Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:01 PM GMT

PDB ID	:	4QIW
Title	:	Crystal structure of euryarchaeal RNA polymerase from Thermococcus kodakarensis
Authors	:	Jun, S.-H.; Murakami, K.S.
Deposited on	:	2014-06-02
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

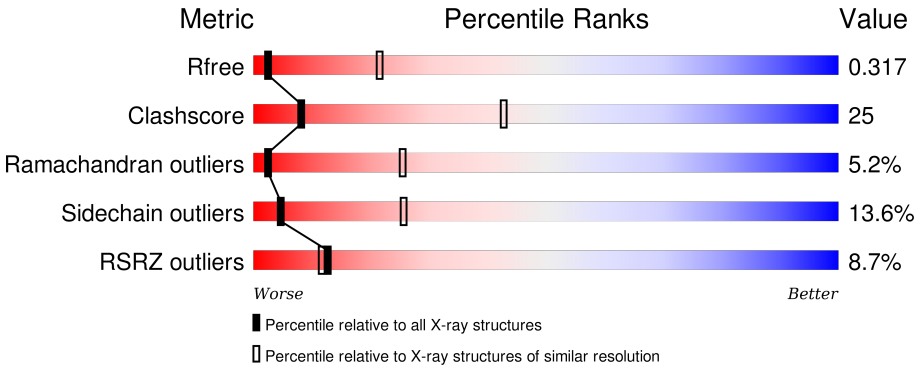
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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

Mol	Chain	Length	Quality of chain
1	A	906	9% 52% 35% 7% • 5%
1	I	906	9% 50% 36% 8% • 5%
2	B	1123	6% 48% 37% 9% • 5%
2	J	1123	4% 47% 39% 9% • 5%
3	C	391	19% 39% 41% 13% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	M	391	19% 38% 43% 12% 6%
4	D	259	10% 71% 25%
4	O	259	5% 70% 27%
5	E	190	13% 63% 28% 5%
5	Q	190	12% 65% 27% 5%
6	F	122	12% 74% 23%
6	R	122	5% 72% 26%
7	H	82	4% 40% 39% 13% 7%
7	S	82	5% 39% 41% 12% 7%
8	K	57	65% 25% 9%
8	T	57	5% 56% 35% 7%
9	L	100	3% 61% 26% 6%
9	U	100	12% 63% 25% 6%
10	N	65	2% 48% 37% 12%
10	V	65	3% 54% 34% 9%
11	P	49	10% 31% 51% 14%
11	W	49	6% 41% 37% 6% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	MG	I	1101	-	-	-	X
13	ZN	J	1301	-	-	-	X

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51069 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	863	Total	C	N	O	S	0	0	0
			6891	4357	1221	1275	38			
1	I	862	Total	C	N	O	S	0	0	0
			6875	4347	1220	1270	38			

- Molecule 2 is a protein called DNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1069	Total	C	N	O	S	0	0	0
			8536	5396	1520	1584	36			
2	J	1069	Total	C	N	O	S	0	0	0
			8536	5396	1520	1584	36			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit A".

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	369	Total	C	N	O	S	0	0	0
			2882	1819	498	555	10			
3	M	369	Total	C	N	O	S	0	0	0
			2879	1816	498	555	10			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	258	Total	C	N	O	S	0	0	0
			2066	1330	341	390	5			
4	O	258	Total	C	N	O	S	0	0	0
			2066	1330	341	390	5			

- Molecule 5 is a protein called DNA-directed RNA polymerase, subunit E'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	181	Total	C	N	O	S	0	0	0
			1465	939	250	267	9			
5	Q	181	Total	C	N	O	S	0	0	0
			1465	939	250	267	9			

- Molecule 6 is a protein called DNA-directed RNA polymerase, subunit F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	122	Total	C	N	O	S	0	0	0
			1020	654	169	193	4			
6	R	122	Total	C	N	O	S	0	0	0
			1020	654	169	193	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	115	ILE	-	EXPRESSION TAG	UNP Q5JI52
F	116	ASP	-	EXPRESSION TAG	UNP Q5JI52
F	117	GLU	-	EXPRESSION TAG	UNP Q5JI52
F	118	TYR	-	EXPRESSION TAG	UNP Q5JI52
F	119	ARG	-	EXPRESSION TAG	UNP Q5JI52
F	120	PRO	-	EXPRESSION TAG	UNP Q5JI52
F	121	LEU	-	EXPRESSION TAG	UNP Q5JI52
F	122	GLU	-	EXPRESSION TAG	UNP Q5JI52
R	115	ILE	-	EXPRESSION TAG	UNP Q5JI52
R	116	ASP	-	EXPRESSION TAG	UNP Q5JI52
R	117	GLU	-	EXPRESSION TAG	UNP Q5JI52
R	118	TYR	-	EXPRESSION TAG	UNP Q5JI52
R	119	ARG	-	EXPRESSION TAG	UNP Q5JI52
R	120	PRO	-	EXPRESSION TAG	UNP Q5JI52
R	121	LEU	-	EXPRESSION TAG	UNP Q5JI52
R	122	GLU	-	EXPRESSION TAG	UNP Q5JI52

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit H.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	H	76	Total	C	N	O	0	0	0
			627	408	105	114			
7	S	76	Total	C	N	O	0	0	0
			627	408	105	114			

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	56	Total	C	N	O	S	0	0	0
			433	284	75	73	1			
8	T	56	Total	C	N	O	S	0	0	0
			433	284	75	73	1			

- Molecule 9 is a protein called DNA-directed RNA polymerase subunit L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	L	94	Total	C	N	O	S	0	0	0
			775	493	134	146	2			
9	U	94	Total	C	N	O	S	0	0	0
			775	493	134	146	2			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	95	HIS	-	EXPRESSION TAG	UNP Q5JE88
L	96	HIS	-	EXPRESSION TAG	UNP Q5JE88
L	97	HIS	-	EXPRESSION TAG	UNP Q5JE88
L	98	HIS	-	EXPRESSION TAG	UNP Q5JE88
L	99	HIS	-	EXPRESSION TAG	UNP Q5JE88
L	100	HIS	-	EXPRESSION TAG	UNP Q5JE88
U	95	HIS	-	EXPRESSION TAG	UNP Q5JE88
U	96	HIS	-	EXPRESSION TAG	UNP Q5JE88
U	97	HIS	-	EXPRESSION TAG	UNP Q5JE88
U	98	HIS	-	EXPRESSION TAG	UNP Q5JE88
U	99	HIS	-	EXPRESSION TAG	UNP Q5JE88
U	100	HIS	-	EXPRESSION TAG	UNP Q5JE88

- Molecule 10 is a protein called DNA-directed RNA polymerase subunit N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	N	63	Total	C	N	O	S	0	0	0
			510	326	87	91	6			
10	V	63	Total	C	N	O	S	0	0	0
			510	326	87	91	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase subunit P.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	42	Total	C	N	O	S	0	0	0
			329	206	65	54	4			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	W	42	Total	C	N	O	S	0	0	0
			329	206	65	54	4			

- Molecule 12 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	I	2	Total	Mg	0	0
			2	2		
12	A	2	Total	Mg	0	0
			2	2		

- Molecule 13 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	P	1	Total	Zn	0	0
			1	1		
13	J	1	Total	Zn	0	0
			1	1		
13	B	1	Total	Zn	0	0
			1	1		
13	I	2	Total	Zn	0	0
			2	2		
13	V	1	Total	Zn	0	0
			1	1		
13	W	1	Total	Zn	0	0
			1	1		
13	A	2	Total	Zn	0	0
			2	2		
13	N	1	Total	Zn	0	0
			1	1		

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	1	Total	O	0	0
			1	1		
14	B	1	Total	O	0	0
			1	1		
14	C	1	Total	O	0	0
			1	1		
14	I	1	Total	O	0	0
			1	1		

Continued on next page...

Continued from previous page...

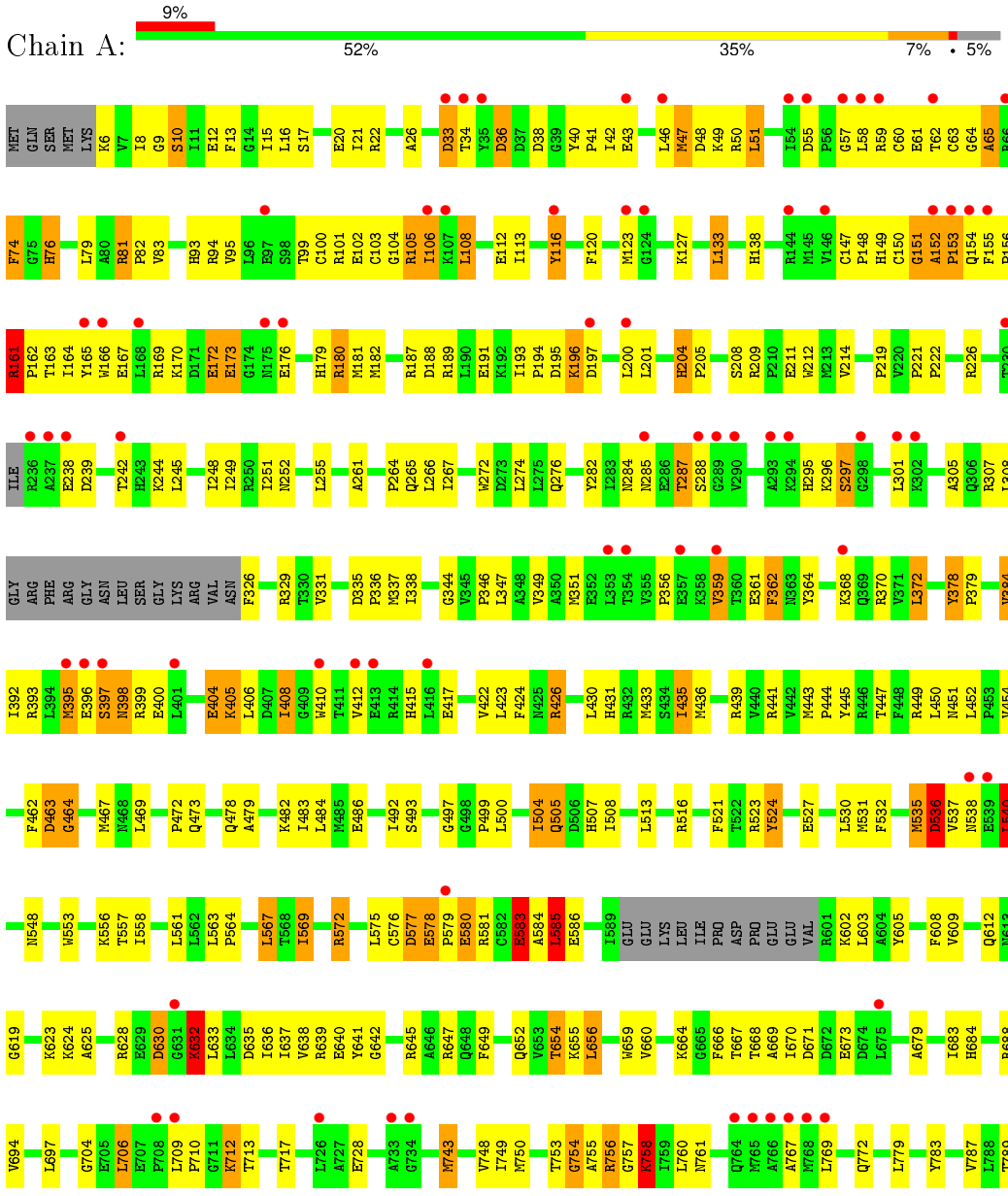
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
14	J	1	Total O 1 1	0	0
14	M	1	Total O 1 1	0	0

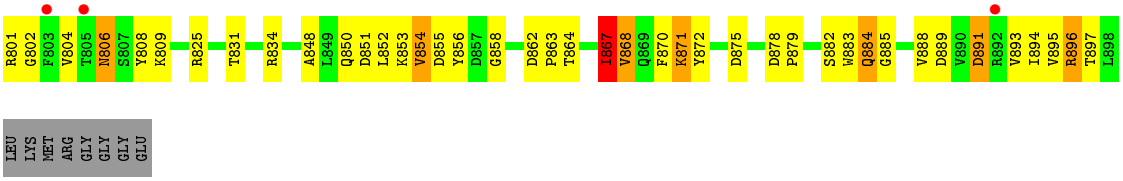
3 Residue-property plots (i)

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

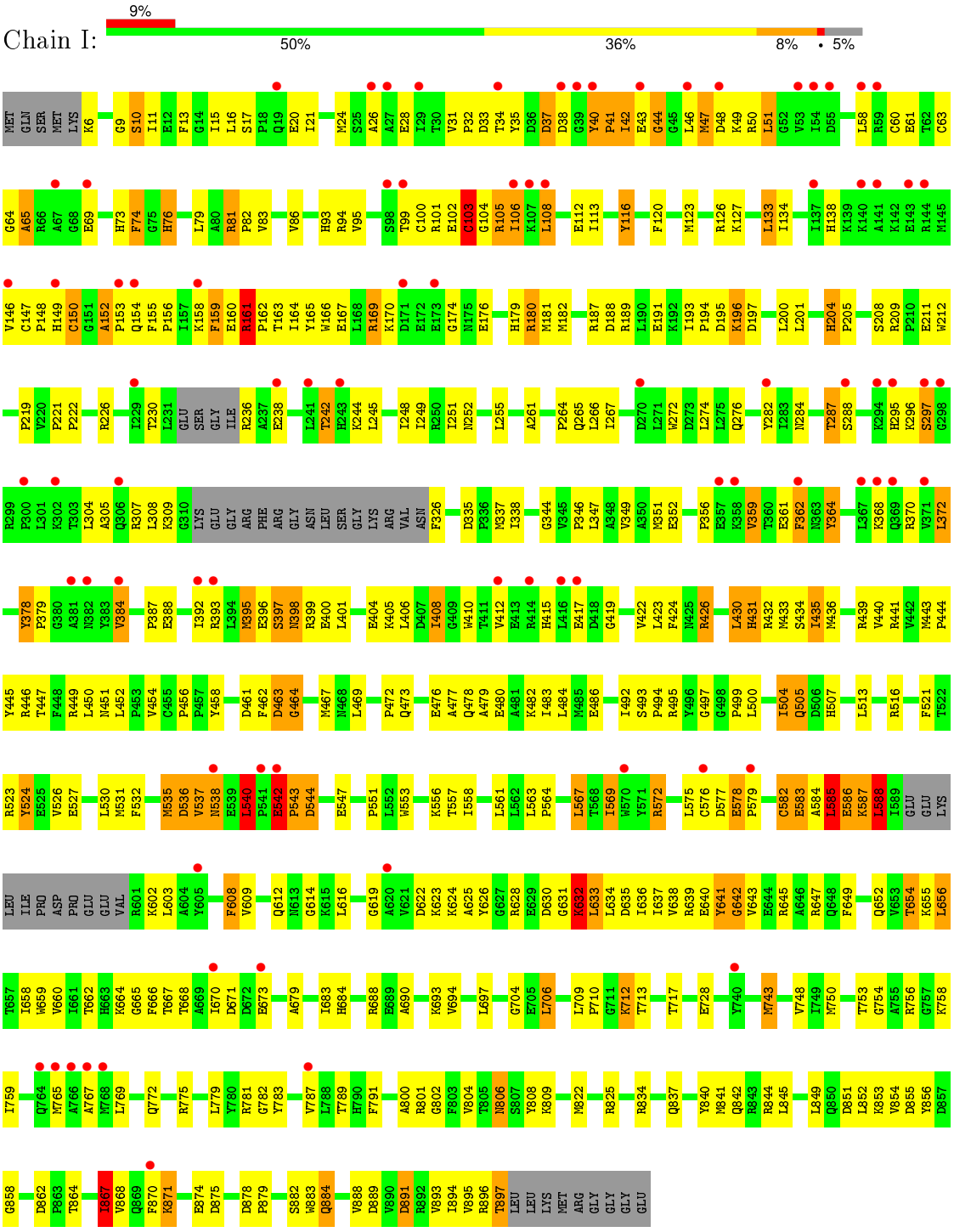
- Molecule 1: DNA-directed RNA polymerase

Chain A:



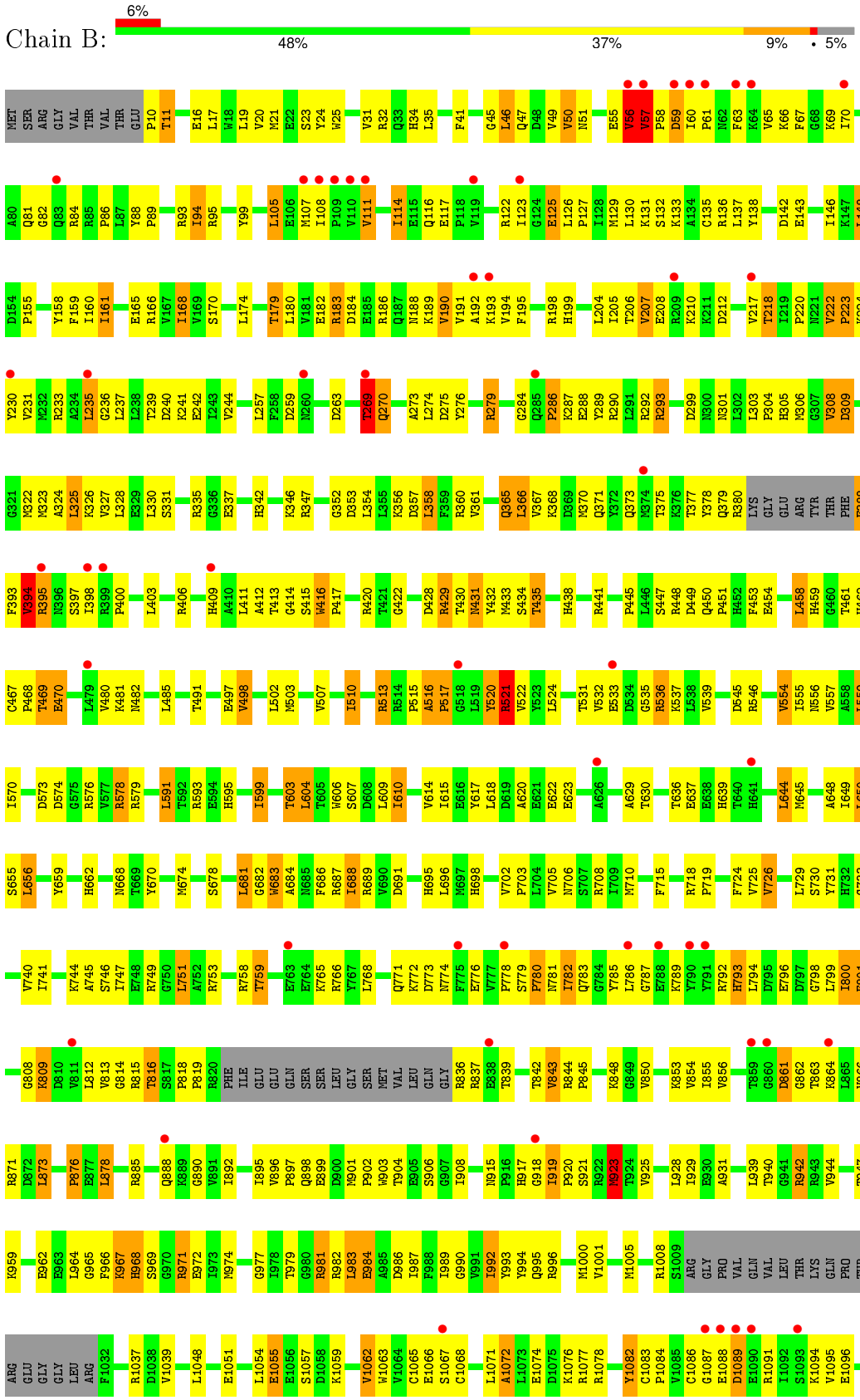


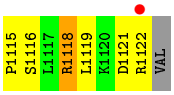
• Molecule 1: DNA-directed RNA polymerase



• Molecule 2: DNA-directed RNA polymerase

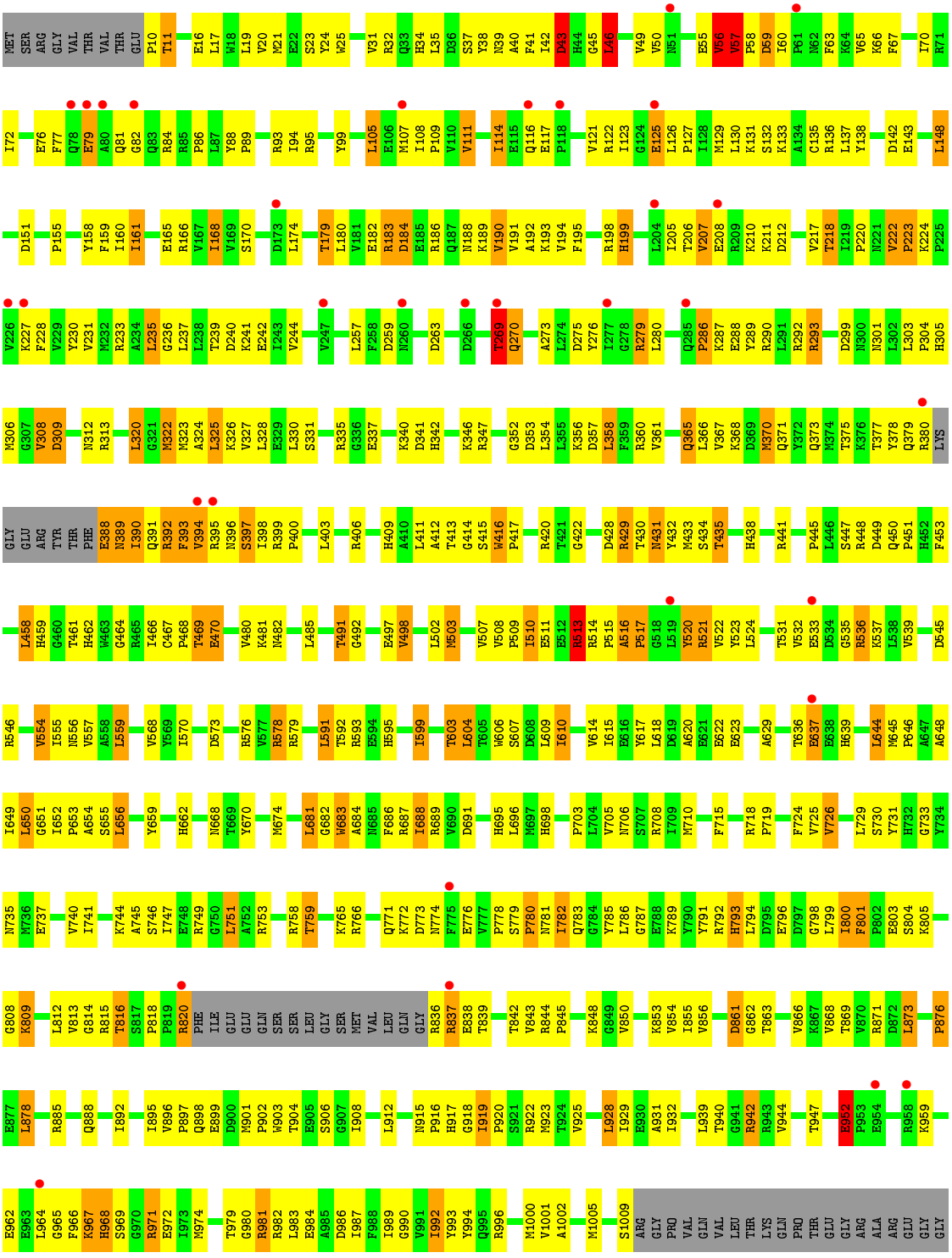
Chain B:

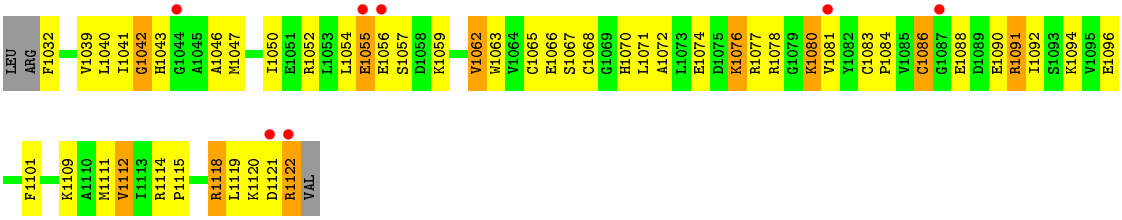




• Molecule 2: DNA-directed RNA polymerase

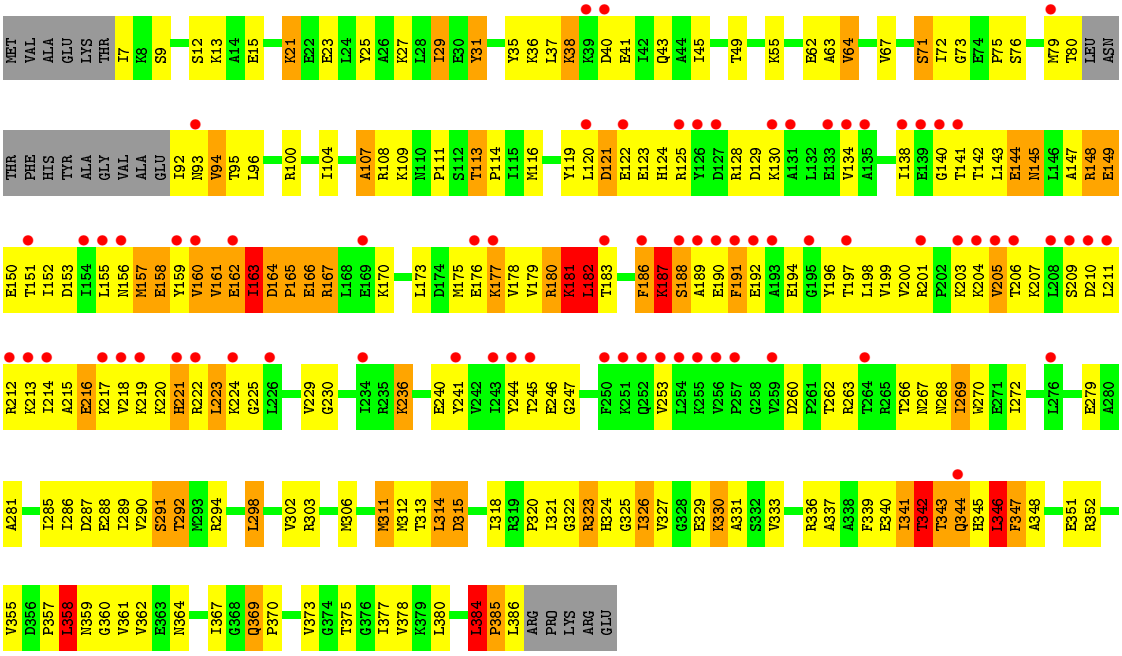
Chain J:





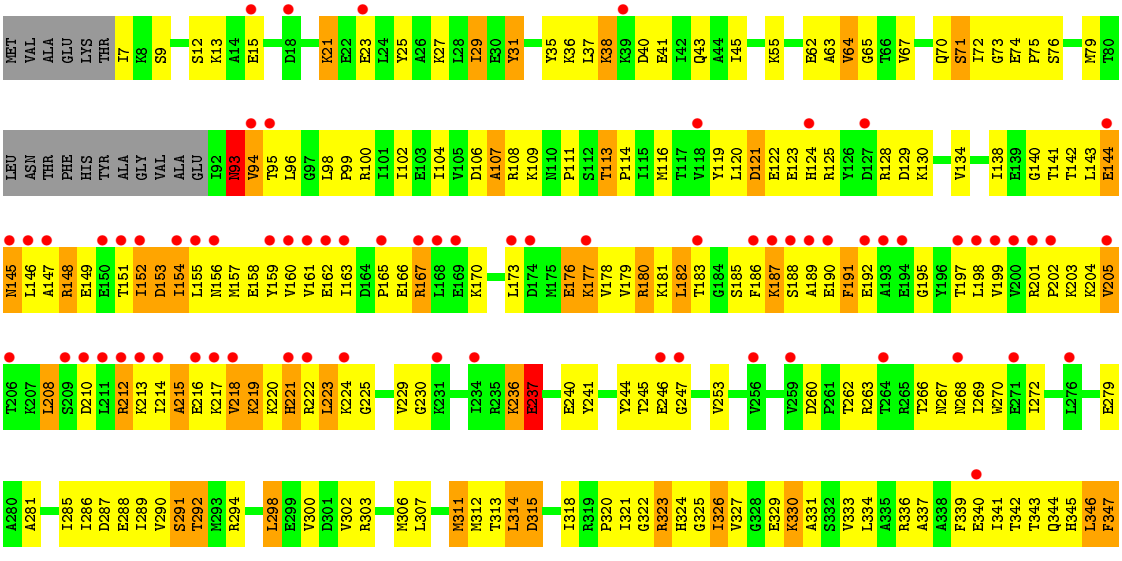
• Molecule 3: DNA-directed RNA polymerase subunit A"

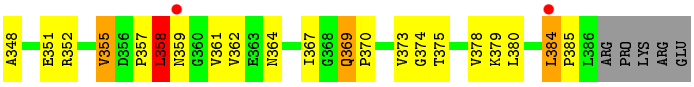
Chain C:



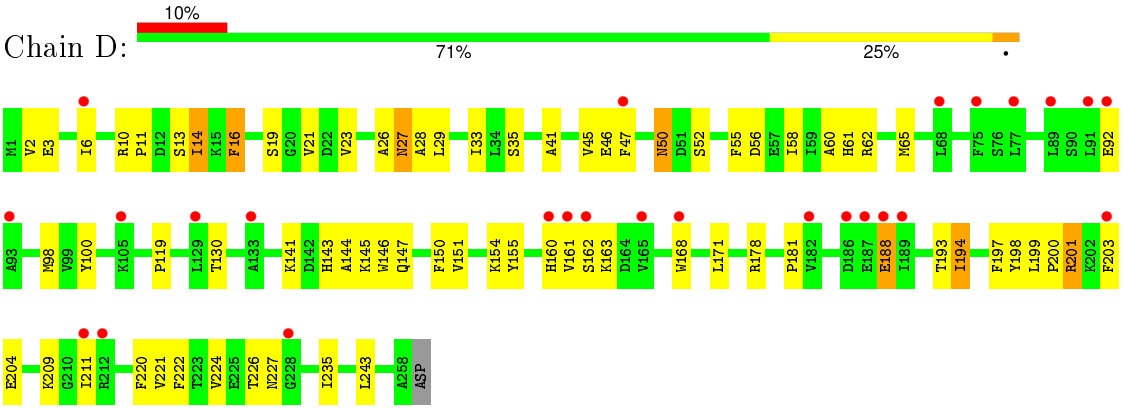
• Molecule 3: DNA-directed RNA polymerase subunit A"

Chain M:

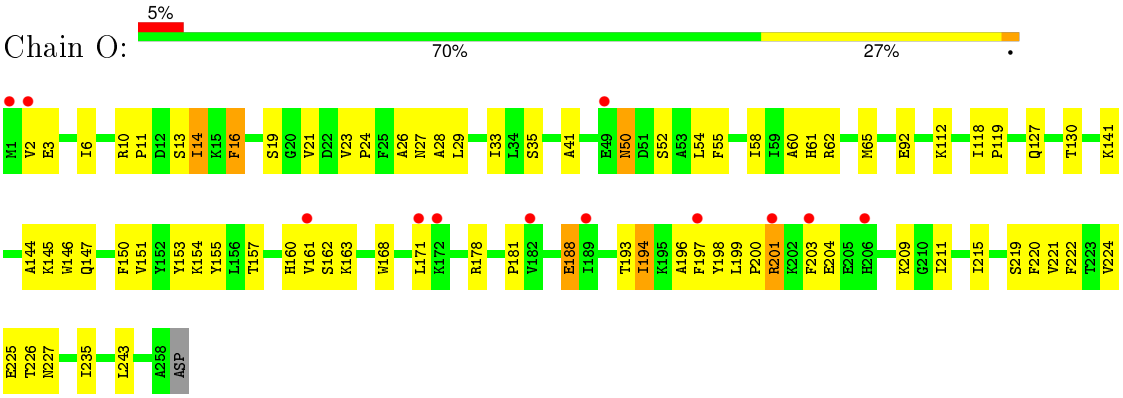




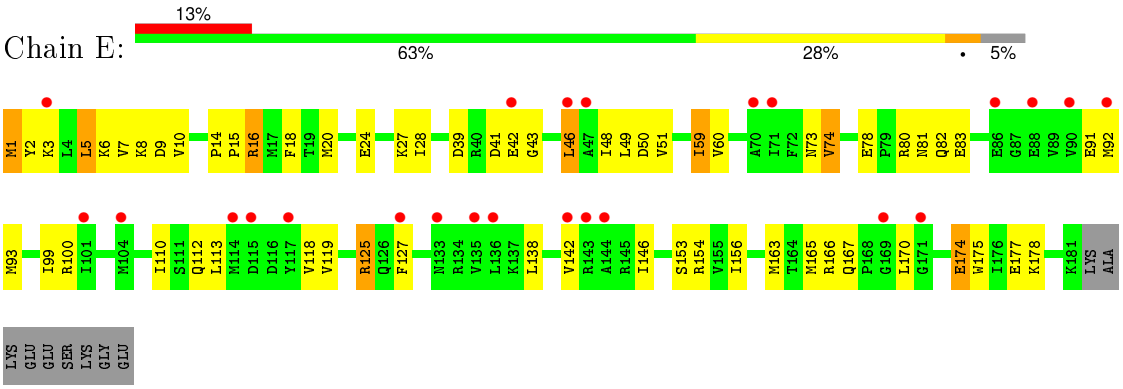
• Molecule 4: DNA-directed RNA polymerase subunit D



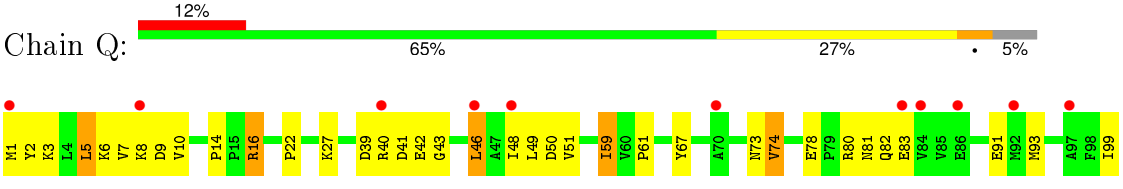
• Molecule 4: DNA-directed RNA polymerase subunit D

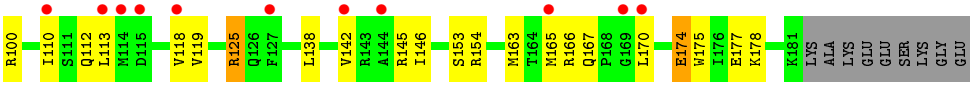


• Molecule 5: DNA-directed RNA polymerase, subunit E'

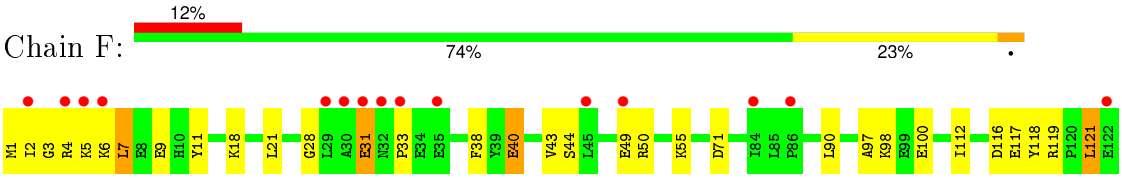


• Molecule 5: DNA-directed RNA polymerase, subunit E'

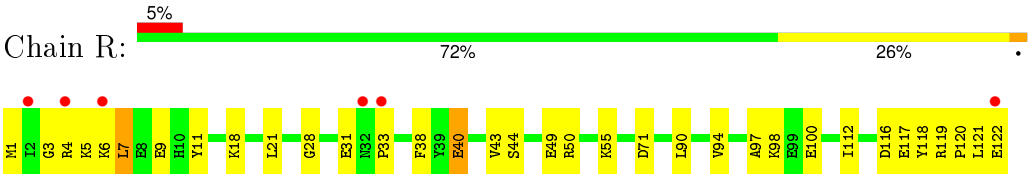




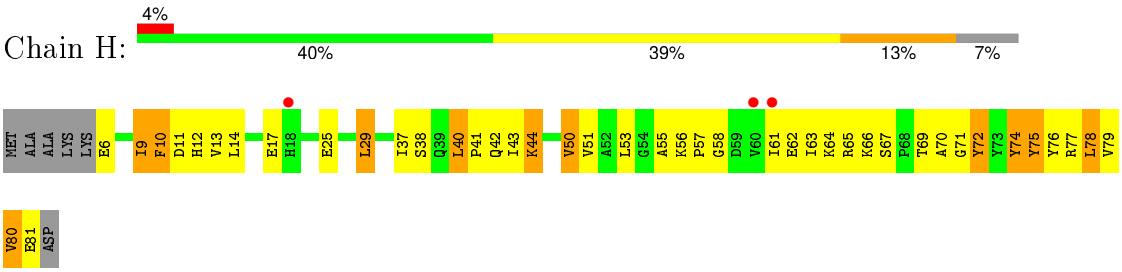
• Molecule 6: DNA-directed RNA polymerase, subunit F



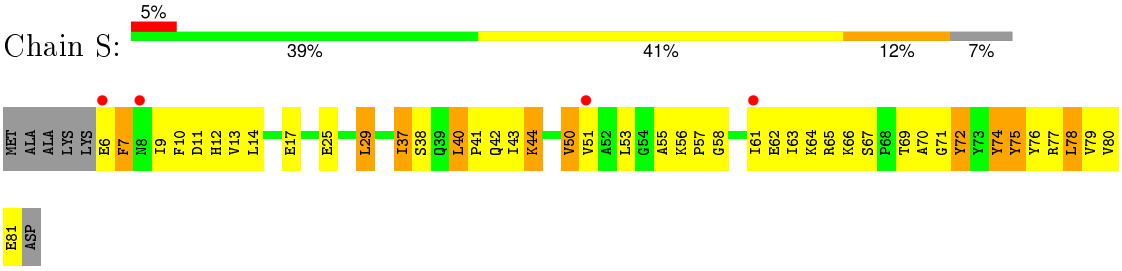
• Molecule 6: DNA-directed RNA polymerase, subunit F



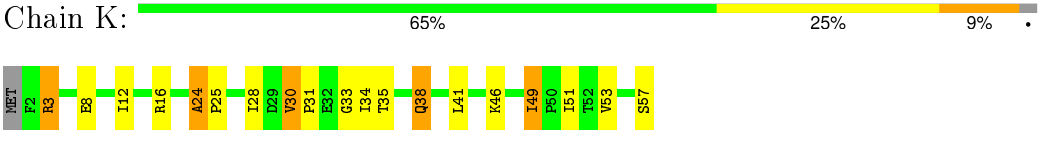
• Molecule 7: DNA-directed RNA polymerase subunit H



