



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 20, 2023 – 03:35 PM JST

PDB ID : 7CO5  
Title : HtrA-type protease AlgW with decapeptide  
Authors : Li, T.; Song, Y.J.; Bao, R.  
Deposited on : 2020-08-03  
Resolution : 2.35 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

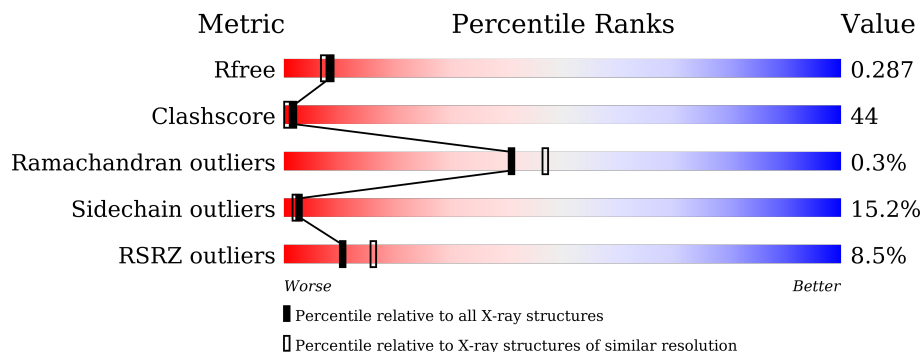
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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

Mol	Chain	Length	Quality of chain
1	A	10	
1	C	10	
1	E	10	
1	G	10	
1	I	10	
1	K	10	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain				
2	B	377	7%	43%	37%	7%	14%
2	D	377	9%	45%	32%	8%	14%
2	F	377	7%	36%	42%	7%	14%
2	H	377	7%	50%	34%	•	14%
2	J	377	5%	45%	34%	6%	• 14%
2	L	377	9%	42%	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
3	IMD	H	401	-	-	X	-
3	IMD	L	401	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15076 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.

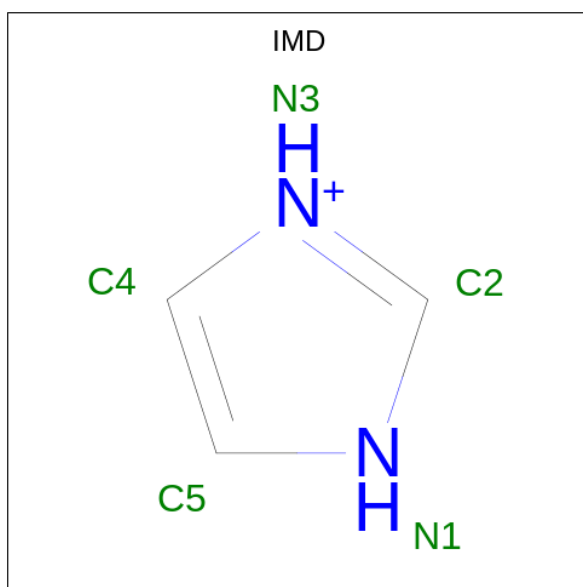
- Molecule 1 is a protein called decapeptide SVRDELRWVF.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	G	6	60	42	10	8	0	0	0
1	A	7	68	46	11	11	0	0	0
1	C	7	68	46	11	11	0	0	0
1	E	6	60	42	10	8	0	0	0
1	I	6	60	42	10	8	0	0	0
1	K	9	86	57	16	13	0	0	0

- Molecule 2 is a protein called AlgW protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	325	2388	1492	427	460	9	0	0	0
2	B	325	2388	1492	427	460	9	0	0	0
2	D	325	2388	1492	427	460	9	0	0	0
2	F	325	2388	1492	427	460	9	0	0	0
2	J	325	2388	1492	427	460	9	0	0	0
2	L	325	2388	1492	427	460	9	0	0	0

- Molecule 3 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total C N 5 3 2	0	0
3	B	1	Total C N 5 3 2	0	0
3	D	1	Total C N 5 3 2	0	0
3	F	1	Total C N 5 3 2	0	0
3	J	1	Total C N 5 3 2	0	0
3	L	1	Total C N 5 3 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	2	Total O 2 2	0	0
4	H	51	Total O 51 51	0	0
4	B	51	Total O 51 51	0	0
4	D	51	Total O 51 51	0	0
4	F	43	Total O 43 43	0	0
4	I	2	Total O 2 2	0	0

*Continued on next page...*

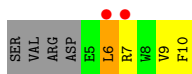
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>	<b>ZeroOcc</b>	<b>AltConf</b>
4	J	44	Total O 44 44	0	0
4	K	1	Total O 1 1	0	0
4	L	71	Total O 71 71	0	0

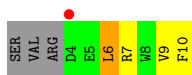
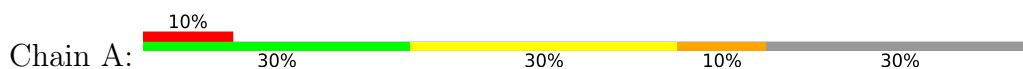
### 3 Residue-property plots [i](#)

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

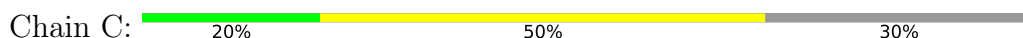
- Molecule 1: decapeptide SVRDELRWVF



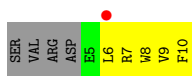
- Molecule 1: decapeptide SVRDELRWVF



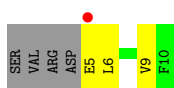
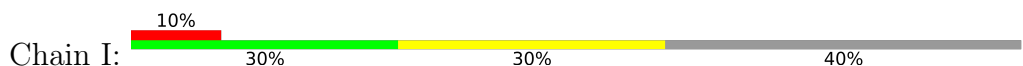
- Molecule 1: decapeptide SVRDELRWVF



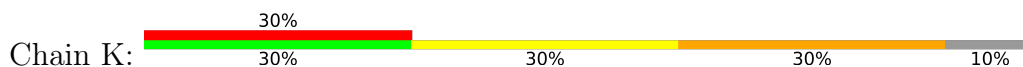
- Molecule 1: decapeptide SVRDELRWVF



- Molecule 1: decapeptide SVRDELRWVF



- Molecule 1: decapeptide SVRDELRWVF











## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.12Å 130.84Å 250.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.50 – 2.35 34.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	84.3 (34.50-2.35) 81.9 (34.50-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 2.34Å)	Xtrriage
Refinement program	PHENIX 1.14_3260	Depositor
R, $R_{free}$	0.268 , 0.289 0.269 , 0.287	Depositor DCC
$R_{free}$ test set	1784 reflections (1.59%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	6.9	Xtrriage
Anisotropy	2.718	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 50.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.75	EDS
Total number of atoms	15076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.18% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.76	0/70	0.83	0/94
1	C	0.67	0/70	1.09	0/94
1	E	0.64	0/62	0.84	0/83
1	G	0.69	0/62	1.07	0/83
1	I	0.83	0/62	0.93	0/83
1	K	0.67	0/88	1.08	0/118
2	B	1.07	2/2422 (0.1%)	1.01	1/3286 (0.0%)
2	D	1.04	1/2422 (0.0%)	1.02	2/3286 (0.1%)
2	F	1.05	1/2422 (0.0%)	1.00	3/3286 (0.1%)
2	H	1.08	0/2422	0.99	1/3286 (0.0%)
2	J	1.07	3/2422 (0.1%)	0.98	1/3286 (0.0%)
2	L	1.08	3/2422 (0.1%)	0.98	2/3286 (0.1%)
All	All	1.06	10/14946 (0.1%)	1.00	10/20271 (0.0%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	370	GLU	CD-OE1	-5.89	1.19	1.25
2	L	213	GLU	CD-OE1	-5.80	1.19	1.25
2	L	341	SER	CA-CB	-5.52	1.44	1.52
2	F	285	GLU	CD-OE2	-5.50	1.19	1.25
2	J	301	GLU	CD-OE1	-5.29	1.19	1.25
2	J	266	GLU	CD-OE1	-5.27	1.19	1.25
2	L	256	GLY	C-O	-5.24	1.15	1.23
2	B	372	GLY	C-O	-5.21	1.15	1.23
2	J	64	PRO	C-O	-5.07	1.13	1.23
2	D	151	GLU	CD-OE1	-5.04	1.20	1.25

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	213	GLU	C-N-CA	-5.72	107.40	121.70
2	D	233	ASP	CB-CA-C	5.70	121.80	110.40
2	F	94	ASP	CB-CA-C	5.58	121.55	110.40
2	H	325	ASP	CB-CA-C	5.38	121.16	110.40
2	D	81	PRO	N-CA-C	5.37	126.06	112.10
2	L	97	PRO	N-CA-C	-5.35	98.19	112.10
2	J	97	PRO	N-CA-CB	-5.30	96.77	102.60
2	F	290	THR	CB-CA-C	-5.16	97.67	111.60
2	B	266	GLU	CB-CA-C	5.10	120.61	110.40
2	L	85	ASP	CB-CA-C	-5.02	100.36	110.40

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	68	0	61	5	0
1	C	68	0	61	10	0
1	E	60	0	57	7	0
1	G	60	0	57	11	0
1	I	60	0	57	0	0
1	K	86	0	83	33	0
2	B	2388	0	2435	220	2
2	D	2388	0	2434	241	0
2	F	2388	0	2434	277	0
2	H	2388	0	2435	197	1
2	J	2388	0	2435	207	1
2	L	2388	0	2435	250	0
3	B	5	0	5	1	0
3	D	5	0	5	3	0
3	F	5	0	5	3	0
3	H	5	0	5	8	0
3	J	5	0	5	1	0
3	L	5	0	5	4	0
4	B	51	0	0	43	0
4	D	51	0	0	32	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	43	0	0	42	0
4	G	2	0	0	0	0
4	H	51	0	0	26	0
4	I	2	0	0	0	0
4	J	44	0	0	23	0
4	K	1	0	0	1	0
4	L	71	0	0	57	0
All	All	15076	0	15014	1320	2

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 44.

All (1320) 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:L:305:ILE:HD11	2:L:327:ILE:CB	1.29	1.60
2:L:305:ILE:CD1	2:L:327:ILE:HB	1.26	1.58
1:K:6:LEU:CD2	2:L:287:LYS:HB3	1.35	1.51
2:B:74:MET:CG	2:B:101:ARG:HE	1.28	1.46
2:J:180:VAL:HA	4:J:518:HOH:O	1.21	1.39
2:F:95:ASN:ND2	2:J:296:SER:O	1.57	1.38
2:J:77:LYS:HE2	2:J:100:LYS:CB	1.50	1.38
2:F:251:GLY:HA3	2:J:253:GLN:NE2	1.41	1.36
2:J:287:LYS:HE2	4:J:521:HOH:O	1.19	1.35
2:J:68:ASN:ND2	2:J:186:ASN:HB2	1.38	1.34
2:H:301:GLU:HG3	2:H:336:SER:O	1.19	1.33
2:H:151:GLU:HG2	4:H:504:HOH:O	1.19	1.33
2:D:297:LEU:HD21	4:D:541:HOH:O	1.14	1.31
2:B:172:SER:HB3	4:B:521:HOH:O	1.29	1.29
2:F:94:ASP:CG	2:F:96:LEU:HD21	1.52	1.29
2:F:154:LEU:HA	4:F:505:HOH:O	1.11	1.28
2:D:141:THR:HG23	4:D:537:HOH:O	1.11	1.27
2:F:94:ASP:OD2	2:F:96:LEU:HD21	1.35	1.27
2:F:142:ILE:HG22	4:F:516:HOH:O	1.28	1.26
2:J:70:TYR:HE1	2:J:132:ILE:CD1	1.49	1.26
2:H:219:ASP:HB3	4:H:503:HOH:O	1.13	1.26
2:B:93:GLY:HA3	4:B:526:HOH:O	1.31	1.25
2:J:117:TYR:CE1	2:J:158:LYS:HD3	1.71	1.25
2:F:284:VAL:HB	4:F:523:HOH:O	1.23	1.25
2:H:97:PRO:HG3	4:D:538:HOH:O	1.38	1.24
1:C:7:ARG:NH1	2:D:287:LYS:HE2	1.51	1.23

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:83:PHE:O	2:L:90:ARG:HD2	1.27	1.23
2:F:172:SER:HB2	4:F:520:HOH:O	1.11	1.23
2:F:83:PHE:HE1	4:L:541:HOH:O	1.22	1.23
2:L:99:GLN:HA	4:L:518:HOH:O	1.08	1.22
2:D:102:MET:HE2	4:K:101:HOH:O	1.37	1.21
2:J:61:ARG:HG2	4:J:515:HOH:O	1.06	1.20
2:L:102:MET:CE	4:L:562:HOH:O	1.84	1.20
1:G:6:LEU:CD1	4:H:518:HOH:O	1.87	1.20
2:L:172:SER:HB2	4:L:521:HOH:O	1.05	1.20
1:K:6:LEU:CD2	2:L:287:LYS:CB	2.20	1.19
2:L:293:LEU:HD21	4:L:561:HOH:O	1.02	1.18
2:F:71:THR:HG22	2:F:106:LEU:CD2	1.72	1.18
2:D:299:LEU:HB2	2:D:302:THR:OG1	1.40	1.18
2:J:70:TYR:CE1	2:J:132:ILE:CD1	2.26	1.17
1:K:6:LEU:HD23	2:L:287:LYS:HB3	1.25	1.17
1:G:6:LEU:HD13	4:H:518:HOH:O	1.45	1.16
2:B:361:ASN:ND2	4:B:501:HOH:O	1.77	1.16
2:D:68:ASN:HB3	4:D:524:HOH:O	1.45	1.16
2:D:325:ASP:OD1	2:D:360:ARG:HD3	1.46	1.16
2:D:188:PHE:CE2	4:L:534:HOH:O	1.98	1.15
2:J:70:TYR:CE1	2:J:132:ILE:HB	1.81	1.15
2:H:279:ARG:NH1	3:H:401:IMD:C5	2.10	1.15
1:K:6:LEU:HD23	2:L:287:LYS:CB	1.76	1.14
2:D:76:SER:HA	2:D:99:GLN:HB3	1.23	1.14
2:D:318:ARG:NH1	4:D:502:HOH:O	1.80	1.14
2:B:74:MET:HG3	2:B:101:ARG:NE	1.61	1.14
2:D:299:LEU:HD12	2:D:302:THR:HG21	1.28	1.14
2:D:103:GLU:OE2	1:K:3:ARG:HB2	1.48	1.13
2:H:301:GLU:CG	2:H:336:SER:O	1.94	1.13
2:J:77:LYS:CE	2:J:100:LYS:CG	2.27	1.13
2:H:94:ASP:HB2	2:H:96:LEU:HG	1.27	1.12
2:H:293:LEU:CB	4:H:501:HOH:O	1.96	1.12
2:F:95:ASN:HB2	2:J:296:SER:HB2	1.30	1.12
2:D:174:GLY:N	4:D:501:HOH:O	1.82	1.12
2:J:68:ASN:ND2	2:J:186:ASN:CB	2.12	1.12
2:J:77:LYS:HE2	2:J:100:LYS:CG	1.79	1.12
2:B:172:SER:CB	4:B:521:HOH:O	1.90	1.11
2:D:115:GLU:O	2:D:158:LYS:HE3	1.50	1.11
2:B:53:VAL:HB	4:B:543:HOH:O	1.49	1.10
2:F:94:ASP:CG	2:F:96:LEU:CD2	2.19	1.10
2:J:77:LYS:CE	2:J:100:LYS:HG2	1.81	1.10

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:LEU:HD22	2:L:287:LYS:HB3	1.10	1.10
2:B:325:ASP:OD2	2:B:360:ARG:NH1	1.85	1.10
2:H:293:LEU:O	2:H:295:GLU:OE1	1.68	1.09
2:J:77:LYS:CE	2:J:100:LYS:HB2	1.81	1.09
2:B:74:MET:CG	2:B:101:ARG:NE	2.13	1.09
2:L:329:THR:CG2	4:L:511:HOH:O	1.98	1.09
2:H:68:ASN:HB3	4:H:525:HOH:O	0.93	1.08
2:J:72:THR:HG22	2:J:130:GLN:OE1	1.53	1.08
2:B:74:MET:HG3	2:B:101:ARG:HE	0.92	1.08
2:D:294:ALA:HB2	4:D:504:HOH:O	1.51	1.08
2:J:353:LYS:HE3	2:J:370:GLU:HG3	1.32	1.08
2:B:246:PHE:HE1	4:B:541:HOH:O	1.32	1.08
2:F:325:ASP:HB3	2:F:358:VAL:HG11	1.36	1.08
2:J:77:LYS:HE3	2:J:100:LYS:HD3	1.36	1.08
2:F:95:ASN:HB2	2:J:296:SER:CB	1.81	1.07
2:D:141:THR:CG2	4:D:537:HOH:O	1.73	1.07
2:B:312:ARG:HB3	4:D:531:HOH:O	1.55	1.07
2:H:279:ARG:NH1	3:H:401:IMD:N1	2.03	1.07
2:D:205:ASN:HB3	4:D:528:HOH:O	1.55	1.07
2:L:75:VAL:HG23	2:L:100:LYS:O	1.53	1.07
2:L:102:MET:HE3	4:L:562:HOH:O	1.45	1.07
2:D:368:THR:CG2	4:D:533:HOH:O	2.03	1.07
2:F:295:GLU:OE2	2:F:296:SER:N	1.87	1.07
2:D:297:LEU:CD2	4:D:541:HOH:O	1.76	1.06
2:H:139:ARG:NH2	2:H:162:LYS:O	1.89	1.06
2:L:85:ASP:HB2	2:L:90:ARG:HH12	1.15	1.06
2:D:85:ASP:OD1	2:D:86:PRO:CD	2.04	1.05
2:J:80:HIS:CD2	2:J:81:PRO:HD2	1.90	1.05
2:B:205:ASN:ND2	2:B:213:GLU:O	1.89	1.05
2:D:100:LYS:HE3	1:K:4:ASP:OD2	1.54	1.05
2:J:77:LYS:HE2	2:J:100:LYS:HB2	1.05	1.05
2:F:95:ASN:HB3	2:J:296:SER:HA	1.38	1.04
2:J:102:MET:HE3	2:J:102:MET:HA	1.40	1.04
2:H:83:PHE:O	2:H:90:ARG:HD2	1.57	1.04
2:D:115:GLU:O	2:D:158:LYS:CE	2.05	1.04
2:D:299:LEU:CD1	2:D:302:THR:HG21	1.88	1.04
2:D:100:LYS:CE	1:K:4:ASP:OD2	2.05	1.03
2:D:171:ARG:O	4:D:501:HOH:O	1.76	1.02
2:J:96:LEU:H	2:J:97:PRO:HD3	1.14	1.02
2:L:93:GLY:CA	4:L:516:HOH:O	2.05	1.02
2:D:294:ALA:CB	4:D:504:HOH:O	2.02	1.02

