



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 08:30 pm BST

PDB ID : 5WQE  
Title : Crystal structure of Alicyclobacillus acidoterrestris C2c1 in complex with single-guide RNA at 3.1 Angstrom resolution  
Authors : Liu, L.; Wang, Y.L.  
Deposited on : 2016-11-26  
Resolution : 3.13 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 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 : 2.11  
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) : 2.11

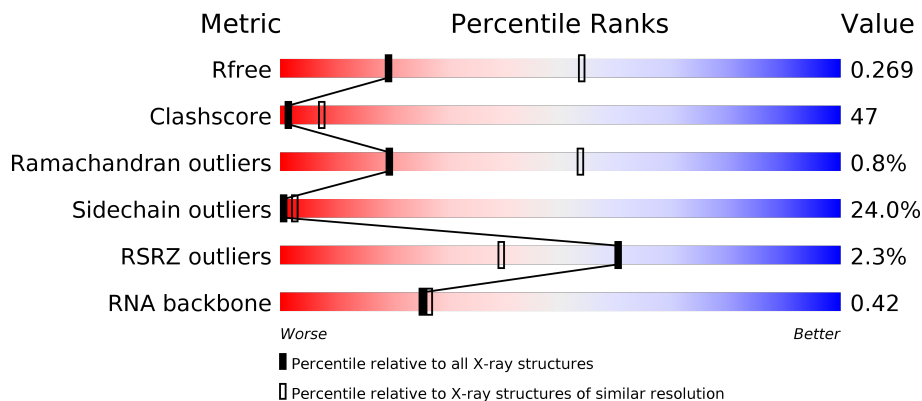
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.13 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	1292 (3.14-3.10)
Clashscore	141614	1389 (3.14-3.10)
Ramachandran outliers	138981	1337 (3.14-3.10)
Sidechain outliers	138945	1337 (3.14-3.10)
RSRZ outliers	127900	1260 (3.14-3.10)
RNA backbone	3102	1134 (3.44-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1137	 2% 38% 39% 11% 11%
2	B	112	 12% 19% 21% 46%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9308 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 CRISPR-associated endonuclease C2c1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	1011	7988	5033	1476	1452	8	19	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1130	LEU	-	expression tag	UNP T0D7A2
A	1131	GLU	-	expression tag	UNP T0D7A2
A	1132	HIS	-	expression tag	UNP T0D7A2
A	1133	HIS	-	expression tag	UNP T0D7A2
A	1134	HIS	-	expression tag	UNP T0D7A2
A	1135	HIS	-	expression tag	UNP T0D7A2
A	1136	HIS	-	expression tag	UNP T0D7A2
A	1137	HIS	-	expression tag	UNP T0D7A2

- Molecule 2 is a RNA chain called RNA (60-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	60	1278	567	241	410	60	0	0	0

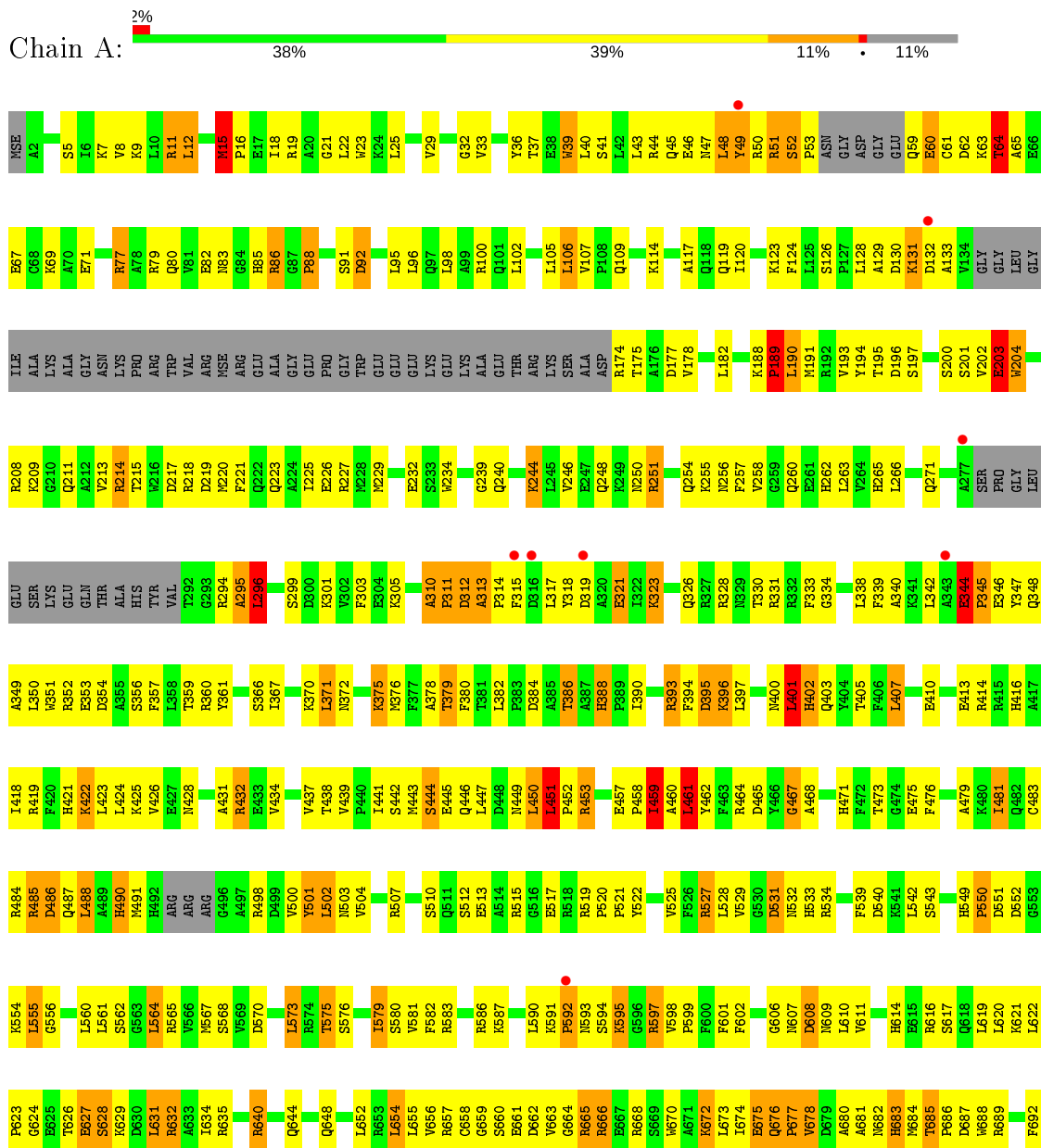
- Molecule 3 is water.

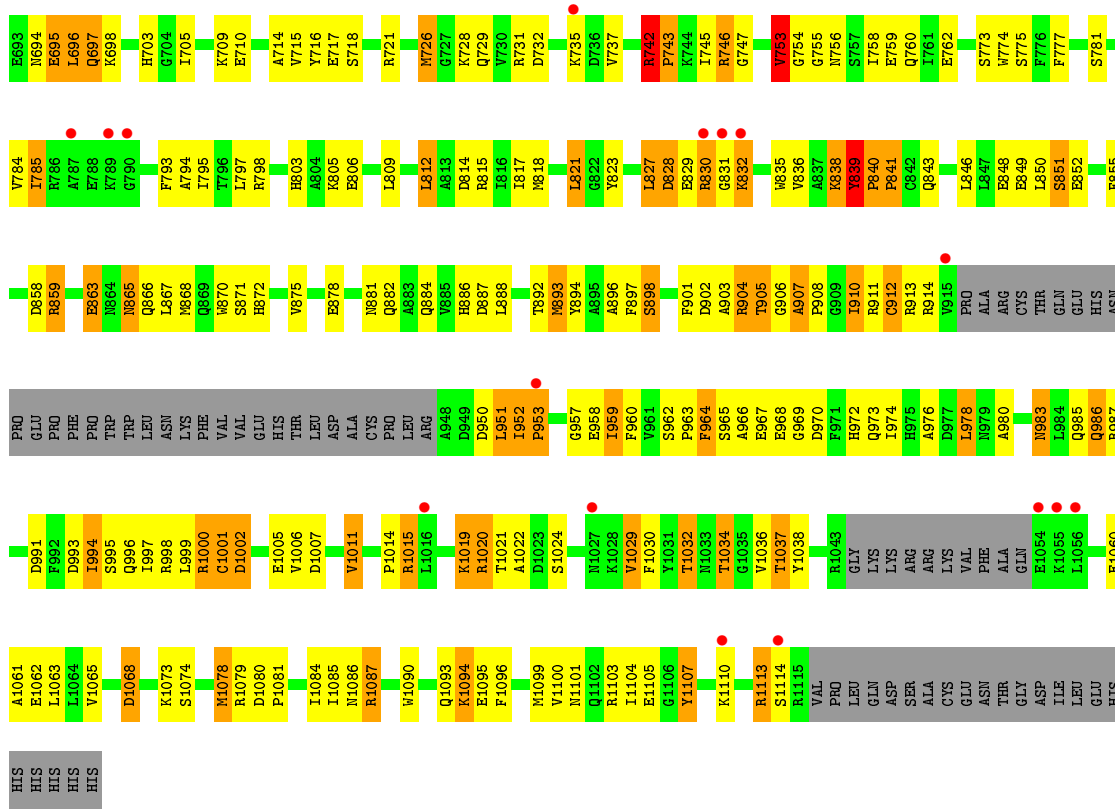
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	39	Total	O	0	0
			39	39		
3	B	3	Total	O	0	0
			3	3		

### 3 Residue-property plots

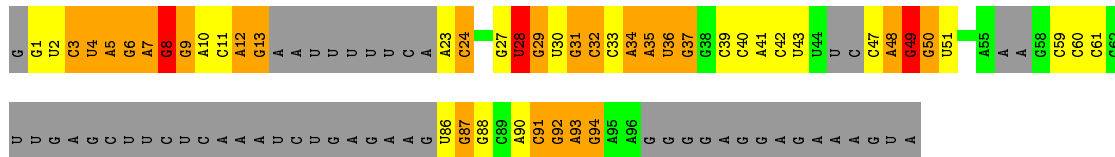
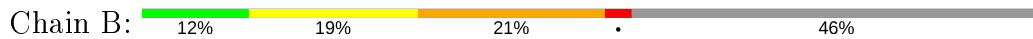
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: CRISPR-associated endonuclease C2c1





• Molecule 2: RNA (60-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	194.55Å 129.84Å 84.00Å 90.00° 110.00° 90.00°	Depositor
Resolution (Å)	48.64 – 3.13 48.64 – 3.13	Depositor EDS
% Data completeness (in resolution range)	79.3 (48.64-3.13) 79.3 (48.64-3.13)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.87 (at 3.12Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.238 , 0.268 0.239 , 0.269	Depositor DCC
$R_{free}$ test set	1340 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtrriage
Anisotropy	0.358	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 21.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	9308	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% 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](#)

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	0.70	12/8134 (0.1%)	0.88	34/10953 (0.3%)
2	B	0.52	1/1427 (0.1%)	0.85	5/2217 (0.2%)
All	All	0.67	13/9561 (0.1%)	0.87	39/13170 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	841	PRO	N-CD	-6.47	1.38	1.47
1	A	677	PRO	N-CD	5.42	1.55	1.47
1	A	345	PRO	N-CD	5.40	1.55	1.47
1	A	88	PRO	N-CD	5.39	1.55	1.47
1	A	520	PRO	N-CD	5.34	1.55	1.47
1	A	311	PRO	N-CD	5.28	1.55	1.47
1	A	189	PRO	N-CD	5.26	1.55	1.47
1	A	592	PRO	N-CD	5.25	1.55	1.47
1	A	521	PRO	N-CD	5.12	1.55	1.47
1	A	743	PRO	N-CD	5.11	1.55	1.47
2	B	49	G	O3'-P	-5.05	1.55	1.61
1	A	840	PRO	N-CD	5.02	1.54	1.47
1	A	314	PRO	N-CD	5.00	1.54	1.47

