Full wwPDB X-ray Structure Validation Report (i)

Sep 17, 2023 – 11:36 AM EDT

PDB ID	:	4Y52
Title	:	Crystal structure of 5-Carboxycytosine Recognition by RNA Polymerase II during Transcription Elongation.
Authors	:	Wang, L.; Chong, J.; Wang, D.
Deposited on	:	2015-02-11
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
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 (i)) were used in the production of this report:

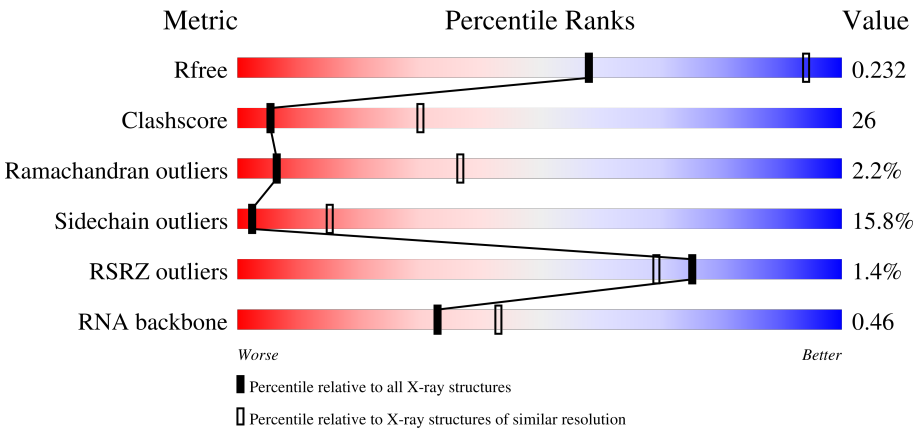
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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% 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	1733	2% 42% 31% 7% 20%
2	B	1224	% 49% 35% 6% • 10%
3	C	318	43% 34% 7% 16%
4	E	215	% 58% 36% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	155	25% 25% • 46%
6	H	146	2% 39% 42% 8% • 9%
7	I	122	43% 40% 14% •
8	J	70	33% 46% 14% 7%
9	K	120	68% 24% • 5%
10	L	70	4% 24% 30% 9% • 36%
11	T	29	24% 14% 72% 14%
12	N	14	14% 14% 79% 7%
13	R	9	56% 22% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	1CC	T	19[A]	-	-	X	-

2 Entry composition (i)

There are 15 unique types of molecules in this entry. The entry contains 29189 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1393	10953	6908	1921	2063	61	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1103	8762	5549	1532	1626	55	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	214	1752	1111	309	321	11	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	84	679	434	115	127	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	133	1068	673	180	211	4	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	119	971	596	179	186	10	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	J	65	532	339	93	94	6	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	K	114	919	590	156	171	2	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	45	358	221	71	62	4	0	0	0

- Molecule 11 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
11	T	29	609	290	111	179	29	0	1	0

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP *GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
12	N	14	284	137	49	85	13	0	0	0

- Molecule 13 is a RNA chain called RNA (5'-D(*AP*UP*GP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
13	R	9	198	89	42	59	8	0	0	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
14	A	2	2	2	0	0
14	B	1	1	1	0	0
14	C	1	1	1	0	0
14	I	2	2	2	0	0
14	J	1	1	1	0	0
14	L	1	1	1	0	0

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

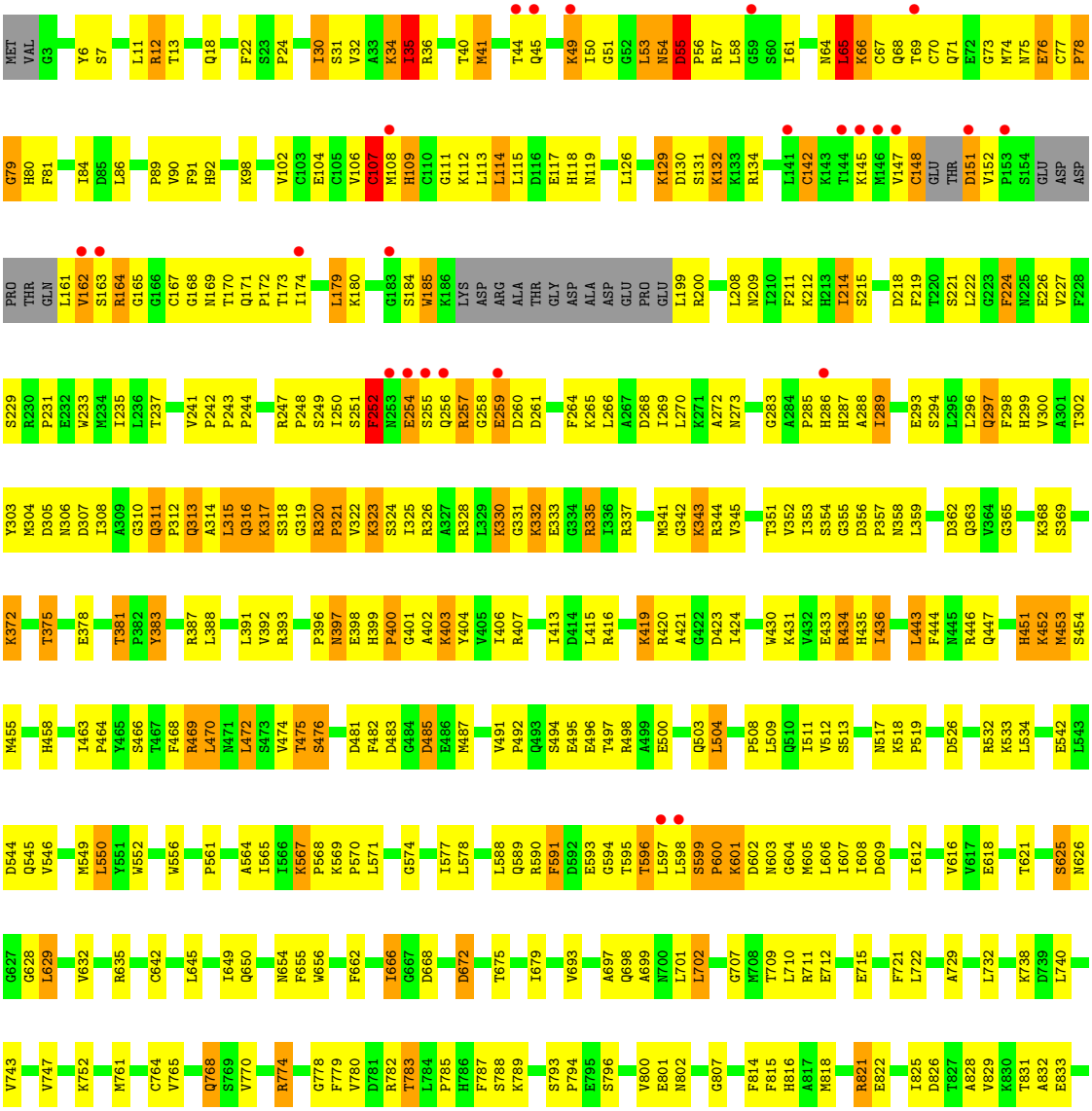
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
15	A	1	1	1	0	0

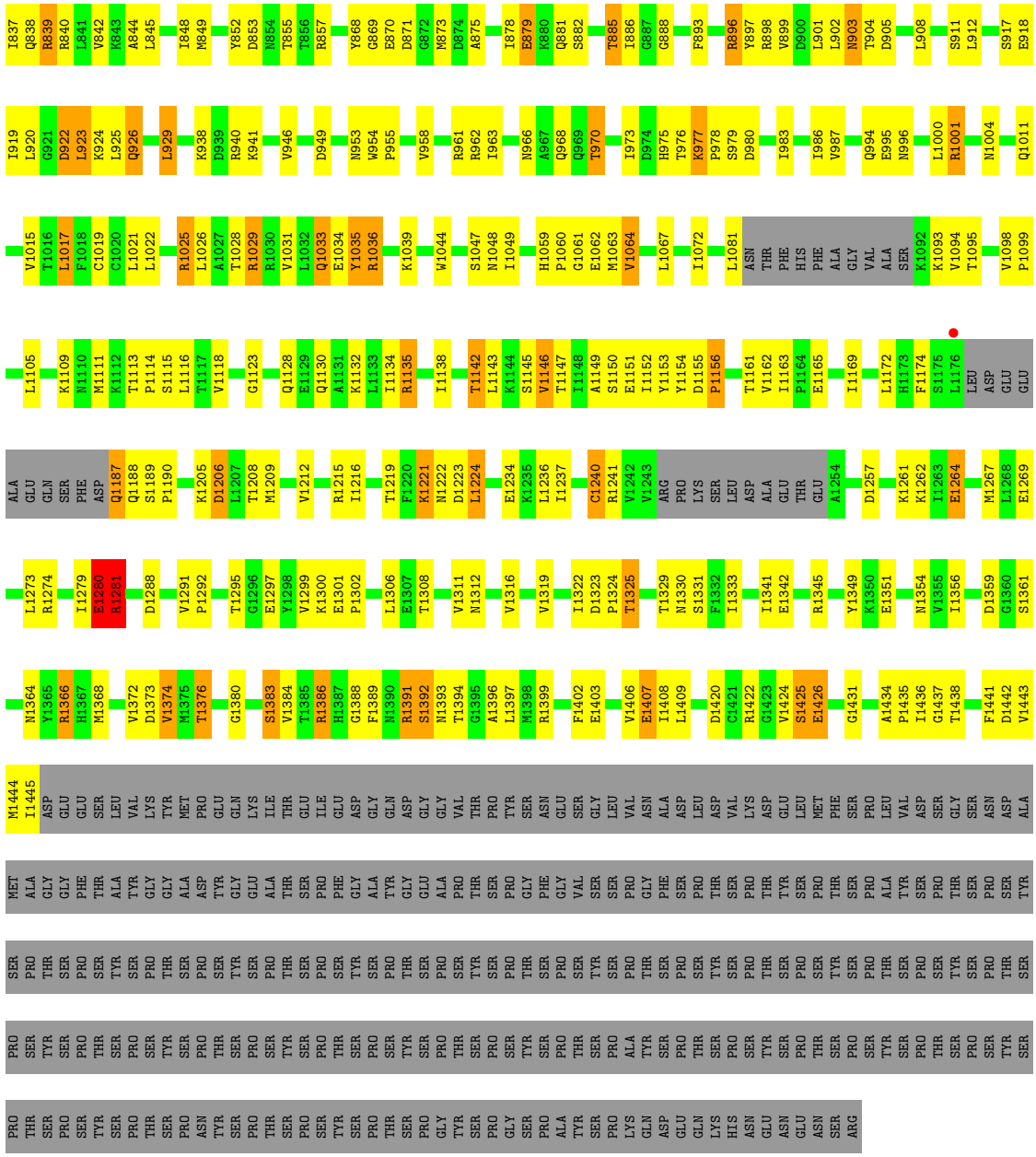
3 Residue-property plots (i)