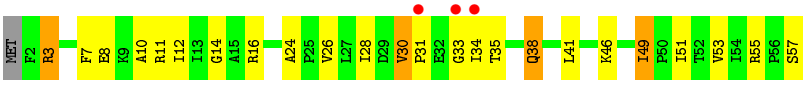
• Molecule 7: DNA-directed RNA polymerase subunit H



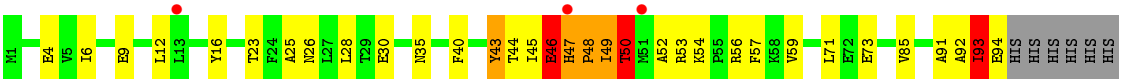
• Molecule 8: DNA-directed RNA polymerase subunit K



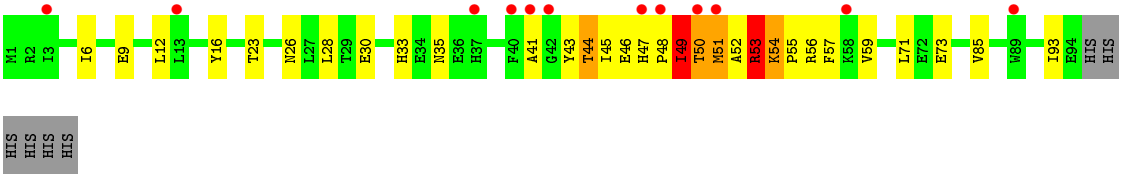
• Molecule 8: DNA-directed RNA polymerase subunit K



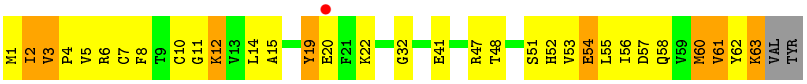
• Molecule 9: DNA-directed RNA polymerase subunit L



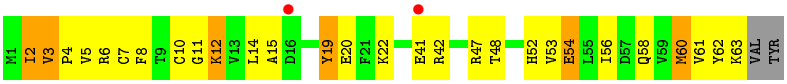
• Molecule 9: DNA-directed RNA polymerase subunit L



• Molecule 10: DNA-directed RNA polymerase subunit N

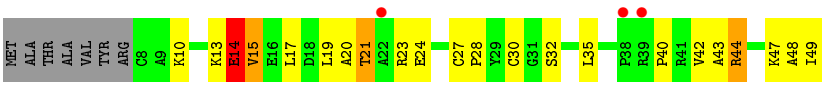


• Molecule 10: DNA-directed RNA polymerase subunit N



• Molecule 11: DNA-directed RNA polymerase subunit P

• Molecule 11: DNA-directed RNA polymerase subunit P



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	112.97Å 206.61Å 365.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 3.50 49.73 – 3.39	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.73-3.50) 93.1 (49.73-3.39)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.26 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, R_{free}	0.277 , 0.316 0.279 , 0.317	Depositor DCC
R_{free} test set	5185 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	84.8	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 105.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.31$, $< L^2 > = 0.15$	Xtriage
Outliers	1 of 113202 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	51069	wwPDB-VP
Average B, all atoms (Å^2)	163.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.26	0/7028	0.50	1/9489 (0.0%)
1	I	0.29	2/7011 (0.0%)	0.52	1/9465 (0.0%)
2	B	0.29	1/8706 (0.0%)	0.53	3/11765 (0.0%)
2	J	0.28	1/8706 (0.0%)	0.52	3/11765 (0.0%)
3	C	0.27	0/2917	0.55	2/3936 (0.1%)
3	M	0.26	0/2914	0.53	1/3932 (0.0%)
4	D	0.27	0/2111	0.43	0/2858
4	O	0.28	0/2111	0.43	0/2858
5	E	0.23	0/1491	0.44	0/2008
5	Q	0.22	0/1491	0.43	0/2008
6	F	0.22	0/1040	0.40	0/1399
6	R	0.22	0/1040	0.40	0/1399
7	H	0.61	4/641 (0.6%)	0.57	0/866
7	S	0.60	4/641 (0.6%)	0.56	0/866
8	K	0.26	0/441	0.52	0/598
8	T	0.26	0/441	0.53	0/598
9	L	0.39	0/790	0.51	1/1066 (0.1%)
9	U	0.41	0/790	0.56	2/1066 (0.2%)
10	N	0.26	0/518	0.57	0/695
10	V	0.27	0/518	0.58	0/695
11	P	0.27	0/333	0.60	0/445
11	W	0.27	0/333	0.56	0/445
All	All	0.29	12/52012 (0.0%)	0.51	14/70222 (0.0%)

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

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	I	0	4
2	J	0	1
All	All	0	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	H	72	TYR	CE2-CZ	7.29	1.48	1.38
7	H	72	TYR	CE1-CZ	7.14	1.47	1.38
7	S	72	TYR	CE2-CZ	7.13	1.47	1.38
7	S	72	TYR	CG-CD1	7.11	1.48	1.39
1	I	150	CYS	CB-SG	-7.05	1.70	1.82
7	H	72	TYR	CG-CD1	6.68	1.47	1.39
7	H	72	TYR	CG-CD2	6.64	1.47	1.39
7	S	72	TYR	CG-CD2	6.42	1.47	1.39
7	S	72	TYR	CE1-CZ	6.42	1.46	1.38
2	B	1086	CYS	CB-SG	-5.84	1.72	1.81
1	I	103	CYS	CB-SG	-5.64	1.72	1.81
2	J	1086	CYS	CB-SG	5.41	1.91	1.82

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	125	GLU	CA-CB-CG	7.21	129.26	113.40
3	C	164	ASP	C-N-CD	-6.97	105.27	120.60
1	I	150	CYS	CB-CA-C	-6.86	96.68	110.40
2	J	57	VAL	C-N-CD	-6.80	105.63	120.60
2	B	57	VAL	C-N-CD	-6.70	105.86	120.60
9	U	47	HIS	C-N-CD	6.07	141.14	128.40
9	L	47	HIS	C-N-CD	6.06	141.13	128.40
9	U	54	LYS	C-N-CD	6.03	141.06	128.40
2	J	952	GLU	CA-CB-CG	5.80	126.16	113.40
3	C	314	LEU	CA-CB-CG	5.79	128.62	115.30
3	M	314	LEU	CA-CB-CG	5.78	128.59	115.30
1	A	642	GLY	N-CA-C	5.65	127.23	113.10
2	J	125	GLU	CA-CB-CG	5.63	125.80	113.40
2	B	923	MET	CG-SD-CE	5.12	108.40	100.20

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	536	ASP	Peptide
1	I	582	CYS	Peptide
1	I	632	LYS	Peptide
1	I	641	TYR	Peptide
1	I	642	GLY	Peptide
2	J	513	ARG	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	6891	0	6945	310	0
1	I	6875	0	6927	382	1
2	B	8536	0	8585	463	10
2	J	8536	0	8583	578	0
3	C	2882	0	2982	305	0
3	M	2879	0	2973	247	0
4	D	2066	0	2080	59	0
4	O	2066	0	2080	66	0
5	E	1465	0	1503	74	2
5	Q	1465	0	1503	68	3
6	F	1020	0	1024	41	12
6	R	1020	0	1024	48	7
7	H	627	0	642	29	0
7	S	627	0	642	34	0
8	K	433	0	466	16	0
8	T	433	0	466	19	0
9	L	775	0	770	51	0
9	U	775	0	770	67	0
10	N	510	0	523	43	0
10	V	510	0	523	26	0
11	P	329	0	356	27	5
11	W	329	0	355	15	0
12	A	2	0	0	0	0
12	I	2	0	0	0	0
13	A	2	0	0	0	0
13	B	1	0	0	0	0
13	I	2	0	0	0	0
13	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
13	N	1	0	0	0	0
13	P	1	0	0	1	0
13	V	1	0	0	0	0
13	W	1	0	0	0	0
14	A	1	0	0	0	0
14	B	1	0	0	1	0
14	C	1	0	0	0	0
14	I	1	0	0	2	0
14	J	1	0	0	0	0
14	M	1	0	0	3	0
All	All	51069	0	51722	2518	20

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 25.

