

Full wwPDB X-ray Structure Validation Report (i)

Jun 3, 2024 – 02:29 PM JST

PDB ID	:	8KAM
Title	:	Crystal structure of SpyCas9 in complex with sgRNA and 16nt target DNA
Authors	:	Chen, Y.; Chen, J.; Liu, L.
Deposited on	:	2023-08-03
Resolution	:	3.91 Å(reported)

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

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

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

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

MolProbity		4.02b-467
	·	4.020-401
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
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)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

The reported resolution of this entry is 3.91 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	1019 (4.18-3.66)
Clashscore	141614	1016 (4.16-3.68)
Ramachandran outliers	138981	1039 (4.18-3.66)
Sidechain outliers	138945	1032 (4.18-3.66)
RNA backbone	3102	1041 (4.84-3.00)

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

Mol	Chain	Length		Quality of chain		
1	А	98	33%	43%	20%	·
2	В	1368	39%	46%	12%	•••
3	С	24	38%	63%		
4	D	11	64%		36%	



8KAM

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 13534 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 RNA chain called RNA (98-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	А	94	Total 2009	C 899	N 362	0 654	Р 94	0	0	0

• Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	1326	Total 10816	C 6890	N 1877	O 2027	S 22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	10	ALA	ASP	engineered mutation	UNP Q99ZW2
В	840	ALA	HIS	engineered mutation	UNP Q99ZW2

• Molecule 3 is a DNA chain called DNA (5'-D(*CP*AP*AP*TP*AP*CP*CP*TP*CP*TP* TP*CP*AP*AP*TP*TP*AP*GP*AP*CP*AP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	С	24	Total 483	C 233	N 88	O 139	Р 23	0	0	0

• Molecule 4 is a DNA chain called DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP* G)-3').

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
4	D	11	Total 225	C 110	N 37	O 68	Р 10	0	0	0

• Molecule 5 is water.



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	В	1	Total O 1 1	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. 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. 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: RNA (98-MER)





• Molecule 4: DNA (5'-D(*TP*TP*TP*AP*GP*GP*TP*AP*TP*TP*G)-3')

38%

G24



• Molecule 3: DNA (5'-D(*CP*AP*AP*TP*AP*CP*CP*TP*CP*TP*TP*CP*AP*AP*TP*TP* AP*GP*AP*AP*CP*AP*CP*G)-3')

63%

Chain C:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	199.03Å 70.39Å 186.96Å	Depositor
a, b, c, α , β , γ	90.00° 109.62° 90.00°	Depositor
Bosolution (Å)	38.78 - 3.91	Depositor
Resolution (A)	48.71 - 3.91	EDS
% Data completeness	36.0 (38.78-3.91)	Depositor
(in resolution range)	47.6(48.71-3.91)	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.86 (at 3.88 \text{\AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
D D	0.260 , 0.290	Depositor
$\mathbf{n}, \mathbf{n}_{free}$	0.260 , 0.290	DCC
R_{free} test set	1138 reflections (10.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	-2.7	Xtriage
Anisotropy	8.165	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.16 , -10.0	EDS
L-test for twinning ²	$ \langle L \rangle = 0.38, \langle L^2 \rangle = 0.21$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.71	EDS
Total number of atoms	13534	wwPDB-VP
Average B, all atoms $(Å^2)$	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.79% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

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

Mal	Chain	Bo	nd lengths	Bond angles		
		RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.25	0/2249	0.81	0/3503	
2	В	0.39	6/11008~(0.1%)	0.71	48/14794~(0.3%)	
3	С	0.64	0/541	1.01	0/831	
4	D	0.55	0/251	1.05	0/387	
All	All	0.39	6/14049~(0.0%)	0.75	48/19515~(0.2%)	

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	В	0	2

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	В	1137	PRO	N-CD	5.32	1.55	1.47
2	В	378	PRO	N-CD	5.26	1.55	1.47
2	В	230	PRO	N-CD	5.15	1.55	1.47
2	В	133	PRO	N-CD	5.07	1.54	1.47
2	В	843	PRO	N-CD	5.07	1.54	1.47
2	В	316	PRO	N-CD	5.04	1.54	1.47

All (6) bond length outliers are listed below:

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	675	SER	CB-CA-C	-19.99	72.11	110.10
2	В	1222	LYS	CB-CA-C	-14.01	82.39	110.40
2	В	284	ASP	CB-CA-C	-10.87	88.67	110.40
2	В	164	PHE	N-CA-C	-10.23	83.39	111.00
2	В	1222	LYS	N-CA-C	9.77	137.38	111.00
2	В	1215	ALA	CB-CA-C	8.25	122.47	110.10



2

2

2

2

В

В

В

В

571

1222

1262

246

LYS

LYS

HIS

LEU

CB-CA-C

C-N-CA

N-CA-C

N-CA-C

Continued from previous page							
Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	В	95	ASP	CB-CA-C	7.77	125.94	110.40
2	В	675	SER	N-CA-C	7.67	131.70	111.00
2	В	905	ARG	CB-CA-C	7.65	125.70	110.40
2	В	675	SER	C-N-CA	7.58	138.21	122.30
2	В	178	ASN	N-CA-C	-7.50	90.74	111.00
2	В	567	ASP	CB-CA-C	7.42	125.24	110.40
2	В	164	PHE	CB-CA-C	7.34	125.08	110.40
2	В	1351	SER	CB-CA-C	-7.05	96.71	110.10
2	В	591	LEU	N-CA-C	-6.73	92.83	111.00
2	В	315	ALA	CB-CA-C	-6.64	100.14	110.10
2	В	455	LEU	N-CA-C	-6.62	93.13	111.00
2	В	879	MET	CB-CA-C	6.49	123.38	110.40
2	В	104	SER	N-CA-CB	6.37	120.05	110.50
2	В	1177	ASN	N-CA-C	-6.34	93.89	111.00
2	В	265	GLN	CB-CA-C	6.23	122.86	110.40
2	В	825	ASP	N-CA-C	6.22	127.78	111.00
2	В	1088	SER	CB-CA-C	6.17	121.82	110.10
2	В	249	THR	C-N-CD	6.15	141.32	128.40
2	В	175	ASN	C-N-CD	6.12	141.24	128.40
2	В	463	ALA	CB-CA-C	-6.06	101.02	110.10
2	В	453	GLY	C-N-CD	5.98	140.96	128.40
2	В	229	LEU	C-N-CD	5.94	140.87	128.40
2	В	572	ILE	CB-CA-C	-5.93	99.74	111.60
2	В	116	HIS	C-N-CD	5.93	140.84	128.40
2	В	1228	LEU	C-N-CD	5.92	140.83	128.40
2	В	870	VAL	C-N-CD	5.85	140.69	128.40
2	В	1191	LYS	CB-CA-C	-5.81	98.79	110.40
2	В	132	TYR	C-N-CD	5.79	140.55	128.40
2	В	842	VAL	C-N-CD	5.79	140.55	128.40
2	В	1177	ASN	CB-CA-C	5.76	121.92	110.40
2	В	1041	ASN	CB-CA-C	5.74	121.87	110.40
2	В	1032	ALA	CB-CA-C	5.70	118.66	110.10
2	В	377	LYS	C-N-CD	5.60	140.17	128.40
2	В	584	GLU	CB-CA-C	-5.58	99.23	110.40
2	В	997	LEU	CB-CA-C	-5.51	99.73	110.20
2	В	1136	SER	C-N-CD	5.44	139.83	128.40
2	В	878	LYS	CB-CA-C	5.39	121.17	110.40
2	В	250	PRO	CA-N-CD	-5.35	104.02	111.50



5.30

5.18

-5.16

-5.13

121.00

133.18

97.06

97.15

110.40

122.30

111.00

111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	В	1222	LYS	Peptide
2	В	675	SER	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	А	2009	0	1009	88	0
2	В	10816	0	10957	1624	3
3	С	483	0	272	48	0
4	D	225	0	129	6	0
5	В	1	0	0	0	0
All	All	13534	0	12367	1663	3

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 64.

All (1663) 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:1204:PHE:CE1	2:B:1347:LEU:HD12	1.32	1.59
2:B:557:ARG:HG2	2:B:595:HIS:CD2	1.33	1.57
2:B:520:VAL:HG21	2:B:591:LEU:CD2	1.32	1.57
2:B:446:PHE:CZ	2:B:478:PHE:CD1	1.92	1.56
2:B:178:ASN:CB	2:B:299:ALA:HA	1.26	1.56
2:B:520:VAL:CG2	2:B:591:LEU:HD23	1.35	1.56
2:B:451:TYR:HA	2:B:491:PHE:CD1	1.41	1.53
2:B:446:PHE:CE1	2:B:478:PHE:HD1	1.26	1.50
2:B:557:ARG:HA	2:B:595:HIS:CD2	1.43	1.50
2:B:178:ASN:CB	2:B:299:ALA:CA	1.87	1.50
2:B:1204:PHE:HD2	2:B:1342:VAL:CG1	1.22	1.49
2:B:340:ARG:NH2	2:B:347:TYR:CE2	1.79	1.48
2:B:1206:LEU:HB3	2:B:1345:ALA:CB	1.40	1.47
2:B:245:SER:CB	2:B:296:LEU:HD23	1.43	1.45



	A l	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:1203:LEU:HD11	2:B:1211:LYS:CD	1.48	1.43
2:B:340:ARG:CZ	2:B:347:TYR:CE2	2.02	1.43
2:B:340:ARG:CZ	2:B:347:TYR:HE2	1.31	1.43
2:B:1204:PHE:CD2	2:B:1342:VAL:CG1	1.99	1.43
2:B:1204:PHE:CD2	2:B:1342:VAL:HG11	1.52	1.41
2:B:1204:PHE:HE1	2:B:1347:LEU:CD1	1.32	1.41
2:B:195:LEU:CD1	2:B:289:LEU:HD12	1.53	1.39
2:B:195:LEU:HD13	2:B:289:LEU:CD1	1.52	1.39
2:B:668:ASN:HD21	2:B:680:LEU:CD2	1.34	1.39
2:B:456:ALA:HB2	2:B:463:ALA:CB	1.51	1.39
2:B:553:PHE:CE2	2:B:559:VAL:HG21	1.57	1.39
2:B:978:ILE:HD11	2:B:1236:LEU:CD1	1.51	1.37
2:B:1348:ILE:HD12	2:B:1359:ARG:NH1	1.37	1.35
2:B:446:PHE:HZ	2:B:478:PHE:CE1	1.44	1.35
2:B:1210:ARG:HG2	2:B:1280:VAL:CG1	1.54	1.35
2:B:379:ILE:O	2:B:383:MET:CG	1.73	1.34
2:B:557:ARG:CA	2:B:595:HIS:CD2	2.07	1.34
2:B:282:ILE:CG2	2:B:286:TYR:CE1	2.12	1.33
2:B:545:LYS:HZ1	2:B:690:ASN:CG	1.29	1.33
2:B:178:ASN:CB	2:B:299:ALA:CB	2.05	1.33
2:B:362:TYR:CD2	2:B:372:PHE:CD2	2.16	1.32
2:B:556:ASN:C	2:B:595:HIS:NE2	1.81	1.32
2:B:557:ARG:CG	2:B:595:HIS:HD2	1.42	1.32
2:B:601:ILE:CD1	2:B:607:LEU:HD21	1.59	1.32
2:B:201:ILE:HD13	2:B:232:GLU:OE1	1.20	1.32
2:B:518:PHE:CE2	2:B:683:LEU:HD12	1.64	1.31
2:B:557:ARG:N	2:B:595:HIS:NE2	1.78	1.31
1:A:58:G:H4'	2:B:457:ARG:CD	1.59	1.31
2:B:557:ARG:CG	2:B:595:HIS:CD2	2.14	1.31
2:B:318:SER:OG	2:B:418:GLU:CD	1.66	1.31
2:B:1139:VAL:HG12	2:B:1167:THR:CA	1.59	1.31
2:B:1224:ASN:ND2	2:B:1280:VAL:HG21	1.46	1.30
2:B:1139:VAL:HB	2:B:1166:ILE:O	1.14	1.29
2:B:553:PHE:CD2	2:B:559:VAL:HG21	1.67	1.29
2:B:1210:ARG:HD2	2:B:1280:VAL:O	1.25	1.29
2:B:245:SER:CB	2:B:296:LEU:CD2	2.13	1.27
2:B:839:ASP:OD1	2:B:864:ARG:NH1	1.64	1.27
2:B:518:PHE:HE2	2:B:683:LEU:CD1	1.46	1.27
1:A:58:G:O2'	2:B:457:ARG:CB	1.82	1.26
2:B:520:VAL:CG2	2:B:591:LEU:CD2	1.98	1.26
2:B:1245:LEU:HD22	2:B:1252:ASN:OD1	1.26	1.26



	A O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:446:PHE:HZ	2:B:478:PHE:CD1	1.35	1.26
2:B:511:HIS:O	2:B:593:THR:HG21	1.36	1.25
2:B:507:VAL:HG11	2:B:660:GLY:O	1.14	1.25
2:B:1210:ARG:CD	2:B:1280:VAL:HA	1.67	1.25
2:B:201:ILE:CD1	2:B:232:GLU:OE1	1.85	1.24
1:A:58:G:C4'	2:B:457:ARG:HD3	1.68	1.22
2:B:318:SER:OG	2:B:418:GLU:OE1	1.55	1.22
2:B:668:ASN:OD1	2:B:680:LEU:HB2	1.10	1.22
2:B:18:TRP:CD1	2:B:49:GLY:C	2.08	1.22
2:B:1210:ARG:HD2	2:B:1280:VAL:C	1.59	1.22
2:B:668:ASN:OD1	2:B:680:LEU:CB	1.87	1.22
2:B:1210:ARG:CG	2:B:1280:VAL:HA	1.68	1.22
2:B:161:MET:O	2:B:164:PHE:O	1.53	1.21
2:B:668:ASN:ND2	2:B:680:LEU:CD2	2.03	1.21
1:A:58:G:O2'	2:B:457:ARG:HB2	1.03	1.19
2:B:107:VAL:HG13	2:B:1131:TYR:CE1	1.76	1.19
2:B:1312:LEU:HD21	2:B:1326:TYR:HD1	1.02	1.19
2:B:116:HIS:NE2	2:B:122:ILE:HB	1.56	1.19
2:B:282:ILE:HG21	2:B:286:TYR:CD1	1.77	1.19
2:B:1297:HIS:CE1	2:B:1327:PHE:HE2	1.59	1.19
2:B:1210:ARG:CG	2:B:1280:VAL:HG13	1.72	1.19
2:B:116:HIS:HD2	2:B:122:ILE:HA	1.06	1.18
2:B:978:ILE:CD1	2:B:1236:LEU:CD1	2.20	1.18
2:B:107:VAL:HG22	2:B:1131:TYR:OH	1.42	1.18
2:B:518:PHE:CZ	2:B:679:ILE:CG2	2.27	1.18
2:B:1212:ARG:NH1	2:B:1336:TYR:CE2	2.13	1.17
2:B:340:ARG:NH2	2:B:347:TYR:HE2	1.23	1.17
2:B:455:LEU:HD23	2:B:473:ILE:CD1	1.74	1.17
2:B:1139:VAL:HG12	2:B:1167:THR:N	1.58	1.17
2:B:107:VAL:N	2:B:1131:TYR:OH	1.76	1.17
2:B:282:ILE:HG21	2:B:286:TYR:CE1	1.73	1.17
2:B:318:SER:OG	2:B:418:GLU:OE2	1.59	1.16
2:B:446:PHE:CE1	2:B:478:PHE:CD1	2.17	1.16
2:B:978:ILE:CD1	2:B:1236:LEU:HD11	1.76	1.16
2:B:1270:ILE:O	2:B:1273:ILE:CG1	1.92	1.16
2:B:1204:PHE:CD2	2:B:1342:VAL:HG12	1.81	1.15
2:B:446:PHE:CZ	2:B:478:PHE:CE1	2.26	1.15
2:B:1270:ILE:HA	2:B:1273:ILE:CD1	1.77	1.15
2:B:282:ILE:CG2	2:B:286:TYR:CD1	2.30	1.14
2:B:1270:ILE:CA	2:B:1273:ILE:HG12	1.78	1.14
2:B:379:ILE:O	2:B:383:MET:HG3	1.37	1.14



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:451:TYR:CA	2:B:491:PHE:CD1	2.30	1.14
2:B:507:VAL:CG1	2:B:660:GLY:O	1.95	1.14
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.18	1.14
2:B:1206:LEU:HB3	2:B:1345:ALA:HB2	1.16	1.14
2:B:557:ARG:HA	2:B:595:HIS:NE2	1.60	1.14
2:B:453:GLY:CA	2:B:464:TRP:HD1	1.60	1.13
2:B:354:GLN:HB2	2:B:361:GLY:HA2	1.14	1.13
2:B:450:TYR:HD2	2:B:491:PHE:CZ	1.66	1.13
2:B:1240:SER:OG	2:B:1307:GLU:HG3	1.45	1.13
2:B:1312:LEU:HD21	2:B:1326:TYR:CD1	1.84	1.12
1:A:58:G:C4'	2:B:457:ARG:CD	2.26	1.12
2:B:446:PHE:CZ	2:B:478:PHE:HD1	1.40	1.11
1:A:58:G:H4'	2:B:457:ARG:HD2	1.12	1.11
2:B:226:ILE:HG22	2:B:229:LEU:HD21	1.25	1.11
2:B:270:THR:O	2:B:274:ASP:HB2	1.51	1.11
2:B:483:ASP:HB3	2:B:486:ALA:HB3	1.32	1.11
2:B:557:ARG:CA	2:B:595:HIS:NE2	2.07	1.11
2:B:456:ALA:CB	2:B:463:ALA:CB	2.29	1.10
2:B:668:ASN:HD21	2:B:680:LEU:HD23	0.99	1.10
2:B:107:VAL:HG13	2:B:1131:TYR:HE1	1.02	1.10
2:B:456:ALA:CB	2:B:463:ALA:HB1	1.82	1.10
2:B:839:ASP:OD2	2:B:864:ARG:HD2	1.51	1.10
2:B:841:ILE:CD1	2:B:900:LEU:HG	1.81	1.10
2:B:18:TRP:NE1	2:B:50:ALA:N	1.87	1.09
2:B:1139:VAL:CB	2:B:1166:ILE:O	1.99	1.09
2:B:1243:GLU:HB3	2:B:1246:LYS:CE	1.82	1.09
2:B:1270:ILE:O	2:B:1273:ILE:HG13	1.48	1.09
2:B:966:PHE:CE1	2:B:970:PHE:CE2	2.40	1.09
2:B:1226:LEU:CD1	2:B:1276:PHE:HB2	1.82	1.09
2:B:762:GLU:OE1	2:B:990:ASN:OD1	1.68	1.09
2:B:134:THR:HB	2:B:137:HIS:ND1	1.67	1.08
2:B:1203:LEU:HD11	2:B:1211:LYS:HD2	1.16	1.08
2:B:601:ILE:HD12	2:B:607:LEU:CD2	1.82	1.08
2:B:379:ILE:O	2:B:383:MET:HG2	1.48	1.08
2:B:1226:LEU:HD13	2:B:1276:PHE:HB2	1.17	1.08
2:B:1270:ILE:C	2:B:1273:ILE:HG12	1.73	1.08
2:B:6:SER:O	2:B:21:ILE:HG13	1.52	1.08
2:B:1203:LEU:HD21	2:B:1211:LYS:HD3	1.12	1.08
2:B:1210:ARG:CG	2:B:1280:VAL:CA	2.31	1.08
2:B:1297:HIS:CG	2:B:1327:PHE:CZ	2.42	1.08
2:B:116:HIS:CD2	2:B:122:ILE:HB	1.87	1.07