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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: DNA-directed RNA polymerase II subunit RPB1

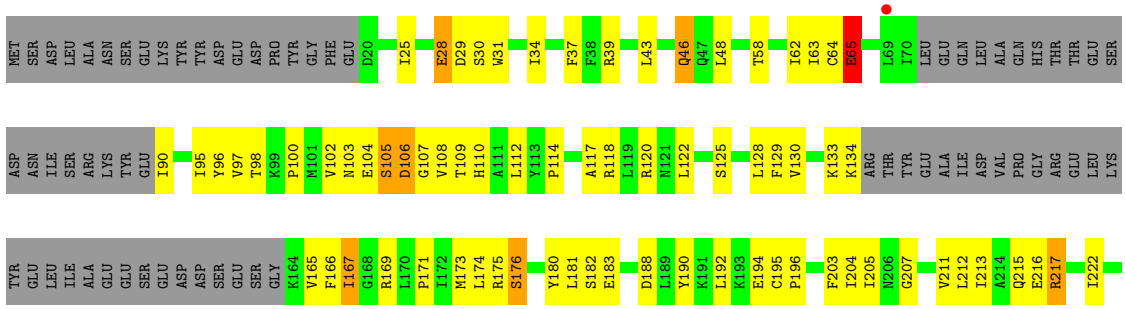
Chain A: 2% 42% 31% 7% 20%

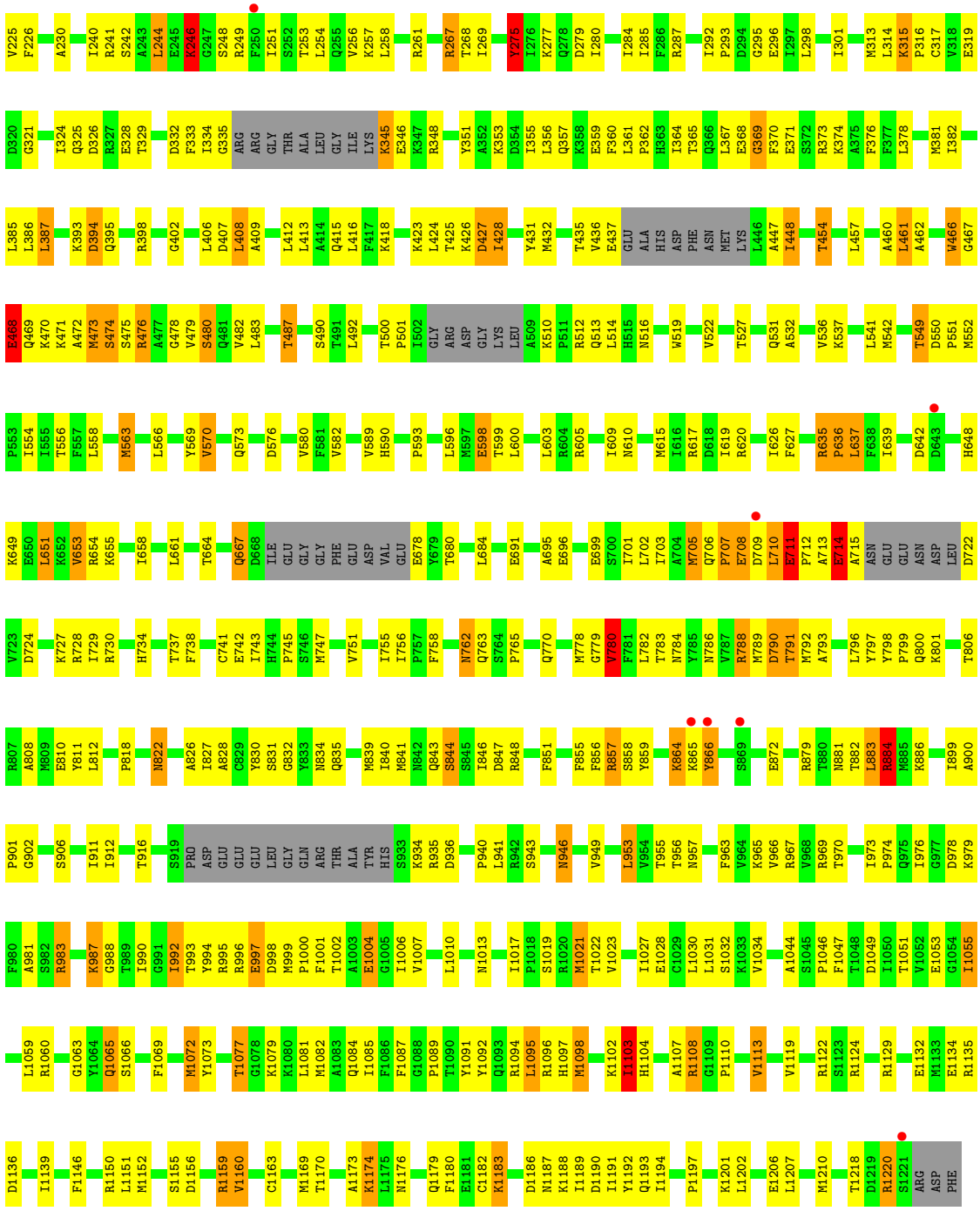




• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

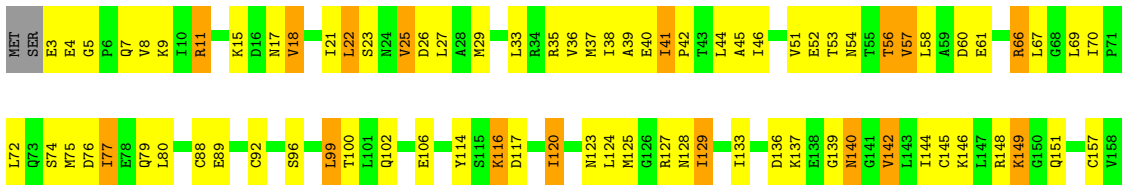
Chain B:

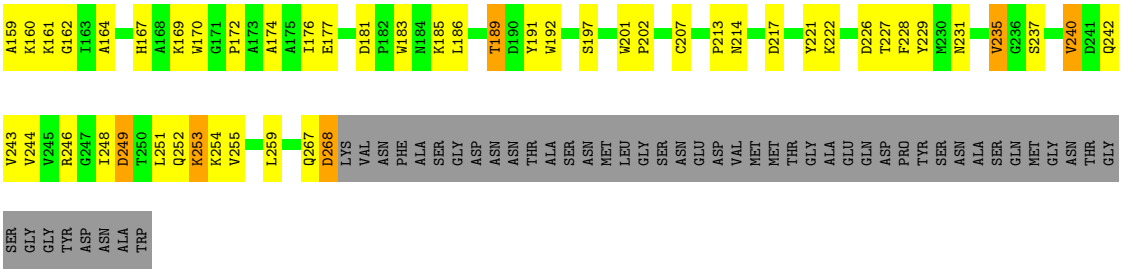




- Molecule 3: DNA-directed RNA polymerase II subunit RPB3

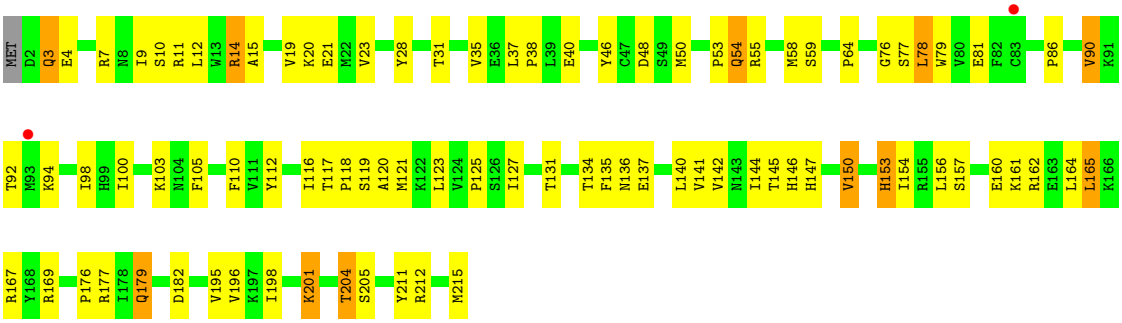
Chain C:





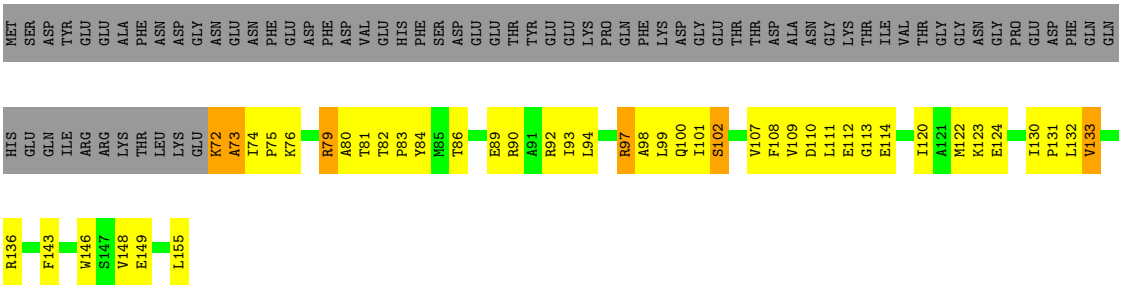
• Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