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	203	GLU	CB-CA-C	-13.91	82.58	110.40

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	LEU	N-CA-CB	13.47	137.34	110.40
1	A	753	VAL	N-CA-C	12.27	144.12	111.00
1	A	295	ALA	N-CA-C	-12.09	78.36	111.00
1	A	421	HIS	N-CA-C	-10.52	82.60	111.00
1	A	953	PRO	CA-N-CD	-8.14	100.11	111.50
2	B	49	G	C2'-C3'-O3'	8.04	127.20	109.50
1	A	204	TRP	N-CA-CB	-7.81	96.54	110.60
1	A	608	ASP	CB-CA-C	-7.26	95.89	110.40
1	A	15	MSE	C-N-CD	6.64	142.35	128.40
2	B	28	U	C2'-C3'-O3'	6.33	123.83	113.70
1	A	549	HIS	C-N-CD	6.23	141.47	128.40
1	A	52	SER	C-N-CD	6.22	141.47	128.40
1	A	685	THR	C-N-CD	6.19	141.41	128.40
1	A	451	LEU	C-N-CD	6.19	141.39	128.40
1	A	457	GLU	C-N-CD	6.17	141.35	128.40
1	A	753	VAL	CB-CA-C	-6.07	99.88	111.40
1	A	107	VAL	C-N-CD	6.03	141.06	128.40
1	A	598	VAL	C-N-CD	6.03	141.06	128.40
1	A	907	ALA	C-N-CD	6.02	141.05	128.40
1	A	841	PRO	N-CD-CG	5.98	112.17	103.20
1	A	422	LYS	N-CA-C	5.86	126.83	111.00
1	A	388	HIS	C-N-CD	5.83	140.65	128.40
1	A	313	ALA	C-N-CD	5.77	140.51	128.40
1	A	742	ARG	C-N-CD	5.76	140.49	128.40
1	A	295	ALA	CB-CA-C	-5.66	101.61	110.10
1	A	310	ALA	C-N-CD	5.65	140.27	128.40
1	A	839	TYR	C-N-CD	5.60	140.16	128.40
1	A	520	PRO	C-N-CD	5.51	139.97	128.40
1	A	344	GLU	C-N-CD	5.46	139.86	128.40
2	B	8	G	C4'-C3'-O3'	-5.37	98.13	109.40
2	B	49	G	N9-C1'-C2'	-5.28	106.20	112.00
1	A	461	LEU	CA-CB-CG	5.26	127.39	115.30
1	A	551	ASP	CB-CG-OD2	5.16	122.94	118.30
2	B	3	C	C4'-C3'-O3'	-5.13	98.63	109.40
1	A	550	PRO	CA-N-CD	-5.12	104.33	111.50
1	A	622	LEU	C-N-CD	5.09	139.09	128.40
1	A	203	GLU	N-CA-C	-5.08	97.28	111.00
1	A	16	PRO	CA-N-CD	-5.04	104.44	111.50

There are no chirality outliers.

All (5) planarity outliers are listed below:



Mol	Chain	Res	Type	Group
1	A	467	GLY	Peptide
1	A	531	ASP	Peptide
1	A	64	THR	Peptide
1	A	784	VAL	Peptide
1	A	912	CYS	Peptide

## 5.2 Too-close contacts [\(i\)](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7988	0	7713	724	0
2	B	1278	0	645	129	0
3	A	39	0	0	3	0
3	B	3	0	0	0	0
All	All	9308	0	8358	825	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 47.

All (825) 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:8:G:H3'	2:B:9:G:C5'	1.71	1.19
1:A:575:THR:CG2	1:A:621:LYS:HE2	1.73	1.18
1:A:758:ILE:HG23	1:A:867:LEU:HD23	1.27	1.14
1:A:1073:LYS:HE2	1:A:1073:LYS:HA	1.15	1.13
2:B:11:C:H2'	2:B:12:A:H5'	1.31	1.11
2:B:8:G:H3'	2:B:9:G:H5'	1.31	1.10
1:A:1062:GLU:HA	1:A:1065:VAL:CG2	1.82	1.08
2:B:47:C:H2'	2:B:48:A:H5''	1.25	1.08
1:A:967:GLU:HA	1:A:1103:ARG:NH2	1.68	1.08
1:A:913:ARG:HB2	1:A:953:PRO:HD2	1.32	1.07
1:A:510:SER:HB2	1:A:513:GLU:HG3	1.33	1.07
2:B:12:A:H2'	2:B:13:G:C8	1.89	1.05
1:A:913:ARG:HB2	1:A:953:PRO:CD	1.87	1.04
1:A:45:GLN:CG	1:A:69:LYS:HD3	1.87	1.04
2:B:11:C:C2'	2:B:12:A:H5'	1.87	1.03

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ARG:HH11	1:A:665:ARG:HB3	1.22	1.02
1:A:11:ARG:HB3	1:A:11:ARG:HH11	1.22	1.02
2:B:9:G:C2	2:B:10:A:C5	2.47	1.02
1:A:131:LYS:HA	1:A:131:LYS:HE3	1.38	1.02
1:A:573:LEU:HD12	1:A:573:LEU:H	1.22	1.02
1:A:491:MSE:SE	1:A:498:ARG:CB	2.59	1.00
1:A:607:ASN:HB3	1:A:610:LEU:HB2	1.42	1.00
1:A:575:THR:HG22	1:A:621:LYS:CE	1.91	0.98
1:A:904:ARG:HG3	1:A:904:ARG:HH11	1.28	0.98
1:A:575:THR:HG22	1:A:621:LYS:HE2	0.99	0.97
1:A:483:CYS:SG	1:A:488:LEU:CD2	2.53	0.97
1:A:303:PHE:CE2	1:A:350:LEU:CB	2.48	0.96
1:A:964:PHE:CE2	1:A:970:ASP:HB3	1.99	0.96
1:A:597:ARG:HB3	1:A:597:ARG:NH1	1.81	0.96
1:A:45:GLN:HG2	1:A:69:LYS:HD3	1.44	0.95
1:A:213:VAL:HG13	1:A:217:ASP:HB2	1.47	0.94
1:A:758:ILE:CG2	1:A:867:LEU:HD23	1.98	0.94
1:A:64:THR:CB	1:A:65:ALA:HB3	1.97	0.94
1:A:758:ILE:HG23	1:A:867:LEU:CD2	1.98	0.93
1:A:726:MSE:HE2	1:A:774:TRP:CZ3	2.04	0.93
1:A:64:THR:HB	1:A:65:ALA:HB3	1.49	0.92
2:B:50:G:H8	2:B:50:G:H5''	1.31	0.92
2:B:8:G:C3'	2:B:9:G:C5'	2.48	0.92
1:A:785:ILE:H	1:A:785:ILE:HD12	1.34	0.92
2:B:47:C:C2'	2:B:48:A:H5''	1.98	0.92
1:A:79:ARG:NH2	1:A:82:GLU:HG2	1.84	0.92
1:A:1062:GLU:CA	1:A:1065:VAL:HG22	1.99	0.91
1:A:1073:LYS:HE2	1:A:1073:LYS:CA	2.01	0.91
1:A:1020:ARG:HG2	1:A:1020:ARG:HH11	1.33	0.91
1:A:674:ILE:HD12	1:A:675:GLU:H	1.36	0.91
1:A:248:GLN:HB3	1:A:1060:GLU:OE2	1.71	0.90
1:A:913:ARG:CB	1:A:953:PRO:HD2	2.00	0.90
1:A:534:ARG:HH11	1:A:534:ARG:HG3	1.36	0.90
1:A:682:ASN:HB3	1:A:683:HIS:ND1	1.86	0.90
1:A:1062:GLU:HA	1:A:1065:VAL:HG22	1.52	0.89
1:A:838:LYS:HB3	1:A:839:TYR:CD1	2.08	0.89
2:B:9:G:C6	2:B:10:A:N6	2.39	0.89
1:A:1062:GLU:C	1:A:1065:VAL:HG22	1.92	0.89
1:A:215:THR:CG2	1:A:422:LYS:NZ	2.36	0.88
1:A:339:PHE:HD1	1:A:342:LEU:HD12	1.36	0.88
1:A:579:ILE:HG21	1:A:620:LEU:HD11	1.55	0.88

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:CG2	1:A:65:ALA:HB3	2.03	0.88
1:A:897:PHE:CZ	1:A:1078:MSE:HE1	2.09	0.88
1:A:79:ARG:HH22	1:A:82:GLU:HG2	1.40	0.87
1:A:371:LEU:HD12	1:A:372:ASN:N	1.90	0.87
1:A:838:LYS:HZ3	1:A:838:LYS:HB2	1.39	0.87
1:A:967:GLU:HA	1:A:1103:ARG:HH22	1.35	0.87
1:A:510:SER:HB2	1:A:513:GLU:CG	2.06	0.86
2:B:8:G:H3'	2:B:9:G:H5''	1.55	0.86
1:A:1095:GLU:O	1:A:1099:MSE:HG3	1.75	0.85
1:A:527:ARG:O	1:A:528:LEU:HD23	1.75	0.85
1:A:33:VAL:O	1:A:37:THR:OG1	1.95	0.85
1:A:485:ARG:HG2	1:A:485:ARG:HH11	1.40	0.84
1:A:665:ARG:HH11	1:A:665:ARG:CB	1.88	0.84
1:A:215:THR:HG21	1:A:422:LYS:NZ	1.93	0.84
1:A:663:VAL:HG12	1:A:664:GLY:H	1.41	0.84
2:B:9:G:N1	2:B:10:A:C6	2.46	0.84
1:A:1062:GLU:HA	1:A:1065:VAL:HG21	1.57	0.84
1:A:677:PRO:O	1:A:678:VAL:CG2	2.26	0.84
1:A:677:PRO:O	1:A:678:VAL:HG22	1.78	0.83
2:B:9:G:C4	2:B:10:A:N7	2.46	0.83
1:A:755:GLY:N	1:A:760:GLN:HG3	1.94	0.83
2:B:47:C:H2'	2:B:48:A:C5'	2.07	0.83
2:B:11:C:H2'	2:B:12:A:C5'	2.09	0.82
1:A:11:ARG:CB	1:A:11:ARG:HH11	1.92	0.82
2:B:31:G:O2'	2:B:32:C:O5'	1.97	0.82
1:A:43:LEU:HD13	1:A:43:LEU:O	1.79	0.82
1:A:1061:ALA:O	1:A:1065:VAL:HG13	1.80	0.81
1:A:49:TYR:CE1	1:A:380:PHE:CD2	2.68	0.81
1:A:48:LEU:H	1:A:48:LEU:HD23	1.44	0.81
1:A:682:ASN:HB3	1:A:683:HIS:CE1	2.15	0.81
1:A:905:THR:OG1	1:A:906:GLY:HA2	1.79	0.81
1:A:36:TYR:CD1	1:A:191:MSE:HE1	2.16	0.81
1:A:59:GLN:NE2	1:A:379:THR:HG23	1.95	0.80
1:A:9:LYS:HD3	2:B:29:G:OP1	1.82	0.80
1:A:396:LYS:H	1:A:396:LYS:HD3	1.47	0.79
1:A:311:PRO:HD3	1:A:351:TRP:CZ2	2.17	0.79
1:A:958:GLU:O	1:A:976:ALA:HB3	1.83	0.79
2:B:5:A:O2'	2:B:6:G:OP1	2.01	0.79
1:A:951:LEU:HG	1:A:952:ILE:HG13	1.65	0.79
1:A:396:LYS:HD3	1:A:396:LYS:N	1.98	0.79
1:A:958:GLU:O	1:A:976:ALA:CB	2.31	0.78

