2:B:833:PRO:HG2	2:B:836:TRP:CZ2	2.52	0.44
5:E:78:LEU:HD13	5:E:107:THR:HB	1.98	0.44
5:E:177:ARG:HD3	5:E:215:MET:HB2	1.99	0.44
15:O:488:HIS:CE1	15:O:489:ASN:OD1	2.71	0.44
1:A:35:PRO:CA	1:A:390:LEU:HD13	2.47	0.44
1:A:257:ASN:OD1	1:A:258:GLU:N	2.51	0.44
1:A:1441:LYS:HB3	1:A:1441:LYS:HE2	1.75	0.44
2:B:107:PRO:HG2	2:B:133:TYR:CZ	2.52	0.44
2:B:468:GLY:O	2:B:484:TYR:HD2	2.01	0.44
2:B:786:ALA:HB1	2:B:928:SER:HB2	1.98	0.44
2:B:1020:GLU:OE2	3:C:61:THR:HG21	2.18	0.44
3:C:230:LEU:CG	3:C:231:PRO:HD2	2.48	0.44
3:C:272:LYS:HA	14:N:175:TYR:CE2	2.53	0.44
1:A:37:VAL:HG12	1:A:38:LEU:HG	2.00	0.44
1:A:891:ILE:HD13	9:I:71:LEU:CB	2.44	0.44
1:A:920:PHE:CD1	1:A:921:PRO:HA	2.52	0.44
1:A:1229:ALA:HB3	1:A:1597:ALA:HB2	1.99	0.44
1:A:1600:ARG:NH2	1:A:1617:THR:OG1	2.48	0.44
3:C:252:PRO:HD2	3:C:255:VAL:HG21	1.99	0.44
4:D:48:GLU:OE2	4:D:90:LYS:NZ	2.51	0.44
10:J:36:LEU:HD13	10:J:47:ARG:HB3	1.98	0.44
15:O:163:ILE:CG2	15:O:211:TYR:HB2	2.38	0.44
15:O:368:PHE:HE2	15:O:382:GLN:HA	1.81	0.44
1:A:1313:LEU:O	1:A:1317:ILE:HD12	2.18	0.44
1:A:1654:PHE:HA	6:F:135:ARG:O	2.17	0.44
2:B:190:ILE:HG13	2:B:191:GLY:N	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:THR:OG1	2:B:912:GLN:NE2	2.51	0.44
2:B:954:PHE:H	2:B:955:PRO:HD2	1.83	0.44
2:B:974:LEU:O	10:J:47:ARG:NH1	2.50	0.44
12:L:63:ARG:HA	12:L:63:ARG:HD2	1.74	0.44
15:O:158:LEU:HD22	15:O:172:HIS:CG	2.52	0.44
15:O:237:ILE:HG22	15:O:381:ILE:CD1	2.34	0.44
1:A:1:MET:CB	2:B:1098:TYR:CG	2.98	0.44
1:A:449:GLY:C	1:A:451:VAL:H	2.23	0.44
1:A:509:GLU:CG	1:A:579:ARG:HE	2.31	0.44
1:A:572:THR:HA	7:G:52:MET:HE1	1.97	0.44
1:A:684:ASP:CG	8:H:20:TYR:HB3	2.42	0.44
1:A:1023:LEU:CD2	1:A:1598:PHE:CE1	3.01	0.44
1:A:1156:LYS:C	1:A:1158:SER:H	2.25	0.44
2:B:938:PHE:CD1	3:C:68:ARG:NH2	2.86	0.44
4:D:28:PRO:HB2	7:G:24:VAL:CG1	2.47	0.44
5:E:93:MET:CG	5:E:120:ALA:HB1	2.46	0.44
15:O:78:VAL:HA	15:O:88:ILE:HG22	2.00	0.44
15:O:241:ASP:CG	15:O:379:ARG:C	2.86	0.44
1:A:1660:VAL:O	7:G:102:GLU:CA	2.50	0.44
2:B:78:PRO:O	2:B:79:LEU:HB3	2.17	0.44
15:O:128:LEU:HB3	15:O:129:PRO:HD2	1.97	0.44
15:O:237:ILE:HD13	15:O:384:ILE:HD11	2.00	0.44
1:A:507:TYR:CD2	1:A:508:PRO:O	2.70	0.44
15:O:76:ASN:O	15:O:80:LEU:HD13	2.18	0.44
15:O:412:GLU:OE1	15:O:412:GLU:HA	2.18	0.44
15:O:458:GLU:CB	15:O:461:VAL:HG21	2.47	0.44
15:O:515:ASN:N	15:O:516:PRO:HD3	2.33	0.44
15:O:521:ASN:CG	15:O:522:GLU:H	2.25	0.44
1:A:1:MET:CB	2:B:1098:TYR:CD1	3.01	0.43
1:A:509:GLU:OE2	1:A:579:ARG:NH2	2.51	0.43
1:A:677:GLY:HA3	1:A:786:TYR:OH	2.18	0.43
1:A:782:ASP:OD2	1:A:931:SER:C	2.58	0.43
3:C:230:LEU:CG	3:C:231:PRO:CD	2.96	0.43
4:D:96:PHE:CE1	7:G:150:HIS:CD2	3.06	0.43
15:O:56:VAL:CG2	15:O:99:ILE:HD12	2.48	0.43
15:O:607:LYS:HE2	15:O:607:LYS:HB2	1.88	0.43
1:A:833:LEU:C	1:A:944:MET:HE3	2.43	0.43
1:A:1028:GLU:HA	1:A:1187:ILE:HG12	2.00	0.43
1:A:1261:VAL:HG21	1:A:1306:TYR:HB3	2.00	0.43
2:B:563:SER:HB2	13:M:73:SER:HB3	2.00	0.43
9:I:26:SER:O	9:I:39:LYS:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:194:LEU:HD21	15:O:225:LEU:HD11	1.96	0.43
15:O:458:GLU:HA	15:O:461:VAL:HG23	0.48	0.43
1:A:36:THR:HG22	1:A:45:VAL:HG21	2.00	0.43
1:A:403:LEU:HD12	1:A:403:LEU:HA	1.79	0.43
1:A:436:ALA:HA	1:A:443:ALA:HB2	1.99	0.43
1:A:509:GLU:OE1	1:A:509:GLU:HA	2.18	0.43
1:A:718:THR:HG21	8:H:118:PHE:O	2.18	0.43
2:B:203:ILE:HB	2:B:405:GLY:HA3	2.00	0.43
2:B:1069:ILE:CG2	2:B:1070:ARG:N	2.73	0.43
14:N:87:TYR:CD1	14:N:141:GLU:HA	2.53	0.43
15:O:391:GLN:CD	15:O:609:TYR:HH	2.26	0.43
15:O:413:ALA:HB1	15:O:415:GLU:OE1	2.18	0.43
1:A:535:GLN:HA	1:A:546:LEU:HG	1.99	0.43
3:C:64:ALA:HB2	3:C:298:PHE:CE2	2.51	0.43
15:O:245:GLN:CG	15:O:378:THR:HG23	2.48	0.43
15:O:383:TYR:O	15:O:386:PHE:N	2.51	0.43
15:O:460:GLU:O	15:O:469:ARG:CZ	2.66	0.43
2:B:209:GLN:CG	2:B:210:ARG:N	2.76	0.43
3:C:84:TYR:CZ	12:L:66:GLN:OE1	2.60	0.43
13:M:8:SER:O	14:N:71:PRO:HA	2.19	0.43
14:N:40:LEU:HD12	14:N:40:LEU:HA	1.84	0.43
14:N:80:MET:HE3	14:N:80:MET:HB2	1.91	0.43
14:N:94:ASP:HB3	14:N:99:LEU:HG	2.00	0.43
15:O:173:HIS:HE1	15:O:214:ASN:O	2.02	0.43
15:O:431:ALA:HB3	15:O:434:LEU:HD21	2.00	0.43
15:O:434:LEU:HD23	15:O:439:ILE:HG13	2.00	0.43
1:A:1089:LEU:CD1	1:A:1175:MET:HE1	2.48	0.43
2:B:893:ASN:O	2:B:895:PHE:HD1	2.01	0.43
2:B:1019:GLY:HA2	3:C:65:ASN:CG	2.44	0.43
15:O:189:PHE:HA	15:O:192:THR:HG23	1.99	0.43
15:O:232:LEU:HA	15:O:232:LEU:HD12	1.74	0.43
15:O:352:LEU:HD23	15:O:358:VAL:HG23	1.85	0.43
1:A:399:LEU:CD1	1:A:423:LEU:HG	2.44	0.43
15:O:224:GLU:N	15:O:224:GLU:CD	2.73	0.43
15:O:377:TYR:O	15:O:377:TYR:CD2	2.70	0.43
1:A:1600:ARG:NH2	1:A:1621:PHE:CE2	2.86	0.43
2:B:29:PRO:O	2:B:177:PRO:HD2	2.18	0.43
2:B:699:ILE:O	2:B:703:LEU:HG	2.19	0.43
2:B:923:GLN:HG2	2:B:949:ILE:CD1	2.47	0.43
3:C:131:THR:CG2	3:C:208:CYS:C	2.92	0.43
7:G:29:ASP:OD1	7:G:30:GLU:N	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:356:GLU:OE1	15:O:356:GLU:HA	2.19	0.43
15:O:487:ARG:NH1	15:O:487:ARG:HG3	2.34	0.43
1:A:477:ASN:C	2:B:1048:SER:O	2.52	0.43
2:B:399:HIS:O	2:B:400:GLN:HG2	2.18	0.43
2:B:555:GLN:N	2:B:646:HIS:NE2	2.67	0.43
4:D:80:THR:HB	15:O:227:PHE:CD2	2.50	0.43
15:O:169:THR:O	15:O:172:HIS:N	2.52	0.43
15:O:175:MET:HB2	15:O:175:MET:HE3	1.81	0.43
1:A:407:GLN:HB3	1:A:409:ASP:OD2	2.19	0.43
1:A:1575:ILE:HG12	9:I:122:ARG:NH1	2.28	0.43
1:A:1657:LEU:HD21	6:F:135:ARG:NH2	2.34	0.43
2:B:742:TYR:CE2	2:B:1037:ARG:HD3	2.54	0.43
15:O:124:LYS:O	15:O:127:GLU:HB2	2.18	0.43
1:A:1172:LEU:O	1:A:1176:ARG:HG2	2.19	0.42