All (2518) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:TYR:CE1	2:B:388:GLU:CA	1.79	1.63
1:I:444:PRO:CG	9:U:50:THR:HG23	1.32	1.58
1:I:444:PRO:HG3	9:U:50:THR:CG2	1.09	1.56
2:J:378:TYR:CE1	2:J:388:GLU:HG3	1.38	1.56
3:C:194:GLU:HB2	3:C:196:TYR:CE2	1.41	1.55
2:J:394:VAL:HB	2:J:395:ARG:CG	1.08	1.54
3:C:161:VAL:CG2	3:C:199:VAL:HG23	1.06	1.53
3:M:148:ARG:CZ	3:M:162:GLU:HB2	1.39	1.51
2:B:378:TYR:CE1	2:B:388:GLU:N	1.69	1.48
2:J:107:MET:HB3	2:J:395:ARG:NH2	1.17	1.47
3:C:161:VAL:CG2	3:C:199:VAL:CG2	1.89	1.46
3:C:161:VAL:HG21	3:C:199:VAL:CG2	1.44	1.45
3:C:162:GLU:CA	3:C:196:TYR:HB2	1.45	1.44
1:I:6:LYS:HE3	2:J:1122:ARG:NH2	1.30	1.44
2:J:378:TYR:HH	2:J:388:GLU:N	0.95	1.43
2:B:378:TYR:CE1	2:B:388:GLU:HA	1.35	1.43
2:B:389:ASN:ND2	2:B:392:ARG:HD3	1.37	1.40
2:J:394:VAL:CB	2:J:395:ARG:HG3	1.54	1.38
1:I:6:LYS:CE	2:J:1122:ARG:HH22	1.35	1.38
1:I:666:PHE:H	2:J:729:LEU:CD1	1.37	1.37
2:J:63:PHE:HZ	2:J:388:GLU:CD	1.28	1.35
3:M:148:ARG:NH2	3:M:162:GLU:CB	1.86	1.35
3:M:148:ARG:NH2	3:M:162:GLU:HB2	1.05	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:394:VAL:CB	2:J:395:ARG:CG	2.05	1.33
2:J:63:PHE:CZ	2:J:388:GLU:CD	2.03	1.30
2:J:107:MET:CB	2:J:395:ARG:NH2	1.95	1.28
1:I:445:TYR:CE2	9:U:49:ILE:CG2	2.17	1.28
2:J:39:ASN:O	2:J:43:ASP:OD1	1.53	1.27
1:I:147:CYS:SG	1:I:152:ALA:HB2	1.73	1.27
2:J:1086:CYS:SG	2:J:1090:GLU:OE1	1.92	1.26
2:B:389:ASN:HD21	2:B:392:ARG:CD	1.48	1.26
2:B:378:TYR:CZ	2:B:388:GLU:HA	1.71	1.24
2:B:378:TYR:CD1	2:B:388:GLU:N	2.05	1.23
1:I:461:ASP:OD2	14:I:1201:HOH:O	1.55	1.23
2:J:107:MET:CB	2:J:395:ARG:CZ	2.08	1.21
2:J:378:TYR:OH	2:J:388:GLU:N	1.67	1.21
3:C:148:ARG:NE	3:C:163:ILE:HG12	1.56	1.20
3:M:165:PRO:HB3	3:M:195:GLY:CA	1.71	1.20
3:C:162:GLU:C	3:C:196:TYR:HB2	1.61	1.20
3:C:161:VAL:HG23	3:C:199:VAL:N	1.56	1.19
5:Q:9:ASP:OD2	6:R:3:GLY:HA2	1.40	1.19
2:J:63:PHE:HZ	2:J:388:GLU:CG	1.56	1.18
2:J:378:TYR:HE1	2:J:388:GLU:CA	1.56	1.18
3:C:148:ARG:HD2	3:C:163:ILE:CG1	1.70	1.18
1:I:100:CYS:SG	1:I:155:PHE:HZ	1.64	1.18
2:J:378:TYR:CE1	2:J:388:GLU:CG	2.26	1.18
2:J:378:TYR:CZ	2:J:388:GLU:N	2.11	1.18
5:E:92:MET:CE	5:E:127:PHE:CD2	2.28	1.17
1:A:100:CYS:SG	1:A:155:PHE:HZ	1.68	1.16
1:I:445:TYR:CE2	9:U:49:ILE:HG21	1.78	1.15
1:I:666:PHE:H	2:J:729:LEU:HD11	1.11	1.15
2:J:389:ASN:HA	2:J:390:ILE:HG23	1.16	1.14
1:I:445:TYR:CD2	9:U:49:ILE:HG21	1.83	1.13
5:E:1:MET:HE3	6:F:11:TYR:CD1	1.84	1.12
3:C:162:GLU:HA	3:C:196:TYR:HB2	1.21	1.11
1:I:666:PHE:N	2:J:729:LEU:CD1	2.11	1.11
2:B:389:ASN:ND2	2:B:392:ARG:CD	2.11	1.11
9:L:49:ILE:HD12	9:L:50:THR:H	1.11	1.11
1:A:666:PHE:O	2:B:729:LEU:HD13	1.51	1.10
5:E:9:ASP:OD2	6:F:3:GLY:HA2	1.51	1.10
1:A:666:PHE:O	2:B:729:LEU:CD1	1.98	1.10
1:I:445:TYR:CE2	9:U:49:ILE:HG23	1.86	1.09
2:J:378:TYR:CE1	2:J:388:GLU:CA	2.35	1.09
1:I:444:PRO:HG3	9:U:50:THR:HG22	1.29	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:CYS:SG	1:I:155:PHE:CZ	2.45	1.09
2:J:378:TYR:HE1	2:J:388:GLU:HA	1.16	1.08
2:J:107:MET:CB	2:J:395:ARG:HH22	1.58	1.08
2:J:1122:ARG:HG3	6:R:4:ARG:HH21	1.15	1.08
3:C:148:ARG:CD	3:C:163:ILE:CG1	2.31	1.07
3:C:194:GLU:CB	3:C:196:TYR:CE2	2.36	1.07
11:P:14:GLU:HG2	11:P:30:CYS:SG	1.94	1.07
2:B:378:TYR:CZ	2:B:388:GLU:CA	2.32	1.07
1:I:444:PRO:HG2	9:U:49:ILE:HB	1.31	1.07
1:A:150:CYS:O	1:A:152:ALA:N	1.86	1.07
5:Q:1:MET:HE3	6:R:11:TYR:CD1	1.90	1.07
2:J:1122:ARG:CD	5:Q:10:VAL:HG11	1.85	1.07
3:C:152:ILE:HG12	3:C:153:ASP:H	1.19	1.06
2:J:107:MET:HB3	2:J:395:ARG:CZ	1.61	1.06
2:J:391:GLN:O	2:J:392:ARG:HG3	1.55	1.06
1:I:666:PHE:N	2:J:729:LEU:HD11	1.67	1.06
2:B:393:PHE:O	2:B:394:VAL:HB	1.49	1.06
1:I:665:GLY:HA2	2:J:729:LEU:HD11	1.32	1.06
3:M:148:ARG:CZ	3:M:162:GLU:CB	2.24	1.05
2:J:1083:CYS:SG	2:J:1086:CYS:HB2	1.96	1.05
2:J:107:MET:HB2	2:J:395:ARG:CZ	1.86	1.05
1:I:6:LYS:HE3	2:J:1122:ARG:CZ	1.86	1.04
2:J:1122:ARG:CG	6:R:4:ARG:HH21	1.70	1.04
3:M:165:PRO:HB3	3:M:195:GLY:HA3	1.06	1.04
2:J:378:TYR:CE1	2:J:388:GLU:N	2.25	1.04
3:C:162:GLU:HA	3:C:196:TYR:CB	1.85	1.04
5:E:92:MET:CE	5:E:127:PHE:CE2	2.40	1.04
2:B:390:ILE:HD12	2:B:391:GLN:H	1.18	1.04
1:I:444:PRO:CG	9:U:50:THR:CG2	2.04	1.04
3:C:162:GLU:CA	3:C:196:TYR:CB	2.36	1.03
1:A:100:CYS:SG	1:A:155:PHE:CZ	2.51	1.03
1:A:758:LYS:O	1:A:761:ASN:OD1	1.76	1.03
2:J:38:TYR:O	2:J:41:PHE:HB3	1.59	1.03
5:E:92:MET:HE1	5:E:127:PHE:CD2	1.92	1.02
2:J:394:VAL:HB	2:J:395:ARG:HG2	1.08	1.02
1:I:103:CYS:SG	1:I:105:ARG:N	2.32	1.02
3:C:161:VAL:HG12	3:C:162:GLU:H	1.22	1.01
2:B:378:TYR:HE1	2:B:388:GLU:CA	1.35	1.01
11:P:14:GLU:CG	11:P:30:CYS:SG	2.49	1.01
1:A:531:MET:HB2	9:L:44:THR:CG2	1.91	1.01
3:M:151:THR:HG22	3:M:152:ILE:H	1.26	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:100:CYS:HB3	1:I:103:CYS:HB3	1.42	1.00
1:I:445:TYR:CZ	9:U:49:ILE:CG2	2.43	1.00
3:C:152:ILE:HG13	3:C:159:TYR:CE2	1.95	1.00
2:J:389:ASN:HA	2:J:390:ILE:CG2	1.92	1.00
2:J:393:PHE:O	2:J:394:VAL:HG22	1.60	0.99
3:C:162:GLU:C	3:C:196:TYR:CB	2.30	0.99
1:I:665:GLY:HA2	2:J:729:LEU:CD1	1.92	0.99
2:B:729:LEU:HD23	2:B:731:TYR:HE1	1.21	0.99
2:B:744:LYS:NZ	9:L:53:ARG:NH2	2.09	0.99
3:C:148:ARG:HD2	3:C:163:ILE:CB	1.91	0.99
1:I:6:LYS:HE2	2:J:1122:ARG:HH12	1.28	0.99
5:E:92:MET:HE3	5:E:127:PHE:CE2	1.96	0.98
2:B:389:ASN:HD21	2:B:392:ARG:HD3	0.84	0.98
3:C:194:GLU:HB2	3:C:196:TYR:CD2	1.98	0.98
3:C:148:ARG:HG2	3:C:149:GLU:HG3	1.41	0.98
3:C:161:VAL:HG22	3:C:199:VAL:CG2	1.92	0.98
5:Q:1:MET:HE3	6:R:11:TYR:HD1	1.21	0.97
11:W:27:CYS:HB3	11:W:30:CYS:SG	2.04	0.97
2:B:391:GLN:O	2:B:393:PHE:N	1.96	0.97
9:U:51:MET:HG2	9:U:53:ARG:HB2	1.46	0.97
2:J:1122:ARG:HD3	5:Q:10:VAL:HG11	1.43	0.97
2:B:744:LYS:HZ3	9:L:53:ARG:NH2	1.63	0.97
1:A:749:ILE:O	1:A:753:THR:HG22	1.65	0.97
2:J:394:VAL:CB	2:J:395:ARG:HG2	1.79	0.97
3:C:162:GLU:HG2	3:C:196:TYR:CD1	1.99	0.96
1:I:147:CYS:SG	1:I:152:ALA:CB	2.53	0.96
1:A:10:SER:HA	3:C:358:LEU:HD21	1.46	0.96
11:P:14:GLU:CD	11:P:30:CYS:SG	2.44	0.96
5:E:3:LYS:NZ	6:F:9:GLU:OE1	1.98	0.96
1:A:753:THR:HG23	1:A:754:GLY:H	1.26	0.96
2:J:378:TYR:CE1	2:J:388:GLU:HA	1.99	0.96
2:J:42:ILE:CG2	2:J:72:ILE:HD13	1.96	0.95
2:J:979:THR:HA	9:U:26:ASN:HD21	1.31	0.95
3:C:148:ARG:NH2	3:C:149:GLU:O	2.00	0.95
3:C:148:ARG:CD	3:C:163:ILE:HG12	1.94	0.95
2:B:744:LYS:HZ3	9:L:53:ARG:HH22	0.99	0.95
9:U:51:MET:HG2	9:U:53:ARG:CB	1.96	0.95
2:J:42:ILE:CG2	2:J:72:ILE:CD1	2.44	0.94
1:I:461:ASP:CG	14:I:1201:HOH:O	1.97	0.94
3:M:165:PRO:CB	3:M:195:GLY:HA3	1.96	0.94
5:Q:3:LYS:NZ	6:R:9:GLU:OE1	2.00	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:ARG:HB2	2:B:186:ARG:HH22	1.33	0.94
1:I:665:GLY:CA	2:J:729:LEU:HD11	1.95	0.94
5:E:1:MET:HE1	6:F:11:TYR:HE1	1.29	0.94
3:M:148:ARG:HH22	3:M:162:GLU:HB2	1.15	0.93
2:J:183:ARG:HB3	2:J:186:ARG:HH22	1.31	0.93
2:J:63:PHE:CZ	2:J:388:GLU:CG	2.46	0.93
2:B:510:ILE:HG22	2:B:513:ARG:HE	1.33	0.93
2:B:1063:TRP:NE1	2:B:1094:LYS:HE3	1.84	0.93
3:M:148:ARG:NH2	3:M:162:GLU:CG	2.31	0.92
2:B:378:TYR:CZ	2:B:388:GLU:N	2.37	0.92
5:Q:9:ASP:OD2	6:R:3:GLY:CA	2.17	0.92
5:Q:1:MET:CE	6:R:11:TYR:CD1	2.50	0.92
2:B:389:ASN:ND2	2:B:392:ARG:HB2	1.83	0.92
5:E:1:MET:HE3	6:F:11:TYR:HD1	1.25	0.92
2:J:378:TYR:CZ	2:J:388:GLU:HG3	2.04	0.92
3:C:148:ARG:NE	3:C:163:ILE:CG1	2.30	0.92
2:J:57:VAL:HG21	2:J:371:GLN:HA	1.52	0.92
5:E:1:MET:CE	6:F:11:TYR:CE1	2.53	0.92
2:B:1063:TRP:CZ3	2:B:1074:GLU:CG	2.53	0.92
3:C:161:VAL:HG23	3:C:199:VAL:HG23	1.47	0.91
5:E:1:MET:CE	6:F:11:TYR:CD1	2.52	0.91
3:C:194:GLU:CB	3:C:196:TYR:HE2	1.80	0.91
3:M:152:ILE:CG2	3:M:159:TYR:HA	2.01	0.91
2:B:57:VAL:HG21	2:B:371:GLN:HA	1.52	0.91
2:J:391:GLN:O	2:J:392:ARG:CG	2.19	0.91
1:I:6:LYS:CE	2:J:1122:ARG:HH12	1.84	0.91
1:A:531:MET:CB	9:L:44:THR:CG2	2.47	0.90
2:B:729:LEU:HD23	2:B:731:TYR:CE1	2.06	0.90
3:C:163:ILE:N	3:C:196:TYR:CB	2.35	0.90
3:C:161:VAL:CG2	3:C:199:VAL:CB	2.48	0.90
2:B:1063:TRP:CE2	2:B:1094:LYS:HE3	2.07	0.90
3:C:163:ILE:HD13	3:C:163:ILE:H	1.34	0.90
2:J:1086:CYS:SG	2:J:1090:GLU:CG	2.60	0.90
1:I:13:PHE:HE2	3:M:333:VAL:HG21	1.36	0.89
3:C:211:LEU:HA	3:C:214:ILE:CD1	2.02	0.89
1:I:40:TYR:H	1:I:41:PRO:HD3	1.37	0.89
1:I:6:LYS:HE3	2:J:1122:ARG:HH22	0.75	0.89
5:E:1:MET:HE1	6:F:11:TYR:CE1	2.07	0.89
2:J:116:GLN:CD	2:J:393:PHE:HD1	1.76	0.89
2:B:394:VAL:HG22	2:B:395:ARG:HG3	1.54	0.89
1:I:443:MET:HB3	9:U:49:ILE:HD12	1.55	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:393:PHE:O	2:J:394:VAL:CG2	2.20	0.89
3:C:148:ARG:HD2	3:C:163:ILE:HB	1.54	0.88
2:J:206:THR:HG1	2:J:218:THR:HG1	1.22	0.88
2:B:1063:TRP:CD1	2:B:1094:LYS:HG3	2.09	0.88
1:I:103:CYS:N	1:I:150:CYS:SG	2.47	0.88
3:M:21:LYS:HD3	7:S:71:GLY:HA3	1.54	0.88
9:U:49:ILE:O	9:U:50:THR:OG1	1.92	0.88
2:J:1086:CYS:SG	2:J:1090:GLU:HG3	2.13	0.88
11:P:30:CYS:SG	13:P:1501:ZN:ZN	1.62	0.88
3:C:216:GLU:O	3:C:220:LYS:HB3	1.72	0.88
2:J:63:PHE:CZ	2:J:388:GLU:OE1	2.27	0.88
2:J:41:PHE:O	2:J:45:GLY:O	1.92	0.87
2:B:391:GLN:OE1	2:B:393:PHE:CD2	2.27	0.87
3:C:163:ILE:N	3:C:196:TYR:HB2	1.89	0.87
5:Q:1:MET:CE	6:R:11:TYR:HD1	1.87	0.87
1:I:126:ARG:NH2	7:S:40:LEU:O	2.07	0.87
1:I:444:PRO:O	9:U:49:ILE:HD13	1.74	0.87
9:L:49:ILE:HD12	9:L:50:THR:N	1.90	0.87
3:M:182:LEU:HD23	3:M:185:SER:CB	2.05	0.87
9:L:92:ALA:O	9:L:94:GLU:N	2.06	0.87
3:C:148:ARG:CD	3:C:163:ILE:HG13	2.05	0.87
2:B:389:ASN:CG	2:B:392:ARG:HD3	1.95	0.86
3:C:163:ILE:HB	3:C:164:ASP:HA	1.56	0.86
10:N:62:TYR:O	10:N:63:LYS:NZ	2.09	0.86
1:I:531:MET:HB2	9:U:44:THR:HG23	1.56	0.86
2:B:1063:TRP:CZ3	2:B:1074:GLU:HG3	2.09	0.86
5:Q:7:VAL:HG13	6:R:5:LYS:O	1.75	0.86
2:J:398:ILE:HG22	2:J:398:ILE:O	1.75	0.85
3:C:21:LYS:HD3	7:H:71:GLY:HA3	1.58	0.85
2:B:1063:TRP:NE1	2:B:1094:LYS:HG3	1.90	0.85
2:J:1122:ARG:HD2	5:Q:10:VAL:HG11	1.55	0.85
2:B:286:PRO:HB2	2:B:289:TYR:HB2	1.58	0.85
1:I:444:PRO:CD	9:U:50:THR:HG23	2.06	0.85
3:C:194:GLU:HB2	3:C:196:TYR:HE2	1.09	0.85
1:I:666:PHE:H	2:J:729:LEU:HD12	1.41	0.85
2:J:286:PRO:HB2	2:J:289:TYR:HB2	1.58	0.85
1:I:666:PHE:N	2:J:729:LEU:HD12	1.92	0.84
3:M:187:LYS:HD2	3:M:202:PRO:HD2	1.58	0.84
5:E:92:MET:HE1	5:E:127:PHE:CE2	2.07	0.84
3:M:163:ILE:O	3:M:195:GLY:O	1.96	0.84
5:Q:1:MET:HE1	6:R:11:TYR:CE1	2.12	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:PHE:O	2:B:394:VAL:CB	2.25	0.84
3:C:216:GLU:O	3:C:220:LYS:CB	2.25	0.84
5:E:81:ASN:O	5:E:82:GLN:HG2	1.77	0.84
3:C:148:ARG:CZ	3:C:163:ILE:HG12	2.06	0.84
3:C:148:ARG:NH1	3:C:163:ILE:O	2.11	0.84
3:C:191:PHE:HB3	3:C:198:LEU:HB2	1.60	0.84
3:C:162:GLU:HA	3:C:196:TYR:CD1	2.13	0.83
3:C:148:ARG:CZ	3:C:149:GLU:O	2.26	0.83
2:J:46:LEU:HD12	2:J:46:LEU:O	1.78	0.83
3:C:212:ARG:HG3	3:C:213:LYS:N	1.91	0.83
2:J:1086:CYS:SG	2:J:1090:GLU:CD	2.57	0.83
9:U:49:ILE:HG22	9:U:50:THR:H	1.42	0.83
2:J:63:PHE:CZ	2:J:388:GLU:HG2	2.12	0.83
1:A:666:PHE:O	2:B:729:LEU:HD12	1.76	0.83
3:C:148:ARG:HD2	3:C:163:ILE:HG13	1.59	0.83
5:Q:1:MET:HE1	6:R:11:TYR:HE1	1.43	0.83
2:J:45:GLY:O	2:J:46:LEU:HB3	1.77	0.82
3:C:151:THR:HG22	3:C:152:ILE:H	1.44	0.82
3:C:163:ILE:CB	3:C:164:ASP:HA	2.09	0.82
1:I:6:LYS:NZ	2:J:1122:ARG:HH22	1.76	0.82
1:A:750:MET:HA	1:A:753:THR:CG2	2.09	0.82
3:C:153:ASP:OD2	3:C:157:MET:HB3	1.78	0.82
1:I:100:CYS:SG	1:I:103:CYS:HB2	2.20	0.82
3:M:148:ARG:NH1	3:M:162:GLU:HB2	1.94	0.82
4:D:2:VAL:HG11	9:L:85:VAL:HA	1.59	0.82
1:I:531:MET:HB3	9:U:44:THR:OG1	1.79	0.82
1:I:103:CYS:HB2	1:I:150:CYS:SG	2.20	0.82
11:W:30:CYS:SG	11:W:32:SER:HB3	2.20	0.81
2:B:1063:TRP:CZ2	2:B:1094:LYS:HE3	2.13	0.81
1:I:445:TYR:CZ	9:U:49:ILE:HG21	2.12	0.81
1:I:563:LEU:HB2	1:I:614:GLY:HA2	1.62	0.81
3:M:160:VAL:HG12	3:M:161:VAL:H	1.43	0.81
1:A:531:MET:CB	9:L:44:THR:HG21	2.10	0.81
2:J:394:VAL:CG2	2:J:395:ARG:HG3	2.11	0.81
2:B:390:ILE:CD1	2:B:391:GLN:H	1.93	0.81
2:J:395:ARG:O	2:J:397:SER:N	2.14	0.81
5:E:7:VAL:HG13	6:F:5:LYS:O	1.80	0.81
1:A:563:LEU:HB2	1:A:614:GLY:HA2	1.63	0.81
2:B:146:ILE:HG21	10:N:61:VAL:HG21	1.61	0.81
1:I:100:CYS:HB3	1:I:103:CYS:CB	2.10	0.80
1:A:79:LEU:HA	1:A:252:ASN:HD21	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:432:ARG:O	2:J:1043:HIS:ND1	2.15	0.80
3:C:162:GLU:HG2	3:C:196:TYR:CG	2.16	0.80
2:J:183:ARG:HG3	2:J:337:GLU:OE2	1.82	0.80
1:A:508:ILE:HG13	1:A:754:GLY:O	1.81	0.80
2:J:952:GLU:N	2:J:952:GLU:OE2	2.15	0.80
3:M:182:LEU:O	3:M:185:SER:HB2	1.82	0.80
2:B:378:TYR:OH	2:B:388:GLU:HA	1.80	0.80
3:M:148:ARG:HG2	3:M:149:GLU:HG3	1.63	0.80
2:J:1122:ARG:HH11	2:J:1122:ARG:HG2	1.47	0.80
2:J:1122:ARG:NH2	5:Q:67:TYR:CE2	2.49	0.80
1:A:531:MET:CB	9:L:44:THR:HG23	2.12	0.80
3:M:204:LYS:HG3	3:M:205:VAL:HG23	1.62	0.80
1:I:452:LEU:HB3	1:I:504:ILE:HD11	1.64	0.80
7:S:41:PRO:HB2	7:S:77:ARG:HG2	1.63	0.79
1:I:384:VAL:HG12	1:I:392:ILE:HB	1.65	0.79
3:C:152:ILE:HG12	3:C:153:ASP:N	1.97	0.79
10:N:57:ASP:HA	10:N:60:MET:HE3	1.62	0.79
8:K:34:ILE:HB	8:K:38:GLN:HG3	1.64	0.79
8:T:34:ILE:HB	8:T:38:GLN:HG3	1.64	0.79
2:J:1122:ARG:HG3	6:R:4:ARG:NH2	1.96	0.79
3:C:162:GLU:CB	3:C:196:TYR:HB2	2.13	0.79
1:I:6:LYS:CE	2:J:1122:ARG:NH1	2.45	0.79
1:I:531:MET:HB2	9:U:44:THR:CG2	2.12	0.79
2:J:391:GLN:O	2:J:392:ARG:CB	2.31	0.79
5:E:9:ASP:OD2	6:F:3:GLY:CA	2.29	0.79
5:Q:1:MET:CE	6:R:11:TYR:CE1	2.66	0.79
4:O:2:VAL:HG11	9:U:85:VAL:HA	1.63	0.79
1:I:6:LYS:CE	2:J:1122:ARG:NH2	2.11	0.78
1:I:103:CYS:SG	1:I:105:ARG:HB2	2.23	0.78
2:J:107:MET:HB3	2:J:395:ARG:HH22	0.76	0.78
1:A:834:ARG:HG3	3:C:80:THR:HG22	1.66	0.78
7:H:41:PRO:HB2	7:H:77:ARG:HG2	1.63	0.78
3:C:162:GLU:C	3:C:196:TYR:CA	2.52	0.78
2:J:1122:ARG:CG	6:R:4:ARG:NH2	2.47	0.78
1:I:79:LEU:HA	1:I:252:ASN:HD21	1.47	0.78
2:B:389:ASN:ND2	2:B:392:ARG:CB	2.45	0.78
2:J:979:THR:HA	9:U:26:ASN:ND2	1.99	0.78
5:E:8:LYS:HE3	6:F:5:LYS:HD2	1.64	0.78
3:C:153:ASP:HB2	3:C:158:GLU:O	1.84	0.78
3:M:187:LYS:O	3:M:188:SER:OG	2.02	0.78
2:J:1122:ARG:HD2	5:Q:10:VAL:CG1	2.13	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:58:GLN:O	10:N:61:VAL:HG12	1.84	0.78
2:B:391:GLN:OE1	2:B:393:PHE:CE2	2.37	0.77
1:A:452:LEU:HB3	1:A:504:ILE:HD11	1.64	0.77
3:C:161:VAL:HG23	3:C:198:LEU:C	2.04	0.77
2:J:63:PHE:HZ	2:J:388:GLU:HG2	1.43	0.77
1:A:384:VAL:HG12	1:A:392:ILE:HB	1.65	0.77
3:M:182:LEU:CD2	3:M:185:SER:HB2	2.14	0.77
3:C:196:TYR:CE1	3:C:198:LEU:HD11	2.20	0.77
3:C:161:VAL:HG23	3:C:199:VAL:CG2	2.10	0.77
2:B:744:LYS:NZ	9:L:53:ARG:HH22	1.74	0.77
2:J:370:MET:SD	2:J:398:ILE:HG12	2.24	0.76
2:J:57:VAL:HB	2:J:58:PRO:HA	1.67	0.76
2:J:394:VAL:HB	2:J:395:ARG:HG3	0.77	0.76
2:B:1063:TRP:HE1	2:B:1094:LYS:HE3	1.48	0.76
3:M:152:ILE:HG23	3:M:159:TYR:HA	1.66	0.76
1:I:147:CYS:SG	1:I:152:ALA:CA	2.74	0.76
2:B:390:ILE:O	2:B:392:ARG:N	2.19	0.76
5:Q:3:LYS:NZ	6:R:9:GLU:CD	2.39	0.76
2:J:361:VAL:HG11	2:J:417:PRO:HG3	1.67	0.76
1:I:632:LYS:HZ2	1:I:634:LEU:H	1.30	0.76
2:B:952:GLU:N	2:B:952:GLU:OE2	2.17	0.76
2:B:390:ILE:HD12	2:B:391:GLN:N	1.99	0.76
3:C:161:VAL:HG23	3:C:199:VAL:CB	2.16	0.75
1:A:531:MET:HB2	9:L:44:THR:HG21	1.66	0.75
1:I:9:GLY:CA	2:J:1120:LYS:HB2	2.15	0.75
4:O:35:SER:HB2	4:O:141:LYS:HB3	1.68	0.75
9:L:46:GLU:OE2	9:L:56:ARG:HD2	1.85	0.75
2:B:361:VAL:HG11	2:B:417:PRO:HG3	1.67	0.75
2:J:1122:ARG:HG2	2:J:1122:ARG:NH1	2.01	0.75
1:I:480:GLU:HA	8:T:10:ALA:HB1	1.68	0.75
1:I:585:LEU:O	1:I:586:GLU:HB3	1.86	0.75
2:B:749:ARG:NH2	4:D:147:GLN:OE1	2.20	0.75
1:I:9:GLY:HA3	2:J:1120:LYS:HB2	1.67	0.75
3:C:194:GLU:OE1	3:C:196:TYR:HE2	1.69	0.75
4:D:35:SER:HB2	4:D:141:LYS:HB3	1.68	0.75
2:J:735:ASN:HB3	2:J:741:ILE:HG13	1.69	0.75
3:C:343:THR:O	3:C:347:PHE:HB3	1.87	0.75
3:M:67:VAL:O	3:M:71:SER:OG	2.05	0.75
2:J:683:TRP:CD1	2:J:686:PHE:HB3	2.22	0.74
2:B:683:TRP:CD1	2:B:686:PHE:HB3	2.22	0.74
2:J:394:VAL:CG1	2:J:395:ARG:HG2	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:183:ARG:HG2	2:B:337:GLU:OE1	1.87	0.74
2:B:735:ASN:HB3	2:B:741:ILE:HG13	1.69	0.74
2:B:57:VAL:HB	2:B:58:PRO:HA	1.67	0.74
2:B:123:ILE:HG22	2:B:403:LEU:HD22	1.69	0.74
1:A:16:LEU:HD11	2:B:1109:LYS:HG3	1.68	0.74
1:A:625:ALA:O	1:A:632:LYS:NZ	2.18	0.74
5:E:92:MET:HE1	5:E:127:PHE:HD2	1.51	0.74
7:H:13:VAL:HG22	7:H:14:LEU:HG	1.70	0.74
2:J:771:GLN:HB3	2:J:818:PRO:HG3	1.69	0.74
1:I:6:LYS:HE3	2:J:1122:ARG:NH1	2.02	0.74
3:C:160:VAL:CG2	3:C:198:LEU:HG	2.18	0.73
2:B:286:PRO:HD2	2:B:290:ARG:HE	1.53	0.73
3:C:67:VAL:O	3:C:71:SER:OG	2.05	0.73
2:B:389:ASN:HD22	2:B:392:ARG:HB2	1.52	0.73
3:C:212:ARG:HG3	3:C:213:LYS:H	1.49	0.73
2:J:996:ARG:HH22	2:J:1000:MET:HE3	1.53	0.73
2:B:239:THR:HB	2:B:242:GLU:HG2	1.70	0.73
2:J:123:ILE:HG22	2:J:403:LEU:HD22	1.69	0.73
2:B:771:GLN:HB3	2:B:818:PRO:HG3	1.69	0.73
3:C:345:HIS:O	3:C:348:ALA:N	2.20	0.73
2:J:286:PRO:HD2	2:J:290:ARG:HE	1.53	0.73
2:J:239:THR:HB	2:J:242:GLU:HG2	1.70	0.73
3:C:134:VAL:HG12	3:C:138:ILE:HD11	1.70	0.73
3:M:134:VAL:HG12	3:M:138:ILE:HD11	1.70	0.73
3:C:164:ASP:CG	3:C:165:PRO:HD2	2.09	0.73
1:I:304:LEU:HB3	2:J:1111:MET:HE2	1.71	0.73
2:J:395:ARG:HB3	2:J:398:ILE:CD1	2.19	0.72
1:A:444:PRO:CD	9:L:50:THR:HG22	2.19	0.72
2:B:744:LYS:HZ1	9:L:53:ARG:NH2	1.87	0.72
1:I:665:GLY:C	2:J:729:LEU:HD11	2.09	0.72
5:E:1:MET:CE	6:F:11:TYR:HD1	1.98	0.72
1:I:445:TYR:CG	9:U:49:ILE:HG21	2.24	0.72
2:J:42:ILE:HG21	2:J:72:ILE:HD13	1.71	0.72
11:W:27:CYS:CB	11:W:30:CYS:SG	2.77	0.72
1:A:671:ASP:OD1	2:B:969:SER:OG	2.07	0.72
2:J:939:LEU:HD11	2:J:966:PHE:HD2	1.54	0.72
1:A:666:PHE:C	2:B:729:LEU:HD13	2.10	0.72
2:B:939:LEU:HD11	2:B:966:PHE:HD2	1.54	0.72
7:S:13:VAL:HG22	7:S:14:LEU:HG	1.71	0.72
1:I:74:PHE:HE1	1:I:222:PRO:HD3	1.54	0.72
2:J:378:TYR:HE1	2:J:388:GLU:CB	2.01	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:14:GLU:CD	11:P:30:CYS:HG	1.92	0.72
2:J:309:ASP:N	2:J:309:ASP:OD1	2.23	0.72
2:J:904:THR:HG22	2:J:906:SER:H	1.55	0.72
2:J:378:TYR:CZ	2:J:388:GLU:CG	2.70	0.72
1:I:666:PHE:H	2:J:729:LEU:CG	2.03	0.72
3:M:153:ASP:CB	3:M:157:MET:HB2	2.20	0.72
2:J:1101:PHE:CG	3:M:367:ILE:HG13	2.25	0.72
2:J:395:ARG:HD3	2:J:398:ILE:HD11	1.72	0.72
2:J:42:ILE:HG23	2:J:72:ILE:HD11	1.72	0.71
3:C:186:PHE:C	3:C:187:LYS:HG2	2.10	0.71
2:B:309:ASP:N	2:B:309:ASP:OD1	2.23	0.71
2:B:904:THR:HG22	2:B:906:SER:H	1.56	0.71
2:B:63:PHE:CD1	2:B:392:ARG:NH2	2.58	0.71
2:J:392:ARG:O	2:J:394:VAL:N	2.22	0.71
3:M:152:ILE:HG23	3:M:160:VAL:H	1.54	0.71
9:L:48:PRO:O	9:L:49:ILE:HG23	1.89	0.71
1:I:13:PHE:CE2	3:M:333:VAL:HG21	2.25	0.71
2:B:996:ARG:HH22	2:B:1000:MET:HE3	1.53	0.71
3:C:163:ILE:HB	3:C:164:ASP:CA	2.20	0.71
2:B:981:ARG:NH2	9:L:30:GLU:OE2	2.22	0.71
3:C:151:THR:HG22	3:C:152:ILE:N	2.04	0.71
2:B:432:TYR:HB2	2:B:682:GLY:HA2	1.73	0.71
2:J:749:ARG:NH2	4:O:147:GLN:OE1	2.24	0.71
2:J:39:ASN:C	2:J:41:PHE:H	1.94	0.71
2:B:146:ILE:CG2	10:N:61:VAL:HG21	2.20	0.71
1:I:670:ILE:HD11	2:J:929:ILE:HG12	1.71	0.71
1:A:181:MET:SD	1:A:189:ARG:NH1	2.64	0.71
3:C:223:LEU:O	3:C:225:GLY:N	2.23	0.71
3:M:165:PRO:HB3	3:M:195:GLY:HA2	1.72	0.71
9:L:25:ALA:HB1	9:L:43:TYR:CE2	2.26	0.71
1:A:749:ILE:O	1:A:753:THR:CG2	2.39	0.71
1:A:564:PRO:HD2	1:A:567:LEU:HD11	1.72	0.71
2:J:1068:CYS:SG	2:J:1070:HIS:CD2	2.84	0.71
1:I:449:ARG:CZ	9:U:49:ILE:HD11	2.21	0.71
3:C:162:GLU:HA	3:C:196:TYR:CG	2.25	0.71
5:Q:9:ASP:OD1	6:R:4:ARG:HG2	1.90	0.71
9:L:49:ILE:CD1	9:L:50:THR:H	1.98	0.71
9:L:25:ALA:HB1	9:L:43:TYR:CD2	2.26	0.71
3:M:145:ASN:OD1	3:M:145:ASN:N	2.24	0.71
5:E:9:ASP:OD1	5:E:10:VAL:N	2.23	0.70
2:B:378:TYR:HE1	2:B:388:GLU:C	1.93	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:LEU:HD12	3:C:177:LYS:HZ2	1.55	0.70
1:A:531:MET:HB3	9:L:44:THR:CG2	2.20	0.70
1:I:822:MET:HG2	2:J:458:LEU:HB3	1.72	0.70
2:J:432:TYR:HB2	2:J:682:GLY:HA2	1.73	0.70
2:B:275:ASP:O	2:B:279:ARG:HB2	1.91	0.70
2:B:47:GLN:HE22	2:B:69:LYS:HA	1.56	0.70
2:J:116:GLN:OE1	2:J:393:PHE:HD1	1.73	0.70
3:M:153:ASP:HB3	3:M:157:MET:HB2	1.73	0.70
1:A:60:CYS:SG	1:A:61:GLU:N	2.64	0.70
1:A:74:PHE:HE1	1:A:222:PRO:HD3	1.57	0.70
1:I:181:MET:SD	1:I:189:ARG:NH1	2.64	0.70
1:I:840:TYR:OH	3:M:323:ARG:NH2	2.25	0.70
3:M:223:LEU:O	3:M:225:GLY:N	2.23	0.70
3:C:196:TYR:O	3:C:196:TYR:CD1	2.45	0.70
2:J:41:PHE:CD1	2:J:42:ILE:HD13	2.27	0.70
1:A:712:LYS:HD2	3:C:92:ILE:HB	1.74	0.70
1:I:476:GLU:OE1	8:T:11:ARG:NH1	2.23	0.70
3:M:152:ILE:O	3:M:160:VAL:HB	1.92	0.69
3:M:120:LEU:O	3:M:125:ARG:NH1	2.26	0.69
1:A:863:PRO:HB3	3:C:360:GLY:HA2	1.75	0.69
2:J:378:TYR:CD1	2:J:388:GLU:HG3	2.22	0.69
3:C:148:ARG:HG2	3:C:149:GLU:CG	2.18	0.69
1:I:564:PRO:HD2	1:I:567:LEU:HD11	1.72	0.69
3:C:342:THR:HB	3:C:345:HIS:HB2	1.73	0.69
2:B:390:ILE:C	2:B:392:ARG:H	1.93	0.69
1:I:60:CYS:SG	1:I:61:GLU:N	2.65	0.69
2:J:63:PHE:CE1	2:J:388:GLU:OE1	2.45	0.69
2:J:42:ILE:HG23	2:J:72:ILE:CD1	2.21	0.69
3:C:145:ASN:OD1	3:C:145:ASN:N	2.25	0.69
5:E:3:LYS:NZ	6:F:9:GLU:CD	2.46	0.69
2:B:730:SER:HA	2:B:735:ASN:HD21	1.58	0.69
1:A:13:PHE:HE1	2:B:1115:PRO:HB3	1.57	0.69
1:A:894:ILE:HG13	3:C:29:ILE:HD12	1.75	0.69
3:C:120:LEU:O	3:C:125:ARG:NH1	2.26	0.69
2:B:389:ASN:HD21	2:B:392:ARG:NE	1.88	0.69
1:I:447:THR:O	1:I:449:ARG:NH1	2.26	0.69
1:A:758:LYS:HG2	1:A:760:LEU:HD21	1.74	0.69
3:C:211:LEU:HA	3:C:214:ILE:HD12	1.73	0.69
10:N:60:MET:O	10:N:62:TYR:N	2.23	0.69
1:I:834:ARG:HH12	3:M:99:PRO:HD3	1.58	0.69
1:I:640:GLU:HG2	1:I:896:ARG:NH1	2.07	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:MET:HB3	9:L:44:THR:HG23	1.72	0.69
5:Q:8:LYS:HE3	6:R:5:LYS:HD2	1.73	0.69
3:M:182:LEU:CD2	3:M:185:SER:CB	2.71	0.69
10:N:57:ASP:HA	10:N:60:MET:CE	2.23	0.69
2:J:275:ASP:O	2:J:279:ARG:HB2	1.91	0.69
3:M:148:ARG:HH12	3:M:162:GLU:C	1.96	0.68
1:I:103:CYS:CA	1:I:150:CYS:SG	2.81	0.68
2:J:378:TYR:CE1	2:J:388:GLU:CB	2.74	0.68
2:J:730:SER:HA	2:J:735:ASN:HD21	1.57	0.68
3:M:153:ASP:OD2	3:M:160:VAL:HG21	1.93	0.68
2:J:395:ARG:HB3	2:J:398:ILE:HD11	1.76	0.68
1:A:872:TYR:CZ	3:C:64:VAL:HG11	2.28	0.68
2:B:719:PRO:HG3	10:N:53:VAL:HG11	1.76	0.68
3:C:161:VAL:HG12	3:C:162:GLU:N	2.03	0.68
5:Q:9:ASP:OD1	5:Q:10:VAL:N	2.23	0.68
3:M:64:VAL:HA	3:M:67:VAL:HG22	1.75	0.68
3:C:161:VAL:HG23	3:C:199:VAL:CA	2.23	0.68
3:C:162:GLU:C	3:C:196:TYR:HA	2.13	0.68
2:J:392:ARG:C	2:J:394:VAL:H	1.96	0.68
2:J:393:PHE:C	2:J:394:VAL:HG22	2.14	0.68
1:A:894:ILE:O	1:A:897:THR:HG23	1.93	0.68
1:A:447:THR:O	1:A:449:ARG:NH1	2.25	0.68
3:M:160:VAL:HG12	3:M:161:VAL:N	2.09	0.68
1:I:671:ASP:OD1	2:J:969:SER:OG	2.11	0.68
1:A:445:TYR:HB2	1:A:449:ARG:HH22	1.59	0.68
3:C:286:ILE:HD13	3:C:306:MET:HG2	1.76	0.68
1:I:100:CYS:CB	1:I:103:CYS:HB3	2.20	0.68
1:A:63:CYS:HG	1:A:73:HIS:HE2	1.42	0.68
3:M:148:ARG:NH1	3:M:162:GLU:C	2.47	0.67
3:C:358:LEU:HD12	3:C:359:ASN:H	1.59	0.67
3:C:64:VAL:HA	3:C:67:VAL:HG22	1.75	0.67
1:I:103:CYS:SG	1:I:105:ARG:CB	2.82	0.67
2:B:731:TYR:CE2	2:B:902:PRO:HG3	2.29	0.67
3:C:55:LYS:HE2	8:K:3:ARG:HH22	1.60	0.67
2:J:56:VAL:HG12	2:J:367:VAL:HG13	1.77	0.67
2:J:42:ILE:CG2	2:J:72:ILE:HD11	2.22	0.67
1:A:753:THR:HG23	1:A:754:GLY:N	2.05	0.67
4:D:6:ILE:HG13	4:D:14:ILE:HD11	1.77	0.67
1:I:775:ARG:HD3	2:J:453:PHE:HD2	1.60	0.67
2:J:211:LYS:HA	3:M:212:ARG:NH2	2.09	0.67
1:I:94:ARG:HG3	1:I:138:HIS:CD2	2.30	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:868:VAL:HG11	3:C:311:MET:HG2	1.77	0.67
1:I:445:TYR:HB2	1:I:449:ARG:HH22	1.60	0.67
5:E:81:ASN:O	5:E:82:GLN:CG	2.43	0.67
2:B:365:GLN:OE1	2:B:406:ARG:NH1	2.28	0.67
5:Q:41:ASP:OD2	6:R:1:MET:SD	2.53	0.67
3:M:286:ILE:HD13	3:M:306:MET:HG2	1.77	0.67
2:B:389:ASN:O	2:B:389:ASN:ND2	2.27	0.67
2:J:41:PHE:CE1	2:J:42:ILE:HD13	2.30	0.67
1:A:94:ARG:HG3	1:A:138:HIS:CD2	2.30	0.67
4:D:56:ASP:HB3	11:P:46:VAL:HG21	1.75	0.67
4:O:6:ILE:HG13	4:O:14:ILE:HD11	1.77	0.67
9:U:51:MET:CG	9:U:53:ARG:HB2	2.24	0.67
2:J:378:TYR:HE1	2:J:388:GLU:HG3	1.34	0.67
2:J:729:LEU:HD23	2:J:730:SER:C	2.15	0.66
1:A:556:LYS:HD2	1:A:616:LEU:HD22	1.77	0.66
1:I:147:CYS:SG	1:I:152:ALA:N	2.68	0.66
3:C:287:ASP:O	3:C:291:SER:OG	2.13	0.66
2:B:856:VAL:HG12	11:P:35:LEU:HB2	1.77	0.66
3:M:287:ASP:O	3:M:291:SER:OG	2.13	0.66
2:B:433:MET:HG3	2:B:656:LEU:HD11	1.78	0.66
1:A:850:GLN:OE1	2:B:1037:ARG:NH1	2.29	0.66
9:U:51:MET:HA	9:U:52:ALA:C	2.15	0.66
2:J:365:GLN:OE1	2:J:406:ARG:NH1	2.28	0.66
1:I:16:LEU:HG	2:J:1114:ARG:HB3	1.77	0.66
2:J:1109:LYS:HD3	2:J:1115:PRO:HD2	1.78	0.66
1:A:508:ILE:HG21	1:A:754:GLY:CA	2.25	0.66
2:J:433:MET:HG3	2:J:656:LEU:HD11	1.78	0.66
1:A:750:MET:HA	1:A:753:THR:HG22	1.76	0.66
2:J:1065:CYS:HB3	2:J:1068:CYS:HB3	1.75	0.66
1:I:775:ARG:HD3	2:J:453:PHE:CD2	2.31	0.66
2:B:56:VAL:HG12	2:B:367:VAL:HG13	1.77	0.66
2:J:43:ASP:OD1	2:J:43:ASP:N	2.28	0.66
2:J:800:ILE:HD11	2:J:812:LEU:HA	1.77	0.66
1:I:894:ILE:HG13	3:M:29:ILE:HD12	1.78	0.66
2:J:546:ARG:NH1	2:J:555:ILE:O	2.29	0.66
9:L:25:ALA:CB	9:L:43:TYR:CE2	2.78	0.66
2:J:174:LEU:HD21	2:J:180:LEU:HD11	1.77	0.66
3:M:321:ILE:HA	3:M:326:ILE:HG13	1.78	0.65
2:J:556:ASN:OD1	2:J:576:ARG:NH1	2.29	0.65
1:A:505:GLN:HB2	2:B:917:HIS:CD2	2.30	0.65
2:J:389:ASN:CA	2:J:390:ILE:HG23	2.11	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:820:ARG:O	2:J:837:ARG:NH1	2.28	0.65
4:O:226:THR:OG1	4:O:227:ASN:N	2.29	0.65
2:B:959:LYS:HA	4:D:201:ARG:HH21	1.61	0.65
1:I:6:LYS:HE2	2:J:1122:ARG:NH1	2.04	0.65
3:M:96:LEU:HB2	3:M:100:ARG:HB2	1.78	0.65
3:C:96:LEU:HB2	3:C:100:ARG:HB2	1.78	0.65
4:O:162:SER:HA	4:O:188:GLU:HB3	1.78	0.65
3:C:162:GLU:CG	3:C:196:TYR:CD1	2.77	0.65
1:A:712:LYS:HZ2	3:C:92:ILE:N	1.95	0.65
3:C:203:LYS:HZ2	3:C:203:LYS:HB2	1.59	0.65
5:Q:100:ARG:CZ	6:R:43:VAL:HG13	2.26	0.65
2:B:556:ASN:OD1	2:B:576:ARG:NH1	2.30	0.65
2:B:546:ARG:NH1	2:B:555:ILE:O	2.29	0.65
2:B:759:THR:HB	2:B:869:THR:HG22	1.79	0.65
2:B:174:LEU:HD21	2:B:180:LEU:HD11	1.78	0.65
1:A:309:LYS:HB3	3:C:341:ILE:HG23	1.77	0.65
2:J:614:VAL:HG13	2:J:615:ILE:HG12	1.79	0.65
2:J:389:ASN:O	2:J:389:ASN:ND2	2.29	0.65
1:A:863:PRO:CB	3:C:360:GLY:HA2	2.27	0.65
2:J:793:HIS:HB3	2:J:800:ILE:HG23	1.79	0.65
2:B:800:ILE:HD11	2:B:812:LEU:HA	1.77	0.65
2:J:759:THR:HB	2:J:869:THR:HG22	1.79	0.65
2:J:198:ARG:HD3	2:J:304:PRO:HB2	1.78	0.65
4:D:162:SER:HA	4:D:188:GLU:HB3	1.78	0.65
1:I:445:TYR:CD2	9:U:49:ILE:CG2	2.61	0.65
3:C:194:GLU:OE1	3:C:196:TYR:CE2	2.48	0.65
1:I:40:TYR:H	1:I:41:PRO:CD	2.10	0.65
2:B:45:GLY:O	2:B:47:GLN:N	2.30	0.65
1:A:248:ILE:HD11	1:A:282:TYR:HB2	1.79	0.65
5:Q:14:PRO:HB3	5:Q:16:ARG:HH11	1.63	0.64
1:I:556:LYS:HD2	1:I:616:LEU:HD22	1.77	0.64
1:I:147:CYS:H	1:I:152:ALA:HB2	1.62	0.64
4:D:200:PRO:HB2	4:D:203:PHE:HD1	1.61	0.64
3:C:164:ASP:OD1	3:C:165:PRO:HD2	1.97	0.64
2:B:614:VAL:HG13	2:B:615:ILE:HG12	1.79	0.64
2:B:793:HIS:HB3	2:B:800:ILE:HG23	1.79	0.64
3:M:148:ARG:NH2	3:M:162:GLU:HG2	2.11	0.64
3:M:151:THR:HG22	3:M:152:ILE:N	2.06	0.64
1:A:750:MET:CA	1:A:753:THR:HG22	2.26	0.64
4:O:154:LYS:NZ	4:O:155:TYR:O	2.31	0.64
3:C:113:THR:OG1	3:C:113:THR:O	2.15	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:198:ARG:HD3	2:B:304:PRO:HB2	1.78	0.64
5:E:14:PRO:HB3	5:E:16:ARG:HH11	1.63	0.64
9:U:52:ALA:O	9:U:53:ARG:HB3	1.96	0.64
2:J:1122:ARG:CD	6:R:4:ARG:HH21	2.11	0.64
3:C:162:GLU:HA	3:C:196:TYR:HD1	1.59	0.64
2:B:183:ARG:NH2	2:B:454:GLU:OE2	2.30	0.64
9:L:93:ILE:O	9:L:94:GLU:HG3	1.97	0.64
2:J:25:TRP:CZ2	2:J:485:LEU:HB3	2.33	0.64
1:I:248:ILE:HD11	1:I:282:TYR:HB2	1.79	0.64
2:J:969:SER:HB3	2:J:971:ARG:HG3	1.80	0.63
3:C:186:PHE:O	3:C:187:LYS:HG2	1.96	0.63
2:J:746:SER:HB3	2:J:751:LEU:HD12	1.80	0.63
3:C:157:MET:O	3:C:158:GLU:HB2	1.96	0.63
1:A:623:LYS:HB2	1:A:754:GLY:HA3	1.80	0.63
2:B:25:TRP:CZ2	2:B:485:LEU:HB3	2.33	0.63
2:J:981:ARG:NH2	9:U:30:GLU:OE2	2.29	0.63
2:B:57:VAL:HG11	2:B:371:GLN:HG3	1.80	0.63
1:I:100:CYS:SG	1:I:103:CYS:CB	2.86	0.63
1:I:492:ILE:HA	1:I:499:PRO:HA	1.79	0.63
4:O:194:ILE:HA	4:O:221:VAL:HG21	1.79	0.63
5:E:5:LEU:CD1	6:F:6:LYS:HD3	2.29	0.63
1:I:895:VAL:O	1:I:897:THR:N	2.31	0.63
3:M:229:VAL:HG21	3:M:245:THR:HG22	1.81	0.63
3:M:358:LEU:HD12	3:M:359:ASN:H	1.62	0.63
3:C:321:ILE:HA	3:C:326:ILE:HG13	1.79	0.63
2:J:57:VAL:HG11	2:J:371:GLN:HG3	1.79	0.63
3:C:160:VAL:CG2	3:C:198:LEU:CG	2.77	0.63
3:M:182:LEU:HD22	3:M:185:SER:HB2	1.80	0.63
4:O:62:ARG:NH2	10:V:2:ILE:O	2.32	0.63
4:O:200:PRO:HB2	4:O:203:PHE:HD1	1.63	0.63
5:E:41:ASP:OD2	6:F:1:MET:SD	2.56	0.63
2:B:532:VAL:HG12	2:B:533:GLU:H	1.64	0.63
3:C:161:VAL:CG2	3:C:198:LEU:C	2.67	0.63
2:J:42:ILE:HG22	2:J:72:ILE:HD13	1.80	0.63
4:D:194:ILE:HA	4:D:221:VAL:HG21	1.79	0.63
4:D:154:LYS:NZ	4:D:155:TYR:O	2.32	0.63
3:C:55:LYS:HG2	8:K:3:ARG:HH21	1.65	0.62
2:B:161:ILE:HG21	2:B:412:ALA:HB2	1.81	0.62
1:A:656:LEU:HD13	1:A:659:TRP:HE1	1.64	0.62
2:J:1063:TRP:HE3	2:J:1092:ILE:HG22	1.64	0.62
1:I:47:MET:O	1:I:49:LYS:N	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:897:THR:HG21	3:C:45:ILE:HD11	1.82	0.62
2:B:979:THR:HA	9:L:26:ASN:HD21	1.64	0.62
7:S:17:GLU:HB2	7:S:64:LYS:HB2	1.81	0.62
2:J:398:ILE:CG2	2:J:398:ILE:O	2.46	0.62
2:J:65:VAL:HG13	2:J:395:ARG:NH2	2.14	0.62
2:B:969:SER:HB3	2:B:971:ARG:HG3	1.81	0.62
3:C:180:ARG:O	3:C:182:LEU:N	2.32	0.62
3:C:229:VAL:HG21	3:C:245:THR:HG22	1.81	0.62
2:J:11:THR:O	2:J:593:ARG:NH2	2.31	0.62
2:B:1109:LYS:HD3	2:B:1115:PRO:HD2	1.81	0.62
3:C:93:ASN:O	3:C:95:THR:N	2.33	0.62
1:I:449:ARG:NH2	9:U:49:ILE:HD11	2.13	0.62
2:B:522:VAL:HG22	2:B:568:VAL:HB	1.82	0.62
1:A:806:ASN:OD1	1:A:806:ASN:N	2.32	0.62
3:M:113:THR:OG1	3:M:113:THR:O	2.15	0.62
9:U:51:MET:HA	9:U:52:ALA:HB3	1.81	0.62
9:U:51:MET:HG2	9:U:53:ARG:HB3	1.77	0.62
1:A:150:CYS:C	1:A:152:ALA:N	2.52	0.62
3:C:211:LEU:HA	3:C:214:ILE:HD11	1.80	0.62
3:M:173:LEU:HB3	3:M:177:LYS:HZ3	1.65	0.62
2:J:532:VAL:HG12	2:J:533:GLU:H	1.64	0.62
5:Q:125:ARG:HE	5:Q:125:ARG:H	1.48	0.62
3:M:191:PHE:HB2	3:M:198:LEU:HB2	1.82	0.62
3:C:187:LYS:NZ	3:C:206:THR:HB	2.15	0.62
2:J:37:SER:O	2:J:41:PHE:HB2	1.99	0.62
1:A:508:ILE:HG21	1:A:754:GLY:C	2.20	0.62
1:A:492:ILE:HA	1:A:499:PRO:HA	1.80	0.62
9:U:44:THR:C	9:U:45:ILE:HG13	2.21	0.62
2:B:11:THR:O	2:B:593:ARG:NH2	2.32	0.62
2:B:190:VAL:HG21	2:B:331:SER:HB3	1.82	0.62
3:C:163:ILE:N	3:C:196:TYR:HB3	2.15	0.61
1:I:665:GLY:CA	2:J:729:LEU:CD1	2.65	0.61
2:J:183:ARG:HG2	2:J:184:ASP:N	2.15	0.61
2:J:330:LEU:HD21	2:J:337:GLU:HG2	1.82	0.61
3:M:339:PHE:O	3:M:341:ILE:N	2.33	0.61
2:B:746:SER:HB3	2:B:751:LEU:HD12	1.81	0.61
2:J:161:ILE:HG21	2:J:412:ALA:HB2	1.81	0.61
2:J:207:VAL:HG12	2:J:217:VAL:HG22	1.81	0.61
7:H:50:VAL:HG13	7:H:55:ALA:HB3	1.81	0.61
2:B:330:LEU:HD21	2:B:337:GLU:HG2	1.82	0.61
2:B:931:ALA:HB1	2:B:990:GLY:HA3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:5:LEU:CD1	6:R:6:LYS:HD3	2.30	0.61
3:C:331:ALA:H	3:C:336:ARG:HH12	1.46	0.61
2:J:93:ARG:HG3	2:J:160:ILE:HD13	1.82	0.61
1:A:463:ASP:HA	2:B:890:GLY:HA2	1.81	0.61
6:R:116:ASP:HA	6:R:119:ARG:HE	1.65	0.61
7:S:50:VAL:HG13	7:S:55:ALA:HB3	1.81	0.61
6:F:116:ASP:HA	6:F:119:ARG:HE	1.65	0.61
5:Q:99:ILE:HD13	5:Q:142:VAL:HG21	1.82	0.61
1:A:47:MET:O	1:A:49:LYS:N	2.33	0.61
3:M:182:LEU:O	3:M:185:SER:CB	2.48	0.61
2:B:979:THR:HA	9:L:26:ASN:ND2	2.16	0.61
7:H:17:GLU:HB2	7:H:64:LYS:HB2	1.81	0.61
3:C:143:LEU:HB2	3:C:222:ARG:HG3	1.81	0.61
3:M:279:GLU:OE1	7:S:65:ARG:NH1	2.34	0.61
2:J:165:GLU:OE1	2:J:429:ARG:NH1	2.33	0.61
2:J:818:PRO:HA	2:J:836:ARG:HB3	1.83	0.61
2:B:276:TYR:O	2:B:279:ARG:HB3	2.01	0.61
3:M:173:LEU:HD12	3:M:177:LYS:HZ2	1.64	0.61
2:J:116:GLN:OE1	2:J:393:PHE:CD1	2.53	0.61
5:E:39:ASP:HA	5:E:154:ARG:HH11	1.66	0.61
1:I:656:LEU:HD13	1:I:659:TRP:HE1	1.64	0.61
5:E:125:ARG:H	5:E:125:ARG:HE	1.48	0.61
7:S:55:ALA:HB1	7:S:79:VAL:HG21	1.82	0.61
2:J:190:VAL:HG21	2:J:331:SER:HB3	1.82	0.61
2:J:931:ALA:HB1	2:J:990:GLY:HA3	1.81	0.61
2:J:971:ARG:HB2	2:J:986:ASP:HB3	1.82	0.61
1:I:103:CYS:HB2	1:I:150:CYS:HG	1.64	0.61
3:C:386:LEU:HD11	5:E:20:MET:C	2.21	0.61
2:J:522:VAL:HG22	2:J:568:VAL:HB	1.81	0.61
2:B:411:LEU:HD12	2:B:416:TRP:HH2	1.66	0.60
2:J:803:GLU:O	11:W:44:ARG:NE	2.34	0.60
5:E:49:LEU:N	5:E:73:ASN:O	2.33	0.60
2:B:971:ARG:HB2	2:B:986:ASP:HB3	1.82	0.60
4:D:50:ASN:HD22	4:D:52:SER:H	1.48	0.60
2:J:233:ARG:NH2	2:J:240:ASP:OD1	2.35	0.60
5:Q:39:ASP:HA	5:Q:154:ARG:HH11	1.66	0.60
3:C:279:GLU:OE1	7:H:65:ARG:NH1	2.34	0.60
1:I:535:MET:HE1	1:I:652:GLN:HE22	1.66	0.60
3:M:378:VAL:HG21	8:T:8:GLU:HG2	1.83	0.60
4:O:50:ASN:HD22	4:O:52:SER:H	1.49	0.60
3:C:160:VAL:HG21	3:C:198:LEU:CG	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:160:VAL:HG23	3:C:198:LEU:HB3	1.82	0.60
2:J:411:LEU:HD12	2:J:416:TRP:HH2	1.66	0.60
2:B:233:ARG:NH2	2:B:240:ASP:OD1	2.34	0.60
2:B:470:GLU:OE2	2:B:482:ASN:ND2	2.35	0.60
1:A:6:LYS:HG2	2:B:1094:LYS:O	2.02	0.60
3:C:217:LYS:HA	3:C:221:HIS:HB2	1.83	0.60
1:A:630:ASP:N	1:A:630:ASP:OD1	2.34	0.60
2:B:818:PRO:HA	2:B:836:ARG:HB3	1.82	0.60
4:O:62:ARG:HH12	10:V:2:ILE:HB	1.66	0.60
7:H:55:ALA:HB1	7:H:79:VAL:HG21	1.82	0.60
2:B:207:VAL:HG12	2:B:217:VAL:HG22	1.82	0.60
2:B:758:ARG:HH11	2:B:844:ARG:HG3	1.66	0.60
1:I:806:ASN:N	1:I:806:ASN:OD1	2.32	0.60
1:A:444:PRO:HD2	9:L:50:THR:HG23	1.82	0.60
2:B:165:GLU:OE1	2:B:429:ARG:NH1	2.34	0.60
1:I:11:ILE:HD12	3:M:358:LEU:CD2	2.32	0.60
2:J:378:TYR:CZ	2:J:388:GLU:OE2	2.55	0.60
1:A:666:PHE:H	2:B:729:LEU:HD13	1.66	0.60
2:J:276:TYR:O	2:J:279:ARG:HB3	2.01	0.60
5:E:5:LEU:HD11	6:F:6:LYS:HD3	1.83	0.60
1:A:62:THR:HG21	2:B:1078:ARG:HH11	1.66	0.60
5:Q:80:ARG:HG3	5:Q:83:GLU:HB2	1.84	0.60
7:H:43:ILE:N	7:H:78:LEU:O	2.29	0.60
2:J:391:GLN:O	2:J:392:ARG:HB2	2.02	0.60
2:B:1065:CYS:HB3	2:B:1068:CYS:HB2	1.83	0.60
1:A:95:VAL:HG22	1:A:201:LEU:HD23	1.84	0.60
2:J:39:ASN:C	2:J:41:PHE:N	2.55	0.60
1:A:444:PRO:HD2	9:L:50:THR:CG2	2.32	0.60
1:I:480:GLU:CD	2:J:1047:MET:HB2	2.22	0.60
4:D:60:ALA:HB1	11:P:48:ALA:HB2	1.82	0.60
9:U:59:VAL:HG21	9:U:71:LEU:HD21	1.83	0.60
2:J:46:LEU:C	2:J:46:LEU:HD12	2.21	0.60
3:M:189:ALA:HB3	3:M:199:VAL:HA	1.83	0.60
5:E:92:MET:HE2	5:E:127:PHE:CD2	2.34	0.60
11:W:30:CYS:SG	11:W:32:SER:CB	2.90	0.60
2:B:146:ILE:CG2	10:N:61:VAL:CG2	2.80	0.60
10:N:61:VAL:HG13	10:N:61:VAL:O	2.02	0.60
3:M:134:VAL:O	3:M:138:ILE:HG13	2.02	0.60
10:V:7:CYS:SG	10:V:8:PHE:N	2.75	0.60
3:C:134:VAL:O	3:C:138:ILE:HG13	2.02	0.59
1:I:756:ARG:HG3	2:J:917:HIS:HB3	1.83	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:758:ARG:HH11	2:J:844:ARG:HG3	1.66	0.59
9:L:59:VAL:HG21	9:L:71:LEU:HD21	1.82	0.59
2:B:394:VAL:CG2	2:B:395:ARG:HG3	2.30	0.59
1:I:449:ARG:NE	9:U:49:ILE:HD11	2.17	0.59
1:A:666:PHE:H	2:B:729:LEU:CD1	2.15	0.59
1:A:63:CYS:O	2:B:1076:LYS:HB2	2.01	0.59
2:J:205:ILE:HD11	2:J:303:LEU:H	1.67	0.59
5:Q:2:TYR:OH	6:R:44:SER:OG	2.17	0.59
5:E:100:ARG:CZ	6:F:43:VAL:HG13	2.31	0.59
2:J:1091:ARG:HD3	2:J:1091:ARG:H	1.67	0.59
3:C:161:VAL:O	3:C:162:GLU:HG3	2.01	0.59
2:J:1122:ARG:HH11	2:J:1122:ARG:CG	2.15	0.59
1:I:666:PHE:O	2:J:729:LEU:HG	2.03	0.59
1:A:758:LYS:HG2	1:A:760:LEU:CD2	2.33	0.59
1:I:63:CYS:HG	1:I:73:HIS:HE2	1.47	0.59
5:Q:5:LEU:HD11	6:R:6:LYS:HD3	1.83	0.59
2:B:789:LYS:HB3	2:B:792:ARG:HB2	1.84	0.59
2:B:93:ARG:HG3	2:B:160:ILE:HD13	1.83	0.59
1:I:690:ALA:HA	1:I:693:LYS:HD2	1.83	0.59
2:J:789:LYS:HB3	2:J:792:ARG:HB2	1.83	0.59
2:B:20:VAL:O	2:B:23:SER:OG	2.18	0.59
5:E:99:ILE:HD13	5:E:142:VAL:HG21	1.83	0.59
2:B:702:VAL:HG23	10:N:53:VAL:HG12	1.84	0.59
1:A:535:MET:HE1	1:A:652:GLN:HE22	1.67	0.59
2:B:49:VAL:HG11	2:B:360:ARG:HA	1.84	0.59
3:M:313:THR:HG22	3:M:318:ILE:HG22	1.85	0.59
1:A:583:GLU:CG	1:A:584:ALA:H	2.15	0.59
2:J:63:PHE:CZ	2:J:388:GLU:OE2	2.55	0.59
3:C:216:GLU:O	3:C:220:LYS:N	2.35	0.59
2:J:599:ILE:HD11	2:J:609:LEU:HD11	1.84	0.59
4:D:145:LYS:NZ	11:P:48:ALA:O	2.31	0.59
5:E:80:ARG:HG3	5:E:83:GLU:HB2	1.84	0.59
3:C:216:GLU:O	3:C:220:LYS:CA	2.51	0.59
5:E:46:LEU:HD22	6:F:21:LEU:HD21	1.84	0.59
4:D:151:VAL:HG22	4:D:224:VAL:HG22	1.84	0.59
3:C:148:ARG:H	3:C:148:ARG:HD3	1.68	0.59
1:A:444:PRO:CD	9:L:50:THR:CG2	2.80	0.59
2:B:599:ILE:HD11	2:B:609:LEU:HD11	1.84	0.59
9:U:43:TYR:HB2	9:U:56:ARG:O	2.03	0.59
2:B:389:ASN:ND2	2:B:392:ARG:CG	2.66	0.59
10:N:2:ILE:HD11	10:N:56:ILE:HD12	1.85	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:20:VAL:O	2:J:23:SER:OG	2.18	0.59
1:I:583:GLU:CG	1:I:584:ALA:H	2.16	0.59
1:I:497:GLY:O	1:I:884:GLN:NE2	2.35	0.59
1:I:444:PRO:HG3	9:U:50:THR:HG23	0.59	0.59
3:C:160:VAL:HG21	3:C:198:LEU:HG	1.83	0.59
3:C:189:ALA:HB3	3:C:199:VAL:HA	1.84	0.59
3:M:148:ARG:HH22	3:M:162:GLU:CB	1.82	0.59
2:J:395:ARG:CD	2:J:398:ILE:HD11	2.32	0.58
1:I:147:CYS:H	1:I:152:ALA:CB	2.16	0.58
1:A:150:CYS:C	1:A:152:ALA:H	2.06	0.58
3:C:229:VAL:HG22	3:C:230:GLY:H	1.68	0.58
3:C:298:LEU:H	3:C:298:LEU:HD13	1.68	0.58
1:A:690:ALA:HA	1:A:693:LYS:HD2	1.84	0.58
2:J:470:GLU:OE2	2:J:482:ASN:ND2	2.35	0.58
2:B:79:GLU:HG2	2:B:95:ARG:HH22	1.68	0.58
3:M:128:ARG:HG3	3:M:241:TYR:CE2	2.38	0.58
3:M:331:ALA:H	3:M:336:ARG:HH12	1.51	0.58
3:M:119:TYR:HD2	3:M:263:ARG:HD2	1.68	0.58
3:C:313:THR:HG22	3:C:318:ILE:HG22	1.85	0.58
10:N:7:CYS:SG	10:N:8:PHE:N	2.76	0.58
2:B:205:ILE:HD11	2:B:303:LEU:H	1.67	0.58
1:A:444:PRO:HD3	9:L:50:THR:HG22	1.83	0.58
4:D:160:HIS:ND1	4:D:188:GLU:OE1	2.27	0.58
4:O:16:PHE:CE1	4:O:222:PHE:HB2	2.38	0.58
2:B:1122:ARG:HG3	5:E:60:VAL:HG21	1.84	0.58
1:I:95:VAL:HG22	1:I:201:LEU:HD23	1.83	0.58
4:O:145:LYS:NZ	11:W:48:ALA:O	2.35	0.58
1:I:783:TYR:CE1	2:J:461:THR:HG22	2.38	0.58
2:J:801:PHE:HB2	11:W:40:PRO:HD3	1.84	0.58
3:C:191:PHE:HD2	3:C:198:LEU:HD13	1.68	0.58
1:I:100:CYS:CB	1:I:103:CYS:CB	2.80	0.58
1:I:870:PHE:CE2	7:S:76:TYR:HD2	2.21	0.58
3:M:358:LEU:CD1	14:M:401:HOH:O	2.51	0.58
1:I:163:THR:HB	1:I:276:GLN:HE21	1.69	0.58
3:M:143:LEU:HB2	3:M:222:ARG:HG3	1.84	0.58
3:M:148:ARG:H	3:M:148:ARG:HD3	1.68	0.58
2:J:45:GLY:O	2:J:46:LEU:CB	2.50	0.58
1:A:875:ASP:HB3	7:H:70:ALA:HB2	1.85	0.58
2:J:508:VAL:O	2:J:513:ARG:NH1	2.36	0.58
3:C:343:THR:OG1	3:C:344:GLN:N	2.35	0.58
2:B:766:ARG:HG2	2:B:772:LYS:HG2	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ARG:HH21	1:A:148:PRO:HB2	1.69	0.58
3:M:55:LYS:HE2	8:T:3:ARG:HH22	1.67	0.58
1:I:449:ARG:NH2	9:U:49:ILE:CD1	2.66	0.58
1:I:103:CYS:CB	1:I:150:CYS:SG	2.91	0.58
3:M:229:VAL:HG22	3:M:230:GLY:H	1.69	0.58
2:J:513:ARG:HG2	2:J:514:ARG:N	2.17	0.58
2:B:151:ASP:HB3	2:B:684:ALA:HB3	1.85	0.58
1:A:497:GLY:O	1:A:884:GLN:NE2	2.36	0.58
3:M:154:ILE:H	3:M:154:ILE:HD12	1.69	0.58
3:M:312:MET:HA	3:M:326:ILE:HD11	1.86	0.58
2:B:789:LYS:HD2	1:I:37:ASP:OD1	2.03	0.58
1:A:163:THR:HB	1:A:276:GLN:HE21	1.68	0.58
10:N:19:TYR:HD1	10:N:20:GLU:H	1.52	0.58
3:M:358:LEU:HD11	14:M:401:HOH:O	2.04	0.58
2:J:79:GLU:HG2	2:J:95:ARG:HH22	1.68	0.58
2:B:378:TYR:HE1	2:B:389:ASN:N	2.00	0.58
9:L:46:GLU:OE2	9:L:56:ARG:CD	2.51	0.58
3:C:157:MET:HA	3:C:157:MET:CE	2.33	0.57
3:M:147:ALA:O	3:M:167:ARG:NH2	2.37	0.57
4:O:151:VAL:HG22	4:O:224:VAL:HG22	1.84	0.57
10:V:19:TYR:HD1	10:V:20:GLU:H	1.52	0.57
3:C:161:VAL:HB	3:C:198:LEU:CA	2.33	0.57
5:E:1:MET:HE3	6:F:11:TYR:CE1	2.24	0.57
1:A:13:PHE:CE1	2:B:1115:PRO:HB3	2.39	0.57
10:V:2:ILE:HD11	10:V:56:ILE:HD12	1.85	0.57
4:D:47:PHE:N	11:P:44:ARG:O	2.34	0.57
3:C:128:ARG:HG3	3:C:241:TYR:CE2	2.39	0.57
3:M:182:LEU:HD23	3:M:185:SER:HB2	1.75	0.57
1:I:74:PHE:CE1	1:I:222:PRO:HD3	2.38	0.57
3:C:177:LYS:HA	3:C:180:ARG:HB2	1.85	0.57
2:B:803:GLU:OE2	2:B:871:ARG:NH2	2.36	0.57
1:I:284:ASN:HB3	1:I:287:THR:HG23	1.86	0.57
5:Q:48:ILE:HD13	5:Q:74:VAL:HG13	1.86	0.57
3:C:216:GLU:HA	3:C:220:LYS:CB	2.33	0.57
2:B:749:ARG:HE	4:D:144:ALA:HB1	1.68	0.57
2:B:237:LEU:HD22	2:B:242:GLU:HB3	1.85	0.57
2:J:237:LEU:HD22	2:J:242:GLU:HB3	1.85	0.57
5:Q:49:LEU:N	5:Q:73:ASN:O	2.36	0.57
4:D:226:THR:OG1	4:D:227:ASN:N	2.29	0.57
3:C:147:ALA:O	3:C:167:ARG:NH2	2.37	0.57
3:M:298:LEU:HD13	3:M:298:LEU:H	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:262:THR:HG22	7:S:12:HIS:CG	2.38	0.57
1:I:159:PHE:HB3	1:I:166:TRP:HE3	1.69	0.57
2:J:38:TYR:C	2:J:41:PHE:HB3	2.23	0.57
1:I:146:VAL:HA	1:I:152:ALA:HB3	1.86	0.57
2:B:731:TYR:HE2	2:B:902:PRO:HG3	1.69	0.57
3:M:217:LYS:HD2	3:M:217:LYS:N	2.19	0.57
8:K:12:ILE:HD11	8:K:53:VAL:HG23	1.87	0.57
1:I:858:GLY:O	1:I:871:LYS:HA	2.05	0.57
1:I:156:PRO:HB3	1:I:169:ARG:HA	1.87	0.57
2:J:151:ASP:HB3	2:J:684:ALA:HB3	1.86	0.57
2:B:378:TYR:OH	2:B:388:GLU:CA	2.48	0.57
3:C:161:VAL:HB	3:C:198:LEU:HA	1.87	0.57
2:J:395:ARG:CB	2:J:398:ILE:CD1	2.83	0.57
1:I:105:ARG:HH21	1:I:148:PRO:HB2	1.69	0.57
2:J:816:THR:HB	2:J:836:ARG:HH21	1.70	0.57
2:J:803:GLU:OE2	2:J:871:ARG:NH2	2.36	0.57
8:T:12:ILE:HD11	8:T:53:VAL:HG23	1.87	0.57
1:I:326:PHE:N	2:J:1052:ARG:HH12	2.03	0.57
1:I:527:GLU:OE2	9:U:41:ALA:N	2.37	0.57
10:N:56:ILE:O	10:N:60:MET:HG3	2.05	0.57
5:E:92:MET:CE	5:E:127:PHE:HD2	2.05	0.57
1:A:709:LEU:HB2	1:A:717:THR:HG22	1.87	0.57
1:A:640:GLU:HG2	1:A:896:ARG:HH12	1.68	0.57
1:A:284:ASN:HB3	1:A:287:THR:HG23	1.86	0.57
2:B:816:THR:HB	2:B:836:ARG:HH21	1.70	0.57
4:D:50:ASN:H	11:P:39:ARG:HD3	1.70	0.57
3:C:114:PRO:HG2	3:C:247:GLY:HA2	1.86	0.57
1:I:445:TYR:CZ	9:U:49:ILE:HG22	2.40	0.56
1:A:750:MET:HA	1:A:753:THR:HG21	1.87	0.56
1:A:885:GLY:HA2	3:C:303:ARG:HH12	1.70	0.56
2:J:211:LYS:HA	3:M:212:ARG:HH21	1.70	0.56
1:I:709:LEU:HB2	1:I:717:THR:HG22	1.87	0.56
1:I:635:ASP:O	1:I:639:ARG:HG3	2.05	0.56
3:C:153:ASP:OD1	3:C:159:TYR:HA	2.05	0.56
1:I:105:ARG:NH2	1:I:148:PRO:HB2	2.20	0.56
1:I:624:LYS:O	1:I:632:LYS:HB3	2.05	0.56
2:J:688:ILE:HD11	10:V:62:TYR:CD1	2.40	0.56
2:J:747:ILE:HG23	2:J:876:PRO:HG2	1.88	0.56
4:O:119:PRO:HD2	10:V:15:ALA:HB1	1.86	0.56
1:A:858:GLY:O	1:A:871:LYS:HA	2.05	0.56
1:I:356:PRO:HG3	1:I:473:GLN:HB3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:58:PRO:HG2	2:J:60:ILE:O	2.05	0.56
3:C:92:ILE:HG13	3:C:93:ASN:H	1.70	0.56
10:V:22:LYS:NZ	10:V:54:GLU:HG2	2.21	0.56
4:D:28:ALA:HB1	4:D:243:LEU:HD21	1.87	0.56
2:J:766:ARG:HG2	2:J:772:LYS:HG2	1.87	0.56
2:B:864:LYS:HG3	11:P:25:VAL:HG11	1.88	0.56
2:J:1088:GLU:OE2	5:Q:40:ARG:HB2	2.05	0.56
3:M:214:ILE:C	3:M:216:GLU:H	2.08	0.56
2:B:58:PRO:HG2	2:B:60:ILE:O	2.05	0.56
3:C:162:GLU:O	3:C:196:TYR:HA	2.05	0.56
2:J:1122:ARG:HD2	6:R:4:ARG:NH2	2.21	0.56
2:B:899:GLU:N	2:B:899:GLU:OE1	2.32	0.56
1:A:74:PHE:CE1	1:A:222:PRO:HD3	2.40	0.56
3:C:312:MET:HA	3:C:326:ILE:HD11	1.86	0.56
2:J:1063:TRP:NE1	2:J:1074:GLU:OE1	2.39	0.56
3:C:119:TYR:CD2	3:C:263:ARG:HB3	2.41	0.56
3:C:119:TYR:HD2	3:C:263:ARG:HB3	1.70	0.56
1:A:769:LEU:HB2	1:A:804:VAL:HG21	1.87	0.56
2:B:65:VAL:HG11	2:B:395:ARG:HH12	1.71	0.56
3:C:160:VAL:HG21	3:C:198:LEU:HD23	1.86	0.56
1:A:150:CYS:SG	1:A:153:PRO:HD3	2.45	0.56
4:O:28:ALA:HB1	4:O:243:LEU:HD21	1.87	0.56
1:A:150:CYS:O	1:A:151:GLY:C	2.44	0.56
2:B:854:VAL:HG13	2:B:868:VAL:HG22	1.87	0.56
3:C:153:ASP:HB2	3:C:158:GLU:C	2.26	0.56
1:I:309:LYS:HE3	3:M:347:PHE:HB2	1.88	0.56
1:I:632:LYS:HD3	1:I:633:LEU:H	1.71	0.56
2:J:986:ASP:C	2:J:987:ILE:HD13	2.26	0.56
3:M:55:LYS:HG2	8:T:3:ARG:HH21	1.70	0.56
1:I:112:GLU:O	1:I:116:TYR:HB2	2.06	0.56
2:B:76:GLU:HG2	2:B:86:PRO:HA	1.88	0.56
2:B:747:ILE:HG23	2:B:876:PRO:HG2	1.88	0.56
1:I:513:LEU:HD13	1:I:664:LYS:HZ2	1.71	0.56
2:J:1042:GLY:O	3:M:70:GLN:NE2	2.35	0.56
2:B:959:LYS:HA	4:D:201:ARG:NH2	2.21	0.56
3:M:111:PRO:HG3	3:M:268:ASN:HA	1.88	0.56
1:A:387:PRO:HD3	1:A:410:TRP:CD1	2.41	0.56
1:A:112:GLU:O	1:A:116:TYR:HB2	2.05	0.56
2:B:683:TRP:O	2:B:683:TRP:HD1	1.89	0.56
2:J:521:ARG:H	2:J:531:THR:HG22	1.71	0.56
1:A:159:PHE:HB3	1:A:166:TRP:HE3	1.69	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:22:LYS:NZ	10:N:54:GLU:HG2	2.21	0.56
2:B:206:THR:OG1	2:B:218:THR:OG1	2.19	0.56
2:B:815:ARG:HD2	2:B:839:THR:HB	1.88	0.55
1:I:10:SER:HA	3:M:358:LEU:HD21	1.87	0.55
2:J:719:PRO:HG3	10:V:53:VAL:HG11	1.88	0.55
3:M:114:PRO:HG2	3:M:247:GLY:HA2	1.87	0.55
5:E:48:ILE:HD13	5:E:74:VAL:HG13	1.88	0.55
2:J:394:VAL:HG11	2:J:395:ARG:HE	1.72	0.55
2:J:39:ASN:O	2:J:41:PHE:N	2.39	0.55
1:A:452:LEU:HD13	2:B:736:MET:SD	2.46	0.55
1:I:625:ALA:O	1:I:632:LYS:NZ	2.21	0.55
3:C:181:LYS:HE3	3:C:188:SER:HB3	1.87	0.55
2:B:606:TRP:CZ2	2:B:615:ILE:HG21	2.41	0.55
1:A:640:GLU:HG2	1:A:896:ARG:NH1	2.22	0.55
5:E:92:MET:HE3	5:E:127:PHE:CD2	2.23	0.55
2:B:967:LYS:HG3	2:B:969:SER:H	1.71	0.55
2:B:227:LYS:HB2	2:B:230:TYR:CD2	2.42	0.55
5:Q:46:LEU:HD22	6:R:21:LEU:HD21	1.87	0.55
2:J:854:VAL:HG13	2:J:868:VAL:HG22	1.87	0.55
4:D:16:PHE:CE1	4:D:222:PHE:HB2	2.41	0.55
3:C:27:LYS:O	3:C:31:TYR:HB2	2.06	0.55
2:J:967:LYS:HG3	2:J:969:SER:H	1.71	0.55
4:O:160:HIS:ND1	4:O:188:GLU:OE1	2.27	0.55
3:C:119:TYR:HD2	3:C:263:ARG:HD2	1.70	0.55
1:I:844:ARG:NH2	3:M:106:ASP:OD2	2.39	0.55
2:J:227:LYS:HB2	2:J:230:TYR:CD2	2.42	0.55
1:I:769:LEU:HB2	1:I:804:VAL:HG21	1.87	0.55
2:B:59:ASP:H	2:B:375:THR:HG22	1.72	0.55
2:B:449:ASP:N	2:B:449:ASP:OD1	2.39	0.55
2:J:968:HIS:ND1	4:O:201:ARG:HG2	2.21	0.55
2:J:1063:TRP:CE2	2:J:1094:LYS:HG3	2.41	0.55
1:A:105:ARG:NH2	1:A:148:PRO:HB2	2.22	0.55
2:J:41:PHE:O	2:J:45:GLY:C	2.44	0.55
2:J:286:PRO:O	2:J:288:GLU:N	2.40	0.55
2:J:606:TRP:CZ2	2:J:615:ILE:HG21	2.42	0.55
2:J:1066:GLU:HG2	2:J:1119:LEU:HD13	1.89	0.55
1:I:387:PRO:HD3	1:I:410:TRP:CD1	2.42	0.55
3:C:160:VAL:HG21	3:C:198:LEU:CD2	2.37	0.55
3:M:151:THR:C	3:M:152:ILE:HG12	2.27	0.55
2:J:815:ARG:HD2	2:J:839:THR:HB	1.89	0.55
1:I:640:GLU:HG2	1:I:896:ARG:HH12	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ILE:HG23	1:A:108:LEU:HB2	1.89	0.55
2:J:513:ARG:HG2	2:J:514:ARG:H	1.70	0.55
2:B:466:ILE:HG21	2:B:481:LYS:HD2	1.88	0.55
1:A:513:LEU:HD13	1:A:664:LYS:HZ2	1.71	0.55
1:I:450:LEU:HD11	1:I:454:VAL:HB	1.89	0.55
2:J:449:ASP:OD1	2:J:449:ASP:N	2.39	0.55
2:B:878:LEU:HD23	2:B:892:ILE:HG22	1.89	0.55
1:A:635:ASP:O	1:A:639:ARG:HG3	2.05	0.55
1:A:450:LEU:HD11	1:A:454:VAL:HB	1.89	0.55
1:I:856:TYR:CE1	8:T:55:ARG:HD3	2.41	0.55
2:J:899:GLU:HG2	4:O:35:SER:HB3	1.89	0.55
2:J:211:LYS:HG3	3:M:212:ARG:CZ	2.37	0.55
2:B:95:ARG:CZ	11:P:33:LYS:HD3	2.36	0.55
3:M:75:PRO:HB3	3:M:298:LEU:HG	1.88	0.55
2:J:76:GLU:HG2	2:J:86:PRO:HA	1.89	0.55
3:C:151:THR:CG2	3:C:152:ILE:H	2.18	0.54
2:B:986:ASP:C	2:B:987:ILE:HD13	2.28	0.54
1:I:783:TYR:HE1	2:J:461:THR:HG22	1.71	0.54
2:J:466:ILE:HG21	2:J:481:LYS:HD2	1.88	0.54
2:B:1063:TRP:NE1	2:B:1094:LYS:CG	2.69	0.54
7:S:43:ILE:N	7:S:78:LEU:O	2.28	0.54
5:Q:8:LYS:HG3	6:R:7:LEU:HD22	1.89	0.54
1:I:585:LEU:O	1:I:586:GLU:CB	2.54	0.54
2:J:683:TRP:O	2:J:683:TRP:HD1	1.89	0.54
2:B:183:ARG:NH1	2:B:337:GLU:OE1	2.40	0.54
2:J:183:ARG:HG3	2:J:337:GLU:CD	2.26	0.54
3:C:181:LYS:C	3:C:183:THR:H	2.09	0.54
2:J:559:LEU:HD22	2:J:568:VAL:HG22	1.90	0.54
2:J:59:ASP:H	2:J:375:THR:HG22	1.72	0.54
2:J:183:ARG:HB3	2:J:186:ARG:NH2	2.13	0.54
2:B:34:HIS:HB3	2:B:129:MET:HE1	1.88	0.54
3:C:380:LEU:HB2	5:E:59:ILE:HB	1.88	0.54
9:U:9:GLU:HB2	9:U:12:LEU:HD22	1.90	0.54
9:U:45:ILE:HG12	9:U:55:PRO:HA	1.88	0.54
2:J:42:ILE:HG22	2:J:72:ILE:CD1	2.36	0.54
7:H:67:SER:N	7:H:71:GLY:O	2.28	0.54
2:J:1063:TRP:NE1	2:J:1094:LYS:HE3	2.23	0.54
3:C:161:VAL:CG2	3:C:199:VAL:HB	2.36	0.54
1:A:13:PHE:CE2	3:C:333:VAL:HG21	2.43	0.54
2:J:962:GLU:O	2:J:965:GLY:N	2.37	0.54
1:I:106:ILE:HG23	1:I:108:LEU:HB2	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:578:GLU:HB3	1:I:579:PRO:HD2	1.88	0.54
3:M:27:LYS:O	3:M:31:TYR:HB2	2.06	0.54
1:A:10:SER:HA	3:C:358:LEU:CD2	2.28	0.54
2:J:959:LYS:HA	4:O:201:ARG:HH21	1.73	0.54
4:D:50:ASN:N	11:P:39:ARG:HH11	2.05	0.54
3:C:75:PRO:HB3	3:C:298:LEU:HG	1.88	0.54
2:J:391:GLN:C	2:J:392:ARG:HG3	2.26	0.54
2:J:182:GLU:N	2:J:191:VAL:O	2.39	0.54
2:B:1063:TRP:HE1	2:B:1094:LYS:CE	2.19	0.54
2:B:939:LEU:HD11	2:B:966:PHE:CD2	2.39	0.54
1:I:61:GLU:O	1:I:63:CYS:N	2.36	0.54
2:B:521:ARG:H	2:B:531:THR:HG22	1.72	0.54
9:U:50:THR:O	9:U:51:MET:HB2	2.08	0.54
1:A:867:ILE:HD13	1:A:870:PHE:HE1	1.73	0.54
1:I:842:GLN:NE2	3:M:70:GLN:HA	2.23	0.54
1:A:361:GLU:HG2	1:A:408:ILE:HD11	1.90	0.54
1:I:609:VAL:HG13	1:I:619:GLY:HA3	1.90	0.54
3:C:111:PRO:HG3	3:C:268:ASN:HA	1.89	0.54
3:M:153:ASP:CG	3:M:157:MET:HB2	2.28	0.54
3:M:279:GLU:HG3	7:S:63:ILE:HG21	1.90	0.54
1:A:308:LEU:HD12	1:A:309:LYS:HG3	1.89	0.54
2:J:793:HIS:NE2	2:J:805:LYS:O	2.40	0.54
2:B:793:HIS:NE2	2:B:805:LYS:O	2.41	0.54
2:B:227:LYS:HB2	2:B:230:TYR:HD2	1.73	0.54
1:I:397:SER:OG	1:I:398:ASN:N	2.40	0.54
1:I:837:GLN:HB3	3:M:102:ILE:HD11	1.90	0.54
1:A:396:GLU:HB3	1:I:40:TYR:OH	2.08	0.53
3:M:262:THR:HG22	7:S:12:HIS:CD2	2.43	0.53
1:I:326:PHE:HB2	2:J:1052:ARG:HH22	1.73	0.53
9:L:9:GLU:HB2	9:L:12:LEU:HD22	1.90	0.53
2:J:438:HIS:HD2	2:J:441:ARG:HE	1.55	0.53
3:C:191:PHE:CD2	3:C:198:LEU:HD22	2.43	0.53
2:B:183:ARG:HB2	2:B:186:ARG:NH2	2.14	0.53
10:N:56:ILE:O	10:N:60:MET:HE3	2.08	0.53
2:B:286:PRO:O	2:B:288:GLU:N	2.40	0.53
1:A:8:ILE:HD13	3:C:367:ILE:HD11	1.90	0.53
1:A:326:PHE:HA	2:B:1008:ARG:O	2.09	0.53
2:J:878:LEU:HD23	2:J:892:ILE:HG22	1.90	0.53
2:J:1076:LYS:O	2:J:1078:ARG:N	2.41	0.53
3:M:266:THR:HG22	3:M:268:ASN:H	1.73	0.53
2:B:1066:GLU:HG2	2:B:1119:LEU:HD13	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:SER:OG	1:A:398:ASN:N	2.41	0.53
11:P:11:CYS:SG	11:P:30:CYS:SG	3.05	0.53
2:B:182:GLU:N	2:B:191:VAL:O	2.40	0.53
2:J:800:ILE:HD11	2:J:812:LEU:HD23	1.90	0.53
1:A:49:LYS:HG3	1:A:50:ARG:HH21	1.74	0.53
3:C:266:THR:HG22	3:C:268:ASN:H	1.73	0.53
3:C:369:GLN:HG3	3:C:370:PRO:HD2	1.90	0.53
3:C:194:GLU:C	3:C:196:TYR:H	2.11	0.53
1:A:667:THR:HG23	2:B:971:ARG:HH21	1.73	0.53
11:W:47:LYS:HB3	11:W:49:ILE:HG13	1.90	0.53
3:C:192:GLU:OE1	3:C:197:THR:HG23	2.09	0.53
2:B:392:ARG:O	2:B:392:ARG:HG2	2.07	0.53
3:C:161:VAL:CG1	3:C:162:GLU:H	2.05	0.53
2:J:1122:ARG:HH11	6:R:4:ARG:NH2	2.07	0.53
2:J:939:LEU:HD11	2:J:966:PHE:CD2	2.39	0.53
2:J:227:LYS:HB2	2:J:230:TYR:HD2	1.73	0.53
1:A:8:ILE:HG13	2:B:1095:VAL:HG11	1.91	0.53
4:D:143:HIS:NE2	11:P:49:ILE:O	2.41	0.53
2:B:299:ASP:HB3	2:B:308:VAL:O	2.09	0.53
1:A:127:LYS:HB2	3:C:330:LYS:HB3	1.91	0.53
4:D:3:GLU:HG3	4:D:19:SER:HB2	1.91	0.53
1:I:462:PHE:O	1:I:464:GLY:N	2.42	0.53
2:B:65:VAL:HG21	2:B:395:ARG:HH12	1.74	0.53
1:A:156:PRO:HG3	1:A:169:ARG:HG3	1.90	0.53
1:A:194:PRO:HB2	1:A:196:LYS:HD2	1.91	0.53
3:M:375:THR:O	3:M:378:VAL:HG12	2.09	0.53
1:A:609:VAL:HG13	1:A:619:GLY:HA3	1.91	0.53
1:A:329:ARG:O	2:B:1005:MET:HA	2.08	0.53
1:I:665:GLY:C	2:J:729:LEU:CD1	2.75	0.53
4:D:62:ARG:HH12	10:N:2:ILE:HD12	1.74	0.53
2:B:962:GLU:O	2:B:965:GLY:N	2.38	0.53
2:B:273:ALA:HA	2:B:276:TYR:CD2	2.44	0.53
2:B:800:ILE:HD11	2:B:812:LEU:HD23	1.90	0.53
1:A:462:PHE:O	1:A:464:GLY:N	2.40	0.53
2:B:1054:LEU:HD22	2:B:1059:LYS:HE3	1.91	0.53
2:J:299:ASP:HB3	2:J:308:VAL:O	2.09	0.53
2:B:438:HIS:HD2	2:B:441:ARG:HE	1.55	0.53
1:I:344:GLY:HA3	1:I:449:ARG:HB2	1.91	0.53
1:I:444:PRO:CD	9:U:50:THR:CG2	2.78	0.53
1:I:194:PRO:HB2	1:I:196:LYS:HD2	1.91	0.53
2:J:968:HIS:CD2	2:J:968:HIS:C	2.82	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:959:LYS:HA	4:O:201:ARG:NH2	2.24	0.53
1:A:404:GLU:O	1:A:406:LEU:N	2.41	0.53
2:J:1054:LEU:HD22	2:J:1059:LYS:HE3	1.91	0.53
2:B:390:ILE:C	2:B:392:ARG:N	2.60	0.53
2:J:392:ARG:C	2:J:394:VAL:N	2.63	0.53
3:M:153:ASP:CB	3:M:157:MET:CB	2.87	0.53
9:L:52:ALA:C	9:L:54:LYS:H	2.13	0.53
3:C:348:ALA:O	3:C:351:GLU:HG2	2.08	0.53
2:J:273:ALA:HA	2:J:276:TYR:CD2	2.44	0.53
3:M:216:GLU:O	3:M:221:HIS:N	2.42	0.53
2:J:116:GLN:CD	2:J:393:PHE:CD1	2.69	0.52
3:C:262:THR:HG22	7:H:12:HIS:CG	2.44	0.52
4:O:3:GLU:HG3	4:O:19:SER:HB2	1.91	0.52
1:I:361:GLU:HG2	1:I:408:ILE:HD11	1.90	0.52
2:J:729:LEU:HD23	2:J:730:SER:N	2.24	0.52
3:M:153:ASP:OD2	3:M:157:MET:HG3	2.09	0.52
3:M:156:ASN:O	3:M:158:GLU:HG2	2.09	0.52
1:A:753:THR:CG2	1:A:754:GLY:H	2.09	0.52
2:B:1063:TRP:CE3	2:B:1074:GLU:HG2	2.44	0.52
1:I:867:ILE:HD11	7:S:40:LEU:HD22	1.91	0.52
1:I:633:LEU:O	1:I:636:ILE:HG12	2.10	0.52
2:J:749:ARG:HE	4:O:144:ALA:HB1	1.74	0.52
2:B:559:LEU:HD22	2:B:568:VAL:HG22	1.90	0.52
1:A:264:PRO:HB2	1:A:267:ILE:HD13	1.91	0.52
1:A:808:TYR:HE2	2:B:923:MET:SD	2.32	0.52
1:A:156:PRO:HB3	1:A:169:ARG:HA	1.90	0.52
4:D:62:ARG:HH22	10:N:2:ILE:HB	1.73	0.52
1:A:630:ASP:HB2	1:A:632:LYS:HE2	1.92	0.52
3:C:178:VAL:O	3:C:181:LYS:HB3	2.09	0.52
1:A:344:GLY:HA3	1:A:449:ARG:HB2	1.91	0.52
3:M:369:GLN:HG3	3:M:370:PRO:HD2	1.92	0.52
4:O:163:LYS:HG2	4:O:168:TRP:CE2	2.44	0.52
1:I:264:PRO:HB2	1:I:267:ILE:HD13	1.91	0.52
5:Q:82:GLN:HB3	6:R:98:LYS:HG3	1.90	0.52
2:B:373:GLN:HG2	2:B:397:SER:HB2	1.91	0.52
3:M:197:THR:HG22	3:M:198:LEU:N	2.24	0.52
4:O:62:ARG:HH22	10:V:2:ILE:HB	1.72	0.52
3:C:192:GLU:HG3	3:C:197:THR:OG1	2.10	0.52
3:M:322:GLY:O	3:M:324:HIS:N	2.42	0.52
3:C:73:GLY:O	3:C:76:SER:OG	2.27	0.52
2:B:94:ILE:HG21	11:P:34:ILE:HG12	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:163:LYS:HG2	4:D:168:TRP:CE2	2.44	0.52
2:J:373:GLN:CG	2:J:397:SER:HB2	2.40	0.52
2:B:1063:TRP:CE3	2:B:1074:GLU:CG	2.93	0.52
2:B:702:VAL:HG23	10:N:53:VAL:CG1	2.40	0.52
2:B:467:CYS:SG	2:B:470:GLU:HB2	2.49	0.52
2:J:462:HIS:HB3	2:J:466:ILE:HB	1.92	0.52
1:I:852:LEU:HD11	3:M:311:MET:HG3	1.91	0.52
3:M:348:ALA:O	3:M:351:GLU:HG2	2.10	0.52
3:C:148:ARG:N	3:C:148:ARG:HD3	2.25	0.52
3:C:160:VAL:HG22	3:C:198:LEU:HG	1.91	0.52
1:A:872:TYR:CE1	3:C:64:VAL:HG11	2.45	0.52
2:J:962:GLU:HA	2:J:966:PHE:O	2.09	0.52
2:J:467:CYS:SG	2:J:470:GLU:HB2	2.50	0.52
1:I:156:PRO:HG3	1:I:169:ARG:HG3	1.92	0.52
1:I:842:GLN:HE21	3:M:70:GLN:HA	1.75	0.52
5:E:2:TYR:HH	6:F:44:SER:HG	1.54	0.52
1:A:187:ARG:NE	1:A:211:GLU:O	2.42	0.52
9:U:49:ILE:C	9:U:50:THR:HG1	2.00	0.52
3:C:161:VAL:H	3:C:199:VAL:H	1.56	0.52
2:J:731:TYR:CE2	2:J:902:PRO:HG3	2.44	0.52
3:M:152:ILE:HG23	3:M:160:VAL:N	2.23	0.52
3:C:104:ILE:HD13	3:C:289:ILE:HG12	1.92	0.52
1:I:431:HIS:HA	3:M:70:GLN:HB3	1.91	0.52
2:B:782:ILE:HG22	2:B:783:GLN:H	1.74	0.52
2:B:888:GLN:NE2	2:B:918:GLY:O	2.43	0.52
2:B:557:VAL:HG22	2:B:570:ILE:HG23	1.92	0.52
1:A:295:HIS:O	1:A:297:SER:N	2.43	0.52
2:B:395:ARG:O	2:B:397:SER:N	2.41	0.52
2:J:730:SER:HB3	2:J:915:ASN:ND2	2.25	0.52
2:J:41:PHE:CE2	2:J:356:LYS:HG2	2.45	0.52
3:C:155:LEU:CD2	3:C:156:ASN:ND2	2.73	0.52
3:C:196:TYR:O	3:C:198:LEU:HD12	2.10	0.52
2:J:1122:ARG:CD	6:R:4:ARG:NH2	2.72	0.52
2:B:968:HIS:C	2:B:968:HIS:CD2	2.82	0.52
1:I:834:ARG:HD2	3:M:98:LEU:HD13	1.92	0.52
2:B:808:GLY:O	2:B:843:VAL:HG12	2.10	0.52
2:J:469:THR:HG21	2:J:668:ASN:HB3	1.92	0.52
3:C:322:GLY:O	3:C:324:HIS:N	2.42	0.52
1:I:445:TYR:HB2	1:I:449:ARG:NH2	2.25	0.51
2:J:107:MET:CA	2:J:395:ARG:HH22	2.20	0.51
1:I:150:CYS:HB3	1:I:153:PRO:HD3	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:P:11:CYS:SG	11:P:14:GLU:OE2	2.68	0.51
2:B:467:CYS:SG	2:B:651:GLY:N	2.78	0.51
2:B:462:HIS:HB3	2:B:466:ILE:HB	1.91	0.51
2:J:888:GLN:NE2	2:J:918:GLY:O	2.43	0.51
1:A:195:ASP:HB3	1:A:205:PRO:HB3	1.92	0.51
2:J:557:VAL:HG22	2:J:570:ILE:HG23	1.92	0.51
3:C:160:VAL:CG2	3:C:198:LEU:CB	2.88	0.51
1:A:508:ILE:HG21	1:A:754:GLY:O	2.10	0.51
3:C:358:LEU:CD1	3:C:359:ASN:H	2.23	0.51
1:I:309:LYS:CE	3:M:347:PHE:HB2	2.40	0.51
7:S:67:SER:N	7:S:71:GLY:O	2.26	0.51
2:J:361:VAL:O	2:J:365:GLN:HG2	2.10	0.51
3:C:203:LYS:NZ	3:C:203:LYS:HB2	2.23	0.51
3:M:104:ILE:HD13	3:M:289:ILE:HG12	1.92	0.51
1:I:849:LEU:O	3:M:65:GLY:HA3	2.09	0.51
2:B:1048:LEU:O	2:B:1051:GLU:HB3	2.10	0.51
2:B:1063:TRP:O	2:B:1072:ALA:N	2.35	0.51
7:S:61:ILE:HG22	7:S:63:ILE:HG13	1.93	0.51
3:C:124:HIS:ND1	3:C:130:LYS:HB3	2.25	0.51
3:C:187:LYS:HD3	3:C:203:LYS:HZ2	1.74	0.51
2:J:982:ARG:HD3	4:O:155:TYR:CD2	2.45	0.51
2:J:789:LYS:HE2	2:J:792:ARG:HB2	1.93	0.51
3:M:119:TYR:CD2	3:M:263:ARG:HB3	2.45	0.51
1:A:356:PRO:HG3	1:A:473:GLN:HB3	1.90	0.51
2:B:390:ILE:HD12	2:B:391:GLN:HB2	1.92	0.51
5:E:9:ASP:OD1	6:F:4:ARG:HG2	2.09	0.51
3:C:217:LYS:O	3:C:218:VAL:HB	2.10	0.51
3:C:216:GLU:C	3:C:220:LYS:HB3	2.31	0.51
2:B:361:VAL:O	2:B:365:GLN:HG2	2.11	0.51
3:M:124:HIS:ND1	3:M:130:LYS:HB3	2.25	0.51
2:B:962:GLU:HA	2:B:966:PHE:O	2.09	0.51
2:J:782:ILE:HG22	2:J:783:GLN:H	1.74	0.51
2:J:414:GLY:O	2:J:422:GLY:N	2.44	0.51
1:A:101:ARG:O	1:A:102:GLU:HB2	2.10	0.51
2:B:389:ASN:HD22	2:B:392:ARG:CB	2.19	0.51
9:U:51:MET:CA	9:U:52:ALA:HB3	2.41	0.51
3:C:216:GLU:HA	3:C:220:LYS:HB2	1.93	0.51
3:M:187:LYS:NZ	3:M:201:ARG:HB3	2.26	0.51
5:E:81:ASN:C	5:E:82:GLN:HG2	2.31	0.51
7:H:61:ILE:HG22	7:H:63:ILE:HG13	1.93	0.51
3:C:375:THR:O	3:C:378:VAL:HG12	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:783:TYR:HE2	1:A:789:THR:HB	1.74	0.51
1:A:99:THR:HG21	1:A:193:ILE:HD11	1.93	0.51
1:I:445:TYR:CE1	9:U:49:ILE:HG21	2.46	0.51
1:I:49:LYS:HG3	1:I:50:ARG:HH21	1.75	0.51