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:189:VAL:HG23	2:B:238:PHE:CZ	1.89	1.07
2:B:453:GLY:HA3	2:B:464:TRP:HD1	1.10	1.07
2:B:1210:ARG:HG3	2:B:1280:VAL:HA	1.33	1.07
2:B:1226:LEU:HD13	2:B:1276:PHE:CB	1.84	1.07
2:B:603:ASP:OD1	2:B:606:PHE:HB2	1.55	1.07
2:B:202:ASN:ND2	2:B:204:SER:OG	1.88	1.07
2:B:451:TYR:CA	2:B:491:PHE:HD1	1.65	1.07
2:B:1203:LEU:CD2	2:B:1211:LYS:HD3	1.83	1.07
2:B:362:TYR:CE2	2:B:372:PHE:CD2	2.42	1.07
2:B:479:GLU:OE1	2:B:484:LYS:NZ	1.88	1.06
2:B:1203:LEU:CD1	2:B:1211:LYS:CD	2.32	1.06
2:B:453:GLY:HA3	2:B:464:TRP:CD1	1.89	1.06
2:B:6:SER:CB	2:B:21:ILE:HD11	1.86	1.06
2:B:453:GLY:CA	2:B:464:TRP:CD1	2.38	1.06
2:B:456:ALA:HB2	2:B:463:ALA:HB1	1.12	1.06
2:B:967:ARG:HB3	2:B:972:PHE:O	1.55	1.06
2:B:516:GLU:HG3	2:B:593:THR:OG1	1.54	1.06
2:B:1139:VAL:HG12	2:B:1167:THR:HA	1.34	1.06
2:B:189:VAL:HG23	2:B:238:PHE:HZ	1.15	1.05
2:B:489:GLN:NE2	2:B:493:GLU:OE2	1.88	1.05
2:B:839:ASP:OD2	2:B:864:ARG:CD	2.04	1.05
2:B:1270:ILE:HA	2:B:1273:ILE:CG1	1.87	1.05
2:B:1297:HIS:CG	2:B:1327:PHE:HZ	1.74	1.05
2:B:853:ASP:O	2:B:896:LYS:HG3	1.55	1.05
2:B:116:HIS:CD2	2:B:122:ILE:CB	2.39	1.05
2:B:320:SER:O	2:B:323:LYS:HB3	1.57	1.05
2:B:360:ALA:O	2:B:364:ASP:N	1.88	1.05
2:B:378:PRO:HG2	2:B:379:ILE:HD12	1.35	1.05
2:B:518:PHE:HZ	2:B:679:ILE:CG2	1.63	1.05
2:B:762:GLU:OE1	2:B:990:ASN:CG	1.95	1.05
2:B:978:ILE:HD11	2:B:1236:LEU:HD11	1.05	1.05
2:B:1203:LEU:HD11	2:B:1211:LYS:CG	1.85	1.04
2:B:762:GLU:OE1	2:B:990:ASN:ND2	1.89	1.04
2:B:1325:LYS:NZ	2:B:1330:THR:OG1	1.88	1.04
2:B:1203:LEU:CD1	2:B:1211:LYS:HD2	1.87	1.04
2:B:22:THR:N	2:B:26:LYS:O	1.90	1.03
2:B:518:PHE:CE2	2:B:683:LEU:CD1	2.32	1.03
2:B:557:ARG:CB	2:B:595:HIS:HD2	1.71	1.03
2:B:1297:HIS:CE1	2:B:1327:PHE:CE2	2.45	1.03
2:B:50:ALA:HB3	2:B:1093:ASN:O	1.58	1.03
2:B:966:PHE:CE1	2:B:970:PHE:HE2	1.74	1.03



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:1206:LEU:CB	2:B:1345:ALA:CB	2.36	1.03
2:B:121:ASN:ND2	2:B:124:ASP:OD2	1.91	1.03
2:B:870:VAL:HG12	2:B:871:PRO:HD2	1.08	1.03
2:B:48:ILE:HD11	2:B:984:ALA:HB1	1.39	1.03
2:B:328:HIS:CD2	2:B:399:LEU:HB3	1.93	1.03
2:B:557:ARG:HG2	2:B:595:HIS:CG	1.91	1.03
2:B:178:ASN:CB	2:B:299:ALA:HB2	1.85	1.03
2:B:869:ASN:OD1	2:B:870:VAL:N	1.92	1.03
2:B:1210:ARG:HD2	2:B:1280:VAL:CA	1.89	1.03
2:B:107:VAL:CG1	2:B:1131:TYR:HE1	1.71	1.02
2:B:376:ILE:CA	2:B:379:ILE:HD13	1.89	1.02
2:B:553:PHE:CE2	2:B:559:VAL:CG2	2.41	1.02
2:B:1063:ILE:HG23	2:B:1074:TRP:O	1.57	1.02
2:B:1236:LEU:HB3	2:B:1310:ILE:HD11	1.41	1.02
2:B:456:ALA:HB2	2:B:463:ALA:HB2	1.39	1.02
2:B:1210:ARG:CD	2:B:1280:VAL:O	2.07	1.02
2:B:508:LEU:HD11	2:B:664:ARG:HB2	1.04	1.01
2:B:945:GLU:OE1	2:B:945:GLU:N	1.93	1.01
2:B:1210:ARG:CD	2:B:1280:VAL:CA	2.36	1.01
2:B:1269:ILE:O	2:B:1273:ILE:HG23	1.60	1.01
2:B:116:HIS:HD2	2:B:122:ILE:CA	1.73	1.01
2:B:508:LEU:CD1	2:B:664:ARG:HB2	1.89	1.01
2:B:567:ASP:O	2:B:571:LYS:CG	2.09	1.01
2:B:1139:VAL:HB	2:B:1166:ILE:C	1.80	1.01
2:B:297:SER:HA	2:B:300:ILE:HG22	1.39	1.01
2:B:478:PHE:HE2	2:B:482:VAL:HG21	1.26	1.01
2:B:1206:LEU:HB3	2:B:1345:ALA:HB1	1.37	1.01
2:B:497:ASN:OD1	3:C:19:DA:OP1	1.79	1.01
2:B:560:THR:N	2:B:563:GLN:OE1	1.94	1.01
2:B:508:LEU:HD11	2:B:664:ARG:CB	1.91	1.00
1:A:58:G:O4'	2:B:457:ARG:HD3	1.60	1.00
2:B:131:LYS:HD3	2:B:132:TYR:HE1	1.23	1.00
2:B:495:MET:HB3	3:C:17:DA:C1'	1.91	1.00
2:B:279:LEU:CD2	2:B:284:ASP:HA	1.91	1.00
1:A:51:A:O2'	2:B:1134:PHE:HE1	1.44	1.00
2:B:1240:SER:OG	2:B:1307:GLU:CG	2.09	1.00
2:B:495:MET:HB2	3:C:17:DA:C4'	1.90	1.00
2:B:719:SER:N	2:B:722:GLU:OE1	1.94	1.00
2:B:520:VAL:HG21	2:B:591:LEU:HD21	1.37	0.99
2:B:668:ASN:ND2	2:B:680:LEU:HD23	1.68	0.99
2:B:245:SER:HB2	2:B:296:LEU:CD2	1.89	0.99



	AL O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:545:LYS:NZ	2:B:690:ASN:CG	2.15	0.99
2:B:189:VAL:CG2	2:B:238:PHE:CZ	2.45	0.99
2:B:853:ASP:HA	2:B:896:LYS:HD2	1.41	0.99
1:A:59:U:OP1	2:B:467:ARG:NH2	1.96	0.98
2:B:839:ASP:CG	2:B:864:ARG:HH11	1.65	0.98
2:B:354:GLN:HB2	2:B:361:GLY:CA	1.94	0.98
2:B:567:ASP:O	2:B:571:LYS:HG3	1.63	0.98
2:B:1297:HIS:ND1	2:B:1327:PHE:CE2	2.31	0.98
2:B:18:TRP:CD1	2:B:49:GLY:O	2.16	0.98
2:B:226:ILE:HA	2:B:229:LEU:CD2	1.94	0.98
2:B:362:TYR:CE2	2:B:372:PHE:HD2	1.77	0.98
2:B:978:ILE:CD1	2:B:1236:LEU:HD12	1.89	0.98
2:B:1270:ILE:HA	2:B:1273:ILE:HG12	1.40	0.98
2:B:455:LEU:CD2	2:B:473:ILE:HD12	1.92	0.98
2:B:116:HIS:CD2	2:B:122:ILE:HA	1.98	0.98
2:B:376:ILE:HA	2:B:379:ILE:HD13	0.99	0.97
2:B:1270:ILE:HD13	2:B:1273:ILE:CD1	1.94	0.97
2:B:870:VAL:HG12	2:B:871:PRO:CD	1.94	0.97
2:B:103:GLU:O	2:B:103:GLU:HG3	1.63	0.97
2:B:354:GLN:CB	2:B:361:GLY:HA2	1.94	0.97
2:B:859:ARG:NE	2:B:860:SER:OG	1.96	0.97
2:B:1312:LEU:HD11	2:B:1326:TYR:CE1	2.00	0.97
2:B:340:ARG:NE	2:B:347:TYR:HE2	1.62	0.96
2:B:18:TRP:O	2:B:48:ILE:CD1	2.13	0.96
2:B:495:MET:CB	3:C:17:DA:C1'	2.44	0.96
2:B:1139:VAL:CG1	2:B:1167:THR:N	2.29	0.96
1:A:60:C:O3'	2:B:460:SER:OG	1.84	0.96
2:B:887:LEU:HB2	2:B:892:ILE:HD11	1.48	0.96
2:B:450:TYR:CD2	2:B:491:PHE:CZ	2.53	0.96
2:B:1203:LEU:HD12	2:B:1212:ARG:O	1.66	0.96
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.45	0.96
2:B:591:LEU:HD12	2:B:594:TYR:HD1	1.27	0.96
2:B:48:ILE:HD12	2:B:49:GLY:N	1.81	0.95
2:B:328:HIS:CE1	2:B:399:LEU:HB2	2.01	0.95
2:B:1206:LEU:CB	2:B:1345:ALA:HB2	1.96	0.95
2:B:226:ILE:HA	2:B:229:LEU:HG	1.48	0.95
2:B:229:LEU:CD1	2:B:232:GLU:HB2	1.96	0.95
2:B:455:LEU:HD23	2:B:473:ILE:HD12	0.96	0.95
2:B:495:MET:CG	3:C:17:DA:O4'	2.13	0.95
2:B:229:LEU:HD13	2:B:232:GLU:HB2	1.49	0.95
2:B:103:GLU:O	2:B:103:GLU:CG	2.13	0.95



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:245:SER:HB3	2:B:296:LEU:HD23	0.97	0.95
2:B:520:VAL:HG22	2:B:591:LEU:HD23	1.44	0.95
2:B:597:LEU:CD1	2:B:607:LEU:HD13	1.97	0.95
2:B:668:ASN:ND2	2:B:680:LEU:HD22	1.78	0.95
2:B:853:ASP:HA	2:B:896:LYS:CD	1.97	0.95
2:B:495:MET:HB3	3:C:17:DA:H1'	1.49	0.95
2:B:450:TYR:HD2	2:B:491:PHE:CE1	1.84	0.94
2:B:518:PHE:HE2	2:B:683:LEU:HD12	0.81	0.94
2:B:495:MET:HB2	3:C:17:DA:H4'	1.45	0.94
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.00	0.94
2:B:1157:LEU:H	2:B:1157:LEU:HD12	1.29	0.94
2:B:597:LEU:HD12	2:B:607:LEU:HD13	1.47	0.94
2:B:1348:ILE:CD1	2:B:1359:ARG:NH1	2.29	0.94
2:B:376:ILE:HA	2:B:379:ILE:CD1	1.95	0.94
2:B:18:TRP:CG	2:B:49:GLY:O	2.21	0.94
2:B:483:ASP:O	2:B:487:SER:OG	1.85	0.94
2:B:686:ASP:OD2	2:B:691:ARG:NE	2.01	0.93
2:B:206:VAL:HG12	2:B:228:GLN:HG3	1.46	0.93
2:B:591:LEU:HD12	2:B:594:TYR:CD1	2.04	0.93
2:B:1359:ARG:HG2	2:B:1359:ARG:HH11	1.33	0.93
2:B:350:ILE:HD11	2:B:375:PHE:HZ	1.34	0.93
2:B:116:HIS:NE2	2:B:122:ILE:CB	2.32	0.93
2:B:495:MET:HG3	3:C:17:DA:O4'	1.66	0.93
2:B:551:LEU:O	2:B:555:THR:OG1	1.85	0.93
2:B:885:GLN:HA	2:B:888:ASN:HB2	1.50	0.93
2:B:559:VAL:HA	2:B:563:GLN:OE1	1.67	0.93
2:B:949:LEU:HD12	2:B:950:ILE:H	1.31	0.93
2:B:1339:THR:O	2:B:1343:LEU:HD21	1.68	0.93
1:A:58:G:HO2'	2:B:457:ARG:HB2	1.26	0.93
2:B:202:ASN:OD1	2:B:204:SER:N	2.01	0.93
2:B:1270:ILE:O	2:B:1273:ILE:HG12	1.64	0.93
2:B:1148:LYS:HD2	2:B:1157:LEU:HD22	1.48	0.93
2:B:1210:ARG:HG3	2:B:1280:VAL:CA	1.95	0.92
2:B:186:ILE:O	2:B:190:GLN:HB3	1.69	0.92
2:B:116:HIS:CD2	2:B:122:ILE:CA	2.52	0.92
2:B:226:ILE:HA	2:B:229:LEU:CG	2.00	0.91
2:B:556:ASN:O	2:B:595:HIS:NE2	2.00	0.91
2:B:557:ARG:CB	2:B:595:HIS:CD2	2.50	0.91
2:B:1236:LEU:HD22	2:B:1310:ILE:CG1	2.00	0.91
2:B:131:LYS:HG2	2:B:132:TYR:CD1	2.06	0.91
2:B:1243:GLU:HB3	2:B:1246:LYS:NZ	1.86	0.91



	A 4 ama 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:1130:LYS:O	2:B:1131:TYR:HD1	1.53	0.90
2:B:1236:LEU:HD22	2:B:1310:ILE:HG13	1.52	0.90
2:B:53:PHE:CD1	2:B:54:ASP:O	2.23	0.90
2:B:116:HIS:HB2	2:B:120:GLY:O	1.71	0.90
2:B:226:ILE:CG2	2:B:229:LEU:HD21	2.02	0.90
2:B:307:ARG:HH22	2:B:323:LYS:HE2	1.35	0.90
2:B:197:GLU:OE1	2:B:197:GLU:N	2.02	0.90
2:B:340:ARG:NE	2:B:347:TYR:CE2	2.35	0.90
2:B:297:SER:HA	2:B:300:ILE:CG2	2.01	0.89
2:B:340:ARG:NH2	2:B:347:TYR:CZ	2.40	0.89
2:B:978:ILE:CG1	2:B:1236:LEU:CD1	2.51	0.89
2:B:446:PHE:HE1	2:B:478:PHE:HD1	1.10	0.89
1:A:43:G:O2'	2:B:363:ILE:HD12	1.72	0.89
2:B:195:LEU:HD13	2:B:289:LEU:HD12	0.89	0.89
2:B:375:PHE:CD2	2:B:376:ILE:HG23	2.08	0.89
2:B:193:ASN:ND2	2:B:201:ILE:O	2.06	0.88
2:B:202:ASN:HB3	2:B:230:PRO:HG3	1.52	0.88
2:B:1297:HIS:CB	2:B:1327:PHE:HZ	1.84	0.88
2:B:523:GLU:OE2	2:B:588:ASN:ND2	2.06	0.88
2:B:1139:VAL:CG1	2:B:1166:ILE:C	2.41	0.88
2:B:1210:ARG:CG	2:B:1280:VAL:CG1	2.42	0.88
1:A:58:G:C2'	2:B:457:ARG:HB2	2.02	0.88
2:B:316:PRO:O	2:B:320:SER:N	2.07	0.88
2:B:1228:LEU:CB	2:B:1233:VAL:HG22	2.04	0.88
2:B:450:TYR:CD2	2:B:491:PHE:CE1	2.62	0.88
2:B:362:TYR:CD2	2:B:372:PHE:CE2	2.62	0.88
2:B:841:ILE:CD1	2:B:900:LEU:CD2	2.51	0.88
1:A:14:A:O2'	2:B:464:TRP:CZ2	2.28	0.87
2:B:338:LEU:CD1	2:B:386:THR:HB	2.04	0.87
2:B:1245:LEU:CD2	2:B:1252:ASN:OD1	2.18	0.87
2:B:553:PHE:HE2	2:B:559:VAL:HG11	1.39	0.87
2:B:569:PHE:O	2:B:574:CYS:N	2.07	0.87
2:B:1105:PHE:O	2:B:1137:PRO:HB3	1.74	0.87
2:B:516:GLU:O	2:B:520:VAL:HG23	1.74	0.87
2:B:491:PHE:HE2	3:C:16:DT:H1'	1.39	0.87
2:B:601:ILE:HD12	2:B:607:LEU:HD21	0.88	0.87
2:B:1270:ILE:HD13	2:B:1273:ILE:HD13	1.57	0.87
2:B:520:VAL:CG2	2:B:591:LEU:HD21	1.93	0.87
2:B:603:ASP:OD1	2:B:606:PHE:CB	2.23	0.87
2:B:1148:LYS:HE2	2:B:1189:GLU:CB	2.04	0.87
2:B:841:ILE:CD1	2:B:900:LEU:CG	2.52	0.86