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:83:PHE:CE1	4:L:541:HOH:O	2.00	1.02
2:B:212:TYR:CD2	2:B:279:ARG:NH1	2.28	1.02
2:J:70:TYR:CE1	2:J:132:ILE:HD13	1.94	1.02
2:D:368:THR:HG22	4:D:533:HOH:O	1.56	1.02
2:F:150:PRO:HD2	4:F:517:HOH:O	0.85	1.02
2:F:303:ALA:HB1	2:F:328:LEU:HA	1.35	1.02
2:L:307:VAL:HG11	4:L:548:HOH:O	1.57	1.01
1:K:10:PHE:O	2:L:282:LEU:N	1.92	1.01
2:H:163:ASN:HB2	4:H:507:HOH:O	1.58	1.01
2:D:70:TYR:CE1	2:D:103:GLU:HB3	1.95	1.01
2:L:303:ALA:HB2	2:L:328:LEU:HD23	1.39	1.01
2:D:151:GLU:HG3	4:D:513:HOH:O	1.59	1.01
2:L:85:ASP:HB2	2:L:90:ARG:NH1	1.76	1.01
2:L:195:THR:HB	4:L:515:HOH:O	0.83	1.00
2:F:322:LEU:HD23	2:F:360:ARG:HH12	1.24	1.00
2:H:94:ASP:HB2	2:H:96:LEU:CG	1.90	1.00
2:J:70:TYR:CE1	2:J:132:ILE:HD12	1.96	1.00
2:B:339:ARG:HD3	4:B:517:HOH:O	1.61	0.99
2:H:70:TYR:CZ	2:H:132:ILE:HG21	1.98	0.99
2:L:53:VAL:HG22	4:L:546:HOH:O	1.61	0.99
2:L:70:TYR:CE2	2:L:132:ILE:HD12	1.97	0.99
2:F:75:VAL:HG22	2:F:100:LYS:O	1.63	0.99
2:L:366:ASN:HB3	4:L:530:HOH:O	0.80	0.98
2:F:251:GLY:HA3	2:J:253:GLN:HE21	1.23	0.98
2:L:329:THR:HG23	4:L:511:HOH:O	1.60	0.98
2:B:74:MET:HG2	2:B:101:ARG:HE	1.27	0.98
2:L:77:LYS:HG3	2:L:78:PRO:HD2	1.47	0.97
2:J:77:LYS:CE	2:J:100:LYS:CB	2.37	0.97
2:L:74:MET:HA	2:L:74:MET:CE	1.94	0.97
2:D:89:ARG:HH11	2:D:89:ARG:HG2	1.27	0.97
2:F:95:ASN:CB	2:J:296:SER:HA	1.93	0.97
2:D:96:LEU:N	2:D:97:PRO:HD2	1.80	0.96
2:J:102:MET:HA	2:J:102:MET:CE	1.94	0.96
2:J:117:TYR:CD1	2:J:158:LYS:HD3	2.00	0.96
2:H:188:PHE:HE1	2:D:248:LYS:HE2	1.27	0.96
2:D:115:GLU:O	2:D:158:LYS:NZ	1.99	0.96
2:J:226:ASN:OD1	4:J:501:HOH:O	1.84	0.95
2:D:85:ASP:OD1	2:D:86:PRO:HD2	1.66	0.95
2:D:188:PHE:CD2	4:L:534:HOH:O	2.15	0.95
2:D:96:LEU:H	2:D:97:PRO:HD2	1.31	0.95
2:D:325:ASP:CG	2:D:360:ARG:HD3	1.87	0.95

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:360:ARG:HH11	2:F:360:ARG:HG3	1.31	0.94
2:H:299:LEU:H	2:H:302:THR:HG21	1.29	0.94
2:F:169:LEU:HD13	2:F:265:LEU:HD11	1.48	0.94
2:J:77:LYS:HE3	2:J:100:LYS:CD	1.97	0.94
1:C:7:ARG:HH12	2:D:287:LYS:HE2	1.25	0.93
2:B:259:ILE:O	4:B:502:HOH:O	1.86	0.93
2:D:303:ALA:HB1	2:D:328:LEU:HD23	1.50	0.93
2:L:322:LEU:HG	2:L:360:ARG:HH21	1.31	0.93
2:D:70:TYR:HE1	2:D:103:GLU:HB3	1.29	0.93
2:B:96:LEU:N	2:B:97:PRO:HD2	1.83	0.92
2:F:71:THR:HG22	2:F:106:LEU:HD21	1.48	0.92
2:L:83:PHE:O	2:L:90:ARG:CD	2.18	0.92
2:J:80:HIS:CG	2:J:81:PRO:HD2	2.04	0.92
2:J:68:ASN:HD21	2:J:186:ASN:HB2	0.94	0.92
2:H:94:ASP:CG	2:H:96:LEU:CD2	2.38	0.92
2:H:188:PHE:CE1	2:D:248:LYS:HE2	2.05	0.92
2:J:141:THR:HG22	4:J:505:HOH:O	1.69	0.92
2:B:200:SER:O	4:B:503:HOH:O	1.88	0.92
2:F:194:VAL:O	2:J:200:SER:OG	1.86	0.92
2:B:212:TYR:CE2	2:B:279:ARG:NH1	2.36	0.91
2:H:70:TYR:CE1	2:H:132:ILE:HG21	2.05	0.91
2:F:71:THR:HG22	2:F:106:LEU:HD22	1.50	0.91
2:F:295:GLU:HB3	4:F:526:HOH:O	1.70	0.91
2:H:198:ILE:HG12	4:H:503:HOH:O	1.70	0.91
2:H:293:LEU:N	4:H:501:HOH:O	2.00	0.91
2:L:205:ASN:HD22	2:L:339:ARG:CD	1.83	0.91
2:L:74:MET:HA	2:L:74:MET:HE2	1.52	0.91
2:D:218:THR:O	4:D:503:HOH:O	1.86	0.91
2:H:279:ARG:HH11	3:H:401:IMD:C5	1.80	0.91
2:J:68:ASN:HD22	2:J:186:ASN:CB	1.84	0.90
2:D:250:GLY:O	2:L:248:LYS:CD	2.19	0.90
2:H:279:ARG:HH12	3:H:401:IMD:HN1	0.94	0.90
1:C:7:ARG:NH1	2:D:287:LYS:CE	2.35	0.90
2:D:250:GLY:O	2:L:248:LYS:HD2	1.71	0.90
2:F:71:THR:CG2	2:F:106:LEU:CD2	2.50	0.90
1:K:7:ARG:HG3	1:K:7:ARG:HH11	1.33	0.90
2:F:295:GLU:HA	4:F:526:HOH:O	1.71	0.90
2:L:344:GLN:NE2	4:L:502:HOH:O	2.02	0.90
2:L:96:LEU:HD11	4:L:559:HOH:O	1.69	0.90
2:L:75:VAL:CG2	2:L:100:LYS:O	2.18	0.89
2:D:195:THR:HG21	2:D:221:ALA:N	1.86	0.89

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:70:TYR:CE1	2:J:132:ILE:CB	2.55	0.89
2:L:77:LYS:CG	2:L:78:PRO:HD2	2.03	0.89
2:D:212:TYR:OH	2:D:279:ARG:HD3	1.73	0.88
2:B:74:MET:SD	2:B:74:MET:N	2.46	0.88
2:L:53:VAL:HG12	4:L:538:HOH:O	1.72	0.88
2:J:77:LYS:HE3	2:J:100:LYS:CG	2.04	0.88
2:B:315:PRO:HA	2:B:318:ARG:HH12	1.39	0.88
2:D:85:ASP:OD1	2:D:86:PRO:HD3	1.70	0.88
2:B:96:LEU:H	2:B:97:PRO:CD	1.85	0.88
2:D:70:TYR:HE1	2:D:103:GLU:CB	1.86	0.88
2:L:307:VAL:HG21	4:L:548:HOH:O	1.74	0.87
2:D:299:LEU:HB2	2:D:302:THR:CB	2.03	0.87
2:J:245:ILE:HG22	2:J:256:GLY:HA2	1.55	0.87
2:B:81:PRO:O	2:B:90:ARG:HD3	1.75	0.87
2:F:250:GLY:HA2	4:F:531:HOH:O	1.73	0.87
2:J:70:TYR:HE1	2:J:132:ILE:HD13	1.28	0.87
2:L:289:LEU:HD23	2:L:306:VAL:CG2	2.05	0.87
2:J:278:ILE:HG23	2:J:373:LEU:HD11	1.56	0.87
2:F:279:ARG:NH1	3:F:401:IMD:C4	2.38	0.87
2:H:279:ARG:NH1	3:H:401:IMD:H5	1.87	0.86
2:D:161:LEU:HB2	2:D:164:LEU:HD13	1.57	0.86
2:D:325:ASP:OD1	2:D:360:ARG:CD	2.23	0.86
2:B:53:VAL:CB	4:B:543:HOH:O	2.11	0.86
2:L:85:ASP:CB	2:L:90:ARG:HH12	1.87	0.86
2:D:80:HIS:CD2	2:D:81:PRO:HD2	2.09	0.86
2:F:195:THR:HG21	2:F:221:ALA:N	1.90	0.86
2:B:350:PRO:HB3	4:B:514:HOH:O	1.73	0.86
2:D:195:THR:HG22	2:D:220:ALA:HB1	1.56	0.86
2:F:74:MET:CE	2:F:74:MET:HA	2.04	0.86
2:J:96:LEU:N	2:J:97:PRO:HD3	1.89	0.86
2:F:210:ASN:N	2:F:213:GLU:OE1	2.07	0.86
2:B:193:THR:HG22	2:F:204:ARG:HH21	1.40	0.85
2:J:72:THR:CG2	2:J:130:GLN:OE1	2.24	0.85
2:D:106:LEU:H	2:D:106:LEU:HD22	1.40	0.85
2:H:218:THR:HG22	2:H:220:ALA:H	1.40	0.85
2:H:295:GLU:HG2	4:H:527:HOH:O	1.76	0.85
2:F:95:ASN:HB2	2:J:296:SER:CA	2.07	0.85
2:L:79:SER:HB2	4:L:523:HOH:O	1.76	0.85
2:B:86:PRO:HA	2:D:312:ARG:HH12	1.38	0.85
2:F:96:LEU:HD23	2:F:96:LEU:H	1.39	0.85
2:B:246:PHE:CE1	4:B:541:HOH:O	2.15	0.85

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ARG:HH12	2:D:287:LYS:CE	1.90	0.84
2:L:93:GLY:HA3	4:L:516:HOH:O	1.66	0.84
2:H:249:SER:HB3	2:L:249:SER:HB2	1.58	0.83
2:B:53:VAL:CG2	4:B:543:HOH:O	2.27	0.83
2:F:267:VAL:HG13	2:F:277:VAL:HG21	1.60	0.83
2:F:352:GLN:NE2	4:F:501:HOH:O	1.92	0.83
2:F:162:LYS:HE3	2:F:162:LYS:HA	1.61	0.83
1:C:8:TRP:HB2	2:D:286:VAL:HG23	1.59	0.83
2:F:162:LYS:HA	2:F:162:LYS:CE	2.09	0.83
2:L:328:LEU:HD12	2:L:357:VAL:HG12	1.59	0.83
2:L:321:LEU:HG	4:L:548:HOH:O	1.77	0.82
2:H:211:THR:HG22	2:H:212:TYR:CD2	2.13	0.82
2:F:325:ASP:HB3	2:F:358:VAL:CG1	2.09	0.82
2:J:85:ASP:O	2:L:312:ARG:NH2	2.11	0.82
2:H:94:ASP:HB2	2:H:96:LEU:CD2	2.10	0.82
2:D:70:TYR:CE1	2:D:103:GLU:CB	2.61	0.82
2:D:76:SER:CA	2:D:99:GLN:HB3	2.07	0.82
2:F:71:THR:CG2	2:F:106:LEU:HD21	2.08	0.82
2:H:91:PHE:HZ	2:F:324:GLY:CA	1.92	0.82
2:F:74:MET:HA	2:F:74:MET:HE3	1.62	0.82
2:F:322:LEU:HD23	2:F:360:ARG:NH1	1.95	0.82
2:L:318:ARG:NH2	4:L:501:HOH:O	1.90	0.82
2:H:72:THR:O	2:H:73:LYS:HE2	1.78	0.82
2:J:139:ARG:NH2	2:J:162:LYS:O	2.12	0.82
2:L:89:ARG:HG2	2:L:89:ARG:HH11	1.44	0.82
2:J:142:ILE:HG12	4:J:504:HOH:O	1.79	0.81
2:J:112:MET:HE1	2:J:119:LEU:HB2	1.61	0.81
2:F:251:GLY:HA3	2:J:253:GLN:HE22	1.44	0.81
2:H:94:ASP:CG	2:H:96:LEU:HD21	1.98	0.81
2:J:70:TYR:CD1	2:J:132:ILE:HB	2.15	0.81
2:L:325:ASP:OD1	2:L:360:ARG:HG3	1.81	0.81
2:B:96:LEU:H	2:B:97:PRO:HD2	1.38	0.81
2:H:299:LEU:H	2:H:302:THR:CG2	1.93	0.81
2:B:315:PRO:CA	2:B:318:ARG:HH12	1.94	0.80
2:H:94:ASP:OD2	2:H:96:LEU:HD23	1.82	0.80
2:F:319:GLY:O	4:F:502:HOH:O	2.00	0.80
2:J:330:ILE:HB	4:J:517:HOH:O	1.80	0.80
2:D:70:TYR:HB3	2:D:132:ILE:HB	1.63	0.80
2:L:176:ARG:HD3	4:L:535:HOH:O	1.82	0.80
2:L:205:ASN:ND2	2:L:339:ARG:NE	2.29	0.80
2:D:96:LEU:H	2:D:97:PRO:CD	1.94	0.79