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:ASP:HB3	1:A:1074:SER:HB2	1.65	0.78
2:B:35:A:H4'	2:B:36:U:OP2	1.82	0.78
2:B:9:G:H2'	2:B:10:A:C8	2.18	0.78
1:A:510:SER:CB	1:A:513:GLU:HG3	2.13	0.78
1:A:423:LEU:O	1:A:434:VAL:HG12	1.82	0.78
1:A:674:ILE:HD12	1:A:675:GLU:N	1.97	0.78
2:B:8:G:C3'	2:B:9:G:H5''	2.11	0.78
2:B:9:G:N3	2:B:10:A:N7	2.31	0.78
1:A:863:GLU:O	1:A:868:MSE:HG3	1.84	0.78
2:B:11:C:C2'	2:B:12:A:C5'	2.63	0.77
2:B:11:C:O2'	2:B:12:A:H5'	1.83	0.77
1:A:660:SER:HB2	1:A:661:GLU:C	2.04	0.77
1:A:827:LEU:HG	1:A:830:ARG:HG2	1.67	0.77
2:B:12:A:H2'	2:B:13:G:H8	1.49	0.77
1:A:1085:ILE:HG21	1:A:1096:PHE:CE1	2.21	0.76
1:A:754:GLY:HA3	1:A:760:GLN:CG	2.14	0.76
1:A:339:PHE:HA	1:A:342:LEU:HD12	1.67	0.76
1:A:904:ARG:NH1	1:A:904:ARG:HG3	1.96	0.76
1:A:12:LEU:HD22	1:A:15:MSE:HG3	1.66	0.76
2:B:9:G:H2'	2:B:10:A:H8	1.50	0.76
1:A:827:LEU:O	1:A:830:ARG:HB3	1.86	0.76
1:A:131:LYS:HE3	1:A:131:LYS:CA	2.14	0.75
1:A:45:GLN:CG	1:A:69:LYS:CD	2.64	0.75
1:A:829:GLU:O	1:A:830:ARG:HG3	1.85	0.75
1:A:1094:LYS:HB2	1:A:1094:LYS:NZ	2.00	0.75
1:A:386:THR:HA	1:A:488:LEU:HD12	1.67	0.75
1:A:579:ILE:HD13	1:A:579:ILE:O	1.86	0.75
1:A:64:THR:HG22	1:A:65:ALA:HB3	1.66	0.75
2:B:23:A:H2'	2:B:24:C:H6	1.50	0.75
2:B:7:A:O2'	2:B:8:G:H5'	1.86	0.75
1:A:617:SER:HB3	1:A:978:LEU:CD1	2.16	0.75
1:A:754:GLY:HA3	1:A:760:GLN:HG3	1.67	0.75
1:A:1062:GLU:O	1:A:1065:VAL:HG22	1.86	0.75
1:A:659:GLY:O	1:A:660:SER:OG	2.04	0.75
1:A:967:GLU:CA	1:A:1103:ARG:HH22	2.00	0.74
1:A:660:SER:HB3	1:A:666:ARG:HB2	1.69	0.74
1:A:215:THR:CG2	1:A:422:LYS:HZ3	1.97	0.74
1:A:555:LEU:HD13	1:A:555:LEU:N	2.01	0.74
2:B:50:G:C8	2:B:50:G:H5''	2.21	0.74
1:A:453:ARG:HD3	1:A:460:ALA:HB1	1.70	0.74
1:A:485:ARG:NH1	1:A:485:ARG:HG2	1.99	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1062:GLU:CA	1:A:1065:VAL:CG2	2.59	0.74
1:A:1062:GLU:O	1:A:1065:VAL:CG2	2.34	0.74
1:A:660:SER:OG	1:A:661:GLU:HA	1.86	0.74
1:A:1032:THR:HG23	1:A:1038:TYR:CD2	2.23	0.73
1:A:453:ARG:CG	1:A:460:ALA:HB1	2.17	0.73
1:A:619:LEU:HD12	2:B:10:A:H5'	1.71	0.73
1:A:44:ARG:HG3	1:A:46:GLU:O	1.88	0.73
1:A:966:ALA:HB1	1:A:1084:ILE:HG12	1.70	0.73
1:A:36:TYR:HD1	1:A:191:MSE:HE1	1.53	0.73
1:A:695:GLU:HG3	1:A:718:SER:OG	1.89	0.73
1:A:215:THR:HG21	1:A:422:LYS:HZ3	1.52	0.73
1:A:670:TRP:CH2	1:A:674:ILE:HG21	2.24	0.73
1:A:528:LEU:HA	1:A:534:ARG:O	1.89	0.72
1:A:573:LEU:HD12	1:A:573:LEU:N	2.01	0.72
2:B:9:G:N3	2:B:10:A:C8	2.57	0.72
1:A:838:LYS:HD2	1:A:839:TYR:CE1	2.25	0.72
1:A:51:ARG:NH2	1:A:52:SER:O	2.23	0.71
1:A:1086:ASN:O	1:A:1087:ARG:HB2	1.88	0.71
1:A:347:TYR:O	1:A:351:TRP:HB2	1.90	0.71
1:A:581:VAL:HG21	1:A:616:ARG:HE	1.56	0.71
1:A:39:TRP:O	1:A:43:LEU:HB2	1.91	0.71
1:A:402:HIS:H	1:A:402:HIS:CD2	2.07	0.71
1:A:215:THR:HG23	1:A:422:LYS:NZ	2.04	0.71
1:A:193:VAL:HG23	1:A:193:VAL:O	1.89	0.71
2:B:93:A:H2'	2:B:94:G:H5'	1.73	0.71
1:A:838:LYS:NZ	1:A:838:LYS:HB2	2.06	0.71
1:A:49:TYR:CD1	1:A:380:PHE:CD2	2.79	0.70
1:A:394:PHE:HE2	1:A:481:ILE:HD11	1.55	0.70
1:A:1032:THR:HG22	1:A:1037:THR:O	1.90	0.70
1:A:1020:ARG:HG2	1:A:1020:ARG:NH1	1.99	0.70
1:A:595:LYS:C	1:A:595:LYS:HD3	2.12	0.70
1:A:400:ASN:O	1:A:401:LEU:HD13	1.91	0.69
2:B:93:A:C2'	2:B:94:G:H5'	2.22	0.69
1:A:126:SER:O	1:A:130:ASP:HB3	1.92	0.69
1:A:338:LEU:O	1:A:342:LEU:HG	1.91	0.69
1:A:262:HIS:CE1	1:A:263:LEU:HG	2.27	0.69
1:A:213:VAL:HG13	1:A:217:ASP:CB	2.23	0.69
1:A:692:PHE:O	1:A:696:LEU:HB2	1.91	0.69
1:A:131:LYS:CE	1:A:132:ASP:H	2.05	0.69
1:A:208:ARG:HG3	1:A:208:ARG:HH11	1.56	0.69
1:A:658:CYS:O	1:A:666:ARG:HG3	1.93	0.69