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:494:ARG:HH11	2:B:494:ARG:HG2	1.39	0.86
2:B:518:PHE:CZ	2:B:679:ILE:HG21	2.10	0.86
2:B:1348:ILE:HD12	2:B:1359:ARG:HH11	1.10	0.86
2:B:6:SER:OG	2:B:21:ILE:HD11	1.75	0.86
2:B:859:ARG:HE	2:B:860:SER:HG	1.18	0.86
2:B:1237:TYR:HA	2:B:1242:TYR:HE1	1.40	0.86
2:B:107:VAL:HG22	2:B:1131:TYR:CZ	2.11	0.86
2:B:452:VAL:O	2:B:465:MET:HB3	1.75	0.86
2:B:1269:ILE:HG22	2:B:1273:ILE:CG2	2.06	0.86
2:B:1139:VAL:HG11	2:B:1165:GLY:O	1.75	0.86
2:B:297:SER:CA	2:B:300:ILE:HG22	2.04	0.86
2:B:841:ILE:HD13	2:B:900:LEU:HG	1.55	0.86
2:B:121:ASN:OD1	2:B:124:ASP:N	2.07	0.86
2:B:340:ARG:CZ	2:B:347:TYR:CD2	2.58	0.86
2:B:1224:ASN:ND2	2:B:1280:VAL:CG2	2.38	0.86
2:B:282:ILE:HG22	2:B:286:TYR:CD1	2.08	0.85
2:B:978:ILE:HD11	2:B:1236:LEU:HD12	1.51	0.85
2:B:1204:PHE:HD2	2:B:1342:VAL:HG11	0.69	0.85
2:B:279:LEU:O	2:B:282:ILE:O	1.92	0.85
2:B:453:GLY:HA2	2:B:464:TRP:CD1	2.10	0.85
2:B:761:ILE:HD13	2:B:931:VAL:HG12	1.57	0.85
2:B:1203:LEU:HD11	2:B:1211:LYS:HG2	1.58	0.85
2:B:338:LEU:HD13	2:B:386:THR:HB	1.57	0.85
2:B:511:HIS:O	2:B:593:THR:CG2	2.24	0.85
2:B:1148:LYS:HE2	2:B:1189:GLU:HG3	1.58	0.85
2:B:135:ILE:HD11	2:B:138:LEU:HD23	1.59	0.85
2:B:206:VAL:HG12	2:B:228:GLN:CG	2.06	0.85
2:B:520:VAL:HG21	2:B:591:LEU:HD23	0.88	0.85
2:B:1312:LEU:HD11	2:B:1326:TYR:HE1	1.41	0.85
1:A:61:C:P	2:B:460:SER:OG	2.34	0.84
2:B:107:VAL:CG2	2:B:1131:TYR:OH	2.25	0.84
2:B:518:PHE:HZ	2:B:679:ILE:HG23	1.41	0.84
2:B:495:MET:HB3	3:C:17:DA:C2'	2.06	0.84
2:B:516:GLU:CG	2:B:593:THR:OG1	2.26	0.84
2:B:545:LYS:HZ1	2:B:690:ASN:ND2	1.76	0.84
2:B:885:GLN:O	2:B:889:ALA:N	2.10	0.84
2:B:186:ILE:O	2:B:190:GLN:CB	2.25	0.84
2:B:1139:VAL:CB	2:B:1166:ILE:C	2.45	0.84
2:B:1203:LEU:HD21	2:B:1211:LYS:CD	2.03	0.84
2:B:518:PHE:CZ	2:B:679:ILE:HG22	2.11	0.84
2:B:720:LEU:CD1	2:B:724:ILE:HG13	2.07	0.84



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:556:ASN:C	2:B:595:HIS:CE1	2.50	0.84
2:B:564:LEU:HD23	2:B:569:PHE:HE2	1.41	0.83
2:B:841:ILE:HD11	2:B:900:LEU:CD2	2.08	0.83
2:B:6:SER:N	2:B:21:ILE:HD11	1.93	0.83
2:B:495:MET:CB	3:C:17:DA:H2"	2.08	0.83
2:B:787:GLY:HA3	2:B:891:LEU:CD2	2.07	0.83
2:B:6:SER:O	2:B:21:ILE:CG1	2.25	0.83
2:B:859:ARG:HG3	2:B:859:ARG:HH11	1.41	0.83
2:B:282:ILE:HG22	2:B:286:TYR:CE1	2.14	0.83
2:B:245:SER:HB3	2:B:296:LEU:CD2	1.93	0.83
2:B:495:MET:CB	3:C:17:DA:C2'	2.56	0.83
2:B:1120:ILE:HD11	2:B:1137:PRO:CD	2.09	0.82
2:B:1148:LYS:HE2	2:B:1189:GLU:CG	2.09	0.82
1:A:43:G:O2'	2:B:363:ILE:CD1	2.27	0.82
2:B:1204:PHE:CE1	2:B:1347:LEU:CD1	2.22	0.82
2:B:1224:ASN:HD22	2:B:1280:VAL:HG21	1.40	0.82
2:B:1361:ASP:OD1	2:B:1363:SER:OG	1.96	0.82
2:B:720:LEU:O	2:B:720:LEU:HD12	1.78	0.82
2:B:841:ILE:HD11	2:B:900:LEU:HG	1.59	0.82
2:B:859:ARG:HD2	2:B:859:ARG:O	1.79	0.82
2:B:1287:LEU:HD12	2:B:1287:LEU:O	1.78	0.82
2:B:317:LEU:CD2	2:B:414:ILE:HD12	2.10	0.82
2:B:1297:HIS:HB3	2:B:1327:PHE:HZ	1.44	0.82
2:B:521:TYR:CE1	2:B:684:LYS:HG2	2.15	0.82
2:B:839:ASP:OD2	2:B:864:ARG:HD3	1.80	0.81
2:B:386:THR:OG1	2:B:389:LEU:HB2	1.80	0.81
2:B:978:ILE:CG1	2:B:1236:LEU:HD11	2.08	0.81
2:B:53:PHE:CE1	2:B:54:ASP:O	2.33	0.81
2:B:491:PHE:CE2	3:C:16:DT:H1'	2.15	0.81
2:B:597:LEU:HD12	2:B:607:LEU:CD1	2.10	0.81
2:B:668:ASN:CG	2:B:680:LEU:CB	2.47	0.81
2:B:1243:GLU:HB3	2:B:1246:LYS:HE2	1.60	0.81
2:B:379:ILE:HD12	2:B:379:ILE:H	1.45	0.81
2:B:841:ILE:HD11	2:B:900:LEU:CG	2.11	0.81
2:B:1210:ARG:CG	2:B:1280:VAL:CB	2.58	0.80
2:B:1348:ILE:HD12	2:B:1359:ARG:HH12	1.41	0.80
1:A:60:C:H5"	2:B:455:LEU:O	1.81	0.80
2:B:194:GLN:N	2:B:194:GLN:OE1	2.15	0.80
2:B:478:PHE:CE2	2:B:482:VAL:HG21	2.16	0.80
2:B:1139:VAL:CG1	2:B:1167:THR:HA	2.11	0.80
2:B:208:ALA:O	2:B:212:LEU:HB2	1.81	0.80



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:362:TYR:CD2	2:B:372:PHE:HD2	1.77	0.80
2:B:545:LYS:NZ	2:B:690:ASN:ND2	2.29	0.80
2:B:131:LYS:HG2	2:B:132:TYR:HD1	1.44	0.80
2:B:294:LYS:NZ	2:B:295:ASN:OD1	2.14	0.80
2:B:839:ASP:OD1	2:B:840:ALA:N	2.15	0.80
2:B:18:TRP:HE1	2:B:50:ALA:N	1.76	0.80
2:B:354:GLN:CB	2:B:361:GLY:CA	2.57	0.80
2:B:362:TYR:CE2	2:B:372:PHE:CE2	2.70	0.79
1:A:61:C:P	2:B:460:SER:HG	2.05	0.79
2:B:334:LEU:CD1	2:B:338:LEU:HD11	2.12	0.79
2:B:369:GLN:O	2:B:373:TYR:HD2	1.64	0.79
2:B:554:LYS:CB	2:B:604:LYS:NZ	2.44	0.79
2:B:591:LEU:HB3	2:B:594:TYR:HB3	1.64	0.79
2:B:520:VAL:CG1	2:B:553:PHE:CD1	2.65	0.79
2:B:265:GLN:O	2:B:271:TYR:CD1	2.35	0.79
2:B:379:ILE:HG22	2:B:383:MET:SD	2.22	0.79
2:B:1108:GLU:O	2:B:1134:PHE:HE2	1.64	0.79
2:B:282:ILE:CG2	2:B:286:TYR:HE1	1.92	0.79
2:B:1148:LYS:CD	2:B:1157:LEU:HD22	2.11	0.79
2:B:189:VAL:O	2:B:193:ASN:N	2.16	0.79
2:B:317:LEU:HD23	2:B:414:ILE:HD12	1.62	0.79
2:B:356:LYS:O	2:B:357:ASN:HB2	1.81	0.79
2:B:392:LYS:HB3	2:B:397:ASP:O	1.82	0.79
2:B:1139:VAL:CG1	2:B:1167:THR:CA	2.54	0.79
2:B:317:LEU:O	2:B:320:SER:OG	2.00	0.79
2:B:967:ARG:CB	2:B:972:PHE:O	2.30	0.79
2:B:307:ARG:NH2	2:B:323:LYS:HE2	1.97	0.79
2:B:1270:ILE:CA	2:B:1273:ILE:CG1	2.53	0.79
2:B:195:LEU:HD12	2:B:289:LEU:HD12	1.63	0.79
2:B:282:ILE:HG23	2:B:286:TYR:CE1	2.18	0.79
2:B:762:GLU:CD	2:B:990:ASN:HD21	1.85	0.79
2:B:131:LYS:HD3	2:B:132:TYR:CE1	2.15	0.78
2:B:720:LEU:HD12	2:B:724:ILE:HG13	1.63	0.78
2:B:1229:PRO:O	2:B:1233:VAL:HG23	1.81	0.78
2:B:591:LEU:CD1	2:B:594:TYR:HB2	2.13	0.78
2:B:1139:VAL:HG21	2:B:1165:GLY:CA	2.13	0.78
2:B:182:ASP:OD1	2:B:209:LYS:HB2	1.84	0.78
2:B:887:LEU:CB	2:B:892:ILE:HD11	2.14	0.78
2:B:362:TYR:HD2	2:B:372:PHE:CD2	1.98	0.78
2:B:195:LEU:HD13	2:B:289:LEU:HD13	1.59	0.78
2:B:316:PRO:HA	2:B:319:ALA:HB3	1.66	0.78



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:493:GLU:O	2:B:496:THR:HG23	1.83	0.78
2:B:545:LYS:HZ1	2:B:690:ASN:CB	1.96	0.78
2:B:686:ASP:CB	2:B:690:ASN:HA	2.13	0.78
2:B:840:ALA:O	2:B:864:ARG:NH1	2.17	0.78
2:B:226:ILE:HA	2:B:229:LEU:HD21	1.66	0.77
2:B:668:ASN:ND2	2:B:680:LEU:HB3	1.99	0.77
2:B:378:PRO:HG2	2:B:379:ILE:CD1	2.12	0.77
2:B:842:VAL:HG12	2:B:854:ASN:OD1	1.83	0.77
2:B:520:VAL:HG11	2:B:553:PHE:HD1	1.50	0.77
2:B:18:TRP:O	2:B:48:ILE:HD12	1.83	0.77
2:B:375:PHE:HD2	2:B:376:ILE:HG23	1.47	0.77
2:B:553:PHE:CD2	2:B:559:VAL:CG2	2.61	0.77
2:B:1270:ILE:HD13	2:B:1273:ILE:HD11	1.64	0.77
2:B:1297:HIS:CG	2:B:1327:PHE:CE2	2.72	0.77
2:B:1245:LEU:HD13	2:B:1252:ASN:HD21	1.50	0.77
2:B:270:THR:O	2:B:274:ASP:CB	2.31	0.77
2:B:315:ALA:HB1	2:B:418:GLU:OE2	1.84	0.76
2:B:350:ILE:HD11	2:B:375:PHE:CZ	2.20	0.76
2:B:359:TYR:CE1	2:B:363:ILE:HG13	2.20	0.76
2:B:564:LEU:HD23	2:B:569:PHE:CE2	2.20	0.76
2:B:567:ASP:O	2:B:571:LYS:HB2	1.84	0.76
2:B:1210:ARG:HG2	2:B:1280:VAL:HG13	0.79	0.76
1:A:51:A:HO2'	2:B:1134:PHE:HE1	0.77	0.76
2:B:686:ASP:HB2	2:B:690:ASN:HD22	1.48	0.76
2:B:1069:THR:OG1	2:B:1071:GLU:HG3	1.85	0.76
2:B:1325:LYS:NZ	2:B:1330:THR:HG1	1.83	0.76
2:B:1327:PHE:HD2	2:B:1328:ASP:H	1.34	0.76
1:A:14:A:O2'	2:B:464:TRP:HZ2	1.68	0.76
2:B:495:MET:HB3	3:C:17:DA:H2"	1.62	0.76
2:B:1130:LYS:O	2:B:1131:TYR:CD1	2.38	0.76
2:B:398:LEU:HG	2:B:399:LEU:HG	1.67	0.76
2:B:520:VAL:HG23	2:B:591:LEU:CD2	2.09	0.76
2:B:567:ASP:O	2:B:571:LYS:CB	2.34	0.76
2:B:1325:LYS:CB	2:B:1330:THR:HA	2.16	0.76
2:B:966:PHE:CE1	2:B:970:PHE:CD2	2.74	0.76
2:B:193:ASN:OD1	2:B:201:ILE:N	2.17	0.76
2:B:350:ILE:CD1	2:B:375:PHE:HZ	1.98	0.75
2:B:1218:GLY:O	2:B:1337:THR:O	2.03	0.75
2:B:1270:ILE:HA	2:B:1273:ILE:HD11	1.65	0.75
2:B:48:ILE:HD12	2:B:49:GLY:H	1.47	0.75
2:B:841:ILE:HD13	2:B:900:LEU:CG	2.15	0.75



	A de pagemi	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:135:ILE:CD1	2:B:138:LEU:HD23	2.16	0.75
2:B:226:ILE:CA	2:B:229:LEU:HG	2.17	0.75
2:B:842:VAL:HG21	2:B:847:LEU:CD2	2.16	0.75
2:B:966:PHE:CD1	2:B:970:PHE:CE2	2.75	0.75
2:B:457:ARG:O	2:B:457:ARG:HG3	1.87	0.75
2:B:245:SER:HB2	2:B:296:LEU:HD21	1.67	0.75
2:B:724:ILE:HD13	2:B:737:ILE:HG22	1.67	0.75
2:B:873:GLU:O	2:B:877:LYS:HG2	1.87	0.75
2:B:566:GLU:O	2:B:571:LYS:HG2	1.85	0.75
2:B:1284:ASP:OD1	2:B:1285:ALA:N	2.20	0.75
2:B:516:GLU:O	2:B:519:THR:HG22	1.86	0.75
2:B:1210:ARG:HG3	2:B:1280:VAL:HG22	1.67	0.75
2:B:495:MET:CB	3:C:17:DA:C4'	2.64	0.74
2:B:279:LEU:HD21	2:B:284:ASP:HA	1.68	0.74
2:B:354:GLN:HA	2:B:361:GLY:HA3	1.69	0.74
2:B:1308:ASN:OD1	2:B:1327:PHE:HB3	1.88	0.74
2:B:520:VAL:CG1	2:B:553:PHE:HD1	1.98	0.74
2:B:328:HIS:CE1	2:B:399:LEU:CB	2.71	0.74
2:B:1119:LEU:HD13	2:B:1119:LEU:N	2.00	0.74
2:B:131:LYS:CD	2:B:132:TYR:HE1	1.98	0.74
2:B:1210:ARG:HG2	2:B:1280:VAL:CB	2.17	0.74
2:B:121:ASN:HD21	2:B:124:ASP:CG	1.91	0.74
2:B:1148:LYS:HE2	2:B:1189:GLU:HB2	1.69	0.74
2:B:761:ILE:HG13	2:B:761:ILE:O	1.87	0.74
1:A:89:G:N1	2:B:1272:GLN:OE1	2.21	0.74
2:B:393:LEU:HD23	2:B:394:ASN:N	2.03	0.74
2:B:668:ASN:HD21	2:B:680:LEU:CG	2.01	0.74
2:B:485:GLY:HA2	2:B:488:ALA:HB3	1.70	0.74
2:B:978:ILE:HG13	2:B:1236:LEU:CD1	2.17	0.74
2:B:275:LEU:O	2:B:279:LEU:N	2.14	0.73
2:B:853:ASP:CA	2:B:896:LYS:HD2	2.16	0.73
2:B:1359:ARG:NH1	2:B:1359:ARG:HG2	1.95	0.73
2:B:178:ASN:HA	2:B:299:ALA:HB2	1.68	0.73
2:B:823:TYR:CE2	2:B:858:THR:HG21	2.23	0.73
2:B:1120:ILE:HD11	2:B:1137:PRO:CG	2.18	0.73
2:B:178:ASN:CA	2:B:299:ALA:HB2	2.17	0.73
2:B:446:PHE:HE1	2:B:478:PHE:CD1	1.88	0.73
2:B:1343:LEU:N	2:B:1343:LEU:HD23	2.03	0.73
2:B:21:ILE:O	2:B:21:ILE:HD12	1.88	0.73
2:B:302:LEU:O	2:B:305:ILE:HG12	1.89	0.73
2:B:312:ILE:HD12	2:B:312:ILE:N	2.03	0.73



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:686:ASP:HB2	2:B:690:ASN:ND2	2.03	0.73
2:B:1207:GLU:OE2	2:B:1210:ARG:NH1	2.22	0.73
2:B:1232:TYR:OH	2:B:1268:GLU:HB3	1.88	0.73
2:B:724:ILE:O	2:B:727:LEU:HG	1.89	0.73
2:B:852:ILE:O	2:B:896:LYS:HD2	1.88	0.73
2:B:1204:PHE:CZ	2:B:1347:LEU:HD12	2.16	0.73
2:B:841:ILE:O	2:B:870:VAL:HG13	1.89	0.73
2:B:1065:THR:OG1	2:B:1071:GLU:O	2.06	0.73
2:B:1203:LEU:CG	2:B:1211:LYS:HD3	2.18	0.73
2:B:359:TYR:HA	2:B:362:TYR:HB3	1.69	0.72
2:B:495:MET:CB	3:C:17:DA:O4'	2.36	0.72
2:B:569:PHE:CE1	2:B:578:VAL:HG11	2.23	0.72
2:B:949:LEU:HD12	2:B:950:ILE:N	2.03	0.72
2:B:1271:GLU:HA	2:B:1274:SER:HB2	1.71	0.72
2:B:307:ARG:HH22	2:B:323:LYS:CE	2.02	0.72
2:B:312:ILE:HD12	2:B:312:ILE:H	1.51	0.72
2:B:1236:LEU:CB	2:B:1310:ILE:HD11	2.19	0.72
2:B:559:VAL:CA	2:B:563:GLN:OE1	2.36	0.72
2:B:1148:LYS:CE	2:B:1189:GLU:HG3	2.19	0.72
2:B:116:HIS:NE2	2:B:122:ILE:HD12	2.04	0.72
2:B:1232:TYR:OH	2:B:1268:GLU:OE1	2.05	0.72
2:B:1290:VAL:HG22	2:B:1331:ILE:CD1	2.19	0.72
2:B:1229:PRO:HD2	2:B:1232:TYR:HD2	1.54	0.72
2:B:1237:TYR:HA	2:B:1242:TYR:CE1	2.24	0.72
2:B:78:ARG:NH1	2:B:162:ILE:O	2.23	0.72
2:B:307:ARG:NH2	2:B:323:LYS:NZ	2.37	0.72
2:B:1120:ILE:CD1	2:B:1137:PRO:CD	2.67	0.72
2:B:379:ILE:HD12	2:B:379:ILE:N	2.04	0.72
2:B:966:PHE:HE1	2:B:970:PHE:HE2	1.35	0.72
2:B:1269:ILE:HG22	2:B:1273:ILE:HG23	1.71	0.72
2:B:265:GLN:O	2:B:271:TYR:HB2	1.90	0.72
2:B:1297:HIS:CB	2:B:1327:PHE:CZ	2.72	0.72
2:B:332:LEU:HD11	2:B:359:TYR:HE2	1.54	0.72
2:B:1229:PRO:CG	2:B:1232:TYR:HD2	2.02	0.72
2:B:1245:LEU:HD22	2:B:1252:ASN:CG	2.08	0.72
2:B:6:SER:CB	2:B:21:ILE:CD1	2.67	0.71
2:B:116:HIS:NE2	2:B:122:ILE:CG1	2.52	0.71
2:B:664:ARG:NH1	2:B:664:ARG:HG3	2.05	0.71
2:B:1269:ILE:O	2:B:1273:ILE:N	2.21	0.71
2:B:455:LEU:CD2	2:B:473:ILE:CD1	2.61	0.71
2:B:1270:ILE:O	2:B:1274:SER:N	2.21	0.71