1:I:867:ILE:HD13	1:I:870:PHE:HE1	1.76	0.51
2:B:812:LEU:HD11	2:B:843:VAL:HG23	1.93	0.51
5:E:39:ASP:O	5:E:43:GLY:N	2.43	0.51
1:I:113:ILE:HG23	1:I:200:LEU:HD11	1.92	0.51
1:A:113:ILE:HG23	1:A:200:LEU:HD11	1.93	0.51
3:C:161:VAL:HG21	3:C:199:VAL:HG23	0.51	0.51
10:N:56:ILE:C	10:N:60:MET:HE3	2.31	0.51
10:N:10:CYS:O	10:N:12:LYS:HG2	2.10	0.51
3:M:119:TYR:HD2	3:M:263:ARG:HB3	1.76	0.51
2:B:885:ARG:HD2	2:B:993:TYR:HB3	1.92	0.51
2:J:885:ARG:HD2	2:J:993:TYR:HB3	1.92	0.51
1:I:308:LEU:HD12	1:I:309:LYS:HG3	1.93	0.51
3:M:186:PHE:O	3:M:187:LYS:HB3	2.11	0.51
2:B:899:GLU:HG2	4:D:35:SER:HB3	1.92	0.51
4:O:26:ALA:HB1	4:O:222:PHE:HZ	1.74	0.51
2:J:459:HIS:ND1	2:J:461:THR:HG23	2.26	0.51
4:D:26:ALA:HB1	4:D:222:PHE:HZ	1.76	0.51
1:I:544:ASP:OD2	1:I:551:PRO:HB2	2.11	0.51
1:I:531:MET:CB	9:U:44:THR:CG2	2.85	0.51
2:J:378:TYR:HE1	2:J:388:GLU:CG	1.93	0.51
7:S:25:GLU:O	7:S:29:LEU:HB2	2.11	0.51
2:J:899:GLU:N	2:J:899:GLU:OE1	2.32	0.51
10:V:2:ILE:HG12	10:V:56:ILE:HG21	1.93	0.51
5:E:42:GLU:HG3	6:F:2:ILE:HG12	1.92	0.51
3:M:148:ARG:HD3	3:M:148:ARG:N	2.26	0.50
2:J:352:GLY:O	2:J:356:LYS:HG3	2.12	0.50
5:E:8:LYS:HG3	6:F:7:LEU:HD22	1.93	0.50
5:E:6:LYS:O	6:F:7:LEU:HD23	2.10	0.50
3:C:279:GLU:HG3	7:H:63:ILE:HG21	1.93	0.50
1:A:61:GLU:O	1:A:63:CYS:N	2.36	0.50
4:D:171:LEU:HD21	4:D:200:PRO:HD2	1.93	0.50
2:B:789:LYS:HE2	2:B:792:ARG:HB2	1.92	0.50
1:I:101:ARG:O	1:I:102:GLU:HB2	2.11	0.50
2:B:326:LYS:HD2	2:B:335:ARG:HE	1.76	0.50
2:B:607:SER:O	2:B:610:ILE:HG13	2.12	0.50
1:A:21:ILE:HD11	2:B:1112:VAL:HG23	1.92	0.50
2:B:554:VAL:HA	2:B:578:ARG:HH12	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1063:TRP:CZ2	2:B:1094:LYS:CE	2.89	0.50
3:M:337:ALA:HA	3:M:346:LEU:HB2	1.93	0.50
2:J:458:LEU:HD11	2:J:468:PRO:HA	1.92	0.50
1:I:83:VAL:HG13	1:I:276:GLN:OE1	2.10	0.50
2:B:70:ILE:HG12	2:B:105:LEU:HG	1.94	0.50
2:J:70:ILE:HG12	2:J:105:LEU:HG	1.94	0.50
6:R:18:LYS:HD2	6:R:49:GLU:HA	1.94	0.50
2:B:458:LEU:HD11	2:B:468:PRO:HA	1.93	0.50
2:J:429:ARG:HB3	2:J:683:TRP:HZ3	1.76	0.50
2:B:429:ARG:HB3	2:B:683:TRP:HZ3	1.76	0.50
1:A:755:ALA:HB1	2:B:917:HIS:CD2	2.46	0.50
2:J:1042:GLY:C	3:M:70:GLN:HE22	2.13	0.50
3:M:178:VAL:HB	3:M:190:GLU:OE2	2.10	0.50
3:M:38:LYS:HG2	3:M:41:GLU:HG3	1.92	0.50
1:A:578:GLU:HB3	1:A:579:PRO:HD2	1.92	0.50
2:B:63:PHE:CG	2:B:392:ARG:NH2	2.80	0.50
1:I:9:GLY:HA3	2:J:1120:LYS:CB	2.39	0.50
2:J:24:TYR:HB2	2:J:606:TRP:NE1	2.27	0.50
3:C:38:LYS:HG2	3:C:41:GLU:HG3	1.92	0.50
2:B:1087:GLY:O	2:B:1089:ASP:N	2.32	0.50
5:E:15:PRO:HB2	8:K:24:ALA:HB2	1.92	0.50
2:B:312:ASN:H	2:B:312:ASN:HD22	1.59	0.50
2:B:390:ILE:CG1	2:B:391:GLN:H	2.24	0.50
2:J:373:GLN:HG2	2:J:397:SER:HB2	1.93	0.50
1:I:308:LEU:HD13	3:M:346:LEU:HD11	1.93	0.50
1:A:633:LEU:O	1:A:636:ILE:HG12	2.11	0.50
4:O:171:LEU:HD21	4:O:200:PRO:HD2	1.94	0.50
2:J:192:ALA:HB3	2:J:207:VAL:HG23	1.94	0.50
1:I:359:VAL:HG22	1:I:408:ILE:HA	1.94	0.50
2:B:50:VAL:HG11	2:B:70:ILE:HG13	1.93	0.50
2:J:779:SER:O	2:J:781:ASN:N	2.44	0.50
1:A:63:CYS:O	1:A:65:ALA:N	2.45	0.50
2:J:808:GLY:O	2:J:843:VAL:HG12	2.10	0.50
2:B:464:GLY:HA3	2:B:579:ARG:HD3	1.94	0.50
1:I:187:ARG:NE	1:I:211:GLU:O	2.42	0.50
1:I:505:GLN:OE1	2:J:737:GLU:N	2.40	0.50
2:B:708:ARG:H	2:B:947:THR:HG1	1.56	0.50
2:J:724:PHE:CD1	2:J:994:TYR:HB2	2.47	0.50
1:A:81:ARG:HG3	1:A:82:PRO:HD2	1.94	0.50
2:B:378:TYR:OH	2:B:388:GLU:CB	2.60	0.50
2:J:312:ASN:H	2:J:312:ASN:HD22	1.60	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:803:GLU:O	11:P:44:ARG:NE	2.45	0.50
1:I:204:HIS:ND1	1:I:205:PRO:HD2	2.27	0.50
2:B:1062:VAL:HG11	2:B:1071:LEU:HD13	1.94	0.50
9:U:51:MET:HA	9:U:52:ALA:CB	2.41	0.50
2:J:368:LYS:O	2:J:371:GLN:HB3	2.12	0.50
5:Q:3:LYS:HD2	6:R:11:TYR:CE1	2.47	0.50
7:H:25:GLU:O	7:H:29:LEU:HB2	2.11	0.50
2:J:464:GLY:HA3	2:J:579:ARG:HD3	1.94	0.50
1:I:195:ASP:HB3	1:I:205:PRO:HB3	1.92	0.50
1:I:99:THR:HG21	1:I:193:ILE:HD11	1.93	0.50
5:Q:146:ILE:HA	5:Q:163:MET:HG2	1.94	0.50
2:J:856:VAL:HG22	2:J:866:VAL:HG22	1.94	0.50
1:I:238:GLU:HG2	1:I:242:THR:HB	1.94	0.50
2:B:469:THR:HG21	2:B:668:ASN:HB3	1.93	0.50
2:J:1062:VAL:HG11	2:J:1071:LEU:HD13	1.93	0.50
2:B:111:VAL:O	2:B:114:ILE:HG12	2.11	0.50
3:C:162:GLU:HB3	3:C:163:ILE:HD13	1.94	0.50
2:J:812:LEU:HD11	2:J:843:VAL:HG23	1.92	0.50
2:B:24:TYR:HB2	2:B:606:TRP:NE1	2.27	0.50
2:J:659:TYR:HB3	2:J:662:HIS:CD2	2.47	0.50
3:C:121:ASP:OD1	3:C:123:GLU:HG2	2.12	0.50
4:O:178:ARG:NH2	4:O:196:ALA:O	2.28	0.50
2:J:326:LYS:HD2	2:J:335:ARG:HE	1.76	0.50
7:S:66:LYS:HG2	7:S:72:TYR:CE1	2.47	0.50
1:I:891:ASP:OD1	1:I:891:ASP:N	2.42	0.50
1:I:44:GLY:HA2	1:I:49:LYS:HG2	1.94	0.49
1:I:867:ILE:HD13	1:I:870:PHE:CE1	2.47	0.49
1:I:9:GLY:N	2:J:1120:LYS:HB2	2.27	0.49
1:A:449:ARG:NH2	2:B:878:LEU:HD12	2.27	0.49
2:B:856:VAL:HG22	2:B:866:VAL:HG22	1.94	0.49
2:J:433:MET:HE1	2:J:652:ILE:HG12	1.93	0.49
2:J:606:TRP:HZ3	2:J:617:TYR:HH	1.58	0.49
2:B:606:TRP:O	2:B:609:LEU:HB2	2.12	0.49
2:J:1091:ARG:HD3	2:J:1091:ARG:N	2.27	0.49
1:A:204:HIS:ND1	1:A:205:PRO:HD2	2.27	0.49
2:B:579:ARG:NH2	2:B:623:GLU:OE2	2.44	0.49
1:I:493:SER:HB3	1:I:500:LEU:HB2	1.94	0.49
2:B:779:SER:O	2:B:781:ASN:N	2.44	0.49
2:J:34:HIS:HB3	2:J:129:MET:HE1	1.94	0.49
3:C:158:GLU:C	3:C:159:TYR:CD1	2.86	0.49
2:J:395:ARG:CB	2:J:398:ILE:HD11	2.40	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:729:LEU:HD22	2:J:731:TYR:CD1	2.47	0.49
1:A:891:ASP:O	1:A:895:VAL:HG23	2.12	0.49
2:J:554:VAL:HA	2:J:578:ARG:HH12	1.76	0.49
1:I:694:VAL:HA	1:I:697:LEU:HD12	1.94	0.49
2:B:659:TYR:HB3	2:B:662:HIS:CD2	2.48	0.49
2:B:57:VAL:HB	2:B:58:PRO:CA	2.35	0.49
2:J:41:PHE:CE2	2:J:356:LYS:CG	2.95	0.49
1:A:105:ARG:HA	1:A:197:ASP:OD2	2.13	0.49
1:A:83:VAL:HG13	1:A:276:GLN:OE1	2.13	0.49
3:M:121:ASP:OD1	3:M:123:GLU:HG2	2.12	0.49
1:I:524:TYR:HD1	1:I:524:TYR:H	1.59	0.49
3:C:159:TYR:O	3:C:160:VAL:HB	2.12	0.49
2:J:652:ILE:HG23	2:J:653:PRO:HD3	1.94	0.49
1:A:867:ILE:HD13	1:A:870:PHE:CE1	2.47	0.49
1:A:694:VAL:HA	1:A:697:LEU:HD12	1.94	0.49
2:J:706:ASN:HB2	2:J:710:MET:SD	2.53	0.49
1:A:245:LEU:O	1:A:249:ILE:HG13	2.13	0.49
2:B:1082:TYR:HD1	2:B:1088:GLU:H	1.59	0.49
1:I:26:ALA:HB3	1:I:51:LEU:HD23	1.95	0.49
1:I:666:PHE:O	2:J:729:LEU:HA	2.12	0.49
7:S:63:ILE:O	7:S:74:TYR:HA	2.12	0.49
7:H:63:ILE:O	7:H:74:TYR:HA	2.12	0.49
2:J:573:ASP:N	2:J:573:ASP:OD1	2.41	0.49
1:I:630:ASP:CG	1:I:631:GLY:H	2.16	0.49
2:J:1078:ARG:HG3	2:J:1080:LYS:HG2	1.94	0.49
3:M:119:TYR:CD2	3:M:263:ARG:HD2	2.48	0.49
3:C:262:THR:HG22	7:H:12:HIS:CD2	2.48	0.49
1:A:783:TYR:CE2	1:A:789:THR:HB	2.48	0.49
1:I:401:LEU:HA	1:I:404:GLU:CG	2.43	0.49
1:I:245:LEU:O	1:I:249:ILE:HG13	2.12	0.49
2:J:413:THR:HG23	2:J:415:SER:H	1.77	0.49
2:B:65:VAL:HG11	2:B:395:ARG:NH1	2.28	0.49
2:J:111:VAL:O	2:J:114:ILE:HG12	2.11	0.49
2:J:41:PHE:CD1	2:J:42:ILE:CD1	2.96	0.49
1:A:531:MET:C	9:L:44:THR:HG21	2.33	0.49
2:J:812:LEU:HD21	2:J:843:VAL:HG23	1.94	0.49
2:B:192:ALA:HB3	2:B:207:VAL:HG23	1.94	0.49
2:J:467:CYS:SG	2:J:651:GLY:N	2.78	0.49
1:I:713:THR:O	1:I:717:THR:HG23	2.12	0.49
1:I:769:LEU:HB2	1:I:804:VAL:CG2	2.43	0.49
2:B:618:LEU:HD22	2:B:622:GLU:HG2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:459:HIS:ND1	2:B:461:THR:HG23	2.28	0.49
3:M:76:SER:HA	3:M:79:MET:HE3	1.94	0.49
3:C:149:GLU:O	3:C:150:GLU:HG2	2.13	0.49
1:I:105:ARG:HA	1:I:197:ASP:OD2	2.13	0.49
1:A:508:ILE:HG21	1:A:754:GLY:HA3	1.93	0.49
2:B:1063:TRP:CZ3	2:B:1074:GLU:HG2	2.46	0.49
1:A:669:ALA:HB2	2:B:971:ARG:NE	2.28	0.49
2:J:591:LEU:HG	2:J:614:VAL:HB	1.95	0.49
2:B:520:TYR:CZ	2:B:532:VAL:HB	2.48	0.49
2:B:982:ARG:HD3	4:D:155:TYR:CD2	2.48	0.49
1:A:536:ASP:HA	1:A:540:LEU:HB2	1.93	0.49
8:K:12:ILE:HG23	8:K:51:ILE:HB	1.95	0.49
1:A:713:THR:O	1:A:717:THR:HG23	2.12	0.49
2:B:885:ARG:HD2	2:B:993:TYR:HD2	1.78	0.49
3:M:73:GLY:O	3:M:76:SER:OG	2.26	0.49
2:J:618:LEU:HD22	2:J:622:GLU:HG2	1.95	0.49
1:A:445:TYR:HB2	1:A:449:ARG:NH2	2.25	0.49
3:C:378:VAL:HG21	8:K:8:GLU:HG2	1.95	0.49
1:I:463:ASP:OD1	1:I:464:GLY:N	2.46	0.49
1:A:21:ILE:HD13	1:A:219:PRO:HD3	1.95	0.49
2:B:88:TYR:CD2	2:B:148:LEU:HD11	2.48	0.49
2:B:428:ASP:OD2	2:B:434:SER:OG	2.31	0.49
2:J:324:ALA:O	2:J:328:LEU:HG	2.13	0.49
2:J:730:SER:HA	2:J:735:ASN:ND2	2.26	0.49
3:M:21:LYS:HB3	3:M:21:LYS:HE3	1.48	0.49
2:B:429:ARG:HE	2:B:435:THR:HG21	1.78	0.49
2:B:730:SER:HB3	2:B:915:ASN:ND2	2.27	0.49
3:C:175:MET:O	3:C:178:VAL:HB	2.13	0.49
2:B:433:MET:HE1	2:B:652:ILE:HG12	1.94	0.49
2:B:606:TRP:HZ3	2:B:617:TYR:HH	1.57	0.49
8:T:12:ILE:HG23	8:T:51:ILE:HB	1.95	0.49
2:B:753:ARG:HA	2:B:876:PRO:HD3	1.95	0.49
1:A:33:ASP:HB3	1:A:43:GLU:OE1	2.12	0.49
2:J:607:SER:O	2:J:610:ILE:HG13	2.12	0.49
1:I:446:ARG:HH21	2:J:1002:ALA:HA	1.77	0.49
4:D:10:ARG:HB2	4:D:13:SER:OG	2.13	0.49
1:I:531:MET:C	9:U:44:THR:HG21	2.33	0.48
2:J:429:ARG:HE	2:J:435:THR:HG21	1.78	0.48
3:C:183:THR:O	3:C:183:THR:HG22	2.12	0.48
1:I:94:ARG:HG3	1:I:138:HIS:HD2	1.74	0.48
2:B:24:TYR:HB2	2:B:606:TRP:CE2	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:354:LEU:HD12	2:J:416:TRP:NE1	2.28	0.48
1:A:439:ARG:NH2	1:A:482:LYS:HE3	2.28	0.48
2:B:414:GLY:O	2:B:422:GLY:N	2.43	0.48
1:I:346:PRO:HB2	1:I:349:VAL:HG23	1.95	0.48
2:J:244:VAL:HG13	2:J:257:LEU:HD12	1.96	0.48
3:C:196:TYR:O	3:C:196:TYR:CG	2.66	0.48
2:B:652:ILE:HG23	2:B:653:PRO:HD3	1.95	0.48
2:B:591:LEU:HG	2:B:614:VAL:HB	1.95	0.48
1:I:10:SER:C	2:J:1118:ARG:HB3	2.34	0.48
3:C:331:ALA:H	3:C:336:ARG:NH1	2.09	0.48
1:I:572:ARG:HD2	1:I:576:CYS:HB3	1.95	0.48
1:I:875:ASP:HB3	7:S:70:ALA:HB2	1.95	0.48
1:A:338:ILE:O	1:A:451:ASN:ND2	2.47	0.48
2:B:629:ALA:HB2	2:B:639:HIS:CG	2.49	0.48
2:J:428:ASP:OD2	2:J:434:SER:OG	2.31	0.48
2:B:368:LYS:O	2:B:371:GLN:HB3	2.12	0.48
2:B:378:TYR:OH	2:B:388:GLU:HB2	2.13	0.48
2:J:731:TYR:CZ	2:J:902:PRO:HG3	2.48	0.48
3:M:122:GLU:HG2	3:M:125:ARG:NH2	2.29	0.48
2:J:606:TRP:O	2:J:609:LEU:HB2	2.12	0.48
2:B:812:LEU:HD21	2:B:843:VAL:HG23	1.94	0.48
2:B:207:VAL:HG21	2:B:323:MET:HB3	1.95	0.48
1:A:493:SER:HB3	1:A:500:LEU:HB2	1.94	0.48
6:F:18:LYS:HD2	6:F:49:GLU:HA	1.94	0.48
1:I:779:LEU:HD12	1:I:802:GLY:HA3	1.95	0.48
1:A:435:ILE:HB	2:B:1039:VAL:HG21	1.94	0.48
2:J:799:LEU:HG	2:J:813:VAL:HG22	1.95	0.48
2:J:159:PHE:HE1	2:J:168:ILE:HG13	1.78	0.48
1:A:572:ARG:HD2	1:A:576:CYS:HB3	1.95	0.48
1:I:6:LYS:NZ	2:J:1122:ARG:NH2	2.48	0.48
10:N:2:ILE:HG12	10:N:56:ILE:HG21	1.94	0.48
4:O:201:ARG:HA	4:O:204:GLU:HG2	1.96	0.48
1:A:463:ASP:OD1	1:A:464:GLY:N	2.46	0.48
3:M:270:TRP:HA	3:M:318:ILE:HD11	1.95	0.48
2:B:724:PHE:CD1	2:B:994:TYR:HB2	2.47	0.48
10:V:10:CYS:O	10:V:12:LYS:HG2	2.12	0.48
2:J:1122:ARG:CD	5:Q:10:VAL:CG1	2.69	0.48
3:M:191:PHE:N	3:M:197:THR:HG23	2.29	0.48
2:B:191:VAL:HG13	2:B:208:GLU:HB3	1.96	0.48
1:I:42:ILE:HG22	1:I:47:MET:HB3	1.96	0.48
5:Q:6:LYS:O	6:R:7:LEU:HD23	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:PRO:HG2	1:A:226:ARG:HE	1.78	0.48
3:M:290:VAL:O	3:M:294:ARG:HG3	2.13	0.48
5:Q:16:ARG:H	5:Q:16:ARG:HD2	1.79	0.48
1:A:769:LEU:HB2	1:A:804:VAL:CG2	2.43	0.48
2:B:536:ARG:HA	2:B:539:VAL:HG22	1.95	0.48
2:J:88:TYR:CD2	2:J:148:LEU:HD11	2.48	0.48
2:B:799:LEU:HG	2:B:813:VAL:HG22	1.95	0.48
2:J:191:VAL:HG13	2:J:208:GLU:HB3	1.96	0.48
2:J:289:TYR:O	2:J:293:ARG:HB2	2.14	0.48
2:J:24:TYR:HB2	2:J:606:TRP:CE2	2.48	0.48
3:C:270:TRP:HA	3:C:318:ILE:HD11	1.95	0.48
2:J:579:ARG:NH2	2:J:623:GLU:OE2	2.46	0.48
1:I:15:ILE:HD12	1:I:208:SER:HB2	1.96	0.48
2:B:785:TYR:CE2	2:B:787:GLY:HA2	2.49	0.48
1:A:346:PRO:HB2	1:A:349:VAL:HG23	1.96	0.48
1:I:21:ILE:HD13	1:I:219:PRO:HD3	1.96	0.48
3:M:321:ILE:O	3:M:327:VAL:HG23	2.14	0.48
1:I:63:CYS:O	1:I:65:ALA:N	2.46	0.48
1:I:11:ILE:HD12	3:M:358:LEU:HD22	1.96	0.48
1:I:783:TYR:HE2	1:I:789:THR:HB	1.79	0.48
2:J:885:ARG:HD2	2:J:993:TYR:HD2	1.79	0.48
1:I:378:TYR:HB2	1:I:379:PRO:HD3	1.95	0.48
2:B:413:THR:HG23	2:B:415:SER:H	1.77	0.48
2:B:794:LEU:HB3	2:B:798:GLY:HA2	1.95	0.48
2:B:159:PHE:HE1	2:B:168:ILE:HG13	1.78	0.48
1:I:81:ARG:HG3	1:I:82:PRO:HD2	1.95	0.48
1:I:444:PRO:CG	9:U:50:THR:HG22	2.10	0.48
1:I:874:GLU:HG3	7:S:67:SER:OG	2.13	0.48
10:N:60:MET:C	10:N:62:TYR:H	2.15	0.48
1:A:443:MET:SD	1:A:449:ARG:HD3	2.53	0.48
3:M:176:GLU:O	3:M:179:VAL:N	2.47	0.48
1:A:535:MET:HB3	1:A:540:LEU:HD12	1.95	0.48
1:A:163:THR:CB	1:A:276:GLN:HE21	2.27	0.48
1:A:779:LEU:HD12	1:A:802:GLY:HA3	1.95	0.48
2:B:706:ASN:HB2	2:B:710:MET:SD	2.53	0.48
4:O:10:ARG:HB2	4:O:13:SER:OG	2.13	0.48
5:E:146:ILE:HA	5:E:163:MET:HG2	1.94	0.48
3:C:160:VAL:HG23	3:C:198:LEU:CB	2.44	0.48
3:C:196:TYR:CE1	3:C:198:LEU:CD1	2.94	0.48
2:J:729:LEU:HD23	2:J:730:SER:O	2.13	0.48
5:Q:3:LYS:HZ2	6:R:9:GLU:CD	2.16	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:SER:HB2	2:B:1118:ARG:HB3	1.94	0.48
3:C:173:LEU:HB3	3:C:177:LYS:NZ	2.28	0.48
3:C:122:GLU:HG2	3:C:125:ARG:NH2	2.29	0.48
2:B:759:THR:HA	2:B:869:THR:HA	1.95	0.48
1:I:535:MET:HB3	1:I:540:LEU:HD12	1.95	0.48
2:J:49:VAL:HG13	2:J:199:HIS:HE1	1.79	0.48
2:J:1122:ARG:NH2	5:Q:67:TYR:HE2	2.08	0.48
3:M:152:ILE:CG2	3:M:159:TYR:CA	2.86	0.48
3:C:290:VAL:O	3:C:294:ARG:HG3	2.13	0.48
2:B:354:LEU:HD12	2:B:416:TRP:NE1	2.28	0.48
1:I:163:THR:CB	1:I:276:GLN:HE21	2.27	0.48
1:I:837:GLN:HB3	3:M:102:ILE:CD1	2.44	0.48
1:A:81:ARG:HG2	1:A:272:TRP:CD2	2.49	0.48
1:I:439:ARG:NH2	1:I:482:LYS:HE3	2.28	0.48
1:A:654:THR:OG1	1:A:655:LYS:N	2.46	0.48
3:M:314:LEU:HD13	3:M:315:ASP:N	2.29	0.48
3:M:148:ARG:HH21	3:M:162:GLU:CG	2.21	0.47
3:C:187:LYS:HB3	3:C:201:ARG:HG2	1.96	0.47
10:V:5:VAL:O	10:V:6:ARG:HB2	2.14	0.47
1:A:359:VAL:HG22	1:A:408:ILE:HA	1.95	0.47
3:C:155:LEU:CD2	3:C:156:ASN:HD22	2.27	0.47
2:B:244:VAL:HG13	2:B:257:LEU:HD12	1.96	0.47
1:A:26:ALA:HB3	1:A:51:LEU:HD23	1.95	0.47
1:I:221:PRO:HG2	1:I:226:ARG:HE	1.79	0.47
2:J:451:PRO:HB2	2:J:453:PHE:CE1	2.49	0.47
2:J:591:LEU:HD13	2:J:595:HIS:CE1	2.49	0.47
2:J:207:VAL:HG21	2:J:323:MET:HB3	1.95	0.47
2:B:766:ARG:NH1	2:B:862:GLY:O	2.47	0.47
2:J:766:ARG:NH1	2:J:862:GLY:O	2.47	0.47
3:C:119:TYR:CD2	3:C:263:ARG:HD2	2.48	0.47
2:B:579:ARG:HH21	2:B:623:GLU:CD	2.18	0.47
3:M:325:GLY:O	3:M:329:GLU:HG2	2.15	0.47
3:C:314:LEU:HD13	3:C:315:ASP:N	2.29	0.47
2:B:352:GLY:O	2:B:356:LYS:HG3	2.13	0.47
8:T:30:VAL:HB	8:T:31:PRO:HD3	1.96	0.47
2:J:794:LEU:HB3	2:J:798:GLY:HA2	1.96	0.47
1:I:623:LYS:HB2	1:I:754:GLY:HA3	1.96	0.47
2:J:395:ARG:CB	2:J:398:ILE:HD12	2.44	0.47
2:J:1122:ARG:NE	5:Q:67:TYR:CD2	2.81	0.47
3:M:151:THR:O	3:M:152:ILE:HD13	2.13	0.47
3:M:163:ILE:HD12	3:M:197:THR:HB	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:236:LYS:HE3	3:M:241:TYR:CE2	2.49	0.47
3:C:236:LYS:HE3	3:C:241:TYR:CE2	2.49	0.47
3:C:155:LEU:HD21	3:C:156:ASN:ND2	2.29	0.47
2:J:536:ARG:HA	2:J:539:VAL:HG22	1.94	0.47
3:M:380:LEU:HB2	5:Q:59:ILE:HB	1.95	0.47
4:O:55:PHE:HB2	4:O:58:ILE:HD12	1.95	0.47
9:L:25:ALA:HB3	9:L:43:TYR:CE2	2.49	0.47
3:C:207:LYS:HE3	3:C:210:ASP:OD1	2.14	0.47
3:C:337:ALA:HA	3:C:346:LEU:HB2	1.97	0.47
5:E:16:ARG:H	5:E:16:ARG:HD2	1.79	0.47
9:U:30:GLU:HA	9:U:33:HIS:HD1	1.79	0.47
1:I:499:PRO:HD2	1:I:630:ASP:HB2	1.96	0.47
2:J:1081:VAL:HG22	2:J:1092:ILE:HD13	1.95	0.47
2:J:520:TYR:CZ	2:J:532:VAL:HB	2.48	0.47
3:M:93:ASN:HB3	3:M:94:VAL:HG22	1.94	0.47
1:A:893:VAL:HG11	3:C:49:THR:HA	1.96	0.47
1:I:338:ILE:O	1:I:451:ASN:ND2	2.47	0.47
1:A:378:TYR:HB2	1:A:379:PRO:HD3	1.95	0.47
1:A:524:TYR:H	1:A:524:TYR:HD1	1.58	0.47
2:B:768:LEU:O	2:J:380:ARG:NH2	2.47	0.47
3:C:161:VAL:HG22	3:C:199:VAL:CB	2.33	0.47
2:J:962:GLU:OE1	4:O:201:ARG:NH1	2.48	0.47
1:I:165:TYR:HB2	1:I:181:MET:HB3	1.97	0.47
2:J:591:LEU:HB3	2:J:595:HIS:CD2	2.50	0.47
2:J:759:THR:HA	2:J:869:THR:HA	1.96	0.47
2:B:591:LEU:HD13	2:B:595:HIS:CE1	2.49	0.47
3:C:321:ILE:O	3:C:327:VAL:HG23	2.15	0.47
3:M:220:LYS:C	3:M:222:ARG:H	2.17	0.47
2:J:753:ARG:HA	2:J:876:PRO:HD3	1.95	0.47
2:B:17:LEU:HD22	2:B:644:LEU:HA	1.97	0.47
2:J:785:TYR:CE2	2:J:787:GLY:HA2	2.49	0.47
2:J:629:ALA:HB2	2:J:639:HIS:CG	2.49	0.47
1:I:352:GLU:OE2	2:J:1009:SER:HB3	2.14	0.47
3:M:180:ARG:HD3	3:M:180:ARG:O	2.15	0.47
2:J:729:LEU:HD22	2:J:731:TYR:CE1	2.49	0.47
5:E:6:LYS:O	6:F:7:LEU:CD2	2.62	0.47
2:J:429:ARG:O	2:J:431:ASN:N	2.48	0.47
1:A:569:ILE:HG13	1:A:636:ILE:HD13	1.97	0.47
2:B:591:LEU:HB3	2:B:595:HIS:CD2	2.50	0.47
7:H:40:LEU:HB2	7:H:78:LEU:HD12	1.97	0.47
2:J:708:ARG:H	2:J:947:THR:HG1	1.57	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:ILE:HD12	1:A:208:SER:HB2	1.96	0.47
2:J:57:VAL:HB	2:J:58:PRO:CA	2.35	0.47
2:B:744:LYS:HB3	2:B:897:PRO:HA	1.97	0.47
2:B:289:TYR:O	2:B:293:ARG:HB2	2.13	0.47
3:M:187:LYS:HE3	3:M:201:ARG:HB3	1.96	0.47
7:H:29:LEU:HD11	7:H:76:TYR:CZ	2.49	0.47
2:B:429:ARG:O	2:B:431:ASN:N	2.48	0.47
2:B:940:THR:O	10:N:32:GLY:HA3	2.14	0.47
1:A:165:TYR:HB2	1:A:181:MET:HB3	1.96	0.47
10:V:8:PHE:HB2	10:V:47:ARG:HH22	1.80	0.47
2:J:681:LEU:HD13	2:J:696:LEU:HD23	1.97	0.47
8:K:30:VAL:HB	8:K:31:PRO:HD3	1.96	0.47
1:A:645:ARG:HB3	1:A:649:PHE:CE2	2.50	0.47
1:I:160:GLU:HA	1:I:164:ILE:O	2.15	0.47
1:A:209:ARG:HB2	1:A:212:TRP:CD2	2.50	0.47
2:B:324:ALA:O	2:B:328:LEU:HG	2.15	0.47
9:U:6:ILE:HD11	9:U:16:TYR:CE2	2.50	0.47
2:B:919:ILE:H	2:B:920:PRO:HD2	1.80	0.47
9:U:50:THR:OG1	9:U:51:MET:N	2.46	0.47
1:A:758:LYS:HA	1:A:758:LYS:HE3	1.96	0.47
7:S:29:LEU:HD11	7:S:76:TYR:CZ	2.49	0.47
3:M:358:LEU:CD1	3:M:359:ASN:H	2.25	0.47
1:A:848:ALA:HB2	3:C:327:VAL:HG22	1.97	0.47
2:J:323:MET:O	2:J:327:VAL:HG23	2.14	0.47
2:B:681:LEU:HD13	2:B:696:LEU:HD23	1.97	0.47
2:J:856:VAL:HG12	11:W:35:LEU:HB2	1.95	0.47
11:W:17:LEU:HD22	11:W:28:PRO:HD2	1.97	0.47
4:D:55:PHE:HB2	4:D:58:ILE:HD12	1.95	0.47
1:I:209:ARG:HB2	1:I:212:TRP:CD2	2.49	0.47
2:B:395:ARG:HD3	2:B:398:ILE:HD11	1.96	0.47
1:I:443:MET:SD	1:I:449:ARG:HD3	2.55	0.47
3:C:161:VAL:HG22	3:C:199:VAL:HB	1.95	0.47
3:M:148:ARG:NH1	3:M:162:GLU:CB	2.66	0.47
1:I:480:GLU:OE2	2:J:1047:MET:HB2	2.14	0.47
1:A:632:LYS:N	1:A:632:LYS:HE3	2.30	0.47
1:I:476:GLU:HA	8:T:14:GLY:HA3	1.96	0.47
6:R:117:GLU:O	6:R:119:ARG:N	2.48	0.47
5:E:125:ARG:H	5:E:125:ARG:NE	2.12	0.47
5:Q:39:ASP:O	5:Q:43:GLY:N	2.43	0.47
10:N:8:PHE:HB2	10:N:47:ARG:HH22	1.80	0.47
2:J:325:LEU:HD23	2:J:326:LYS:HG2	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1122:ARG:HD2	6:R:4:ARG:HH21	1.77	0.47
3:M:160:VAL:HG11	3:M:198:LEU:HD12	1.96	0.47
1:I:305:ALA:O	1:I:309:LYS:HD2	2.14	0.47
3:C:181:LYS:O	3:C:183:THR:N	2.48	0.47
2:B:323:MET:O	2:B:327:VAL:HG23	2.15	0.47
1:I:783:TYR:CE2	1:I:789:THR:HB	2.50	0.47
3:M:266:THR:HB	3:M:272:ILE:HD11	1.97	0.47
2:B:325:LEU:HD23	2:B:326:LYS:HG2	1.97	0.47
2:B:636:THR:H	2:B:639:HIS:HD2	1.63	0.47
2:B:31:VAL:CG2	2:B:155:PRO:HB2	2.45	0.47
9:L:6:ILE:HD11	9:L:16:TYR:CE2	2.50	0.47
1:A:585:LEU:O	1:A:586:GLU:HB3	2.15	0.47
2:B:373:GLN:CG	2:B:397:SER:HB2	2.45	0.46
5:Q:6:LYS:O	6:R:7:LEU:CD2	2.63	0.46
3:M:187:LYS:CE	3:M:201:ARG:HB3	2.45	0.46
3:M:323:ARG:H	3:M:327:VAL:HB	1.80	0.46
2:J:151:ASP:HB2	2:J:718:ARG:HH22	1.80	0.46
9:U:28:LEU:HD23	9:U:57:PHE:HE2	1.79	0.46
2:B:925:VAL:HA	2:B:928:LEU:HD12	1.97	0.46
1:I:430:LEU:HD23	3:M:74:GLU:HG3	1.96	0.46
3:C:189:ALA:HB3	3:C:199:VAL:HG13	1.97	0.46
3:C:220:LYS:C	3:C:222:ARG:H	2.18	0.46
10:N:56:ILE:HG12	10:N:60:MET:CG	2.45	0.46
3:M:187:LYS:O	3:M:187:LYS:HG3	2.15	0.46
1:I:435:ILE:O	2:J:1043:HIS:CE1	2.68	0.46
2:B:986:ASP:O	2:B:987:ILE:HD13	2.15	0.46
4:D:201:ARG:HA	4:D:204:GLU:HG2	1.96	0.46
2:B:574:ASP:OD1	14:B:1301:HOH:O	2.20	0.46
3:C:323:ARG:H	3:C:327:VAL:HB	1.79	0.46
3:M:128:ARG:HG3	3:M:241:TYR:HE2	1.77	0.46
3:C:330:LYS:HD3	3:C:330:LYS:H	1.80	0.46
4:O:178:ARG:HH12	4:O:197:PHE:HA	1.80	0.46
1:I:81:ARG:HG2	1:I:272:TRP:CD2	2.50	0.46
3:C:325:GLY:O	3:C:329:GLU:HG2	2.14	0.46
2:B:342:HIS:HE1	2:B:620:ALA:HB1	1.81	0.46
3:C:194:GLU:CG	3:C:196:TYR:HE2	2.29	0.46
10:N:57:ASP:CA	10:N:60:MET:HE3	2.38	0.46
5:Q:8:LYS:CG	6:R:7:LEU:HD22	2.45	0.46
2:J:513:ARG:HA	2:J:514:ARG:HH11	1.81	0.46
2:J:861:ASP:HB3	2:J:863:THR:HG23	1.98	0.46
1:I:645:ARG:HB3	1:I:649:PHE:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1083:CYS:HG	2:J:1086:CYS:HB2	1.76	0.46
1:I:477:ALA:HA	2:J:1047:MET:HB3	1.97	0.46
2:B:683:TRP:O	2:B:683:TRP:CD1	2.67	0.46
1:A:462:PHE:HB2	2:B:737:GLU:O	2.15	0.46
2:J:744:LYS:HB3	2:J:897:PRO:HA	1.97	0.46
2:B:603:THR:HB	2:B:604:LEU:HD23	1.98	0.46
1:A:426:ARG:HB2	1:A:467:MET:HE3	1.98	0.46
3:M:116:MET:HE1	3:M:253:VAL:HG21	1.97	0.46
2:J:342:HIS:HE1	2:J:620:ALA:HB1	1.81	0.46
1:A:12:GLU:N	2:B:1116:SER:O	2.29	0.46
2:J:683:TRP:CD1	2:J:683:TRP:O	2.66	0.46
2:B:904:THR:HG21	2:B:972:GLU:OE1	2.15	0.46
3:C:303:ARG:HA	3:C:306:MET:HE2	1.96	0.46
2:B:205:ILE:CD1	2:B:303:LEU:H	2.29	0.46
11:P:43:ALA:O	11:P:44:ARG:HD3	2.16	0.46
3:M:216:GLU:O	3:M:221:HIS:HB2	2.15	0.46
2:J:726:VAL:HG11	2:J:992:ILE:HG12	1.98	0.46
2:J:636:THR:H	2:J:639:HIS:HD2	1.63	0.46
5:Q:27:LYS:HD3	5:Q:51:VAL:HG23	1.97	0.46
2:J:21:MET:SD	2:J:645:MET:HB3	2.55	0.46
2:J:650:LEU:HB2	2:J:654:ALA:HB3	1.97	0.46
8:K:49:ILE:H	8:K:49:ILE:HG13	1.46	0.46
1:A:160:GLU:HA	1:A:164:ILE:O	2.15	0.46
2:B:269:THR:HB	2:B:270:GLN:H	1.55	0.46
1:A:347:LEU:HD22	1:A:444:PRO:HA	1.97	0.46
1:I:569:ILE:HG13	1:I:636:ILE:HD13	1.97	0.46
3:C:342:THR:CB	3:C:345:HIS:HB2	2.43	0.46
4:D:200:PRO:HB2	4:D:203:PHE:CD1	2.48	0.46
3:C:128:ARG:HG3	3:C:241:TYR:HE2	1.78	0.46
9:U:28:LEU:HD23	9:U:57:PHE:CE2	2.51	0.46
3:M:215:ALA:HA	3:M:219:LYS:HG3	1.98	0.46
2:B:861:ASP:HB3	2:B:863:THR:HG23	1.97	0.46
3:C:116:MET:HE1	3:C:253:VAL:HG21	1.98	0.46
2:J:235:LEU:HD13	2:J:313:ARG:HB3	1.97	0.46
2:J:17:LEU:HD22	2:J:644:LEU:HA	1.97	0.46
1:A:405:LYS:HE3	1:A:405:LYS:HB2	1.72	0.46
7:S:75:TYR:HD1	7:S:76:TYR:H	1.64	0.46
7:S:40:LEU:HB2	7:S:78:LEU:HD12	1.98	0.46
3:C:187:LYS:HD3	3:C:203:LYS:NZ	2.30	0.46
1:I:756:ARG:HH12	2:J:922:ARG:HH12	1.64	0.46
2:B:766:ARG:HD3	2:B:772:LYS:HE2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:654:THR:OG1	1:I:655:LYS:N	2.47	0.46
2:J:31:VAL:CG2	2:J:155:PRO:HB2	2.45	0.46
10:N:5:VAL:O	10:N:6:ARG:HB2	2.15	0.46
1:I:750:MET:HE1	2:J:916:PRO:O	2.16	0.46
2:J:902:PRO:HB2	2:J:974:MET:CG	2.46	0.46
1:I:103:CYS:SG	1:I:105:ARG:CA	3.03	0.46
3:M:152:ILE:HG21	3:M:158:GLU:O	2.16	0.46
1:A:666:PHE:N	2:B:729:LEU:HD13	2.30	0.46
2:B:731:TYR:OH	2:B:902:PRO:HG3	2.16	0.46
2:B:432:TYR:O	2:B:435:THR:HG23	2.16	0.46
2:B:730:SER:HA	2:B:735:ASN:ND2	2.27	0.46
1:A:624:LYS:O	1:A:632:LYS:HD3	2.14	0.46
2:J:986:ASP:O	2:J:987:ILE:HD13	2.16	0.46
1:I:670:ILE:HG21	2:J:932:ILE:HD11	1.97	0.46
3:M:303:ARG:HA	3:M:306:MET:HE2	1.97	0.46
1:A:94:ARG:HG3	1:A:138:HIS:HD2	1.75	0.46
5:Q:125:ARG:H	5:Q:125:ARG:NE	2.12	0.46
3:C:76:SER:HA	3:C:79:MET:HE3	1.98	0.46
2:B:447:SER:HB2	2:B:450:GLN:HG2	1.98	0.46
2:B:451:PRO:HB2	2:B:453:PHE:CE1	2.50	0.46
3:M:374:GLY:HA2	8:T:7:PHE:CE2	2.51	0.46
1:A:580:GLU:H	1:A:580:GLU:HG3	1.63	0.46
1:A:59:ARG:HH12	11:W:21:THR:HG21	1.81	0.46
4:D:29:LEU:O	4:D:33:ILE:HG13	2.16	0.46
1:I:347:LEU:HD22	1:I:444:PRO:HA	1.97	0.46
1:A:757:GLY:O	1:A:758:LYS:HD2	2.16	0.46
9:L:45:ILE:C	9:L:47:HIS:H	2.19	0.46
2:B:749:ARG:HE	4:D:144:ALA:CB	2.27	0.46
2:J:429:ARG:HA	2:J:429:ARG:HD2	1.78	0.46
2:J:968:HIS:HD2	2:J:969:SER:CA	2.29	0.46
2:B:161:ILE:HD12	2:B:411:LEU:HB3	1.97	0.46
2:B:416:TRP:HB2	2:B:420:ARG:HG3	1.98	0.46
6:F:117:GLU:O	6:F:119:ARG:N	2.48	0.46
1:A:584:ALA:O	1:A:605:TYR:OH	2.23	0.46
2:J:513:ARG:NH1	2:J:531:THR:OG1	2.48	0.46
1:I:639:ARG:NH2	1:I:882:SER:O	2.48	0.46
1:I:446:ARG:HB3	2:J:1005:MET:SD	2.56	0.46
4:D:46:GLU:HA	11:P:45:ARG:HA	1.97	0.46
1:A:336:PRO:HD2	2:B:734:TYR:CE1	2.51	0.46
11:P:17:LEU:HD22	11:P:28:PRO:HD2	1.97	0.46
3:M:286:ILE:O	3:M:290:VAL:HG23	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:100:ARG:HH21	3:M:288:GLU:HG2	1.81	0.46
10:V:56:ILE:HG12	10:V:60:MET:HG2	1.97	0.46
3:C:269:ILE:HG22	3:C:270:TRP:H	1.80	0.46
4:D:178:ARG:HH12	4:D:197:PHE:HA	1.80	0.46
1:A:670:ILE:HG21	2:B:958:ARG:HD3	1.97	0.46
4:O:127:GLN:HE21	10:V:63:LYS:HG2	1.81	0.46
2:J:228:PHE:CE1	2:J:320:LEU:HD22	2.51	0.46
2:B:21:MET:SD	2:B:645:MET:HB3	2.55	0.46
1:I:542:GLU:H	1:I:542:GLU:HG2	1.49	0.46
2:B:56:VAL:CG2	2:B:65:VAL:HB	2.46	0.45
1:I:443:MET:CB	9:U:49:ILE:HD12	2.38	0.45
1:I:665:GLY:HA2	2:J:729:LEU:HD13	1.91	0.45
2:B:744:LYS:HG3	2:B:895:ILE:HD11	1.98	0.45
1:A:305:ALA:O	1:A:309:LYS:HD2	2.16	0.45
2:J:1101:PHE:CD2	3:M:367:ILE:HG13	2.52	0.45
2:J:925:VAL:HA	2:J:928:LEU:HD12	1.97	0.45
5:Q:100:ARG:NE	6:R:43:VAL:HG13	2.31	0.45
11:W:43:ALA:O	11:W:44:ARG:HD3	2.15	0.45
3:C:266:THR:HB	3:C:272:ILE:HD11	1.97	0.45
2:J:1059:LYS:HE2	2:J:1096:GLU:HG2	1.98	0.45
3:C:155:LEU:HD23	3:C:156:ASN:HD22	1.81	0.45
1:I:426:ARG:HB2	1:I:467:MET:HE3	1.97	0.45
1:I:787:VAL:HG23	1:I:801:ARG:HH11	1.81	0.45
3:M:62:GLU:HG3	3:M:63:ALA:H	1.81	0.45
1:I:6:LYS:CE	2:J:1122:ARG:CZ	2.63	0.45
3:M:160:VAL:HG11	3:M:198:LEU:CD1	2.46	0.45
3:C:333:VAL:O	3:C:337:ALA:N	2.50	0.45
2:J:904:THR:HG21	2:J:972:GLU:OE1	2.15	0.45
2:J:211:LYS:HG3	3:M:212:ARG:NH2	2.31	0.45
3:M:173:LEU:HB3	3:M:177:LYS:NZ	2.30	0.45
2:J:358:LEU:HD23	2:J:416:TRP:CE2	2.51	0.45
2:J:205:ILE:CD1	2:J:303:LEU:H	2.29	0.45
1:I:507:HIS:NE2	1:I:654:THR:HB	2.32	0.45
1:A:167:GLU:HG3	1:A:179:HIS:HB3	1.98	0.45
2:J:603:THR:HB	2:J:604:LEU:HD23	1.99	0.45
1:I:134:ILE:HD13	1:I:134:ILE:HA	1.82	0.45
2:B:378:TYR:HE1	2:B:388:GLU:HA	0.95	0.45
1:I:750:MET:HA	1:I:753:THR:HG22	1.97	0.45
10:N:62:TYR:C	10:N:63:LYS:HZ2	2.10	0.45
2:J:432:TYR:O	2:J:435:THR:HG23	2.16	0.45
2:J:968:HIS:HD2	2:J:969:SER:N	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:O:226:THR:HB	4:O:235:ILE:HD11	1.99	0.45
3:M:104:ILE:HD12	3:M:288:GLU:HB3	1.98	0.45
5:E:5:LEU:HD13	6:F:6:LYS:CD	2.46	0.45
2:J:579:ARG:HH21	2:J:623:GLU:CD	2.19	0.45
2:B:1059:LYS:HE2	2:B:1096:GLU:HG2	1.98	0.45
1:A:264:PRO:O	1:A:266:LEU:N	2.50	0.45
2:B:636:THR:N	2:B:639:HIS:HD2	2.14	0.45
2:B:126:LEU:HD12	2:B:127:PRO:HD2	1.99	0.45
2:J:269:THR:HB	2:J:270:GLN:H	1.55	0.45
1:A:577:ASP:HA	1:A:581:ARG:HG3	1.97	0.45
2:J:637:GLU:H	2:J:637:GLU:HG2	1.42	0.45
2:B:389:ASN:OD1	2:B:392:ARG:HD3	2.15	0.45
3:C:194:GLU:CB	3:C:196:TYR:CD2	2.84	0.45
2:J:731:TYR:OH	2:J:902:PRO:HG3	2.17	0.45
2:B:902:PRO:HB2	2:B:974:MET:CG	2.46	0.45
1:A:150:CYS:O	1:A:153:PRO:HD3	2.16	0.45
3:C:62:GLU:HG3	3:C:63:ALA:H	1.81	0.45
2:J:189:LYS:NZ	3:M:212:ARG:NH1	2.64	0.45
2:J:25:TRP:HZ2	2:J:485:LEU:HB3	1.80	0.45
6:F:112:ILE:O	6:F:116:ASP:N	2.49	0.45
4:D:50:ASN:ND2	4:D:52:SER:H	2.13	0.45
3:M:331:ALA:H	3:M:336:ARG:NH1	2.15	0.45
1:A:639:ARG:NH2	1:A:882:SER:O	2.49	0.45
2:J:919:ILE:H	2:J:920:PRO:HD2	1.80	0.45
2:B:122:ARG:HE	2:B:400:PRO:HG3	1.82	0.45
2:B:942:ARG:HB2	2:B:942:ARG:CZ	2.47	0.45
2:J:56:VAL:CG2	2:J:65:VAL:HB	2.46	0.45
1:I:666:PHE:O	2:J:916:PRO:HG3	2.16	0.45
9:L:46:GLU:C	9:L:47:HIS:CG	2.89	0.45
2:J:485:LEU:HD12	2:J:648:ALA:HA	1.98	0.45
3:M:177:LYS:C	3:M:179:VAL:H	2.19	0.45
2:J:766:ARG:HD3	2:J:772:LYS:HE2	1.99	0.45
2:J:636:THR:N	2:J:639:HIS:HD2	2.14	0.45
2:B:778:PRO:HD3	2:B:814:GLY:HA3	1.99	0.45
3:M:330:LYS:HD3	3:M:330:LYS:H	1.82	0.45
2:B:228:PHE:CE1	2:B:320:LEU:HD22	2.51	0.45
1:I:445:TYR:CD1	9:U:49:ILE:HG21	2.51	0.45
2:J:67:PHE:CD1	2:J:107:MET:HG2	2.52	0.45
3:M:153:ASP:CG	3:M:157:MET:HG3	2.37	0.45
1:A:632:LYS:H	1:A:632:LYS:HE3	1.81	0.45
3:C:286:ILE:O	3:C:290:VAL:HG23	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:609:LEU:HD22	2:B:614:VAL:HG11	1.97	0.45
2:J:416:TRP:HB2	2:J:420:ARG:HG3	1.98	0.45
2:J:89:PRO:HG3	2:J:99:TYR:CE2	2.51	0.45
3:C:386:LEU:HA	3:C:386:LEU:HD12	1.66	0.45
1:A:783:TYR:OH	2:B:623:GLU:OE2	2.31	0.45
2:B:726:VAL:HG11	2:B:992:ILE:HG12	1.98	0.45
2:J:744:LYS:HG3	2:J:895:ILE:HD11	1.98	0.45
2:B:131:LYS:N	2:B:135:CYS:SG	2.90	0.45
2:B:231:VAL:O	2:B:235:LEU:HB2	2.17	0.45
2:B:235:LEU:HD13	2:B:313:ARG:HB3	1.98	0.45
1:I:791:PHE:CE2	1:I:800:ALA:HA	2.52	0.45
2:J:942:ARG:CZ	2:J:942:ARG:HB2	2.47	0.45
2:B:939:LEU:HB2	2:B:964:LEU:HD13	1.99	0.45
2:B:878:LEU:HD23	2:B:878:LEU:HA	1.74	0.45
5:E:5:LEU:HD13	6:F:6:LYS:HD3	1.98	0.45
5:Q:5:LEU:HD13	6:R:6:LYS:CD	2.47	0.45
6:R:112:ILE:O	6:R:116:ASP:N	2.49	0.45
3:M:269:ILE:HG22	3:M:270:TRP:H	1.80	0.45
2:B:151:ASP:HB2	2:B:718:ARG:HH22	1.81	0.45
5:E:42:GLU:O	5:E:78:GLU:HB2	2.17	0.45
2:J:1121:ASP:OD2	3:M:379:LYS:HE3	2.17	0.45
1:I:167:GLU:HG3	1:I:179:HIS:HB3	1.99	0.45
1:I:870:PHE:HE2	7:S:75:TYR:HD1	1.64	0.45
2:J:239:THR:HG22	2:J:241:LYS:H	1.82	0.45
2:J:161:ILE:HD12	2:J:411:LEU:HB3	1.97	0.45
4:D:226:THR:HB	4:D:235:ILE:HD11	1.98	0.45
8:K:24:ALA:HA	8:K:25:PRO:HD2	1.84	0.45
1:A:507:HIS:NE2	1:A:654:THR:HB	2.32	0.45
2:J:231:VAL:O	2:J:235:LEU:HB2	2.16	0.45
2:J:447:SER:HB2	2:J:450:GLN:HG2	1.98	0.45
4:O:29:LEU:O	4:O:33:ILE:HG13	2.16	0.45
2:J:63:PHE:HD1	2:J:111:VAL:HG13	1.82	0.45
2:J:107:MET:C	2:J:395:ARG:NH2	2.71	0.45
3:M:157:MET:O	3:M:158:GLU:HB2	2.17	0.45
11:P:10:LYS:O	11:P:35:LEU:HA	2.17	0.45
4:O:50:ASN:ND2	4:O:52:SER:H	2.13	0.45
1:A:147:CYS:HA	1:A:148:PRO:HD3	1.81	0.45
1:A:187:ARG:O	1:A:191:GLU:HG3	2.17	0.45
1:A:161:ARG:HA	1:A:162:PRO:C	2.38	0.45
1:A:543:PRO:O	1:A:544:ASP:HB2	2.15	0.45
2:B:67:PHE:CD1	2:B:107:MET:HG2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:180:ARG:NH1	1:I:182:MET:SD	2.89	0.45
2:B:650:LEU:HB2	2:B:654:ALA:HB3	1.97	0.45
2:B:63:PHE:HD1	2:B:111:VAL:HG13	1.82	0.45
2:J:41:PHE:HD1	2:J:42:ILE:HD13	1.79	0.45
1:I:103:CYS:SG	1:I:104:GLY:N	2.89	0.45
2:B:815:ARG:HG2	2:B:816:THR:H	1.82	0.45
1:A:895:VAL:O	1:A:897:THR:N	2.50	0.45
2:B:89:PRO:HG3	2:B:99:TYR:CE2	2.51	0.45
5:E:27:LYS:HD3	5:E:51:VAL:HG23	1.98	0.45
2:J:791:TYR:OH	2:J:838:GLU:OE2	2.25	0.45
1:A:791:PHE:CE2	1:A:800:ALA:HA	2.52	0.45
3:M:281:ALA:O	3:M:285:ILE:HG12	2.17	0.45
2:J:503:MET:HA	2:J:507:VAL:HB	1.99	0.45
1:I:161:ARG:HA	1:I:162:PRO:C	2.38	0.45
3:M:153:ASP:HB2	3:M:160:VAL:HG23	1.98	0.44
1:I:867:ILE:H	1:I:867:ILE:HG13	1.27	0.44
7:H:75:TYR:HD1	7:H:76:TYR:H	1.64	0.44
2:B:773:ASP:OD2	2:B:815:ARG:NH1	2.44	0.44
3:C:104:ILE:HD12	3:C:288:GLU:HB3	1.98	0.44
2:J:609:LEU:HD22	2:J:614:VAL:HG11	1.98	0.44
2:J:1080:LYS:HB3	5:Q:154:ARG:HD3	1.99	0.44
11:W:10:LYS:O	11:W:35:LEU:HA	2.17	0.44
5:Q:42:GLU:O	5:Q:78:GLU:HB2	2.17	0.44
4:D:27:ASN:HD22	4:D:27:ASN:HA	1.51	0.44
10:N:56:ILE:HG23	10:N:60:MET:HE2	1.99	0.44
4:D:150:PHE:HD1	10:N:12:LYS:HZ1	1.65	0.44
2:B:968:HIS:HD2	2:B:969:SER:CA	2.30	0.44
3:C:173:LEU:HB3	3:C:177:LYS:HZ3	1.81	0.44
4:D:201:ARG:HG3	4:D:201:ARG:H	1.18	0.44
3:C:385:PRO:HA	3:C:386:LEU:CD1	2.48	0.44
3:C:107:ALA:HB1	3:C:270:TRP:CZ2	2.52	0.44
9:U:45:ILE:HD13	9:U:53:ARG:NH1	2.32	0.44
3:C:210:ASP:O	3:C:214:ILE:HG13	2.17	0.44
9:L:46:GLU:O	9:L:47:HIS:CG	2.71	0.44
2:B:358:LEU:HD23	2:B:416:TRP:CE2	2.51	0.44
2:B:10:PRO:O	2:B:11:THR:OG1	2.24	0.44
2:B:357:ASP:HA	2:B:360:ARG:NH1	2.32	0.44
1:I:187:ARG:O	1:I:191:GLU:HG3	2.17	0.44
1:I:404:GLU:O	1:I:406:LEU:HG	2.17	0.44
1:I:758:LYS:HB3	1:I:759:ILE:H	1.53	0.44
2:J:179:THR:HA	2:J:194:VAL:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:305:HIS:CE1	2:J:306:MET:HG2	2.53	0.44
9:L:52:ALA:O	9:L:53:ARG:HB2	2.17	0.44
1:I:309:LYS:HZ1	3:M:346:LEU:HG	1.82	0.44
7:S:42:GLN:HA	7:S:78:LEU:H	1.82	0.44
2:B:286:PRO:HD2	2:B:290:ARG:NE	2.29	0.44
1:A:632:LYS:HZ2	1:A:633:LEU:H	1.66	0.44
3:C:348:ALA:O	3:C:352:ARG:HG2	2.16	0.44
3:C:187:LYS:HZ1	3:C:206:THR:HB	1.83	0.44
2:B:853:LYS:HE2	2:B:869:THR:HG21	2.00	0.44
4:D:181:PRO:HD3	4:D:194:ILE:HD13	1.99	0.44
3:M:154:ILE:N	3:M:154:ILE:HD12	2.32	0.44
1:I:588:LEU:CD2	1:I:588:LEU:C	2.86	0.44
2:B:222:VAL:HA	2:B:223:PRO:HD2	1.79	0.44
2:B:503:MET:HA	2:B:507:VAL:HB	2.00	0.44
1:A:787:VAL:HG23	1:A:801:ARG:HH11	1.82	0.44
5:Q:113:LEU:HD12	5:Q:118:VAL:HG11	2.00	0.44
2:J:729:LEU:HB3	2:J:731:TYR:HE1	1.82	0.44
2:B:182:GLU:HG3	2:B:183:ARG:H	1.82	0.44
1:I:41:PRO:HB2	1:I:42:ILE:HD13	2.00	0.44
5:E:8:LYS:CG	6:F:7:LEU:HD22	2.47	0.44
2:B:239:THR:HG22	2:B:241:LYS:H	1.82	0.44
2:J:1068:CYS:SG	2:J:1070:HIS:CG	3.11	0.44
2:J:25:TRP:CH2	2:J:485:LEU:HD22	2.52	0.44
2:B:485:LEU:HD12	2:B:648:ALA:HA	1.99	0.44
4:O:50:ASN:ND2	4:O:52:SER:OG	2.42	0.44
1:A:542:GLU:HG2	1:A:542:GLU:H	1.49	0.44
1:A:704:GLY:C	1:A:706:LEU:H	2.21	0.44
2:J:131:LYS:N	2:J:135:CYS:SG	2.89	0.44
1:A:251:ILE:HD13	1:A:274:LEU:HD22	2.00	0.44
2:B:649:ILE:HD13	2:B:649:ILE:HA	1.80	0.44
2:J:809:LYS:H	2:J:809:LYS:HG2	1.52	0.44
1:I:445:TYR:HD2	2:J:878:LEU:HD12	1.83	0.44
1:I:667:THR:HA	2:J:916:PRO:HB3	1.99	0.44
1:I:152:ALA:HA	1:I:153:PRO:HD2	1.79	0.44
5:E:3:LYS:CE	6:F:9:GLU:OE1	2.64	0.44
2:B:902:PRO:HB2	2:B:974:MET:HG2	1.99	0.44
2:B:745:ALA:HB1	2:B:749:ARG:CZ	2.48	0.44
3:C:177:LYS:H	3:C:177:LYS:HG3	1.64	0.44
2:B:25:TRP:CH2	2:B:485:LEU:HD22	2.53	0.44
4:D:50:ASN:ND2	4:D:52:SER:OG	2.41	0.44
10:V:6:ARG:HB3	10:V:7:CYS:H	1.44	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Q:112:GLN:HA	5:Q:166:ARG:HG3	2.00	0.44
2:B:703:PRO:HG3	2:B:715:PHE:HE2	1.83	0.44
1:A:180:ARG:NH1	1:A:182:MET:SD	2.90	0.44
1:A:743:MET:HA	1:A:748:VAL:HG11	2.00	0.44
7:S:37:ILE:H	7:S:37:ILE:HG12	1.31	0.44
3:C:216:GLU:HA	3:C:220:LYS:HB3	2.00	0.44
3:M:364:ASN:O	3:M:367:ILE:HG22	2.18	0.44
3:C:204:LYS:C	3:C:206:THR:N	2.71	0.44
1:A:891:ASP:N	1:A:891:ASP:OD1	2.42	0.44
1:I:244:LYS:HE3	1:I:244:LYS:HB2	1.66	0.44
3:M:107:ALA:HB1	3:M:270:TRP:CZ2	2.52	0.44
2:J:122:ARG:HE	2:J:400:PRO:HG3	1.82	0.44
4:D:199:LEU:HD21	4:D:211:ILE:HG21	1.99	0.44
5:E:112:GLN:HA	5:E:166:ARG:HG3	2.00	0.44
2:J:35:LEU:CD2	2:J:132:SER:HA	2.48	0.44
1:I:295:HIS:O	1:I:297:SER:N	2.49	0.44
2:J:393:PHE:O	2:J:394:VAL:HG23	2.13	0.44
2:J:902:PRO:HB2	2:J:974:MET:HG2	2.00	0.44
2:J:41:PHE:HE2	2:J:356:LYS:CG	2.31	0.44
11:P:14:GLU:OE2	11:P:30:CYS:SG	2.75	0.44
1:I:74:PHE:CE1	1:I:221:PRO:HA	2.53	0.44
2:B:573:ASP:OD1	2:B:576:ARG:NE	2.40	0.44
1:I:756:ARG:NH2	2:J:922:ARG:HH22	2.16	0.44
1:I:93:HIS:NE2	1:I:160:GLU:HB2	2.33	0.44
1:A:93:HIS:CE1	1:A:160:GLU:HB2	2.53	0.44
11:W:14:GLU:HB2	11:W:15:VAL:H	1.59	0.44
2:J:126:LEU:HD12	2:J:127:PRO:HD2	1.99	0.44
5:E:113:LEU:HD12	5:E:118:VAL:HG11	2.00	0.44
1:I:704:GLY:C	1:I:706:LEU:H	2.21	0.44
3:M:384:LEU:O	5:Q:22:PRO:HG3	2.18	0.44
1:I:673:GLU:CB	1:I:809:LYS:HD2	2.48	0.44
3:C:144:GLU:HG2	3:C:144:GLU:H	1.54	0.44
1:I:104:GLY:O	1:I:194:PRO:HD2	2.18	0.44
3:M:160:VAL:CG1	3:M:161:VAL:H	2.21	0.44
1:A:100:CYS:O	1:A:103:CYS:SG	2.75	0.44
1:A:104:GLY:O	1:A:194:PRO:HD2	2.17	0.44
7:S:41:PRO:HG2	7:S:75:TYR:CE1	2.53	0.44
5:Q:61:PRO:HA	8:T:11:ARG:NH2	2.33	0.44
1:A:852:LEU:HD11	3:C:311:MET:HG3	1.99	0.44
3:C:100:ARG:HH21	3:C:288:GLU:HG2	1.81	0.44
4:O:54:LEU:HD11	10:V:2:ILE:HD12	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:1063:TRP:HE1	2:J:1094:LYS:HE3	1.82	0.44
1:I:106:ILE:HD13	1:I:201:LEU:HD11	2.00	0.44
2:B:539:VAL:HG12	2:B:557:VAL:HG12	1.99	0.44
9:U:35:ASN:ND2	9:U:73:GLU:OE1	2.51	0.44
3:C:281:ALA:O	3:C:285:ILE:HG12	2.18	0.44
2:J:778:PRO:HD3	2:J:814:GLY:HA3	1.99	0.44
1:I:351:MET:HG2	1:I:415:HIS:ND1	2.33	0.44
2:J:357:ASP:HA	2:J:360:ARG:NH1	2.32	0.44
3:C:163:ILE:CD1	3:C:163:ILE:H	2.08	0.43
2:J:182:GLU:HG3	2:J:183:ARG:H	1.82	0.43
2:B:688:ILE:HD11	10:N:62:TYR:CD1	2.52	0.43
2:B:365:GLN:HB3	2:B:365:GLN:HE21	1.56	0.43
2:B:968:HIS:HD2	2:B:969:SER:N	2.16	0.43
3:M:288:GLU:O	3:M:292:THR:OG1	2.35	0.43
4:O:181:PRO:HD3	4:O:194:ILE:HD13	1.99	0.43
4:O:62:ARG:HH12	10:V:2:ILE:HD12	1.83	0.43
1:I:536:ASP:HA	1:I:540:LEU:HB2	2.00	0.43
1:A:867:ILE:H	1:A:867:ILE:HG13	1.28	0.43
7:H:42:GLN:HA	7:H:78:LEU:H	1.82	0.43
3:M:269:ILE:H	3:M:269:ILE:HG13	1.57	0.43
1:I:852:LEU:HD13	3:M:307:LEU:HD21	1.99	0.43
2:J:992:ILE:HD11	2:J:994:TYR:CE1	2.53	0.43
1:A:93:HIS:NE2	1:A:160:GLU:HB2	2.33	0.43
5:Q:167:GLN:HB2	5:Q:170:LEU:HD12	1.99	0.43
2:J:491:THR:HB	2:J:492:GLY:H	1.58	0.43
1:A:172:GLU:OE1	1:A:173:GLU:N	2.51	0.43
2:J:222:VAL:HA	2:J:223:PRO:HD2	1.79	0.43
2:J:322:MET:HE1	2:J:523:TYR:HE2	1.83	0.43
9:L:35:ASN:ND2	9:L:73:GLU:OE1	2.52	0.43
6:R:120:PRO:O	6:R:122:GLU:N	2.44	0.43
3:C:384:LEU:HD21	5:E:18:PHE:HA	2.00	0.43
2:J:745:ALA:HB1	2:J:749:ARG:CZ	2.48	0.43
2:J:925:VAL:O	2:J:929:ILE:HG13	2.18	0.43
1:I:894:ILE:HD13	3:M:45:ILE:HD13	2.00	0.43
8:K:8:GLU:HB3	8:K:53:VAL:HG21	2.00	0.43
1:A:664:LYS:HG2	2:B:984:GLU:OE2	2.18	0.43
1:I:264:PRO:O	1:I:266:LEU:N	2.49	0.43
4:O:199:LEU:HD21	4:O:211:ILE:HG21	1.99	0.43
5:E:167:GLN:HB2	5:E:170:LEU:HD12	1.99	0.43
2:B:179:THR:HA	2:B:194:VAL:HG22	2.00	0.43
2:J:280:LEU:HA	2:J:280:LEU:HD23	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:GLN:HE22	2:B:393:PHE:HE2	1.65	0.43
2:J:391:GLN:HB3	2:J:392:ARG:H	1.67	0.43
1:A:155:PHE:HA	1:A:156:PRO:HD2	1.75	0.43
5:E:3:LYS:HZ2	6:F:9:GLU:CD	2.21	0.43
2:B:574:ASP:N	2:B:574:ASP:OD1	2.51	0.43
2:J:853:LYS:HE2	2:J:869:THR:HG21	2.00	0.43
3:M:336:ARG:HB3	3:M:345:HIS:HB3	2.00	0.43
1:A:163:THR:HB	1:A:276:GLN:NE2	2.33	0.43
2:J:539:VAL:HG12	2:J:557:VAL:HG12	1.99	0.43
2:B:148:LEU:HD13	2:B:148:LEU:HA	1.63	0.43
3:M:385:PRO:HA	5:Q:22:PRO:HD3	1.99	0.43
5:E:174:GLU:HG3	5:E:175:TRP:N	2.33	0.43
1:I:765:MET:HG3	2:J:923:MET:HG2	1.99	0.43
4:D:119:PRO:HD2	10:N:15:ALA:HB1	2.00	0.43
1:A:673:GLU:CB	1:A:809:LYS:HD2	2.48	0.43
1:A:10:SER:CB	2:B:1118:ARG:HB3	2.48	0.43
3:M:359:ASN:OD1	14:M:401:HOH:O	2.21	0.43
3:M:236:LYS:O	3:M:237:GLU:HB3	2.18	0.43
2:J:1040:LEU:O	2:J:1042:GLY:N	2.49	0.43
1:I:127:LYS:HB2	3:M:330:LYS:HB3	2.01	0.43
1:A:527:GLU:HG3	9:L:40:PHE:CD1	2.53	0.43
4:D:92:GLU:HB2	4:D:130:THR:HG23	2.00	0.43
1:I:444:PRO:O	9:U:49:ILE:CD1	2.58	0.43
3:C:152:ILE:HG13	3:C:159:TYR:CD2	2.48	0.43
1:A:757:GLY:O	1:A:758:LYS:HB2	2.17	0.43
9:L:91:ALA:C	9:L:94:GLU:OE1	2.57	0.43
2:J:749:ARG:HE	4:O:144:ALA:CB	2.30	0.43
2:B:702:VAL:O	10:N:51:SER:HB2	2.19	0.43
2:B:25:TRP:HZ2	2:B:485:LEU:HB3	1.80	0.43
2:B:485:LEU:HD11	2:B:655:SER:OG	2.19	0.43
1:A:8:ILE:HB	3:C:369:GLN:OE1	2.19	0.43
2:B:992:ILE:HD11	2:B:994:TYR:CE1	2.53	0.43
2:J:46:LEU:O	2:J:50:VAL:HG12	2.19	0.43
7:S:43:ILE:HG22	7:S:44:LYS:N	2.34	0.43
3:C:187:LYS:CE	3:C:206:THR:HB	2.48	0.43
1:A:885:GLY:O	3:C:303:ARG:NH2	2.46	0.43
5:Q:5:LEU:CD1	6:R:6:LYS:CD	2.96	0.43
1:A:635:ASP:O	1:A:638:VAL:HG22	2.18	0.43
1:I:93:HIS:CE1	1:I:160:GLU:HB2	2.53	0.43
1:A:351:MET:HG2	1:A:415:HIS:ND1	2.33	0.43
2:B:35:LEU:CD2	2:B:132:SER:HA	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:333:VAL:O	3:M:337:ALA:N	2.51	0.43
7:H:41:PRO:HG2	7:H:75:TYR:CE1	2.54	0.43
1:I:834:ARG:NH1	3:M:99:PRO:HD3	2.30	0.43
1:A:106:ILE:HD13	1:A:201:LEU:HD11	2.01	0.43
2:B:99:TYR:HB2	2:B:160:ILE:HB	2.01	0.43
2:B:1066:GLU:HA	2:B:1119:LEU:HD22	2.00	0.43
4:O:225:GLU:OE2	10:V:42:ARG:NH2	2.51	0.43
2:B:305:HIS:CE1	2:B:306:MET:HG2	2.53	0.43
1:I:436:MET:HB2	1:I:458:TYR:OH	2.19	0.43
1:I:150:CYS:CB	1:I:153:PRO:HD3	2.48	0.43
8:T:38:GLN:HG2	8:T:38:GLN:H	1.37	0.43
2:B:749:ARG:NH1	4:D:150:PHE:HZ	2.17	0.43
3:M:100:ARG:O	3:M:104:ILE:HG22	2.19	0.43
2:J:780:PRO:HA	2:J:785:TYR:CZ	2.54	0.43
1:I:582:CYS:HB2	1:I:608:PHE:CE1	2.54	0.43
2:B:698:HIS:HE1	2:B:873:LEU:HD21	1.84	0.43
2:B:516:ALA:HA	2:B:517:PRO:HA	1.72	0.43
1:A:684:HIS:O	1:A:688:ARG:HG3	2.19	0.43
1:I:251:ILE:HD13	1:I:274:LEU:HD22	2.00	0.43
1:I:447:THR:HG22	2:J:1001:VAL:HG21	2.00	0.43
2:J:378:TYR:C	2:J:380:ARG:H	2.22	0.43
1:A:103:CYS:SG	1:A:104:GLY:N	2.91	0.43
1:I:632:LYS:NZ	1:I:634:LEU:H	2.08	0.43
2:J:429:ARG:HG3	2:J:683:TRP:CZ3	2.54	0.43
3:M:100:ARG:NH2	3:M:267:ASN:O	2.52	0.43
3:M:177:LYS:C	3:M:179:VAL:N	2.72	0.43
10:V:22:LYS:HZ3	10:V:54:GLU:HG2	1.82	0.43
1:I:543:PRO:O	1:I:544:ASP:HB2	2.18	0.43
1:I:370:ARG:HD3	1:I:379:PRO:O	2.19	0.43
1:I:808:TYR:HE2	2:J:923:MET:SD	2.42	0.43
4:O:92:GLU:HB2	4:O:130:THR:HG23	1.99	0.43
3:C:13:LYS:HE2	3:C:13:LYS:HB2	1.82	0.43
2:J:41:PHE:HD1	2:J:42:ILE:CD1	2.32	0.43
7:S:43:ILE:HG22	7:S:44:LYS:H	1.84	0.43
3:M:205:VAL:HG12	3:M:205:VAL:O	2.19	0.43
1:I:564:PRO:HB2	1:I:567:LEU:HD21	2.01	0.43
5:E:100:ARG:NE	6:F:43:VAL:HG13	2.34	0.43
2:B:780:PRO:HA	2:B:785:TYR:CZ	2.54	0.43
1:I:743:MET:HA	1:I:748:VAL:HG11	2.00	0.43
7:S:56:LYS:O	7:S:58:GLY:N	2.51	0.43
2:B:393:PHE:O	2:B:394:VAL:CG1	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:CYS:SG	1:A:153:PRO:CD	3.07	0.42
10:N:62:TYR:O	10:N:63:LYS:HG3	2.20	0.42
1:I:626:TYR:HA	1:I:632:LYS:NZ	2.34	0.42
2:J:165:GLU:OE2	2:J:689:ARG:NH2	2.52	0.42
7:H:13:VAL:HG13	7:H:14:LEU:H	1.84	0.42
2:J:939:LEU:HB2	2:J:964:LEU:HD13	1.99	0.42
2:J:1101:PHE:CD1	3:M:367:ILE:HG13	2.54	0.42
4:D:45:VAL:O	11:P:46:VAL:N	2.47	0.42
2:J:591:LEU:HD22	2:J:595:HIS:NE2	2.34	0.42
2:B:591:LEU:HD22	2:B:595:HIS:NE2	2.34	0.42
3:C:385:PRO:HA	3:C:386:LEU:HD13	2.01	0.42
8:T:8:GLU:HB3	8:T:53:VAL:HG21	2.00	0.42
1:I:159:PHE:HD1	1:I:159:PHE:HA	1.78	0.42
2:J:1066:GLU:HA	2:J:1119:LEU:HD22	2.00	0.42
3:M:178:VAL:O	3:M:190:GLU:OE1	2.37	0.42
2:B:1087:GLY:C	2:B:1089:ASP:H	2.18	0.42
1:A:370:ARG:HD3	1:A:379:PRO:O	2.19	0.42
2:B:17:LEU:HB3	2:B:644:LEU:O	2.19	0.42
2:J:220:PRO:HD2	2:J:301:ASN:HB3	2.01	0.42
4:D:98:MET:HG2	4:D:100:TYR:HE1	1.84	0.42
1:I:17:SER:HB3	1:I:20:GLU:HG3	2.00	0.42
3:C:179:VAL:HG22	3:C:190:GLU:OE2	2.19	0.42
2:J:703:PRO:HG3	2:J:715:PHE:HE2	1.83	0.42
7:H:56:LYS:O	7:H:58:GLY:N	2.51	0.42
1:I:444:PRO:CB	9:U:50:THR:HG22	2.48	0.42
3:C:214:ILE:HG22	3:C:218:VAL:HB	2.01	0.42
2:B:429:ARG:HG3	2:B:683:TRP:CZ3	2.54	0.42
2:J:815:ARG:HG2	2:J:816:THR:H	1.83	0.42
1:A:221:PRO:O	1:A:226:ARG:NH2	2.49	0.42
2:J:573:ASP:OD1	2:J:576:ARG:NE	2.40	0.42
3:C:100:ARG:O	3:C:104:ILE:HG22	2.19	0.42
4:O:50:ASN:HD22	4:O:50:ASN:C	2.22	0.42
3:M:262:THR:HA	7:S:12:HIS:HB3	2.01	0.42
3:C:364:ASN:O	3:C:367:ILE:HG22	2.19	0.42
2:B:41:PHE:HD1	2:B:356:LYS:HG2	1.83	0.42
5:Q:174:GLU:HG3	5:Q:175:TRP:N	2.33	0.42
6:R:38:PHE:CD2	6:R:40:GLU:HG2	2.54	0.42
1:A:120:PHE:CD2	1:A:133:LEU:HD11	2.54	0.42
9:L:28:LEU:HD23	9:L:57:PHE:HE2	1.84	0.42
2:J:649:ILE:HD13	2:J:649:ILE:HA	1.79	0.42
3:C:160:VAL:CG2	3:C:198:LEU:HB3	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:N:56:ILE:C	10:N:58:GLN:H	2.23	0.42
7:H:65:ARG:NH1	7:H:75:TYR:HD2	2.18	0.42
2:J:749:ARG:HH21	4:O:144:ALA:HB1	1.83	0.42
2:B:573:ASP:HB2	2:B:574:ASP:H	1.63	0.42
2:J:99:TYR:HB2	2:J:160:ILE:HB	2.01	0.42
1:I:495:ARG:HG2	3:M:300:VAL:HG23	2.02	0.42
1:I:684:HIS:O	1:I:688:ARG:HG3	2.19	0.42
2:J:903:TRP:HE1	4:O:153:TYR:H	1.67	0.42
2:J:498:VAL:O	2:J:502:LEU:HG	2.19	0.42
1:I:889:ASP:O	1:I:893:VAL:HG23	2.20	0.42
1:A:9:GLY:O	3:C:358:LEU:HD11	2.19	0.42
3:M:182:LEU:HA	3:M:185:SER:OG	2.19	0.42
2:J:365:GLN:H	2:J:365:GLN:HG2	1.66	0.42
10:V:56:ILE:C	10:V:58:GLN:H	2.23	0.42
7:H:43:ILE:HG22	7:H:44:LYS:H	1.84	0.42
4:O:60:ALA:HB1	11:W:48:ALA:HB2	2.00	0.42
2:J:510:ILE:HA	2:J:513:ARG:NH2	2.34	0.42
10:N:52:HIS:CE1	10:N:54:GLU:H	2.38	0.42
1:I:364:TYR:OH	1:I:406:LEU:HB3	2.19	0.42
5:Q:174:GLU:O	5:Q:178:LYS:HB2	2.19	0.42
2:B:220:PRO:HD2	2:B:301:ASN:HB3	2.01	0.42
1:A:17:SER:HB3	1:A:20:GLU:HG3	2.01	0.42
1:I:878:ASP:HA	1:I:879:PRO:HD2	1.85	0.42
8:T:49:ILE:H	8:T:49:ILE:HG13	1.46	0.42
1:I:31:VAL:HA	1:I:32:PRO:HD3	1.86	0.42
5:Q:145:ARG:NH2	6:R:94:VAL:HG23	2.35	0.42
2:B:378:TYR:CE1	2:B:389:ASN:N	2.83	0.42
3:M:160:VAL:CG1	3:M:161:VAL:N	2.79	0.42
1:A:750:MET:C	1:A:753:THR:HG22	2.40	0.42
3:M:130:LYS:O	3:M:134:VAL:HG23	2.19	0.42
3:C:187:LYS:O	3:C:188:SER:HB2	2.20	0.42
3:M:213:LYS:O	3:M:216:GLU:HG3	2.18	0.42
1:I:712:LYS:HD2	3:M:93:ASN:OD1	2.20	0.42
2:B:925:VAL:O	2:B:929:ILE:HG13	2.20	0.42
9:L:28:LEU:HD23	9:L:57:PHE:CE2	2.55	0.42
6:F:38:PHE:CD2	6:F:40:GLU:HG2	2.54	0.42
1:I:456:PRO:HB3	1:I:628:ARG:NH1	2.35	0.42
2:B:58:PRO:HG3	2:B:63:PHE:HB2	2.02	0.42
9:U:49:ILE:HG22	9:U:50:THR:N	2.21	0.42
4:D:161:VAL:HG11	4:D:171:LEU:HD12	2.01	0.42
3:M:109:LYS:HA	3:M:270:TRP:CD1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:404:GLU:HG2	1:I:404:GLU:H	1.69	0.42
5:E:174:GLU:O	5:E:178:LYS:HB2	2.19	0.42
2:B:498:VAL:O	2:B:502:LEU:HG	2.19	0.42
3:M:343:THR:OG1	3:M:344:GLN:OE1	2.34	0.42
2:B:378:TYR:C	2:B:380:ARG:H	2.22	0.42
1:I:44:GLY:HA2	1:I:49:LYS:HD3	2.01	0.42
7:S:65:ARG:NH1	7:S:75:TYR:HD2	2.17	0.42
1:I:9:GLY:HA3	2:J:1120:LYS:CG	2.50	0.42
1:A:456:PRO:HB3	1:A:628:ARG:NH1	2.35	0.42
1:A:462:PHE:CD2	2:B:737:GLU:HB2	2.55	0.42
1:I:756:ARG:NH1	2:J:922:ARG:HH12	2.17	0.42
1:I:635:ASP:O	1:I:638:VAL:HG22	2.18	0.42
2:B:554:VAL:HA	2:B:578:ARG:NH1	2.35	0.42
1:I:370:ARG:HH21	1:I:417:GLU:CD	2.22	0.42
1:I:439:ARG:NH1	1:I:486:GLU:OE2	2.52	0.42
1:I:658:ILE:HD13	2:J:733:GLY:HA3	2.02	0.42
1:I:120:PHE:CD2	1:I:133:LEU:HD11	2.54	0.42
1:A:863:PRO:HB2	3:C:360:GLY:HA2	2.02	0.42
4:O:24:PRO:HB3	9:U:30:GLU:OE1	2.19	0.42
2:B:189:LYS:HB3	2:B:190:VAL:H	1.60	0.42
2:B:681:LEU:O	2:B:718:ARG:HB3	2.20	0.42
5:Q:48:ILE:HA	5:Q:74:VAL:HG13	2.01	0.42
3:M:214:ILE:C	3:M:216:GLU:N	2.73	0.42
3:M:348:ALA:O	3:M:352:ARG:HG2	2.18	0.42
2:B:31:VAL:HG21	2:B:155:PRO:HB2	2.02	0.42
2:J:645:MET:HA	2:J:646:PRO:HD2	1.95	0.42
1:I:781:ARG:HH22	2:J:341:ASP:HB2	1.84	0.42
1:I:368:LYS:O	1:I:372:LEU:HB2	2.20	0.42
2:B:77:PHE:HD1	2:B:77:PHE:HA	1.67	0.42
3:C:72:ILE:HA	3:C:72:ILE:HD12	1.89	0.42
2:B:63:PHE:HB3	2:B:392:ARG:NH2	2.34	0.42
3:C:163:ILE:HG22	3:C:165:PRO:HD3	2.02	0.42
1:I:147:CYS:SG	1:I:152:ALA:HA	2.58	0.42
2:B:365:GLN:HG2	2:B:365:GLN:H	1.67	0.42
3:C:120:LEU:C	3:C:260:ASP:HB2	2.40	0.42
2:J:485:LEU:HD11	2:J:655:SER:OG	2.19	0.42
1:I:656:LEU:O	1:I:660:VAL:HG23	2.20	0.42
2:J:17:LEU:HB3	2:J:644:LEU:O	2.19	0.42
1:I:587:LYS:HB2	1:I:588:LEU:H	1.72	0.42
8:T:16:ARG:HG2	8:T:49:ILE:HG22	2.02	0.42
2:J:898:GLN:O	2:J:901:MET:HB2	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:366:LEU:HD21	2:B:398:ILE:O	2.20	0.42
9:U:44:THR:C	9:U:45:ILE:CG1	2.88	0.42
1:A:150:CYS:O	1:A:152:ALA:CA	2.65	0.42
1:I:432:ARG:O	1:I:434:SER:N	2.53	0.42
3:C:177:LYS:HE2	3:C:178:VAL:N	2.34	0.42
3:M:120:LEU:C	3:M:260:ASP:HB2	2.40	0.42
4:D:50:ASN:C	4:D:50:ASN:HD22	2.23	0.42
7:H:43:ILE:HG22	7:H:44:LYS:N	2.34	0.42
2:J:758:ARG:NH1	2:J:844:ARG:HG3	2.34	0.42
3:C:109:LYS:HA	3:C:270:TRP:CD1	2.55	0.42
1:A:439:ARG:NH1	1:A:486:GLU:OE2	2.52	0.42
1:A:772:GLN:HB2	1:A:779:LEU:HD11	2.02	0.42
1:A:370:ARG:HH21	1:A:417:GLU:CD	2.22	0.42
2:J:31:VAL:HG21	2:J:155:PRO:HB2	2.02	0.42
1:I:553:TRP:HB3	1:I:558:ILE:HD11	2.01	0.42
1:A:521:PHE:CD1	1:A:521:PHE:N	2.88	0.42
3:C:165:PRO:HG2	3:C:166:GLU:OE2	2.20	0.41
3:M:153:ASP:CG	3:M:157:MET:CB	2.87	0.41
2:B:510:ILE:HA	2:B:513:ARG:HG3	2.01	0.41
1:A:656:LEU:O	1:A:660:VAL:HG23	2.20	0.41
1:A:463:ASP:HA	2:B:890:GLY:CA	2.49	0.41
1:I:782:GLY:O	2:J:459:HIS:HE1	2.03	0.41
2:J:681:LEU:O	2:J:718:ARG:HB3	2.20	0.41
4:O:61:HIS:O	4:O:65:MET:HG2	2.20	0.41
4:D:23:VAL:HA	4:D:220:PHE:HE2	1.85	0.41
2:B:801:PHE:O	2:B:804:SER:OG	2.36	0.41
2:B:731:TYR:HE2	2:B:902:PRO:CG	2.31	0.41
2:J:286:PRO:HD2	2:J:290:ARG:NE	2.28	0.41
2:B:165:GLU:OE2	2:B:689:ARG:NH2	2.52	0.41
2:J:749:ARG:NH1	4:O:150:PHE:HZ	2.18	0.41
1:I:63:CYS:SG	1:I:73:HIS:NE2	2.77	0.41
3:C:288:GLU:O	3:C:292:THR:OG1	2.35	0.41
2:J:554:VAL:HA	2:J:578:ARG:NH1	2.35	0.41
2:J:148:LEU:HA	2:J:148:LEU:HD13	1.63	0.41
2:J:498:VAL:HG12	2:J:502:LEU:HD11	2.02	0.41
2:B:130:LEU:HD22	2:B:158:TYR:CZ	2.55	0.41
7:H:66:LYS:HG2	7:H:72:TYR:CE1	2.55	0.41
1:A:756:ARG:HB3	2:B:921:SER:HB3	2.01	0.41
4:O:112:LYS:HB3	4:O:112:LYS:HE2	1.89	0.41
2:B:809:LYS:H	2:B:809:LYS:HG2	1.52	0.41
5:E:3:LYS:HD2	6:F:11:TYR:CE1	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:21:LYS:HE3	3:C:21:LYS:HB3	1.41	0.41
1:A:309:LYS:HZ1	3:C:343:THR:HA	1.85	0.41
1:A:854:VAL:CG2	3:C:62:GLU:HB3	2.50	0.41
2:J:940:THR:OG1	2:J:964:LEU:HD11	2.20	0.41
2:B:940:THR:OG1	2:B:964:LEU:HD11	2.20	0.41
1:A:441:ARG:O	1:A:443:MET:HG3	2.20	0.41
3:C:100:ARG:NH2	3:C:267:ASN:O	2.52	0.41
4:O:161:VAL:HG11	4:O:171:LEU:HD12	2.01	0.41
1:I:536:ASP:O	1:I:537:VAL:C	2.59	0.41
5:E:48:ILE:HA	5:E:74:VAL:HG13	2.03	0.41
1:I:31:VAL:HG11	1:I:43:GLU:OE1	2.20	0.41
1:A:553:TRP:HB3	1:A:558:ILE:HD11	2.02	0.41
1:I:521:PHE:N	1:I:521:PHE:CD1	2.88	0.41
3:C:215:ALA:O	3:C:220:LYS:HB2	2.19	0.41
4:D:201:ARG:HA	4:D:204:GLU:CG	2.50	0.41
1:A:244:LYS:O	1:A:248:ILE:HG13	2.21	0.41
2:J:592:THR:HB	2:J:593:ARG:H	1.64	0.41
2:J:801:PHE:O	2:J:804:SER:OG	2.37	0.41
3:M:143:LEU:HA	3:M:146:LEU:HB2	2.03	0.41
2:J:508:VAL:HA	2:J:509:PRO:HD2	1.88	0.41
3:M:55:LYS:HG2	8:T:3:ARG:NH2	2.35	0.41
1:I:709:LEU:H	1:I:717:THR:HG21	1.85	0.41
1:A:635:ASP:OD1	1:A:639:ARG:NE	2.50	0.41
1:A:889:ASP:O	1:A:893:VAL:HG23	2.20	0.41
1:A:878:ASP:HA	1:A:879:PRO:HD2	1.85	0.41
1:A:331:VAL:HG23	2:B:1001:VAL:HG23	2.01	0.41
4:D:61:HIS:O	4:D:65:MET:HG2	2.20	0.41
1:A:368:LYS:O	1:A:372:LEU:HB2	2.20	0.41
3:M:160:VAL:C	3:M:161:VAL:HG23	2.40	0.41
1:I:13:PHE:HB2	3:M:355:VAL:O	2.20	0.41
1:A:854:VAL:HG22	3:C:64:VAL:HG23	2.03	0.41
3:C:130:LYS:O	3:C:134:VAL:HG23	2.19	0.41
4:O:201:ARG:HA	4:O:204:GLU:CG	2.50	0.41
7:S:13:VAL:HG13	7:S:14:LEU:H	1.84	0.41
3:C:55:LYS:HG2	8:K:3:ARG:NH2	2.33	0.41
5:Q:5:LEU:HD13	6:R:6:LYS:HD3	2.02	0.41
1:I:635:ASP:OD1	1:I:639:ARG:NE	2.50	0.41
10:V:52:HIS:CE1	10:V:54:GLU:H	2.38	0.41
5:E:2:TYR:OH	6:F:44:SER:OG	2.27	0.41
1:I:209:ARG:HB2	1:I:212:TRP:CE2	2.56	0.41
5:Q:27:LYS:HD2	5:Q:50:ASP:HA	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:385:PRO:HA	5:Q:22:PRO:CD	2.50	0.41
2:B:670:TYR:O	2:B:674:MET:HB2	2.20	0.41
1:A:238:GLU:HG2	1:A:239:ASP:N	2.35	0.41
4:O:41:ALA:HB3	4:O:146:TRP:CD1	2.56	0.41
2:B:1083:CYS:HB2	2:B:1084:PRO:HD2	2.02	0.41
1:A:679:ALA:O	1:A:683:ILE:HG12	2.21	0.41
2:B:983:LEU:HG	2:B:983:LEU:H	1.65	0.41
2:B:274:LEU:HD12	2:B:274:LEU:HA	1.89	0.41
3:C:189:ALA:HB2	3:C:200:VAL:O	2.21	0.41
3:M:191:PHE:HA	3:M:191:PHE:HD1	1.69	0.41
1:A:307:ARG:C	1:A:309:LYS:H	2.23	0.41
1:A:456:PRO:HB3	1:A:628:ARG:HH11	1.85	0.41
1:I:244:LYS:O	1:I:248:ILE:HG13	2.21	0.41
2:B:193:LYS:HE3	2:B:204:LEU:HD11	2.03	0.41
1:A:709:LEU:H	1:A:717:THR:HG21	1.85	0.41
1:I:456:PRO:HB3	1:I:628:ARG:HH11	1.86	0.41
1:A:472:PRO:HG2	1:A:478:GLN:HG2	2.03	0.41
2:J:912:LEU:HD23	2:J:912:LEU:HA	1.89	0.41
2:J:373:GLN:HE21	2:J:397:SER:HA	1.84	0.41
2:B:731:TYR:C	2:B:733:GLY:H	2.23	0.41
9:L:43:TYR:O	9:L:44:THR:HG22	2.21	0.41
1:A:74:PHE:CE1	1:A:221:PRO:HA	2.55	0.41
2:J:189:LYS:HZ2	3:M:212:ARG:NH1	2.19	0.41
2:J:174:LEU:HD11	2:J:340:LYS:HB2	2.02	0.41
2:B:591:LEU:HD13	2:B:595:HIS:ND1	2.35	0.41
1:A:867:ILE:HD12	7:H:40:LEU:HA	2.03	0.41
10:N:7:CYS:HB2	10:N:14:LEU:HD12	2.03	0.41
2:B:116:GLN:HE21	2:B:117:GLU:HB3	1.86	0.41
2:B:678:SER:OG	2:B:995:GLN:OE1	2.29	0.41
2:J:16:GLU:HA	2:J:19:LEU:HD12	2.03	0.41
6:F:121:LEU:HD23	6:F:121:LEU:HA	1.91	0.41
3:M:157:MET:HB3	3:M:160:VAL:CG2	2.51	0.41
2:J:773:ASP:OD2	2:J:815:ARG:NH1	2.44	0.41
2:B:691:ASP:O	2:B:759:THR:HG23	2.21	0.41
1:A:244:LYS:HE3	1:A:244:LYS:HB2	1.66	0.41
1:A:848:ALA:HB2	3:C:327:VAL:CG2	2.51	0.41
1:A:62:THR:HA	2:B:1077:ARG:HH11	1.85	0.41
2:B:1082:TYR:HD1	2:B:1088:GLU:N	2.18	0.41
1:I:772:GLN:HB2	1:I:779:LEU:HD11	2.01	0.41
9:L:4:GLU:HB2	9:L:16:TYR:HB2	2.03	0.41
2:J:135:CYS:O	2:J:137:LEU:N	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:898:GLN:O	2:B:901:MET:HB2	2.20	0.41
4:O:219:SER:C	4:O:220:PHE:HD1	2.24	0.41
3:M:144:GLU:HG2	3:M:144:GLU:H	1.56	0.41
3:M:72:ILE:HD12	3:M:72:ILE:HA	1.88	0.41
1:I:472:PRO:HG2	1:I:478:GLN:HG2	2.02	0.41
1:I:441:ARG:O	1:I:443:MET:HG3	2.20	0.41
3:C:194:GLU:CD	3:C:196:TYR:HE2	2.22	0.41
2:J:116:GLN:HE21	2:J:117:GLU:HB3	1.86	0.41
3:M:157:MET:C	3:M:159:TYR:H	2.24	0.41
2:B:731:TYR:CZ	2:B:902:PRO:HG3	2.55	0.41
9:L:43:TYR:C	9:L:44:THR:CG2	2.89	0.41
10:N:61:VAL:O	10:N:61:VAL:HG22	2.21	0.41
8:K:38:GLN:HG2	8:K:38:GLN:H	1.37	0.41
3:C:187:LYS:HB2	3:C:188:SER:H	1.73	0.41
1:A:564:PRO:HB2	1:A:567:LEU:HD21	2.02	0.41
2:J:691:ASP:O	2:J:759:THR:HG23	2.21	0.41
2:J:520:TYR:OH	2:J:535:GLY:HA2	2.21	0.41
1:A:583:GLU:HG3	1:A:584:ALA:H	1.86	0.41
1:A:159:PHE:HD1	1:A:159:PHE:HA	1.78	0.41
2:J:1054:LEU:O	2:J:1056:GLU:N	2.54	0.41
4:O:225:GLU:HG3	10:V:12:LYS:NZ	2.36	0.41
2:B:135:CYS:O	2:B:137:LEU:N	2.54	0.41
1:A:542:GLU:HA	1:A:543:PRO:HA	1.90	0.41
2:B:498:VAL:HG12	2:B:502:LEU:HD11	2.02	0.41
4:O:23:VAL:HA	4:O:220:PHE:HE2	1.85	0.41
2:J:980:GLY:HA3	4:O:23:VAL:HG13	2.03	0.41
1:I:679:ALA:O	1:I:683:ILE:HG12	2.21	0.41
1:I:230:THR:HG22	1:I:236:ARG:HD3	2.03	0.41
2:B:16:GLU:HA	2:B:19:LEU:HD12	2.03	0.41
2:B:903:TRP:HZ3	2:B:977:GLY:HA2	1.86	0.41
1:I:479:ALA:O	1:I:483:ILE:HG12	2.21	0.41
1:A:22:ARG:HA	1:A:76:HIS:ND1	2.36	0.41
1:A:285:ASN:ND2	1:A:301:LEU:O	2.43	0.41
2:J:698:HIS:HE1	2:J:873:LEU:HD21	1.84	0.41
1:I:24:MET:HA	2:J:1084:PRO:CB	2.50	0.41
1:A:479:ALA:O	1:A:483:ILE:HG12	2.21	0.41
2:J:109:PRO:HG2	2:J:116:GLN:OE1	2.21	0.41
3:M:148:ARG:CZ	3:M:162:GLU:HB3	2.38	0.41
1:I:307:ARG:C	1:I:309:LYS:H	2.24	0.41
2:B:968:HIS:CD2	2:B:969:SER:N	2.89	0.41
2:B:47:GLN:HE21	2:B:51:ASN:ND2	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:189:LYS:NZ	3:M:212:ARG:HH12	2.19	0.41
2:B:520:TYR:OH	2:B:535:GLY:HA2	2.21	0.41
2:B:204:LEU:HD23	2:B:205:ILE:N	2.36	0.41
1:I:789:THR:HG21	2:J:623:GLU:OE2	2.21	0.41
1:I:86:VAL:HG11	1:I:287:THR:HG21	2.03	0.41
3:M:217:LYS:C	3:M:218:VAL:HG23	2.41	0.41
2:J:1050:ILE:HD11	3:M:370:PRO:CA	2.50	0.41
1:I:493:SER:HA	1:I:494:PRO:HD3	1.92	0.41
1:A:209:ARG:HB2	1:A:212:TRP:CE2	2.56	0.41
8:K:16:ARG:HG2	8:K:49:ILE:HG22	2.02	0.41
11:P:17:LEU:HD11	11:P:27:CYS:HA	2.03	0.41
1:A:856:TYR:HE2	3:C:377:ILE:O	2.04	0.41
2:J:1122:ARG:NE	2:J:1122:ARG:C	2.75	0.40
1:I:662:THR:HG23	2:J:731:TYR:HA	2.03	0.40
1:I:147:CYS:HA	1:I:148:PRO:HD3	1.83	0.40
5:E:3:LYS:CE	6:F:9:GLU:CD	2.90	0.40
3:M:183:THR:C	3:M:185:SER:N	2.75	0.40
3:M:183:THR:O	3:M:185:SER:N	2.53	0.40
10:N:60:MET:C	10:N:62:TYR:N	2.73	0.40
1:A:362:PHE:HD2	8:K:34:ILE:O	2.03	0.40
1:I:622:ASP:OD1	1:I:624:LYS:HB2	2.21	0.40
2:J:968:HIS:CD2	2:J:969:SER:N	2.89	0.40
3:C:96:LEU:CB	3:C:100:ARG:HB2	2.49	0.40
2:J:520:TYR:CZ	2:J:535:GLY:HA2	2.56	0.40
10:V:7:CYS:HB2	10:V:14:LEU:HD12	2.03	0.40
3:C:107:ALA:HB1	3:C:270:TRP:HZ2	1.86	0.40
2:J:521:ARG:N	2:J:531:THR:HG22	2.36	0.40
5:E:27:LYS:HD2	5:E:50:ASP:HA	2.03	0.40
2:J:130:LEU:HD22	2:J:158:TYR:CZ	2.55	0.40
2:J:58:PRO:HG3	2:J:63:PHE:HB2	2.02	0.40
1:A:831:THR:HA	3:C:80:THR:HG21	2.03	0.40
1:A:628:ARG:O	1:A:630:ASP:N	2.46	0.40
2:J:309:ASP:HB2	2:J:312:ASN:ND2	2.37	0.40
7:H:43:ILE:O	7:H:80:VAL:N	2.53	0.40
1:I:841:MET:O	1:I:845:LEU:HG	2.22	0.40
2:J:670:TYR:O	2:J:674:MET:HB2	2.20	0.40
4:O:157:THR:HG22	4:O:215:ILE:HA	2.03	0.40
1:A:55:ASP:O	1:A:57:GLY:N	2.52	0.40
10:N:1:MET:H1	10:N:55:LEU:N	2.18	0.40
5:E:156:ILE:H	5:E:156:ILE:HG13	1.68	0.40
2:B:114:ILE:HG12	2:B:114:ILE:H	1.79	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:334:LEU:HA	3:M:337:ALA:HB3	2.03	0.40
2:B:429:ARG:HD2	2:B:429:ARG:HA	1.78	0.40
6:F:117:GLU:C	6:F:119:ARG:H	2.24	0.40
3:M:107:ALA:HB1	3:M:270:TRP:HZ2	1.87	0.40
2:B:95:ARG:NH2	11:P:33:LYS:HD3	2.37	0.40
1:A:187:ARG:HD2	1:A:214:VAL:HB	2.03	0.40
3:M:320:PRO:O	3:M:325:GLY:HA3	2.21	0.40
3:C:320:PRO:O	3:C:325:GLY:HA3	2.22	0.40
4:O:219:SER:O	4:O:220:PHE:HD1	2.05	0.40
5:E:24:GLU:O	5:E:28:ILE:HG13	2.22	0.40
4:D:41:ALA:HB3	4:D:146:TRP:CD1	2.56	0.40
1:A:436:MET:HB2	1:A:458:TYR:OH	2.21	0.40
1:I:362:PHE:CZ	8:T:26:VAL:HG21	2.57	0.40
2:B:153:LYS:HD2	2:B:153:LYS:HA	1.86	0.40
3:M:160:VAL:HG13	3:M:199:VAL:H	1.86	0.40
4:O:141:LYS:HE3	4:O:141:LYS:HB2	1.96	0.40
10:N:12:LYS:HB3	10:N:12:LYS:HE3	1.65	0.40
3:C:55:LYS:HE2	8:K:3:ARG:NH2	2.32	0.40
2:J:591:LEU:HD13	2:J:595:HIS:ND1	2.35	0.40
6:R:117:GLU:C	6:R:119:ARG:H	2.24	0.40
2:J:509:PRO:C	2:J:511:GLU:H	2.24	0.40
1:I:709:LEU:HD12	1:I:717:THR:HA	2.04	0.40
4:O:118:ILE:HG23	10:V:15:ALA:HB3	2.04	0.40
2:J:121:VAL:HG12	2:J:122:ARG:O	2.21	0.40
1:I:526:VAL:HG21	1:I:553:TRP:CD1	2.57	0.40
2:J:193:LYS:HE2	2:J:195:PHE:CE2	2.56	0.40
1:I:419:GLY:N	1:I:440:VAL:O	2.52	0.40
3:M:13:LYS:HE2	3:M:13:LYS:HB2	1.83	0.40
9:L:43:TYR:C	9:L:44:THR:HG23	2.41	0.40
3:C:204:LYS:HG3	3:C:205:VAL:N	2.36	0.40
2:J:10:PRO:O	2:J:11:THR:OG1	2.24	0.40
2:B:193:LYS:HE2	2:B:195:PHE:CE2	2.56	0.40
2:J:459:HIS:CE1	2:J:461:THR:HG23	2.57	0.40
1:I:28:GLU:HB2	1:I:76:HIS:HE2	1.87	0.40
2:J:516:ALA:HA	2:J:517:PRO:HA	1.72	0.40