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:VAL:O	1:A:753:VAL:HG23	1.92	0.69
1:A:849:GLU:HG3	1:A:894:TYR:HA	1.75	0.69
1:A:1002:ASP:OD1	1:A:1002:ASP:N	2.23	0.69
1:A:1094:LYS:HG3	1:A:1095:GLU:OE1	1.93	0.69
1:A:225:ILE:HG22	1:A:229:MSE:HE3	1.75	0.68
1:A:597:ARG:HB3	1:A:597:ARG:HH11	1.57	0.68
1:A:677:PRO:C	1:A:678:VAL:HG23	2.14	0.68
1:A:555:LEU:H	1:A:555:LEU:HD13	1.59	0.68
1:A:479:ALA:HB2	1:A:504:VAL:HG12	1.76	0.68
1:A:483:CYS:SG	1:A:488:LEU:HD23	2.33	0.68
1:A:838:LYS:HB3	1:A:839:TYR:HD1	1.57	0.68
1:A:668:ARG:O	1:A:672:LYS:HG2	1.94	0.68
1:A:755:GLY:H	1:A:760:GLN:HG3	1.56	0.68
1:A:86:ARG:HH11	1:A:86:ARG:HG2	1.58	0.68
2:B:1:G:H2'	2:B:2:U:H6	1.58	0.68
1:A:579:ILE:HD13	1:A:579:ILE:C	2.14	0.68
1:A:130:ASP:OD2	1:A:132:ASP:HA	1.94	0.68
1:A:326:GLN:O	1:A:330:THR:HB	1.93	0.68
1:A:444:SER:HB2	2:B:29:G:C8	2.29	0.68
1:A:447:LEU:O	1:A:450:LEU:HD22	1.94	0.68
1:A:794:ALA:HB1	1:A:797:LEU:HB3	1.76	0.67
1:A:1000:ARG:CZ	1:A:1065:VAL:HB	2.24	0.67
1:A:1085:ILE:CG2	1:A:1096:PHE:CE1	2.77	0.67
1:A:215:THR:OG1	1:A:402:HIS:HD2	1.77	0.67
1:A:64:THR:HG22	1:A:65:ALA:CB	2.23	0.67
1:A:131:LYS:HD3	1:A:133:ALA:H	1.59	0.67
1:A:964:PHE:HD1	1:A:965:SER:HB3	1.58	0.67
1:A:48:LEU:N	1:A:48:LEU:HD23	2.10	0.67
1:A:994:ILE:H	1:A:994:ILE:HD12	1.59	0.67
1:A:785:ILE:HD12	1:A:785:ILE:N	2.03	0.67
1:A:865:ASN:HD22	1:A:867:LEU:H	1.43	0.67
1:A:737:VAL:HA	1:A:742:ARG:HH21	1.58	0.66
1:A:597:ARG:HB3	1:A:597:ARG:CZ	2.25	0.66
1:A:45:GLN:HG3	1:A:69:LYS:CD	2.25	0.66
1:A:601:PHE:CD2	1:A:611:VAL:HG21	2.30	0.66
1:A:213:VAL:CG1	1:A:217:ASP:HB2	2.24	0.66
1:A:591:LYS:N	1:A:592:PRO:HD2	2.10	0.66
1:A:731:ARG:HD3	1:A:735:LYS:NZ	2.11	0.66
1:A:453:ARG:CD	1:A:460:ALA:HB1	2.26	0.66
2:B:40:C:H2'	2:B:41:A:H8	1.59	0.66
1:A:1011:VAL:HG11	1:A:1029:VAL:CG1	2.26	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:PHE:CD1	1:A:342:LEU:HD12	2.25	0.66
1:A:1001:CYS:HB3	1:A:1014:PRO:HA	1.78	0.65
1:A:967:GLU:HA	1:A:1103:ARG:CZ	2.26	0.65
1:A:458:PRO:C	1:A:459:ILE:HG23	2.17	0.65
1:A:579:ILE:HG21	1:A:620:LEU:CD1	2.27	0.65
1:A:51:ARG:CZ	1:A:52:SER:O	2.44	0.65
1:A:564:LEU:HD13	1:A:565:ARG:N	2.11	0.65
1:A:36:TYR:CD1	1:A:191:MSE:CE	2.79	0.65
1:A:131:LYS:HD3	1:A:132:ASP:N	2.11	0.65
2:B:40:C:H2'	2:B:41:A:C8	2.31	0.65
1:A:865:ASN:HD22	1:A:867:LEU:N	1.94	0.65
1:A:967:GLU:CA	1:A:1103:ARG:NH2	2.51	0.65
1:A:467:GLY:N	1:A:468:ALA:O	2.30	0.65
1:A:534:ARG:NH1	1:A:534:ARG:HG3	2.05	0.65
1:A:575:THR:CG2	1:A:621:LYS:CE	2.62	0.64
1:A:594:SER:HB2	1:A:597:ARG:O	1.97	0.64
1:A:213:VAL:HG12	1:A:214:ARG:O	1.96	0.64
1:A:694:ASN:O	1:A:697:GLN:HG3	1.98	0.64
1:A:680:ALA:O	1:A:684:MSE:HE3	1.98	0.64
1:A:726:MSE:HE2	1:A:774:TRP:CE3	2.32	0.64
2:B:36:U:H4'	2:B:37:G:OP2	1.98	0.64
1:A:193:VAL:CG2	1:A:196:ASP:HB3	2.28	0.64
1:A:340:ALA:HB1	1:A:668:ARG:NH2	2.12	0.64
2:B:23:A:H2'	2:B:24:C:C6	2.30	0.64
1:A:215:THR:CG2	1:A:422:LYS:HZ1	2.11	0.64
1:A:339:PHE:HD1	1:A:342:LEU:CD1	2.10	0.63
1:A:670:TRP:NE1	1:A:703:HIS:CE1	2.66	0.63
1:A:407:LEU:CD2	1:A:410:GLU:OE1	2.45	0.63
1:A:450:LEU:C	1:A:450:LEU:HD23	2.19	0.63
1:A:902:ASP:HB3	1:A:905:THR:OG1	1.99	0.63
1:A:1101:ASN:O	1:A:1105:GLU:HB2	1.98	0.63
1:A:33:VAL:HG21	1:A:390:ILE:CD1	2.28	0.63
1:A:539:PHE:HB3	1:A:606:GLY:HA3	1.80	0.63
1:A:483:CYS:SG	1:A:488:LEU:HD22	2.36	0.63
1:A:994:ILE:HD12	1:A:994:ILE:N	2.13	0.63
1:A:450:LEU:HD23	1:A:450:LEU:O	1.98	0.63
1:A:53:PRO:HG3	1:A:60:GLU:OE2	1.99	0.63
1:A:677:PRO:C	1:A:678:VAL:CG2	2.65	0.63
1:A:458:PRO:O	1:A:459:ILE:HG23	1.99	0.63
1:A:515:ARG:NH2	1:A:517:GLU:OE1	2.30	0.63
1:A:64:THR:OG1	1:A:67:GLU:HG3	1.98	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:993:ASP:HB2	1:A:1020:ARG:HE	1.64	0.62
1:A:746:ARG:NH1	2:B:60:C:OP1	2.31	0.62
1:A:586:ARG:HA	1:A:609:ASN:O	1.99	0.62
1:A:1002:ASP:CG	1:A:1015:ARG:NH1	2.53	0.62
1:A:803:HIS:HB3	2:B:31:G:O2'	1.99	0.62
2:B:31:G:H2'	2:B:32:C:H6	1.65	0.62
2:B:9:G:C2	2:B:10:A:C6	2.87	0.62
1:A:296:LEU:H	1:A:334:GLY:HA3	1.65	0.62
1:A:479:ALA:HB1	1:A:502:LEU:HD22	1.80	0.62
1:A:86:ARG:CG	1:A:86:ARG:HH11	2.12	0.61
2:B:50:G:H8	2:B:50:G:C5'	2.09	0.61
1:A:208:ARG:O	1:A:209:LYS:HB2	2.00	0.61
1:A:968:GLU:OE2	1:A:1107:TYR:CD2	2.53	0.61
1:A:418:ILE:HD13	1:A:502:LEU:HD12	1.83	0.61
1:A:486:ASP:N	1:A:486:ASP:OD1	2.33	0.61
1:A:838:LYS:HB3	1:A:839:TYR:CE1	2.35	0.61
1:A:897:PHE:CE2	1:A:1078:MSE:HE1	2.35	0.61
2:B:9:G:C2	2:B:10:A:N7	2.69	0.61
1:A:426:VAL:HG12	1:A:431:ALA:CB	2.31	0.61
1:A:953:PRO:O	1:A:953:PRO:HD2	2.01	0.61
2:B:59:C:H2'	2:B:60:C:H6	1.66	0.61
2:B:49:G:O2'	2:B:50:G:OP1	2.19	0.60
1:A:912:CYS:O	1:A:959:ILE:HG13	2.01	0.60
2:B:1:G:C4	2:B:2:U:C5	2.89	0.60
1:A:619:LEU:HD21	1:A:978:LEU:HD23	1.82	0.60
2:B:5:A:HO2'	2:B:6:G:P	2.21	0.60
1:A:670:TRP:HE1	1:A:703:HIS:CE1	2.19	0.60
2:B:1:G:H2'	2:B:2:U:C6	2.35	0.60
1:A:1085:ILE:CG2	1:A:1096:PHE:HE1	2.13	0.60
1:A:624:GLY:HA3	1:A:754:GLY:O	2.02	0.60
1:A:215:THR:OG1	1:A:402:HIS:CD2	2.54	0.60
1:A:968:GLU:HA	1:A:969:GLY:C	2.22	0.60
1:A:568:SER:OG	1:A:580:SER:HB3	2.02	0.59
1:A:396:LYS:H	1:A:396:LYS:CD	2.14	0.59
1:A:865:ASN:HD21	1:A:867:LEU:CB	2.14	0.59
2:B:23:A:O5'	2:B:23:A:H8	1.85	0.59
1:A:838:LYS:CD	1:A:839:TYR:CE1	2.85	0.59
1:A:407:LEU:HD23	1:A:410:GLU:OE1	2.01	0.59
1:A:838:LYS:CG	1:A:839:TYR:CE1	2.85	0.59
1:A:838:LYS:HD2	1:A:839:TYR:HE1	1.67	0.59
1:A:983:ASN:O	1:A:987:ARG:HG3	2.02	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:G:N2	2:B:10:A:C4	2.70	0.59
1:A:695:GLU:CG	1:A:718:SER:OG	2.50	0.59
1:A:812:LEU:HD13	1:A:875:VAL:HG21	1.85	0.59
2:B:43:U:C2	2:B:50:G:N2	2.69	0.59
1:A:1085:ILE:HG22	1:A:1096:PHE:HE1	1.68	0.59
1:A:257:PHE:O	1:A:260:GLN:HG2	2.02	0.59
1:A:614:HIS:ND1	2:B:6:G:OP1	2.35	0.59
1:A:991:ASP:O	1:A:1020:ARG:NH2	2.36	0.59
1:A:993:ASP:O	1:A:996:GLN:HG3	2.02	0.59
1:A:315:PHE:CE1	1:A:319:ASP:HB2	2.37	0.59
1:A:958:GLU:O	1:A:976:ALA:HB2	2.03	0.59
1:A:371:LEU:HD12	1:A:372:ASN:H	1.65	0.59
1:A:458:PRO:O	1:A:459:ILE:HG12	2.02	0.59
1:A:775:SER:OG	2:B:48:A:H8	1.85	0.59
1:A:901:PHE:CE2	1:A:908:PRO:HG3	2.38	0.59
1:A:258:VAL:O	1:A:258:VAL:HG12	2.01	0.58
2:B:92:G:H2'	2:B:93:A:O4'	2.02	0.58
2:B:9:G:C2'	2:B:10:A:H8	2.14	0.58
2:B:60:C:H2'	2:B:61:C:H6	1.67	0.58
1:A:11:ARG:CG	1:A:11:ARG:HH11	2.14	0.58
1:A:655:LEU:O	1:A:658:CYS:HB2	2.04	0.58
1:A:994:ILE:H	1:A:994:ILE:CD1	2.16	0.58
1:A:386:THR:HG22	1:A:488:LEU:O	2.04	0.58
1:A:839:TYR:OH	2:B:8:G:OP1	2.12	0.58
1:A:208:ARG:HG2	1:A:209:LYS:N	2.18	0.57
1:A:705:ILE:N	1:A:705:ILE:HD13	2.19	0.57
1:A:648:GLN:OE1	1:A:685:THR:HB	2.05	0.57
1:A:952:ILE:N	1:A:953:PRO:HD3	2.18	0.57
1:A:1062:GLU:O	1:A:1065:VAL:HG23	2.04	0.57
1:A:175:THR:O	1:A:178:VAL:N	2.36	0.57
2:B:4:U:HO2'	2:B:5:A:P	2.28	0.57
1:A:215:THR:HG21	1:A:422:LYS:HZ1	1.66	0.57
1:A:305:LYS:HD3	1:A:321:GLU:HG3	1.87	0.57
1:A:677:PRO:O	1:A:678:VAL:HG23	2.04	0.57
1:A:743:PRO:HG2	2:B:34:A:C5	2.40	0.57
2:B:9:G:C2	2:B:10:A:C4	2.93	0.57
1:A:200:SER:OG	1:A:202:VAL:HG12	2.05	0.57
1:A:266:LEU:HD21	1:A:346:GLU:HG3	1.85	0.57
1:A:303:PHE:CD2	1:A:350:LEU:CB	2.88	0.57
1:A:830:ARG:H	1:A:832:LYS:N	2.01	0.57
1:A:330:THR:HA	1:A:331:ARG:C	2.24	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:HIS:HE1	1:A:88:PRO:O	1.88	0.57
1:A:913:ARG:HA	1:A:953:PRO:O	2.04	0.57
1:A:665:ARG:HH11	1:A:665:ARG:CG	2.15	0.57
1:A:775:SER:OG	2:B:48:A:H1'	2.05	0.57
1:A:528:LEU:C	1:A:529:VAL:HG23	2.24	0.57
1:A:951:LEU:CG	1:A:952:ILE:HG13	2.33	0.57
1:A:1019:LYS:HB3	1:A:1022:ALA:HB3	1.86	0.56
1:A:225:ILE:O	1:A:229:MSE:HG3	2.05	0.56
1:A:244:LYS:HG3	1:A:248:GLN:OE1	2.05	0.56
1:A:117:ALA:CB	1:A:226:GLU:HG3	2.34	0.56
1:A:587:LYS:N	1:A:609:ASN:O	2.36	0.56
1:A:665:ARG:NH1	1:A:665:ARG:HB3	2.06	0.56
1:A:208:ARG:HG2	1:A:209:LYS:H	1.70	0.56
1:A:910:ILE:HD11	1:A:1104:ILE:HB	1.86	0.56
1:A:775:SER:CB	1:A:793:PHE:HZ	2.17	0.56
1:A:775:SER:CB	2:B:48:A:H8	2.19	0.56
1:A:973:GLN:O	2:B:4:U:H5'	2.06	0.56
1:A:203:GLU:HB3	1:A:432:ARG:HA	1.87	0.56
1:A:413:GLU:O	1:A:414:ARG:HB2	2.05	0.56
1:A:660:SER:HB2	1:A:661:GLU:O	2.05	0.56
1:A:965:SER:N	1:A:966:ALA:HA	2.20	0.56
1:A:539:PHE:HA	1:A:542:LEU:CD1	2.35	0.56
1:A:661:GLU:HG2	1:A:662:ASP:N	2.20	0.56
1:A:754:GLY:CA	1:A:760:GLN:HG3	2.35	0.56
1:A:838:LYS:CB	1:A:839:TYR:CD1	2.87	0.56
1:A:193:VAL:CG2	1:A:193:VAL:O	2.54	0.56
2:B:87:G:O2'	2:B:88:G:OP2	2.19	0.56
1:A:323:LYS:HE3	1:A:672:LYS:HE2	1.86	0.56
1:A:685:THR:HG21	1:A:729:GLN:NE2	2.21	0.56
2:B:11:C:O2'	2:B:12:A:C5'	2.51	0.56
1:A:36:TYR:CE1	1:A:191:MSE:CE	2.89	0.56
1:A:402:HIS:N	1:A:402:HIS:CD2	2.75	0.55
1:A:39:TRP:O	1:A:43:LEU:N	2.38	0.55
1:A:528:LEU:O	1:A:529:VAL:CG2	2.54	0.55
1:A:839:TYR:CD1	1:A:839:TYR:N	2.73	0.55
1:A:44:ARG:NH2	1:A:232:GLU:OE2	2.39	0.55
1:A:737:VAL:O	1:A:742:ARG:NH2	2.39	0.55
1:A:1000:ARG:HB3	1:A:1000:ARG:HH11	1.72	0.55
1:A:131:LYS:HA	1:A:131:LYS:CE	2.25	0.55
1:A:43:LEU:C	1:A:43:LEU:HD13	2.26	0.55
1:A:18:ILE:O	1:A:21:GLY:N	2.40	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:TRP:CE3	1:A:378:ALA:HB1	2.42	0.55
1:A:120:ILE:HD12	1:A:229:MSE:CE	2.37	0.55
1:A:347:TYR:O	1:A:351:TRP:N	2.31	0.55
2:B:59:C:H2'	2:B:60:C:C6	2.42	0.55
1:A:219:ASP:O	1:A:223:GLN:HG3	2.06	0.55
1:A:602:PHE:CE2	1:A:986:GLN:HB2	2.41	0.55
1:A:45:GLN:HG2	1:A:69:LYS:CD	2.29	0.55
1:A:418:ILE:CD1	1:A:502:LEU:HD12	2.37	0.55
1:A:775:SER:OG	2:B:48:A:C8	2.59	0.54
1:A:865:ASN:HD21	1:A:867:LEU:HB3	1.73	0.54
1:A:1006:VAL:HG23	1:A:1007:ASP:N	2.22	0.54
1:A:660:SER:CB	1:A:661:GLU:CA	2.85	0.54
1:A:105:LEU:HD22	1:A:175:THR:HG22	1.90	0.54
1:A:36:TYR:HD1	1:A:191:MSE:CE	2.16	0.54
1:A:49:TYR:CD1	1:A:380:PHE:HD2	2.23	0.54
1:A:330:THR:OG1	1:A:331:ARG:HA	2.08	0.54
2:B:31:G:C2'	2:B:32:C:O5'	2.55	0.54
1:A:208:ARG:HG3	1:A:208:ARG:NH1	2.21	0.54
1:A:347:TYR:O	1:A:351:TRP:CB	2.56	0.54
1:A:670:TRP:O	1:A:674:ILE:HG13	2.07	0.54
1:A:754:GLY:HA3	1:A:760:GLN:HG2	1.87	0.54
1:A:63:LYS:HE2	1:A:71:GLU:OE1	2.07	0.54
1:A:904:ARG:HH11	1:A:904:ARG:CG	2.11	0.54
1:A:1086:ASN:HB2	1:A:1099:MSE:HE1	1.89	0.54
2:B:60:C:H2'	2:B:61:C:C6	2.42	0.54
1:A:1000:ARG:NH2	1:A:1065:VAL:HB	2.23	0.53
1:A:260:GLN:HG3	1:A:260:GLN:O	2.08	0.53
1:A:339:PHE:O	1:A:342:LEU:HB2	2.08	0.53
1:A:483:CYS:SG	1:A:488:LEU:HD21	2.48	0.53
1:A:528:LEU:C	1:A:529:VAL:CG2	2.77	0.53
1:A:597:ARG:CZ	1:A:597:ARG:CB	2.86	0.53
1:A:670:TRP:CH2	1:A:674:ILE:CG2	2.89	0.53
1:A:617:SER:HB3	1:A:978:LEU:HD13	1.89	0.53
2:B:50:G:C8	2:B:50:G:C5'	2.88	0.53
1:A:310:ALA:O	1:A:313:ALA:HB3	2.09	0.53
1:A:681:ALA:HA	1:A:689:ARG:HD2	1.91	0.53
1:A:905:THR:CB	1:A:906:GLY:HA2	2.37	0.53
1:A:951:LEU:CD1	1:A:952:ILE:HG13	2.38	0.53
1:A:1019:LYS:HA	1:A:1022:ALA:H	1.73	0.53
1:A:809:LEU:HD23	1:A:870:TRP:CH2	2.43	0.53
1:A:913:ARG:HG3	1:A:914:ARG:N	2.23	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:ASP:HB3	1:A:356:SER:OG	2.08	0.53
1:A:533:HIS:O	1:A:892:THR:HG23	2.08	0.53
1:A:534:ARG:HH12	1:A:893:MSE:HE2	1.73	0.53
1:A:339:PHE:HA	1:A:342:LEU:CD1	2.38	0.53
1:A:528:LEU:O	1:A:529:VAL:HG22	2.09	0.53
1:A:52:SER:HB3	1:A:59:GLN:HG2	1.89	0.53
1:A:1011:VAL:HB	1:A:1029:VAL:HG13	1.91	0.53
1:A:865:ASN:C	1:A:865:ASN:HD22	2.12	0.53
1:A:964:PHE:C	1:A:966:ALA:HA	2.29	0.53
1:A:221:PHE:CE2	1:A:225:ILE:HD11	2.43	0.52
1:A:344:GLU:CB	1:A:345:PRO:HD2	2.38	0.52
1:A:591:LYS:N	1:A:592:PRO:CD	2.72	0.52
1:A:830:ARG:N	1:A:831:GLY:CA	2.73	0.52
1:A:41:SER:HB2	1:A:49:TYR:CZ	2.44	0.52
2:B:92:G:HO2'	2:B:93:A:P	2.31	0.52
1:A:131:LYS:HE2	1:A:132:ASP:H	1.74	0.52
1:A:46:GLU:CB	1:A:47:ASN:ND2	2.73	0.52
1:A:821:LEU:HB3	1:A:823:TYR:CE2	2.43	0.52
1:A:972:HIS:NE2	2:B:4:U:H5''	2.24	0.52
2:B:49:G:C2'	2:B:50:G:OP1	2.57	0.52
1:A:1005:GLU:O	1:A:1005:GLU:HG3	2.08	0.52
1:A:48:LEU:CD2	1:A:48:LEU:N	2.73	0.52
1:A:674:ILE:HG22	1:A:696:LEU:CD1	2.39	0.52
2:B:49:G:H2'	2:B:50:G:O4'	2.09	0.52
1:A:534:ARG:NH1	1:A:534:ARG:CG	2.73	0.52
1:A:851:SER:CB	1:A:852:GLU:HA	2.39	0.52
1:A:262:HIS:HE1	1:A:263:LEU:HG	1.75	0.52
1:A:660:SER:HG	1:A:661:GLU:HA	1.75	0.52
1:A:248:GLN:CB	1:A:1060:GLU:OE2	2.52	0.52
1:A:299:SER:O	1:A:303:PHE:HB2	2.09	0.52
1:A:423:LEU:HB3	1:A:437:VAL:HG21	1.91	0.52
1:A:682:ASN:CB	1:A:683:HIS:CE1	2.90	0.52
1:A:965:SER:OG	1:A:965:SER:O	2.28	0.52
1:A:815:ARG:NH2	2:B:8:G:O6	2.43	0.52
2:B:92:G:OP2	2:B:92:G:H4'	2.10	0.52
1:A:913:ARG:CB	1:A:953:PRO:CD	2.70	0.51
2:B:39:C:H2'	2:B:40:C:C6	2.45	0.51
1:A:555:LEU:HA	1:A:840:PRO:HA	1.92	0.51
1:A:964:PHE:CE2	1:A:970:ASP:CB	2.84	0.51
1:A:1061:ALA:O	1:A:1065:VAL:CG1	2.56	0.51
1:A:405:THR:HA	3:A:1202:HOH:O	2.10	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:PRO:HD2	1:A:756:ASN:HD22	1.76	0.51
1:A:660:SER:CB	1:A:661:GLU:HA	2.40	0.51
1:A:829:GLU:HB2	1:A:831:GLY:HA3	1.91	0.51
1:A:993:ASP:HB2	1:A:1020:ARG:NE	2.25	0.51
1:A:665:ARG:CG	1:A:665:ARG:NH1	2.73	0.51
1:A:830:ARG:N	1:A:831:GLY:HA3	2.25	0.51
1:A:86:ARG:CG	1:A:86:ARG:NH1	2.73	0.51
1:A:893:MSE:O	1:A:894:TYR:C	2.44	0.51
1:A:964:PHE:CD1	1:A:965:SER:HB3	2.44	0.51
1:A:59:GLN:HE21	1:A:379:THR:HG23	1.71	0.51
1:A:552:ASP:HB2	1:A:562:SER:HB2	1.92	0.51
1:A:674:ILE:HD13	1:A:675:GLU:HB2	1.92	0.51
1:A:654:LEU:O	1:A:657:ARG:HB2	2.11	0.51
1:A:827:LEU:CG	1:A:830:ARG:HG2	2.40	0.51
1:A:896:ALA:H	1:A:987:ARG:HH12	1.57	0.51
2:B:9:G:N1	2:B:10:A:N6	2.55	0.51
1:A:19:ARG:NH1	1:A:498:ARG:O	2.44	0.50
1:A:670:TRP:CZ3	1:A:674:ILE:HG23	2.46	0.50
1:A:570:ASP:CG	1:A:859:ARG:HH22	2.15	0.50
1:A:174:ARG:NH1	1:A:177:ASP:OD2	2.45	0.50
1:A:394:PHE:CD1	1:A:402:HIS:HB2	2.46	0.50
1:A:818:MSE:HG2	1:A:835:TRP:CZ2	2.47	0.50
1:A:1020:ARG:HH11	1:A:1020:ARG:CG	2.13	0.50
1:A:485:ARG:CG	1:A:485:ARG:HH11	2.13	0.50
1:A:830:ARG:HD2	1:A:830:ARG:O	2.11	0.50
1:A:851:SER:HB3	1:A:852:GLU:HA	1.94	0.50
1:A:1036:VAL:HG13	1:A:1095:GLU:HG2	1.93	0.50
1:A:1034:THR:HB	1:A:1036:VAL:H	1.76	0.50
1:A:907:ALA:HB2	1:A:1084:ILE:HD12	1.93	0.50
1:A:225:ILE:CG2	1:A:229:MSE:HE3	2.41	0.50
1:A:25:LEU:O	1:A:29:VAL:HG23	2.11	0.50
1:A:726:MSE:HB3	1:A:774:TRP:CH2	2.47	0.50
1:A:902:ASP:OD1	1:A:903:ALA:N	2.44	0.50
1:A:912:CYS:O	1:A:959:ILE:N	2.39	0.50
1:A:190:LEU:HB3	1:A:191:MSE:HG3	1.94	0.50
1:A:348:GLN:HA	1:A:351:TRP:HB3	1.94	0.50
1:A:451:LEU:O	1:A:462:TYR:N	2.44	0.50
1:A:200:SER:OG	1:A:202:VAL:CG1	2.60	0.50
1:A:315:PHE:C	1:A:315:PHE:CD1	2.85	0.50
1:A:384:ASP:HB3	1:A:388:HIS:H	1.76	0.50
1:A:490:HIS:ND1	1:A:490:HIS:O	2.45	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:ARG:N	1:A:832:LYS:N	2.60	0.50
1:A:45:GLN:HG3	1:A:96:LEU:HD13	1.93	0.50
1:A:296:LEU:O	1:A:296:LEU:HG	2.11	0.49
1:A:459:ILE:HA	1:A:476:PHE:HD2	1.75	0.49
1:A:656:VAL:HG21	1:A:777:PHE:CE1	2.47	0.49
1:A:836:VAL:O	1:A:836:VAL:HG23	2.11	0.49
1:A:865:ASN:ND2	1:A:867:LEU:CB	2.75	0.49
1:A:1085:ILE:HG23	1:A:1099:MSE:CE	2.42	0.49
1:A:344:GLU:C	1:A:346:GLU:H	2.14	0.49
1:A:453:ARG:HB3	1:A:462:TYR:CE1	2.47	0.49
1:A:128:LEU:O	1:A:190:LEU:N	2.46	0.49
1:A:353:GLU:HA	1:A:354:ASP:C	2.32	0.49
1:A:23:TRP:CH2	1:A:491:MSE:HB2	2.47	0.49
1:A:120:ILE:HD12	1:A:229:MSE:HE1	1.94	0.49
1:A:442:SER:HB3	2:B:29:G:H5''	1.94	0.49
1:A:453:ARG:CG	1:A:460:ALA:CB	2.88	0.49
1:A:662:ASP:O	1:A:665:ARG:HG2	2.12	0.49
1:A:846:LEU:HD22	1:A:893:MSE:HB2	1.94	0.49
1:A:959:ILE:O	1:A:959:ILE:HG13	2.11	0.49
2:B:48:A:N3	2:B:48:A:H5'	2.27	0.49
2:B:92:G:H2'	2:B:93:A:O5'	2.13	0.49
1:A:1107:TYR:CD1	1:A:1107:TYR:C	2.86	0.49
1:A:131:LYS:CE	1:A:132:ASP:N	2.73	0.49
1:A:579:ILE:CG2	1:A:620:LEU:CD1	2.90	0.49
1:A:964:PHE:CD1	1:A:964:PHE:C	2.85	0.49
1:A:1113:ARG:NH1	1:A:1113:ARG:HG3	2.27	0.49
1:A:129:ALA:HB1	1:A:193:VAL:HG12	1.95	0.49
1:A:193:VAL:HG23	1:A:196:ASP:HB3	1.94	0.49
1:A:257:PHE:N	1:A:257:PHE:CD1	2.81	0.49
1:A:11:ARG:NH1	1:A:11:ARG:HB3	2.07	0.49
1:A:11:ARG:NH1	1:A:11:ARG:CG	2.73	0.49
1:A:315:PHE:O	1:A:318:TYR:HB2	2.13	0.49
1:A:344:GLU:CB	1:A:345:PRO:CD	2.91	0.49
1:A:731:ARG:HD3	1:A:735:LYS:CE	2.42	0.49
2:B:92:G:C2'	2:B:93:A:O5'	2.61	0.49
1:A:1094:LYS:HZ1	1:A:1094:LYS:HB2	1.76	0.48
1:A:326:GLN:O	1:A:330:THR:N	2.46	0.48
2:B:8:G:C2'	2:B:9:G:H5''	2.43	0.48
1:A:41:SER:HB2	1:A:49:TYR:CE2	2.48	0.48
1:A:601:PHE:HD2	1:A:611:VAL:HG21	1.73	0.48
2:B:39:C:H2'	2:B:40:C:H6	1.77	0.48