	A de pagenn	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:380:LEU:HA	2:B:383:MET:HG3	1.72	0.71
2:B:668:ASN:CG	2:B:680:LEU:HB3	2.11	0.71
2:B:1277:SER:OG	2:B:1287:LEU:HD22	1.91	0.71
1:A:83:C:H42	1:A:95:G:H1	1.36	0.71
2:B:861:ASP:OD2	2:B:861:ASP:N	2.23	0.71
2:B:1139:VAL:HA	2:B:1167:THR:HA	1.73	0.71
2:B:307:ARG:HH21	2:B:323:LYS:NZ	1.88	0.71
2:B:348:LYS:HA	2:B:352:PHE:HD1	1.56	0.71
2:B:489:GLN:HE21	2:B:493:GLU:CD	1.93	0.71
2:B:70:ARG:HH22	2:B:462:PHE:HE2	1.38	0.71
2:B:203:ALA:O	2:B:206:VAL:HG13	1.89	0.71
2:B:1325:LYS:HB2	2:B:1329:THR:O	1.91	0.71
2:B:315:ALA:O	2:B:319:ALA:HB2	1.91	0.71
2:B:465:MET:CE	2:B:482:VAL:HG22	2.21	0.71
2:B:1210:ARG:HG3	2:B:1280:VAL:CB	2.21	0.71
2:B:107:VAL:HG22	2:B:1131:TYR:HH	1.56	0.71
2:B:307:ARG:NH2	2:B:323:LYS:CE	2.54	0.71
2:B:1139:VAL:CG1	2:B:1167:THR:HG22	2.21	0.71
2:B:45:LYS:HB3	2:B:1091:GLN:HE22	1.56	0.70
2:B:174:LEU:HD23	2:B:302:LEU:HD21	1.73	0.70
2:B:870:VAL:CG1	2:B:871:PRO:HD2	2.03	0.70
2:B:961:LYS:NZ	2:B:965:ASP:OD2	2.21	0.70
2:B:1312:LEU:HA	2:B:1324:PHE:CE2	2.26	0.70
1:A:44:U:H5'	2:B:363:ILE:HD13	1.73	0.70
2:B:201:ILE:HD11	2:B:232:GLU:OE1	1.88	0.70
2:B:1114:ARG:NH1	4:D:9:DA:H5'	2.06	0.70
2:B:495:MET:HB2	3:C:17:DA:C2'	2.21	0.70
2:B:963:VAL:HG21	2:B:990:ASN:OD1	1.91	0.70
2:B:992:VAL:O	2:B:996:ALA:N	2.21	0.70
2:B:1105:PHE:O	2:B:1137:PRO:CB	2.39	0.70
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.74	0.70
2:B:1205:GLU:OE1	2:B:1359:ARG:NH2	2.24	0.70
2:B:1270:ILE:CD1	2:B:1273:ILE:HD11	2.22	0.70
2:B:317:LEU:HD23	2:B:414:ILE:CD1	2.21	0.70
2:B:225:LEU:HD13	2:B:229:LEU:HD23	1.72	0.70
2:B:495:MET:SD	3:C:17:DA:H1'	2.30	0.70
2:B:668:ASN:ND2	2:B:680:LEU:CB	2.54	0.70
2:B:851:SER:O	2:B:855:LYS:HG3	1.91	0.70
2:B:1269:ILE:HG22	2:B:1273:ILE:HG21	1.72	0.70
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.73	0.70
2:B:478:PHE:HE2	2:B:482:VAL:CG2	2.02	0.70



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:492:ILE:HD12	2:B:625:LEU:O	1.91	0.70
2:B:279:LEU:HD23	2:B:284:ASP:HA	1.73	0.70
2:B:1297:HIS:ND1	2:B:1327:PHE:CZ	2.56	0.70
2:B:664:ARG:HG3	2:B:664:ARG:HH11	1.55	0.69
2:B:1348:ILE:CD1	2:B:1359:ARG:HH11	1.99	0.69
2:B:518:PHE:CE2	2:B:683:LEU:HD11	2.26	0.69
2:B:841:ILE:HD11	2:B:900:LEU:HD21	1.74	0.69
2:B:1206:LEU:HD12	2:B:1206:LEU:O	1.91	0.69
2:B:442:LYS:HE2	2:B:476:TRP:HA	1.74	0.69
2:B:522:ASN:HA	2:B:525:THR:OG1	1.93	0.69
2:B:686:ASP:HB3	2:B:689:ALA:O	1.92	0.69
2:B:1139:VAL:HG21	2:B:1165:GLY:C	2.12	0.69
1:A:58:G:C5'	2:B:457:ARG:HH11	2.05	0.69
2:B:956:ILE:HD11	2:B:998:ILE:HD13	1.75	0.69
2:B:245:SER:OG	2:B:296:LEU:CD2	2.39	0.69
2:B:359:TYR:O	2:B:362:TYR:HB3	1.91	0.69
2:B:187:GLN:O	2:B:191:THR:HG23	1.92	0.69
2:B:328:HIS:CD2	2:B:399:LEU:CB	2.74	0.69
1:A:61:C:OP1	2:B:460:SER:OG	2.11	0.69
2:B:556:ASN:O	2:B:595:HIS:CE1	2.46	0.69
2:B:1204:PHE:CE1	2:B:1347:LEU:CG	2.76	0.69
2:B:188:LEU:HD11	2:B:238:PHE:CE1	2.28	0.69
2:B:489:GLN:HG2	2:B:493:GLU:OE1	1.92	0.69
2:B:790:GLU:CD	2:B:889:ALA:HA	2.13	0.69
2:B:1245:LEU:HD12	2:B:1245:LEU:C	2.13	0.69
2:B:1281:ILE:HG22	2:B:1283:ALA:HB2	1.74	0.69
2:B:369:GLN:OE1	2:B:400:ARG:NH1	2.24	0.68
2:B:5:TYR:OH	2:B:754:HIS:O	2.10	0.68
2:B:1239:ALA:HB1	2:B:1306:ALA:HB2	1.76	0.68
2:B:328:HIS:CG	2:B:399:LEU:HB3	2.29	0.68
2:B:563:GLN:O	2:B:567:ASP:HB2	1.93	0.68
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.26	0.68
2:B:1297:HIS:HB3	2:B:1327:PHE:CZ	2.28	0.68
1:A:43:G:HO2'	2:B:363:ILE:HD12	1.59	0.68
2:B:118:ILE:HG22	2:B:119:PHE:CE1	2.27	0.68
2:B:317:LEU:CD2	2:B:414:ILE:CD1	2.71	0.68
2:B:1204:PHE:HE1	2:B:1347:LEU:CG	2.06	0.68
1:A:77:A:OP1	2:B:721:HIS:CD2	2.46	0.68
2:B:6:SER:CA	2:B:21:ILE:HD11	2.23	0.68
2:B:885:GLN:CA	2:B:888:ASN:HB2	2.24	0.68
2:B:53:PHE:HD1	2:B:54:ASP:O	1.72	0.68



	A l O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:841:ILE:HD13	2:B:900:LEU:CD2	2.24	0.68
2:B:1065:THR:HB	2:B:1072:ILE:HA	1.75	0.68
2:B:1269:ILE:CG2	2:B:1273:ILE:CG2	2.71	0.67
2:B:1312:LEU:HA	2:B:1324:PHE:CD2	2.29	0.67
2:B:666:LEU:O	2:B:666:LEU:HD23	1.94	0.67
2:B:1271:GLU:O	2:B:1275:GLU:N	2.26	0.67
2:B:309:ASN:ND2	2:B:312:ILE:HD13	2.09	0.67
2:B:551:LEU:HD12	2:B:551:LEU:C	2.15	0.67
2:B:465:MET:HE1	2:B:482:VAL:HG22	1.76	0.67
2:B:1215:ALA:HB2	2:B:1221:GLN:HG3	1.74	0.67
2:B:18:TRP:N	2:B:49:GLY:O	2.27	0.67
2:B:143:VAL:O	2:B:425:ARG:NE	2.27	0.67
2:B:188:LEU:O	2:B:191:THR:OG1	2.13	0.67
2:B:296:LEU:O	2:B:300:ILE:N	2.22	0.67
2:B:524:LEU:O	2:B:524:LEU:HD23	1.94	0.67
2:B:565:LYS:HG2	2:B:578:VAL:HG12	1.77	0.67
2:B:1032:ALA:HA	2:B:1035:LYS:HB3	1.75	0.67
2:B:1324:PHE:O	2:B:1331:ILE:N	2.24	0.67
2:B:188:LEU:CD1	2:B:238:PHE:HE1	2.08	0.67
2:B:283:GLY:O	2:B:286:TYR:HD1	1.78	0.67
2:B:300:ILE:HD12	2:B:300:ILE:O	1.94	0.67
2:B:1229:PRO:CD	2:B:1232:TYR:HD2	2.06	0.67
2:B:1308:ASN:OD1	2:B:1327:PHE:CA	2.43	0.67
2:B:317:LEU:HB3	2:B:414:ILE:HD12	1.77	0.67
2:B:661:ARG:NH1	2:B:661:ARG:HG3	2.10	0.67
2:B:188:LEU:C	2:B:188:LEU:HD13	2.15	0.67
2:B:348:LYS:CG	2:B:352:PHE:HB2	2.25	0.67
2:B:1139:VAL:HG21	2:B:1165:GLY:HA3	1.75	0.67
2:B:597:LEU:O	2:B:601:ILE:HG12	1.95	0.67
2:B:1269:ILE:CG2	2:B:1273:ILE:HG23	2.25	0.67
2:B:895:ARG:HD2	2:B:895:ARG:C	2.15	0.66
2:B:1120:ILE:HD11	2:B:1137:PRO:HG3	1.76	0.66
2:B:1240:SER:HB3	2:B:1242:TYR:CE1	2.31	0.66
2:B:1308:ASN:OD1	2:B:1327:PHE:CB	2.43	0.66
2:B:229:LEU:HD12	2:B:229:LEU:C	2.15	0.66
2:B:393:LEU:HD23	2:B:393:LEU:C	2.16	0.66
2:B:591:LEU:HD13	2:B:594:TYR:HB2	1.76	0.66
2:B:857:LEU:C	2:B:857:LEU:HD23	2.15	0.66
2:B:1231:LYS:HD2	2:B:1265:TYR:OH	1.95	0.66
2:B:284:ASP:OD2	2:B:284:ASP:N	2.29	0.66
2:B:477:ASN:O	2:B:481:VAL:HG23	1.96	0.66



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:564:LEU:CD2	2:B:569:PHE:HE2	2.09	0.66
2:B:1210:ARG:HG3	2:B:1280:VAL:CG2	2.25	0.66
2:B:1276:PHE:CZ	2:B:1281:ILE:HD11	2.31	0.66
2:B:229:LEU:HD11	2:B:232:GLU:HB2	1.75	0.66
2:B:282:ILE:N	2:B:282:ILE:HD12	2.10	0.66
2:B:455:LEU:HD21	2:B:473:ILE:HG21	1.77	0.66
2:B:446:PHE:CZ	2:B:478:PHE:HE1	2.08	0.66
2:B:1229:PRO:HD2	2:B:1232:TYR:CD2	2.30	0.66
2:B:303:SER:O	2:B:306:LEU:O	2.14	0.66
2:B:554:LYS:CB	2:B:604:LYS:HZ3	2.06	0.66
2:B:115:ARG:HG3	2:B:116:HIS:HD1	1.60	0.65
2:B:495:MET:CG	3:C:17:DA:C1'	2.74	0.65
2:B:1204:PHE:CE2	2:B:1342:VAL:HG11	2.26	0.65
2:B:1207:GLU:OE1	2:B:1208:ASN:N	2.27	0.65
2:B:1226:LEU:HD13	2:B:1276:PHE:CG	2.30	0.65
2:B:1206:LEU:CB	2:B:1345:ALA:HB1	2.16	0.65
2:B:1229:PRO:HG2	2:B:1232:TYR:CD2	2.31	0.65
2:B:696:LEU:HD13	2:B:702:LEU:HD13	1.78	0.65
2:B:1120:ILE:CD1	2:B:1137:PRO:HG3	2.26	0.65
1:A:14:A:O2'	2:B:464:TRP:CH2	2.49	0.65
1:A:58:G:H5'	2:B:457:ARG:NH1	2.12	0.65
2:B:887:LEU:CA	2:B:892:ILE:HD11	2.27	0.65
2:B:1204:PHE:CD1	2:B:1347:LEU:HB2	2.31	0.65
2:B:6:SER:N	2:B:21:ILE:CD1	2.59	0.65
2:B:115:ARG:HG3	2:B:116:HIS:ND1	2.12	0.65
2:B:350:ILE:CD1	2:B:375:PHE:CZ	2.79	0.65
2:B:516:GLU:HG3	2:B:593:THR:CB	2.27	0.65
2:B:691:ARG:HB2	2:B:696:LEU:CD2	2.27	0.65
2:B:720:LEU:HD11	2:B:724:ILE:CD1	2.27	0.65
2:B:354:GLN:CA	2:B:361:GLY:HA3	2.26	0.65
2:B:1203:LEU:CD1	2:B:1211:LYS:HD3	2.21	0.65
2:B:1347:LEU:C	2:B:1347:LEU:HD23	2.16	0.65
2:B:553:PHE:HE2	2:B:559:VAL:CG1	2.08	0.65
2:B:602:LYS:O	2:B:602:LYS:HG3	1.97	0.65
2:B:6:SER:HB2	2:B:21:ILE:HD11	1.78	0.65
2:B:189:VAL:HG22	2:B:238:PHE:CZ	2.31	0.65
2:B:975:VAL:HG11	2:B:978:ILE:HG13	1.77	0.65
2:B:1308:ASN:OD1	2:B:1327:PHE:N	2.30	0.65
2:B:597:LEU:HD13	2:B:607:LEU:HD13	1.79	0.64
2:B:601:ILE:CD1	2:B:607:LEU:CD2	2.56	0.64
2:B:195:LEU:CD1	2:B:289:LEU:CD1	2.37	0.64



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:843:PRO:HD2	2:B:846:PHE:CD2	2.31	0.64
2:B:35:LEU:HB2	2:B:1358:THR:HG22	1.78	0.64
2:B:188:LEU:CD1	2:B:238:PHE:CE1	2.80	0.64
2:B:297:SER:OG	2:B:301:LEU:HD11	1.96	0.64
2:B:1270:ILE:C	2:B:1273:ILE:CG1	2.47	0.64
2:B:362:TYR:HD2	2:B:372:PHE:CE2	2.11	0.64
2:B:902:LYS:HG3	2:B:907:GLY:HA2	1.80	0.64
2:B:6:SER:HB2	2:B:21:ILE:CD1	2.27	0.64
2:B:466:THR:C	2:B:467:ARG:HG3	2.18	0.64
2:B:553:PHE:CE2	2:B:559:VAL:CB	2.79	0.64
2:B:1120:ILE:CD1	2:B:1137:PRO:HD3	2.28	0.64
2:B:6:SER:HB2	2:B:21:ILE:HG12	1.79	0.64
2:B:229:LEU:HD12	2:B:229:LEU:O	1.97	0.64
2:B:1269:ILE:O	2:B:1273:ILE:CG2	2.41	0.64
2:B:136:TYR:HE2	2:B:402:GLN:HB3	1.60	0.64
2:B:18:TRP:CD1	2:B:50:ALA:N	2.49	0.64
2:B:354:GLN:HA	2:B:361:GLY:CA	2.26	0.64
2:B:557:ARG:CA	2:B:595:HIS:HD2	1.72	0.64
1:A:56:U:O2	1:A:58:G:N2	2.31	0.64
2:B:861:ASP:O	2:B:864:ARG:HG2	1.98	0.64
2:B:513:LEU:O	2:B:517:TYR:N	2.28	0.64
2:B:851:SER:O	2:B:855:LYS:CG	2.46	0.64
1:A:41:A:H2'	1:A:42:A:H5"	1.80	0.63
2:B:131:LYS:HG2	2:B:132:TYR:CE1	2.33	0.63
2:B:167:HIS:HD2	2:B:169:LEU:HD12	1.63	0.63
2:B:184:LEU:O	2:B:187:GLN:N	2.30	0.63
2:B:334:LEU:HD13	2:B:338:LEU:HD11	1.80	0.63
2:B:1327:PHE:HD2	2:B:1328:ASP:N	1.95	0.63
2:B:521:TYR:HE1	2:B:684:LYS:HG2	1.60	0.63
2:B:665:LYS:O	2:B:669:GLY:N	2.32	0.63
2:B:334:LEU:HD13	2:B:338:LEU:CD1	2.28	0.63
2:B:1203:LEU:CD2	2:B:1211:LYS:CD	2.71	0.63
2:B:277:ASN:HB3	2:B:653:ARG:HE	1.62	0.63
2:B:379:ILE:CD1	2:B:379:ILE:H	2.10	0.63
2:B:594:TYR:HD2	2:B:594:TYR:O	1.80	0.63
2:B:668:ASN:HD21	2:B:680:LEU:CB	2.10	0.63
3:C:13:DA:H2'	3:C:14:DA:H8	1.62	0.63
2:B:188:LEU:O	2:B:188:LEU:HD22	1.97	0.63
2:B:495:MET:HG3	3:C:17:DA:C4'	2.29	0.63
2:B:859:ARG:HG3	2:B:859:ARG:NH1	2.11	0.63
2:B:1245:LEU:HD12	2:B:1245:LEU:O	1.99	0.63



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:48:A:H2'	1:A:49:A:C8	2.34	0.63
2:B:378:PRO:O	2:B:382:LYS:N	2.32	0.63
2:B:483:ASP:CB	2:B:486:ALA:HB3	2.18	0.63
2:B:591:LEU:HD12	2:B:594:TYR:HB2	1.79	0.63
2:B:1240:SER:OG	2:B:1307:GLU:HG2	1.98	0.63
1:A:63:U:OP2	2:B:69:ARG:NH2	2.32	0.63
2:B:524:LEU:HD11	2:B:548:ILE:HD12	1.80	0.63
2:B:36:GLY:HA3	2:B:1359:ARG:O	1.99	0.63
2:B:348:LYS:O	2:B:352:PHE:N	2.32	0.63
1:A:52:A:OP2	1:A:62:G:N2	2.32	0.62
2:B:491:PHE:HE2	3:C:16:DT:C1'	2.10	0.62
2:B:761:ILE:HD13	2:B:931:VAL:CG1	2.28	0.62
2:B:116:HIS:CD2	2:B:122:ILE:CG1	2.82	0.62
2:B:869:ASN:OD1	2:B:870:VAL:HG23	1.99	0.62
2:B:6:SER:HB2	2:B:21:ILE:CG1	2.29	0.62
2:B:423:LEU:HD13	2:B:437:ARG:HG3	1.81	0.62
2:B:93:VAL:O	2:B:152:ARG:NH1	2.33	0.62
2:B:94:ASP:HB2	2:B:152:ARG:HH11	1.63	0.62
2:B:282:ILE:HG22	2:B:283:GLY:N	2.15	0.62
2:B:495:MET:SD	3:C:17:DA:C1'	2.88	0.62
2:B:720:LEU:HD11	2:B:724:ILE:HG13	1.80	0.62
2:B:975:VAL:HG11	2:B:1236:LEU:CD1	2.29	0.62
2:B:1139:VAL:HG12	2:B:1167:THR:CG2	2.29	0.62
2:B:1243:GLU:HB3	2:B:1246:LYS:CD	2.29	0.62
2:B:316:PRO:O	2:B:319:ALA:HB3	2.00	0.62
2:B:520:VAL:HG13	2:B:553:PHE:CE1	2.33	0.62
2:B:572:ILE:O	2:B:572:ILE:HG22	1.99	0.62
2:B:591:LEU:HB3	2:B:594:TYR:CB	2.30	0.62
2:B:328:HIS:NE2	2:B:399:LEU:CB	2.63	0.62
2:B:859:ARG:HD2	2:B:859:ARG:C	2.20	0.62
2:B:1120:ILE:HD12	2:B:1137:PRO:HD3	1.82	0.62
2:B:83:GLN:O	2:B:87:SER:N	2.33	0.61
2:B:664:ARG:HH11	2:B:664:ARG:CG	2.13	0.61
2:B:1203:LEU:CD1	2:B:1211:LYS:HG2	2.28	0.61
1:A:67:C:OP1	2:B:739:GLN:NE2	2.32	0.61
2:B:181:VAL:HG21	2:B:209:LYS:HA	1.83	0.61
2:B:187:GLN:O	2:B:191:THR:CG2	2.48	0.61
2:B:545:LYS:NZ	2:B:690:ASN:CB	2.59	0.61
2:B:1106:SER:HB2	2:B:1135:ASP:O	2.00	0.61
2:B:1243:GLU:CB	2:B:1246:LYS:HE2	2.28	0.61
2:B:1273:ILE:HG13	2:B:1274:SER:N	2.14	0.61