Chain E:



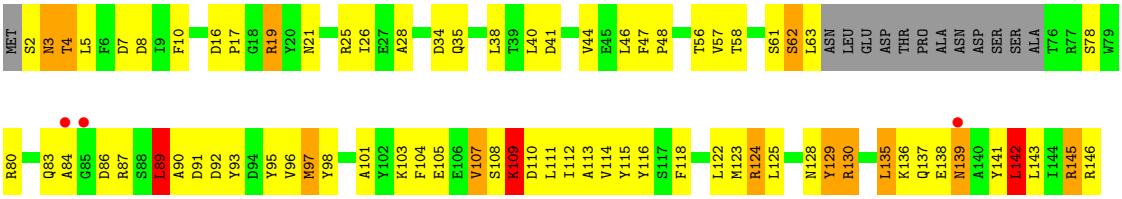
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2

Chain F:



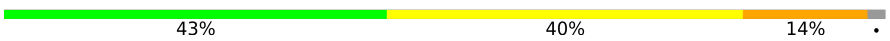
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3

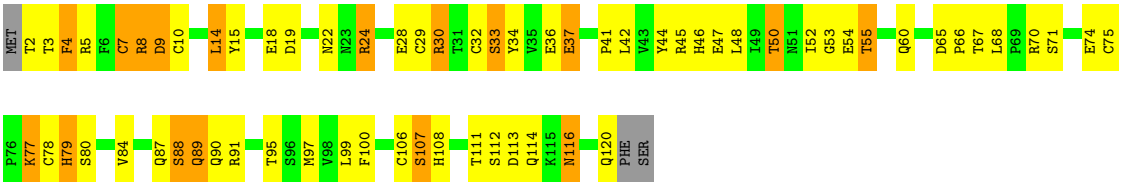
Chain H:



• Molecule 7: DNA-directed RNA polymerase II subunit RPB9

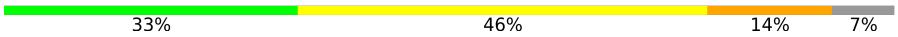
Chain I:

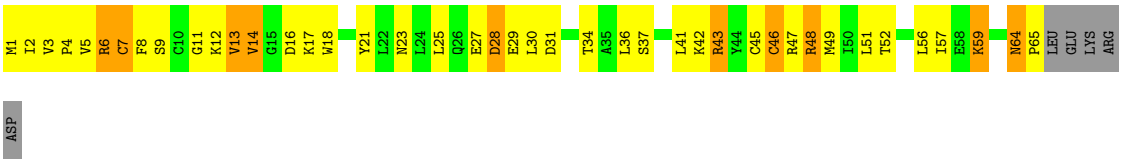




• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5

Chain J:



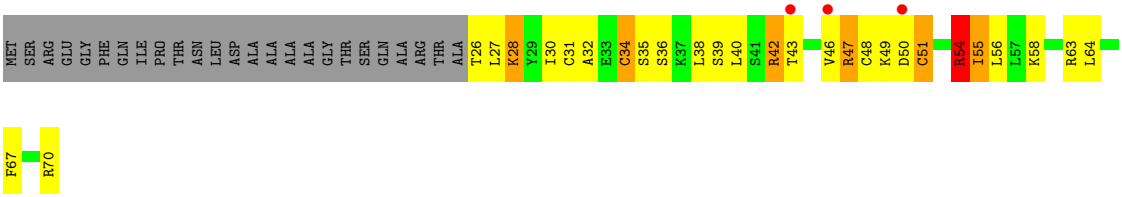


• Molecule 9: DNA-directed RNA polymerase II subunit RPB11

Chain K:

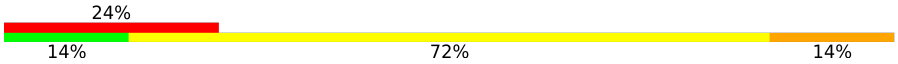
• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4

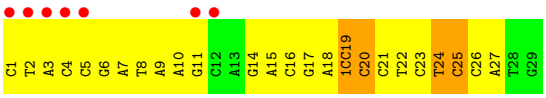
Chain L:



• Molecule 11: DNA (29-MER)

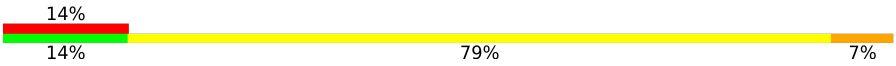
Chain T:

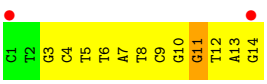




• Molecule 12: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')

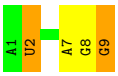
Chain N:





• Molecule 13: RNA (5'-D(*AP*UP*GP*GP*AP*GP*AP*GP*G)-3')

Chain R:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	166.70Å 221.64Å 192.41Å 90.00° 100.35° 90.00°	Depositor
Resolution (Å)	49.27 – 3.50 49.27 – 3.50	Depositor EDS
% Data completeness (in resolution range)	94.1 (49.27-3.50) 94.2 (49.27-3.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 3.48Å)	Xtriage
Refinement program	PHENIX, REFMAC	Depositor
R, R_{free}	0.201 , 0.232 0.201 , 0.232	Depositor DCC
R_{free} test set	4090 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	75.7	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 70.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	29189	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1CC, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.44	2/11146 (0.0%)	0.67	5/15066 (0.0%)
2	B	0.46	0/8932	0.68	5/12045 (0.0%)
3	C	0.48	0/2133	0.70	0/2891
4	E	0.41	1/1788 (0.1%)	0.56	0/2406
5	F	0.41	0/691	0.64	0/933
6	H	0.37	0/1086	0.65	4/1470 (0.3%)
7	I	0.41	0/989	0.58	0/1331
8	J	0.48	0/541	0.73	0/727
9	K	0.47	0/937	0.64	0/1265
10	L	0.37	0/360	0.63	0/478
11	T	0.59	0/632	1.09	6/969 (0.6%)
12	N	0.39	0/317	0.99	1/488 (0.2%)
13	R	0.57	0/223	1.00	0/348
All	All	0.45	3/29775 (0.0%)	0.68	21/40417 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	38	PRO	N-CD	5.30	1.55	1.47
1	A	400	PRO	N-CD	5.14	1.55	1.47
1	A	321	PRO	N-CD	5.08	1.54	1.47

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	77	CYS	C-N-CD	-15.50	86.50	120.60
2	B	474	SER	N-CA-CB	-7.60	99.10	110.50
11	T	24	DT	N3-C4-O4	7.25	124.25	119.90
11	T	24	DT	P-O5'-C5'	-6.69	110.20	120.90
11	T	25	DC	O4'-C4'-C3'	-6.24	102.01	104.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	793	ALA	N-CA-CB	6.23	118.82	110.10
1	A	79	GLY	N-CA-C	-6.15	97.72	113.10
1	A	171	GLN	C-N-CD	6.04	141.08	128.40
6	H	142	LEU	N-CA-CB	5.97	122.34	110.40
11	T	26	DC	O4'-C1'-N1	5.79	112.05	108.00
1	A	603	ASN	N-CA-CB	-5.66	100.42	110.60
6	H	142	LEU	N-CA-C	-5.66	95.73	111.00
2	B	734	HIS	N-CA-CB	-5.39	100.90	110.60
11	T	24	DT	C5-C4-O4	-5.33	121.17	124.90
12	N	11	DG	O4'-C4'-C3'	-5.27	102.39	104.50
1	A	403	LYS	CB-CA-C	-5.17	100.05	110.40
11	T	20	DC	OP2-P-O3'	5.17	116.56	105.20
6	H	4	THR	N-CA-CB	5.11	120.02	110.30
2	B	705	MET	CB-CA-C	-5.09	100.22	110.40
2	B	780	VAL	CB-CA-C	-5.08	101.74	111.40
6	H	89	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

There are no planarity outliers.

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	10953	0	11053	638	0
2	B	8762	0	8797	428	0
3	C	2095	0	2051	101	0
4	E	1752	0	1776	67	0
5	F	679	0	701	30	0
6	H	1068	0	1040	102	0
7	I	971	0	927	82	0
8	J	532	0	542	54	0
9	K	919	0	929	24	0
10	L	358	0	381	35	0
11	T	609	0	337	96	0
12	N	284	0	161	30	0
13	R	198	0	100	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	1	0	0	0	0
All	All	29189	0	28795	1511	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 26.