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:70:TYR:HE1	2:J:132:ILE:CB	1.94	0.79
2:F:95:ASN:CB	2:J:296:SER:CA	2.59	0.79
2:L:279:ARG:HE	3:L:401:IMD:H4	1.45	0.79
2:F:295:GLU:CB	4:F:526:HOH:O	2.27	0.79
2:J:212:TYR:CE2	2:J:279:ARG:NH1	2.51	0.79
2:D:299:LEU:HB2	2:D:302:THR:CG2	2.12	0.79
2:L:205:ASN:HD22	2:L:339:ARG:NE	1.80	0.79
2:F:313:ASP:OD1	2:F:318:ARG:NH1	2.17	0.78
2:B:315:PRO:HA	2:B:318:ARG:NH1	1.97	0.78
2:F:85:ASP:HB2	2:F:90:ARG:HH12	1.47	0.78
2:J:180:VAL:HG22	4:J:518:HOH:O	1.83	0.78
2:D:193:THR:HG22	2:L:204:ARG:HH21	1.48	0.78
2:H:94:ASP:CG	2:H:96:LEU:HD23	2.03	0.78
2:B:289:LEU:O	2:B:289:LEU:HD12	1.83	0.78
2:L:177:THR:HA	2:L:199:ILE:HG22	1.63	0.78
2:F:71:THR:CG2	2:F:106:LEU:HD22	2.14	0.78
2:B:108:SER:O	2:B:228:GLY:C	2.23	0.77
2:D:186:ASN:O	2:D:225:GLY:O	2.02	0.77
2:B:96:LEU:N	2:B:97:PRO:CD	2.43	0.77
2:H:87:MET:SD	2:F:311:TYR:CE1	2.78	0.77
2:J:70:TYR:HE1	2:J:132:ILE:CG1	1.98	0.77
3:B:401:IMD:H2	4:B:531:HOH:O	1.84	0.77
2:D:143:ALA:HB2	2:D:159:ILE:CD1	2.14	0.76
2:H:219:ASP:CB	4:H:503:HOH:O	1.92	0.76
2:D:195:THR:HG21	2:D:221:ALA:H	1.46	0.76
2:H:94:ASP:CB	2:H:96:LEU:CD2	2.64	0.76
2:L:70:TYR:CE2	2:L:103:GLU:OE1	2.39	0.76
2:F:77:LYS:HE3	2:F:96:LEU:CD1	2.16	0.75
2:F:139:ARG:NH2	2:F:162:LYS:O	2.19	0.75
2:L:70:TYR:CE2	2:L:132:ILE:CD1	2.70	0.75
2:L:328:LEU:HD12	2:L:357:VAL:CG1	2.16	0.75
2:D:186:ASN:O	2:D:186:ASN:ND2	2.20	0.75
2:F:123:HIS:ND1	2:F:153:ASP:OD2	2.16	0.75
2:H:87:MET:SD	2:F:311:TYR:OH	2.43	0.74
2:H:68:ASN:OD1	2:H:186:ASN:HB2	1.87	0.74
2:B:80:HIS:CD2	2:B:81:PRO:HD2	2.22	0.74
2:L:77:LYS:CD	2:L:78:PRO:HD2	2.17	0.74
2:L:330:ILE:HB	4:L:502:HOH:O	1.86	0.74
2:B:139:ARG:NH2	2:B:162:LYS:O	2.20	0.74
2:D:303:ALA:CB	2:D:328:LEU:HD23	2.18	0.74
2:B:89:ARG:HG2	2:B:89:ARG:HH11	1.51	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:175:ILE:HD13	2:L:199:ILE:HG12	1.69	0.74
2:L:243:THR:HG21	2:L:259:ILE:CD1	2.18	0.74
2:F:135:LEU:N	2:F:135:LEU:HD23	2.02	0.73
1:C:10:PHE:HE2	2:D:286:VAL:HG21	1.52	0.73
2:H:85:ASP:HB2	2:H:86:PRO:CD	2.17	0.73
2:D:76:SER:HA	2:D:99:GLN:CB	2.11	0.73
2:J:71:THR:OG1	2:J:129:ASP:OD1	2.06	0.73
2:F:77:LYS:NZ	2:F:100:LYS:HG2	2.03	0.73
2:B:54:SER:OG	2:F:179:ASP:OD1	2.05	0.73
2:B:108:SER:O	2:B:228:GLY:O	2.07	0.73
2:F:96:LEU:CD2	2:F:96:LEU:H	2.00	0.73
2:F:301:GLU:O	2:F:336:SER:HB2	1.89	0.73
2:L:322:LEU:CG	2:L:360:ARG:HH21	2.02	0.73
2:B:312:ARG:HD3	2:D:87:MET:HA	1.70	0.73
2:D:65:ALA:HB3	2:D:167:MET:HE1	1.70	0.73
2:D:116:GLY:HA3	2:D:159:ILE:O	1.89	0.73
2:J:69:LEU:HD11	2:J:109:ALA:HB2	1.69	0.73
2:F:74:MET:HE3	2:F:100:LYS:O	1.89	0.72
2:H:293:LEU:HB2	4:H:501:HOH:O	1.71	0.72
2:B:177:THR:HA	2:B:199:ILE:HG22	1.71	0.72
2:D:74:MET:HA	2:D:74:MET:CE	2.18	0.72
2:F:68:ASN:HB3	4:F:514:HOH:O	1.87	0.72
2:L:305:ILE:HD12	2:L:305:ILE:O	1.89	0.72
2:D:282:LEU:O	2:D:316:ALA:HB2	1.90	0.72
2:D:305:ILE:HD13	2:D:335:ALA:HB1	1.71	0.72
2:F:289:LEU:HD21	2:F:294:ALA:HB2	1.71	0.72
2:J:316:ALA:HB1	2:J:321:LEU:HB2	1.72	0.72
1:K:6:LEU:HD23	2:L:287:LYS:HD3	1.71	0.72
2:B:361:ASN:N	2:B:361:ASN:HD22	1.88	0.72
2:F:284:VAL:HG13	2:F:316:ALA:CB	2.19	0.72
2:B:134:ALA:HB2	2:B:140:GLU:HG2	1.71	0.72
2:D:121:ASN:HB2	2:D:124:VAL:HG23	1.71	0.72
2:D:65:ALA:HB3	2:D:167:MET:CE	2.19	0.72
2:F:261:THR:HG22	2:F:265:LEU:HD12	1.72	0.72
2:H:87:MET:SD	2:F:311:TYR:CZ	2.83	0.72
2:B:74:MET:HG2	2:B:101:ARG:HH11	1.54	0.72
2:B:121:ASN:ND2	2:B:153:ASP:O	2.23	0.72
2:J:250:GLY:HA2	4:J:519:HOH:O	1.90	0.72
2:H:74:MET:HA	2:H:101:ARG:HA	1.72	0.71
2:H:153:ASP:OD2	4:H:502:HOH:O	2.06	0.71
2:F:77:LYS:HE3	2:F:96:LEU:HD12	1.72	0.71

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:98:GLN:NE2	2:J:98:GLN:HA	2.03	0.71
1:K:6:LEU:HD13	1:K:6:LEU:O	1.90	0.71
2:L:325:ASP:OD1	2:L:360:ARG:CG	2.37	0.71
2:L:175:ILE:HD11	2:L:202:THR:HG22	1.70	0.71
2:F:226:ASN:OD1	4:F:503:HOH:O	2.08	0.71
2:J:96:LEU:N	2:J:97:PRO:CD	2.52	0.71
2:H:112:MET:HE2	2:H:119:LEU:HB3	1.71	0.71
2:B:350:PRO:CB	4:B:514:HOH:O	2.36	0.71
2:H:299:LEU:N	2:H:302:THR:HG21	2.01	0.71
4:F:511:HOH:O	2:L:82:LEU:CD1	2.38	0.71
2:D:294:ALA:N	4:D:504:HOH:O	2.23	0.71
2:F:71:THR:CB	2:F:106:LEU:HD21	2.21	0.71
2:J:94:ASP:OD1	2:J:94:ASP:N	2.23	0.71
1:E:8:TRP:HH2	2:F:206:GLN:HG2	1.54	0.71
2:B:72:THR:OG1	2:B:130:GLN:NE2	2.24	0.71
2:B:68:ASN:OD1	2:B:108:SER:OG	2.08	0.71
2:F:286:VAL:HG12	4:F:523:HOH:O	1.90	0.70
2:H:94:ASP:CB	2:H:96:LEU:HD23	2.21	0.70
2:B:231:LEU:HB2	2:B:242:ASN:HD21	1.56	0.70
2:H:70:TYR:CE1	2:H:132:ILE:CG2	2.74	0.70
2:F:77:LYS:HD2	2:F:100:LYS:HG3	1.72	0.70
2:F:301:GLU:O	2:F:336:SER:CB	2.39	0.70
2:D:75:VAL:HG21	2:D:102:MET:SD	2.31	0.70
4:B:503:HOH:O	2:J:192:GLN:O	2.09	0.70
2:D:195:THR:CG2	2:D:221:ALA:H	2.05	0.70
2:F:77:LYS:CE	2:F:96:LEU:HD12	2.22	0.70
2:J:325:ASP:OD2	2:J:360:ARG:NH2	2.23	0.70
2:H:279:ARG:NH1	3:H:401:IMD:HN1	1.73	0.70
2:H:70:TYR:HE1	2:H:132:ILE:HD13	1.57	0.70
2:H:299:LEU:C	2:H:302:THR:HG22	2.12	0.70
2:D:75:VAL:HG21	2:D:102:MET:CE	2.21	0.69
2:D:282:LEU:O	2:D:316:ALA:CB	2.40	0.69
2:J:96:LEU:H	2:J:97:PRO:CD	1.96	0.69
2:L:96:LEU:CD1	4:L:559:HOH:O	2.31	0.69
2:L:289:LEU:HD23	2:L:306:VAL:HG23	1.74	0.69
2:L:293:LEU:HD12	2:L:295:GLU:OE2	1.92	0.69
2:B:301:GLU:OE2	2:B:302:THR:N	2.25	0.69
2:B:313:ASP:O	2:B:318:ARG:NH2	2.25	0.69
1:G:6:LEU:HD12	1:G:6:LEU:O	1.93	0.69
2:H:81:PRO:O	2:H:90:ARG:HD3	1.92	0.69
2:D:103:GLU:OE2	1:K:3:ARG:CB	2.35	0.69

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:301:GLU:N	2:F:301:GLU:OE2	2.24	0.69
2:D:212:TYR:CZ	2:D:279:ARG:HD3	2.27	0.69
2:F:132:ILE:HG21	4:F:541:HOH:O	1.92	0.69
2:L:243:THR:HG21	2:L:259:ILE:HG13	1.75	0.69
2:B:200:SER:HB3	2:J:193:THR:HG23	1.73	0.69
2:D:175:ILE:HD11	2:D:216:ILE:HD12	1.74	0.69
2:D:299:LEU:CB	2:D:302:THR:CG2	2.70	0.69
1:K:7:ARG:HG3	1:K:7:ARG:NH1	1.95	0.69
2:D:290:THR:O	4:D:504:HOH:O	2.10	0.69
2:F:94:ASP:CB	2:F:96:LEU:HD21	2.23	0.69
2:J:184:ILE:HG12	2:J:194:VAL:HG13	1.73	0.69
2:D:83:PHE:HA	2:D:92:PHE:O	1.93	0.68
2:J:112:MET:CE	2:J:119:LEU:HB2	2.23	0.68
2:H:299:LEU:O	2:H:302:THR:HG22	1.93	0.68
2:B:259:ILE:HB	4:B:502:HOH:O	1.92	0.68
2:D:140:GLU:HB2	4:D:517:HOH:O	1.92	0.68
2:F:94:ASP:CB	2:F:96:LEU:CD2	2.71	0.68
2:J:95:ASN:HB2	2:J:96:LEU:HD22	1.73	0.68
2:L:289:LEU:CD2	2:L:306:VAL:CG2	2.71	0.68
2:H:70:TYR:HD2	4:H:545:HOH:O	1.75	0.68
4:F:542:HOH:O	2:J:246:PHE:HD2	1.76	0.68
2:H:214:ASP:O	2:H:260:PRO:CD	2.41	0.68
2:H:296:SER:HB3	4:H:527:HOH:O	1.93	0.68
2:F:173:ASP:O	4:F:504:HOH:O	2.11	0.68
2:H:85:ASP:HB2	2:H:86:PRO:HD3	1.76	0.68
2:H:295:GLU:CG	4:H:527:HOH:O	2.37	0.68
2:B:196:MET:HE1	2:J:196:MET:CE	2.23	0.68
2:F:212:TYR:CE2	2:F:279:ARG:NH1	2.62	0.68
2:J:198:ILE:HG22	4:J:518:HOH:O	1.94	0.68
2:H:293:LEU:HB3	4:H:501:HOH:O	1.73	0.68
2:F:325:ASP:CB	2:F:358:VAL:HG11	2.18	0.68
2:J:77:LYS:NZ	2:J:100:LYS:HG2	2.09	0.68
2:L:217:GLN:HG3	2:L:257:PHE:CE1	2.29	0.68
2:B:74:MET:HG3	2:B:101:ARG:CD	2.24	0.67
2:B:289:LEU:N	4:B:509:HOH:O	2.26	0.67
2:J:63:ALA:N	2:J:64:PRO:HD2	2.09	0.67
2:L:136:ARG:NH1	4:L:505:HOH:O	2.26	0.67
2:F:96:LEU:HD23	2:F:96:LEU:N	2.10	0.67
2:L:205:ASN:ND2	2:L:339:ARG:CD	2.57	0.67
2:F:132:ILE:CG2	4:F:541:HOH:O	2.43	0.67
2:F:169:LEU:CD1	2:F:265:LEU:HD11	2.24	0.67