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:189:VAL:CG2	2:B:238:PHE:HZ	1.92	0.61
2:B:723:HIS:NE2	2:B:934:ILE:HD11	2.15	0.61
2:B:348:LYS:HG3	2:B:352:PHE:CB	2.30	0.61
2:B:358:GLY:O	2:B:362:TYR:N	2.32	0.61
2:B:850:ASP:O	2:B:855:LYS:CD	2.48	0.61
2:B:1270:ILE:HA	2:B:1273:ILE:HD13	1.81	0.61
2:B:165:ARG:NH2	2:B:446:PHE:O	2.34	0.61
2:B:297:SER:C	2:B:300:ILE:HG22	2.21	0.61
2:B:720:LEU:HD11	2:B:724:ILE:HD11	1.82	0.61
2:B:1348:ILE:HD11	2:B:1357:GLU:CD	2.21	0.61
2:B:247:GLY:O	2:B:248:LEU:HD23	2.00	0.61
2:B:886:LEU:N	2:B:886:LEU:HD23	2.15	0.61
2:B:1239:ALA:HB1	2:B:1306:ALA:CB	2.30	0.61
2:B:282:ILE:HG22	2:B:283:GLY:O	2.01	0.61
2:B:557:ARG:N	2:B:595:HIS:CD2	2.47	0.61
2:B:748:VAL:HG12	2:B:753:ARG:HA	1.82	0.61
2:B:1139:VAL:HG12	2:B:1167:THR:CB	2.29	0.61
2:B:182:ASP:OD1	2:B:209:LYS:CB	2.48	0.61
2:B:518:PHE:CE1	2:B:679:ILE:HG21	2.36	0.61
2:B:1257:LEU:O	2:B:1261:GLN:N	2.31	0.61
2:B:359:TYR:CE1	2:B:363:ILE:HD11	2.37	0.60
2:B:502:LEU:HD23	2:B:505:GLU:HG3	1.84	0.60
2:B:354:GLN:CA	2:B:361:GLY:CA	2.78	0.60
2:B:647:VAL:O	2:B:651:LEU:N	2.34	0.60
2:B:841:ILE:CD1	2:B:900:LEU:HD23	2.30	0.60
2:B:188:LEU:HD11	2:B:238:PHE:HE1	1.64	0.60
2:B:188:LEU:HD13	2:B:189:VAL:N	2.16	0.60
2:B:842:VAL:HG21	2:B:847:LEU:HD21	1.83	0.60
2:B:1109:SER:OG	3:C:9:DC:OP2	2.16	0.60
2:B:51:LEU:O	2:B:52:LEU:HD22	2.01	0.60
2:B:253:LYS:O	2:B:257:ASP:N	2.33	0.60
2:B:369:GLN:O	2:B:373:TYR:CD2	2.51	0.60
2:B:395:ARG:C	2:B:396:GLU:HG3	2.21	0.60
2:B:877:LYS:HG3	2:B:878:LYS:H	1.66	0.60
1:A:27:G:H1'	2:B:129:HIS:CD2	2.36	0.60
2:B:553:PHE:CE2	2:B:559:VAL:HG11	2.28	0.60
2:B:809:GLU:HA	2:B:812:TYR:HB3	1.82	0.60
1:A:43:G:N2	2:B:360:ALA:HB2	2.17	0.60
2:B:90:MET:HG2	2:B:98:PHE:CE1	2.36	0.60
2:B:520:VAL:HG13	2:B:553:PHE:CD1	2.36	0.60
2:B:889:ALA:O	2:B:890:LYS:HB2	2.01	0.60



	A 1 O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:901:THR:O	2:B:905:ARG:NH2	2.34	0.60
2:B:1224:ASN:HD22	2:B:1280:VAL:CG2	2.10	0.60
2:B:178:ASN:CA	2:B:299:ALA:CB	2.75	0.60
2:B:841:ILE:HD13	2:B:900:LEU:HD23	1.83	0.60
2:B:1063:ILE:CG2	2:B:1074:TRP:O	2.43	0.60
1:A:42:A:O2'	1:A:43:G:OP1	2.18	0.59
2:B:197:GLU:H	2:B:197:GLU:CD	1.98	0.59
2:B:850:ASP:O	2:B:855:LYS:HG3	2.01	0.59
2:B:279:LEU:CD2	2:B:284:ASP:CA	2.76	0.59
2:B:721:HIS:CE1	2:B:738:LEU:HD21	2.37	0.59
2:B:68:ALA:HA	2:B:71:ARG:HB3	1.84	0.59
2:B:118:ILE:CG2	2:B:119:PHE:CE1	2.86	0.59
2:B:601:ILE:HD11	2:B:607:LEU:HD11	1.83	0.59
2:B:842:VAL:HG12	2:B:854:ASN:CG	2.22	0.59
2:B:845:SER:O	2:B:920:GLN:NE2	2.35	0.59
2:B:174:LEU:CD2	2:B:302:LEU:HD21	2.32	0.59
2:B:208:ALA:O	2:B:212:LEU:CB	2.50	0.59
2:B:593:THR:O	2:B:597:LEU:HG	2.02	0.59
2:B:1229:PRO:CG	2:B:1232:TYR:CD2	2.85	0.59
2:B:11:ILE:HD13	2:B:740:THR:HG21	1.84	0.59
2:B:116:HIS:NE2	2:B:122:ILE:CD1	2.65	0.59
2:B:569:PHE:CD1	2:B:578:VAL:HG11	2.37	0.59
2:B:942:LYS:N	2:B:942:LYS:HD3	2.18	0.59
2:B:967:ARG:CA	2:B:972:PHE:O	2.50	0.59
2:B:495:MET:HB2	3:C:17:DA:H2"	1.81	0.59
2:B:720:LEU:HD12	2:B:720:LEU:C	2.23	0.59
2:B:763:MET:HG3	2:B:928:THR:HB	1.84	0.59
2:B:121:ASN:OD1	2:B:123:VAL:HG13	2.03	0.59
2:B:893:THR:HG23	2:B:896:LYS:HB2	1.85	0.59
2:B:1148:LYS:HA	2:B:1159:SER:HA	1.84	0.59
2:B:1240:SER:CB	2:B:1242:TYR:CE1	2.85	0.59
2:B:139:ARG:HH11	2:B:161:MET:HG2	1.66	0.59
2:B:131:LYS:CG	2:B:132:TYR:CE1	2.86	0.59
2:B:186:ILE:O	2:B:190:GLN:HB2	2.03	0.59
2:B:359:TYR:CE1	2:B:363:ILE:CD1	2.85	0.59
2:B:857:LEU:HD23	2:B:857:LEU:O	2.03	0.59
2:B:1228:LEU:CB	2:B:1233:VAL:CG2	2.79	0.59
2:B:312:ILE:H	2:B:312:ILE:CD1	2.16	0.58
2:B:386:THR:HG1	2:B:389:LEU:HB2	1.66	0.58
2:B:661:ARG:HH11	2:B:661:ARG:CG	2.15	0.58
2:B:723:HIS:CE1	2:B:727:LEU:CD2	2.86	0.58



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:979:ASN:OD1	2:B:980:ASN:N	2.36	0.58
2:B:1207:GLU:CD	2:B:1208:ASN:H	2.07	0.58
2:B:18:TRP:CZ3	2:B:49:GLY:CA	2.70	0.58
2:B:317:LEU:CB	2:B:414:ILE:HD12	2.33	0.58
2:B:552:LEU:HD21	2:B:563:GLN:NE2	2.17	0.58
2:B:592:GLY:O	2:B:596:ASP:N	2.32	0.58
2:B:661:ARG:HG3	2:B:661:ARG:HH11	1.66	0.58
2:B:823:TYR:HE2	2:B:858:THR:HG21	1.68	0.58
2:B:1130:LYS:C	2:B:1131:TYR:CD1	2.76	0.58
2:B:381:GLU:O	2:B:382:LYS:HD3	2.03	0.58
2:B:749:LYS:HG3	2:B:753:ARG:HH12	1.67	0.58
2:B:821:ASP:OD2	2:B:859:ARG:HB2	2.02	0.58
2:B:1045:PHE:O	2:B:1076:LYS:NZ	2.25	0.58
2:B:1157:LEU:HD12	2:B:1157:LEU:N	2.03	0.58
3:C:1:DC:H42	4:D:12:DG:H1	1.51	0.58
1:A:33:G:N2	1:A:36:A:OP2	2.36	0.58
2:B:378:PRO:CG	2:B:379:ILE:HD12	2.23	0.58
2:B:359:TYR:CE1	2:B:363:ILE:CG1	2.86	0.58
2:B:297:SER:O	2:B:300:ILE:HG22	2.02	0.58
2:B:328:HIS:NE2	2:B:399:LEU:HB3	2.18	0.58
2:B:522:ASN:O	2:B:525:THR:OG1	2.22	0.58
2:B:544:GLN:O	2:B:548:ILE:HG13	2.04	0.58
2:B:718:ASP:HB3	2:B:722:GLU:HB2	1.86	0.58
2:B:288:ASP:HA	2:B:291:LEU:HD22	1.84	0.58
2:B:1222:LYS:NZ	2:B:1314:THR:O	2.37	0.58
3:C:17:DA:H2'	3:C:18:DG:H8	1.69	0.58
2:B:850:ASP:O	2:B:855:LYS:CG	2.52	0.57
2:B:348:LYS:HG3	2:B:352:PHE:HB2	1.85	0.57
2:B:494:ARG:HH11	2:B:494:ARG:CG	2.12	0.57
2:B:202:ASN:HD21	2:B:204:SER:HA	1.69	0.57
2:B:307:ARG:NH2	2:B:323:LYS:HZ1	2.01	0.57
2:B:328:HIS:CG	2:B:399:LEU:CB	2.87	0.57
2:B:634:GLU:HA	2:B:637:LYS:HE2	1.85	0.57
2:B:973:TYR:N	2:B:973:TYR:CD2	2.73	0.57
2:B:1224:ASN:HB2	2:B:1280:VAL:HG11	1.85	0.57
2:B:307:ARG:HH21	2:B:323:LYS:HZ1	1.51	0.57
2:B:564:LEU:CD2	2:B:569:PHE:CE2	2.86	0.57
2:B:1269:ILE:O	2:B:1273:ILE:HG12	2.05	0.57
2:B:1142:SER:HA	2:B:1165:GLY:HA2	1.86	0.57
2:B:334:LEU:O	2:B:338:LEU:HG	2.05	0.57
2:B:340:ARG:HH21	2:B:347:TYR:HE2	1.24	0.57



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:384:ASP:N	2:B:384:ASP:OD1	2.35	0.57
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.22	0.57
2:B:6:SER:H	2:B:21:ILE:CD1	2.18	0.57
2:B:494:ARG:HG2	2:B:494:ARG:NH1	2.16	0.57
2:B:720:LEU:HD11	2:B:724:ILE:CG1	2.34	0.57
2:B:755:LYS:NZ	2:B:942:LYS:HE2	2.19	0.57
2:B:1127:ASP:HB3	2:B:1130:LYS:HG3	1.87	0.57
2:B:237:LEU:HD13	2:B:256:PHE:CE1	2.40	0.57
2:B:265:GLN:O	2:B:271:TYR:HD1	1.86	0.57
2:B:540:LEU:O	2:B:545:LYS:HE3	2.04	0.57
2:B:1315:LEU:HD13	2:B:1324:PHE:HE1	1.70	0.57
2:B:8:GLY:HA3	2:B:991:ALA:HB2	1.86	0.57
2:B:178:ASN:CB	2:B:299:ALA:HB1	2.22	0.57
2:B:348:LYS:O	2:B:352:PHE:HB2	2.05	0.57
2:B:1062:LEU:HD23	2:B:1062:LEU:H	1.70	0.57
2:B:1108:GLU:HB2	3:C:9:DC:H5"	1.87	0.57
2:B:1281:ILE:CG2	2:B:1283:ALA:HB2	2.35	0.57
2:B:484:LYS:O	2:B:488:ALA:N	2.37	0.56
2:B:842:VAL:CG2	2:B:847:LEU:CD2	2.82	0.56
2:B:483:ASP:HB3	2:B:486:ALA:CB	2.20	0.56
2:B:1225:GLU:HA	2:B:1225:GLU:OE1	2.05	0.56
2:B:315:ALA:CB	2:B:418:GLU:HG2	2.35	0.56
2:B:499:ASP:CB	2:B:502:LEU:O	2.53	0.56
2:B:522:ASN:HD22	2:B:523:GLU:N	2.02	0.56
2:B:895:ARG:HH11	2:B:899:ASN:ND2	2.04	0.56
2:B:944:ASP:OD1	2:B:944:ASP:N	2.37	0.56
2:B:1139:VAL:CG1	2:B:1167:THR:CG2	2.83	0.56
2:B:1198:LEU:HD13	2:B:1204:PHE:HZ	1.69	0.56
2:B:1270:ILE:CA	2:B:1273:ILE:CD1	2.70	0.56
2:B:100:ARG:NE	2:B:117:PRO:O	2.37	0.56
2:B:325:TYR:O	2:B:329:HIS:N	2.34	0.56
2:B:516:GLU:CD	2:B:593:THR:OG1	2.44	0.56
2:B:1206:LEU:O	2:B:1207:GLU:HG3	2.06	0.56
2:B:1236:LEU:HD22	2:B:1310:ILE:CD1	2.35	0.56
1:A:13:A:H5"	2:B:59:ALA:HB3	1.86	0.56
2:B:18:TRP:CE3	2:B:49:GLY:N	2.69	0.56
2:B:169:LEU:HD21	3:C:13:DA:H2"	1.88	0.56
2:B:217:SER:OG	2:B:220:ARG:NH1	2.39	0.56
2:B:686:ASP:OD2	2:B:690:ASN:HA	2.05	0.56
2:B:897:PHE:CZ	2:B:901:THR:HG21	2.40	0.56
2:B:1041:ASN:O	2:B:1044:ASN:HB2	2.06	0.56



	A construction of the cons	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:1146:VAL:HG13	2:B:1191:LYS:HG3	1.86	0.56
2:B:161:MET:C	2:B:164:PHE:O	2.39	0.56
2:B:761:ILE:CD1	2:B:931:VAL:HG12	2.35	0.56
2:B:856:VAL:HG22	2:B:857:LEU:N	2.20	0.56
2:B:975:VAL:HG11	2:B:1236:LEU:HD13	1.87	0.56
2:B:1119:LEU:HD13	2:B:1119:LEU:H	1.69	0.56
2:B:1123:LYS:HB2	2:B:1126:TRP:CE3	2.41	0.56
2:B:1240:SER:CB	2:B:1242:TYR:CZ	2.88	0.56
2:B:245:SER:OG	2:B:296:LEU:HD22	2.04	0.56
2:B:252:PHE:CZ	2:B:264:LEU:HD13	2.41	0.56
2:B:594:TYR:HA	2:B:597:LEU:HD11	1.88	0.56
2:B:1210:ARG:HD3	2:B:1280:VAL:HA	1.76	0.56
2:B:18:TRP:CZ3	2:B:47:LEU:O	2.59	0.56
2:B:107:VAL:CG1	2:B:1131:TYR:CE1	2.60	0.56
2:B:135:ILE:HG23	2:B:136:TYR:N	2.20	0.56
2:B:887:LEU:N	2:B:892:ILE:HD11	2.21	0.56
2:B:749:LYS:HG3	2:B:753:ARG:NH1	2.21	0.56
2:B:1297:HIS:NE2	2:B:1327:PHE:HE2	2.01	0.56
2:B:451:TYR:CB	2:B:491:PHE:CD1	2.89	0.55
2:B:520:VAL:HG11	2:B:553:PHE:CD1	2.34	0.55
2:B:721:HIS:ND1	2:B:738:LEU:HD11	2.21	0.55
2:B:1243:GLU:CB	2:B:1246:LYS:NZ	2.66	0.55
2:B:484:LYS:O	2:B:488:ALA:HB2	2.06	0.55
2:B:31:LYS:HG3	2:B:44:LYS:HB2	1.87	0.55
1:A:58:G:H5'	2:B:457:ARG:HH11	1.71	0.55
2:B:107:VAL:HG22	2:B:1131:TYR:CE1	2.42	0.55
2:B:132:TYR:CD1	2:B:132:TYR:N	2.73	0.55
2:B:279:LEU:HD21	2:B:284:ASP:CA	2.37	0.55
2:B:886:LEU:HB2	2:B:892:ILE:HD13	1.87	0.55
2:B:343:LEU:O	2:B:343:LEU:HG	2.07	0.55
2:B:379:ILE:CG2	2:B:383:MET:SD	2.95	0.55
2:B:749:LYS:HD2	2:B:753:ARG:HH22	1.71	0.55
2:B:1204:PHE:CD1	2:B:1347:LEU:CB	2.89	0.55
2:B:393:LEU:HD23	2:B:394:ASN:CA	2.37	0.55
2:B:1114:ARG:HH12	4:D:9:DA:P	2.30	0.55
2:B:1287:LEU:HD12	2:B:1287:LEU:C	2.26	0.55
2:B:288:ASP:HA	2:B:291:LEU:CD2	2.36	0.55
2:B:300:ILE:HG23	2:B:301:LEU:N	2.21	0.55
2:B:456:ALA:CB	2:B:463:ALA:HB2	2.19	0.55
2:B:328:HIS:NE2	2:B:399:LEU:HB2	2.21	0.54
2:B:497:ASN:OD1	3:C:19:DA:P	2.65	0.54



	h h o	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:1349:HIS:HB2	2:B:1358:THR:OG1	2.06	0.54
2:B:222:LEU:O	2:B:226:ILE:HG12	2.06	0.54
2:B:853:ASP:C	2:B:896:LYS:HG3	2.25	0.54
2:B:967:ARG:NH1	2:B:986:ASP:OD1	2.40	0.54
2:B:47:LEU:O	2:B:48:ILE:C	2.45	0.54
2:B:513:LEU:O	2:B:516:GLU:HB2	2.08	0.54
2:B:531:THR:HG22	2:B:534:MET:SD	2.47	0.54
2:B:941:THR:C	2:B:942:LYS:HD3	2.28	0.54
2:B:972:PHE:N	2:B:972:PHE:CD1	2.73	0.54
1:A:15:U:OP2	2:B:66:ARG:NH2	2.40	0.54
2:B:520:VAL:CG1	2:B:553:PHE:CE1	2.90	0.54
2:B:978:ILE:HD12	2:B:1236:LEU:HD12	1.86	0.54
2:B:1207:GLU:CG	2:B:1208:ASN:H	2.20	0.54
1:A:92:G:OP1	2:B:40:ARG:NH2	2.41	0.54
2:B:316:PRO:HD2	2:B:317:LEU:H	1.73	0.54
2:B:473:ILE:HG12	2:B:481:VAL:HG11	1.89	0.54
2:B:22:THR:OG1	2:B:26:LYS:O	2.26	0.54
2:B:107:VAL:N	2:B:1131:TYR:CZ	2.64	0.54
2:B:338:LEU:HD13	2:B:386:THR:CB	2.35	0.54
2:B:843:PRO:HD2	2:B:846:PHE:HD2	1.71	0.54
2:B:1325:LYS:HA	2:B:1330:THR:HA	1.89	0.54
2:B:318:SER:CB	2:B:418:GLU:OE2	2.53	0.54
2:B:680:LEU:O	2:B:684:LYS:HG3	2.07	0.54
2:B:879:MET:O	2:B:882:TYR:N	2.40	0.54
2:B:131:LYS:CD	2:B:132:TYR:CE1	2.86	0.54
2:B:482:VAL:HG12	2:B:483:ASP:N	2.22	0.54
2:B:1243:GLU:O	2:B:1246:LYS:HD2	2.07	0.54
2:B:666:LEU:HD23	2:B:666:LEU:C	2.29	0.54
2:B:727:LEU:O	2:B:734:LYS:HD3	2.08	0.54
2:B:895:ARG:NH1	2:B:899:ASN:ND2	2.54	0.54
2:B:682:PHE:CG	2:B:696:LEU:HD11	2.43	0.53
2:B:686:ASP:HB2	2:B:690:ASN:HA	1.88	0.53
1:A:68:A:H2'	1:A:69:A:C8	2.43	0.53
2:B:115:ARG:CG	2:B:116:HIS:HD1	2.21	0.53
2:B:359:TYR:CA	2:B:362:TYR:HB3	2.38	0.53
2:B:361:GLY:HA2	2:B:365:GLY:H	1.74	0.53
2:B:465:MET:HE2	2:B:482:VAL:HG22	1.91	0.53
2:B:554:LYS:CB	2:B:604:LYS:HZ1	2.19	0.53
2:B:316:PRO:CD	2:B:317:LEU:H	2.21	0.53
2:B:455:LEU:CD2	2:B:473:ILE:HG21	2.38	0.53
2:B:553:PHE:HE2	2:B:559:VAL:HG21	1.52	0.53