All (1511) 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)
1:A:315:LEU:HD23	1:A:316:GLN:CG	1.22	1.56
1:A:315:LEU:CD2	1:A:316:GLN:HG3	1.43	1.44
1:A:315:LEU:HB3	1:A:316:GLN:CB	1.54	1.37
1:A:315:LEU:CD2	1:A:316:GLN:CG	1.96	1.36
11:T:1:DC:H2"	11:T:2:DT:C5'	1.63	1.27
11:T:19[A]:1CC:C2'	11:T:20:DC:H5'	1.66	1.24
11:T:8:DT:H2"	11:T:9:DA:C8	1.70	1.24
11:T:9:DA:H2"	11:T:10:DA:C8	1.75	1.20
2:B:711:GLU:HG3	2:B:712:PRO:CD	1.70	1.20
6:H:128:ASN:O	6:H:129:TYR:CD2	1.95	1.19
1:A:315:LEU:HB3	1:A:316:GLN:CA	1.69	1.18
11:T:19[A]:1CC:C2'	11:T:20:DC:C5'	2.23	1.17
11:T:1:DC:C2'	11:T:2:DT:H5'	1.75	1.17
11:T:19[A]:1CC:H7	11:T:20:DC:H5"	1.26	1.17
1:A:711:ARG:HG3	7:I:97:MET:CE	1.75	1.16
2:B:475:SER:HB3	2:B:476:ARG:HG3	1.18	1.14
1:A:326:ARG:HE	1:A:1406:VAL:HG11	0.99	1.13
12:N:8:DT:H2"	12:N:9:DC:C5	1.85	1.11
1:A:711:ARG:CG	7:I:97:MET:HE3	1.79	1.11
10:L:47:ARG:HB3	10:L:54:ARG:HA	1.12	1.11
11:T:19[A]:1CC:H7	11:T:20:DC:C5'	1.78	1.11
1:A:317:LYS:HB3	1:A:319:GLY:HA3	1.11	1.11
1:A:55:ASP:HB3	1:A:56:PRO:HA	1.22	1.08
11:T:3:DA:H2"	11:T:4:DC:C5'	1.82	1.08
11:T:1:DC:H2"	11:T:2:DT:H5'	1.29	1.08
1:A:315:LEU:HD22	1:A:316:GLN:HG3	1.36	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:47:ARG:HB3	10:L:54:ARG:CA	1.83	1.07
1:A:58:LEU:O	1:A:79:GLY:HA2	1.54	1.06
1:A:50:ILE:HG12	1:A:51:GLY:H	1.18	1.06
2:B:475:SER:CB	2:B:476:ARG:HG3	1.83	1.06
11:T:19[A]:1CC:H8	11:T:20:DC:H5'	1.08	1.06
2:B:711:GLU:HG3	2:B:712:PRO:HD3	1.07	1.05
1:A:1063:MET:CG	1:A:1436:ILE:HG23	1.85	1.05
2:B:472:ALA:N	2:B:473:MET:HA	1.67	1.04
1:A:315:LEU:HB3	1:A:316:GLN:CG	1.86	1.04
2:B:364:ILE:CG2	2:B:374:LYS:HE2	1.87	1.03
1:A:298:PHE:HE1	1:A:312:PRO:HB2	1.23	1.03
2:B:708:GLU:HA	2:B:710:LEU:H	1.21	1.03
2:B:711:GLU:CG	2:B:712:PRO:HD3	1.88	1.03
1:A:53:LEU:HD23	1:A:54:ASN:H	1.25	1.02
1:A:310:GLY:C	1:A:312:PRO:HD3	1.79	1.02
2:B:471:LYS:HB2	2:B:472:ALA:HA	1.39	1.01
1:A:40:THR:HG22	1:A:41:MET:HG3	1.42	1.01
7:I:106:CYS:SG	7:I:108:HIS:HB3	2.00	1.01
1:A:597:LEU:HD12	6:H:115:TYR:CE2	1.96	1.00
8:J:7:CYS:O	8:J:11:GLY:HA2	1.60	1.00
1:A:598:LEU:HD22	6:H:25:ARG:HH11	1.26	1.00
11:T:4:DC:H2"	11:T:5:DC:C5	1.96	0.99
10:L:34:CYS:HB2	10:L:51:CYS:SG	2.01	0.99
6:H:56:THR:HB	6:H:145:ARG:HG2	1.45	0.98
6:H:129:TYR:OH	6:H:130:ARG:NH2	1.95	0.98
6:H:128:ASN:O	6:H:129:TYR:HD2	1.35	0.98
11:T:16:DC:H1'	11:T:17:DG:H5"	1.43	0.98
1:A:306:ASN:HD21	1:A:313:GLN:HB3	1.24	0.97
2:B:246:LYS:HA	2:B:246:LYS:HE3	1.47	0.96
12:N:4:DC:H2"	12:N:5:DT:H5'	1.46	0.96
7:I:15:TYR:CE1	7:I:30:ARG:HD3	2.01	0.96
1:A:326:ARG:NE	1:A:1406:VAL:HG11	1.81	0.96
7:I:15:TYR:CD1	7:I:30:ARG:HD3	2.01	0.96
11:T:3:DA:H2'	11:T:4:DC:C6	2.00	0.96
2:B:637:LEU:HD21	2:B:742:GLU:HA	1.48	0.95
10:L:48:CYS:SG	10:L:49:LYS:N	2.37	0.95
11:T:8:DT:H2"	11:T:9:DA:H8	1.08	0.95
2:B:364:ILE:HG21	2:B:374:LYS:HG2	1.47	0.95
1:A:265:LYS:HZ1	1:A:302:THR:HG23	1.31	0.95
6:H:107:VAL:HG12	6:H:108:SER:H	1.31	0.95
1:A:317:LYS:CB	1:A:319:GLY:HA3	1.96	0.95