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:LEU:O	1:A:461:LEU:HA	2.13	0.48
1:A:479:ALA:HB1	1:A:502:LEU:CD2	2.43	0.48
1:A:656:VAL:HG21	1:A:777:PHE:HE1	1.78	0.48
1:A:697:GLN:HG3	1:A:698:LYS:N	2.28	0.48
1:A:262:HIS:ND1	1:A:263:LEU:N	2.60	0.48
1:A:312:ASP:N	1:A:312:ASP:OD1	2.47	0.48
1:A:98:LEU:HD11	1:A:178:VAL:HG13	1.96	0.48
1:A:838:LYS:NZ	1:A:838:LYS:CB	2.73	0.48
1:A:973:GLN:C	1:A:974:ILE:HG13	2.33	0.48
1:A:747:GLY:HA2	2:B:88:G:O4'	2.13	0.48
1:A:194:TYR:O	1:A:197:SER:HB3	2.14	0.48
1:A:531:ASP:HA	1:A:533:HIS:HD2	1.79	0.48
1:A:731:ARG:HD3	1:A:735:LYS:HE3	1.95	0.48
1:A:865:ASN:ND2	1:A:867:LEU:H	2.09	0.48
2:B:31:G:H2'	2:B:32:C:C6	2.46	0.48
1:A:208:ARG:O	1:A:211:GLN:HG2	2.13	0.48
1:A:262:HIS:CG	1:A:263:LEU:N	2.82	0.48
1:A:550:PRO:O	1:A:562:SER:O	2.31	0.48
1:A:673:LEU:HD11	1:A:692:PHE:CE2	2.49	0.48
1:A:865:ASN:ND2	1:A:867:LEU:N	2.60	0.48
1:A:805:LYS:HG2	1:A:870:TRP:CH2	2.49	0.48
1:A:827:LEU:HD12	1:A:830:ARG:HD3	1.96	0.48
2:B:9:G:N1	2:B:10:A:C5	2.75	0.48
1:A:973:GLN:HB2	2:B:3:C:O2'	2.14	0.48
1:A:256:ASN:HD22	1:A:360:ARG:HD2	1.77	0.48
1:A:131:LYS:CD	1:A:132:ASP:N	2.77	0.47
1:A:295:ALA:O	1:A:296:LEU:CD2	2.62	0.47
1:A:617:SER:HB3	1:A:978:LEU:HD11	1.95	0.47
2:B:31:G:O2'	2:B:32:C:P	2.72	0.47
1:A:174:ARG:CZ	1:A:177:ASP:OD2	2.62	0.47
1:A:501:TYR:N	1:A:501:TYR:CD1	2.82	0.47
1:A:827:LEU:HD23	1:A:828:ASP:H	1.80	0.47
1:A:303:PHE:HE2	1:A:350:LEU:CB	2.20	0.47
1:A:1032:THR:HG23	1:A:1038:TYR:CG	2.49	0.47
1:A:211:GLN:O	1:A:211:GLN:HG3	2.14	0.47
1:A:266:LEU:HD21	1:A:346:GLU:CG	2.44	0.47
1:A:564:LEU:HA	1:A:843:GLN:OE1	2.14	0.47
1:A:1061:ALA:O	1:A:1065:VAL:HG22	2.14	0.47
2:B:47:C:C2'	2:B:48:A:C5'	2.80	0.47
1:A:394:PHE:HD1	1:A:402:HIS:HB2	1.78	0.47
1:A:614:HIS:CE1	2:B:6:G:OP1	2.67	0.47