	A i a	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:362:TYR:HD1	2:B:362:TYR:O	1.92	0.53
2:B:395:ARG:O	2:B:396:GLU:HG3	2.07	0.53
2:B:1229:PRO:HD2	2:B:1232:TYR:HB2	1.91	0.53
3:C:17:DA:H2'	3:C:18:DG:C8	2.43	0.53
2:B:374:LYS:HA	2:B:374:LYS:CE	2.37	0.53
2:B:686:ASP:H	2:B:690:ASN:ND2	2.06	0.53
2:B:1207:GLU:HG2	2:B:1210:ARG:HH12	1.71	0.53
2:B:241:LEU:HD21	2:B:290:PHE:HE2	1.74	0.53
2:B:379:ILE:C	2:B:383:MET:HG3	2.22	0.53
2:B:1351:SER:OG	2:B:1356:TYR:HB2	2.08	0.53
3:C:1:DC:N4	4:D:12:DG:H1	2.06	0.53
2:B:116:HIS:CD2	2:B:122:ILE:HG13	2.44	0.53
2:B:609:ASN:ND2	2:B:612:ASN:OD1	2.34	0.53
2:B:850:ASP:O	2:B:855:LYS:HD2	2.09	0.53
2:B:884:ARG:O	2:B:888:ASN:N	2.32	0.53
2:B:1276:PHE:HE2	2:B:1316:THR:HA	1.74	0.53
1:A:51:A:O2'	2:B:1134:PHE:CE1	2.37	0.53
2:B:359:TYR:OH	2:B:363:ILE:HD11	2.09	0.53
2:B:131:LYS:CG	2:B:132:TYR:CD1	2.88	0.53
2:B:226:ILE:O	2:B:229:LEU:HG	2.09	0.53
2:B:266:LEU:HD21	2:B:294:LYS:HA	1.90	0.53
2:B:334:LEU:CD1	2:B:338:LEU:CD1	2.85	0.53
2:B:63:ARG:O	2:B:67:THR:OG1	2.20	0.52
2:B:335:LEU:O	2:B:339:VAL:HG23	2.10	0.52
2:B:478:PHE:CE2	2:B:482:VAL:CG2	2.86	0.52
2:B:1202:SER:O	2:B:1214:LEU:N	2.28	0.52
2:B:297:SER:O	2:B:301:LEU:HD12	2.10	0.52
2:B:315:ALA:HB2	2:B:418:GLU:HG2	1.90	0.52
2:B:398:LEU:HG	2:B:399:LEU:H	1.75	0.52
2:B:600:ILE:N	2:B:600:ILE:CD1	2.73	0.52
2:B:942:LYS:O	2:B:950:ILE:HB	2.09	0.52
2:B:356:LYS:O	2:B:357:ASN:CB	2.53	0.52
2:B:1207:GLU:OE1	2:B:1208:ASN:HB3	2.10	0.52
3:C:11:DT:H2'	3:C:12:DC:O4'	2.09	0.52
3:C:13:DA:H2'	3:C:14:DA:C8	2.41	0.52
2:B:312:ILE:N	2:B:312:ILE:CD1	2.73	0.52
2:B:454:PRO:O	2:B:456:ALA:N	2.42	0.52
2:B:1315:LEU:HD13	2:B:1324:PHE:CE1	2.44	0.52
2:B:282:ILE:HG22	2:B:286:TYR:HD1	1.68	0.52
2:B:966:PHE:CZ	2:B:970:PHE:HD2	2.28	0.52
2:B:1107:LYS:HD3	3:C:8:DT:H4'	1.92	0.52



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:1325:LYS:CA	2:B:1330:THR:HA	2.40	0.52
2:B:1347:LEU:HD23	2:B:1347:LEU:O	2.10	0.52
2:B:189:VAL:HA	2:B:192:TYR:HB3	1.92	0.52
2:B:1325:LYS:HB3	2:B:1330:THR:OG1	2.10	0.52
2:B:1348:ILE:HD11	2:B:1357:GLU:CG	2.40	0.52
3:C:18:DG:H2'	3:C:19:DA:C8	2.45	0.52
2:B:134:THR:CB	2:B:137:HIS:ND1	2.58	0.52
2:B:236:GLY:O	2:B:240:ASN:ND2	2.42	0.52
2:B:303:SER:O	2:B:306:LEU:C	2.48	0.52
2:B:359:TYR:O	2:B:363:ILE:N	2.38	0.52
2:B:1339:THR:O	2:B:1343:LEU:CD2	2.50	0.52
2:B:374:LYS:CE	2:B:374:LYS:CA	2.86	0.51
2:B:1119:LEU:H	2:B:1119:LEU:HD22	1.75	0.51
2:B:78:ARG:CZ	2:B:165:ARG:HD2	2.40	0.51
2:B:308:VAL:HG12	2:B:309:ASN:N	2.25	0.51
2:B:509:PRO:HB3	2:B:624:THR:HG21	1.91	0.51
2:B:851:SER:C	2:B:855:LYS:HG3	2.31	0.51
2:B:70:ARG:NH2	2:B:462:PHE:CD2	2.78	0.51
2:B:115:ARG:CG	2:B:116:HIS:ND1	2.73	0.51
2:B:245:SER:OG	2:B:296:LEU:HD23	2.02	0.51
2:B:523:GLU:OE1	2:B:589:ALA:HB2	2.10	0.51
2:B:1236:LEU:O	2:B:1240:SER:HB2	2.11	0.51
1:A:81:G:N1	2:B:1356:TYR:HB3	2.26	0.51
2:B:686:ASP:CB	2:B:690:ASN:ND2	2.73	0.51
2:B:713:VAL:O	2:B:716:GLN:N	2.32	0.51
2:B:853:ASP:HA	2:B:896:LYS:CG	2.40	0.51
2:B:1127:ASP:O	2:B:1131:TYR:N	2.37	0.51
2:B:115:ARG:HG3	2:B:116:HIS:CE1	2.45	0.51
2:B:134:THR:HG22	2:B:136:TYR:H	1.75	0.51
2:B:887:LEU:N	2:B:892:ILE:CD1	2.73	0.51
2:B:1243:GLU:OE1	2:B:1243:GLU:HA	2.11	0.51
2:B:1245:LEU:HD13	2:B:1252:ASN:ND2	2.23	0.51
2:B:114:GLU:HG2	2:B:120:GLY:HA2	1.92	0.51
2:B:520:VAL:HG21	2:B:591:LEU:CG	2.27	0.51
2:B:591:LEU:HD12	2:B:594:TYR:CB	2.40	0.51
2:B:966:PHE:CZ	2:B:970:PHE:CD2	2.99	0.51
2:B:999:LYS:HB3	2:B:1073:VAL:HG11	1.92	0.51
2:B:1207:GLU:CG	2:B:1208:ASN:N	2.73	0.51
2:B:336:LYS:O	2:B:340:ARG:HG2	2.11	0.51
2:B:569:PHE:HA	2:B:573:GLU:HB2	1.92	0.51
2:B:226:ILE:C	2:B:229:LEU:HG	2.31	0.51



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:790:GLU:OE2	2:B:888:ASN:O	2.28	0.51
2:B:1224:ASN:HD21	2:B:1280:VAL:HG21	1.60	0.51
2:B:45:LYS:CB	2:B:1091:GLN:HE22	2.22	0.51
2:B:282:ILE:N	2:B:282:ILE:CD1	2.73	0.51
2:B:347:TYR:C	2:B:347:TYR:CD1	2.84	0.51
2:B:433:LEU:O	2:B:437:ARG:N	2.44	0.51
2:B:879:MET:O	2:B:880:LYS:C	2.49	0.51
2:B:936:ASP:CG	2:B:951:ARG:HE	2.14	0.51
2:B:1062:LEU:O	2:B:1076:LYS:HG3	2.11	0.51
2:B:1100:VAL:HG13	2:B:1140:ALA:HB1	1.92	0.51
1:A:22:U:H2'	1:A:23:U:C6	2.46	0.51
2:B:465:MET:SD	2:B:467:ARG:HG3	2.51	0.51
2:B:679:ILE:HG12	2:B:704:PHE:CE1	2.46	0.51
2:B:1120:ILE:HD11	2:B:1137:PRO:HD2	1.91	0.51
2:B:1343:LEU:HD23	2:B:1343:LEU:H	1.72	0.51
1:A:8:G:O2'	1:A:9:U:OP1	2.27	0.50
2:B:334:LEU:HD12	2:B:389:LEU:HD11	1.93	0.50
2:B:780:ARG:HD3	2:B:812:TYR:CE2	2.46	0.50
2:B:691:ARG:HB2	2:B:696:LEU:HD22	1.94	0.50
2:B:1348:ILE:HG23	2:B:1348:ILE:O	2.11	0.50
2:B:135:ILE:O	2:B:138:LEU:HB3	2.11	0.50
2:B:661:ARG:N	2:B:661:ARG:CD	2.73	0.50
2:B:1220:LEU:CD2	2:B:1342:VAL:HG21	2.42	0.50
2:B:1363:SER:O	2:B:1364:GLN:HB3	2.12	0.50
2:B:620:VAL:HG13	2:B:656:TYR:CE2	2.46	0.50
2:B:970:PHE:O	2:B:971:GLN:HB2	2.11	0.50
2:B:48:ILE:HG21	2:B:1092:VAL:HG22	1.92	0.50
2:B:60:GLU:HG3	2:B:63:ARG:HH22	1.76	0.50
2:B:202:ASN:OD1	2:B:203:ALA:N	2.45	0.50
2:B:457:ARG:HG2	2:B:459:ASN:ND2	2.26	0.50
2:B:552:LEU:O	2:B:555:THR:OG1	2.29	0.50
2:B:559:VAL:C	2:B:563:GLN:OE1	2.49	0.50
2:B:760:VAL:HG11	2:B:990:ASN:O	2.11	0.50
2:B:118:ILE:C	2:B:119:PHE:CD1	2.85	0.50
2:B:509:PRO:HA	2:B:659:TRP:HA	1.93	0.50
2:B:192:TYR:C	2:B:192:TYR:CD2	2.85	0.50
2:B:277:ASN:O	2:B:281:GLN:OE1	2.30	0.50
2:B:291:LEU:O	2:B:294:LYS:HD3	2.11	0.50
2:B:359:TYR:HE1	2:B:363:ILE:CG1	2.25	0.50
2:B:666:LEU:HA	2:B:670:ILE:HG12	1.94	0.50
2:B:940:ASN:HB3	2:B:950:ILE:O	2.11	0.50



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:1270:ILE:CA	2:B:1273:ILE:HD11	2.40	0.50
2:B:53:PHE:CD1	2:B:53:PHE:C	2.85	0.49
2:B:121:ASN:OD1	2:B:124:ASP:HB2	2.11	0.49
2:B:202:ASN:ND2	2:B:204:SER:CB	2.74	0.49
2:B:491:PHE:C	2:B:491:PHE:CD2	2.85	0.49
2:B:495:MET:CB	3:C:17:DA:H1'	2.22	0.49
2:B:522:ASN:ND2	2:B:523:GLU:N	2.60	0.49
1:A:70:C:H2'	1:A:71:U:C6	2.47	0.49
2:B:648:MET:HA	2:B:651:LEU:HB2	1.94	0.49
2:B:1204:PHE:CE2	2:B:1342:VAL:CG1	2.85	0.49
2:B:1235:PHE:CD1	2:B:1258:PHE:CE2	3.00	0.49
2:B:1348:ILE:CD1	2:B:1359:ARG:HH12	2.10	0.49
2:B:491:PHE:HD2	2:B:492:ILE:HG12	1.77	0.49
2:B:495:MET:HB2	3:C:17:DA:C3'	2.42	0.49
2:B:1309:ILE:HG12	2:B:1326:TYR:OH	2.12	0.49
1:A:58:G:C5'	2:B:457:ARG:NH1	2.71	0.49
2:B:373:TYR:O	2:B:376:ILE:HD12	2.13	0.49
1:A:15:U:H4'	2:B:464:TRP:HE1	1.77	0.49
2:B:282:ILE:CG2	2:B:283:GLY:N	2.75	0.49
2:B:331:ASP:HB3	2:B:398:LEU:HD11	1.94	0.49
2:B:334:LEU:HD12	2:B:389:LEU:CD1	2.42	0.49
2:B:787:GLY:O	2:B:791:LEU:N	2.32	0.49
2:B:1120:ILE:CD1	2:B:1137:PRO:CG	2.84	0.49
1:A:8:G:O4'	2:B:894:GLN:OE1	2.30	0.49
2:B:11:ILE:HG22	2:B:12:GLY:H	1.77	0.49
2:B:201:ILE:HG22	2:B:202:ASN:N	2.27	0.49
2:B:1279:ARG:HG2	2:B:1280:VAL:HG23	1.94	0.49
2:B:1325:LYS:HB3	2:B:1330:THR:HA	1.90	0.49
1:A:32:A:H61	1:A:37:U:H3	1.60	0.49
2:B:218:LYS:H	2:B:218:LYS:HD2	1.78	0.49
2:B:450:TYR:HD2	2:B:491:PHE:HZ	1.45	0.49
2:B:513:LEU:HB2	2:B:617:GLU:OE2	2.12	0.49
2:B:545:LYS:HZ2	2:B:690:ASN:ND2	2.08	0.49
2:B:279:LEU:HD11	2:B:287:ALA:HB2	1.95	0.49
2:B:359:TYR:CD1	2:B:359:TYR:C	2.85	0.49
2:B:401:LYS:HB2	2:B:404:THR:CG2	2.43	0.49
2:B:733:ILE:HD11	2:B:763:MET:HE3	1.94	0.49
2:B:128:TYR:CD1	2:B:153:LEU:HD21	2.48	0.49
2:B:362:TYR:CD1	2:B:362:TYR:C	2.85	0.49
1:A:27:G:N2	1:A:44:U:OP2	2.46	0.48
2:B:1239:ALA:CB	2:B:1306:ALA:HB1	2.43	0.48



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:A:45:U:H2'	1:A:46:A:C8	2.47	0.48
1:A:59:U:P	2:B:467:ARG:HH22	2.36	0.48
2:B:377:LYS:O	2:B:381:GLU:HB2	2.13	0.48
2:B:1204:PHE:CE1	2:B:1347:LEU:HB2	2.48	0.48
1:A:8:G:HO2'	1:A:9:U:P	2.37	0.48
2:B:186:ILE:HD12	2:B:203:ALA:HB2	1.95	0.48
2:B:1276:PHE:CE2	2:B:1316:THR:HB	2.49	0.48
2:B:512:SER:O	2:B:516:GLU:HG2	2.12	0.48
2:B:524:LEU:HD23	2:B:524:LEU:C	2.34	0.48
2:B:316:PRO:CA	2:B:319:ALA:HB3	2.39	0.48
2:B:746:GLU:HA	2:B:749:LYS:HB3	1.95	0.48
2:B:1262:HIS:HD2	2:B:1265:TYR:CZ	2.30	0.48
1:A:33:G:H2'	1:A:34:A:H5"	1.95	0.48
1:A:49:A:H1'	2:B:1122:ARG:NH1	2.29	0.48
2:B:720:LEU:CD1	2:B:724:ILE:CG1	2.86	0.48
2:B:949:LEU:CD1	2:B:950:ILE:N	2.73	0.48
2:B:169:LEU:HD22	3:C:14:DA:H5'	1.95	0.48
2:B:275:LEU:HD11	2:B:290:PHE:CD1	2.49	0.48
2:B:362:TYR:HE2	2:B:372:PHE:CE2	2.29	0.48
1:A:45:U:H2'	1:A:46:A:H8	1.78	0.48
1:A:65:A:OP1	2:B:57:GLU:N	2.46	0.48
2:B:206:VAL:HG12	2:B:228:GLN:HG2	1.94	0.48
2:B:975:VAL:HG21	2:B:1236:LEU:HB2	1.96	0.48
2:B:1229:PRO:HG2	2:B:1232:TYR:CE2	2.48	0.48
2:B:332:LEU:HD11	2:B:359:TYR:CE2	2.42	0.48
2:B:869:ASN:CG	2:B:870:VAL:N	2.65	0.48
2:B:93:VAL:HG12	2:B:152:ARG:NH1	2.28	0.48
2:B:343:LEU:O	2:B:343:LEU:CG	2.62	0.48
2:B:393:LEU:HD23	2:B:394:ASN:HA	1.94	0.48
2:B:1240:SER:HB3	2:B:1242:TYR:CZ	2.49	0.48
3:C:3:DA:H2'	3:C:4:DT:H71	1.95	0.48
2:B:270:THR:OG1	2:B:629:ARG:NH1	2.47	0.47
2:B:668:ASN:HD21	2:B:680:LEU:HB3	1.67	0.47
2:B:975:VAL:HG11	2:B:1236:LEU:HD12	1.94	0.47
2:B:1206:LEU:HB3	2:B:1345:ALA:HB3	1.71	0.47
2:B:1334:LYS:NZ	3:C:2:DA:O3'	2.46	0.47
1:A:43:G:H22	2:B:360:ALA:HB2	1.79	0.47
2:B:121:ASN:ND2	2:B:124:ASP:HB2	2.29	0.47
2:B:347:TYR:C	2:B:347:TYR:HD1	2.17	0.47
2:B:489:GLN:O	2:B:493:GLU:HB2	2.14	0.47
2:B:897:PHE:HA	2:B:900:LEU:HB2	1.96	0.47