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:360:ARG:HE	2:F:365:VAL:HG21	1.59	0.67
2:J:222:ILE:O	2:J:252:SER:HB2	1.94	0.67
1:K:6:LEU:CD2	2:L:287:LYS:HD3	2.25	0.67
2:L:292:GLU:O	2:L:295:GLU:OE1	2.12	0.67
2:B:209:LEU:HB2	2:B:213:GLU:OE1	1.93	0.67
1:C:10:PHE:CE2	2:D:286:VAL:HG21	2.30	0.67
2:L:80:HIS:CG	2:L:81:PRO:HD2	2.29	0.67
2:L:296:SER:OG	2:L:297:LEU:HD12	1.93	0.67
2:H:94:ASP:OD2	2:H:96:LEU:CD2	2.43	0.67
2:D:299:LEU:CB	2:D:302:THR:HG23	2.25	0.67
2:D:301:GLU:O	2:D:301:GLU:HG2	1.95	0.67
2:F:77:LYS:HD2	2:F:100:LYS:CG	2.25	0.67
2:H:70:TYR:CZ	2:H:132:ILE:CG2	2.77	0.66
2:D:299:LEU:CB	2:D:302:THR:OG1	2.31	0.66
2:H:204:ARG:HB2	2:H:215:PHE:HB2	1.75	0.66
2:F:106:LEU:N	2:F:106:LEU:HD23	2.10	0.66
2:F:331:ASP:HB2	2:F:354:ILE:HG21	1.77	0.66
2:H:112:MET:CE	2:H:119:LEU:HB3	2.25	0.66
2:B:98:GLN:HG3	2:B:99:GLN:HG3	1.76	0.66
2:F:303:ALA:CB	2:F:328:LEU:HA	2.19	0.66
2:H:96:LEU:HD12	2:H:96:LEU:O	1.96	0.66
2:H:91:PHE:CZ	2:F:324:GLY:CA	2.77	0.66
2:H:163:ASN:CB	4:H:507:HOH:O	2.27	0.66
2:H:303:ALA:O	2:H:328:LEU:HA	1.95	0.66
2:D:70:TYR:CZ	2:D:103:GLU:HB3	2.31	0.66
2:L:303:ALA:HB2	2:L:328:LEU:CD2	2.20	0.66
2:D:177:THR:HA	2:D:199:ILE:HG22	1.77	0.66
1:K:6:LEU:HD21	2:L:287:LYS:NZ	2.11	0.66
2:H:83:PHE:O	2:H:90:ARG:CD	2.41	0.66
2:H:188:PHE:HE1	2:D:248:LYS:CE	2.04	0.66
2:H:217:GLN:HE22	2:L:193:THR:CG2	2.08	0.66
2:D:71:THR:HG22	2:D:104:SER:O	1.96	0.66
2:D:80:HIS:CD2	2:D:81:PRO:CD	2.79	0.66
2:F:94:ASP:CG	2:F:96:LEU:HD23	2.12	0.66
2:L:53:VAL:HA	4:L:538:HOH:O	1.95	0.66
4:F:542:HOH:O	2:J:246:PHE:CD2	2.49	0.66
2:B:241:ILE:N	4:B:502:HOH:O	2.05	0.66
2:B:325:ASP:CG	2:B:360:ARG:HH11	1.94	0.65
2:D:232:VAL:HG13	2:D:236:GLY:HA2	1.77	0.65
2:F:85:ASP:HB2	2:F:90:ARG:NH1	2.11	0.65
2:F:195:THR:HG22	2:F:220:ALA:HB1	1.77	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:VAL:HG21	4:B:543:HOH:O	1.93	0.65
2:F:286:VAL:CG1	4:F:523:HOH:O	2.43	0.65
2:L:321:LEU:HD12	2:L:358:VAL:HG21	1.78	0.65
2:J:278:ILE:HG23	2:J:373:LEU:CD1	2.27	0.65
2:J:305:ILE:HD13	2:J:305:ILE:N	2.11	0.65
2:F:322:LEU:CD2	2:F:360:ARG:HH12	2.05	0.65
2:J:180:VAL:CG2	4:J:518:HOH:O	2.42	0.65
2:F:141:THR:OG1	2:F:161:LEU:HD11	1.96	0.65
2:F:203:GLY:HA2	2:F:214:ASP:OD1	1.96	0.65
2:F:331:ASP:CG	2:F:354:ILE:HG21	2.17	0.65
2:L:279:ARG:HE	3:L:401:IMD:C4	2.09	0.65
2:B:169:LEU:HD13	2:B:265:LEU:HD11	1.78	0.65
2:D:106:LEU:H	2:D:106:LEU:CD2	2.10	0.65
1:E:9:VAL:HG22	2:F:285:GLU:HG2	1.79	0.65
2:F:188:PHE:HE1	2:F:224:PRO:HG2	1.62	0.65
2:L:293:LEU:HD11	4:L:561:HOH:O	1.97	0.65
2:B:289:LEU:HG	4:B:509:HOH:O	1.97	0.65
2:H:116:GLY:O	2:H:118:LEU:HD12	1.97	0.64
2:B:241:ILE:HB	4:B:502:HOH:O	1.96	0.64
2:B:289:LEU:HD12	4:B:509:HOH:O	1.97	0.64
2:D:100:LYS:HD2	2:D:101:ARG:H	1.63	0.64
2:F:195:THR:CG2	2:F:221:ALA:N	2.59	0.64
2:B:217:GLN:HG3	2:B:257:PHE:CE1	2.33	0.64
2:D:251:GLY:HA3	2:L:253:GLN:NE2	2.12	0.64
2:D:279:ARG:NE	3:D:401:IMD:HN3	1.95	0.64
2:B:74:MET:HG2	2:B:101:ARG:NH1	2.12	0.64
2:L:143:ALA:HB2	2:L:159:ILE:HD11	1.79	0.64
2:F:195:THR:CG2	2:F:221:ALA:H	2.10	0.64
2:L:307:VAL:CG1	4:L:548:HOH:O	2.30	0.64
2:B:297:LEU:N	2:B:297:LEU:HD12	2.13	0.64
2:D:284:VAL:HG21	4:D:548:HOH:O	1.97	0.64
2:J:70:TYR:CD1	2:J:132:ILE:HD12	2.33	0.64
2:D:100:LYS:NZ	1:K:4:ASP:OD2	2.31	0.64
2:D:143:ALA:HB2	2:D:159:ILE:HD11	1.80	0.64
2:D:210:ASN:N	2:D:213:GLU:OE2	2.19	0.64
2:F:243:THR:HG21	2:F:259:ILE:HG13	1.79	0.64
1:K:10:PHE:HA	4:L:514:HOH:O	1.97	0.64
2:L:312:ARG:NH1	4:L:507:HOH:O	2.29	0.64
1:K:6:LEU:HD23	2:L:287:LYS:HB2	1.74	0.64
2:H:279:ARG:HH12	3:H:401:IMD:C5	1.92	0.64
2:H:282:LEU:O	2:H:316:ALA:HB2	1.98	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:HG22	2:D:285:GLU:HG2	1.79	0.64
2:J:71:THR:CG2	2:J:106:LEU:HD21	2.27	0.64
2:F:106:LEU:HD23	2:F:106:LEU:H	1.63	0.64
2:B:90:ARG:NH2	2:D:285:GLU:OE2	2.31	0.63
2:J:262:LYS:O	4:J:502:HOH:O	2.15	0.63
2:B:74:MET:HG2	2:B:101:ARG:NE	1.95	0.63
2:H:214:ASP:O	2:H:260:PRO:HD3	1.98	0.63
2:B:168:THR:OG1	4:B:505:HOH:O	2.11	0.63
2:D:289:LEU:HD12	2:D:304:GLY:HA2	1.81	0.63
2:F:360:ARG:HG3	2:F:360:ARG:NH1	2.07	0.63
2:F:75:VAL:HG23	2:F:100:LYS:HB2	1.81	0.63
2:B:69:LEU:HD11	2:B:109:ALA:HB2	1.81	0.63
2:B:122:ASN:ND2	2:B:150:PRO:HG3	2.14	0.63
2:L:77:LYS:HG3	2:L:78:PRO:CD	2.26	0.63
2:H:307:VAL:HG12	2:H:323:PRO:HA	1.81	0.63
2:F:207:LEU:HD13	4:F:513:HOH:O	1.97	0.63
2:L:219:ASP:OD1	4:L:503:HOH:O	2.15	0.63
2:D:96:LEU:N	2:D:97:PRO:CD	2.46	0.63
2:B:289:LEU:CD1	4:B:509:HOH:O	2.47	0.63
2:J:175:ILE:HD12	2:J:199:ILE:HD13	1.80	0.63
2:J:309:GLY:HA2	2:L:89:ARG:O	1.99	0.63
2:L:315:PRO:HB3	2:L:370:GLU:O	1.98	0.63
4:B:503:HOH:O	2:J:193:THR:HA	1.99	0.62
2:J:278:ILE:CG2	2:J:373:LEU:CD1	2.76	0.62
2:L:77:LYS:HD2	2:L:78:PRO:HD2	1.80	0.62
2:H:181:CYS:SG	2:H:218:THR:HG23	2.39	0.62
2:D:89:ARG:HG2	2:D:89:ARG:NH1	2.06	0.62
2:H:290:THR:HB	4:H:501:HOH:O	2.00	0.62
2:D:116:GLY:HA2	2:D:164:LEU:CD2	2.29	0.62
2:F:151:GLU:HG2	4:F:517:HOH:O	1.98	0.62
2:J:94:ASP:HB2	2:J:97:PRO:HD2	1.82	0.62
2:L:360:ARG:CZ	4:L:513:HOH:O	2.47	0.62
2:B:196:MET:HE1	2:J:196:MET:HE3	1.81	0.62
2:F:305:ILE:HG13	2:F:327:ILE:HB	1.81	0.62
2:J:214:ASP:O	2:J:260:PRO:CD	2.48	0.62
2:L:285:GLU:HG2	2:L:308:ALA:HB3	1.80	0.62
1:K:6:LEU:CD2	2:L:287:LYS:CG	2.76	0.62
2:L:283:GLY:HA3	2:L:311:TYR:HB2	1.82	0.62
2:B:68:ASN:OD1	2:B:186:ASN:HB2	2.00	0.62
2:F:74:MET:SD	2:F:101:ARG:HB3	2.39	0.62
2:F:291:PRO:HA	2:F:294:ALA:HB3	1.81	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:214:ASP:O	2:J:260:PRO:HD3	2.00	0.62
2:H:87:MET:O	2:F:311:TYR:HA	2.00	0.62
2:B:80:HIS:CG	2:B:81:PRO:HD2	2.35	0.62
2:D:161:LEU:HB2	2:D:164:LEU:CD1	2.28	0.62
2:D:279:ARG:HE	3:D:401:IMD:HN3	1.48	0.62
2:F:278:ILE:HD12	2:F:278:ILE:O	1.98	0.62
2:F:293:LEU:O	2:F:293:LEU:HG	1.98	0.62
2:D:205:ASN:HD22	2:D:339:ARG:NE	1.98	0.61
2:H:182:LEU:HB2	2:H:232:VAL:HG12	1.82	0.61
2:H:299:LEU:HB2	2:H:302:THR:CG2	2.30	0.61
2:B:82:LEU:N	2:B:82:LEU:HD23	2.15	0.61
2:L:80:HIS:CE1	2:L:81:PRO:HD2	2.35	0.61
2:H:143:ALA:HB2	2:H:159:ILE:HD13	1.82	0.61
2:F:94:ASP:OD2	2:F:96:LEU:CD2	2.28	0.61
2:F:279:ARG:NH1	3:F:401:IMD:H4	2.16	0.61
2:F:279:ARG:HH12	3:F:401:IMD:C4	2.13	0.61
2:F:282:LEU:O	2:F:316:ALA:HB2	2.00	0.61
2:D:195:THR:HG23	2:L:219:ASP:OD1	2.00	0.61
2:B:251:GLY:HA3	2:F:253:GLN:NE2	2.15	0.61
2:L:80:HIS:CG	2:L:81:PRO:CD	2.84	0.61
2:L:296:SER:C	2:L:297:LEU:HD12	2.20	0.61
2:B:63:ALA:N	2:B:64:PRO:HD2	2.15	0.61
2:H:65:ALA:O	2:H:111:ILE:HG13	2.00	0.61
2:H:151:GLU:N	4:H:504:HOH:O	2.16	0.61
2:J:71:THR:HB	2:J:106:LEU:HD21	1.83	0.61
2:L:177:THR:HA	2:L:199:ILE:CG2	2.29	0.61
2:F:251:GLY:CA	2:J:253:GLN:HE21	2.07	0.60
2:B:61:ARG:NH2	2:B:168:THR:HG21	2.16	0.60
2:D:299:LEU:HB3	2:D:302:THR:HG23	1.83	0.60
2:J:329:THR:HB	2:J:357:VAL:CG2	2.31	0.60
2:J:331:ASP:HB2	2:J:354:ILE:HB	1.83	0.60
2:L:303:ALA:CB	2:L:328:LEU:HD23	2.23	0.60
2:D:187:PRO:HA	2:D:225:GLY:HA3	1.84	0.60
2:F:71:THR:HB	2:F:106:LEU:HD21	1.83	0.60
1:G:6:LEU:HD11	4:H:518:HOH:O	1.72	0.60
2:B:82:LEU:HD12	2:B:92:PHE:CE2	2.37	0.60
2:L:282:LEU:HB3	2:L:284:VAL:HG23	1.84	0.60
2:H:83:PHE:CD2	2:H:94:ASP:OD1	2.55	0.60
2:D:71:THR:CG2	2:D:104:SER:O	2.49	0.60
2:D:284:VAL:HB	4:D:548:HOH:O	2.01	0.60
2:F:188:PHE:CE1	2:F:224:PRO:HG2	2.37	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:83:PHE:O	2:H:90:ARG:HB2	2.01	0.60
2:B:121:ASN:HB2	2:B:124:VAL:HG23	1.83	0.60
2:L:80:HIS:ND1	2:L:81:PRO:HD2	2.15	0.60
2:L:141:THR:OG1	2:L:161:LEU:HD21	2.02	0.60
2:H:91:PHE:HZ	2:F:324:GLY:HA2	1.66	0.60
2:B:188:PHE:HE1	2:F:248:LYS:HE2	1.66	0.60
2:B:195:THR:HG21	2:B:221:ALA:HB3	1.82	0.60
1:K:10:PHE:HD2	2:L:342:MET:HG3	1.66	0.60
2:D:207:LEU:HB3	2:D:209:LEU:HD12	1.84	0.60
2:F:120:THR:O	4:F:505:HOH:O	2.15	0.59
2:J:131:ILE:HG22	2:J:143:ALA:HB3	1.82	0.59
2:L:243:THR:HG21	2:L:259:ILE:CG1	2.32	0.59
2:L:334:GLU:O	2:L:334:GLU:HG2	1.99	0.59
2:D:141:THR:OG1	2:D:161:LEU:HD11	2.02	0.59
2:F:172:SER:CB	4:F:520:HOH:O	1.95	0.59
2:H:71:THR:HB	2:H:106:LEU:HD11	1.85	0.59
2:F:91:PHE:N	2:F:91:PHE:CD1	2.71	0.59
2:J:195:THR:HG21	2:J:221:ALA:O	2.02	0.59
2:L:293:LEU:HD12	2:L:293:LEU:O	2.02	0.59
2:B:95:ASN:HB3	2:B:97:PRO:HD2	1.85	0.59
2:F:74:MET:HE3	2:F:101:ARG:HA	1.83	0.59
2:L:283:GLY:CA	2:L:311:TYR:HB2	2.33	0.59
2:D:279:ARG:NE	3:D:401:IMD:N3	2.50	0.59
2:J:176:ARG:HG2	2:J:176:ARG:HH11	1.68	0.59
2:H:196:MET:HB2	2:D:198:ILE:HG12	1.85	0.59
2:D:115:GLU:HB3	2:D:158:LYS:HZ1	1.68	0.59
2:L:83:PHE:C	2:L:90:ARG:HB2	2.23	0.59
2:B:193:THR:HG22	2:F:204:ARG:NH2	2.12	0.59
2:F:77:LYS:HE2	2:F:97:PRO:O	2.03	0.59
2:F:243:THR:CG2	2:F:259:ILE:HG13	2.32	0.58
2:H:68:ASN:CB	4:H:525:HOH:O	1.76	0.58
2:F:295:GLU:CA	4:F:526:HOH:O	2.32	0.58
2:F:331:ASP:CB	2:F:354:ILE:HG21	2.31	0.58
2:L:262:LYS:HD3	4:L:557:HOH:O	2.02	0.58
2:H:261:THR:CG2	2:H:265:LEU:HD12	2.34	0.58
2:B:297:LEU:CD1	2:B:297:LEU:H	2.16	0.58
2:H:261:THR:O	2:H:265:LEU:HB2	2.03	0.58
2:J:117:TYR:CD1	2:J:158:LYS:CD	2.82	0.58
2:H:152:THR:HG21	2:H:263:LEU:HD11	1.86	0.58
2:D:193:THR:HG21	2:L:217:GLN:HE22	1.69	0.58
2:D:214:ASP:O	2:D:260:PRO:HD3	2.04	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:305:ILE:HD11	2:L:327:ILE:CA	2.24	0.58
2:B:335:ALA:HB2	4:B:522:HOH:O	2.03	0.58
2:L:242:ASN:HD22	2:L:258:ALA:HB2	1.69	0.58
2:D:182:LEU:HD23	2:D:194:VAL:CG1	2.34	0.58
2:F:278:ILE:HD12	2:F:278:ILE:C	2.24	0.58
2:L:231:LEU:HB2	2:L:242:ASN:HD21	1.69	0.58
2:F:94:ASP:HB2	2:F:96:LEU:CD2	2.33	0.58
2:J:118:LEU:HB2	2:J:157:LEU:HB2	1.86	0.58
2:D:328:LEU:HB2	2:D:357:VAL:HG12	1.86	0.57
2:F:136:ARG:N	4:F:508:HOH:O	2.37	0.57
2:J:195:THR:CG2	2:J:221:ALA:N	2.67	0.57
1:K:10:PHE:C	2:L:282:LEU:H	2.03	0.57
1:G:6:LEU:HB3	2:H:287:LYS:CB	2.34	0.57
2:F:118:LEU:HB2	2:F:157:LEU:HB2	1.85	0.57
2:F:175:ILE:O	4:F:504:HOH:O	2.17	0.57
2:J:184:ILE:O	4:J:501:HOH:O	2.17	0.57
2:D:70:TYR:OH	2:D:103:GLU:HB3	2.04	0.57
1:E:7:ARG:NH1	2:F:287:LYS:HB2	2.19	0.57
2:F:299:LEU:HD13	2:F:302:THR:HB	1.84	0.57
2:F:356:ILE:O	2:F:367:LEU:HB2	2.03	0.57
2:J:129:ASP:OD1	2:J:129:ASP:N	2.36	0.57
2:B:198:ILE:HG12	2:J:196:MET:HB2	1.86	0.57
2:B:289:LEU:CG	4:B:509:HOH:O	2.52	0.57
2:D:106:LEU:HD22	2:D:106:LEU:N	2.15	0.57
2:L:337:ASP:HB3	2:L:340:ARG:HG3	1.86	0.57
2:B:315:PRO:N	2:B:318:ARG:HH12	2.02	0.57
2:D:143:ALA:CB	2:D:159:ILE:CD1	2.81	0.57
2:D:284:VAL:CB	4:D:548:HOH:O	2.52	0.57
2:F:85:ASP:CB	2:F:90:ARG:HH12	2.13	0.57
2:J:84:ASP:OD1	2:J:90:ARG:N	2.29	0.57
2:J:175:ILE:CD1	2:J:199:ILE:HD13	2.34	0.57
1:G:6:LEU:HB3	2:H:287:LYS:HB3	1.87	0.57
2:H:211:THR:HG22	2:H:212:TYR:CE2	2.38	0.57
2:J:95:ASN:OD1	2:J:95:ASN:N	2.36	0.57
2:L:74:MET:HA	2:L:74:MET:HE3	1.82	0.57
2:H:85:ASP:CB	2:H:86:PRO:CD	2.81	0.57
2:H:198:ILE:HD13	2:L:196:MET:HB2	1.87	0.57
2:B:74:MET:HG2	2:B:101:ARG:CZ	2.35	0.57
2:F:154:LEU:HD23	4:F:505:HOH:O	2.04	0.57
2:L:304:GLY:HA3	2:L:336:SER:O	2.05	0.57
2:H:193:THR:HG23	2:D:200:SER:HB3	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:284:VAL:CG2	4:D:548:HOH:O	2.50	0.57
2:B:311:TYR:HD1	2:D:88:PHE:CE1	2.23	0.56
2:D:321:LEU:CD2	2:D:367:LEU:HD22	2.34	0.56
2:B:86:PRO:CA	2:D:312:ARG:HH12	2.12	0.56
2:L:293:LEU:CD1	4:L:561:HOH:O	2.53	0.56
2:H:217:GLN:HE22	2:L:193:THR:HG21	1.70	0.56
2:B:169:LEU:HD11	2:B:265:LEU:HD21	1.86	0.56
2:F:115:GLU:O	2:F:158:LYS:HE2	2.05	0.56
1:K:6:LEU:CD2	2:L:287:LYS:CD	2.83	0.56
2:L:293:LEU:CD2	4:L:561:HOH:O	1.87	0.56
2:L:305:ILE:HD13	2:L:327:ILE:HD12	1.87	0.56
2:H:299:LEU:N	2:H:302:THR:CG2	2.65	0.56
2:J:175:ILE:HD12	2:J:199:ILE:CD1	2.35	0.56
2:D:69:LEU:O	2:D:106:LEU:HD22	2.05	0.56
2:F:75:VAL:O	2:F:99:GLN:HA	2.06	0.56
2:H:94:ASP:OD1	2:H:94:ASP:N	2.39	0.56
2:D:299:LEU:CD1	2:D:302:THR:CG2	2.73	0.56
2:F:207:LEU:CD1	4:F:513:HOH:O	2.53	0.56
2:D:69:LEU:HB3	2:D:106:LEU:HD21	1.88	0.56
2:F:347:ARG:HG2	2:F:347:ARG:HH11	1.71	0.56
2:H:223:ASN:HB3	2:H:224:PRO:HD2	1.86	0.56
2:H:302:THR:HG23	2:H:302:THR:O	2.05	0.56
2:B:167:MET:HG2	2:B:238:LEU:HD13	1.88	0.56
2:B:249:SER:HB3	2:J:249:SER:HB2	1.86	0.56
2:D:115:GLU:CB	2:D:158:LYS:HZ1	2.19	0.56
2:D:195:THR:CG2	2:D:221:ALA:N	2.62	0.56
2:J:121:ASN:HB2	2:J:124:VAL:HG23	1.86	0.56
2:D:113:SER:HB3	2:D:117:TYR:HB2	1.88	0.56
2:J:77:LYS:HE2	2:J:100:LYS:HG2	1.57	0.55
2:L:139:ARG:NH2	2:L:162:LYS:O	2.40	0.55
2:H:149:ASP:OD2	2:H:279:ARG:NH2	2.38	0.55
2:H:276:GLN:HE21	2:H:278:ILE:HD11	1.70	0.55
2:D:112:MET:HE3	2:D:119:LEU:HB2	1.87	0.55
2:F:77:LYS:HG3	2:F:100:LYS:HG3	1.88	0.55
2:F:303:ALA:CB	2:F:328:LEU:HD23	2.36	0.55
1:K:2:VAL:HG23	1:K:2:VAL:O	2.06	0.55
2:L:341:SER:O	2:L:345:VAL:HG23	2.06	0.55
2:B:111:ILE:HD11	2:B:135:LEU:HD22	1.89	0.55
2:J:77:LYS:CD	2:J:100:LYS:HB2	2.36	0.55
2:L:172:SER:CB	4:L:521:HOH:O	1.87	0.55
2:H:299:LEU:HB2	2:H:302:THR:HG21	1.86	0.55