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:HIS:ND1	1:A:683:HIS:N	2.62	0.47
1:A:898:SER:O	1:A:980:ALA:HA	2.15	0.47
1:A:564:LEU:HD13	1:A:564:LEU:C	2.34	0.47
1:A:715:VAL:O	1:A:716:TYR:C	2.53	0.47
1:A:195:THR:HG22	1:A:204:TRP:CZ2	2.50	0.47
1:A:515:ARG:HB2	1:A:517:GLU:HG3	1.96	0.47
1:A:568:SER:HG	1:A:580:SER:HB3	1.78	0.47
1:A:581:VAL:HG21	1:A:616:ARG:NE	2.27	0.47
1:A:827:LEU:HD23	1:A:828:ASP:N	2.30	0.47
1:A:818:MSE:HG2	1:A:835:TRP:CH2	2.50	0.47
1:A:85:HIS:CE1	1:A:88:PRO:O	2.67	0.47
1:A:92:ASP:C	1:A:92:ASP:OD1	2.52	0.47
1:A:953:PRO:O	1:A:953:PRO:CD	2.63	0.47
1:A:1036:VAL:CG1	1:A:1095:GLU:HG2	2.45	0.46
1:A:12:LEU:CD1	1:A:19:ARG:HA	2.44	0.46
1:A:579:ILE:CG2	1:A:620:LEU:HG	2.45	0.46
1:A:556:GLY:O	1:A:841:PRO:HD3	2.15	0.46
1:A:908:PRO:HG2	1:A:1096:PHE:CZ	2.50	0.46
2:B:9:G:C6	2:B:10:A:C6	2.96	0.46
2:B:33:C:OP2	2:B:35:A:O2'	2.18	0.46
1:A:858:ASP:CG	1:A:897:PHE:H	2.19	0.46
2:B:9:G:O2'	2:B:10:A:O5'	2.31	0.46
1:A:79:ARG:HD2	1:A:79:ARG:HA	1.66	0.46
1:A:838:LYS:HG2	1:A:839:TYR:CE1	2.51	0.46
2:B:92:G:O2'	2:B:93:A:P	2.73	0.46
1:A:106:LEU:HD13	1:A:106:LEU:HA	1.80	0.46
1:A:257:PHE:HD1	1:A:257:PHE:N	2.14	0.46
1:A:851:SER:CB	1:A:852:GLU:CA	2.94	0.46
1:A:855:PHE:CE2	1:A:998:ARG:CZ	2.98	0.46
1:A:426:VAL:HG12	1:A:431:ALA:HA	1.98	0.46
1:A:246:VAL:O	1:A:250:ASN:HB2	2.16	0.46
1:A:674:ILE:CD1	1:A:675:GLU:N	2.73	0.46
1:A:587:LYS:HB3	1:A:587:LYS:HE2	1.78	0.46
1:A:579:ILE:HG23	1:A:620:LEU:HG	1.97	0.46
1:A:775:SER:OG	1:A:793:PHE:HZ	1.99	0.46
1:A:1032:THR:HG23	1:A:1038:TYR:CE2	2.51	0.46
1:A:1073:LYS:CE	1:A:1073:LYS:HA	2.09	0.46
1:A:208:ARG:CG	1:A:209:LYS:N	2.79	0.46
1:A:663:VAL:HG12	1:A:664:GLY:N	2.20	0.46
1:A:1002:ASP:CG	1:A:1015:ARG:HH11	2.19	0.45
1:A:333:PHE:CE1	1:A:339:PHE:CE2	3.03	0.45