All (20) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:98:LYS:NZ	5:Q:82:GLN:NE2[3_445]	1.00	1.20

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PRO:C	6:F:31:GLU:OE1[1_655]	1.06	1.14
2:B:61:PRO:O	6:F:31:GLU:OE1[1_655]	1.11	1.09
2:B:61:PRO:CB	6:F:31:GLU:CD[1_655]	1.35	0.85
2:B:61:PRO:CA	6:F:31:GLU:OE1[1_655]	1.41	0.79
2:B:61:PRO:CA	6:F:31:GLU:CD[1_655]	1.59	0.61
11:P:29:TYR:CD2	6:R:122:GLU:CD[1_655]	1.66	0.54
2:B:61:PRO:CB	6:F:31:GLU:OE2[1_655]	1.66	0.54
2:B:61:PRO:CA	6:F:31:GLU:OE2[1_655]	1.70	0.50
11:P:29:TYR:CD2	6:R:122:GLU:OE1[1_655]	1.73	0.47
11:P:29:TYR:CD2	6:R:122:GLU:OE2[1_655]	1.75	0.45
11:P:29:TYR:CG	6:R:122:GLU:OE1[1_655]	1.77	0.43
6:F:98:LYS:NZ	5:Q:82:GLN:CD[3_445]	1.86	0.34
2:B:61:PRO:CB	6:F:31:GLU:OE1[1_655]	1.97	0.23
6:F:97:ALA:O	5:Q:81:ASN:ND2[3_445]	2.05	0.15
2:B:61:PRO:CB	6:F:31:GLU:CG[1_655]	2.08	0.12
5:E:81:ASN:ND2	6:R:97:ALA:O[3_445]	2.08	0.12
11:P:29:TYR:CB	6:R:122:GLU:OE1[1_655]	2.08	0.12
5:E:82:GLN:OE1	6:R:98:LYS:CD[3_445]	2.08	0.12
2:B:284:GLY:N	1:I:150:CYS:O[3_545]	2.17	0.03