2:B:883:GLU:HG3	2:B:906:ARG:HB2	2.01	0.42
14:N:63:ASP:OD2	14:N:66:LYS:NZ	2.35	0.42
15:O:390:GLN:NE2	15:O:431:ALA:HA	2.34	0.42
2:B:550:ARG:HA	2:B:550:ARG:HD3	1.80	0.42
6:F:66:ARG:NH1	7:G:90:LEU:CD1	2.82	0.42
12:L:32:ALA:HB3	12:L:55:ILE:HG23	2.01	0.42
15:O:96:LEU:O	15:O:100:LEU:HG	2.20	0.42
15:O:147:ILE:C	15:O:149:LYS:N	2.73	0.42
15:O:156:MET:HG2	15:O:197:PHE:CZ	2.53	0.42
15:O:199:PRO:HD3	15:O:211:TYR:CG	2.54	0.42
15:O:457:ARG:HA	15:O:460:GLU:CG	2.49	0.42
1:A:550:SER:OG	1:A:553:GLN:HG3	2.19	0.42
1:A:938:VAL:HG22	9:I:82:ILE:HD13	2.00	0.42
1:A:953:GLU:CA	1:A:1205:PHE:CD2	2.97	0.42
2:B:300:SER:OG	9:I:49:THR:HG23	2.17	0.42
2:B:569:GLY:CA	14:N:140:SER:OG	2.66	0.42
3:C:55:ASP:HB3	3:C:297:HIS:HE2	1.80	0.42
15:O:173:HIS:NE2	15:O:217:LYS:HB3	2.35	0.42
15:O:336:LEU:HD11	15:O:380:SER:O	2.19	0.42
15:O:383:TYR:O	15:O:384:ILE:C	2.60	0.42
1:A:998:HIS:NE2	2:B:712:SER:N	2.55	0.42
1:A:1034:TYR:HA	1:A:1181:PRO:CB	2.49	0.42
1:A:1606:SER:HB3	1:A:1611:MET:CE	2.47	0.42
2:B:243:GLN:O	2:B:411:MET:HE2	2.20	0.42
3:C:57:ILE:HB	3:C:297:HIS:CE1	2.55	0.42
6:F:93:ILE:HA	6:F:93:ILE:HD13	1.70	0.42
14:N:70:LEU:HA	14:N:71:PRO:HD3	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:404:ILE:CD1	15:O:442:VAL:HG11	2.49	0.42
15:O:430:ARG:HH22	15:O:596:PRO:CD	2.25	0.42
15:O:515:ASN:HD21	15:O:547:ASN:HD21	1.67	0.42
15:O:584:GLN:CD	15:O:584:GLN:H	2.13	0.42
1:A:1072:ASN:O	1:A:1073:TYR:C	2.61	0.42
2:B:211:ARG:CB	2:B:239:VAL:CG1	2.98	0.42
2:B:809:VAL:HG13	2:B:901:VAL:HB	2.01	0.42
2:B:1082:HIS:HB3	2:B:1084:THR:HG23	2.01	0.42
3:C:31:TRP:CE3	11:K:82:LYS:CB	3.02	0.42
4:D:44:ILE:HG21	4:D:90:LYS:CE	2.45	0.42
7:G:160:ASN:OD1	7:G:160:ASN:N	2.52	0.42
9:I:60:LEU:CA	9:I:63:LYS:HG3	2.45	0.42
15:O:125:TRP:C	15:O:127:GLU:N	2.77	0.42
1:A:475:ARG:NH1	2:B:1061:LYS:HA	2.35	0.42
1:A:990:ILE:CB	1:A:994:GLU:HB2	2.41	0.42
1:A:1655:ASP:HB2	6:F:135:ARG:CG	2.49	0.42
2:B:57:ASP:OD1	2:B:57:ASP:N	2.52	0.42
2:B:890:ASP:O	12:L:54:ARG:CD	2.68	0.42
15:O:124:LYS:HD3	15:O:127:GLU:OE2	2.20	0.42
15:O:202:ASN:N	15:O:202:ASN:OD1	2.52	0.42
15:O:234:ILE:HA	15:O:234:ILE:HD13	1.74	0.42
15:O:468:GLU:HG2	15:O:469:ARG:N	2.33	0.42
1:A:999:CYS:SG	2:B:531:VAL:HG22	2.59	0.42
2:B:33:SER:C	2:B:35:PHE:N	2.77	0.42
11:K:50:LEU:O	11:K:54:THR:HG23	2.20	0.42
13:M:102:SER:O	13:M:106:LYS:CB	2.56	0.42
15:O:156:MET:CE	15:O:193:TYR:CE1	3.00	0.42
1:A:478:TYR:HA	2:B:1048:SER:HA	0.57	0.42
1:A:1003:ARG:HD2	2:B:520:LEU:HB3	2.02	0.42
1:A:1575:ILE:CG1	9:I:122:ARG:HH22	2.32	0.42
2:B:469:ASN:HA	2:B:482:SER:HA	2.00	0.42
2:B:478:LEU:HB3	2:B:484:TYR:OH	2.20	0.42
2:B:697:LEU:HB2	2:B:702:ASN:ND2	2.35	0.42
2:B:938:PHE:CE2	3:C:68:ARG:HD2	2.54	0.42
15:O:447:THR:HB	15:O:505:PHE:CZ	2.55	0.42
15:O:447:THR:HG21	15:O:480:LEU:HD21	2.02	0.42
1:A:477:ASN:C	1:A:479:ALA:H	2.28	0.42
1:A:660:PRO:O	1:A:1057:ILE:HG21	2.20	0.42
2:B:467:THR:C	2:B:469:ASN:N	2.73	0.42
2:B:881:TYR:CZ	12:L:67:PHE:HE1	2.37	0.42
3:C:116:VAL:HG11	3:C:125:LYS:HE3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:66:ASN:ND2	15:O:111:ARG:CZ	2.83	0.42
15:O:77:GLN:HG2	15:O:88:ILE:HB	2.01	0.42
15:O:129:PRO:HD2	15:O:132:THR:CB	2.25	0.42
15:O:409:ALA:O	15:O:417:LYS:HE2	2.20	0.42
15:O:467:MET:CG	15:O:519:PHE:CZ	2.96	0.42
2:B:938:PHE:CE1	3:C:68:ARG:CD	3.03	0.42
2:B:1017:ALA:O	3:C:65:ASN:ND2	2.53	0.42
3:C:57:ILE:HG13	3:C:297:HIS:HB2	2.02	0.42
4:D:28:PRO:CB	7:G:24:VAL:CG1	2.98	0.42
7:G:158:LYS:C	15:O:105:ASN:ND2	2.78	0.42
15:O:370:THR:O	15:O:374:PRO:HG3	2.19	0.42
1:A:692:TYR:O	1:A:696:ILE:HG12	2.19	0.41
1:A:1648:ASN:O	1:A:1652:GLY:O	2.38	0.41
2:B:211:ARG:HH21	2:B:239:VAL:HG21	1.81	0.41
3:C:236:LEU:HD11	3:C:290:LYS:HG3	2.02	0.41
15:O:173:HIS:CG	15:O:217:LYS:HG3	2.55	0.41
15:O:417:LYS:HD3	15:O:472:HIS:CE1	2.33	0.41
1:A:385:LEU:HA	1:A:385:LEU:HD23	1.88	0.41
1:A:507:TYR:CE2	1:A:508:PRO:O	2.73	0.41
1:A:874:GLU:OE2	1:A:878:ARG:HD2	2.20	0.41
2:B:1090:ASP:HA	2:B:1094:ASN:HB2	2.02	0.41
5:E:26:ARG:O	5:E:75:MET:HE1	2.20	0.41
8:H:105:GLU:HG2	8:H:115:TYR:HE1	1.84	0.41
14:N:81:THR:HG22	14:N:86:ASP:HB3	2.01	0.41
15:O:56:VAL:HG23	15:O:57:LYS:N	2.35	0.41
15:O:430:ARG:O	15:O:610:TYR:HA	2.20	0.41
1:A:451:VAL:HA	1:A:452:PRO:HD3	1.95	0.41
1:A:680:LEU:O	1:A:728:GLY:HA3	2.21	0.41
2:B:478:LEU:CB	2:B:484:TYR:OH	2.69	0.41
2:B:656:LEU:HD21	2:B:689:VAL:HG12	2.01	0.41
3:C:64:ALA:HB1	3:C:298:PHE:CD2	2.56	0.41
15:O:150:TRP:O	15:O:154:VAL:HG23	2.21	0.41
15:O:234:ILE:HG22	15:O:371:HIS:CD2	2.42	0.41
15:O:458:GLU:HG2	15:O:461:VAL:HG21	2.02	0.41
15:O:592:PHE:HA	15:O:593:PRO:HD3	1.91	0.41
1:A:854:GLY:HA3	1:A:974:THR:O	2.21	0.41
1:A:891:ILE:HD12	9:I:71:LEU:N	2.35	0.41
1:A:1009:THR:C	1:A:1011:VAL:N	2.78	0.41
1:A:1248:ASP:OD1	1:A:1517:ARG:NH1	2.49	0.41
1:A:1499:ARG:HG2	1:A:1500:GLN:N	2.35	0.41
2:B:143:TRP:CE3	2:B:446:MET:HG3	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:GLN:HB3	9:I:32:GLN:HE21	1.84	0.41
2:B:1094:ASN:O	2:B:1096:SER:N	2.41	0.41
7:G:223:GLU:H	7:G:223:GLU:HG3	1.71	0.41
15:O:108:GLU:HB2	15:O:147:ILE:CD1	2.47	0.41
15:O:201:LYS:H	15:O:201:LYS:HG3	1.59	0.41
15:O:352:LEU:CD2	15:O:358:VAL:CG2	2.56	0.41
15:O:413:ALA:HB1	15:O:415:GLU:CD	2.44	0.41
15:O:423:TYR:CE1	15:O:593:PRO:HB2	2.55	0.41
1:A:990:ILE:HB	1:A:994:GLU:CD	2.45	0.41
1:A:1242:ILE:HG22	1:A:1536:ILE:HG22	2.01	0.41
1:A:1348:VAL:HA	1:A:1349:PRO:HD3	1.93	0.41
2:B:464:PHE:O	2:B:468:GLY:N	2.49	0.41
3:C:84:TYR:CE2	12:L:66:GLN:HB2	2.47	0.41
3:C:84:TYR:HD2	12:L:66:GLN:CB	2.30	0.41