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ILE:HA	1:A:370:LYS:HE3	1.98	0.45
1:A:77:ARG:NH1	1:A:80:GLN:OE1	2.49	0.45
1:A:952:ILE:HG22	1:A:952:ILE:O	2.17	0.45
2:B:48:A:C2'	2:B:49:G:O5'	2.64	0.45
1:A:1019:LYS:HA	1:A:1021:THR:N	2.30	0.45
1:A:193:VAL:HG21	1:A:196:ASP:HB3	1.98	0.45
1:A:251:ARG:O	1:A:254:GLN:N	2.49	0.45
1:A:263:LEU:HD21	1:A:349:ALA:HA	1.98	0.45
1:A:663:VAL:CG1	1:A:664:GLY:H	2.21	0.45
1:A:911:ARG:C	1:A:912:CYS:SG	2.95	0.45
1:A:962:SER:HA	1:A:963:PRO:HD3	1.79	0.45
2:B:5:A:O2'	2:B:6:G:P	2.71	0.45
1:A:208:ARG:CG	1:A:209:LYS:H	2.30	0.45
1:A:423:LEU:HD12	1:A:423:LEU:HA	1.84	0.45
1:A:473:THR:HG23	3:A:1217:HOH:O	2.16	0.45
1:A:479:ALA:HA	1:A:503:ASN:O	2.16	0.45
1:A:632:ARG:NH1	1:A:635:ARG:HD2	2.32	0.45
2:B:42:C:C2	2:B:43:U:C5	3.05	0.45
2:B:7:A:O2'	2:B:9:G:H5'	2.16	0.45
1:A:654:LEU:HA	1:A:657:ARG:HG3	1.98	0.45
1:A:957:GLY:HA2	1:A:958:GLU:HA	1.79	0.45
1:A:1011:VAL:HG11	1:A:1029:VAL:HG11	1.96	0.45
1:A:215:THR:O	1:A:218:ARG:HB2	2.17	0.45
1:A:446:GLN:O	1:A:449:ASN:HB2	2.17	0.45
1:A:502:LEU:HA	1:A:502:LEU:HD23	1.82	0.45
1:A:905:THR:N	1:A:906:GLY:HA2	2.31	0.45
1:A:913:ARG:CG	1:A:914:ARG:N	2.79	0.45
1:A:12:LEU:HD12	1:A:22:LEU:HD12	1.99	0.45
1:A:375:LYS:HA	1:A:375:LYS:HD3	1.69	0.45
1:A:504:VAL:HG23	1:A:504:VAL:O	2.17	0.45
1:A:515:ARG:HE	1:A:517:GLU:CD	2.19	0.45
1:A:564:LEU:C	1:A:564:LEU:CD1	2.85	0.45
1:A:315:PHE:CE1	1:A:319:ASP:OD2	2.70	0.45
1:A:46:GLU:CB	1:A:47:ASN:CG	2.86	0.45
1:A:418:ILE:HD13	1:A:502:LEU:CD1	2.45	0.45
1:A:594:SER:HB3	1:A:599:PRO:HD3	1.98	0.45
1:A:964:PHE:CD1	1:A:964:PHE:O	2.70	0.45
1:A:12:LEU:HD22	1:A:15:MSE:CG	2.42	0.44
1:A:459:ILE:O	1:A:459:ILE:HG13	2.17	0.44
1:A:662:ASP:OD1	1:A:663:VAL:O	2.35	0.44
1:A:7:LYS:NZ	2:B:94:G:OP1	2.50	0.44

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:ARG:NH2	1:A:1065:VAL:HG12	2.32	0.44
1:A:1030:PHE:HE2	1:A:1090:TRP:CD1	2.35	0.44
1:A:1113:ARG:CG	1:A:1113:ARG:HH11	2.29	0.44
1:A:131:LYS:HD3	1:A:131:LYS:C	2.37	0.44
1:A:305:LYS:CD	1:A:321:GLU:HG3	2.47	0.44
1:A:1002:ASP:OD2	1:A:1015:ARG:NH1	2.51	0.44
1:A:422:LYS:HE3	1:A:422:LYS:HB2	1.81	0.44
1:A:555:LEU:C	1:A:555:LEU:CD2	2.85	0.44
1:A:960:PHE:CE2	1:A:962:SER:HB3	2.53	0.44
2:B:50:G:C5	2:B:51:U:C5	3.05	0.44
1:A:119:GLN:O	1:A:123:LYS:HG2	2.17	0.44
1:A:339:PHE:CD1	1:A:342:LEU:CD1	2.93	0.44
1:A:407:LEU:HD22	1:A:410:GLU:OE1	2.16	0.44
1:A:676:GLN:HA	1:A:677:PRO:HA	1.82	0.44
1:A:326:GLN:O	1:A:330:THR:CB	2.63	0.44
1:A:512:SER:HB2	1:A:515:ARG:NH2	2.32	0.44
1:A:619:LEU:HD12	2:B:10:A:C5'	2.44	0.44
1:A:628:SER:HB3	1:A:631:LEU:HB2	1.99	0.44
1:A:972:HIS:CE1	2:B:4:U:C5'	3.01	0.44
1:A:1084:ILE:HG22	1:A:1085:ILE:HD12	1.99	0.44
1:A:894:TYR:CE2	1:A:896:ALA:HB2	2.52	0.44
1:A:1107:TYR:O	1:A:1107:TYR:CD1	2.70	0.44
1:A:419:ARG:HA	1:A:437:VAL:O	2.18	0.44
1:A:451:LEU:O	1:A:461:LEU:HB2	2.18	0.44
1:A:590:LEU:O	1:A:593:ASN:N	2.50	0.44
1:A:830:ARG:CA	1:A:831:GLY:C	2.85	0.44
1:A:5:SER:HB3	2:B:92:G:H1'	1.99	0.44
1:A:627:GLU:OE1	1:A:628:SER:N	2.51	0.44
1:A:965:SER:N	1:A:966:ALA:CA	2.81	0.44
2:B:43:U:O5'	2:B:43:U:H6	2.01	0.44
1:A:994:ILE:CD1	1:A:994:ILE:N	2.77	0.44
2:B:27:G:O2'	2:B:28:U:H5'	2.18	0.44
1:A:515:ARG:NE	1:A:517:GLU:OE1	2.51	0.43
1:A:670:TRP:NE1	1:A:703:HIS:ND1	2.65	0.43
1:A:812:LEU:HD13	1:A:875:VAL:CG2	2.47	0.43
1:A:959:ILE:HA	1:A:976:ALA:HB2	2.00	0.43
1:A:15:MSE:H	1:A:15:MSE:HG2	1.57	0.43
1:A:380:PHE:CZ	1:A:382:LEU:CD2	3.01	0.43
1:A:219:ASP:OD1	1:A:393:ARG:NH1	2.51	0.43
1:A:567:MSE:SE	1:A:579:ILE:HG13	2.68	0.43
1:A:587:LYS:CE	1:A:608:ASP:O	2.66	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:LYS:CE	1:A:672:LYS:HE2	2.48	0.43
1:A:838:LYS:CB	1:A:839:TYR:CE1	3.00	0.43
1:A:1107:TYR:O	1:A:1107:TYR:HD1	2.00	0.43
1:A:400:ASN:O	1:A:401:LEU:HB2	2.18	0.43
1:A:203:GLU:OE2	1:A:432:ARG:HD2	2.17	0.43
1:A:50:ARG:HA	1:A:61:CYS:HA	1.99	0.43
1:A:1019:LYS:HA	1:A:1020:ARG:C	2.39	0.43
1:A:1113:ARG:HB3	1:A:1114:SER:H	1.43	0.43
1:A:531:ASP:HA	1:A:533:HIS:CD2	2.54	0.43
1:A:972:HIS:HE2	2:B:4:U:H3'	1.84	0.43
1:A:814:ASP:O	1:A:818:MSE:HB2	2.19	0.43
2:B:12:A:O2'	2:B:13:G:O5'	2.36	0.43
1:A:552:ASP:HB3	1:A:554:LYS:H	1.84	0.43
1:A:805:LYS:HE2	3:A:1215:HOH:O	2.19	0.43
1:A:865:ASN:ND2	1:A:867:LEU:HB2	2.33	0.43
1:A:188:LYS:HA	1:A:189:PRO:HA	1.81	0.42
1:A:239:GLY:HA2	1:A:376:MSE:O	2.19	0.42
1:A:555:LEU:HD22	1:A:556:GLY:N	2.34	0.42
1:A:567:MSE:SE	1:A:579:ILE:CG1	3.17	0.42
1:A:660:SER:HB2	1:A:661:GLU:CA	2.48	0.42
1:A:968:GLU:OE1	1:A:968:GLU:HA	2.19	0.42
2:B:27:G:H2'	2:B:28:U:C6	2.54	0.42
1:A:582:PHE:CE2	1:A:614:HIS:HB2	2.54	0.42
1:A:102:LEU:HG	1:A:106:LEU:HD23	2.00	0.42
1:A:45:GLN:HE21	1:A:69:LYS:CD	2.31	0.42
1:A:672:LYS:H	1:A:672:LYS:HG2	1.66	0.42
1:A:907:ALA:CB	1:A:1084:ILE:HD12	2.48	0.42
1:A:407:LEU:HD22	1:A:410:GLU:CD	2.39	0.42
1:A:5:SER:H	2:B:92:G:H1'	1.85	0.42
1:A:64:THR:HB	1:A:65:ALA:CB	2.34	0.42
1:A:48:LEU:HD22	1:A:65:ALA:CA	2.49	0.42
1:A:69:LYS:HD2	1:A:96:LEU:HD13	2.02	0.42
1:A:754:GLY:CA	1:A:760:GLN:CG	2.92	0.42
2:B:23:A:C2'	2:B:24:C:O5'	2.67	0.42
1:A:109:GLN:OE1	1:A:109:GLN:N	2.53	0.42
1:A:32:GLY:HA3	1:A:220:MSE:SE	2.70	0.42
1:A:357:PHE:O	1:A:361:TYR:HB2	2.20	0.42
1:A:686:PRO:O	1:A:689:ARG:N	2.53	0.42
1:A:963:PRO:HB2	1:A:1084:ILE:HG21	2.02	0.42
2:B:4:U:O2'	2:B:5:A:O5'	2.35	0.42
1:A:602:PHE:CE2	1:A:986:GLN:CB	3.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:ARG:HG2	1:A:735:LYS:HE3	2.01	0.42
1:A:45:GLN:NE2	1:A:96:LEU:HD13	2.35	0.42
1:A:694:ASN:O	1:A:697:GLN:CG	2.66	0.42
1:A:966:ALA:CB	1:A:1084:ILE:HG12	2.46	0.42
1:A:395:ASP:O	1:A:403:GLN:HA	2.19	0.42
1:A:817:ILE:O	1:A:821:LEU:HD22	2.20	0.42
1:A:865:ASN:C	1:A:865:ASN:ND2	2.73	0.42
2:B:92:G:C4'	2:B:92:G:OP2	2.68	0.42
1:A:48:LEU:HD22	1:A:65:ALA:HB2	2.01	0.41
2:B:36:U:HO2'	2:B:37:G:P	2.42	0.41
1:A:794:ALA:N	2:B:50:G:OP2	2.52	0.41
2:B:9:G:C2'	2:B:10:A:C8	2.92	0.41
1:A:366:SER:O	1:A:370:LYS:HE3	2.20	0.41
1:A:12:LEU:HD23	1:A:439:VAL:HG13	2.01	0.41
1:A:809:LEU:CD1	1:A:878:GLU:HG3	2.50	0.41
1:A:131:LYS:HD3	1:A:133:ALA:N	2.32	0.41
1:A:670:TRP:CZ3	1:A:674:ILE:CG2	3.03	0.41
1:A:904:ARG:NH1	1:A:904:ARG:CG	2.73	0.41
1:A:911:ARG:C	1:A:912:CYS:HG	2.24	0.41
1:A:968:GLU:OE2	1:A:1107:TYR:CE2	2.73	0.41
1:A:999:LEU:HA	1:A:999:LEU:HD23	1.92	0.41
1:A:490:HIS:C	1:A:490:HIS:ND1	2.73	0.41
1:A:41:SER:HA	1:A:49:TYR:OH	2.20	0.41
1:A:717:GLU:O	1:A:721:ARG:HG3	2.20	0.41
1:A:913:ARG:HB2	1:A:953:PRO:HD3	1.89	0.41
2:B:4:U:O2'	2:B:5:A:P	2.78	0.41
1:A:710:GLU:O	1:A:714:ALA:HB2	2.20	0.41
1:A:728:LYS:O	1:A:732:ASP:CG	2.59	0.41
1:A:743:PRO:O	2:B:34:A:C8	2.73	0.41
2:B:40:C:C2	2:B:41:A:N7	2.88	0.41
1:A:416:HIS:CD2	1:A:447:LEU:HD13	2.54	0.41
2:B:90:A:C2'	2:B:91:C:H5'	2.51	0.41
1:A:1085:ILE:HG23	1:A:1099:MSE:HE3	2.01	0.41
1:A:1096:PHE:O	1:A:1100:VAL:HG23	2.20	0.41
1:A:120:ILE:O	1:A:124:PHE:HB2	2.21	0.41
1:A:512:SER:HA	1:A:515:ARG:CZ	2.51	0.41
1:A:640:ARG:O	1:A:644:GLN:HG3	2.21	0.41
2:B:9:G:O6	2:B:10:A:N6	2.49	0.41
1:A:1113:ARG:CG	1:A:1113:ARG:NH1	2.84	0.41
1:A:12:LEU:CD1	1:A:22:LEU:HD12	2.50	0.41
1:A:1068:ASP:HB3	1:A:1074:SER:CB	2.44	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ILE:HA	1:A:696:LEU:HD11	2.02	0.41
1:A:797:LEU:HD13	2:B:36:U:C6	2.56	0.41
1:A:12:LEU:HA	1:A:12:LEU:HD23	1.86	0.41
1:A:256:ASN:ND2	1:A:360:ARG:HD2	2.36	0.41
1:A:484:ARG:HB2	1:A:487:GLN:HG2	2.03	0.41
1:A:560:LEU:HA	1:A:560:LEU:HD23	1.79	0.41
1:A:61:CYS:O	1:A:61:CYS:SG	2.79	0.41
1:A:628:SER:O	1:A:632:ARG:HB2	2.21	0.41
1:A:1080:ASP:OD1	1:A:1081:PRO:HD2	2.21	0.40
1:A:234:TRP:CZ3	1:A:378:ALA:HB1	2.56	0.40
1:A:555:LEU:C	1:A:555:LEU:HD22	2.42	0.40
1:A:570:ASP:OD1	1:A:859:ARG:NH2	2.54	0.40
1:A:295:ALA:O	1:A:296:LEU:HD22	2.22	0.40
1:A:36:TYR:O	1:A:39:TRP:HB2	2.21	0.40
1:A:655:LEU:HD12	1:A:692:PHE:HE1	1.87	0.40
2:B:27:G:H2'	2:B:28:U:H6	1.87	0.40
1:A:174:ARG:CZ	1:A:177:ASP:CG	2.89	0.40
1:A:451:LEU:O	1:A:461:LEU:CA	2.69	0.40
1:A:570:ASP:OD2	1:A:859:ARG:NH2	2.47	0.40
1:A:340:ALA:CB	1:A:668:ARG:NH2	2.83	0.40
1:A:758:ILE:O	1:A:762:GLU:HB2	2.20	0.40
1:A:855:PHE:HE2	1:A:998:ARG:CZ	2.34	0.40
2:B:92:G:H8	2:B:92:G:H5''	1.85	0.40
1:A:459:ILE:O	1:A:475:GLU:HA	2.21	0.40
1:A:952:ILE:O	1:A:952:ILE:CG2	2.70	0.40
2:B:9:G:HO2'	2:B:10:A:C5'	2.35	0.40
2:B:9:G:HO2'	2:B:10:A:H8	1.67	0.40
1:A:1037:THR:HB	1:A:1086:ASN:HD21	1.86	0.40
1:A:400:ASN:O	1:A:401:LEU:CB	2.69	0.40
1:A:865:ASN:ND2	1:A:868:MSE:H	2.19	0.40
1:A:968:GLU:N	1:A:969:GLY:HA3	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	997/1137 (88%)	965 (97%)	24 (2%)	8 (1%)	19	53