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:877:LYS:HG3	2:B:878:LYS:N	2.29	0.47
1:A:47:A:O2'	2:B:104:SER:OG	2.23	0.47
2:B:372:PHE:CD1	2:B:372:PHE:C	2.85	0.47
2:B:484:LYS:HA	2:B:487:SER:OG	2.14	0.47
2:B:495:MET:CG	3:C:17:DA:C4'	2.88	0.47
2:B:601:ILE:HD11	2:B:607:LEU:HD21	1.80	0.47
2:B:1065:THR:CB	2:B:1072:ILE:HA	2.42	0.47
2:B:1276:PHE:HE2	2:B:1316:THR:CA	2.27	0.47
2:B:485:GLY:HA2	2:B:488:ALA:CB	2.41	0.47
2:B:755:LYS:HZ2	2:B:942:LYS:HE2	1.80	0.47
2:B:1118:LYS:HA	2:B:1118:LYS:HD3	1.73	0.47
2:B:1139:VAL:CA	2:B:1167:THR:HA	2.43	0.47
2:B:1297:HIS:CD2	2:B:1327:PHE:CE2	3.03	0.47
2:B:119:PHE:HD2	2:B:124:ASP:O	1.98	0.47
2:B:317:LEU:HD22	2:B:414:ILE:CD1	2.43	0.47
2:B:340:ARG:NE	2:B:347:TYR:CD2	2.77	0.47
2:B:375:PHE:CE2	2:B:376:ILE:HG23	2.48	0.47
2:B:380:LEU:CA	2:B:383:MET:HG3	2.44	0.47
2:B:431:PRO:O	2:B:434:LYS:HG2	2.14	0.47
2:B:494:ARG:CG	2:B:494:ARG:NH1	2.73	0.47
2:B:679:ILE:HG12	2:B:704:PHE:HE1	1.80	0.47
2:B:778:ARG:NH1	3:C:11:DT:OP1	2.48	0.47
2:B:825:ASP:CG	2:B:825:ASP:O	2.53	0.47
2:B:887:LEU:HA	2:B:892:ILE:HG12	1.97	0.47
2:B:1045:PHE:HB2	2:B:1064:GLU:CD	2.35	0.47
2:B:1075:ASP:OD1	2:B:1078:ARG:N	2.33	0.47
2:B:1139:VAL:HG11	2:B:1165:GLY:C	2.32	0.47
2:B:1144:LEU:HB3	2:B:1196:ILE:HB	1.95	0.47
2:B:1148:LYS:HB2	2:B:1157:LEU:HB2	1.96	0.47
2:B:1203:LEU:CD1	2:B:1212:ARG:O	2.53	0.47
2:B:1236:LEU:CG	2:B:1310:ILE:HD11	2.45	0.47
2:B:1239:ALA:CB	2:B:1306:ALA:CB	2.92	0.47
2:B:1270:ILE:HG13	2:B:1294:TYR:CE2	2.50	0.47
2:B:1281:ILE:O	2:B:1336:TYR:OH	2.26	0.47
2:B:328:HIS:CG	2:B:399:LEU:HA	2.49	0.47
2:B:465:MET:SD	2:B:467:ARG:CG	3.02	0.47
2:B:491:PHE:CD2	2:B:492:ILE:HG12	2.49	0.47
2:B:518:PHE:CZ	2:B:679:ILE:HG23	2.25	0.47
2:B:942:LYS:N	2:B:942:LYS:CD	2.73	0.47
2:B:86:PHE:HE2	2:B:155:TYR:HB2	1.79	0.47
2:B:572:ILE:O	2:B:572:ILE:CG2	2.63	0.47



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
3:C:2:DA:H2"	3:C:3:DA:C8	2.50	0.47
2:B:421:ALA:O	2:B:425:ARG:N	2.48	0.47
2:B:478:PHE:C	2:B:478:PHE:CD2	2.85	0.47
2:B:516:GLU:HA	2:B:519:THR:HG22	1.97	0.47
2:B:721:HIS:HE1	2:B:738:LEU:HD21	1.79	0.47
2:B:784:ILE:HG22	2:B:796:LEU:HD11	1.96	0.47
2:B:954:LYS:HD2	2:B:998:ILE:HD12	1.97	0.47
2:B:121:ASN:CG	2:B:124:ASP:HB2	2.35	0.46
2:B:949:LEU:CG	2:B:950:ILE:N	2.78	0.46
2:B:969:ASP:OD1	2:B:969:ASP:N	2.47	0.46
2:B:686:ASP:HB3	2:B:690:ASN:HA	1.95	0.46
2:B:959:LYS:HD2	2:B:960:SER:H	1.79	0.46
2:B:1236:LEU:HD22	2:B:1310:ILE:HD11	1.96	0.46
2:B:453:GLY:HA2	2:B:464:TRP:NE1	2.30	0.46
2:B:822:MET:HG2	2:B:856:VAL:HG21	1.97	0.46
2:B:887:LEU:HA	2:B:892:ILE:CG1	2.45	0.46
1:A:58:G:C4'	2:B:457:ARG:HD2	2.04	0.46
1:A:61:C:H5'	2:B:460:SER:OG	2.16	0.46
1:A:70:C:H2'	1:A:71:U:H6	1.79	0.46
2:B:9:LEU:HD12	2:B:761:ILE:HG22	1.98	0.46
2:B:135:ILE:CG2	2:B:136:TYR:N	2.78	0.46
2:B:197:GLU:O	2:B:198:GLU:C	2.51	0.46
2:B:315:ALA:O	2:B:319:ALA:CB	2.62	0.46
2:B:518:PHE:CD2	2:B:683:LEU:HD12	2.38	0.46
2:B:668:ASN:O	2:B:678:THR:HG21	2.15	0.46
2:B:1231:LYS:CD	2:B:1265:TYR:OH	2.62	0.46
2:B:1243:GLU:O	2:B:1246:LYS:NZ	2.27	0.46
2:B:94:ASP:OD1	2:B:97:PHE:N	2.48	0.46
2:B:616:LEU:HA	2:B:619:ILE:HG22	1.98	0.46
2:B:677:LYS:HB2	2:B:682:PHE:CE2	2.51	0.46
2:B:308:VAL:CG1	2:B:309:ASN:N	2.79	0.46
2:B:374:LYS:HA	2:B:374:LYS:HE3	1.96	0.46
2:B:530:VAL:O	2:B:578:VAL:HG22	2.15	0.46
2:B:597:LEU:HG	2:B:597:LEU:H	1.52	0.46
2:B:914:ALA:HB3	2:B:1032:ALA:HB1	1.95	0.46
2:B:515:TYR:HD2	2:B:515:TYR:O	1.98	0.46
2:B:967:ARG:C	2:B:972:PHE:O	2.53	0.46
2:B:986:ASP:O	2:B:990:ASN:ND2	2.48	0.46
2:B:1139:VAL:HG13	2:B:1167:THR:HG22	1.94	0.46
2:B:297:SER:O	2:B:301:LEU:HG	2.15	0.46
2:B:518:PHE:HZ	2:B:679:ILE:HG21	1.54	0.46



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:520:VAL:HG23	2:B:591:LEU:HD21	1.80	0.46
2:B:949:LEU:HD11	2:B:950:ILE:O	2.15	0.46
2:B:348:LYS:HG2	2:B:352:PHE:HB2	1.96	0.46
2:B:794:GLN:CD	2:B:794:GLN:H	2.19	0.46
2:B:859:ARG:NE	2:B:860:SER:HG	1.98	0.46
2:B:1274:SER:O	2:B:1277:SER:HB3	2.16	0.46
2:B:1348:ILE:HD11	2:B:1357:GLU:OE1	2.15	0.46
2:B:245:SER:HA	2:B:297:SER:HB2	1.97	0.46
2:B:1224:ASN:CB	2:B:1280:VAL:HG11	2.46	0.46
2:B:746:GLU:OE1	2:B:1352:ILE:HG22	2.15	0.45
2:B:1045:PHE:O	2:B:1064:GLU:OE2	2.33	0.45
2:B:1065:THR:HB	2:B:1072:ILE:HG12	1.98	0.45
2:B:1211:LYS:NZ	2:B:1211:LYS:CB	2.78	0.45
1:A:8:G:C4'	2:B:894:GLN:OE1	2.64	0.45
1:A:67:C:OP1	2:B:742:LYS:NZ	2.47	0.45
2:B:128:TYR:OH	2:B:135:ILE:HD13	2.16	0.45
2:B:859:ARG:NH1	2:B:859:ARG:CG	2.75	0.45
2:B:557:ARG:HG2	2:B:595:HIS:CB	2.46	0.45
2:B:1212:ARG:NH1	2:B:1336:TYR:CD2	2.77	0.45
2:B:111:LYS:HD3	2:B:115:ARG:HA	1.99	0.45
2:B:188:LEU:C	2:B:188:LEU:HD22	2.33	0.45
2:B:201:ILE:HG23	2:B:230:PRO:HD2	1.98	0.45
2:B:348:LYS:HG3	2:B:352:PHE:CG	2.52	0.45
2:B:895:ARG:HD2	2:B:895:ARG:O	2.16	0.45
2:B:966:PHE:CD1	2:B:970:PHE:CD2	3.04	0.45
2:B:971:GLN:C	2:B:972:PHE:HD1	2.19	0.45
2:B:20:VAL:O	2:B:27:VAL:HB	2.16	0.45
2:B:37:ASN:OD1	2:B:1360:ILE:HG23	2.17	0.45
2:B:193:ASN:CG	2:B:201:ILE:H	2.14	0.45
1:A:49:A:H1'	2:B:1122:ARG:HH11	1.81	0.45
1:A:91:C:H2'	2:B:44:LYS:O	2.16	0.45
2:B:372:PHE:CD1	2:B:372:PHE:O	2.70	0.45
2:B:687:GLY:O	2:B:689:ALA:N	2.48	0.45
2:B:478:PHE:CD2	2:B:478:PHE:O	2.70	0.45
2:B:823:TYR:CD1	2:B:875:VAL:HG11	2.52	0.45
2:B:1270:ILE:HG23	2:B:1273:ILE:HD11	1.97	0.45
2:B:1308:ASN:CG	2:B:1327:PHE:HB3	2.36	0.45
2:B:350:ILE:O	2:B:359:TYR:N	2.47	0.45
2:B:362:TYR:O	2:B:362:TYR:CD1	2.70	0.45
2:B:723:HIS:CE1	2:B:727:LEU:HD21	2.51	0.45
2:B:762:GLU:CD	2:B:990:ASN:ND2	2.57	0.45



	At 0	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:B:933:GLN:OE1	2:B:934:ILE:HG13	2.16	0.45
2:B:1078:ARG:O	2:B:1082:THR:HG23	2.16	0.45
2:B:1105:PHE:CE2	2:B:1169:MET:HG3	2.52	0.45
2:B:226:ILE:CA	2:B:229:LEU:HD21	2.44	0.45
2:B:304:ASP:OD1	2:B:304:ASP:N	2.45	0.45
2:B:597:LEU:HB2	2:B:601:ILE:CD1	2.47	0.45
2:B:664:ARG:CD	2:B:664:ARG:C	2.86	0.45
2:B:686:ASP:CG	2:B:691:ARG:CZ	2.85	0.45
2:B:746:GLU:O	2:B:750:VAL:N	2.48	0.45
2:B:874:GLU:O	2:B:877:LYS:HG3	2.17	0.45
2:B:53:PHE:HE1	2:B:54:ASP:O	1.94	0.44
2:B:225:LEU:CD1	2:B:229:LEU:HD23	2.46	0.44
2:B:376:ILE:CD1	2:B:376:ILE:C	2.86	0.44
2:B:686:ASP:N	2:B:690:ASN:ND2	2.64	0.44
2:B:817:GLN:OE1	2:B:857:LEU:O	2.35	0.44
2:B:1139:VAL:CA	2:B:1166:ILE:O	2.63	0.44
2:B:1243:GLU:CG	2:B:1246:LYS:HE2	2.47	0.44
2:B:1325:LYS:HB3	2:B:1330:THR:CB	2.47	0.44
1:A:24:U:H2'	1:A:25:U:O4'	2.17	0.44
1:A:48:A:H2'	1:A:49:A:H8	1.81	0.44
2:B:139:ARG:NH1	2:B:161:MET:HG2	2.32	0.44
2:B:1232:TYR:CZ	2:B:1268:GLU:HB3	2.52	0.44
2:B:1276:PHE:CE2	2:B:1316:THR:HA	2.51	0.44
1:A:42:A:HO2'	1:A:43:G:P	2.39	0.44
2:B:265:GLN:O	2:B:271:TYR:CB	2.63	0.44
2:B:265:GLN:C	2:B:271:TYR:CD1	2.90	0.44
2:B:1276:PHE:CD1	2:B:1276:PHE:O	2.70	0.44
2:B:103:GLU:OE2	2:B:113:HIS:HB2	2.18	0.44
2:B:158:LEU:O	2:B:162:ILE:HG13	2.17	0.44
2:B:270:THR:O	2:B:270:THR:OG1	2.34	0.44
2:B:277:ASN:ND2	2:B:649:LYS:O	2.50	0.44
2:B:359:TYR:CZ	2:B:363:ILE:HD11	2.52	0.44
2:B:975:VAL:CG1	2:B:978:ILE:HG13	2.47	0.44
2:B:1116:SER:O	2:B:1119:LEU:HD22	2.18	0.44
2:B:316:PRO:CG	2:B:317:LEU:N	2.81	0.44
2:B:359:TYR:O	2:B:359:TYR:CD1	2.70	0.44
2:B:466:THR:O	2:B:467:ARG:HG3	2.17	0.44
2:B:612:ASN:O	2:B:616:LEU:HG	2.17	0.44
2:B:51:LEU:HD13	2:B:1352:ILE:O	2.18	0.44
2:B:181:VAL:HG23	2:B:182:ASP:OD1	2.18	0.44
2:B:730:SER:O	2:B:733:ILE:HG22	2.18	0.44



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:887:LEU:HD23	2:B:887:LEU:O	2.16	0.44
2:B:450:TYR:C	2:B:491:PHE:HE1	2.20	0.44
2:B:478:PHE:O	2:B:478:PHE:HD2	2.01	0.44
2:B:552:LEU:HD22	2:B:559:VAL:HG22	1.99	0.44
2:B:811:LEU:HD13	2:B:811:LEU:O	2.18	0.44
2:B:1206:LEU:CA	2:B:1345:ALA:HB1	2.46	0.44
2:B:1217:ALA:O	2:B:1339:THR:HG21	2.18	0.44
2:B:666:LEU:C	2:B:666:LEU:CD2	2.85	0.44
2:B:790:GLU:OE1	2:B:889:ALA:HA	2.17	0.44
2:B:1039:TYR:O	2:B:1042:ILE:HG22	2.18	0.44
2:B:255:ASN:OD1	2:B:256:PHE:CD1	2.70	0.44
2:B:761:ILE:CD1	2:B:931:VAL:CG1	2.95	0.44
2:B:859:ARG:C	2:B:859:ARG:CD	2.86	0.44
2:B:6:SER:OG	2:B:21:ILE:CD1	2.59	0.43
2:B:134:THR:CG2	2:B:136:TYR:CD2	3.01	0.43
2:B:386:THR:HG23	2:B:386:THR:O	2.18	0.43
2:B:518:PHE:CD1	2:B:667:ILE:HG12	2.52	0.43
2:B:553:PHE:CE2	2:B:559:VAL:CG1	2.93	0.43
2:B:1207:GLU:HG2	2:B:1210:ARG:NH1	2.33	0.43
2:B:780:ARG:HD3	2:B:812:TYR:CZ	2.52	0.43
2:B:966:PHE:O	2:B:970:PHE:HB2	2.19	0.43
2:B:1240:SER:HB2	2:B:1242:TYR:CE1	2.53	0.43
2:B:1272:GLN:HE21	2:B:1272:GLN:C	2.19	0.43
2:B:265:GLN:O	2:B:271:TYR:CG	2.70	0.43
2:B:552:LEU:CD2	2:B:563:GLN:NE2	2.80	0.43
2:B:569:PHE:N	2:B:569:PHE:CD2	2.86	0.43
2:B:602:LYS:HE3	2:B:602:LYS:HB2	1.64	0.43
2:B:1204:PHE:CD1	2:B:1347:LEU:CG	3.01	0.43
2:B:1235:PHE:HD1	2:B:1258:PHE:CE2	2.37	0.43
1:A:15:U:O2'	2:B:450:TYR:O	2.30	0.43
1:A:58:G:C1'	2:B:457:ARG:HB2	2.47	0.43
2:B:18:TRP:O	2:B:48:ILE:HD13	2.07	0.43
2:B:135:ILE:HG21	2:B:160:HIS:CD2	2.53	0.43
2:B:181:VAL:CG2	2:B:209:LYS:HB2	2.48	0.43
2:B:266:LEU:H	2:B:266:LEU:HD12	1.84	0.43
2:B:202:ASN:ND2	2:B:204:SER:HA	2.33	0.43
2:B:1123:LYS:HD2	2:B:1123:LYS:HA	1.85	0.43
1:A:27:G:H4'	1:A:28:A:OP2	2.18	0.43
1:A:94:U:H2'	1:A:95:G:C8	2.52	0.43
2:B:320:SER:O	2:B:323:LYS:CB	2.47	0.43
2:B:334:LEU:HD11	2:B:338:LEU:HD11	1.97	0.43