4:D:82:LEU:O	4:D:86:ILE:HG23	2.20	0.41
7:G:24:VAL:O	7:G:25:THR:O	2.39	0.41
9:I:20:PRO:C	9:I:22:ALA:H	2.29	0.41
15:O:358:VAL:C	15:O:362:ASN:HD21	2.27	0.41
1:A:1:MET:HB2	2:B:1098:TYR:CD2	2.54	0.41
1:A:248:PHE:HD1	1:A:442:LYS:O	2.01	0.41
1:A:1056:ASP:HB3	1:A:1059:LYS:HB2	2.02	0.41
1:A:1305:GLU:HG3	9:I:60:LEU:HG	2.03	0.41
2:B:211:ARG:O	2:B:212:ASN:HB2	2.21	0.41
2:B:286:ARG:HD2	2:B:286:ARG:HA	1.88	0.41
3:C:272:LYS:HG3	14:N:175:TYR:CZ	2.55	0.41
7:G:139:ILE:CD1	15:O:178:TYR:OH	2.68	0.41
14:N:25:ILE:HA	14:N:26:PRO:HD3	1.84	0.41
1:A:1070:LEU:C	1:A:1072:ASN:N	2.78	0.41
2:B:206:LEU:HD23	2:B:206:LEU:HA	1.81	0.41
3:C:80:ALA:HB3	3:C:102:GLY:HA2	2.03	0.41
7:G:28:ILE:HG23	7:G:34:THR:O	2.20	0.41
8:H:95:TYR:HD2	8:H:144:ILE:HD12	1.86	0.41
12:L:33:GLU:HG3	12:L:53:HIS:ND1	2.36	0.41
15:O:241:ASP:CG	15:O:380:SER:N	2.78	0.41
15:O:241:ASP:HA	15:O:380:SER:CB	2.46	0.41
1:A:437:PHE:C	1:A:439:ASP:N	2.78	0.41
3:C:57:ILE:HB	3:C:297:HIS:ND1	2.35	0.41
4:D:23:HIS:CD2	6:F:58:PHE:CE1	3.08	0.41
11:K:54:THR:HG22	11:K:62:SER:H	1.86	0.41
15:O:107:ILE:O	15:O:107:ILE:CG2	2.69	0.41
15:O:115:LEU:O	15:O:119:ILE:HG13	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:237:ILE:HG21	15:O:381:ILE:CG1	2.51	0.41
15:O:241:ASP:CG	15:O:378:THR:CG2	2.78	0.41
1:A:315:ILE:HG13	1:A:319:GLU:HB2	2.03	0.41
1:A:509:GLU:CG	1:A:579:ARG:CD	2.99	0.41
1:A:1074:TYR:CE2	1:A:1159:ASP:HB3	2.54	0.41
1:A:1195:GLU:HB3	1:A:1196:PRO:HD3	2.03	0.41
1:A:1262:LEU:HD22	1:A:1497:ILE:HG12	2.03	0.41
1:A:1317:ILE:O	1:A:1322:ILE:HG12	2.21	0.41
1:A:1575:ILE:HG13	9:I:122:ARG:NH2	2.36	0.41
1:A:1606:SER:CB	1:A:1611:MET:HE3	2.49	0.41
2:B:262:PHE:CE1	2:B:357:ILE:HD13	2.56	0.41
2:B:279:ALA:HB2	2:B:326:VAL:HG12	2.03	0.41
2:B:527:PHE:CE2	2:B:666:PRO:HA	2.55	0.41
2:B:545:PHE:CZ	2:B:551:ILE:HD11	2.56	0.41
2:B:1043:LYS:HE2	2:B:1063:ARG:HD2	2.01	0.41
7:G:50:ALA:HA	7:G:113:PHE:CD2	2.56	0.41
8:H:41:ASP:HB2	8:H:121:LEU:HB3	2.02	0.41
9:I:2:SER:HA	9:I:9:PHE:O	2.21	0.41
15:O:107:ILE:CD1	15:O:115:LEU:HD23	2.51	0.41
15:O:147:ILE:HG22	15:O:149:LYS:CB	2.51	0.41
15:O:163:ILE:HD12	15:O:207:LYS:HG2	2.02	0.41
15:O:182:MET:HE2	15:O:183:ILE:HG13	2.03	0.41
15:O:369:LYS:HZ3	15:O:369:LYS:CB	2.21	0.41
15:O:521:ASN:CG	15:O:522:GLU:N	2.79	0.41
1:A:700:ILE:HD13	1:A:700:ILE:HA	1.81	0.41
1:A:964:LYS:HB3	1:A:964:LYS:HE2	1.83	0.41
1:A:1037:SER:HA	1:A:1049:MET:HA	2.03	0.41
2:B:42:VAL:O	2:B:46:ILE:CG1	2.69	0.41
2:B:371:PHE:CE2	2:B:375:LEU:HD11	2.56	0.41
2:B:401:GLU:CG	2:B:402:VAL:N	2.73	0.41
2:B:699:ILE:HD13	2:B:760:TYR:CD1	2.55	0.41
2:B:736:ARG:NH1	2:B:738:ASP:OD1	2.54	0.41
2:B:1069:ILE:CG2	2:B:1070:ARG:H	2.20	0.41
15:O:194:LEU:O	15:O:232:LEU:CD2	2.57	0.41
15:O:447:THR:O	15:O:450:LEU:CA	2.68	0.41
1:A:411:VAL:CG2	1:A:412:SER:H	2.26	0.40
1:A:1006:LEU:CD2	2:B:535:ASP:CB	2.99	0.40
2:B:416:LYS:HA	2:B:416:LYS:HD3	1.87	0.40
3:C:31:TRP:NE1	11:K:78:TYR:HH	2.19	0.40
4:D:95:ASP:CG	7:G:151:ASP:HB2	2.46	0.40
15:O:198:PHE:HD2	15:O:232:LEU:CD2	2.32	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:365:THR:O	1:A:367:PHE:N	2.54	0.40
1:A:516:ILE:HG12	15:O:376:TYR:HE2	1.73	0.40
1:A:556:ALA:HA	15:O:246:ASN:HD22	1.85	0.40
1:A:1055:ILE:HG21	1:A:1060:GLU:CG	2.34	0.40
1:A:1229:ALA:HB1	1:A:1595:TYR:CE2	2.56	0.40
2:B:219:ARG:HA	2:B:220:PRO:HD2	1.73	0.40
2:B:427:GLN:OE1	2:B:452:ARG:NH1	2.54	0.40
2:B:555:GLN:CB	2:B:646:HIS:CE1	3.04	0.40
7:G:41:VAL:HA	7:G:42:PRO:HD3	1.92	0.40
8:H:7:ASP:HA	8:H:57:VAL:O	2.21	0.40
11:K:135:PHE:CE2	11:K:139:ILE:HD11	2.56	0.40
15:O:128:LEU:HD13	15:O:132:THR:HG22	2.02	0.40
15:O:244:LEU:HD23	15:O:244:LEU:O	2.20	0.40
1:A:487:ASP:HB2	1:A:615:ARG:HB3	2.02	0.40
1:A:756:LYS:HD2	9:I:85:LYS:HZ2	1.61	0.40
1:A:1661:PRO:HA	7:G:101:SER:O	2.21	0.40
2:B:472:SER:C	2:B:474:SER:N	2.77	0.40
2:B:937:PRO:HB2	2:B:1013:MET:HE2	2.04	0.40
3:C:128:ASP:OD1	3:C:128:ASP:N	2.54	0.40
4:D:25:THR:HB	6:F:59:GLN:HG3	2.02	0.40
7:G:71:MET:HE1	7:G:153:PHE:CE1	2.56	0.40
15:O:505:PHE:O	15:O:509:MET:HG2	2.21	0.40
2:B:467:THR:HB	2:B:469:ASN:HD21	1.81	0.40
2:B:491:ILE:HB	2:B:495:ARG:HD2	2.03	0.40
3:C:45:SER:HB3	3:C:271:ARG:HH22	1.80	0.40
15:O:237:ILE:HB	15:O:381:ILE:HD11	1.92	0.40
15:O:422:GLN:HB3	15:O:593:PRO:HD3	2.02	0.40
15:O:505:PHE:CD1	15:O:505:PHE:C	2.99	0.40
1:A:389:VAL:O	1:A:393:SER:HB2	2.22	0.40
1:A:498:PRO:HA	1:A:499:PRO:HD3	1.81	0.40
1:A:1048:PHE:HD2	5:E:210:SER:HG	1.69	0.40
2:B:168:ASN:O	2:B:169:ARG:HD3	2.21	0.40
4:D:23:HIS:CB	6:F:58:PHE:CD2	3.04	0.40
8:H:39:THR:O	8:H:123:MET:HA	2.22	0.40
9:I:87:PRO:HG2	9:I:119:TYR:CE2	2.56	0.40
15:O:342:HIS:NE2	15:O:346:GLN:HG3	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1464/1664 (88%)	1370 (94%)	82 (6%)	12 (1%)	16	52
2	B	1166/1203 (97%)	1086 (93%)	56 (5%)	24 (2%)	5	29
3	C	303/335 (90%)	278 (92%)	18 (6%)	7 (2%)	5	28
4	D	54/137 (39%)	50 (93%)	2 (4%)	2 (4%)	2	19
5	E	210/215 (98%)	197 (94%)	11 (5%)	2 (1%)	12	47
6	F	98/155 (63%)	94 (96%)	4 (4%)	0	100	100
7	G	189/326 (58%)	171 (90%)	13 (7%)	5 (3%)	4	25
8	H	127/146 (87%)	121 (95%)	6 (5%)	0	100	100
9	I	101/125 (81%)	89 (88%)	9 (9%)	3 (3%)	3	22
10	J	67/70 (96%)	63 (94%)	4 (6%)	0	100	100
11	K	99/142 (70%)	92 (93%)	7 (7%)	0	100	100
12	L	41/70 (59%)	32 (78%)	6 (15%)	3 (7%)	1	11
13	M	103/415 (25%)	93 (90%)	8 (8%)	2 (2%)	6	32
14	N	139/233 (60%)	123 (88%)	13 (9%)	3 (2%)	5	28
15	O	457/627 (73%)	400 (88%)	38 (8%)	19 (4%)	2	17
All	All	4618/5863 (79%)	4259 (92%)	277 (6%)	82 (2%)	9	33