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:LEU:HG	2:B:293:LEU:O	2.06	0.55
2:F:77:LYS:NZ	2:F:96:LEU:HD12	2.21	0.55
2:F:77:LYS:CE	2:F:96:LEU:CD1	2.83	0.55
2:F:80:HIS:CG	2:F:81:PRO:HD2	2.41	0.55
2:L:289:LEU:HG	2:L:303:ALA:O	2.07	0.55
2:H:329:THR:CG2	2:H:357:VAL:HG23	2.36	0.55
2:B:337:ASP:HB2	2:B:340:ARG:HH21	1.71	0.55
2:F:68:ASN:OD1	2:F:186:ASN:HB2	2.07	0.55
2:B:195:THR:CG2	2:B:221:ALA:H	2.20	0.55
2:F:77:LYS:CD	2:F:100:LYS:HG3	2.36	0.55
2:L:89:ARG:HH11	2:L:89:ARG:CG	2.19	0.55
2:D:172:SER:C	4:D:501:HOH:O	2.45	0.55
2:D:329:THR:OG1	2:D:357:VAL:HB	2.06	0.55
2:F:106:LEU:O	2:F:124:VAL:HG13	2.07	0.55
2:H:53:VAL:HG21	4:L:546:HOH:O	2.08	0.54
2:F:77:LYS:CB	2:F:78:PRO:CD	2.85	0.54
2:F:282:LEU:O	2:F:316:ALA:CB	2.56	0.54
2:J:65:ALA:HB3	2:J:167:MET:HE1	1.89	0.54
2:L:93:GLY:HA2	4:L:516:HOH:O	1.92	0.54
2:H:77:LYS:HB2	2:H:98:GLN:O	2.08	0.54
2:F:77:LYS:HZ2	2:F:100:LYS:HG2	1.72	0.54
2:L:243:THR:CG2	2:L:259:ILE:HG13	2.36	0.54
2:B:169:LEU:CD1	2:B:265:LEU:HD11	2.37	0.54
2:B:303:ALA:O	2:B:328:LEU:HD22	2.08	0.54
2:D:83:PHE:HZ	2:J:92:PHE:CE2	2.26	0.54
2:D:83:PHE:HZ	2:J:92:PHE:HE2	1.55	0.54
2:D:89:ARG:HH11	2:D:89:ARG:CG	2.07	0.54
2:D:303:ALA:CB	2:D:328:LEU:CD2	2.86	0.54
2:J:70:TYR:CB	2:J:105:SER:HA	2.36	0.54
2:H:56:ALA:HB1	2:D:176:ARG:HH11	1.71	0.54
2:J:358:VAL:HG12	2:J:365:VAL:HB	1.89	0.54
2:L:80:HIS:CB	4:L:541:HOH:O	2.55	0.54
2:H:96:LEU:HD12	2:H:96:LEU:C	2.28	0.54
2:H:55:TYR:CE1	2:H:180:VAL:HG11	2.43	0.54
2:H:195:THR:HG21	2:H:221:ALA:N	2.22	0.54
2:B:315:PRO:HB3	2:B:370:GLU:O	2.08	0.54
2:D:95:ASN:HB3	2:D:97:PRO:HD2	1.89	0.54
2:B:231:LEU:HB2	2:B:242:ASN:ND2	2.23	0.54
2:B:297:LEU:HD12	2:B:297:LEU:H	1.73	0.54
2:B:315:PRO:CA	2:B:318:ARG:NH1	2.64	0.54
2:J:241:ILE:O	2:J:258:ALA:HB1	2.07	0.54