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	855/906 (94%)	689 (81%)	116 (14%)	50 (6%)	2 23
1	I	853/906 (94%)	692 (81%)	110 (13%)	51 (6%)	2 21
2	B	1061/1123 (94%)	872 (82%)	141 (13%)	48 (4%)	3 30
2	J	1061/1123 (94%)	864 (81%)	143 (14%)	54 (5%)	2 26
3	C	365/391 (93%)	258 (71%)	73 (20%)	34 (9%)	1 11
3	M	365/391 (93%)	266 (73%)	75 (20%)	24 (7%)	1 19
4	D	256/259 (99%)	241 (94%)	12 (5%)	3 (1%)	16 61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	O	256/259 (99%)	242 (94%)	11 (4%)	3 (1%)	16 61
5	E	179/190 (94%)	161 (90%)	18 (10%)	0	100 100
5	Q	179/190 (94%)	161 (90%)	18 (10%)	0	100 100
6	F	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	5 39
6	R	120/122 (98%)	108 (90%)	8 (7%)	4 (3%)	5 39
7	H	74/82 (90%)	59 (80%)	10 (14%)	5 (7%)	1 19
7	S	74/82 (90%)	60 (81%)	10 (14%)	4 (5%)	2 25
8	K	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1 16
8	T	54/57 (95%)	43 (80%)	7 (13%)	4 (7%)	1 16
9	L	92/100 (92%)	74 (80%)	12 (13%)	6 (6%)	1 20
9	U	92/100 (92%)	75 (82%)	10 (11%)	7 (8%)	1 15
10	N	61/65 (94%)	44 (72%)	11 (18%)	6 (10%)	1 10
10	V	61/65 (94%)	44 (72%)	11 (18%)	6 (10%)	1 10
11	P	40/49 (82%)	24 (60%)	10 (25%)	6 (15%)	0 3
11	W	40/49 (82%)	22 (55%)	11 (28%)	7 (18%)	0 2
All	All	6312/6688 (94%)	5150 (82%)	832 (13%)	330 (5%)	2 25