	A h o	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:882:TYR:HD2	2:B:883:TRP:HD1	1.66	0.43
2:B:895:ARG:C	2:B:895:ARG:CD	2.85	0.43
2:B:1211:LYS:HZ3	2:B:1211:LYS:HB2	1.84	0.43
2:B:1220:LEU:HD21	2:B:1342:VAL:HG21	2.00	0.43
2:B:1310:ILE:HA	2:B:1313:PHE:CD2	2.53	0.43
2:B:1359:ARG:HH11	2:B:1359:ARG:CG	2.11	0.43
2:B:34:VAL:HG11	2:B:1359:ARG:HD3	1.99	0.43
2:B:86:PHE:CE2	2:B:155:TYR:HB2	2.54	0.43
2:B:256:PHE:CD1	2:B:256:PHE:N	2.85	0.43
2:B:450:TYR:C	2:B:491:PHE:CE1	2.92	0.43
2:B:520:VAL:HG13	2:B:553:PHE:HE1	1.81	0.43
2:B:1119:LEU:N	2:B:1119:LEU:CD1	2.73	0.43
1:A:71:U:H2'	1:A:72:U:H6	1.83	0.43
2:B:298:ASP:O	2:B:302:LEU:HG	2.19	0.43
2:B:361:GLY:O	2:B:365:GLY:N	2.52	0.43
2:B:823:TYR:CE2	2:B:864:ARG:HB3	2.54	0.43
2:B:1203:LEU:HA	2:B:1212:ARG:O	2.18	0.43
2:B:1325:LYS:HB2	2:B:1330:THR:HA	2.00	0.43
1:A:58:G:O2'	2:B:457:ARG:CA	2.58	0.43
2:B:118:ILE:HG22	2:B:119:PHE:HE1	1.77	0.43
2:B:672:ASP:HB2	2:B:704:PHE:HE2	1.84	0.43
1:A:58:G:O4'	2:B:457:ARG:CD	2.46	0.43
2:B:18:TRP:HE1	2:B:50:ALA:H	1.61	0.43
2:B:256:PHE:CE2	2:B:282:ILE:HG12	2.54	0.43
2:B:307:ARG:HE	2:B:307:ARG:HB2	1.69	0.43
2:B:1143:VAL:HG12	2:B:1164:LEU:O	2.18	0.43
2:B:1324:PHE:N	2:B:1324:PHE:CD1	2.86	0.43
2:B:24:GLU:O	2:B:25:TYR:HB2	2.19	0.42
2:B:106:LEU:HA	2:B:1131:TYR:CE2	2.54	0.42
2:B:229:LEU:HD11	2:B:232:GLU:CB	2.45	0.42
2:B:282:ILE:HG23	2:B:286:TYR:HE1	1.72	0.42
2:B:317:LEU:HA	2:B:320:SER:OG	2.19	0.42
2:B:541:SER:N	2:B:544:GLN:OE1	2.48	0.42
2:B:594:TYR:CE2	2:B:607:LEU:HD12	2.54	0.42
2:B:1308:ASN:O	2:B:1311:HIS:HB2	2.18	0.42
1:A:93:G:H2'	1:A:94:U:C6	2.54	0.42
2:B:193:ASN:OD1	2:B:200:PRO:HA	2.19	0.42
2:B:202:ASN:ND2	2:B:204:SER:CA	2.82	0.42
2:B:1000:LYS:HB2	2:B:1073:VAL:HG21	2.01	0.42
2:B:22:THR:HG22	2:B:23:ASP:H	1.84	0.42
2:B:723:HIS:ND1	2:B:723:HIS:C	2.73	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:1222:LYS:O	2:B:1318:LEU:HA	2.19	0.42
2:B:1235:PHE:CE1	2:B:1258:PHE:CE2	3.07	0.42
2:B:229:LEU:CD1	2:B:229:LEU:C	2.85	0.42
2:B:513:LEU:O	2:B:516:GLU:N	2.53	0.42
2:B:573:GLU:HA	2:B:573:GLU:OE1	2.18	0.42
2:B:817:GLN:HB3	2:B:820:ARG:O	2.20	0.42
2:B:1157:LEU:N	2:B:1157:LEU:CD1	2.73	0.42
2:B:1163:LEU:HD12	2:B:1339:THR:HB	2.02	0.42
2:B:1211:LYS:NZ	2:B:1211:LYS:HB2	2.35	0.42
2:B:594:TYR:C	2:B:594:TYR:CD2	2.93	0.42
2:B:672:ASP:HB2	2:B:704:PHE:CE2	2.54	0.42
2:B:1154:SER:HB2	2:B:1156:LYS:HG3	2.01	0.42
2:B:1333:ARG:HD2	2:B:1335:ARG:HG3	2.02	0.42
2:B:191:THR:HG1	2:B:192:TYR:N	2.18	0.42
2:B:201:ILE:HG22	2:B:202:ASN:H	1.85	0.42
2:B:482:VAL:CG1	2:B:483:ASP:N	2.83	0.42
2:B:495:MET:SD	3:C:17:DA:O4'	2.77	0.42
2:B:522:ASN:ND2	2:B:522:ASN:C	2.73	0.42
2:B:603:ASP:OD1	2:B:606:PHE:N	2.53	0.42
2:B:1239:ALA:HB3	2:B:1306:ALA:HB1	2.01	0.42
2:B:555:THR:C	2:B:556:ASN:ND2	2.73	0.42
2:B:560:THR:OG1	2:B:563:GLN:HG3	2.19	0.42
2:B:569:PHE:N	2:B:569:PHE:HD2	2.17	0.42
2:B:594:TYR:HD2	2:B:594:TYR:C	2.23	0.42
2:B:818:ASN:O	2:B:818:ASN:ND2	2.52	0.42
2:B:843:PRO:HG2	2:B:846:PHE:CE2	2.55	0.42
2:B:1036:TYR:O	2:B:1040:SER:HB3	2.20	0.42
2:B:1210:ARG:CG	2:B:1280:VAL:HG22	2.44	0.42
2:B:60:GLU:HA	2:B:63:ARG:NH1	2.35	0.42
2:B:178:ASN:HA	2:B:299:ALA:CB	2.41	0.42
2:B:465:MET:HE1	2:B:467:ARG:HG2	2.02	0.42
2:B:465:MET:SD	2:B:465:MET:C	2.98	0.42
2:B:495:MET:H	2:B:495:MET:HG2	1.52	0.42
2:B:672:ASP:HA	2:B:703:THR:HG22	2.02	0.42
2:B:733:ILE:O	2:B:737:ILE:HG13	2.18	0.42
2:B:920:GLN:OE1	2:B:961:LYS:HE3	2.20	0.42
1:A:40:C:H2'	1:A:41:A:C8	2.55	0.42
2:B:10:ALA:O	2:B:17:GLY:N	2.52	0.42
2:B:219:SER:O	2:B:223:GLU:HG3	2.20	0.42
2:B:316:PRO:CD	2:B:317:LEU:N	2.83	0.42
2:B:518:PHE:HD1	2:B:667:ILE:CD1	2.32	0.42



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
2:B:652:LYS:HE2	2:B:652:LYS:HB2	1.82	0.42
2:B:389:LEU:O	2:B:392:LYS:N	2.53	0.42
2:B:704:PHE:O	2:B:708:ILE:HG12	2.20	0.42
2:B:810:LYS:HE2	2:B:838:VAL:HG23	2.02	0.42
2:B:883:TRP:CZ3	2:B:900:LEU:HD22	2.54	0.42
2:B:1364:GLN:O	2:B:1364:GLN:HG2	2.19	0.42
2:B:135:ILE:HG21	2:B:160:HIS:NE2	2.34	0.41
2:B:197:GLU:O	2:B:200:PRO:HD3	2.19	0.41
2:B:374:LYS:HE3	2:B:374:LYS:O	2.20	0.41
2:B:398:LEU:CG	2:B:399:LEU:H	2.30	0.41
2:B:27:VAL:HG12	2:B:1086:VAL:HG22	2.02	0.41
2:B:202:ASN:CG	2:B:204:SER:N	2.73	0.41
2:B:256:PHE:N	2:B:256:PHE:HD1	2.18	0.41
2:B:492:ILE:HG23	3:C:17:DA:H5'	2.02	0.41
2:B:555:THR:C	2:B:556:ASN:HD22	2.23	0.41
2:B:591:LEU:HD12	2:B:594:TYR:CG	2.54	0.41
2:B:359:TYR:C	2:B:362:TYR:HB3	2.39	0.41
2:B:361:GLY:CA	2:B:365:GLY:H	2.32	0.41
2:B:625:LEU:HD13	2:B:659:TRP:HZ2	1.86	0.41
2:B:760:VAL:HG13	2:B:956:ILE:CG2	2.50	0.41
2:B:882:TYR:O	2:B:886:LEU:HG	2.21	0.41
2:B:266:LEU:HG	2:B:271:TYR:CZ	2.55	0.41
2:B:668:ASN:OD1	2:B:680:LEU:HB3	1.96	0.41
2:B:905:ARG:NH1	3:C:24:DG:OP1	2.54	0.41
2:B:1149:VAL:HG23	2:B:1149:VAL:O	2.20	0.41
2:B:1207:GLU:CD	2:B:1210:ARG:NH1	2.73	0.41
2:B:313:THR:HG23	2:B:313:THR:O	2.20	0.41
2:B:331:ASP:HB3	2:B:398:LEU:CD1	2.49	0.41
2:B:451:TYR:HA	2:B:491:PHE:CE1	2.30	0.41
2:B:519:THR:HG23	2:B:520:VAL:N	2.36	0.41
2:B:551:LEU:HD12	2:B:552:LEU:N	2.36	0.41
2:B:686:ASP:CG	2:B:691:ARG:NH2	2.73	0.41
2:B:48:ILE:HG13	2:B:1092:VAL:HG13	2.01	0.41
2:B:376:ILE:HD12	2:B:376:ILE:N	2.36	0.41
2:B:512:SER:OG	2:B:617:GLU:OE1	2.24	0.41
1:A:64:U:O3'	2:B:57:GLU:HB2	2.21	0.41
2:B:181:VAL:HG23	2:B:182:ASP:N	2.36	0.41
2:B:492:ILE:CG2	3:C:17:DA:H5'	2.51	0.41
2:B:846:PHE:HB3	2:B:916:PHE:HD2	1.85	0.41
2:B:855:LYS:HB3	2:B:855:LYS:HE2	1.76	0.41
2:B:1105:PHE:CZ	2:B:1169:MET:HG3	2.56	0.41



	A L O	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:67:C:P	2:B:739:GLN:HE22	2.43	0.41
2:B:315:ALA:HB1	2:B:418:GLU:HG2	2.01	0.41
2:B:376:ILE:HD12	2:B:376:ILE:H	1.85	0.41
2:B:563:GLN:O	2:B:567:ASP:N	2.48	0.41
2:B:846:PHE:O	2:B:920:GLN:NE2	2.44	0.41
2:B:1229:PRO:CD	2:B:1232:TYR:CD2	2.94	0.41
1:A:23:U:H3	1:A:48:A:H2	1.66	0.41
2:B:18:TRP:CA	2:B:49:GLY:O	2.69	0.41
2:B:27:VAL:HG12	2:B:1086:VAL:CG2	2.51	0.41
2:B:37:ASN:OD1	2:B:1360:ILE:HA	2.21	0.41
2:B:48:ILE:CG1	2:B:1092:VAL:HG13	2.51	0.41
2:B:188:LEU:O	2:B:192:TYR:N	2.46	0.41
2:B:328:HIS:ND1	2:B:399:LEU:CB	2.84	0.41
2:B:398:LEU:C	2:B:398:LEU:HD12	2.41	0.41
2:B:530:VAL:O	2:B:578:VAL:CG2	2.69	0.41
2:B:624:THR:HA	2:B:656:TYR:HB2	2.02	0.41
2:B:686:ASP:H	2:B:690:ASN:HD21	1.68	0.41
2:B:724:ILE:HD12	2:B:738:LEU:HG	2.03	0.41
2:B:857:LEU:C	2:B:857:LEU:CD2	2.86	0.41
2:B:1276:PHE:CD2	2:B:1316:THR:HB	2.56	0.41
1:A:7:U:O2'	2:B:894:GLN:OE1	2.28	0.41
1:A:31:U:H2'	1:A:32:A:O4'	2.20	0.41
2:B:79:ILE:H	2:B:79:ILE:HG12	1.68	0.41
2:B:300:ILE:CG2	2:B:301:LEU:N	2.83	0.41
2:B:421:ALA:HA	2:B:424:ARG:HB2	2.03	0.41
2:B:465:MET:SD	2:B:465:MET:O	2.79	0.41
2:B:1050:ILE:HG13	2:B:1059:LYS:N	2.36	0.41
2:B:100:ARG:HD2	2:B:117:PRO:HA	2.03	0.40
2:B:451:TYR:HA	2:B:491:PHE:HD1	0.68	0.40
2:B:969:ASP:C	2:B:970:PHE:HD1	2.25	0.40
4:D:3:DT:H2"	4:D:4:DT:H71	2.03	0.40
2:B:154:ILE:O	2:B:158:LEU:HG	2.21	0.40
2:B:681:ASP:HA	2:B:684:LYS:HE2	2.03	0.40
2:B:686:ASP:CG	2:B:690:ASN:HA	2.42	0.40
1:A:58:G:O2'	2:B:457:ARG:HB3	2.03	0.40
2:B:27:VAL:HG11	2:B:1086:VAL:HG13	2.02	0.40
2:B:301:LEU:O	2:B:304:ASP:OD1	2.39	0.40
2:B:518:PHE:CE1	2:B:679:ILE:CG2	2.91	0.40
2:B:1235:PHE:CE1	2:B:1259:VAL:HA	2.56	0.40
2:B:215:ARG:O	2:B:215:ARG:NE	2.44	0.40
2:B:557:ARG:HA	2:B:595:HIS:HD2	1.32	0.40



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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:755:LYS:HZ1	2:B:942:LYS:HE2	1.87	0.40
2:B:939:MET:HG3	2:B:953:VAL:HG11	2.04	0.40
2:B:963:VAL:CG2	2:B:990:ASN:OD1	2.66	0.40
2:B:1183:GLU:HG2	2:B:1187:TYR:O	2.21	0.40
2:B:88:ASN:O	2:B:92:LYS:HE3	2.21	0.40
2:B:188:LEU:HA	2:B:191:THR:OG1	2.22	0.40
2:B:350:ILE:CD1	2:B:350:ILE:N	2.84	0.40
2:B:489:GLN:CG	2:B:493:GLU:CD	2.89	0.40
2:B:823:TYR:CD2	2:B:858:THR:HG21	2.56	0.40

All (3) 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:B:232:GLU:O	2:B:573:GLU:OE2[4_445]	1.99	0.21
2:B:226:ILE:CD1	2:B:574:CYS:SG[4_445]	2.08	0.12
2:B:611:GLU:O	2:B:859:ARG:NH2[1_565]	2.12	0.08

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
2	В	1318/1368~(96%)	1254 (95%)	62~(5%)	2~(0%)	47 79

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	В	250	PRO
2	В	316	PRO



5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	В	1183/1225~(97%)	997~(84%)	186 (16%)	2 17

All (186) residues with a non-rotameric sidechain are listed below:

\mathbf{Mol}	Chain	Res	Type
2	В	26	LYS
2	В	48	ILE
2	В	53	PHE
2	В	86	PHE
2	В	104	SER
2	В	114	GLU
2	В	115	ARG
2	В	116	HIS
2	В	125	GLU
2	В	129	HIS
2	В	132	TYR
2	В	144	ASP
2	В	167	HIS
2	В	177	ASP
2	В	182	ASP
2	В	185	PHE
2	В	188	LEU
2	В	189	VAL
2	В	194	GLN
2	В	196	PHE
2	В	197	GLU
2	В	204	SER
2	В	215	ARG
2	В	232	GLU
2	В	233	LYS
2	В	246	LEU
2	В	248	LEU
2	В	252	PHE
2	В	253	LYS
2	В	258	LEU



Mol	Chain	Res	Type
2	В	260	GLU
2	В	261	ASP
2	В	267	SER
2	В	281	GLN
2	В	284	ASP
2	В	291	LEU
2	В	294	LYS
2	В	296	LEU
2	В	300	ILE
2	В	303	SER
2	В	307	ARG
2	В	310	THR
2	В	311	GLU
2	В	317	LEU
2	В	318	SER
2	В	341	GLN
2	В	342	GLN
2	В	343	LEU
2	В	347	TYR
2	В	350	ILE
2	В	355	SER
2	В	362	TYR
2	В	372	PHE
2	В	374	LYS
2	В	376	ILE
2	В	383	MET
2	В	384	ASP
2	В	387	GLU
2	В	390	LEU
2	В	393	LEU
2	В	397	ASP
2	В	398	LEU
2	В	399	LEU
2	В	400	ARG
2	В	425	ARG
2	В	432	PHE
2	В	460	SER
2	B	461	ARG
2	B	464	TRP
2	B	465	MET
2	B	478	PHE
2	В	480	GLU



Mol	Chain	Res	Type
2	В	491	PHE
2	В	492	ILE
2	В	494	ARG
2	В	495	MET
2	В	506	LYS
2	В	518	PHE
2	В	521	TYR
2	В	522	ASN
2	В	529	TYR
2	В	535	ARG
2	В	546	LYS
2	В	550	ASP
2	В	551	LEU
2	В	552	LEU
2	В	555	THR
2	В	557	ARG
2	В	564	LEU
2	В	576	ASP
2	В	577	SER
2	В	591	LEU
2	В	593	THR
2	В	594	TYR
2	В	597	LEU
2	В	598	LEU
2	В	600	ILE
2	В	602	LYS
2	В	621	LEU
2	В	631	MET
2	В	661	ARG
2	В	662	LEU
2	В	664	ARG
2	В	665	LYS
2	В	686	ASP
2	В	691	ARG
2	B	719	SER
2	В	720	LEU
2	В	723	HIS
2	В	727	LEU
2	B	751	MET
2	В	763	MET
2	В	820	ARG
2	В	821	ASP



Mol	Chain	Res	Type
2	В	826	GLN
2	В	829	ASP
2	В	855	LYS
2	В	858	THR
2	В	859	ARG
2	В	860	SER
2	В	861	ASP
2	В	868	ASP
2	В	873	GLU
2	В	885	GLN
2	В	887	LEU
2	В	893	THR
2	В	895	ARG
2	В	905	ARG
2	В	926	GLN
2	В	933	GLN
2	В	936	ASP
2	В	937	SER
2	В	944	ASP
2	В	948	LYS
2	В	949	LEU
2	В	964	SER
2	В	968	LYS
2	В	969	ASP
2	В	971	GLN
2	В	973	TYR
2	В	974	LYS
2	В	980	ASN
2	В	1031	LYS
2	В	1037	PHE
2	В	1045	PHE
2	В	1065	THR
2	В	1080	PHE
2	В	1091	GLN
2	В	1116	SER
2	В	1119	LEU
2	В	1123	LYS
2	В	1134	PHE
2	В	1138	THR
2	В	1148	LYS
2	В	1154	SER
2	В	1157	LEU



Mol	Chain	Res	Type
2	В	1158	LYS
2	В	1159	SER
2	В	1206	LEU
2	В	1207	GLU
2	В	1210	ARG
2	В	1211	LYS
2	В	1212	ARG
2	В	1231	LYS
2	В	1235	PHE
2	В	1240	SER
2	В	1243	GLU
2	В	1244	LYS
2	В	1245	LEU
2	В	1246	LYS
2	В	1248	SER
2	В	1255	LYS
2	В	1272	GLN
2	В	1274	SER
2	В	1287	LEU
2	В	1325	LYS
2	В	1326	TYR
2	В	1327	PHE
2	В	1328	ASP
2	В	1329	THR
2	В	1340	LYS
2	В	1341	GLU
2	B	1343	LEU
2	В	1347	LEU
2	В	1359	ARG
2	В	1364	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	\mathbf{Res}	Type
2	В	190	GLN
2	В	202	ASN
2	В	342	GLN
2	В	459	ASN
2	В	522	ASN
2	В	668	ASN
2	В	690	ASN
2	В	980	ASN



Continued from previous page...

Mol	Chain	Res	Type
2	В	990	ASN
2	В	1091	GLN
2	В	1224	ASN
2	В	1262	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	А	93/98~(94%)	27~(29%)	4 (4%)

All (27) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	А	9	U
1	А	11	С
1	А	27	G
1	А	28	А
1	А	29	G
1	А	34	А
1	А	37	U
1	А	38	А
1	А	40	С
1	A	42	А
1	А	43	G
1	А	51	А
1	А	56	U
1	А	57	А
1	А	59	U
1	А	60	С
1	А	63	U
1	А	68	А
1	А	69	А
1	A	74	А
1	A	77	A
1	А	82	G
1	A	87	G
1	А	89	G
1	A	90	U
1	A	91	С
1	А	92	G



All (4) RNA pucker outliers are listed below:

Mol	Chain	\mathbf{Res}	Type
1	А	8	G
1	А	27	G
1	А	42	А
1	А	68	А

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