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:303:ALA:HB1	2:L:326:VAL:HG13	1.89	0.54
1:G:10:PHE:HB3	2:H:342:MET:HG3	1.90	0.54
2:B:196:MET:HE1	2:J:196:MET:HE1	1.89	0.54
2:F:70:TYR:HD2	4:F:541:HOH:O	1.89	0.54
2:F:331:ASP:CG	2:F:354:ILE:CG2	2.75	0.54
2:F:332:LYS:O	2:F:332:LYS:HG2	2.07	0.54
2:J:70:TYR:HB2	2:J:105:SER:HA	1.89	0.54
2:H:303:ALA:HA	2:H:334:GLU:HG3	1.90	0.54
2:B:162:LYS:HA	4:B:534:HOH:O	2.08	0.54
2:D:321:LEU:HD22	2:D:367:LEU:HD22	1.90	0.54
2:J:143:ALA:HA	2:J:159:ILE:CD1	2.38	0.54
2:H:219:ASP:OD1	2:L:195:THR:HG23	2.07	0.53
2:J:195:THR:HG21	2:J:221:ALA:N	2.23	0.53
2:H:163:ASN:ND2	4:H:507:HOH:O	2.32	0.53
2:J:119:LEU:HD23	2:J:241:ILE:HD11	1.90	0.53
2:H:303:ALA:O	2:H:328:LEU:HD23	2.08	0.53
2:B:86:PRO:HA	2:D:312:ARG:NH1	2.17	0.53
2:F:281:TRP:CE3	2:F:374:ARG:HG3	2.43	0.53
2:J:135:LEU:HD12	2:J:139:ARG:HB2	1.89	0.53
2:D:207:LEU:HB2	2:D:213:GLU:OE1	2.08	0.53
2:L:89:ARG:HG2	2:L:89:ARG:NH1	2.21	0.53
2:B:162:LYS:H	2:B:162:LYS:HD3	1.74	0.53
2:J:71:THR:HG22	2:J:106:LEU:HD21	1.90	0.53
2:J:321:LEU:HD22	2:J:367:LEU:HD12	1.91	0.53
1:A:7:ARG:HD2	2:B:285:GLU:OE2	2.08	0.53
2:D:305:ILE:CD1	2:D:335:ALA:HB1	2.38	0.53
2:J:243:THR:OG1	2:J:259:ILE:HG13	2.08	0.53
2:H:116:GLY:CA	2:H:159:ILE:HG22	2.39	0.53
2:B:289:LEU:HD12	2:B:289:LEU:C	2.29	0.53
2:B:313:ASP:O	2:B:318:ARG:CZ	2.57	0.53
2:F:310:VAL:CG1	2:F:317:ALA:HB2	2.39	0.53
2:B:89:ARG:HG2	2:B:89:ARG:NH1	2.23	0.53
2:D:96:LEU:HD23	2:D:96:LEU:C	2.28	0.53
2:H:350:PRO:HA	2:H:371:VAL:HG12	1.90	0.53
2:F:315:PRO:HB3	2:F:370:GLU:O	2.09	0.53
2:B:141:THR:HB	2:B:159:ILE:HD11	1.91	0.53
2:F:75:VAL:CG2	2:F:100:LYS:O	2.46	0.53
2:J:325:ASP:HB3	2:J:358:VAL:CG2	2.39	0.53
2:L:66:VAL:HG11	2:L:184:ILE:HG22	1.91	0.52
2:D:69:LEU:CB	2:D:106:LEU:HD21	2.39	0.52
2:F:303:ALA:HB1	2:F:328:LEU:CA	2.25	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:70:TYR:CD2	2:L:132:ILE:HD12	2.43	0.52
2:B:82:LEU:HD12	2:B:92:PHE:HE2	1.74	0.52
2:B:172:SER:HB2	4:B:521:HOH:O	1.80	0.52
2:H:72:THR:C	2:H:73:LYS:HE2	2.30	0.52
2:H:186:ASN:O	2:H:225:GLY:HA3	2.09	0.52
1:A:10:PHE:CE1	2:B:284:VAL:CG2	2.93	0.52
2:D:203:GLY:HA2	2:D:214:ASP:OD1	2.10	0.52
2:J:98:GLN:NE2	4:J:509:HOH:O	2.42	0.52
2:L:195:THR:HG21	2:L:221:ALA:N	2.25	0.52
2:B:255:ILE:HD11	2:J:223:ASN:ND2	2.25	0.52
2:D:175:ILE:CD1	2:D:216:ILE:HD12	2.38	0.52
2:H:83:PHE:HE1	2:B:83:PHE:CE1	2.27	0.52
2:H:287:LYS:HG2	2:H:306:VAL:HB	1.92	0.52
2:B:307:VAL:HG23	2:B:325:ASP:O	2.09	0.52
2:F:113:SER:HB3	2:F:117:TYR:HB2	1.90	0.52
2:H:83:PHE:CE2	2:H:94:ASP:OD1	2.62	0.52
2:B:68:ASN:CG	2:B:186:ASN:HB2	2.30	0.52
2:F:85:ASP:OD1	2:F:86:PRO:HD2	2.10	0.52
2:J:119:LEU:HD21	2:J:264:ALA:HB1	1.92	0.52
2:L:53:VAL:CG1	4:L:538:HOH:O	2.45	0.52
1:A:10:PHE:CE1	2:B:284:VAL:HG21	2.45	0.52
2:F:353:LYS:CE	2:F:370:GLU:HB2	2.40	0.52
2:B:89:ARG:NH1	2:B:89:ARG:CG	2.72	0.51
2:B:281:TRP:HB2	2:B:374:ARG:HA	1.93	0.51
2:D:74:MET:SD	2:D:75:VAL:N	2.83	0.51
2:J:70:TYR:C	2:J:70:TYR:HD1	2.14	0.51
2:L:321:LEU:CD1	2:L:358:VAL:HG21	2.41	0.51
2:J:285:GLU:HB2	2:L:88:PHE:CE1	2.46	0.51
2:B:241:ILE:CA	4:B:502:HOH:O	2.54	0.51
2:D:279:ARG:HA	2:D:346:ALA:O	2.11	0.51
2:F:89:ARG:NH2	4:F:506:HOH:O	2.32	0.51
2:L:85:ASP:CG	2:L:90:ARG:HH12	2.13	0.51
2:L:195:THR:HG22	2:L:220:ALA:HB1	1.92	0.51
2:L:365:VAL:HG12	2:L:367:LEU:CD1	2.40	0.51
2:H:69:LEU:CD2	2:H:133:VAL:HG22	2.40	0.51
2:F:251:GLY:CA	2:J:253:GLN:NE2	2.38	0.51
2:B:138:GLY:HA2	4:B:508:HOH:O	2.11	0.51
2:B:184:ILE:CG2	2:B:192:GLN:HE21	2.22	0.51
2:F:77:LYS:HZ3	2:F:100:LYS:HG2	1.74	0.51
2:J:70:TYR:HA	2:J:106:LEU:HG	1.91	0.51
2:L:320:GLY:O	2:L:360:ARG:NH2	2.43	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:ASP:HB2	4:B:528:HOH:O	2.10	0.51
2:B:310:VAL:HG22	2:D:89:ARG:HB3	1.92	0.51
2:J:68:ASN:HD22	2:J:186:ASN:CG	2.13	0.51
2:J:266:GLU:HG3	4:J:502:HOH:O	2.11	0.51
2:B:325:ASP:OD1	2:B:360:ARG:HD2	2.11	0.51
2:F:353:LYS:HE3	2:F:370:GLU:HB2	1.91	0.51
2:L:123:HIS:CE1	2:L:227:SER:HB3	2.45	0.51
2:L:175:ILE:HD11	2:L:202:THR:CG2	2.37	0.51
2:L:294:ALA:HB1	2:L:298:GLY:HA3	1.92	0.51
2:H:195:THR:HG23	2:D:219:ASP:OD1	2.10	0.51
2:B:216:ILE:HD11	2:B:260:PRO:HB3	1.93	0.51
2:H:222:ILE:HG23	2:H:226:ASN:CB	2.41	0.51
2:D:85:ASP:HB2	2:D:90:ARG:NH1	2.25	0.51
2:D:250:GLY:O	2:L:248:LYS:HD3	2.05	0.51
2:D:174:GLY:CA	4:D:501:HOH:O	2.46	0.51
1:K:10:PHE:CD1	2:L:345:VAL:HG21	2.46	0.51
2:L:283:GLY:HA3	2:L:311:TYR:CB	2.40	0.51
2:L:322:LEU:HD11	2:L:360:ARG:HE	1.76	0.51
2:B:85:ASP:OD1	2:B:86:PRO:CD	2.59	0.50
2:B:350:PRO:CA	4:B:514:HOH:O	2.56	0.50
2:F:70:TYR:HB2	4:F:541:HOH:O	2.11	0.50
2:J:108:SER:O	2:J:228:GLY:HA3	2.11	0.50
2:L:94:ASP:N	4:L:516:HOH:O	2.42	0.50
2:H:329:THR:HG21	2:H:357:VAL:HG23	1.94	0.50
2:B:286:VAL:HG11	2:B:305:ILE:HD12	1.93	0.50
2:D:217:GLN:HG3	2:D:257:PHE:CE1	2.46	0.50
2:J:70:TYR:CD1	2:J:70:TYR:C	2.84	0.50
2:F:312:ARG:HD2	2:F:312:ARG:O	2.09	0.50
2:D:74:MET:HA	2:D:74:MET:HE2	1.90	0.50
1:E:8:TRP:CH2	2:F:206:GLN:HG2	2.41	0.50
2:F:261:THR:HG22	2:F:265:LEU:CD1	2.40	0.50
2:J:195:THR:CG2	2:J:221:ALA:H	2.25	0.50
2:B:87:MET:HG3	2:D:311:TYR:CE1	2.46	0.50
2:B:241:ILE:CB	4:B:502:HOH:O	2.57	0.50
2:D:69:LEU:HB2	2:D:106:LEU:HD23	1.94	0.50
2:J:89:ARG:CD	4:L:507:HOH:O	2.58	0.50
2:J:325:ASP:OD2	2:J:360:ARG:NE	2.42	0.50
2:J:330:ILE:HD12	4:J:517:HOH:O	2.11	0.50
1:K:6:LEU:HD23	2:L:287:LYS:CD	2.39	0.50
2:B:122:ASN:HD21	2:B:150:PRO:HG3	1.77	0.50
1:G:9:VAL:HG23	1:G:9:VAL:O	2.12	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:TYR:CE1	2:B:158:LYS:HD3	2.47	0.50
2:B:297:LEU:N	2:B:297:LEU:CD1	2.73	0.50
2:F:141:THR:OG1	2:F:161:LEU:CD1	2.60	0.50
2:H:70:TYR:OH	2:H:132:ILE:HG21	2.10	0.49
2:H:78:PRO:HD3	2:H:100:LYS:NZ	2.26	0.49
2:F:193:THR:HG21	2:J:217:GLN:HE22	1.76	0.49
2:F:295:GLU:CD	2:F:296:SER:H	2.11	0.49
2:F:321:LEU:CD1	2:F:358:VAL:HG21	2.42	0.49
2:L:231:LEU:HB2	2:L:242:ASN:ND2	2.27	0.49
2:H:141:THR:HG22	2:H:142:ILE:O	2.11	0.49
2:J:175:ILE:CG1	2:J:199:ILE:HD13	2.43	0.49
2:L:216:ILE:HD11	2:L:260:PRO:HB3	1.93	0.49
2:H:223:ASN:HB3	2:H:224:PRO:CD	2.42	0.49
2:L:74:MET:HA	2:L:101:ARG:HA	1.94	0.49
2:L:156:VAL:HG22	2:L:268:MET:HG3	1.94	0.49
2:H:295:GLU:HG2	2:H:296:SER:N	2.25	0.49
2:D:106:LEU:CD2	2:D:106:LEU:N	2.72	0.49
2:F:142:ILE:HG23	2:F:142:ILE:O	2.12	0.49
2:J:71:THR:CB	2:J:106:LEU:HD21	2.42	0.49
2:B:95:ASN:HD22	2:B:96:LEU:HD12	1.77	0.49
2:B:312:ARG:HG3	2:B:312:ARG:O	2.13	0.49
2:J:64:PRO:HD3	2:J:136:ARG:NH2	2.28	0.49
2:J:141:THR:CG2	4:J:505:HOH:O	2.43	0.49
2:L:284:VAL:HG12	2:L:286:VAL:HG13	1.94	0.49
2:B:209:LEU:HD21	4:B:541:HOH:O	2.11	0.49
2:D:297:LEU:O	2:D:297:LEU:HG	2.11	0.49
2:F:95:ASN:CB	2:J:296:SER:CB	2.71	0.49
2:F:281:TRP:N	2:F:372:GLY:O	2.42	0.49
2:F:360:ARG:NH1	2:F:360:ARG:CG	2.72	0.49
2:B:268:MET:HG2	2:B:272:ILE:HD12	1.94	0.49
2:F:213:GLU:HG2	2:F:215:PHE:HE2	1.77	0.49
2:J:89:ARG:HD3	4:L:507:HOH:O	2.11	0.49
2:H:83:PHE:CZ	2:B:80:HIS:CE1	3.00	0.49
2:B:112:MET:N	2:B:112:MET:HE2	2.27	0.49
2:D:69:LEU:HB2	2:D:106:LEU:CD2	2.42	0.49
2:H:279:ARG:HH11	3:H:401:IMD:H5	1.57	0.49
2:F:73:LYS:HB2	2:F:73:LYS:NZ	2.28	0.49
2:J:143:ALA:HA	2:J:159:ILE:HD13	1.94	0.49
2:J:180:VAL:CB	4:J:518:HOH:O	2.43	0.49
2:B:216:ILE:CD1	2:B:216:ILE:N	2.76	0.49
2:B:314:GLY:C	2:B:318:ARG:NH1	2.67	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:74:MET:CE	2:F:100:LYS:O	2.60	0.49
2:H:222:ILE:O	2:H:252:SER:HB2	2.13	0.48
2:D:133:VAL:HG12	2:D:133:VAL:O	2.12	0.48
2:F:75:VAL:O	2:F:100:LYS:N	2.46	0.48
2:F:287:LYS:CG	2:F:306:VAL:HB	2.43	0.48
2:J:180:VAL:CA	4:J:518:HOH:O	2.02	0.48
2:L:85:ASP:HB3	2:L:88:PHE:H	1.77	0.48
2:L:374:ARG:NH2	4:L:514:HOH:O	2.42	0.48
1:G:7:ARG:O	1:G:7:ARG:HD3	2.13	0.48
2:B:134:ALA:CB	2:B:140:GLU:HG2	2.42	0.48
1:K:6:LEU:HD21	2:L:287:LYS:CD	2.42	0.48
2:D:195:THR:HG22	2:D:220:ALA:CB	2.36	0.48
2:D:249:SER:H	2:D:253:GLN:HE22	1.61	0.48
2:L:347:ARG:HG3	3:L:401:IMD:H5	1.94	0.48
2:B:85:ASP:CB	2:B:86:PRO:CD	2.91	0.48
2:F:85:ASP:HB3	2:F:88:PHE:H	1.78	0.48
2:J:329:THR:HB	2:J:357:VAL:HG23	1.95	0.48
1:E:10:PHE:HD2	2:F:342:MET:HG2	1.78	0.48
2:F:135:LEU:N	2:F:135:LEU:CD2	2.74	0.48
2:F:299:LEU:CD1	2:F:302:THR:HB	2.43	0.48
2:J:111:ILE:HA	2:J:118:LEU:HD23	1.94	0.48
2:L:80:HIS:HB2	4:L:541:HOH:O	2.12	0.48
2:B:334:GLU:O	2:B:335:ALA:HB3	2.14	0.48
2:H:281:TRP:HB3	2:H:372:GLY:O	2.13	0.48
2:B:170:GLY:O	2:B:261:THR:HG21	2.14	0.48
2:B:361:ASN:HD22	2:B:361:ASN:H	1.61	0.48
2:H:261:THR:HG22	2:H:265:LEU:HD12	1.96	0.48
2:B:280:GLY:HA2	4:B:514:HOH:O	2.13	0.48
1:E:7:ARG:CZ	2:F:287:LYS:HE3	2.43	0.48
2:F:71:THR:N	2:F:106:LEU:HD21	2.29	0.48
2:J:66:VAL:HG11	2:J:184:ILE:HG22	1.95	0.48
2:J:111:ILE:HG13	2:J:118:LEU:CD2	2.44	0.48
1:G:6:LEU:CB	2:H:287:LYS:HB3	2.42	0.47
2:H:116:GLY:HA2	2:H:164:LEU:CD1	2.44	0.47
2:H:299:LEU:O	2:H:302:THR:CG2	2.61	0.47
1:A:6:LEU:HD12	1:A:6:LEU:O	2.14	0.47
2:B:361:ASN:ND2	2:B:361:ASN:N	2.59	0.47
2:J:177:THR:HA	2:J:199:ILE:HG22	1.96	0.47
2:L:367:LEU:N	2:L:367:LEU:HD13	2.29	0.47
2:D:195:THR:CG2	2:D:220:ALA:HB1	2.37	0.47
2:F:287:LYS:HG3	2:F:306:VAL:HB	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:LEU:CD2	2:B:133:VAL:HG22	2.44	0.47
2:B:212:TYR:HD2	2:B:279:ARG:HH12	1.56	0.47
2:D:69:LEU:O	2:D:106:LEU:CD2	2.62	0.47
2:D:214:ASP:O	2:D:260:PRO:CD	2.61	0.47
2:F:112:MET:HG2	2:F:268:MET:SD	2.54	0.47
2:F:175:ILE:HD12	2:F:199:ILE:HD12	1.96	0.47
2:L:248:LYS:H	2:L:253:GLN:HE21	1.62	0.47
2:H:94:ASP:CB	2:H:96:LEU:HG	2.20	0.47
2:B:162:LYS:H	2:B:162:LYS:CD	2.27	0.47
2:J:326:VAL:HB	2:J:359:LEU:HB3	1.96	0.47
2:J:348:THR:HG21	2:J:371:VAL:HG21	1.96	0.47
1:K:6:LEU:HD21	2:L:287:LYS:HZ3	1.76	0.47
2:H:303:ALA:HA	2:H:334:GLU:O	2.15	0.47
2:H:329:THR:HB	2:H:357:VAL:HB	1.96	0.47
2:B:255:ILE:HD13	2:J:188:PHE:CD2	2.50	0.47
2:D:70:TYR:CE1	2:D:103:GLU:HB2	2.47	0.47
2:F:150:PRO:CD	4:F:517:HOH:O	1.73	0.47
2:F:230:ALA:HB1	2:F:238:LEU:HD12	1.96	0.47
2:J:321:LEU:HD22	2:J:367:LEU:CD1	2.44	0.47
2:H:94:ASP:HB2	2:H:96:LEU:HD23	1.87	0.47
2:H:196:MET:CB	2:D:198:ILE:HG12	2.45	0.47
2:D:207:LEU:HD22	2:D:246:PHE:CZ	2.50	0.47
2:F:331:ASP:HB2	2:F:354:ILE:CG2	2.45	0.47
2:J:70:TYR:HD1	2:J:70:TYR:O	1.97	0.47
2:J:332:LYS:N	4:J:508:HOH:O	2.40	0.47
2:J:355:SER:O	2:J:355:SER:OG	2.31	0.47
1:K:10:PHE:CD2	2:L:342:MET:HA	2.49	0.47
2:L:102:MET:HE1	4:L:562:HOH:O	1.81	0.47
2:L:112:MET:HE1	2:L:169:LEU:HD21	1.97	0.47
2:L:223:ASN:N	4:L:509:HOH:O	2.47	0.47
2:L:243:THR:HG21	2:L:259:ILE:HD11	1.94	0.47
2:H:299:LEU:CA	2:H:302:THR:CG2	2.92	0.47
2:F:121:ASN:HB2	2:F:124:VAL:HG23	1.97	0.47
2:F:175:ILE:HD11	2:F:216:ILE:HD12	1.96	0.47
2:F:212:TYR:CD2	2:F:279:ARG:NH1	2.82	0.47
2:L:322:LEU:CD2	2:L:360:ARG:NH2	2.77	0.47
2:D:112:MET:HG2	2:D:268:MET:CE	2.45	0.47
2:F:162:LYS:HA	2:F:162:LYS:HE2	1.94	0.47
2:J:175:ILE:HG13	2:J:199:ILE:HD13	1.96	0.47
2:H:211:THR:CG2	2:H:212:TYR:CE2	2.98	0.46
2:H:333:GLN:HB2	4:H:515:HOH:O	2.15	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:91:PHE:HZ	2:F:324:GLY:HA3	1.76	0.46
2:H:295:GLU:CD	4:H:527:HOH:O	2.52	0.46
2:H:299:LEU:CA	2:H:302:THR:HG22	2.45	0.46
2:F:74:MET:CE	2:F:100:LYS:C	2.83	0.46
2:F:213:GLU:HG2	2:F:215:PHE:CE2	2.50	0.46
2:F:305:ILE:CG1	2:F:327:ILE:HB	2.45	0.46
2:B:242:ASN:HD22	2:B:258:ALA:HB2	1.80	0.46
2:D:267:VAL:HG22	4:D:544:HOH:O	2.15	0.46
2:J:353:LYS:CE	2:J:370:GLU:HG3	2.23	0.46
2:B:214:ASP:O	2:B:260:PRO:HD3	2.15	0.46
1:C:5:GLU:O	1:C:5:GLU:HG3	2.14	0.46
2:D:212:TYR:CE2	2:D:279:ARG:NE	2.83	0.46
2:F:74:MET:CE	2:F:101:ARG:HA	2.45	0.46
2:L:321:LEU:CD2	4:L:548:HOH:O	2.63	0.46
2:H:271:ILE:O	2:H:274:HIS:O	2.33	0.46
2:H:287:LYS:CG	2:H:306:VAL:HB	2.45	0.46
2:B:64:PRO:HD3	2:B:136:ARG:NH1	2.31	0.46
2:D:158:LYS:HD2	2:D:159:ILE:H	1.79	0.46
2:H:335:ALA:HA	2:H:341:SER:OG	2.15	0.46
2:B:195:THR:HG21	2:B:221:ALA:N	2.30	0.46
2:J:252:SER:HA	4:J:506:HOH:O	2.14	0.46
2:L:118:LEU:HB2	2:L:157:LEU:HB2	1.97	0.46
2:L:153:ASP:HB2	2:L:210:ASN:OD1	2.15	0.46
2:D:89:ARG:NH1	2:D:89:ARG:CG	2.71	0.46
2:D:100:LYS:HE3	1:K:4:ASP:CG	2.32	0.46
2:F:376:PRO:CB	4:F:519:HOH:O	2.63	0.46
2:L:328:LEU:O	2:L:335:ALA:HB3	2.14	0.46
2:D:252:SER:HB3	2:L:253:GLN:O	2.16	0.46
2:L:305:ILE:CD1	2:L:327:ILE:CB	2.22	0.46
2:B:85:ASP:OD1	2:B:86:PRO:HD3	2.16	0.46
2:F:74:MET:CE	2:F:74:MET:CA	2.85	0.46
2:F:196:MET:HB2	2:J:198:ILE:HD13	1.96	0.46