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	296	LEU
1	A	401	LEU
1	A	459	ILE
1	A	952	ILE
1	A	344	GLU
1	A	859	ARG
1	A	678	VAL
1	A	452	PRO

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	804/955 (84%)	611 (76%)	193 (24%)	0	2

All (193) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	VAL
1	A	11	ARG
1	A	12	LEU
1	A	15	MSE
1	A	39	TRP
1	A	40	LEU
1	A	48	LEU
1	A	49	TYR
1	A	51	ARG
1	A	60	GLU
1	A	62	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	64	THR
1	A	77	ARG
1	A	83	ASN
1	A	86	ARG
1	A	91	SER
1	A	92	ASP
1	A	95	LEU
1	A	100	ARG
1	A	106	LEU
1	A	114	LYS
1	A	131	LYS
1	A	182	LEU
1	A	189	PRO
1	A	190	LEU
1	A	201	SER
1	A	203	GLU
1	A	214	ARG
1	A	227	ARG
1	A	240	GLN
1	A	244	LYS
1	A	251	ARG
1	A	255	LYS
1	A	265	HIS
1	A	271	GLN
1	A	294	ARG
1	A	296	LEU
1	A	301	LYS
1	A	312	ASP
1	A	317	LEU
1	A	321	GLU
1	A	323	LYS
1	A	328	ARG
1	A	352	ARG
1	A	359	THR
1	A	371	LEU
1	A	375	LYS
1	A	379	THR
1	A	386	THR
1	A	393	ARG
1	A	395	ASP
1	A	396	LYS
1	A	397	LEU

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	401	LEU
1	A	402	HIS
1	A	407	LEU
1	A	424	LEU
1	A	425	LYS
1	A	428	ASN
1	A	432	ARG
1	A	438	THR
1	A	441	ILE
1	A	443	MSE
1	A	444	SER
1	A	445	GLU
1	A	450	LEU
1	A	451	LEU
1	A	453	ARG
1	A	459	ILE
1	A	461	LEU
1	A	464	ARG
1	A	465	ASP
1	A	471	HIS
1	A	481	ILE
1	A	485	ARG
1	A	486	ASP
1	A	488	LEU
1	A	490	HIS
1	A	500	VAL
1	A	501	TYR
1	A	502	LEU
1	A	507	ARG
1	A	519	ARG
1	A	522	TYR
1	A	525	VAL
1	A	527	ARG
1	A	532	ASN
1	A	540	ASP
1	A	543	SER
1	A	555	LEU
1	A	561	LEU
1	A	564	LEU
1	A	573	LEU
1	A	575	THR
1	A	576	SER

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	579	ILE
1	A	583	ARG
1	A	595	LYS
1	A	597	ARG
1	A	626	THR
1	A	627	GLU
1	A	628	SER
1	A	629	LYS
1	A	631	LEU
1	A	632	ARG
1	A	634	ILE
1	A	640	ARG
1	A	652	LEU
1	A	654	LEU
1	A	665	ARG
1	A	666	ARG
1	A	672	LYS
1	A	675	GLU
1	A	676	GLN
1	A	683	HIS
1	A	687	ASP
1	A	688	TRP
1	A	695	GLU
1	A	696	LEU
1	A	697	GLN
1	A	709	LYS
1	A	726	MSE
1	A	742	ARG
1	A	745	ILE
1	A	746	ARG
1	A	753	VAL
1	A	759	GLU
1	A	773	SER
1	A	781	SER
1	A	785	ILE
1	A	795	ILE
1	A	798	ARG
1	A	806	GLU
1	A	812	LEU
1	A	821	LEU
1	A	827	LEU
1	A	828	ASP

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	830	ARG
1	A	832	LYS
1	A	838	LYS
1	A	839	TYR
1	A	848	GLU
1	A	850	LEU
1	A	851	SER
1	A	863	GLU
1	A	865	ASN
1	A	866	GLN
1	A	871	SER
1	A	872	HIS
1	A	881	ASN
1	A	882	GLN
1	A	884	GLN
1	A	886	HIS
1	A	887	ASP
1	A	888	LEU
1	A	893	MSE
1	A	898	SER
1	A	904	ARG
1	A	905	THR
1	A	910	ILE
1	A	950	ASP
1	A	951	LEU
1	A	959	ILE
1	A	964	PHE
1	A	978	LEU
1	A	983	ASN
1	A	985	GLN
1	A	986	GLN
1	A	994	ILE
1	A	995	SER
1	A	997	ILE
1	A	1000	ARG
1	A	1001	CYS
1	A	1002	ASP
1	A	1011	VAL
1	A	1015	ARG
1	A	1019	LYS
1	A	1020	ARG
1	A	1024	SER

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1029	VAL
1	A	1032	THR
1	A	1034	THR
1	A	1037	THR
1	A	1063	LEU
1	A	1068	ASP
1	A	1078	MSE
1	A	1079	ARG
1	A	1087	ARG
1	A	1093	GLN
1	A	1094	LYS
1	A	1107	TYR
1	A	1110	LYS
1	A	1113	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	45	GLN
1	A	47	ASN
1	A	85	HIS
1	A	119	GLN
1	A	256	ASN
1	A	260	GLN
1	A	336	HIS
1	A	400	ASN
1	A	402	HIS
1	A	487	GLN
1	A	533	HIS
1	A	618	GLN
1	A	648	GLN
1	A	697	GLN
1	A	703	HIS
1	A	729	GLN
1	A	756	ASN
1	A	800	HIS
1	A	857	ASN
1	A	865	ASN
1	A	877	GLN
1	A	881	ASN
1	A	1093	GLN

## 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	55/112 (49%)	25 (45%)	9 (16%)

All (25) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	4	U
2	B	5	A
2	B	6	G
2	B	7	A
2	B	8	G
2	B	9	G
2	B	12	A
2	B	13	G
2	B	24	C
2	B	29	G
2	B	30	U
2	B	31	G
2	B	32	C
2	B	34	A
2	B	35	A
2	B	36	U
2	B	37	G
2	B	48	A
2	B	49	G
2	B	50	G
2	B	87	G
2	B	91	C
2	B	92	G
2	B	93	A
2	B	94	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	5	A
2	B	8	G
2	B	28	U
2	B	31	G
2	B	36	U
2	B	49	G
2	B	50	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	86	U
2	B	92	G

#### 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 carbohydrates 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

### 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	992/1137 (87%)	-0.21	24 (2%) 59 37	11, 41, 87, 134	6 (0%)
2	B	60/112 (53%)	-0.35	0 100 100	22, 61, 124, 146	0
All	All	1052/1249 (84%)	-0.22	24 (2%) 60 39	11, 43, 90, 146	6 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	831	GLY	7.4
1	A	790	GLY	6.6
1	A	1055	LYS	5.3
1	A	830	ARG	4.2
1	A	316	ASP	3.7
1	A	953	PRO	3.7
1	A	832	LYS	3.1
1	A	319	ASP	2.8
1	A	315	PHE	2.7
1	A	735	LYS	2.7
1	A	1027	ASN	2.7
1	A	1054	GLU	2.7
1	A	789	LYS	2.6
1	A	1056	LEU	2.5
1	A	1114	SER	2.5
1	A	787	ALA	2.4
1	A	915	VAL	2.3
1	A	1016	LEU	2.2
1	A	343	ALA	2.1
1	A	1110	LYS	2.1
1	A	49	TYR	2.1
1	A	132	ASP	2.1
1	A	277	ALA	2.0
1	A	592	PRO	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.