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:475:SER:HB3	2:B:476:ARG:CG	1.96	0.94
11:T:8:DT:C2'	11:T:9:DA:C8	2.49	0.94
1:A:828:ALA:O	1:A:831:THR:HG22	1.66	0.94
1:A:315:LEU:HD23	1:A:316:GLN:HG2	0.97	0.94
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.48	0.93
1:A:41:MET:HB3	1:A:49:LYS:HG3	1.48	0.92
1:A:78:PRO:HB3	2:B:1201:LYS:CE	1.99	0.92
6:H:112:ILE:HG22	6:H:113:ALA:H	1.31	0.92
11:T:17:DG:H2"	11:T:18:DA:H5"	1.52	0.92
11:T:19[A]:1CC:H8	11:T:20:DC:C5'	1.91	0.91
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.53	0.91
11:T:1:DC:C2'	11:T:2:DT:C5'	2.43	0.90
1:A:57:ARG:HG2	1:A:68:GLN:HG2	1.51	0.90
2:B:364:ILE:HG23	2:B:365:THR:N	1.84	0.90
1:A:257:ARG:HG2	1:A:257:ARG:HH11	1.36	0.90
10:L:38:LEU:HD11	10:L:49:LYS:HB2	1.53	0.90
1:A:298:PHE:CE1	1:A:312:PRO:HB2	2.06	0.90
1:A:315:LEU:CB	1:A:316:GLN:CA	2.50	0.89
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.37	0.89
1:A:35:ILE:HD13	1:A:53:LEU:HA	1.54	0.89
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.53	0.88
1:A:315:LEU:HB3	1:A:316:GLN:HA	1.53	0.88
1:A:315:LEU:CB	1:A:316:GLN:CG	2.51	0.88
2:B:883:LEU:O	2:B:884:ARG:HB2	1.73	0.88
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.53	0.88
1:A:315:LEU:HB3	1:A:316:GLN:HB2	1.57	0.87
1:A:310:GLY:C	1:A:311:GLN:HG2	1.93	0.87
11:T:4:DC:H2"	11:T:5:DC:C6	2.08	0.87
11:T:16:DC:C1'	11:T:17:DG:H5"	2.04	0.87
3:C:142:VAL:H	8:J:16:ASP:HB3	1.40	0.86
1:A:147:VAL:HG22	1:A:148:CYS:H	1.41	0.86
1:A:315:LEU:CD2	1:A:316:GLN:HG2	1.81	0.86
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.38	0.86
1:A:1434:ALA:CB	1:A:1436:ILE:HD13	2.06	0.86
1:A:711:ARG:HG3	7:I:97:MET:HE3	0.90	0.86
1:A:1116:LEU:H	1:A:1308:THR:HB	1.40	0.86
11:T:1:DC:C3'	11:T:2:DT:H5'	2.05	0.86
1:A:306:ASN:ND2	1:A:313:GLN:HB3	1.91	0.85
2:B:470:LYS:HB2	2:B:472:ALA:HB2	1.56	0.85
1:A:50:ILE:CG1	1:A:51:GLY:H	1.88	0.85
1:A:53:LEU:HD23	1:A:54:ASN:N	1.91	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:364:ILE:HG23	2:B:365:THR:H	1.38	0.84
1:A:40:THR:HG22	1:A:41:MET:CG	2.07	0.84
1:A:35:ILE:HD12	1:A:241:VAL:HG11	1.60	0.84
1:A:315:LEU:CB	1:A:316:GLN:HG3	2.08	0.84
1:A:55:ASP:CB	1:A:56:PRO:HA	1.99	0.84
1:A:315:LEU:CB	1:A:316:GLN:CB	2.49	0.84
1:A:164:ARG:CD	1:A:165:GLY:H	1.91	0.84
11:T:21:DC:C5	11:T:22:DT:H71	2.12	0.84
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.13	0.83
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.61	0.83
11:T:1:DC:C4'	11:T:2:DT:H5'	2.09	0.83
6:H:62:SER:CB	6:H:63:LEU:HA	2.07	0.83
1:A:1132:LYS:HG3	1:A:1135:ARG:HH12	1.44	0.82
1:A:315:LEU:CB	1:A:316:GLN:HA	2.08	0.82
1:A:50:ILE:HG12	1:A:51:GLY:N	1.93	0.82
1:A:599:SER:HB2	6:H:122:LEU:HD12	1.61	0.82
1:A:1063:MET:HG3	1:A:1436:ILE:HG23	1.60	0.82
11:T:9:DA:H2"	11:T:10:DA:H8	1.41	0.82
12:N:8:DT:H2"	12:N:9:DC:C6	2.14	0.82
11:T:1:DC:H2"	11:T:2:DT:O5'	1.77	0.82
1:A:315:LEU:CG	1:A:316:GLN:HG3	2.10	0.82
2:B:364:ILE:CG2	2:B:365:THR:H	1.93	0.82
2:B:708:GLU:HA	2:B:710:LEU:N	1.95	0.82
1:A:49:LYS:H	1:A:49:LYS:HD2	1.44	0.82
10:L:46:VAL:HB	10:L:47:ARG:HG3	1.61	0.82
2:B:357:GLN:NE2	2:B:368:GLU:HA	1.94	0.81
11:T:8:DT:C4	11:T:9:DA:N6	2.48	0.81
11:T:9:DA:C2'	11:T:10:DA:C8	2.61	0.81
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.94	0.81
2:B:468:GLU:OE2	2:B:469:GLN:N	2.13	0.81
2:B:706:GLN:HB2	2:B:710:LEU:HD22	1.61	0.81
1:A:1224:LEU:HD12	1:A:1240:CYS:HB3	1.63	0.81
1:A:316:GLN:C	1:A:318:SER:HB3	2.00	0.81
7:I:15:TYR:CD1	7:I:30:ARG:CD	2.64	0.80
1:A:65:LEU:HA	1:A:73:GLY:HA2	1.64	0.80
11:T:3:DA:H2"	11:T:4:DC:O5'	1.78	0.80
1:A:164:ARG:HD3	1:A:165:GLY:H	1.47	0.80
11:T:1:DC:H2'	11:T:2:DT:C6	2.16	0.80
11:T:8:DT:C2	11:T:9:DA:C5	2.70	0.80
12:N:4:DC:C2'	12:N:5:DT:H5'	2.10	0.80
2:B:435:THR:HG22	2:B:435:THR:O	1.81	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LEU:CD2	1:A:54:ASN:H	1.95	0.80
1:A:298:PHE:HE1	1:A:312:PRO:CB	1.93	0.80
11:T:16:DC:C2'	11:T:17:DG:H5"	2.12	0.80
2:B:843:GLN:HB2	2:B:993:THR:HB	1.61	0.79
11:T:1:DC:H1'	11:T:2:DT:O4'	1.81	0.79
2:B:471:LYS:CB	2:B:472:ALA:HA	2.06	0.79
2:B:364:ILE:CG2	2:B:374:LYS:CE	2.60	0.79
2:B:637:LEU:CD2	2:B:742:GLU:HA	2.12	0.79
12:N:8:DT:C2'	12:N:9:DC:C5	2.66	0.79
1:A:372:LYS:HE2	1:A:397:ASN:O	1.83	0.79
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.47	0.79
2:B:792:MET:HA	2:B:856:PHE:O	1.83	0.79
2:B:169:ARG:H	2:B:454:THR:HG23	1.48	0.78
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.64	0.78
6:H:98:TYR:CE1	6:H:139:ASN:HA	2.17	0.78
2:B:467:GLY:C	2:B:468:GLU:HG3	2.04	0.78
1:A:315:LEU:CG	1:A:316:GLN:CG	2.61	0.78
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.22	0.78
2:B:467:GLY:O	2:B:468:GLU:HG3	1.84	0.78
1:A:315:LEU:HD23	1:A:316:GLN:CD	2.03	0.78
3:C:52:GLU:HA	10:L:64:LEU:HD11	1.65	0.78
3:C:56:THR:HG23	3:C:58:LEU:H	1.48	0.78
3:C:142:VAL:H	8:J:16:ASP:CB	1.97	0.77
1:A:317:LYS:HE3	1:A:317:LYS:HA	1.64	0.77
6:H:83:GLN:HB3	6:H:86:ASP:HB3	1.66	0.77
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.66	0.77
2:B:1173:ALA:HA	2:B:1180:PHE:HD1	1.48	0.77
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.64	0.77
1:A:598:LEU:HD22	6:H:25:ARG:NH1	2.00	0.77
11:T:3:DA:H2"	11:T:4:DC:H5'	1.67	0.77
11:T:3:DA:H2"	11:T:4:DC:O4'	1.85	0.76
1:A:304:MET:HG2	2:B:1210:MET:HG3	1.67	0.76
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.67	0.76
1:A:316:GLN:CA	1:A:318:SER:HB3	2.16	0.76
2:B:708:GLU:HB3	2:B:709:ASP:HA	1.66	0.76
1:A:1224:LEU:CD1	1:A:1240:CYS:HB3	2.15	0.76
2:B:364:ILE:HG21	2:B:374:LYS:HE2	1.65	0.76
11:T:6:DG:H2"	11:T:7:DA:C8	2.21	0.76
1:A:55:ASP:HB3	1:A:56:PRO:CA	2.10	0.75
2:B:364:ILE:HG21	2:B:374:LYS:CG	2.17	0.75
2:B:470:LYS:HB2	2:B:472:ALA:CB	2.15	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:123:MET:HE1	6:H:142:LEU:HD13	1.68	0.75
1:A:78:PRO:HB3	2:B:1201:LYS:HE3	1.66	0.75
2:B:864:LYS:HD2	2:B:866:TYR:H	1.52	0.75
6:H:112:ILE:HG22	6:H:113:ALA:N	2.02	0.75
1:A:57:ARG:HG2	1:A:68:GLN:CG	2.16	0.75
6:H:4:THR:HG22	6:H:5:LEU:H	1.52	0.75
10:L:38:LEU:HD11	10:L:49:LYS:CB	2.17	0.75
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.69	0.74
1:A:1434:ALA:HB3	1:A:1436:ILE:HD13	1.67	0.74
2:B:848:ARG:HD3	8:J:7:CYS:O	1.87	0.74
2:B:1104:HIS:HB2	2:B:1122:ARG:HG3	1.68	0.74
2:B:257:LYS:NZ	2:B:279:ASP:OD2	2.20	0.74
1:A:1063:MET:HG3	1:A:1436:ILE:CG2	2.17	0.74
2:B:364:ILE:CG2	2:B:365:THR:N	2.49	0.74
6:H:128:ASN:O	6:H:129:TYR:CG	2.40	0.74
2:B:471:LYS:C	2:B:473:MET:HA	2.07	0.74
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.51	0.74
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.34	0.74
2:B:791:THR:O	2:B:857:ARG:HA	1.88	0.74
1:A:821:ARG:O	1:A:825:ILE:HG12	1.87	0.73
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.51	0.73
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.52	0.73
1:A:311:GLN:N	1:A:312:PRO:CD	2.51	0.73
1:A:57:ARG:CG	1:A:68:GLN:HG2	2.18	0.73
1:A:79:GLY:HA3	1:A:243:PRO:HB2	1.70	0.73
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.70	0.73
1:A:1035:TYR:O	1:A:1036:ARG:HB2	1.88	0.73
1:A:259:GLU:HG3	1:A:264:PHE:CZ	2.23	0.73
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	1.71	0.73
2:B:353:LYS:O	2:B:357:GLN:HG2	1.89	0.73
2:B:471:LYS:HB2	2:B:472:ALA:CA	2.16	0.73
8:J:7:CYS:O	8:J:11:GLY:CA	2.35	0.73
2:B:364:ILE:HG21	2:B:374:LYS:CE	2.19	0.73
12:N:13:DA:C6	12:N:14:DG:C6	2.76	0.73
1:A:310:GLY:O	1:A:311:GLN:HG2	1.89	0.73
6:H:4:THR:HG21	6:H:58:THR:CG2	2.19	0.73
2:B:620:ARG:CZ	7:I:68:LEU:HD21	2.19	0.72
7:I:89:GLN:HE21	7:I:89:GLN:HA	1.54	0.72