2:J:71:THR:HG22	2:J:106:LEU:CD2	2.46	0.46
2:L:68:ASN:CG	2:L:186:ASN:ND2	2.69	0.46
2:L:101:ARG:O	2:L:101:ARG:HG2	2.16	0.46
2:B:227:SER:HA	2:B:242:ASN:O	2.16	0.46
2:D:230:ALA:HB1	2:D:238:LEU:HD12	1.97	0.46
2:F:187:PRO:O	2:F:187:PRO:HG2	2.16	0.46
2:F:310:VAL:HG12	2:F:317:ALA:HB2	1.98	0.46
2:J:325:ASP:HB3	2:J:358:VAL:HG21	1.98	0.46
2:H:303:ALA:HB1	2:H:328:LEU:HB3	1.98	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:172:SER:O	2:J:175:ILE:HG23	2.16	0.45
2:J:242:ASN:ND2	4:J:501:HOH:O	2.49	0.45
2:L:296:SER:O	2:L:297:LEU:HD12	2.16	0.45
1:C:8:TRP:HB2	2:D:286:VAL:CG2	2.39	0.45
2:F:65:ALA:HB3	2:F:167:MET:CE	2.46	0.45
2:B:137:ASP:HB3	4:B:516:HOH:O	2.17	0.45
2:F:284:VAL:CG1	2:F:316:ALA:CB	2.92	0.45
2:B:209:LEU:N	2:B:213:GLU:OE1	2.48	0.45
2:D:65:ALA:HB3	2:D:167:MET:HE2	1.97	0.45
2:D:265:LEU:HD12	2:D:265:LEU:HA	1.80	0.45
2:F:121:ASN:HA	4:F:505:HOH:O	2.16	0.45
2:F:216:ILE:HD11	2:F:260:PRO:HB3	1.98	0.45
2:J:159:ILE:HD13	2:J:159:ILE:HA	1.75	0.45
2:H:145:LEU:HA	2:H:145:LEU:HD12	1.83	0.45
2:H:195:THR:HG21	2:H:221:ALA:HB3	1.98	0.45
2:H:303:ALA:HB1	2:H:328:LEU:O	2.17	0.45
2:D:292:GLU:H	2:D:292:GLU:HG2	1.42	0.45
2:B:181:CYS:SG	2:B:199:ILE:HD12	2.56	0.45
2:D:231:LEU:HD12	2:D:231:LEU:HA	1.75	0.45
2:F:214:ASP:O	2:F:260:PRO:HD3	2.17	0.45
2:F:267:VAL:HG13	2:F:277:VAL:CG2	2.39	0.45
2:F:303:ALA:HB1	2:F:328:LEU:HD23	1.98	0.45
2:F:304:GLY:H	2:F:336:SER:HA	1.82	0.45
2:L:305:ILE:HD11	2:L:327:ILE:CG2	2.27	0.45
2:H:91:PHE:CZ	2:F:324:GLY:N	2.84	0.45
2:H:151:GLU:OE1	2:H:211:THR:CB	2.65	0.45
2:H:289:LEU:HD12	2:H:293:LEU:HD23	1.97	0.45
2:B:112:MET:HE2	2:B:112:MET:CA	2.47	0.45
2:B:259:ILE:CA	4:B:502:HOH:O	2.65	0.45
2:F:193:THR:CG2	2:J:217:GLN:HE22	2.29	0.45
2:F:331:ASP:CB	2:F:354:ILE:CG2	2.95	0.45
2:L:307:VAL:CG2	4:L:548:HOH:O	2.43	0.45
2:H:91:PHE:CZ	2:F:324:GLY:HA3	2.50	0.45
2:B:281:TRP:CZ2	2:B:283:GLY:HA2	2.51	0.45
2:D:251:GLY:HA3	2:L:253:GLN:CD	2.36	0.45
2:F:75:VAL:CG2	2:F:100:LYS:HB2	2.46	0.45
2:F:231:LEU:HD22	2:F:258:ALA:HB3	1.99	0.45
2:L:142:ILE:HD13	4:L:549:HOH:O	2.16	0.45
2:B:72:THR:HG1	2:B:130:GLN:NE2	2.15	0.45
2:D:299:LEU:HD13	2:D:302:THR:HG21	1.88	0.45
2:F:284:VAL:HG13	2:F:316:ALA:HB2	1.99	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:267:VAL:HG13	2:J:277:VAL:CG2	2.47	0.45
2:H:214:ASP:O	2:H:260:PRO:HG3	2.17	0.45
2:B:312:ARG:NH2	2:D:87:MET:CE	2.78	0.45
2:D:65:ALA:CB	2:D:167:MET:HE2	2.47	0.45
2:J:217:GLN:HG3	2:J:257:PHE:CE1	2.52	0.45
2:L:205:ASN:C	2:L:206:GLN:HG3	2.37	0.45
2:L:322:LEU:CD2	2:L:360:ARG:HH21	2.29	0.45
2:L:325:ASP:OD1	2:L:360:ARG:HG2	2.13	0.45
2:H:309:GLY:HA2	2:H:323:PRO:HB3	2.00	0.44
2:B:119:LEU:HA	2:B:119:LEU:HD12	1.82	0.44
2:D:101:ARG:HE	2:D:101:ARG:HB2	1.67	0.44
2:H:85:ASP:HB2	2:H:86:PRO:HD2	1.98	0.44
2:D:175:ILE:HD12	2:D:199:ILE:HD13	1.99	0.44
2:F:110:VAL:HB	2:F:112:MET:HE1	1.99	0.44
2:F:116:GLY:O	2:F:159:ILE:HB	2.17	0.44
2:F:347:ARG:HG2	2:F:347:ARG:NH1	2.33	0.44
2:L:115:GLU:O	2:L:158:LYS:HE2	2.18	0.44
2:H:299:LEU:HD13	2:H:299:LEU:HA	1.79	0.44
2:D:141:THR:HG22	4:D:537:HOH:O	1.71	0.44
2:H:83:PHE:CE1	2:B:83:PHE:CE1	3.04	0.44
2:D:76:SER:CB	2:D:99:GLN:HB3	2.46	0.44
2:D:83:PHE:CZ	2:J:92:PHE:CE2	3.06	0.44
2:D:115:GLU:C	2:D:158:LYS:NZ	2.70	0.44
2:J:65:ALA:HB3	2:J:167:MET:CE	2.46	0.44
1:K:4:ASP:OD1	1:K:4:ASP:N	2.50	0.44
2:B:314:GLY:HA3	4:B:511:HOH:O	2.17	0.44
2:D:96:LEU:HD23	2:D:97:PRO:N	2.32	0.44
2:L:187:PRO:HD2	2:L:193:THR:HG23	1.99	0.44
2:H:96:LEU:C	2:H:96:LEU:CD1	2.85	0.44
2:B:89:ARG:HD2	2:B:89:ARG:HA	1.79	0.44
2:B:196:MET:CE	2:J:196:MET:HE1	2.47	0.44
2:D:95:ASN:HD22	2:D:95:ASN:HA	1.49	0.44
2:F:142:ILE:C	2:F:142:ILE:HD13	2.37	0.44
2:B:85:ASP:OD1	2:B:86:PRO:HD2	2.18	0.44
2:L:289:LEU:CD2	2:L:306:VAL:HG22	2.45	0.44
2:H:263:LEU:HD12	2:H:263:LEU:O	2.18	0.44
2:B:74:MET:HG3	2:B:101:ARG:HD3	2.00	0.44
2:J:68:ASN:ND2	2:J:186:ASN:CG	2.68	0.44
2:L:70:TYR:OH	2:L:140:GLU:OE2	2.35	0.44
2:L:321:LEU:CG	4:L:548:HOH:O	2.52	0.44
2:F:119:LEU:HD12	2:F:119:LEU:HA	1.60	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:326:VAL:O	2:F:358:VAL:HG13	2.18	0.44
2:H:70:TYR:CE1	2:H:132:ILE:HD13	2.44	0.43
2:H:282:LEU:O	2:H:316:ALA:CB	2.66	0.43
2:B:111:ILE:HG21	2:B:165:PRO:O	2.18	0.43
2:D:150:PRO:HD2	4:D:513:HOH:O	2.18	0.43
2:D:315:PRO:HD3	4:D:534:HOH:O	2.18	0.43
2:L:164:LEU:HD23	2:L:164:LEU:HA	1.83	0.43
2:L:307:VAL:HG12	2:L:323:PRO:HA	2.00	0.43
2:H:326:VAL:HB	2:H:359:LEU:HB3	2.01	0.43
2:B:106:LEU:O	2:B:124:VAL:HG13	2.18	0.43
2:J:133:VAL:CG2	2:J:143:ALA:HB2	2.49	0.43
2:J:176:ARG:HG2	2:J:176:ARG:NH1	2.31	0.43
2:J:297:LEU:CD1	2:J:306:VAL:HG21	2.48	0.43
2:L:118:LEU:HD11	2:L:159:ILE:CG1	2.48	0.43
2:L:281:TRP:HB3	2:L:372:GLY:HA3	2.00	0.43
2:B:118:LEU:HB2	2:B:157:LEU:HB2	2.01	0.43
2:B:153:ASP:OD2	2:B:243:THR:CG2	2.65	0.43
2:B:186:ASN:O	2:B:225:GLY:HA3	2.18	0.43
2:J:195:THR:HG21	2:J:221:ALA:CA	2.48	0.43
2:L:96:LEU:N	2:L:97:PRO:HD3	2.33	0.43
2:L:135:LEU:N	2:L:135:LEU:HD12	2.33	0.43
2:H:223:ASN:O	2:H:226:ASN:HB2	2.19	0.43
2:D:69:LEU:CD2	2:D:133:VAL:HG22	2.48	0.43
2:D:103:GLU:H	2:D:103:GLU:HG3	1.55	0.43
2:D:182:LEU:HD23	2:D:194:VAL:HG11	2.00	0.43
2:F:337:ASP:HB3	2:F:340:ARG:HB2	1.99	0.43
2:J:245:ILE:HG22	2:J:256:GLY:CA	2.39	0.43
2:D:69:LEU:CB	2:D:106:LEU:CD2	2.96	0.43
2:F:119:LEU:CD1	2:F:156:VAL:HG22	2.49	0.43
2:F:182:LEU:HD23	2:F:194:VAL:HG12	2.01	0.43
2:J:161:LEU:HD23	2:J:161:LEU:HA	1.64	0.43
2:J:325:ASP:HB3	2:J:358:VAL:HG22	2.00	0.43
2:L:162:LYS:HD3	2:L:162:LYS:HA	1.61	0.43
2:B:223:ASN:O	2:B:226:ASN:HB2	2.19	0.43
2:B:325:ASP:OD1	2:B:360:ARG:CD	2.66	0.43
2:F:77:LYS:CG	2:F:100:LYS:HG3	2.49	0.43
2:F:147:GLY:HA3	2:F:271:ILE:HG23	2.00	0.43
2:L:281:TRP:HA	2:L:281:TRP:CE3	2.54	0.43
2:H:68:ASN:CA	4:H:525:HOH:O	2.41	0.43
2:H:72:THR:O	2:H:72:THR:OG1	2.30	0.43
2:J:158:LYS:HD2	2:J:158:LYS:HA	1.64	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:63:ALA:N	2:L:64:PRO:CD	2.82	0.43
2:L:80:HIS:CD2	2:L:81:PRO:HD2	2.54	0.43
2:L:151:GLU:OE1	2:L:151:GLU:HA	2.19	0.43
2:D:63:ALA:N	2:D:64:PRO:CD	2.82	0.43
2:D:143:ALA:HA	2:D:159:ILE:HD12	1.99	0.43
2:D:205:ASN:CB	4:D:528:HOH:O	2.35	0.43
2:F:143:ALA:HB2	2:F:159:ILE:HD11	1.99	0.43
2:F:281:TRP:HB2	2:F:374:ARG:HA	2.00	0.43
1:K:6:LEU:HD21	2:L:287:LYS:CG	2.49	0.43
2:L:347:ARG:CG	3:L:401:IMD:H5	2.49	0.43
2:H:151:GLU:OE2	2:H:377:PRO:HG3	2.19	0.43
2:B:195:THR:HG22	2:B:221:ALA:H	1.84	0.43
2:D:74:MET:SD	2:D:74:MET:C	2.97	0.43
2:D:96:LEU:HD23	2:D:97:PRO:CD	2.49	0.43
2:D:96:LEU:HD23	2:D:97:PRO:HD3	2.00	0.43
2:F:98:GLN:OE1	2:F:98:GLN:HA	2.19	0.43
2:J:143:ALA:HB2	2:J:159:ILE:HD11	2.01	0.43
2:L:68:ASN:CG	2:L:186:ASN:HD22	2.21	0.43
2:L:118:LEU:HD11	2:L:159:ILE:HG13	2.01	0.43
2:L:167:MET:HE2	2:L:167:MET:HB2	1.89	0.43
2:B:193:THR:HG21	2:F:217:GLN:HE22	1.83	0.42
2:F:73:LYS:HB2	2:F:73:LYS:HZ2	1.84	0.42
2:F:74:MET:CE	2:F:101:ARG:CA	2.96	0.42
2:F:77:LYS:HB3	2:F:78:PRO:CD	2.48	0.42
2:F:281:TRP:CZ2	2:F:283:GLY:HA2	2.54	0.42
2:L:321:LEU:CD1	2:L:358:VAL:CG2	2.97	0.42
1:A:9:VAL:HA	2:B:284:VAL:O	2.18	0.42
2:D:54:SER:OG	2:L:179:ASP:OD1	2.26	0.42
2:D:115:GLU:C	2:D:158:LYS:HZ1	2.22	0.42
1:E:7:ARG:NH2	2:F:287:LYS:HE3	2.35	0.42
2:F:77:LYS:HB3	2:F:78:PRO:HD2	2.00	0.42
2:F:137:ASP:N	4:F:508:HOH:O	2.42	0.42
1:K:7:ARG:HH11	1:K:7:ARG:CG	2.12	0.42
2:L:337:ASP:HB3	2:L:340:ARG:CG	2.48	0.42
2:D:295:GLU:O	2:D:295:GLU:HG2	2.16	0.42
2:J:343:ASN:HD22	3:J:401:IMD:HN3	1.66	0.42
2:L:124:VAL:CG2	2:L:227:SER:HB2	2.49	0.42
2:B:280:GLY:HA3	2:B:345:VAL:O	2.19	0.42
2:F:136:ARG:HB3	4:F:508:HOH:O	2.19	0.42
2:B:112:MET:CA	2:B:112:MET:CE	2.93	0.42
2:L:89:ARG:CG	2:L:89:ARG:NH1	2.80	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:322:LEU:HD12	2:D:360:ARG:HD2	2.01	0.42
2:J:69:LEU:CD1	2:J:109:ALA:HB2	2.44	0.42
2:H:112:MET:HG2	2:H:268:MET:SD	2.60	0.42
2:H:269:GLN:H	2:H:269:GLN:HG2	1.69	0.42
2:J:292:GLU:H	2:J:292:GLU:HG3	1.74	0.42
2:L:103:GLU:H	2:L:103:GLU:HG2	1.54	0.42
2:H:204:ARG:HB2	2:H:215:PHE:CB	2.44	0.42
2:L:159:ILE:CG2	2:L:161:LEU:HG	2.50	0.42
1:G:6:LEU:HB3	2:H:287:LYS:HB2	2.01	0.42
2:H:281:TRP:H	2:H:371:VAL:HG13	1.84	0.42
2:B:90:ARG:HG2	2:D:308:ALA:O	2.19	0.42
2:B:111:ILE:O	2:B:111:ILE:HG22	2.19	0.42
2:F:117:TYR:CE1	2:F:272:ILE:HD13	2.55	0.42
2:L:75:VAL:HG22	2:L:100:LYS:O	2.15	0.42
2:B:172:SER:OG	2:B:261:THR:HG22	2.19	0.42
2:B:195:THR:HG21	2:B:221:ALA:H	1.81	0.42
2:B:310:VAL:HG22	2:D:89:ARG:CB	2.50	0.42
2:F:248:LYS:HB2	2:F:253:GLN:HE22	1.85	0.42
2:L:305:ILE:HD12	2:L:305:ILE:C	2.40	0.42
2:H:87:MET:SD	2:F:311:TYR:HE1	2.38	0.41
2:D:280:GLY:HA3	2:D:345:VAL:O	2.19	0.41
4:F:511:HOH:O	2:L:82:LEU:HD12	2.12	0.41
2:J:80:HIS:CG	2:J:81:PRO:CD	2.91	0.41
2:B:230:ALA:HB1	2:B:238:LEU:CD1	2.50	0.41
2:F:55:TYR:CE2	2:F:180:VAL:HG11	2.56	0.41
2:F:69:LEU:N	4:F:514:HOH:O	2.52	0.41
2:F:70:TYR:HD1	2:F:105:SER:HA	1.85	0.41
2:L:204:ARG:HG2	2:L:204:ARG:HH11	1.85	0.41
2:H:299:LEU:CB	2:H:302:THR:CG2	2.98	0.41
2:B:182:LEU:HA	2:B:195:THR:O	2.20	0.41
2:D:302:THR:O	2:D:303:ALA:HB3	2.20	0.41
2:L:96:LEU:HD13	2:L:96:LEU:O	2.19	0.41
2:L:289:LEU:HD21	2:L:306:VAL:HG22	2.01	0.41
2:H:80:HIS:HB3	2:H:83:PHE:HB2	2.01	0.41
2:B:133:VAL:O	2:B:140:GLU:HA	2.20	0.41
2:B:216:ILE:HD12	4:B:506:HOH:O	2.20	0.41
2:B:312:ARG:O	2:B:312:ARG:CG	2.68	0.41
2:D:112:MET:HG2	2:D:268:MET:HE2	2.02	0.41
2:J:325:ASP:OD2	2:J:360:ARG:CZ	2.68	0.41
2:H:169:LEU:HD13	2:H:265:LEU:HD11	2.01	0.41
2:H:280:GLY:HA3	2:H:345:VAL:O	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:112:MET:HE3	2:B:112:MET:HB2	1.69	0.41
2:B:226:ASN:ND2	4:B:504:HOH:O	1.93	0.41
2:L:94:ASP:HB3	2:L:97:PRO:CD	2.51	0.41
2:H:69:LEU:HD21	2:H:133:VAL:HG22	2.01	0.41
2:H:219:ASP:CG	2:L:195:THR:HG23	2.40	0.41
2:B:337:ASP:HB3	2:B:340:ARG:HE	1.86	0.41
2:F:85:ASP:OD1	2:F:86:PRO:CD	2.69	0.41
2:F:353:LYS:HE3	2:F:370:GLU:HG3	2.02	0.41
2:J:63:ALA:N	2:J:64:PRO:CD	2.81	0.41
2:L:158:LYS:HD2	2:L:159:ILE:H	1.85	0.41
2:L:195:THR:CB	4:L:515:HOH:O	1.75	0.41
2:B:301:GLU:O	2:B:302:THR:C	2.59	0.41
2:L:205:ASN:HD22	2:L:339:ARG:HD2	1.74	0.41
2:L:360:ARG:NE	4:L:513:HOH:O	2.53	0.41
2:H:214:ASP:O	2:H:260:PRO:CG	2.67	0.41
2:H:283:GLY:O	2:H:311:TYR:HB2	2.21	0.41
2:B:181:CYS:HB3	2:B:199:ILE:HD11	2.01	0.41
2:F:116:GLY:HA2	2:F:164:LEU:CD1	2.51	0.41
2:J:253:GLN:N	4:J:506:HOH:O	2.35	0.41
2:B:177:THR:HG23	2:B:199:ILE:O	2.20	0.41
2:D:161:LEU:CB	2:D:164:LEU:HD13	2.38	0.41
2:D:186:ASN:ND2	2:D:186:ASN:C	2.75	0.41
2:F:94:ASP:OD1	2:F:96:LEU:HD23	2.21	0.41
2:J:98:GLN:HA	2:J:98:GLN:HE21	1.83	0.41
2:L:68:ASN:OD1	2:L:186:ASN:ND2	2.52	0.41
2:B:273:GLU:HG2	2:B:274:HIS:CD2	2.56	0.41
2:B:289:LEU:CD1	2:B:289:LEU:C	2.89	0.41
2:F:164:LEU:HD23	2:F:164:LEU:HA	1.72	0.41
2:F:243:THR:HG21	2:F:259:ILE:CG1	2.48	0.41
2:L:133:VAL:O	2:L:140:GLU:HA	2.21	0.41
2:H:151:GLU:OE1	2:H:211:THR:HB	2.21	0.40
2:H:376:PRO:HA	2:H:377:PRO:HD3	1.87	0.40
2:B:82:LEU:HD12	2:B:92:PHE:CD2	2.56	0.40
2:B:138:GLY:C	4:B:508:HOH:O	2.60	0.40
2:B:221:ALA:HA	2:B:252:SER:OG	2.21	0.40
2:D:196:MET:HE3	2:D:196:MET:HB3	1.97	0.40
2:D:327:ILE:HA	2:D:358:VAL:HG23	2.03	0.40
2:F:85:ASP:CG	2:F:90:ARG:HH12	2.24	0.40
2:F:291:PRO:HA	2:F:294:ALA:CB	2.50	0.40
4:F:511:HOH:O	2:L:82:LEU:HD11	2.12	0.40
2:J:195:THR:HG22	2:J:220:ALA:HB1	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:331:ASP:CB	2:J:354:ILE:HB	2.51	0.40
2:L:156:VAL:CG2	2:L:268:MET:HG3	2.50	0.40
2:L:260:PRO:HB2	4:L:521:HOH:O	2.21	0.40
2:L:349:ARG:HH21	2:L:349:ARG:HD3	1.66	0.40
2:B:66:VAL:HG11	2:B:184:ILE:HG22	2.04	0.40
2:F:96:LEU:HB2	2:F:97:PRO:HD2	2.03	0.40
2:F:377:PRO:CD	4:F:519:HOH:O	2.69	0.40
2:J:85:ASP:HB3	2:J:88:PHE:HB2	2.04	0.40
2:J:98:GLN:NE2	2:J:98:GLN:CA	2.74	0.40
2:L:173:ASP:OD2	2:L:262:LYS:HE2	2.21	0.40
2:D:175:ILE:N	4:D:501:HOH:O	2.46	0.40
2:D:251:GLY:HA3	2:L:253:GLN:HE22	1.86	0.40
2:F:190:VAL:O	2:F:190:VAL:CG1	2.70	0.40
2:J:64:PRO:O	2:J:165:PRO:HG2	2.21	0.40
2:D:232:VAL:CG1	2:D:236:GLY:HA2	2.48	0.40
2:L:65:ALA:HB3	2:L:167:MET:HE1	2.02	0.40
2:L:96:LEU:CD1	2:L:96:LEU:O	2.69	0.40
2:B:85:ASP:HB2	2:B:90:ARG:HH12	1.86	0.40
2:B:182:LEU:O	2:B:231:LEU:HD12	2.21	0.40
2:D:100:LYS:HD2	2:D:101:ARG:N	2.33	0.40
2:F:121:ASN:HD21	2:F:243:THR:HG22	1.86	0.40
2:L:222:ILE:HD13	2:L:242:ASN:HB3	2.02	0.40
2:L:305:ILE:CD1	2:L:327:ILE:CG1	2.96	0.40