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1606	SER
2	B	111	ASP
2	B	117	VAL
2	B	895	PHE
2	B	1069	ILE
3	C	224	THR
4	D	99	LEU
7	G	25	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	41	GLN
15	O	165	PRO
15	O	226	GLY
15	O	325	ILE
15	O	380	SER
15	O	431	ALA
15	O	489	ASN
15	O	521	ASN
1	A	448	SER
1	A	783	LYS
1	A	1533	GLU
2	B	473	GLN
2	B	817	ARG
2	B	1140	LYS
4	D	98	GLY
5	E	50	MET
7	G	27	PRO
9	I	5	GLY
12	L	62	LYS
15	O	374	PRO
15	O	488	HIS
15	O	540	CYS
1	A	450	LYS
1	A	1050	TYR
2	B	34	ALA
2	B	78	PRO
2	B	208	VAL
2	B	209	GLN
2	B	1044	PHE
2	B	1070	ARG
2	B	1095	SER
2	B	1098	TYR
3	C	297	HIS
5	E	146	HIS
7	G	99	ASP
9	I	21	ASN
12	L	46	VAL
13	M	85	LYS
15	O	82	SER
15	O	130	PRO
15	O	457	ARG
15	O	469	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	834	LYS
2	B	1094	ASN
3	C	295	ARG
7	G	100	THR
12	L	43	THR
13	M	36	THR
14	N	115	SER
15	O	148	PRO
15	O	187	MET
1	A	439	ASP
1	A	451	VAL
1	A	564	PRO
1	A	581	ILE
1	A	1049	MET
2	B	80	ASN
2	B	1062	GLY
2	B	1096	SER
3	C	32	ASN
3	C	296	ASN
15	O	377	TYR
1	A	1512	PRO
2	B	1063	ARG
3	C	222	VAL
15	O	147	ILE
3	C	221	PRO
14	N	70	LEU
15	O	128	LEU
2	B	468	GLY
14	N	39	PRO
7	G	28	ILE
2	B	833	PRO
2	B	954	PHE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	1307/1465 (89%)	1215 (93%)	92 (7%)	14	36
2	B	1027/1053 (98%)	957 (93%)	70 (7%)	14	36
3	C	269/296 (91%)	251 (93%)	18 (7%)	15	37
4	D	55/116 (47%)	50 (91%)	5 (9%)	9	28
5	E	194/197 (98%)	180 (93%)	14 (7%)	13	35
6	F	90/137 (66%)	86 (96%)	4 (4%)	25	47
7	G	170/291 (58%)	158 (93%)	12 (7%)	13	35
8	H	115/128 (90%)	107 (93%)	8 (7%)	14	36
9	I	97/110 (88%)	90 (93%)	7 (7%)	13	35
10	J	64/65 (98%)	56 (88%)	8 (12%)	4	17
11	K	91/130 (70%)	82 (90%)	9 (10%)	7	24
12	L	38/57 (67%)	33 (87%)	5 (13%)	4	16
13	M	95/371 (26%)	83 (87%)	12 (13%)	4	17
14	N	135/220 (61%)	128 (95%)	7 (5%)	21	43
15	O	427/576 (74%)	374 (88%)	53 (12%)	4	18
All	All	4174/5212 (80%)	3850 (92%)	324 (8%)	14	32