11:T:19[A]:1CC:C2'	11:T:20:DC:H5"	2.02	0.72
1:A:919:ILE:CG2	1:A:925:LEU:HD12	2.18	0.72
2:B:855:PHE:HZ	2:B:857:ARG:NH1	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.72	0.72
1:A:40:THR:HG22	1:A:41:MET:SD	2.30	0.72
1:A:975:HIS:HA	1:A:1036:ARG:HD2	1.71	0.72
2:B:778:MET:HE1	2:B:1094:ARG:HD3	1.71	0.72
7:I:106:CYS:SG	7:I:108:HIS:CB	2.77	0.71
1:A:164:ARG:CG	1:A:165:GLY:H	2.04	0.71
2:B:213:ILE:O	2:B:215:GLN:NE2	2.23	0.71
7:I:78:CYS:C	7:I:80:SER:H	1.93	0.71
1:A:853:ASP:OD1	1:A:855:THR:HB	1.90	0.71
12:N:6:DT:H2"	12:N:7:DA:C8	2.26	0.71
7:I:77:LYS:HB2	7:I:108:HIS:CD2	2.26	0.71
6:H:128:ASN:O	6:H:129:TYR:CB	2.39	0.71
8:J:9:SER:OG	8:J:45:CYS:HB2	1.90	0.71
1:A:147:VAL:HG22	1:A:148:CYS:N	2.05	0.71
2:B:642:ASP:HA	2:B:649:LYS:HA	1.73	0.71
3:C:142:VAL:N	8:J:16:ASP:HB3	2.05	0.70
10:L:47:ARG:CB	10:L:54:ARG:HA	2.06	0.70
11:T:1:DC:C2'	11:T:2:DT:C6	2.73	0.70
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.06	0.70
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.72	0.70
7:I:8:ARG:HG3	7:I:34:TYR:CE2	2.26	0.70
2:B:468:GLU:CD	2:B:469:GLN:H	1.94	0.70
1:A:332:LYS:HG3	1:A:333:GLU:H	1.54	0.70
1:A:899:VAL:HB	1:A:929:LEU:CG	2.22	0.70
2:B:708:GLU:CB	2:B:709:ASP:HA	2.21	0.70
2:B:711:GLU:HG3	2:B:712:PRO:HD2	1.69	0.70
6:H:25:ARG:HD3	6:H:41:ASP:OD1	1.92	0.70
2:B:364:ILE:HG22	2:B:374:LYS:HE2	1.74	0.70
11:T:8:DT:N3	11:T:9:DA:N6	2.40	0.70
1:A:310:GLY:C	1:A:312:PRO:CD	2.59	0.69
4:E:79:TRP:HB2	4:E:105:PHE:HD2	1.54	0.69
2:B:882:THR:HG23	2:B:934:LYS:HB2	1.74	0.69
3:C:41:ILE:HG13	3:C:172:PRO:HG3	1.74	0.69
6:H:93:TYR:HD1	6:H:145:ARG:HB3	1.57	0.69
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.69
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.74	0.69
1:A:134:ARG:HD3	1:A:221:SER:O	1.92	0.69
6:H:25:ARG:HG2	6:H:25:ARG:HH21	1.55	0.69
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.75	0.69
1:A:1329:THR:HB	1:A:1331:SER:H	1.56	0.69
1:A:1438:THR:HG23	5:F:92:ARG:HB2	1.74	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:LEU:CD2	2:B:457:LEU:HD23	2.23	0.69
1:A:316:GLN:HA	1:A:318:SER:HB3	1.75	0.69
2:B:287:ARG:NH1	2:B:324:ILE:O	2.26	0.69
2:B:378:LEU:O	2:B:382:ILE:HG12	1.92	0.69
2:B:416:LEU:HD23	2:B:457:LEU:HD23	1.74	0.69
1:A:1434:ALA:HB1	1:A:1436:ILE:CD1	2.23	0.69
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.74	0.69
4:E:28:TYR:HE1	4:E:76:GLY:O	1.76	0.69
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.24	0.68
6:H:63:LEU:HD23	6:H:63:LEU:H	1.56	0.68
7:I:111:THR:HG22	7:I:113:ASP:H	1.56	0.68
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	1.93	0.68
1:A:49:LYS:H	1:A:49:LYS:CD	2.06	0.68
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.29	0.68
1:A:1356:ILE:HG22	1:A:1361:SER:HB2	1.74	0.68
12:N:5:DT:H2"	12:N:6:DT:OP2	1.93	0.68
1:A:332:LYS:HG3	1:A:333:GLU:N	2.09	0.68
4:E:46:TYR:CD1	4:E:58:MET:HG2	2.28	0.68
9:K:47:ARG:HD2	9:K:60:ALA:HA	1.75	0.68
1:A:904:THR:HG23	1:A:905:ASP:OD1	1.94	0.68
10:L:28:LYS:HA	10:L:39:SER:HA	1.76	0.68
1:A:304:MET:CG	2:B:1210:MET:HG3	2.23	0.68
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.76	0.68
2:B:216:GLU:HG3	2:B:406:LEU:CD2	2.23	0.68
1:A:304:MET:O	1:A:326:ARG:HB2	1.94	0.68
1:A:326:ARG:HE	1:A:1406:VAL:CG1	1.92	0.68
2:B:1031:LEU:HD13	2:B:1055:ILE:HD13	1.76	0.67
7:I:78:CYS:O	7:I:80:SER:N	2.27	0.67
6:H:62:SER:CB	6:H:63:LEU:CA	2.71	0.67
11:T:3:DA:H2"	11:T:4:DC:C4'	2.24	0.67
2:B:428:ILE:HD11	2:B:448:ILE:HA	1.76	0.67
1:A:55:ASP:OD2	1:A:61:ILE:HG12	1.94	0.67
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.76	0.67
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.77	0.67
11:T:11:DG:H4'	11:T:11:DG:OP1	1.93	0.67
1:A:1134:ILE:O	1:A:1138:ILE:HG12	1.95	0.67
11:T:8:DT:N3	11:T:9:DA:C6	2.63	0.67
1:A:1406:VAL:HG13	1:A:1407:GLU:OE2	1.95	0.67
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.43	0.67
8:J:14:VAL:HA	8:J:17:LYS:HG3	1.76	0.67
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HG21	1:A:466:SER:O	1.95	0.67
1:A:1436:ILE:N	1:A:1436:ILE:HD12	2.11	0.66
2:B:706:GLN:CB	2:B:710:LEU:HD22	2.25	0.66
1:A:1279:ILE:HG23	1:A:1308:THR:HG23	1.78	0.66
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.78	0.66
4:E:135:PHE:HD2	4:E:140:LEU:HD21	1.60	0.66
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.61	0.66
1:A:1221:LYS:O	1:A:1222:ASN:ND2	2.28	0.66
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.10	0.66
3:C:116:LYS:HD3	3:C:140:ASN:HB3	1.77	0.66
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.77	0.66
11:T:3:DA:C2'	11:T:4:DC:O5'	2.44	0.66
1:A:485:ASP:N	1:A:485:ASP:OD1	2.27	0.66
2:B:471:LYS:HB3	2:B:473:MET:HB2	1.78	0.66
1:A:78:PRO:HB3	2:B:1201:LYS:HE2	1.77	0.66
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.78	0.66
1:A:343:LYS:O	1:A:345:VAL:HG13	1.96	0.66
1:A:392:VAL:HG13	1:A:415:LEU:CD1	2.25	0.66
7:I:32:CYS:SG	7:I:33:SER:N	2.68	0.65
8:J:9:SER:CB	8:J:45:CYS:HB2	2.26	0.65
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.96	0.65
11:T:20:DC:H2'	11:T:21:DC:C6	2.32	0.65
1:A:403:LYS:HB3	1:A:404:TYR:CD1	2.32	0.65
1:A:1149:ALA:HA	7:I:47:GLU:HA	1.77	0.65
3:C:57:VAL:HG12	3:C:58:LEU:HD23	1.79	0.65
5:F:107:VAL:HG11	5:F:111:LEU:HD21	1.77	0.65
1:A:595:THR:O	1:A:596:THR:HG23	1.97	0.65
1:A:1434:ALA:HB1	1:A:1436:ILE:HD13	1.78	0.65
1:A:469:ARG:HB3	1:A:469:ARG:HH11	1.62	0.65
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.29	0.65
2:B:806:THR:HG22	2:B:808:ALA:H	1.61	0.65
6:H:56:THR:HB	6:H:145:ARG:CG	2.24	0.65
3:C:52:GLU:HA	10:L:64:LEU:CD1	2.26	0.65
1:A:325:ILE:O	1:A:328:ARG:HB2	1.98	0.64
1:A:594:GLY:O	1:A:600:PRO:HG3	1.96	0.64
2:B:822:ASN:O	8:J:48:ARG:NH1	2.30	0.64
11:T:6:DG:H1'	11:T:7:DA:C8	2.31	0.64
11:T:21:DC:C5	11:T:22:DT:C7	2.80	0.64
7:I:34:TYR:HE1	7:I:36:GLU:HB3	1.63	0.64
12:N:10:DG:C2	12:N:11:DG:C6	2.85	0.64
1:A:783:THR:HG21	1:A:796:SER:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:MET:CG	1:A:1436:ILE:CG2	2.69	0.64
8:J:14:VAL:HG12	8:J:41:LEU:HD21	1.78	0.64
1:A:1162:VAL:CG1	7:I:41:PRO:HG3	2.27	0.64
2:B:996:ARG:NH2	3:C:174:ALA:O	2.31	0.64
4:E:117:THR:O	4:E:120:ALA:N	2.31	0.64
6:H:129:TYR:OH	6:H:130:ARG:CZ	2.45	0.64
12:N:8:DT:H2"	12:N:9:DC:H5	1.60	0.64
1:A:629:LEU:HD13	1:A:645:LEU:HD21	1.78	0.64
1:A:888:GLY:O	1:A:940:ARG:NH2	2.31	0.64
2:B:471:LYS:CB	2:B:473:MET:CB	2.76	0.64
4:E:46:TYR:CE1	4:E:58:MET:HG2	2.32	0.64
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.63	0.64
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.32	0.64
2:B:801:LYS:O	8:J:52:THR:HG23	1.98	0.64
2:B:1187:ASN:ND2	2:B:1190:ASP:O	2.29	0.64
1:A:1147:THR:HB	7:I:48:LEU:HD12	1.80	0.64
3:C:60:ASP:HB3	10:L:67:PHE:CE2	2.33	0.64
11:T:4:DC:C2'	11:T:5:DC:C5	2.79	0.64
12:N:3:DG:H2"	12:N:4:DC:H5"	1.80	0.64
1:A:254:GLU:CB	2:B:916:THR:HG21	2.28	0.63
1:A:341:MET:HE1	1:A:1425:SER:HB3	1.80	0.63
4:E:79:TRP:HB2	4:E:105:PHE:CD2	2.32	0.63
1:A:599:SER:HB2	6:H:122:LEU:CD1	2.28	0.63
2:B:301:ILE:HG21	2:B:314:LEU:HD11	1.81	0.63
6:H:128:ASN:O	6:H:129:TYR:HB3	1.99	0.63
1:A:311:GLN:N	1:A:312:PRO:HD3	2.12	0.63
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.80	0.63
3:C:66:ARG:NH2	8:J:3:VAL:O	2.31	0.63
1:A:977:LYS:HG3	1:A:978:PRO:HD2	1.81	0.63
2:B:1032:SER:HB3	2:B:1089:PRO:HB2	1.81	0.63
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.62	0.63
10:L:30:ILE:HG22	10:L:36:SER:O	1.99	0.63
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.34	0.62
3:C:35:ARG:NH1	9:K:41:THR:OG1	2.31	0.62
6:H:62:SER:OG	6:H:63:LEU:HA	1.98	0.62