All (330) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	ASP
1	A	151	GLY
1	A	153	PRO
1	A	154	GLN
1	A	398	ASN
1	A	400	GLU
1	A	430	LEU
1	A	463	ASP
1	A	537	VAL
1	A	583	GLU
1	A	630	ASP
2	B	57	VAL
2	B	183	ARG
2	B	286	PRO
2	B	287	LYS
2	B	391	GLN
2	B	392	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	394	VAL
2	B	430	THR
2	B	513	ARG
2	B	515	PRO
2	B	521	ARG
2	B	845	PRO
3	C	161	VAL
3	C	162	GLU
3	C	165	PRO
3	C	181	LYS
3	C	224	LYS
4	D	209	LYS
7	H	9	ILE
7	H	11	ASP
8	K	28	ILE
8	K	30	VAL
9	L	49	ILE
9	L	93	ILE
10	N	2	ILE
10	N	61	VAL
11	P	19	LEU
11	P	20	ALA
1	I	40	TYR
1	I	41	PRO
1	I	48	ASP
1	I	154	GLN
1	I	395	MET
1	I	397	SER
1	I	398	ASN
1	I	400	GLU
1	I	430	LEU
1	I	463	ASP
1	I	537	VAL
1	I	583	GLU
1	I	587	LYS
1	I	642	GLY
1	I	643	VAL
2	J	43	ASP
2	J	57	VAL
2	J	183	ARG
2	J	286	PRO
2	J	287	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	392	ARG
2	J	393	PHE
2	J	394	VAL
2	J	396	ASN
2	J	430	THR
2	J	515	PRO
2	J	521	ARG
2	J	845	PRO
3	M	152	ILE
3	M	205	VAL
3	M	224	LYS
3	M	237	GLU
3	M	340	GLU
4	O	209	LYS
7	S	11	ASP
8	T	28	ILE
8	T	30	VAL
9	U	93	ILE
10	V	2	ILE
1	A	64	GLY
1	A	65	ALA
1	A	296	LYS
1	A	297	SER
1	A	405	LYS
1	A	578	GLU
1	A	585	LEU
1	A	608	PHE
1	A	758	LYS
2	B	56	VAL
2	B	79	GLU
2	B	138	TYR
2	B	390	ILE
2	B	944	VAL
2	B	1055	GLU
2	B	1057	SER
2	B	1082	TYR
3	C	94	VAL
3	C	160	VAL
3	C	209	SER
3	C	323	ARG
3	C	342	THR
3	C	343	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	346	LEU
3	C	357	PRO
3	C	358	LEU
3	C	361	VAL
3	C	385	PRO
10	N	11	GLY
11	P	13	LYS
11	P	14	GLU
1	I	35	TYR
1	I	64	GLY
1	I	65	ALA
1	I	103	CYS
1	I	174	GLY
1	I	297	SER
1	I	585	LEU
1	I	586	GLU
1	I	608	PHE
2	J	40	ALA
2	J	56	VAL
2	J	79	GLU
2	J	138	TYR
2	J	944	VAL
2	J	1055	GLU
2	J	1057	SER
2	J	1077	ARG
3	M	93	ASN
3	M	323	ARG
3	M	357	PRO
3	M	358	LEU
3	M	361	VAL
7	S	7	PHE
9	U	48	PRO
10	V	11	GLY
11	W	13	LYS
11	W	14	GLU
1	A	172	GLU
1	A	173	GLU
1	A	261	ALA
1	A	378	TYR
1	A	395	MET
1	A	397	SER
1	A	404	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	548	ASN
1	A	710	PRO
1	A	754	GLY
1	A	896	ARG
2	B	136	ARG
2	B	212	ASP
2	B	222	VAL
2	B	591	LEU
2	B	780	PRO
2	B	819	PRO
3	C	35	TYR
3	C	36	LYS
3	C	108	ARG
3	C	140	GLY
3	C	158	GLU
3	C	182	LEU
3	C	188	SER
3	C	191	PHE
3	C	221	HIS
9	L	23	THR
9	L	50	THR
1	I	261	ALA
1	I	378	TYR
1	I	396	GLU
1	I	433	MET
1	I	578	GLU
1	I	710	PRO
2	J	136	ARG
2	J	212	ASP
2	J	222	VAL
2	J	397	SER
2	J	591	LEU
2	J	780	PRO
2	J	1042	GLY
2	J	1076	LYS
3	M	35	TYR
3	M	36	LYS
3	M	108	ARG
3	M	140	GLY
3	M	208	LEU
3	M	215	ALA
3	M	218	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	221	HIS
9	U	23	THR
9	U	50	THR
1	A	69	GLU
1	A	152	ALA
1	A	161	ARG
1	A	265	GLN
1	A	433	MET
1	A	544	ASP
1	A	767	ALA
1	A	871	LYS
2	B	82	GLY
2	B	188	ASN
2	B	223	PRO
2	B	236	GLY
2	B	269	THR
2	B	379	GLN
2	B	774	ASN
2	B	919	ILE
2	B	923	MET
3	C	107	ALA
3	C	121	ASP
3	C	142	THR
3	C	163	ILE
3	C	344	GLN
6	F	28	GLY
6	F	31	GLU
6	F	118	TYR
7	H	57	PRO
11	P	24	GLU
1	I	69	GLU
1	I	161	ARG
1	I	265	GLN
1	I	405	LYS
1	I	538	ASN
1	I	588	LEU
1	I	632	LYS
1	I	767	ALA
2	J	46	LEU
2	J	82	GLY
2	J	188	ASN
2	J	223	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	236	GLY
2	J	269	THR
2	J	379	GLN
2	J	774	ASN
2	J	919	ILE
3	M	107	ALA
3	M	121	ASP
3	M	142	THR
3	M	187	LYS
6	R	28	GLY
6	R	31	GLU
6	R	118	TYR
7	S	57	PRO
11	W	21	THR
11	W	24	GLU
1	A	535	MET
1	A	540	LEU
1	A	542	GLU
1	A	632	LYS
1	A	756	ARG
1	A	867	ILE
1	A	888	VAL
2	B	11	THR
2	B	32	ARG
2	B	224	LYS
2	B	445	PRO
2	B	498	VAL
2	B	516	ALA
2	B	837	ARG
2	B	876	PRO
2	B	1072	ALA
3	C	187	LYS
3	C	341	ILE
3	C	384	LEU
4	D	11	PRO
7	H	10	PHE
9	L	48	PRO
10	N	41	GLU
11	P	42	VAL
1	I	44	GLY
1	I	152	ALA
1	I	296	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	540	LEU
1	I	542	GLU
1	I	544	ASP
1	I	867	ILE
1	I	871	LYS
1	I	888	VAL
2	J	11	THR
2	J	32	ARG
2	J	224	LYS
2	J	399	ARG
2	J	498	VAL
2	J	516	ALA
2	J	837	ARG
2	J	876	PRO
2	J	1046	ALA
2	J	1072	ALA
3	M	203	LYS
4	O	11	PRO
10	V	41	GLU
11	W	19	LEU
11	W	42	VAL
1	A	36	ASP
1	A	464	GLY
2	B	46	LEU
2	B	1112	VAL
7	H	80	VAL
8	K	24	ALA
9	L	46	GLU
10	N	3	VAL
10	N	4	PRO
1	I	464	GLY
1	I	535	MET
1	I	633	LEU
2	J	445	PRO
2	J	1041	ILE
2	J	1112	VAL
3	M	95	THR
7	S	80	VAL
8	T	24	ALA
9	U	51	MET
9	U	53	ARG
10	V	3	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	V	4	PRO
11	W	20	ALA
2	B	705	VAL
4	D	21	VAL
2	J	705	VAL
4	O	21	VAL
9	U	49	ILE
10	V	61	VAL
1	A	543	PRO
2	B	517	PRO
3	C	205	VAL
6	F	33	PRO
1	I	543	PRO
2	J	517	PRO
6	R	33	PRO
1	A	41	PRO
8	K	33	GLY
2	J	390	ILE
8	T	33	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	743/779 (95%)	639 (86%)	104 (14%)	4 24
1	I	740/779 (95%)	636 (86%)	104 (14%)	4 24
2	B	923/969 (95%)	788 (85%)	135 (15%)	4 22
2	J	923/969 (95%)	787 (85%)	136 (15%)	4 22
3	C	314/334 (94%)	252 (80%)	62 (20%)	1 9
3	M	313/334 (94%)	250 (80%)	63 (20%)	1 9
4	D	227/228 (100%)	218 (96%)	9 (4%)	38 75
4	O	227/228 (100%)	218 (96%)	9 (4%)	38 75
5	E	160/167 (96%)	144 (90%)	16 (10%)	9 41

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
5	Q	160/167 (96%)	145 (91%)	15 (9%)	11 44
6	F	107/107 (100%)	99 (92%)	8 (8%)	17 55
6	R	107/107 (100%)	99 (92%)	8 (8%)	17 55
7	H	68/72 (94%)	51 (75%)	17 (25%)	1 4
7	S	68/72 (94%)	50 (74%)	18 (26%)	0 4
8	K	45/46 (98%)	38 (84%)	7 (16%)	3 20
8	T	45/46 (98%)	38 (84%)	7 (16%)	3 20
9	L	81/87 (93%)	77 (95%)	4 (5%)	31 70
9	U	81/87 (93%)	76 (94%)	5 (6%)	23 63
10	N	57/59 (97%)	50 (88%)	7 (12%)	6 29
10	V	57/59 (97%)	51 (90%)	6 (10%)	8 38
11	P	35/40 (88%)	30 (86%)	5 (14%)	4 24
11	W	35/40 (88%)	31 (89%)	4 (11%)	7 33
All	All	5516/5776 (96%)	4767 (86%)	749 (14%)	5 26