All (324) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	GLU
1	A	40	ASN
1	A	61	LEU
1	A	83	VAL
1	A	136	LEU
1	A	174	SER
1	A	186	SER
1	A	202	THR
1	A	230	ARG
1	A	257	ASN
1	A	262	THR
1	A	266	VAL
1	A	271	ARG
1	A	272	GLN
1	A	312	SER
1	A	315	ILE
1	A	346	SER
1	A	357	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	373	LEU
1	A	379	GLU
1	A	393	SER
1	A	403	LEU
1	A	408	LYS
1	A	412	SER
1	A	413	LEU
1	A	439	ASP
1	A	447	THR
1	A	451	VAL
1	A	503	VAL
1	A	518	GLU
1	A	524	ILE
1	A	555	LYS
1	A	582	LYS
1	A	611	GLU
1	A	627	ASP
1	A	661	THR
1	A	666	VAL
1	A	670	ILE
1	A	684	ASP
1	A	700	ILE
1	A	708	THR
1	A	709	ARG
1	A	739	VAL
1	A	747	ILE
1	A	758	GLU
1	A	783	LYS
1	A	794	VAL
1	A	815	ARG
1	A	878	ARG
1	A	955	ARG
1	A	957	VAL
1	A	966	LEU
1	A	988	SER
1	A	999	CYS
1	A	1004	GLU
1	A	1021	ARG
1	A	1026	GLN
1	A	1033	SER
1	A	1085	LEU
1	A	1098	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1102	LEU
1	A	1118	VAL
1	A	1123	VAL
1	A	1131	LYS
1	A	1136	VAL
1	A	1150	LYS
1	A	1159	ASP
1	A	1162	ASN
1	A	1204	THR
1	A	1215	VAL
1	A	1226	VAL
1	A	1273	THR
1	A	1275	THR
1	A	1276	THR
1	A	1310	LYS
1	A	1314	GLN
1	A	1320	GLN
1	A	1441	LYS
1	A	1455	ARG
1	A	1508	VAL
1	A	1518	VAL
1	A	1531	ASP
1	A	1533	GLU
1	A	1536	ILE
1	A	1601	GLN
1	A	1604	GLU
1	A	1605	THR
1	A	1607	THR
1	A	1609	SER
1	A	1611	MET
1	A	1633	GLN
1	A	1635	ASP
2	B	13	THR
2	B	17	ARG
2	B	22	GLU
2	B	37	LEU
2	B	53	THR
2	B	57	ASP
2	B	65	VAL
2	B	70	GLU
2	B	79	LEU
2	B	81	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	87	ASN
2	B	97	VAL
2	B	187	SER
2	B	202	LEU
2	B	211	ARG
2	B	221	SER
2	B	228	SER
2	B	231	HIS
2	B	236	ILE
2	B	239	VAL
2	B	276	ILE
2	B	281	CYS
2	B	305	ARG
2	B	306	LEU
2	B	311	ARG
2	B	315	LYS
2	B	357	ILE
2	B	486	VAL
2	B	490	LYS
2	B	523	GLU
2	B	537	SER
2	B	583	LEU
2	B	622	ILE
2	B	658	LEU
2	B	720	GLN
2	B	725	THR
2	B	731	VAL
2	B	753	LYS
2	B	782	ASP
2	B	811	LEU
2	B	813	LEU
2	B	822	THR
2	B	824	HIS
2	B	829	ASN
2	B	833	PRO
2	B	835	GLU
2	B	858	ILE
2	B	871	ILE
2	B	883	GLU
2	B	897	GLU
2	B	977	ILE
2	B	998	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1026	ILE
2	B	1043	LYS
2	B	1047	ARG
2	B	1060	VAL
2	B	1064	LYS
2	B	1069	ILE
2	B	1070	ARG
2	B	1075	GLU
2	B	1097	ASP
2	B	1100	GLN
2	B	1103	VAL
2	B	1125	THR
2	B	1136	GLU
2	B	1141	LEU
2	B	1153	ILE
2	B	1163	GLN
2	B	1165	ASN
2	B	1174	THR
3	C	38	LYS
3	C	43	ASN
3	C	61	THR
3	C	77	SER
3	C	91	VAL
3	C	97	LEU
3	C	118	SER
3	C	131	THR
3	C	138	VAL
3	C	142	ARG
3	C	181	ASP
3	C	193	LEU
3	C	222	VAL
3	C	224	THR
3	C	232	GLN
3	C	243	SER
3	C	277	ARG
3	C	279	VAL
4	D	15	THR
4	D	29	GLN
4	D	38	GLN
4	D	80	THR
4	D	99	LEU
5	E	4	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	31	THR
5	E	33	GLU
5	E	74	ASP
5	E	90	VAL
5	E	92	THR
5	E	93	MET
5	E	107	THR
5	E	131	THR
5	E	136	ASN
5	E	142	VAL
5	E	162	ARG
5	E	163	GLU
5	E	177	ARG
6	F	59	GLN
6	F	87	LYS
6	F	99	LEU
6	F	109	VAL
7	G	21	LYS
7	G	24	VAL
7	G	35	SER
7	G	39	VAL
7	G	139	ILE
7	G	147	LEU
7	G	167	THR
7	G	169	VAL
7	G	223	GLU
7	G	230	ARG
7	G	239	THR
7	G	243	VAL
8	H	3	ASN
8	H	9	ILE
8	H	39	THR
8	H	108	SER
8	H	111	LEU
8	H	112	ILE
8	H	114	VAL
8	H	121	LEU
9	I	2	SER
9	I	3	VAL
9	I	15	ASP
9	I	45	LEU
9	I	70	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	74	ASN
9	I	81	THR
10	J	3	VAL
10	J	9	SER
10	J	10	CYS
10	J	14	VAL
10	J	27	GLU
10	J	34	THR
10	J	45	CYS
10	J	48	ARG
11	K	44	ARG
11	K	45	GLU
11	K	51	THR
11	K	68	GLU
11	K	99	ASN
11	K	103	ILE
11	K	118	GLN
11	K	123	ASP
11	K	133	SER
12	L	38	LEU
12	L	41	SER
12	L	55	ILE
12	L	57	LEU
12	L	66	GLN
13	M	17	ASP
13	M	18	GLN
13	M	31	ARG
13	M	44	LYS
13	M	48	LYS
13	M	52	VAL
13	M	63	GLU
13	M	65	TYR
13	M	77	VAL
13	M	84	GLU
13	M	98	SER
13	M	109	ARG
14	N	51	GLN
14	N	89	ILE
14	N	124	THR
14	N	135	LYS
14	N	153	VAL
14	N	167	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
14	N	178	GLU
15	O	66	ASN
15	O	67	ASP
15	O	69	THR
15	O	78	VAL
15	O	80	LEU
15	O	87	ARG
15	O	101	SER
15	O	110	SER
15	O	111	ARG
15	O	117	GLN
15	O	149	LYS
15	O	171	CYS
15	O	175	MET
15	O	180	LEU
15	O	181	ARG
15	O	190	ILE
15	O	192	THR
15	O	194	LEU
15	O	202	ASN
15	O	203	ASP
15	O	204	THR
15	O	205	ARG
15	O	212	THR
15	O	213	SER
15	O	215	LEU
15	O	228	GLN
15	O	232	LEU
15	O	234	ILE
15	O	245	GLN
15	O	248	LEU
15	O	325	ILE
15	O	341	THR
15	O	350	GLU
15	O	354	SER
15	O	363	THR
15	O	368	PHE
15	O	369	LYS
15	O	382	GLN
15	O	395	LEU
15	O	415	GLU
15	O	437	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	454	VAL
15	O	457	ARG
15	O	487	ARG
15	O	489	ASN
15	O	494	THR
15	O	522	GLU
15	O	526	LEU
15	O	543	ILE
15	O	581	THR
15	O	584	GLN
15	O	597	LEU
15	O	602	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	382	GLN
1	A	432	ASN
1	A	435	ASN
1	A	470	HIS
1	A	580	HIS
1	A	590	ASN
1	A	671	GLN
1	A	863	ASN
1	A	1162	ASN
1	A	1180	ASN
2	B	87	ASN
2	B	328	GLN
2	B	422	GLN
2	B	462	GLN
2	B	646	HIS
2	B	893	ASN
2	B	912	GLN
2	B	1038	HIS
2	B	1163	GLN
2	B	1199	ASN
3	C	99	HIS
3	C	323	ASN
4	D	23	HIS
4	D	93	GLN
5	E	5	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	32	GLN
6	F	59	GLN
6	F	78	GLN
7	G	56	ASN
7	G	126	GLN
7	G	150	HIS
7	G	154	ASN
9	I	32	GLN
12	L	66	GLN
13	M	18	GLN
13	M	82	ASN
14	N	61	ASN
14	N	85	HIS
14	N	132	GLN
15	O	66	ASN
15	O	105	ASN
15	O	117	GLN
15	O	172	HIS
15	O	173	HIS
15	O	245	GLN
15	O	346	GLN
15	O	362	ASN
15	O	371	HIS
15	O	390	GLN
15	O	472	HIS
15	O	497	ASN
15	O	507	GLN
15	O	521	ASN
15	O	547	ASN
15	O	549	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