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.80	0.62
11:T:3:DA:C2'	11:T:4:DC:O4'	2.47	0.62
3:C:167:HIS:HD2	3:C:169:LYS:H	1.46	0.62
1:A:483:ASP:HB2	2:B:987:LYS:HG2	1.80	0.62
11:T:6:DG:C4	11:T:7:DA:C5	2.88	0.62
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.82	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1406:VAL:CG1	1:A:1407:GLU:OE2	2.48	0.62
1:A:106:VAL:HG13	1:A:112:LYS:N	2.14	0.62
1:A:472:LEU:O	1:A:475:THR:HB	1.99	0.62
1:A:899:VAL:HB	1:A:929:LEU:HG	1.82	0.62
2:B:244:LEU:HD12	2:B:244:LEU:H	1.64	0.62
1:A:247:ARG:N	1:A:248:PRO:HD3	2.15	0.62
1:A:265:LYS:NZ	1:A:302:THR:HG23	2.09	0.62
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.82	0.62
2:B:471:LYS:HB2	2:B:473:MET:HB3	1.82	0.62
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.81	0.61
2:B:471:LYS:HB2	2:B:473:MET:CB	2.29	0.61
2:B:416:LEU:HD23	2:B:457:LEU:CD2	2.31	0.61
1:A:919:ILE:HG23	1:A:925:LEU:HD12	1.82	0.61
2:B:1084:GLN:NE2	3:C:192:TRP:H	1.95	0.61
1:A:112:LYS:HG2	1:A:113:LEU:N	2.16	0.61
1:A:283:GLY:O	1:A:285:PRO:HD3	2.00	0.61
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.33	0.61
6:H:47:PHE:HB3	6:H:95:TYR:CD2	2.35	0.61
1:A:650:GLN:O	1:A:654:ASN:HB2	2.00	0.61
2:B:639:ILE:HD11	2:B:691:GLU:CG	2.29	0.61
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.35	0.61
6:H:105:GLU:HB3	6:H:113:ALA:HB3	1.81	0.61
11:T:16:DC:H2"	11:T:17:DG:H5"	1.81	0.61
6:H:57:VAL:HG13	6:H:142:LEU:HD11	1.81	0.61
1:A:69:THR:O	1:A:69:THR:HG22	2.00	0.61
8:J:28:ASP:OD1	8:J:28:ASP:N	2.32	0.61
1:A:147:VAL:HA	1:A:170:THR:HA	1.83	0.61
1:A:259:GLU:CG	1:A:264:PHE:CZ	2.83	0.61
6:H:25:ARG:HG2	6:H:25:ARG:NH2	2.15	0.61
1:A:322:VAL:HG22	1:A:323:LYS:N	2.15	0.61
1:A:699:ALA:HA	7:I:112:SER:O	2.00	0.61
1:A:869:GLY:O	4:E:204:THR:HG21	2.01	0.61
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.81	0.61
1:A:597:LEU:CD1	6:H:115:TYR:CE2	2.81	0.61
1:A:919:ILE:HG21	1:A:925:LEU:HD12	1.81	0.61
1:A:148:CYS:HB2	1:A:168:GLY:HA2	1.83	0.60
1:A:257:ARG:HG2	1:A:257:ARG:NH1	2.08	0.60
1:A:355:GLY:CA	1:A:482:PHE:CZ	2.84	0.60
1:A:381:THR:HG23	1:A:383:TYR:H	1.66	0.60
4:E:77:SER:HB2	4:E:105:PHE:CD1	2.36	0.60
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:25:ARG:CD	6:H:41:ASP:OD1	2.49	0.60
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.82	0.60
1:A:107:CYS:SG	1:A:108:MET:N	2.75	0.60
1:A:357:PRO:HG3	2:B:832:GLY:O	2.02	0.60
1:A:919:ILE:O	1:A:919:ILE:HG22	2.02	0.60
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.84	0.60
2:B:884:ARG:O	2:B:936:ASP:HB3	2.02	0.60
1:A:1187:GLN:NE2	1:A:1188:GLN:OE1	2.35	0.60
5:F:108:PHE:O	5:F:109:VAL:HG22	2.02	0.60
2:B:605:ARG:HG2	2:B:691:GLU:OE2	2.01	0.60
8:J:9:SER:OG	8:J:48:ARG:NH2	2.34	0.60
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.66	0.60
6:H:91:ASP:OD1	6:H:92:ASP:N	2.35	0.60
2:B:473:MET:O	2:B:473:MET:HG2	2.01	0.59
2:B:792:MET:HE3	2:B:857:ARG:NH1	2.17	0.59
7:I:24:ARG:CG	7:I:24:ARG:HH11	2.14	0.59
11:T:6:DG:C1'	11:T:7:DA:C8	2.85	0.59
1:A:92:HIS:CE1	1:A:304:MET:SD	2.95	0.59
3:C:235:VAL:CG1	8:J:13:VAL:HG13	2.32	0.59
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.83	0.59
5:F:109:VAL:HG21	5:F:124:GLU:HA	1.83	0.59
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.68	0.59
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.84	0.59
11:T:1:DC:H2"	11:T:2:DT:C4'	2.30	0.59
1:A:304:MET:HG2	2:B:1210:MET:CG	2.32	0.59
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.38	0.59
6:H:61:SER:HB2	6:H:139:ASN:ND2	2.16	0.59
11:T:1:DC:O2	11:T:2:DT:C2	2.54	0.59
1:A:711:ARG:HH11	7:I:97:MET:HE3	1.68	0.59
1:A:1155:ASP:O	1:A:1241:ARG:NH1	2.35	0.59
6:H:107:VAL:HG12	6:H:108:SER:N	2.10	0.59
1:A:32:VAL:HG21	1:A:57:ARG:O	2.03	0.59
1:A:55:ASP:OD1	1:A:55:ASP:N	2.36	0.59
1:A:565:ILE:O	1:A:570:PRO:HA	2.03	0.59
2:B:30:SER:OG	2:B:743:ILE:O	2.21	0.59
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.84	0.59
12:N:13:DA:N6	12:N:14:DG:O6	2.35	0.59
1:A:977:LYS:HE3	1:A:977:LYS:HA	1.84	0.59
2:B:246:LYS:HA	2:B:246:LYS:CE	2.19	0.59
3:C:38:ILE:HG13	3:C:176:ILE:HD11	1.84	0.59
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:15:TYR:HD1	7:I:30:ARG:CD	2.15	0.59
12:N:13:DA:H2"	12:N:14:DG:H5'	1.85	0.59
1:A:482:PHE:HD2	2:B:835:GLN:O	1.85	0.59
2:B:472:ALA:N	2:B:473:MET:CA	2.53	0.59
1:A:1154:TYR:OH	7:I:18:GLU:HG3	2.02	0.58
2:B:216:GLU:HG3	2:B:406:LEU:HD23	1.85	0.58
2:B:696:GLU:O	2:B:699:GLU:HB2	2.03	0.58
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.84	0.58
1:A:711:ARG:CG	7:I:97:MET:CE	2.57	0.58
1:A:1221:LYS:O	1:A:1222:ASN:CG	2.41	0.58
6:H:129:TYR:CZ	6:H:130:ARG:NE	2.70	0.58
8:J:42:LYS:HG3	8:J:43:ARG:H	1.68	0.58
1:A:899:VAL:HB	1:A:929:LEU:CD1	2.33	0.58
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.17	0.58
2:B:110:HIS:CE1	10:L:54:ARG:HH12	2.20	0.58
2:B:707:PRO:C	2:B:708:GLU:HG3	2.22	0.58
7:I:24:ARG:HH12	7:I:37:GLU:CD	2.06	0.58
1:A:79:GLY:HA3	1:A:243:PRO:CB	2.32	0.58
2:B:435:THR:O	2:B:435:THR:CG2	2.51	0.58
2:B:487:THR:HG22	2:B:490:SER:H	1.68	0.58
1:A:455:MET:HE3	2:B:1134:GLU:HG3	1.86	0.58
7:I:113:ASP:OD2	7:I:116:ASN:ND2	2.37	0.58
8:J:45:CYS:SG	8:J:46:CYS:N	2.76	0.58
11:T:19[B]:1CC:O2	11:T:19[B]:1CC:H8	2.04	0.58
2:B:475:SER:HB3	2:B:476:ARG:CD	2.33	0.58
2:B:883:LEU:O	2:B:884:ARG:CB	2.48	0.58
1:A:70:CYS:HA	2:B:1174:LYS:HD3	1.84	0.58
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.39	0.58
1:A:1151:GLU:HA	7:I:44:TYR:O	2.04	0.58
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.85	0.58
6:H:7:ASP:OD1	6:H:8:ASP:N	2.37	0.58
11:T:6:DG:H2"	11:T:7:DA:H8	1.69	0.58
2:B:635:ARG:HG2	2:B:635:ARG:O	2.04	0.57
2:B:706:GLN:CG	2:B:710:LEU:HD22	2.34	0.57
11:T:16:DC:H2"	11:T:17:DG:C5'	2.34	0.57
1:A:591:PHE:HB3	1:A:595:THR:HB	1.87	0.57
6:H:104:PHE:CD1	6:H:114:VAL:HG12	2.38	0.57
8:J:43:ARG:HG2	8:J:46:CYS:SG	2.44	0.57
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.86	0.57
1:A:372:LYS:CE	1:A:397:ASN:O	2.52	0.57
1:A:1386:ARG:HE	1:A:1403:GLU:CD	2.07	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:112:ILE:CG2	6:H:113:ALA:H	2.11	0.57
1:A:173:THR:HB	1:A:184:SER:HB3	1.85	0.57
2:B:58:THR:O	2:B:62:ILE:HG12	2.05	0.57
2:B:1051:THR:HG22	2:B:1053:GLU:N	2.19	0.57
1:A:250:ILE:HD11	2:B:1113:VAL:HG21	1.85	0.57
2:B:864:LYS:HB3	2:B:872:GLU:H	1.69	0.57
2:B:471:LYS:HB3	2:B:473:MET:CB	2.34	0.57
6:H:103:LYS:HB3	6:H:115:TYR:HD2	1.69	0.57
4:E:28:TYR:CE1	4:E:76:GLY:O	2.57	0.57
2:B:31:TRP:HA	2:B:34:ILE:HD12	1.87	0.57
2:B:280:ILE:HB	2:B:285:ILE:HD11	1.87	0.57
2:B:1129:ARG:N	11:T:22:DT:OP1	2.35	0.57
3:C:148:ARG:HG2	3:C:149:LYS:H	1.70	0.57
1:A:413:ILE:HG21	1:A:424:ILE:HD11	1.86	0.56
6:H:4:THR:HG21	6:H:58:THR:HG22	1.86	0.56
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.87	0.56
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.87	0.56
11:T:6:DG:C5	11:T:7:DA:C6	2.93	0.56
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.87	0.56
2:B:394:ASP:N	2:B:394:ASP:OD1	2.37	0.56
2:B:470:LYS:C	2:B:472:ALA:HB2	2.26	0.56
2:B:784:ASN:O	2:B:788:ARG:HD2	2.04	0.56
2:B:857:ARG:NH1	2:B:857:ARG:HG3	2.19	0.56
2:B:1081:LEU:O	3:C:189:THR:HG23	2.05	0.56
2:B:1173:ALA:HA	2:B:1180:PHE:CD1	2.34	0.56
6:H:62:SER:HB2	6:H:63:LEU:CA	2.34	0.56
12:N:6:DT:H2"	12:N:7:DA:H8	1.69	0.56
1:A:1152:ILE:HB	7:I:44:TYR:HB3	1.86	0.56
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.86	0.56
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.87	0.56
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.87	0.56