All (749) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	33	ASP
1	A	34	THR
1	A	36	ASP
1	A	38	ASP
1	A	40	TYR
1	A	42	ILE
1	A	46	LEU
1	A	47	MET
1	A	51	LEU
1	A	58	LEU
1	A	74	PHE
1	A	76	HIS
1	A	81	ARG
1	A	105	ARG
1	A	106	ILE
1	A	108	LEU
1	A	116	TYR
1	A	123	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	133	LEU
1	A	149	HIS
1	A	158	LYS
1	A	159	PHE
1	A	161	ARG
1	A	170	LYS
1	A	176	GLU
1	A	180	ARG
1	A	188	ASP
1	A	196	LYS
1	A	204	HIS
1	A	242	THR
1	A	255	LEU
1	A	287	THR
1	A	288	SER
1	A	335	ASP
1	A	337	MET
1	A	359	VAL
1	A	362	PHE
1	A	364	TYR
1	A	372	LEU
1	A	384	VAL
1	A	388	GLU
1	A	393	ARG
1	A	395	MET
1	A	399	ARG
1	A	408	ILE
1	A	412	VAL
1	A	422	VAL
1	A	423	LEU
1	A	424	PHE
1	A	426	ARG
1	A	431	HIS
1	A	435	ILE
1	A	469	LEU
1	A	484	LEU
1	A	504	ILE
1	A	505	GLN
1	A	516	ARG
1	A	523	ARG
1	A	524	TYR
1	A	530	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	532	PHE
1	A	536	ASP
1	A	538	ASN
1	A	540	LEU
1	A	542	GLU
1	A	557	THR
1	A	561	LEU
1	A	567	LEU
1	A	569	ILE
1	A	572	ARG
1	A	575	LEU
1	A	577	ASP
1	A	580	GLU
1	A	583	GLU
1	A	585	LEU
1	A	602	LYS
1	A	603	LEU
1	A	612	GLN
1	A	632	LYS
1	A	637	ILE
1	A	641	TYR
1	A	647	ARG
1	A	654	THR
1	A	656	LEU
1	A	668	THR
1	A	706	LEU
1	A	712	LYS
1	A	728	GLU
1	A	743	MET
1	A	758	LYS
1	A	806	ASN
1	A	825	ARG
1	A	851	ASP
1	A	853	LYS
1	A	854	VAL
1	A	855	ASP
1	A	862	ASP
1	A	864	THR
1	A	867	ILE
1	A	868	VAL
1	A	883	TRP
1	A	884	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	891	ASP
2	B	46	LEU
2	B	50	VAL
2	B	55	GLU
2	B	56	VAL
2	B	57	VAL
2	B	59	ASP
2	B	66	LYS
2	B	77	PHE
2	B	81	GLN
2	B	84	ARG
2	B	94	ILE
2	B	105	LEU
2	B	108	ILE
2	B	111	VAL
2	B	114	ILE
2	B	125	GLU
2	B	133	LYS
2	B	142	ASP
2	B	143	GLU
2	B	148	LEU
2	B	161	ILE
2	B	166	ARG
2	B	168	ILE
2	B	170	SER
2	B	179	THR
2	B	184	ASP
2	B	190	VAL
2	B	199	HIS
2	B	207	VAL
2	B	210	LYS
2	B	218	THR
2	B	235	LEU
2	B	259	ASP
2	B	263	ASP
2	B	269	THR
2	B	270	GLN
2	B	279	ARG
2	B	292	ARG
2	B	293	ARG
2	B	308	VAL
2	B	309	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	320	LEU
2	B	322	MET
2	B	325	LEU
2	B	346	LYS
2	B	347	ARG
2	B	353	ASP
2	B	358	LEU
2	B	365	GLN
2	B	366	LEU
2	B	370	MET
2	B	377	THR
2	B	388	GLU
2	B	389	ASN
2	B	394	VAL
2	B	395	ARG
2	B	409	HIS
2	B	416	TRP
2	B	429	ARG
2	B	431	ASN
2	B	435	THR
2	B	448	ARG
2	B	458	LEU
2	B	469	THR
2	B	470	GLU
2	B	480	VAL
2	B	491	THR
2	B	497	GLU
2	B	510	ILE
2	B	520	TYR
2	B	521	ARG
2	B	524	LEU
2	B	536	ARG
2	B	537	LYS
2	B	545	ASP
2	B	554	VAL
2	B	559	LEU
2	B	578	ARG
2	B	599	ILE
2	B	603	THR
2	B	604	LEU
2	B	610	ILE
2	B	630	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	637	GLU
2	B	644	LEU
2	B	650	LEU
2	B	656	LEU
2	B	681	LEU
2	B	683	TRP
2	B	687	ARG
2	B	688	ILE
2	B	695	HIS
2	B	725	VAL
2	B	726	VAL
2	B	740	VAL
2	B	751	LEU
2	B	759	THR
2	B	765	LYS
2	B	776	GLU
2	B	782	ILE
2	B	786	LEU
2	B	793	HIS
2	B	796	GLU
2	B	800	ILE
2	B	801	PHE
2	B	809	LYS
2	B	816	THR
2	B	842	THR
2	B	843	VAL
2	B	848	LYS
2	B	850	VAL
2	B	855	ILE
2	B	861	ASP
2	B	873	LEU
2	B	878	LEU
2	B	896	VAL
2	B	908	ILE
2	B	942	ARG
2	B	952	GLU
2	B	967	LYS
2	B	968	HIS
2	B	971	ARG
2	B	981	ARG
2	B	983	LEU
2	B	984	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	989	ILE
2	B	992	ILE
2	B	1055	GLU
2	B	1062	VAL
2	B	1067	SER
2	B	1089	ASP
2	B	1091	ARG
2	B	1112	VAL
2	B	1118	ARG
2	B	1121	ASP
3	C	7	ILE
3	C	9	SER
3	C	12	SER
3	C	15	GLU
3	C	21	LYS
3	C	23	GLU
3	C	25	TYR
3	C	29	ILE
3	C	31	TYR
3	C	37	LEU
3	C	38	LYS
3	C	40	ASP
3	C	43	GLN
3	C	64	VAL
3	C	71	SER
3	C	94	VAL
3	C	113	THR
3	C	129	ASP
3	C	141	THR
3	C	144	GLU
3	C	145	ASN
3	C	148	ARG
3	C	149	GLU
3	C	157	MET
3	C	163	ILE
3	C	166	GLU
3	C	167	ARG
3	C	170	LYS
3	C	176	GLU
3	C	177	LYS
3	C	180	ARG
3	C	181	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	182	LEU
3	C	186	PHE
3	C	187	LYS
3	C	216	GLU
3	C	219	LYS
3	C	223	LEU
3	C	236	LYS
3	C	240	GLU
3	C	244	TYR
3	C	246	GLU
3	C	269	ILE
3	C	291	SER
3	C	292	THR
3	C	298	LEU
3	C	302	VAL
3	C	311	MET
3	C	315	ASP
3	C	326	ILE
3	C	330	LYS
3	C	339	PHE
3	C	340	GLU
3	C	342	THR
3	C	346	LEU
3	C	347	PHE
3	C	355	VAL
3	C	358	LEU
3	C	362	VAL
3	C	369	GLN
3	C	373	VAL
3	C	384	LEU
4	D	14	ILE
4	D	16	PHE
4	D	27	ASN
4	D	50	ASN
4	D	188	GLU
4	D	193	THR
4	D	194	ILE
4	D	198	TYR
4	D	201	ARG
5	E	1	MET
5	E	5	LEU
5	E	16	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	46	LEU
5	E	59	ILE
5	E	74	VAL
5	E	91	GLU
5	E	93	MET
5	E	110	ILE
5	E	119	VAL
5	E	125	ARG
5	E	138	LEU
5	E	153	SER
5	E	165	MET
5	E	174	GLU
5	E	177	GLU
6	F	7	LEU
6	F	40	GLU
6	F	50	ARG
6	F	55	LYS
6	F	71	ASP
6	F	90	LEU
6	F	100	GLU
6	F	121	LEU
7	H	6	GLU
7	H	9	ILE
7	H	10	PHE
7	H	29	LEU
7	H	37	ILE
7	H	38	SER
7	H	40	LEU
7	H	44	LYS
7	H	50	VAL
7	H	51	VAL
7	H	53	LEU
7	H	62	GLU
7	H	69	THR
7	H	74	TYR
7	H	75	TYR
7	H	78	LEU
7	H	81	GLU
8	K	3	ARG
8	K	35	THR
8	K	38	GLN
8	K	41	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	K	46	LYS
8	K	49	ILE
8	K	57	SER
9	L	43	TYR
9	L	46	GLU
9	L	50	THR
9	L	93	ILE
10	N	3	VAL
10	N	12	LYS
10	N	19	TYR
10	N	48	THR
10	N	54	GLU
10	N	60	MET
10	N	63	LYS
11	P	14	GLU
11	P	15	VAL
11	P	21	THR
11	P	23	ARG
11	P	44	ARG
1	I	10	SER
1	I	33	ASP
1	I	34	THR
1	I	37	ASP
1	I	38	ASP
1	I	42	ILE
1	I	46	LEU
1	I	47	MET
1	I	51	LEU
1	I	58	LEU
1	I	74	PHE
1	I	76	HIS
1	I	81	ARG
1	I	105	ARG
1	I	106	ILE
1	I	108	LEU
1	I	116	TYR
1	I	123	MET
1	I	133	LEU
1	I	149	HIS
1	I	158	LYS
1	I	159	PHE
1	I	161	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	169	ARG
1	I	170	LYS
1	I	176	GLU
1	I	180	ARG
1	I	188	ASP
1	I	196	LYS
1	I	204	HIS
1	I	242	THR
1	I	255	LEU
1	I	287	THR
1	I	288	SER
1	I	335	ASP
1	I	337	MET
1	I	359	VAL
1	I	362	PHE
1	I	364	TYR
1	I	372	LEU
1	I	384	VAL
1	I	388	GLU
1	I	393	ARG
1	I	395	MET
1	I	399	ARG
1	I	408	ILE
1	I	412	VAL
1	I	422	VAL
1	I	423	LEU
1	I	424	PHE
1	I	426	ARG
1	I	431	HIS
1	I	435	ILE
1	I	469	LEU
1	I	484	LEU
1	I	504	ILE
1	I	505	GLN
1	I	516	ARG
1	I	523	ARG
1	I	524	TYR
1	I	530	LEU
1	I	532	PHE
1	I	536	ASP
1	I	538	ASN
1	I	540	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	542	GLU
1	I	547	GLU
1	I	557	THR
1	I	561	LEU
1	I	567	LEU
1	I	569	ILE
1	I	572	ARG
1	I	575	LEU
1	I	577	ASP
1	I	585	LEU
1	I	588	LEU
1	I	602	LYS
1	I	603	LEU
1	I	612	GLN
1	I	632	LYS
1	I	637	ILE
1	I	641	TYR
1	I	647	ARG
1	I	654	THR
1	I	656	LEU
1	I	668	THR
1	I	706	LEU
1	I	712	LYS
1	I	728	GLU
1	I	743	MET
1	I	806	ASN
1	I	825	ARG
1	I	851	ASP
1	I	853	LYS
1	I	854	VAL
1	I	855	ASP
1	I	862	ASP
1	I	864	THR
1	I	867	ILE
1	I	868	VAL
1	I	883	TRP
1	I	884	GLN
1	I	891	ASP
1	I	897	THR
2	J	43	ASP
2	J	46	LEU
2	J	55	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	56	VAL
2	J	57	VAL
2	J	59	ASP
2	J	66	LYS
2	J	77	PHE
2	J	81	GLN
2	J	84	ARG
2	J	94	ILE
2	J	105	LEU
2	J	108	ILE
2	J	111	VAL
2	J	114	ILE
2	J	125	GLU
2	J	133	LYS
2	J	142	ASP
2	J	143	GLU
2	J	148	LEU
2	J	161	ILE
2	J	166	ARG
2	J	168	ILE
2	J	170	SER
2	J	179	THR
2	J	184	ASP
2	J	190	VAL
2	J	199	HIS
2	J	207	VAL
2	J	210	LYS
2	J	218	THR
2	J	235	LEU
2	J	259	ASP
2	J	263	ASP
2	J	269	THR
2	J	270	GLN
2	J	279	ARG
2	J	292	ARG
2	J	293	ARG
2	J	308	VAL
2	J	309	ASP
2	J	320	LEU
2	J	322	MET
2	J	325	LEU
2	J	346	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	347	ARG
2	J	353	ASP
2	J	358	LEU
2	J	365	GLN
2	J	366	LEU
2	J	370	MET
2	J	377	THR
2	J	388	GLU
2	J	389	ASN
2	J	409	HIS
2	J	416	TRP
2	J	429	ARG
2	J	431	ASN
2	J	435	THR
2	J	448	ARG
2	J	458	LEU
2	J	469	THR
2	J	470	GLU
2	J	480	VAL
2	J	491	THR
2	J	497	GLU
2	J	503	MET
2	J	510	ILE
2	J	513	ARG
2	J	520	TYR
2	J	524	LEU
2	J	536	ARG
2	J	537	LYS
2	J	545	ASP
2	J	554	VAL
2	J	559	LEU
2	J	578	ARG
2	J	599	ILE
2	J	603	THR
2	J	604	LEU
2	J	610	ILE
2	J	637	GLU
2	J	644	LEU
2	J	650	LEU
2	J	656	LEU
2	J	681	LEU
2	J	683	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	687	ARG
2	J	688	ILE
2	J	695	HIS
2	J	725	VAL
2	J	726	VAL
2	J	740	VAL
2	J	751	LEU
2	J	759	THR
2	J	765	LYS
2	J	776	GLU
2	J	782	ILE
2	J	786	LEU
2	J	793	HIS
2	J	796	GLU
2	J	800	ILE
2	J	801	PHE
2	J	809	LYS
2	J	816	THR
2	J	820	ARG
2	J	842	THR
2	J	848	LYS
2	J	850	VAL
2	J	855	ILE
2	J	861	ASP
2	J	873	LEU
2	J	878	LEU
2	J	896	VAL
2	J	908	ILE
2	J	928	LEU
2	J	942	ARG
2	J	952	GLU
2	J	967	LYS
2	J	968	HIS
2	J	971	ARG
2	J	981	ARG
2	J	983	LEU
2	J	984	GLU
2	J	989	ILE
2	J	992	ILE
2	J	1032	PHE
2	J	1039	VAL
2	J	1055	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	1062	VAL
2	J	1067	SER
2	J	1080	LYS
2	J	1091	ARG
2	J	1112	VAL
2	J	1118	ARG
2	J	1122	ARG
3	M	7	ILE
3	M	9	SER
3	M	12	SER
3	M	15	GLU
3	M	21	LYS
3	M	23	GLU
3	M	25	TYR
3	M	29	ILE
3	M	31	TYR
3	M	37	LEU
3	M	38	LYS
3	M	40	ASP
3	M	43	GLN
3	M	64	VAL
3	M	71	SER
3	M	93	ASN
3	M	94	VAL
3	M	113	THR
3	M	129	ASP
3	M	141	THR
3	M	144	GLU
3	M	145	ASN
3	M	148	ARG
3	M	153	ASP
3	M	154	ILE
3	M	155	LEU
3	M	166	GLU
3	M	167	ARG
3	M	170	LYS
3	M	176	GLU
3	M	177	LYS
3	M	180	ARG
3	M	181	LYS
3	M	182	LEU
3	M	191	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	M	192	GLU
3	M	208	LEU
3	M	210	ASP
3	M	212	ARG
3	M	219	LYS
3	M	223	LEU
3	M	236	LYS
3	M	237	GLU
3	M	240	GLU
3	M	244	TYR
3	M	246	GLU
3	M	291	SER
3	M	292	THR
3	M	298	LEU
3	M	302	VAL
3	M	311	MET
3	M	315	ASP
3	M	326	ILE
3	M	330	LYS
3	M	342	THR
3	M	346	LEU
3	M	347	PHE
3	M	355	VAL
3	M	358	LEU
3	M	362	VAL
3	M	369	GLN
3	M	373	VAL
3	M	384	LEU
4	O	14	ILE
4	O	16	PHE
4	O	27	ASN
4	O	50	ASN
4	O	188	GLU
4	O	193	THR
4	O	194	ILE
4	O	198	TYR
4	O	201	ARG
5	Q	5	LEU
5	Q	16	ARG
5	Q	46	LEU
5	Q	59	ILE
5	Q	74	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Q	91	GLU
5	Q	93	MET
5	Q	110	ILE
5	Q	119	VAL
5	Q	125	ARG
5	Q	138	LEU
5	Q	153	SER
5	Q	165	MET
5	Q	174	GLU
5	Q	177	GLU
6	R	7	LEU
6	R	40	GLU
6	R	50	ARG
6	R	55	LYS
6	R	71	ASP
6	R	90	LEU
6	R	100	GLU
6	R	121	LEU
7	S	6	GLU
7	S	7	PHE
7	S	9	ILE
7	S	10	PHE
7	S	29	LEU
7	S	37	ILE
7	S	38	SER
7	S	40	LEU
7	S	44	LYS
7	S	50	VAL
7	S	51	VAL
7	S	53	LEU
7	S	62	GLU
7	S	69	THR
7	S	74	TYR
7	S	75	TYR
7	S	78	LEU
7	S	81	GLU
8	T	3	ARG
8	T	35	THR
8	T	38	GLN
8	T	41	LEU
8	T	46	LYS
8	T	49	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	T	57	SER
9	U	44	THR
9	U	46	GLU
9	U	49	ILE
9	U	53	ARG
9	U	54	LYS
10	V	3	VAL
10	V	12	LYS
10	V	19	TYR
10	V	48	THR
10	V	54	GLU
10	V	60	MET
11	W	14	GLU
11	W	15	VAL
11	W	23	ARG
11	W	44	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	252	ASN
1	A	648	GLN
1	A	884	GLN
2	B	47	GLN
2	B	312	ASN
2	B	389	ASN
2	B	391	GLN
2	B	639	HIS
2	B	968	HIS
3	C	43	GLN
3	C	156	ASN
4	D	27	ASN
4	D	50	ASN
5	E	68	HIS
9	L	26	ASN
10	N	52	HIS
1	I	138	HIS
1	I	252	ASN
1	I	648	GLN
1	I	842	GLN
1	I	884	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	J	51	ASN
2	J	312	ASN
2	J	639	HIS
2	J	1070	HIS
3	M	43	GLN
4	O	27	ASN
4	O	50	ASN
5	Q	68	HIS
10	V	52	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 14 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	863/906 (95%)	0.42	82 (9%) 10 10	41, 157, 264, 370	0
1	I	862/906 (95%)	0.44	83 (9%) 10 9	54, 163, 263, 381	0
2	B	1069/1123 (95%)	0.27	62 (5%) 26 21	46, 149, 253, 402	0
2	J	1069/1123 (95%)	0.12	40 (3%) 45 36	39, 139, 248, 360	0
3	C	369/391 (94%)	0.92	74 (20%) 1 2	68, 192, 319, 372	0
3	M	369/391 (94%)	1.02	73 (19%) 1 2	71, 193, 327, 419	0
4	D	258/259 (99%)	0.49	26 (10%) 9 9	71, 143, 235, 295	0
4	O	258/259 (99%)	0.14	12 (4%) 35 28	63, 136, 226, 319	0
5	E	181/190 (95%)	0.66	24 (13%) 4 5	69, 159, 250, 398	0
5	Q	181/190 (95%)	0.61	22 (12%) 5 6	90, 163, 244, 317	0
6	F	122/122 (100%)	0.58	15 (12%) 5 6	133, 165, 244, 447	0
6	R	122/122 (100%)	0.31	6 (4%) 33 25	142, 184, 257, 324	0
7	H	76/82 (92%)	0.20	3 (3%) 43 35	105, 157, 228, 268	0
7	S	76/82 (92%)	0.51	4 (5%) 30 23	114, 166, 248, 293	0
8	K	56/57 (98%)	0.08	0 100 100	88, 131, 196, 288	0
8	T	56/57 (98%)	0.16	3 (5%) 29 23	62, 119, 227, 330	0
9	L	94/100 (94%)	0.34	3 (3%) 51 42	78, 142, 221, 331	0
9	U	94/100 (94%)	0.54	12 (12%) 5 5	83, 149, 223, 474	0
10	N	63/65 (96%)	-0.03	1 (1%) 74 65	81, 141, 218, 281	0
10	V	63/65 (96%)	0.08	2 (3%) 51 42	69, 131, 196, 232	0
11	P	42/49 (85%)	0.50	5 (11%) 6 6	125, 173, 254, 294	0
11	W	42/49 (85%)	0.34	3 (7%) 19 15	90, 147, 201, 253	0
All	All	6385/6688 (95%)	0.40	555 (8%) 13 12	39, 156, 270, 474	0

All (555) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1089	ASP	14.0
3	M	200	VAL	12.6
3	M	340	GLU	11.1
5	E	92	MET	9.7
3	M	209	SER	9.7
2	B	1087	GLY	8.4
3	M	246	GLU	8.1
3	C	209	SER	8.0
2	B	1088	GLU	7.8
9	L	51	MET	7.6
1	A	579	PRO	7.6
3	M	188	SER	7.3
3	M	152	ILE	7.1
1	I	298	GLY	7.0
3	M	173	LEU	6.9
3	M	194	GLU	6.7
5	Q	92	MET	6.5
3	C	218	VAL	6.5
6	F	29	LEU	6.5
3	C	151	THR	6.5
1	I	59	ARG	6.5
1	I	141	ALA	6.5
1	A	154	GLN	6.3
3	C	160	VAL	6.2
1	I	144	ARG	6.2
6	F	122	GLU	6.2
1	A	765	MET	6.0
3	C	210	ASP	6.0
1	I	154	GLN	5.9
6	F	33	PRO	5.9
3	C	211	LEU	5.8
2	B	63	PHE	5.8
3	M	212	ARG	5.8
2	B	109	PRO	5.7
1	A	767	ALA	5.7
3	C	264	THR	5.7
1	I	294	LYS	5.7
1	I	54	ILE	5.6
3	C	122	GLU	5.6
6	F	30	ALA	5.6
5	E	133	ASN	5.5
2	B	119	VAL	5.4
3	C	203	LYS	5.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	201	ARG	5.4
2	B	860	GLY	5.3
3	C	134	VAL	5.3
3	C	126	TYR	5.3
3	C	259	VAL	5.3
6	R	32	ASN	5.3
2	J	1122	ARG	5.2
2	B	518	GLY	5.2
3	M	15	GLU	5.2
1	A	766	ALA	5.2
3	M	189	ALA	5.1
3	M	155	LEU	5.1
6	F	35	GLU	5.1
1	I	297	SER	5.1
3	C	221	HIS	5.1
1	A	395	MET	5.0
1	A	293	ALA	5.0
1	A	176	GLU	5.0
3	M	224	LYS	5.0
4	D	161	VAL	5.0
2	B	64	LYS	5.0
3	M	201	ARG	4.9
3	M	217	LYS	4.9
1	I	579	PRO	4.9
1	A	675	LEU	4.9
3	C	212	ARG	4.8
6	F	32	ASN	4.8
3	M	197	THR	4.8
5	Q	1	MET	4.7
2	B	285	GLN	4.7
2	B	59	ASP	4.5
2	J	79	GLU	4.5
1	I	767	ALA	4.5
4	O	1	MET	4.5
4	D	228	GLY	4.5
1	I	302	LYS	4.5
3	C	197	THR	4.4
3	M	214	ILE	4.4
1	I	764	GLN	4.4
6	F	49	GLU	4.4
6	F	31	GLU	4.4
11	P	41	ARG	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	380	ARG	4.3
1	I	238	GLU	4.3
1	A	708	PRO	4.2
3	C	204	LYS	4.2
1	A	106	ILE	4.2
1	A	123	MET	4.2
3	C	120	LEU	4.2
4	D	203	PHE	4.1
1	I	766	ALA	4.1
3	C	250	PHE	4.1
5	E	143	ARG	4.1
5	Q	165	MET	4.1
4	D	188	GLU	4.1
9	U	51	MET	4.1
1	I	243	HIS	4.1
3	M	218	VAL	4.0
3	M	210	ASP	4.0
3	C	222	ARG	4.0
3	M	144	GLU	4.0
2	J	1087	GLY	4.0
4	D	189	ILE	4.0
1	A	34	THR	4.0
1	A	396	GLU	3.9
3	C	217	LYS	3.9
3	C	205	VAL	3.9
2	B	811	VAL	3.9
1	A	288	SER	3.9
1	A	768	MET	3.9
3	M	174	ASP	3.9
1	I	542	GLU	3.9
3	C	135	ALA	3.9
3	M	147	ALA	3.8
3	M	222	ARG	3.8
1	A	59	ARG	3.8
1	A	107	LYS	3.8
3	M	264	THR	3.8
5	Q	83	GLU	3.8
1	I	27	ALA	3.8
2	J	820	ARG	3.8
1	A	116	TYR	3.8
6	F	2	ILE	3.8
3	C	140	GLY	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	412	VAL	3.8
2	B	110	VAL	3.8
3	C	139	GLU	3.8
3	M	18	ASP	3.8
4	O	197	PHE	3.8
1	A	46	LEU	3.7
5	E	46	LEU	3.7
1	A	298	GLY	3.7
1	I	229	ILE	3.7
5	E	136	LEU	3.7
2	B	123	ILE	3.7
1	I	295	HIS	3.7
3	M	187	LYS	3.7
7	H	61	ILE	3.7
1	I	300	PRO	3.7
4	O	2	VAL	3.7
3	M	259	VAL	3.7
9	U	50	THR	3.7
2	B	193	LYS	3.7
3	M	234	ILE	3.7
3	C	191	PHE	3.7
1	I	357	GLU	3.6
1	I	367	LEU	3.6
1	I	870	PHE	3.6
3	M	165	PRO	3.6
3	M	94	VAL	3.6
3	M	190	GLU	3.6
1	I	107	LYS	3.6
1	A	289	GLY	3.6
3	C	131	ALA	3.6
1	I	146	VAL	3.6
2	J	285	GLN	3.5
3	C	155	LEU	3.5
1	A	124	GLY	3.5
3	C	169	GLU	3.5
6	R	6	LYS	3.5
3	C	257	PRO	3.5
3	C	125	ARG	3.5
1	A	764	GLN	3.5
3	M	186	PHE	3.5
3	M	151	THR	3.5
1	I	137	ILE	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	34	THR	3.4
3	C	244	TYR	3.4
2	B	398	ILE	3.4
2	J	107	MET	3.4
3	M	127	ASP	3.4
5	Q	113	LEU	3.4
1	A	302	LYS	3.4
3	M	118	VAL	3.4
2	B	61	PRO	3.4
3	M	271	GLU	3.4
5	Q	169	GLY	3.4
4	D	212	ARG	3.3
6	R	2	ILE	3.3
7	S	6	GLU	3.3
2	B	567	GLU	3.3
3	M	213	LYS	3.3
1	A	709	LEU	3.3
3	C	224	LYS	3.3
1	A	301	LEU	3.3
3	M	154	ILE	3.3
6	R	4	ARG	3.3
2	B	1093	SER	3.3
3	C	159	TYR	3.3
1	A	237	ALA	3.3
2	B	775	PHE	3.3
2	J	637	GLU	3.3
3	C	245	THR	3.3
1	I	67	ALA	3.3
3	C	141	THR	3.2
3	C	186	PHE	3.2
2	J	61	PRO	3.2
1	I	108	LEU	3.2
6	R	122	GLU	3.2
1	I	143	GLU	3.2
4	D	68	LEU	3.2
2	B	56	VAL	3.2
11	P	18	ASP	3.2
3	M	161	VAL	3.2
2	J	519	LEU	3.2
3	C	192	GLU	3.2
3	C	241	TYR	3.2
2	J	125	GLU	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	91	LEU	3.2
9	L	47	HIS	3.2
3	C	138	ILE	3.2
4	D	93	ALA	3.2
1	A	359	VAL	3.2
1	A	769	LEU	3.1
1	I	173	GLU	3.1
1	I	288	SER	3.1
1	I	538	ASN	3.1
9	U	42	GLY	3.1
3	C	177	LYS	3.1
9	U	13	LEU	3.1
5	Q	115	ASP	3.1
9	U	48	PRO	3.1
4	D	165	VAL	3.1
4	D	182	VAL	3.1
3	C	234	ILE	3.1
1	A	175	ASN	3.1
6	R	33	PRO	3.1
5	E	86	GLU	3.1
1	A	538	ASN	3.1
2	B	395	ARG	3.1
4	D	133	ALA	3.1
4	D	186	ASP	3.1
5	Q	86	GLU	3.1
1	I	140	LYS	3.1
3	C	255	LYS	3.0
5	E	90	VAL	3.0
11	P	36	TYR	3.0
3	C	344	GLN	3.0
1	I	46	LEU	3.0
1	A	33	ASP	3.0
2	B	107	MET	3.0
3	C	190	GLU	3.0
3	M	202	PRO	3.0
4	O	172	LYS	3.0
1	A	416	LEU	3.0
3	C	206	THR	3.0
2	B	399	ARG	3.0
3	C	256	VAL	3.0
3	C	156	ASN	3.0
5	E	169	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	D	211	ILE	3.0
1	I	43	GLU	3.0
1	I	358	LYS	3.0
2	B	641	HIS	3.0
5	E	144	ALA	3.0
1	A	158	LYS	3.0
3	M	192	GLU	3.0
1	I	765	MET	3.0
1	A	153	PRO	2.9
3	M	193	ALA	2.9
3	M	211	LEU	2.9
4	O	203	PHE	2.9
1	I	40	TYR	2.9
4	D	77	LEU	2.9
1	A	144	ARG	2.9
5	E	142	VAL	2.9
3	C	93	ASN	2.9
1	I	48	ASP	2.9
3	M	168	LEU	2.9
2	B	791	TYR	2.9
2	B	788	GLU	2.9
11	P	40	PRO	2.9
3	M	160	VAL	2.9
5	Q	114	MET	2.9
1	A	157	ILE	2.9
3	C	176	GLU	2.9
1	A	734	GLY	2.9
2	J	266	ASP	2.9
4	D	160	HIS	2.9
3	M	206	THR	2.9
1	A	892	ARG	2.9
1	I	53	VAL	2.9
2	B	260	ASN	2.9
3	M	146	LEU	2.9
2	J	208	GLU	2.9
6	F	6	LYS	2.9
1	I	26	ALA	2.9
3	C	189	ALA	2.8
1	A	66	ARG	2.8
1	A	236	ARG	2.8
3	C	243	ILE	2.8
1	I	69	GLU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	M	162	GLU	2.8
1	I	38	ASP	2.8
5	E	115	ASP	2.8
3	C	188	SER	2.8
3	C	214	ILE	2.8
4	D	162	SER	2.8
1	A	803	PHE	2.8
3	C	79	MET	2.8
3	C	127	ASP	2.8
3	M	167	ARG	2.8
1	A	62	THR	2.8
1	I	55	ASP	2.8
3	M	199	VAL	2.8
1	I	768	MET	2.8
4	O	49	GLU	2.8
5	E	42	GLU	2.8
1	I	541	PRO	2.7
3	M	150	GLU	2.7
5	Q	97	ALA	2.7
7	S	8	ASN	2.7
11	W	22	ALA	2.7
1	A	539	GLU	2.7
3	M	198	LEU	2.7
4	D	105	LYS	2.7
5	E	71	ILE	2.7
1	I	393	ARG	2.7
3	C	130	LYS	2.7
3	C	183	THR	2.7
2	B	229	VAL	2.7
4	O	201	ARG	2.7
2	J	958	ARG	2.7
1	I	371	VAL	2.7
2	B	859	THR	2.7
4	D	89	LEU	2.7
3	C	154	ILE	2.7
1	A	401	LEU	2.7
4	D	129	LEU	2.7
2	J	1121	ASP	2.7
1	A	200	LEU	2.6
2	J	227	LYS	2.6
3	M	231	LYS	2.6
1	A	155	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	135	VAL	2.6
1	I	362	PHE	2.6
1	A	152	ALA	2.6
2	B	864	LYS	2.6
5	E	117	TYR	2.6
5	Q	144	ALA	2.6
1	A	413	GLU	2.6
2	J	1081	VAL	2.6
3	M	124	HIS	2.6
1	I	740	TYR	2.6
9	U	58	LYS	2.6
5	Q	142	VAL	2.6
1	I	99	THR	2.6
2	J	1044	GLY	2.6
1	I	158	LYS	2.6
2	B	228	PHE	2.6
9	U	41	ALA	2.6
9	U	47	HIS	2.6
3	M	177	LYS	2.6
1	A	397	SER	2.6
2	B	1067	SER	2.5
3	M	145	ASN	2.5
1	I	98	SER	2.5
4	D	187	GLU	2.5
2	J	247	VAL	2.5
1	I	414	ARG	2.5
10	V	41	GLU	2.5
2	B	1122	ARG	2.5
1	I	153	PRO	2.5
2	B	192	ALA	2.5
2	B	235	LEU	2.5
3	M	39	LYS	2.5
5	Q	70	ALA	2.5
5	E	114	MET	2.5
1	A	58	LEU	2.5
3	C	254	LEU	2.5
1	A	168	LEU	2.5
1	A	631	GLY	2.5
1	I	29	ILE	2.5
1	A	35	TYR	2.5
1	A	310	GLY	2.5
2	B	626	ALA	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	260	ASN	2.5
4	D	47	PHE	2.5
2	B	479	LEU	2.4
1	A	54	ILE	2.4
3	M	169	GLU	2.4
3	C	252	GLN	2.4
2	B	57	VAL	2.4
1	I	241	LEU	2.4
3	M	163	ILE	2.4
2	B	533	GLU	2.4
4	D	75	PHE	2.4
5	Q	127	PHE	2.4
2	J	204	LEU	2.4
9	U	40	PHE	2.4
1	I	368	LYS	2.4
5	Q	46	LEU	2.4
9	L	13	LEU	2.4
5	E	104	MET	2.4
1	A	354	THR	2.4
5	E	70	ALA	2.4
1	A	57	GLY	2.4
1	I	787	VAL	2.4
3	M	205	VAL	2.4
9	U	3	ILE	2.4
1	A	357	GLU	2.4
4	O	182	VAL	2.4
5	E	171	GLY	2.4
7	H	18	HIS	2.4
5	Q	40	ARG	2.4
6	F	4	ARG	2.4
3	M	276	LEU	2.4
2	B	918	GLY	2.4
2	J	1055	GLU	2.4
1	I	670	ILE	2.4
3	M	359	ASN	2.4
4	O	189	ILE	2.4
1	I	19	GLN	2.4
8	T	31	PRO	2.4
3	C	195	GLY	2.3
2	J	954	GLU	2.3
2	B	111	VAL	2.3
1	A	368	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	1090	GLU	2.3
3	C	133	GLU	2.3
5	Q	118	VAL	2.3
11	W	38	PRO	2.3
3	C	226	LEU	2.3
3	M	159	TYR	2.3
1	A	55	ASP	2.3
1	I	149	HIS	2.3
3	M	247	GLY	2.3
1	A	805	THR	2.3
2	B	838	GLU	2.3
3	M	95	THR	2.3
3	C	208	LEU	2.3
5	Q	84	VAL	2.3
7	S	61	ILE	2.3
1	I	306	GLN	2.3
2	B	389	ASN	2.3
5	E	47	ALA	2.3
1	I	270	ASP	2.3
2	B	269	THR	2.3
1	I	382	ASN	2.3
6	F	45	LEU	2.3
3	M	183	THR	2.3
3	M	268	ASN	2.3
1	I	605	TYR	2.3
3	M	216	GLU	2.3
3	C	213	LYS	2.3
1	I	673	GLU	2.3
2	B	790	TYR	2.3
2	J	118	PRO	2.2
2	B	392	ARG	2.2
2	J	116	GLN	2.2
1	A	230	THR	2.2
1	I	282	TYR	2.2
2	J	395	ARG	2.2
3	C	253	VAL	2.2
7	S	51	VAL	2.2
2	B	230	TYR	2.2
1	I	416	LEU	2.2
2	B	786	LEU	2.2
9	U	89	TRP	2.2
3	M	156	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
5	E	101	ILE	2.2
2	B	374	MET	2.2
2	J	775	PHE	2.2
3	M	221	HIS	2.2
1	I	620	ALA	2.2
8	T	33	GLY	2.2
2	J	394	VAL	2.2
4	O	161	VAL	2.2
2	B	778	PRO	2.2
1	A	159	PHE	2.2
1	A	242	THR	2.2
1	A	353	LEU	2.2
2	J	82	GLY	2.2
2	J	837	ARG	2.2
1	A	146	VAL	2.2
3	C	40	ASP	2.2
3	M	384	LEU	2.2
1	A	238	GLU	2.2
1	I	417	GLU	2.2
2	B	108	ILE	2.2
3	C	193	ALA	2.2
3	M	256	VAL	2.2
4	D	92	GLU	2.2
5	E	127	PHE	2.2
1	I	576	CYS	2.2
2	B	60	ILE	2.2
2	J	80	ALA	2.2
3	M	23	GLU	2.2
6	F	86	PRO	2.2
4	O	206	HIS	2.2
1	A	410	TRP	2.2
2	B	79	GLU	2.2
3	C	276	LEU	2.1
2	B	888	GLN	2.1
4	D	6	ILE	2.1
2	J	226	VAL	2.1
1	I	412	VAL	2.1
1	A	285	ASN	2.1
1	I	58	LEU	2.1
2	B	70	ILE	2.1
1	A	290	VAL	2.1
1	A	197	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	J	78	GLN	2.1
7	H	60	VAL	2.1
3	C	219	LYS	2.1
11	P	35	LEU	2.1
2	J	533	GLU	2.1
2	J	51	ASN	2.1
5	E	88	GLU	2.1
2	B	217	VAL	2.1
5	Q	110	ILE	2.1
1	A	165	TYR	2.1
1	I	171	ASP	2.1
4	D	168	TRP	2.1
11	W	39	ARG	2.1
5	Q	8	LYS	2.1
5	Q	170	LEU	2.1
1	A	166	TRP	2.1
2	B	209	ARG	2.1
1	A	294	LYS	2.1
2	B	763	GLU	2.1
1	A	726	LEU	2.1
4	O	171	LEU	2.1
1	A	733	ALA	2.1
1	I	106	ILE	2.1
1	I	384	VAL	2.1
2	J	173	ASP	2.1
5	Q	48	ILE	2.1
5	E	3	LYS	2.1
1	I	392	ILE	2.0
9	U	37	HIS	2.0
1	A	97	GLU	2.0
2	J	1056	GLU	2.0
1	I	39	GLY	2.0
2	B	83	GLN	2.0
2	J	277	ILE	2.0
8	T	34	ILE	2.0
1	A	69	GLU	2.0
2	J	964	LEU	2.0
3	C	39	LYS	2.0
3	C	162	GLU	2.0
3	C	251	LYS	2.0
2	J	269	THR	2.0
1	A	43	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	I	369	GLN	2.0
6	F	84	ILE	2.0
10	N	20	GLU	2.0
2	B	409	HIS	2.0
1	I	570	TRP	2.0
6	F	5	LYS	2.0
1	I	381	ALA	2.0
10	V	16	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
13	ZN	J	1301	1/1	0.89	0.49	3.87	521,521,521,521	0
12	MG	I	1101	1/1	0.72	0.39	2.22	175,175,175,175	0
13	ZN	B	1201	1/1	0.93	0.28	1.00	364,364,364,364	0
13	ZN	V	1601	1/1	0.99	0.24	0.30	210,210,210,210	0
13	ZN	P	1501	1/1	0.72	0.26	-0.21	354,354,354,354	0
13	ZN	A	1003	1/1	0.59	0.18	-0.93	488,488,488,488	0
13	ZN	W	1701	1/1	0.97	0.08	-1.00	94,94,94,94	0
13	ZN	A	1002	1/1	0.88	0.20	-1.00	137,137,137,137	0
13	ZN	I	1102	1/1	0.89	0.10	-1.08	147,147,147,147	0
13	ZN	I	1103	1/1	0.78	0.17	-1.44	527,527,527,527	0
13	ZN	N	1401	1/1	0.74	0.20	-1.48	127,127,127,127	0
12	MG	I	1104	1/1	0.87	0.82	-	54,54,54,54	0
12	MG	A	1001	1/1	0.89	0.35	-	52,52,52,52	0
12	MG	A	1004	1/1	0.89	0.62	-	58,58,58,58	0

6.5 Other polymers (i)

There are no such residues in this entry.