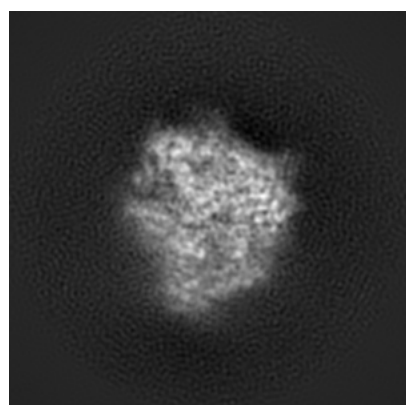
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3439. These allow visual inspection of the internal detail of the map and identification of artifacts.

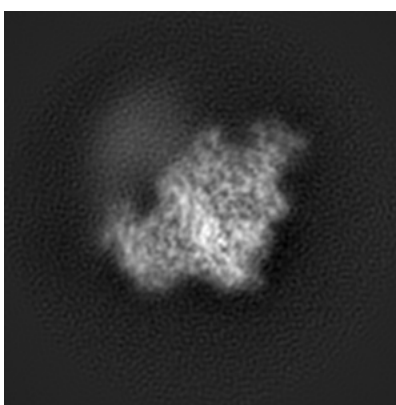
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

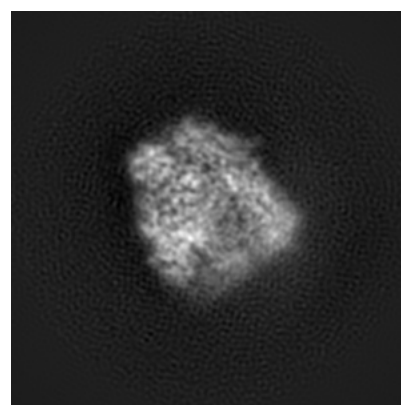
6.1.1 Primary map



X



Y

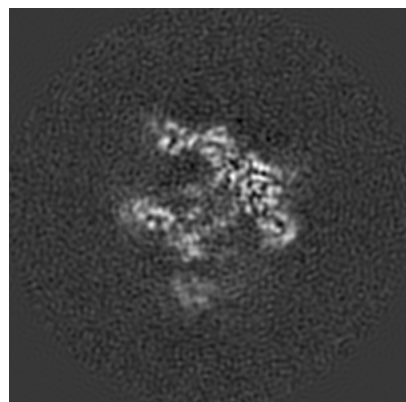


Z

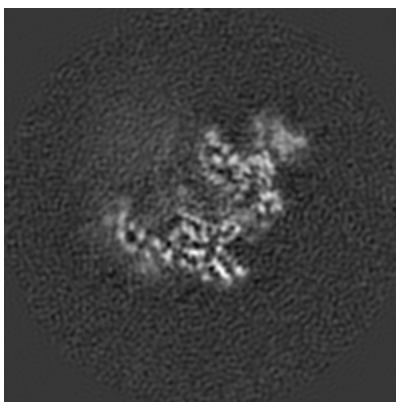
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

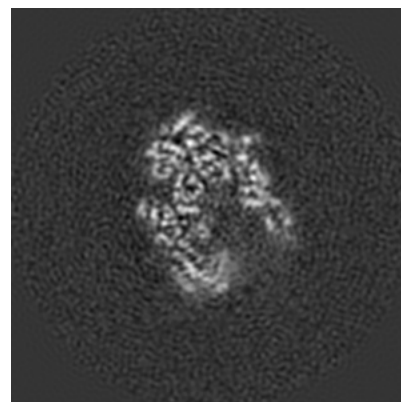
6.2.1 Primary map



X Index: 120



Y Index: 120

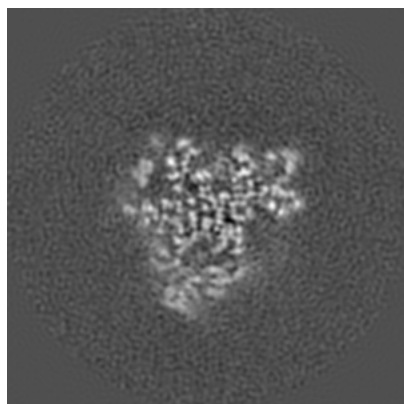


Z Index: 120

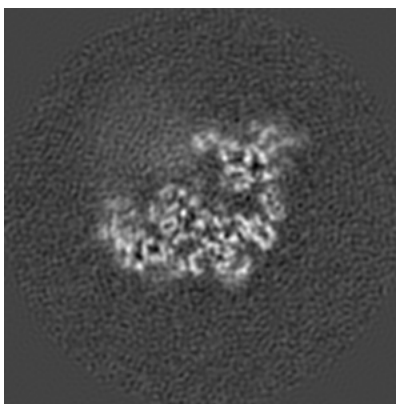
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

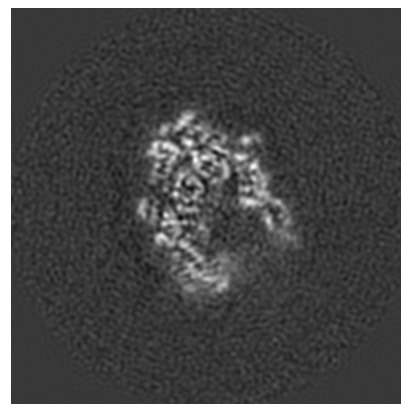
6.3.1 Primary map



X Index: 106



Y Index: 106

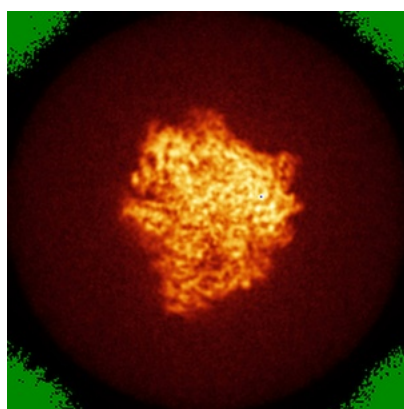


Z Index: 121

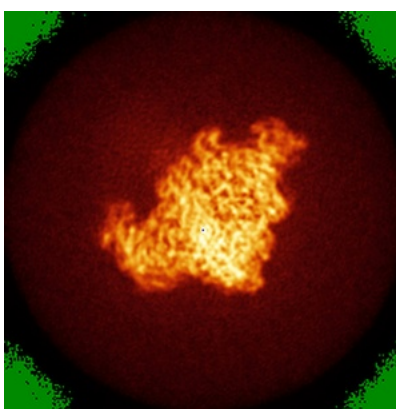
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

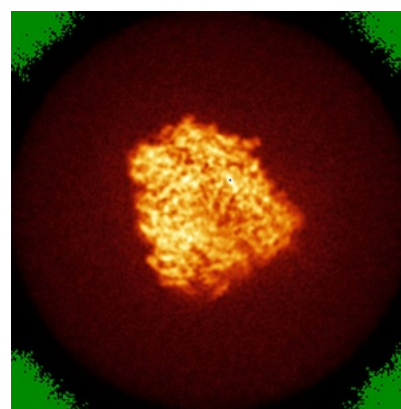
6.4.1 Primary map



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

This section was not generated.