All (2) 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)
2:H:89:ARG:NH1	2:B:296:SER:O[1_655]	1.87	0.33
2:B:61:ARG:NH1	2:J:301:GLU:OE2[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	5/10 (50%)	5 (100%)	0	0	100	100
1	C	5/10 (50%)	5 (100%)	0	0	100	100
1	E	4/10 (40%)	4 (100%)	0	0	100	100
1	G	4/10 (40%)	4 (100%)	0	0	100	100
1	I	4/10 (40%)	4 (100%)	0	0	100	100
1	K	7/10 (70%)	7 (100%)	0	0	100	100
2	B	323/377 (86%)	316 (98%)	6 (2%)	1 (0%)	41	47
2	D	323/377 (86%)	318 (98%)	4 (1%)	1 (0%)	41	47
2	F	323/377 (86%)	318 (98%)	5 (2%)	0	100	100
2	H	323/377 (86%)	309 (96%)	14 (4%)	0	100	100
2	J	323/377 (86%)	316 (98%)	5 (2%)	2 (1%)	25	26
2	L	323/377 (86%)	318 (98%)	3 (1%)	2 (1%)	25	26
All	All	1967/2322 (85%)	1924 (98%)	37 (2%)	6 (0%)	41	47

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	J	97	PRO
2	B	96	LEU
2	J	96	LEU
2	D	96	LEU
2	L	97	PRO
2	L	186	ASN

### 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	7/10 (70%)	6 (86%)	1 (14%)	3	2
1	C	7/10 (70%)	7 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	6/10 (60%)	5 (83%)	1 (17%)	2	1
1	G	6/10 (60%)	5 (83%)	1 (17%)	2	1
1	I	6/10 (60%)	3 (50%)	3 (50%)	0	0
1	K	9/10 (90%)	6 (67%)	3 (33%)	0	0
2	B	253/298 (85%)	213 (84%)	40 (16%)	2	1
2	D	253/298 (85%)	210 (83%)	43 (17%)	2	1
2	F	253/298 (85%)	209 (83%)	44 (17%)	2	1
2	H	253/298 (85%)	233 (92%)	20 (8%)	12	12
2	J	253/298 (85%)	209 (83%)	44 (17%)	2	1
2	L	253/298 (85%)	216 (85%)	37 (15%)	3	2
All	All	1559/1848 (84%)	1322 (85%)	237 (15%)	3	2

All (237) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	6	LEU
2	H	84	ASP
2	H	94	ASP
2	H	96	LEU
2	H	144	GLN
2	H	148	SER
2	H	175	ILE
2	H	186	ASN
2	H	209	LEU
2	H	232	VAL
2	H	246	PHE
2	H	248	LYS
2	H	265	LEU
2	H	266	GLU
2	H	269	GLN
2	H	286	VAL
2	H	302	THR
2	H	329	THR
2	H	337	ASP
2	H	358	VAL
2	H	368	THR
1	A	6	LEU
2	B	53	VAL

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	71	THR
2	B	72	THR
2	B	74	MET
2	B	82	LEU
2	B	85	ASP
2	B	87	MET
2	B	89	ARG
2	B	94	ASP
2	B	95	ASN
2	B	98	GLN
2	B	100	LYS
2	B	104	SER
2	B	113	SER
2	B	135	LEU
2	B	136	ARG
2	B	151	GLU
2	B	162	LYS
2	B	176	ARG
2	B	196	MET
2	B	211	THR
2	B	216	ILE
2	B	227	SER
2	B	232	VAL
2	B	261	THR
2	B	273	GLU
2	B	274	HIS
2	B	282	LEU
2	B	287	LYS
2	B	289	LEU
2	B	295	GLU
2	B	301	GLU
2	B	313	ASP
2	B	328	LEU
2	B	329	THR
2	B	332	LYS
2	B	352	GLN
2	B	358	VAL
2	B	361	ASN
2	B	363	GLN
2	D	60	SER
2	D	70	TYR
2	D	71	THR

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	D	73	LYS
2	D	74	MET
2	D	77	LYS
2	D	89	ARG
2	D	91	PHE
2	D	95	ASN
2	D	96	LEU
2	D	99	GLN
2	D	100	LYS
2	D	101	ARG
2	D	103	GLU
2	D	104	SER
2	D	106	LEU
2	D	113	SER
2	D	130	GLN
2	D	141	THR
2	D	142	ILE
2	D	144	GLN
2	D	159	ILE
2	D	172	SER
2	D	186	ASN
2	D	204	ARG
2	D	227	SER
2	D	239	ILE
2	D	253	GLN
2	D	261	THR
2	D	265	LEU
2	D	285	GLU
2	D	286	VAL
2	D	289	LEU
2	D	292	GLU
2	D	295	GLU
2	D	301	GLU
2	D	305	ILE
2	D	321	LEU
2	D	333	GLN
2	D	357	VAL
2	D	358	VAL
2	D	359	LEU
2	D	368	THR
1	E	6	LEU
2	F	53	VAL

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	54	SER
2	F	61	ARG
2	F	66	VAL
2	F	73	LYS
2	F	74	MET
2	F	76	SER
2	F	77	LYS
2	F	85	ASP
2	F	91	PHE
2	F	102	MET
2	F	103	GLU
2	F	106	LEU
2	F	118	LEU
2	F	141	THR
2	F	142	ILE
2	F	148	SER
2	F	160	ASP
2	F	162	LYS
2	F	171	ARG
2	F	176	ARG
2	F	190	VAL
2	F	207	LEU
2	F	209	LEU
2	F	219	ASP
2	F	232	VAL
2	F	243	THR
2	F	262	LYS
2	F	278	ILE
2	F	282	LEU
2	F	285	GLU
2	F	287	LYS
2	F	290	THR
2	F	295	GLU
2	F	301	GLU
2	F	302	THR
2	F	312	ARG
2	F	322	LEU
2	F	332	LYS
2	F	342	MET
2	F	349	ARG
2	F	354	ILE
2	F	355	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	F	360	ARG
1	I	5	GLU
1	I	6	LEU
1	I	9	VAL
2	J	53	VAL
2	J	61	ARG
2	J	70	TYR
2	J	75	VAL
2	J	87	MET
2	J	89	ARG
2	J	94	ASP
2	J	95	ASN
2	J	102	MET
2	J	104	SER
2	J	106	LEU
2	J	112	MET
2	J	129	ASP
2	J	141	THR
2	J	158	LYS
2	J	159	ILE
2	J	162	LYS
2	J	168	THR
2	J	172	SER
2	J	175	ILE
2	J	182	LEU
2	J	192	GLN
2	J	200	SER
2	J	205	ASN
2	J	206	GLN
2	J	226	ASN
2	J	255	ILE
2	J	263	LEU
2	J	265	LEU
2	J	276	GLN
2	J	289	LEU
2	J	292	GLU
2	J	293	LEU
2	J	299	LEU
2	J	301	GLU
2	J	305	ILE
2	J	307	VAL
2	J	334	GLU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	J	336	SER
2	J	339	ARG
2	J	350	PRO
2	J	358	VAL
2	J	363	GLN
2	J	368	THR
1	K	4	ASP
1	K	6	LEU
1	K	7	ARG
2	L	53	VAL
2	L	61	ARG
2	L	74	MET
2	L	75	VAL
2	L	76	SER
2	L	85	ASP
2	L	87	MET
2	L	89	ARG
2	L	95	ASN
2	L	96	LEU
2	L	98	GLN
2	L	100	LYS
2	L	103	GLU
2	L	113	SER
2	L	145	LEU
2	L	172	SER
2	L	175	ILE
2	L	192	GLN
2	L	193	THR
2	L	199	ILE
2	L	209	LEU
2	L	237	ASN
2	L	243	THR
2	L	249	SER
2	L	276	GLN
2	L	278	ILE
2	L	289	LEU
2	L	297	LEU
2	L	313	ASP
2	L	322	LEU
2	L	328	LEU
2	L	329	THR
2	L	334	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	L	342	MET
2	L	359	LEU
2	L	363	GLN
2	L	367	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	95	ASN
2	H	186	ASN
2	H	217	GLN
2	H	253	GLN
2	H	276	GLN
2	H	344	GLN
2	B	80	HIS
2	B	95	ASN
2	B	122	ASN
2	B	130	GLN
2	B	163	ASN
2	B	223	ASN
2	B	242	ASN
2	B	276	GLN
2	B	343	ASN
2	B	344	GLN
2	B	352	GLN
2	B	361	ASN
2	B	363	GLN
2	D	80	HIS
2	D	95	ASN
2	D	276	GLN
2	D	343	ASN
2	D	361	ASN
2	F	226	ASN
2	F	276	GLN
2	F	343	ASN
2	F	361	ASN
2	J	68	ASN
2	J	98	GLN
2	J	186	ASN
2	J	242	ASN
2	J	276	GLN
2	J	343	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	J	344	GLN
2	L	99	GLN
2	L	186	ASN
2	L	205	ASN
2	L	242	ASN
2	L	253	GLN
2	L	276	GLN
2	L	344	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	IMD	F	401	-	3,5,5	0.69	0	4,5,5	0.29	0
3	IMD	L	401	-	3,5,5	0.71	0	4,5,5	0.72	0
3	IMD	J	401	-	3,5,5	0.60	0	4,5,5	0.57	0
3	IMD	B	401	-	3,5,5	0.63	0	4,5,5	0.51	0
3	IMD	D	401	-	3,5,5	0.51	0	4,5,5	0.64	0
3	IMD	H	401	-	3,5,5	0.62	0	4,5,5	0.42	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	IMD	F	401	-	-	-	0/1/1/1
3	IMD	L	401	-	-	-	0/1/1/1
3	IMD	J	401	-	-	-	0/1/1/1
3	IMD	B	401	-	-	-	0/1/1/1
3	IMD	D	401	-	-	-	0/1/1/1
3	IMD	H	401	-	-	-	0/1/1/1

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.

6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	401	IMD	3	0
3	L	401	IMD	4	0
3	J	401	IMD	1	0
3	B	401	IMD	1	0
3	D	401	IMD	3	0
3	H	401	IMD	8	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	7/10 (70%)	1.29	1 (14%) 2 4	20, 41, 53, 70	0
1	C	7/10 (70%)	0.64	0 100 100	18, 33, 67, 72	0
1	E	6/10 (60%)	1.44	1 (16%) 1 2	32, 45, 66, 69	0
1	G	6/10 (60%)	1.53	2 (33%) 0 0	20, 34, 59, 64	0
1	I	6/10 (60%)	1.13	1 (16%) 1 2	19, 29, 40, 71	0
1	K	9/10 (90%)	2.02	3 (33%) 0 0	29, 69, 85, 94	0
2	B	325/377 (86%)	0.70	25 (7%) 13 20	9, 27, 77, 101	0
2	D	325/377 (86%)	0.77	35 (10%) 5 9	6, 27, 76, 116	0
2	F	325/377 (86%)	0.62	25 (7%) 13 20	8, 31, 63, 97	0
2	H	325/377 (86%)	0.65	25 (7%) 13 20	8, 25, 70, 100	0
2	J	325/377 (86%)	0.61	18 (5%) 25 34	9, 27, 65, 114	0
2	L	325/377 (86%)	0.68	33 (10%) 6 11	7, 27, 73, 99	0
All	All	1991/2322 (85%)	0.68	169 (8%) 10 16	6, 27, 73, 116	0

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	74	MET	10.0
2	J	96	LEU	8.5
2	D	75	VAL	8.4
2	B	297	LEU	8.3
2	D	96	LEU	7.7
2	L	303	ALA	7.0
2	J	100	LYS	7.0
2	D	94	ASP	6.9
2	J	99	GLN	6.6
2	J	95	ASN	6.5
2	B	303	ALA	6.2

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	J	78	PRO	5.9
2	L	96	LEU	5.7
2	H	297	LEU	5.7
2	H	98	GLN	5.7
2	F	300	GLY	5.7
2	J	74	MET	5.7
2	D	73	LYS	5.5
2	B	98	GLN	5.4
2	H	95	ASN	5.3
2	L	300	GLY	5.3
2	L	297	LEU	5.2
2	B	302	THR	5.1
2	D	102	MET	5.0
2	B	78	PRO	5.0
2	B	94	ASP	5.0
2	L	304	GLY	4.9
2	B	76	SER	4.9
2	D	98	GLN	4.8
2	J	97	PRO	4.8
2	F	302	THR	4.7
2	B	299	LEU	4.6
2	F	301	GLU	4.6
2	H	78	PRO	4.6
2	B	101	ARG	4.5
2	H	87	MET	4.5
2	L	76	SER	4.4
2	D	99	GLN	4.3
2	B	97	PRO	4.3
2	D	100	LYS	4.3
2	D	93	GLY	4.3
2	L	292	GLU	4.3
1	K	2	VAL	4.2
2	D	95	ASN	4.1
1	I	5	GLU	3.9
2	B	74	MET	3.9
2	L	290	THR	3.9
2	H	76	SER	3.8
2	J	75	VAL	3.8
2	J	77	LYS	3.8
2	J	76	SER	3.8
2	H	303	ALA	3.7
2	H	97	PRO	3.7

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	H	302	THR	3.7
2	L	95	ASN	3.6
2	H	74	MET	3.6
2	B	79	SER	3.6
2	F	79	SER	3.6
2	D	72	THR	3.6
2	F	299	LEU	3.5
2	L	282	LEU	3.5
1	K	6	LEU	3.5
1	G	7	ARG	3.5
1	E	6	LEU	3.4
2	B	96	LEU	3.4
2	L	301	GLU	3.4
2	D	297	LEU	3.4
2	D	97	PRO	3.4
2	D	91	PHE	3.4
2	L	302	THR	3.3
2	D	304	GLY	3.3
2	B	75	VAL	3.3
1	G	6	LEU	3.3
2	D	299	LEU	3.2
2	D	302	THR	3.2
2	H	299	LEU	3.2
2	H	77	LYS	3.2
2	L	77	LYS	3.2
2	D	88	PHE	3.1
2	F	75	VAL	3.1
2	L	78	PRO	3.1
2	D	70	TYR	3.1
2	D	87	MET	3.1
2	L	313	ASP	3.1
2	D	78	PRO	3.1
2	B	93	GLY	3.1
2	L	299	LEU	3.0
2	H	101	ARG	3.0
2	D	101	ARG	3.0
2	B	73	LYS	2.9
2	F	98	GLN	2.9
2	F	293	LEU	2.8
2	J	70	TYR	2.8
2	H	79	SER	2.8
2	B	99	GLN	2.8

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	J	276	GLN	2.8
2	D	303	ALA	2.8
2	F	102	MET	2.8
2	B	77	LYS	2.8
2	F	370	GLU	2.7
2	D	106	LEU	2.7
2	L	75	VAL	2.7
2	H	129	ASP	2.7
2	L	321	LEU	2.7
2	H	102	MET	2.7
2	F	95	ASN	2.6
2	H	73	LYS	2.6
2	D	129	ASP	2.6
2	J	79	SER	2.6
1	A	4	ASP	2.6
2	L	305	ILE	2.6
2	H	99	GLN	2.6
2	L	73	LYS	2.5
1	K	4	ASP	2.5
2	J	93	GLY	2.5
2	H	127	GLY	2.5
2	H	83	PHE	2.4
2	B	70	TYR	2.4
2	J	206	GLN	2.4
2	L	102	MET	2.4
2	D	83	PHE	2.4
2	F	96	LEU	2.4
2	D	76	SER	2.4
2	L	289	LEU	2.4
2	B	334	GLU	2.4
2	H	91	PHE	2.4
2	D	282	LEU	2.4
2	F	145	LEU	2.4
2	F	101	ARG	2.3
2	L	99	GLN	2.3
2	F	100	LYS	2.3
2	H	128	ALA	2.3
2	F	303	ALA	2.3
2	B	102	MET	2.3
2	H	75	VAL	2.3
2	H	301	GLU	2.3
2	H	94	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	F	76	SER	2.3
2	D	89	ARG	2.3
2	B	269	GLN	2.3
2	L	353	LYS	2.3
2	L	369	ALA	2.3
2	L	129	ASP	2.2
2	F	321	LEU	2.2
2	J	102	MET	2.2
2	L	100	LYS	2.2
2	F	324	GLY	2.2
2	D	305	ILE	2.2
2	D	293	LEU	2.2
2	L	298	GLY	2.2
2	D	212	TYR	2.1
2	L	94	ASP	2.1
2	L	357	VAL	2.1
2	F	246	PHE	2.1
2	D	77	LYS	2.1
2	F	129	ASP	2.1
2	F	330	ILE	2.1
2	L	79	SER	2.1
2	B	293	LEU	2.1
2	L	334	GLU	2.1
2	B	95	ASN	2.1
2	L	358	VAL	2.1
2	J	246	PHE	2.1
2	B	83	PHE	2.1
2	F	277	VAL	2.0
2	J	87	MET	2.0
2	F	363	GLN	2.0
2	D	86	PRO	2.0
2	F	352	GLN	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
3	IMD	L	401	5/5	0.81	0.31	24,26,32,34	0
3	IMD	H	401	5/5	0.87	0.20	32,33,39,42	0
3	IMD	B	401	5/5	0.88	0.16	29,29,39,43	0
3	IMD	J	401	5/5	0.91	0.19	24,25,41,50	0
3	IMD	D	401	5/5	0.91	0.16	24,26,31,31	0
3	IMD	F	401	5/5	0.93	0.15	25,32,36,38	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.