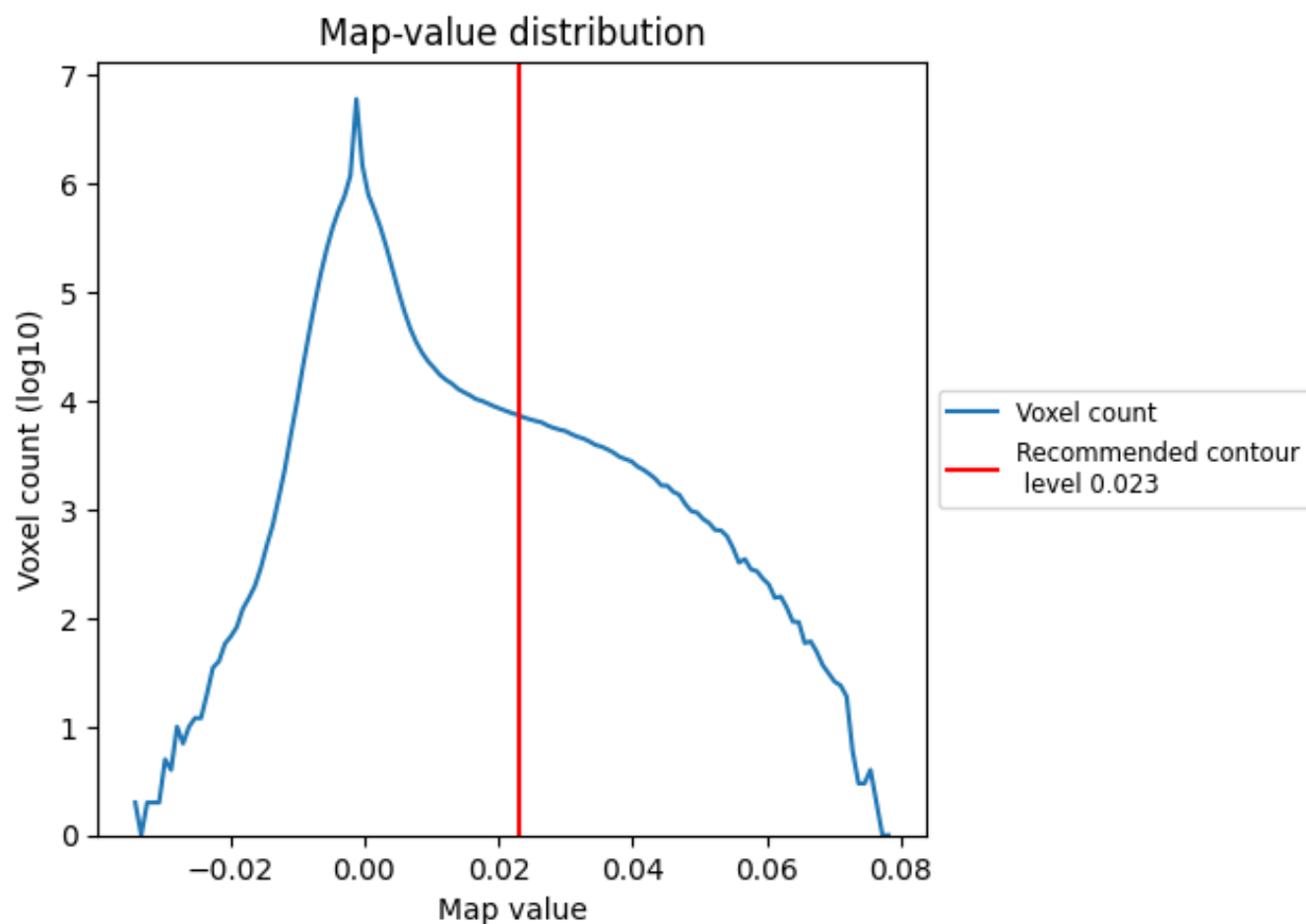
6.6 Mask visualisation

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

7 Map analysis [i](#)

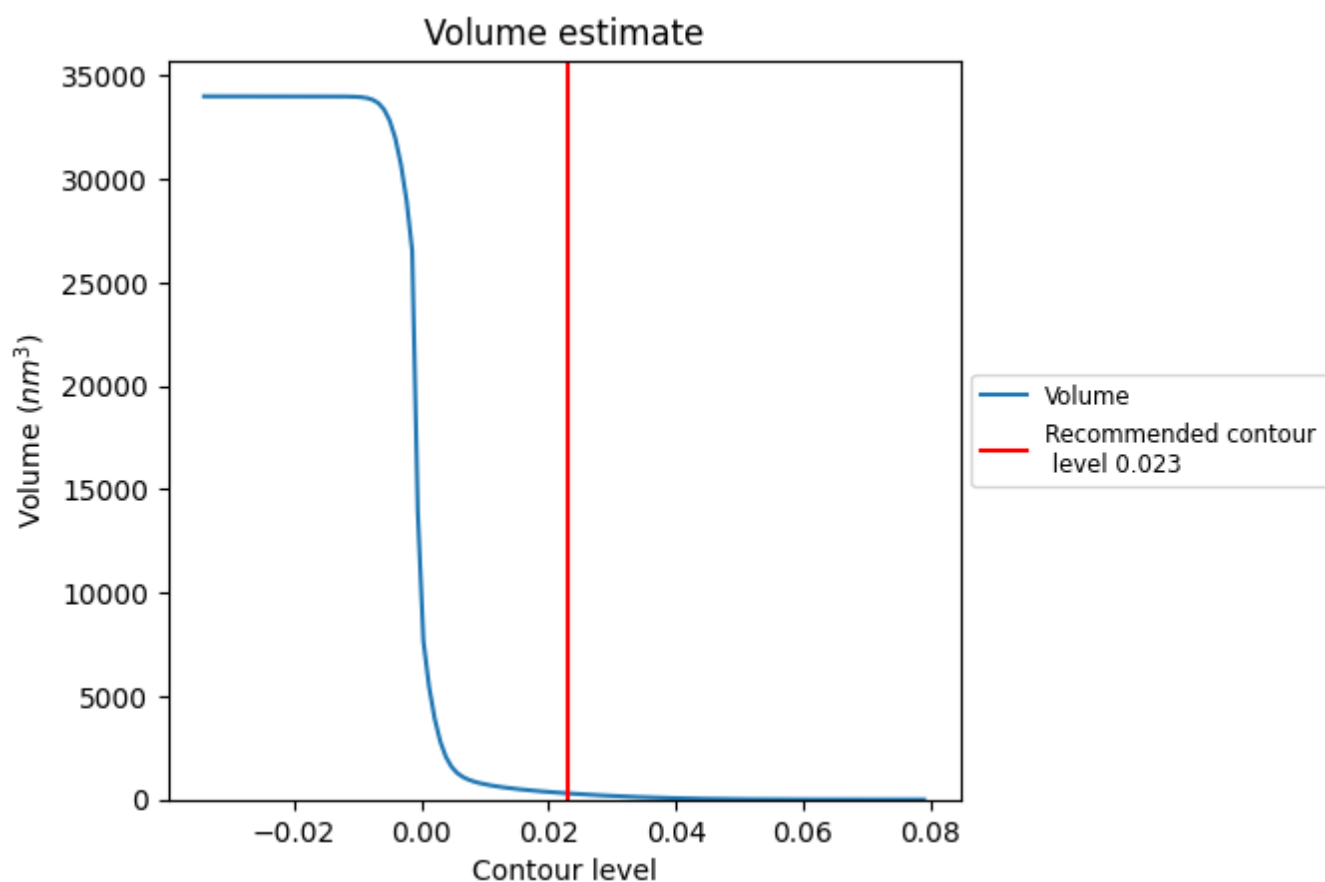
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

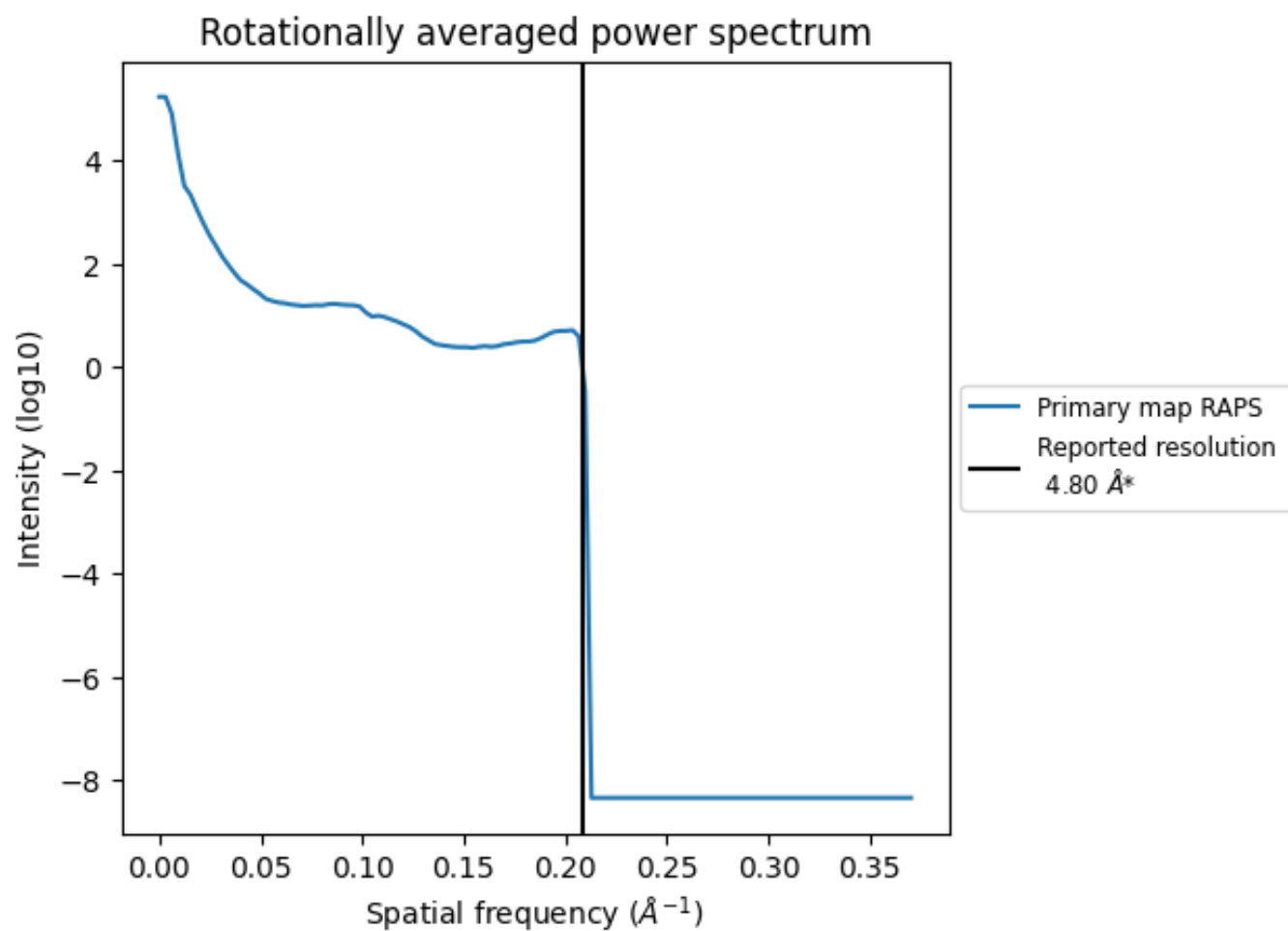
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 300 nm³; this corresponds to an approximate mass of 271 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.208 Å⁻¹

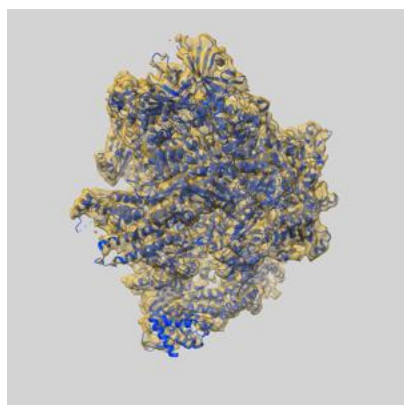
8 Fourier-Shell correlation

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

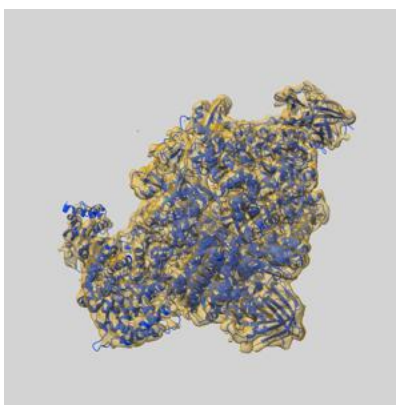
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3439 and PDB model 5G5L. Per-residue inclusion information can be found in section [3](#) on page [7](#).

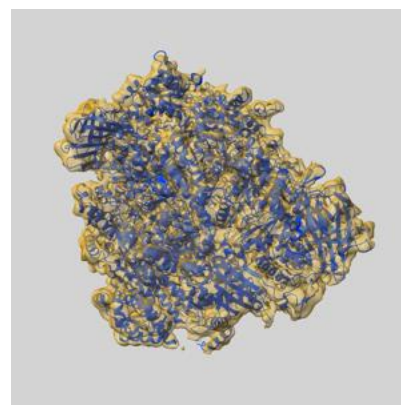
9.1 Map-model overlay [i](#)



X



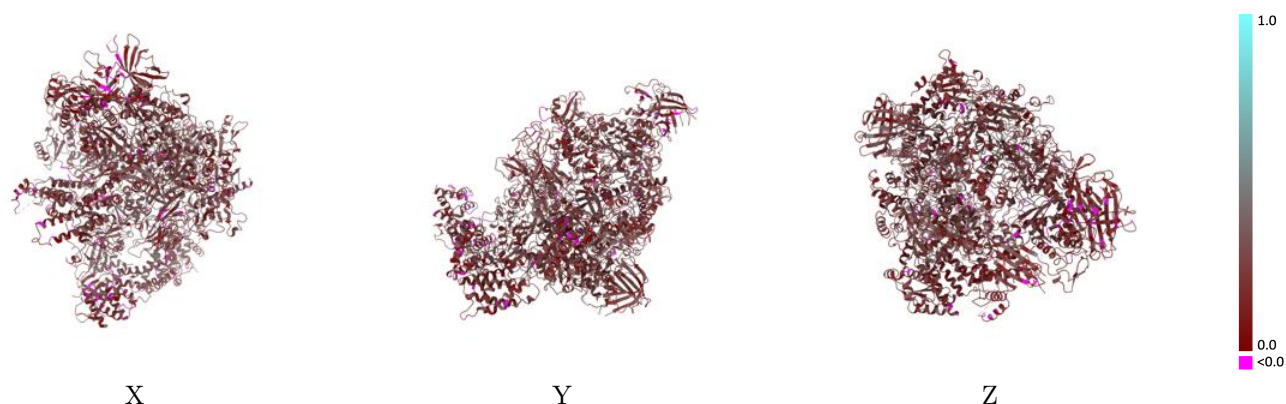
Y



Z

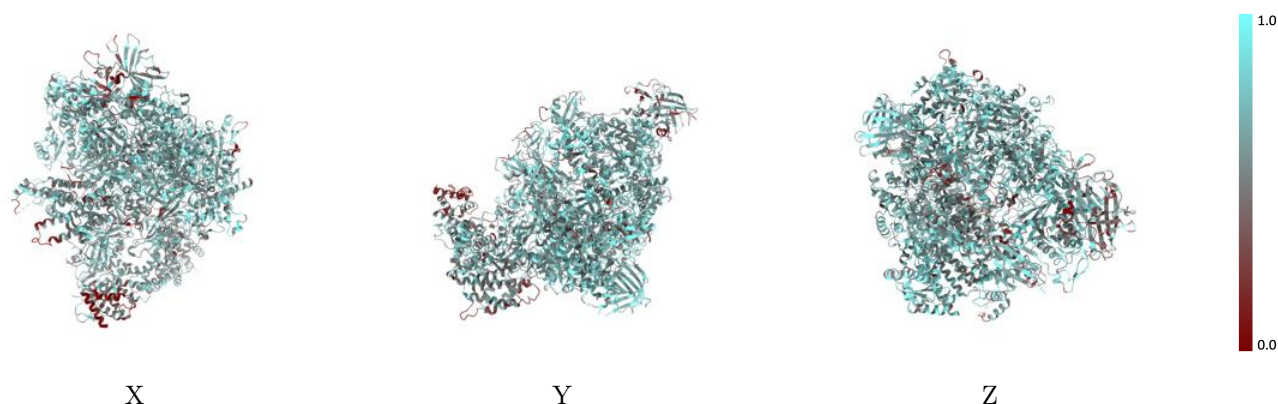
The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



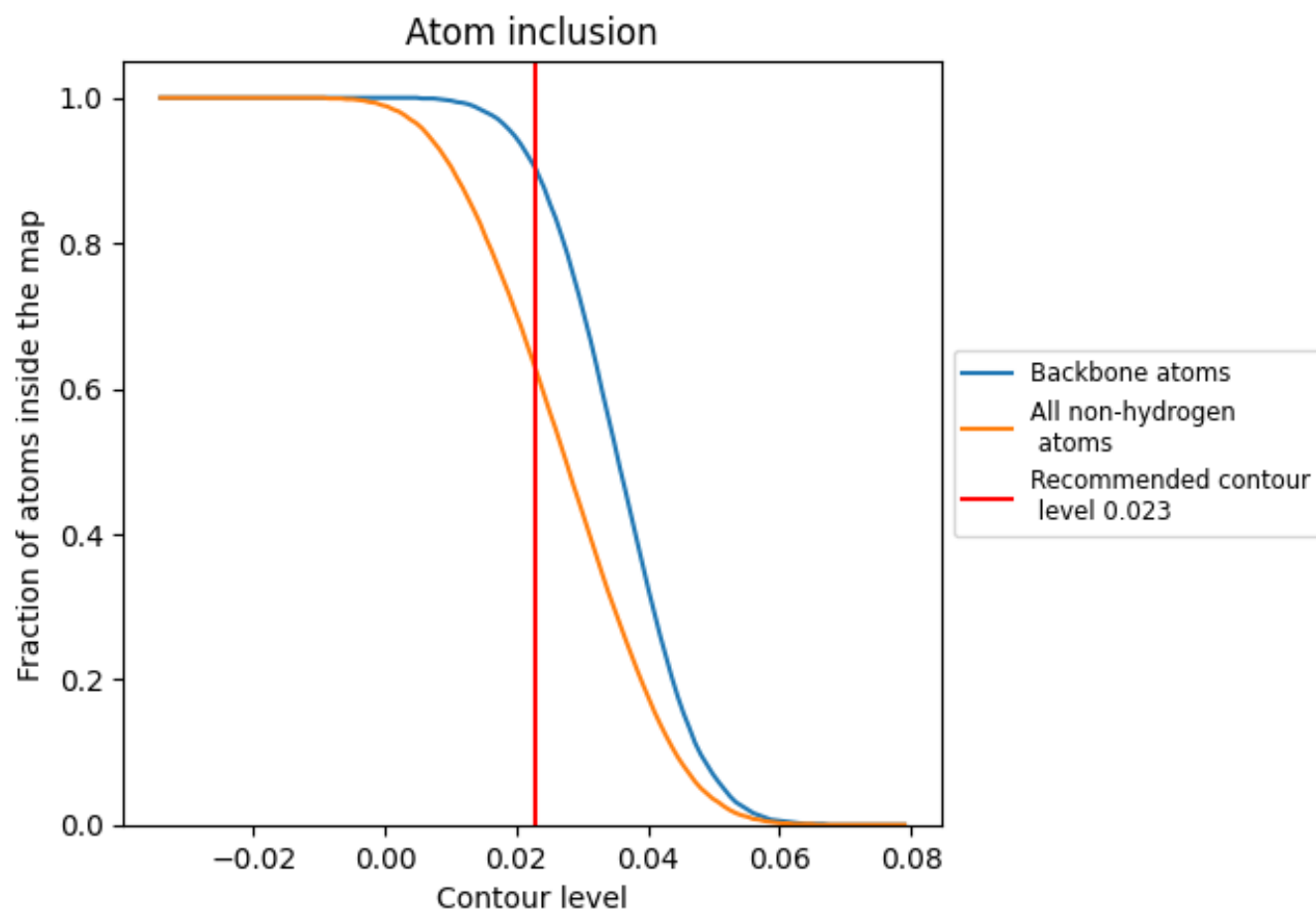
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.023).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 62% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6250	0.2290
A	0.6390	0.2330
B	0.6490	0.2420
C	0.6940	0.2360
D	0.6020	0.2160
E	0.7100	0.2390
F	0.6600	0.2600
G	0.6350	0.2230
H	0.7140	0.2510
I	0.5270	0.2350
J	0.6790	0.2400
K	0.6620	0.2310
L	0.6730	0.2440
M	0.4990	0.1990
N	0.4510	0.1930
O	0.4920	0.1840

1.0

0.0

<0.0