1:A:152:VAL:HG11	1:A:161:LEU:CB	2.36	0.56
1:A:172:PRO:HB3	1:A:185:TRP:CZ2	2.40	0.56
1:A:268:ASP:O	1:A:299:HIS:ND1	2.34	0.56
2:B:470:LYS:CB	2:B:472:ALA:HB2	2.33	0.56
6:H:38:LEU:HD13	6:H:125:LEU:HD13	1.88	0.56
7:I:77:LYS:HB2	7:I:108:HIS:HD2	1.66	0.56
10:L:47:ARG:HB3	10:L:54:ARG:N	2.21	0.56
11:T:6:DG:C2'	11:T:7:DA:C8	2.88	0.56
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.45	0.56
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.86	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:SER:HA	1:A:482:PHE:CD1	2.41	0.56
1:A:591:PHE:HA	1:A:595:THR:HG21	1.86	0.56
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.20	0.56
3:C:88:CYS:SG	3:C:92:CYS:HB3	2.45	0.56
4:E:157:SER:N	4:E:160:GLU:OE1	2.30	0.56
7:I:55:THR:HG21	7:I:120:GLN:HB3	1.88	0.56
1:A:402:ALA:HA	1:A:434:ARG:HA	1.86	0.56
1:A:546:VAL:HG13	1:A:577:ILE:HG21	1.87	0.56
7:I:89:GLN:HA	7:I:89:GLN:NE2	2.21	0.56
1:A:248:PRO:O	1:A:260:ASP:HB2	2.06	0.56
2:B:361:LEU:O	2:B:364:ILE:HG22	2.06	0.56
2:B:711:GLU:CG	2:B:712:PRO:CD	2.60	0.56
7:I:8:ARG:CG	7:I:34:TYR:CE2	2.88	0.56
7:I:24:ARG:HG3	7:I:24:ARG:NH1	2.21	0.56
11:T:1:DC:C1'	11:T:2:DT:H5'	2.33	0.56
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.87	0.56
7:I:65:ASP:OD1	7:I:67:THR:OG1	2.20	0.56
12:N:5:DT:H2"	12:N:6:DT:H72	1.88	0.56
1:A:419:LYS:HG3	1:A:420:ARG:H	1.70	0.55
2:B:788:ARG:HB3	2:B:788:ARG:HH11	1.69	0.55
1:A:303:TYR:O	1:A:303:TYR:CG	2.58	0.55
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.87	0.55
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.06	0.55
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.88	0.55
2:B:129:PHE:CE1	2:B:166:PHE:HB2	2.42	0.55
2:B:714:GLU:CD	2:B:715:ALA:H	2.09	0.55
3:C:251:LEU:O	3:C:255:VAL:HG23	2.05	0.55
7:I:47:GLU:HG2	7:I:50:THR:HG23	1.87	0.55
1:A:597:LEU:HD12	6:H:115:TYR:CD2	2.41	0.55
1:A:901:LEU:HD13	1:A:919:ILE:HG22	1.89	0.55
2:B:95:ILE:HD12	2:B:130:VAL:HG22	1.87	0.55
6:H:63:LEU:HG	6:H:90:ALA:HB3	1.88	0.55
1:A:593:GLU:OE1	1:A:593:GLU:HA	2.06	0.55
10:L:38:LEU:HD22	10:L:48:CYS:HA	1.89	0.55
1:A:852:TYR:O	5:F:81:THR:HG22	2.07	0.55
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.15	0.55
2:B:790:ASP:N	2:B:790:ASP:OD1	2.37	0.55
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.89	0.55
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.88	0.55
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.07	0.55
11:T:8:DT:C2	11:T:9:DA:C6	2.95	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:N	1:A:318:SER:HA	2.21	0.55
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.89	0.55
2:B:1097:HIS:HA	2:B:1102:LYS:HE3	1.89	0.55
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.89	0.55
1:A:152:VAL:HG11	1:A:161:LEU:HB3	1.89	0.55
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.88	0.55
1:A:589:GLN:HG2	1:A:591:PHE:HE1	1.70	0.55
1:A:1116:LEU:HD22	1:A:1311:VAL:HG22	1.88	0.55
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.88	0.55
11:T:3:DA:C2'	11:T:4:DC:C6	2.85	0.55
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.88	0.55
2:B:62:ILE:HD12	2:B:418:LYS:HG3	1.89	0.55
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.89	0.55
5:F:97:ARG:HE	5:F:124:GLU:CD	2.10	0.55
1:A:922:ASP:C	1:A:924:LYS:H	2.10	0.54
1:A:949:ASP:OD1	1:A:949:ASP:N	2.40	0.54
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.88	0.54
1:A:342:GLY:C	1:A:343:LYS:HG3	2.27	0.54
1:A:1434:ALA:CB	1:A:1436:ILE:CD1	2.80	0.54
1:A:783:THR:HG22	1:A:787:PHE:CD2	2.43	0.54
2:B:345:LYS:HG2	2:B:348:ARG:HH12	1.73	0.54
1:A:1435:PRO:C	1:A:1436:ILE:HD12	2.28	0.54
2:B:590:HIS:HD2	2:B:596:LEU:HD22	1.72	0.54
6:H:89:LEU:HD23	6:H:92:ASP:H	1.72	0.54
6:H:110:ASP:O	6:H:111:LEU:HG	2.08	0.54
1:A:114:LEU:HB3	1:A:145:LYS:HG3	1.90	0.54
1:A:148:CYS:CB	1:A:167:CYS:O	2.54	0.54
4:E:179:GLN:O	4:E:182:ASP:HB2	2.08	0.54
6:H:98:TYR:CD1	6:H:141:TYR:CZ	2.96	0.54
2:B:620:ARG:HD2	7:I:68:LEU:HD11	1.89	0.54
1:A:310:GLY:CA	1:A:312:PRO:HD3	2.37	0.54
6:H:35:GLN:HB2	6:H:111:LEU:HD21	1.90	0.54
7:I:15:TYR:HD1	7:I:30:ARG:HD2	1.71	0.54
7:I:19:ASP:HB3	7:I:24:ARG:HG2	1.89	0.54
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.89	0.54
1:A:420:ARG:NH2	1:A:423:ASP:O	2.38	0.54
1:A:494:SER:H	1:A:497:THR:CG2	2.21	0.54
2:B:549:THR:HG21	2:B:610:ASN:HD22	1.73	0.54
1:A:591:PHE:CD1	1:A:591:PHE:N	2.74	0.54
1:A:1063:MET:HG2	1:A:1436:ILE:HG23	1.84	0.54
3:C:162:GLY:HA3	3:C:170:TRP:CE2	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:13:VAL:HG23	8:J:13:VAL:O	2.08	0.54
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.90	0.54
1:A:40:THR:CG2	1:A:41:MET:SD	2.96	0.53
1:A:90:VAL:HB	1:A:297:GLN:NE2	2.24	0.53
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.88	0.53
2:B:364:ILE:O	2:B:365:THR:HG23	2.08	0.53
7:I:15:TYR:CE1	7:I:30:ARG:CD	2.82	0.53
1:A:308:ILE:HD12	1:A:308:ILE:H	1.73	0.53
1:A:1031:VAL:O	1:A:1031:VAL:HG12	2.07	0.53
4:E:15:ALA:O	4:E:19:VAL:HG23	2.08	0.53
11:T:22:DT:C2'	11:T:23:DC:H5'	2.39	0.53
1:A:343:LYS:NZ	2:B:1155:SER:HB3	2.22	0.53
2:B:1084:GLN:HE22	3:C:192:TRP:N	2.04	0.53
1:A:242:PRO:O	1:A:247:ARG:NH2	2.40	0.53
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.88	0.53
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.89	0.53
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.91	0.53
1:A:492:PRO:HB2	1:A:497:THR:HG23	1.89	0.53
2:B:953:LEU:HD11	10:L:55:ILE:HG23	1.90	0.53
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.09	0.53
1:A:315:LEU:CG	1:A:316:GLN:HG2	2.34	0.53
1:A:503:GLN:OE1	5:F:90:ARG:NH2	2.42	0.53
1:A:564:ALA:O	6:H:97:MET:HB3	2.08	0.53
2:B:361:LEU:N	2:B:362:PRO:HD3	2.22	0.53
3:C:75:MET:O	3:C:246:ARG:NH2	2.41	0.53
12:N:12:DT:H2"	12:N:13:DA:C8	2.44	0.53
1:A:161:LEU:O	1:A:162:VAL:CG1	2.57	0.53
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.16	0.53
1:A:844:ALA:HB2	1:A:1389:PHE:CE1	2.44	0.53
1:A:1142:THR:O	1:A:1145:SER:OG	2.26	0.53
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.24	0.53
8:J:30:LEU:HD22	8:J:34:THR:HG21	1.91	0.53
1:A:50:ILE:CG1	1:A:51:GLY:N	2.57	0.53
1:A:372:LYS:HG2	1:A:397:ASN:O	2.09	0.53
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.91	0.53
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.53
1:A:32:VAL:HG21	1:A:80:HIS:HB2	1.90	0.52
11:T:1:DC:C1'	11:T:2:DT:O4'	2.54	0.52
1:A:789:LYS:HG3	7:I:67:THR:HB	1.91	0.52
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.90	0.52
2:B:711:GLU:H	2:B:712:PRO:HD2	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:839:ARG:HH11	1:A:1402:PHE:HD1	1.56	0.52
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.49	0.52
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.90	0.52
7:I:89:GLN:HE21	7:I:89:GLN:CA	2.17	0.52
7:I:116:ASN:OD1	7:I:116:ASN:N	2.41	0.52
11:T:1:DC:H4'	11:T:2:DT:H5'	1.89	0.52
1:A:317:LYS:HA	1:A:317:LYS:CE	2.29	0.52
1:A:401:GLY:O	1:A:435:HIS:CD2	2.63	0.52
3:C:76:ASP:OD2	3:C:128:ASN:N	2.35	0.52
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.45	0.52
1:A:244:PRO:O	1:A:248:PRO:HD3	2.09	0.52
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.90	0.52
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.91	0.52
7:I:19:ASP:CB	7:I:24:ARG:HG2	2.39	0.52
11:T:21:DC:C4	11:T:22:DT:C7	2.92	0.52
1:A:257:ARG:NH1	1:A:257:ARG:CG	2.73	0.52
2:B:857:ARG:HG3	2:B:857:ARG:HH11	1.74	0.52
7:I:15:TYR:CD1	7:I:30:ARG:HD2	2.45	0.52
10:L:47:ARG:N	10:L:47:ARG:CD	2.73	0.52
11:T:21:DC:H2'	11:T:22:DT:O4'	2.09	0.52
1:A:164:ARG:CG	1:A:165:GLY:N	2.73	0.52
6:H:115:TYR:CE1	6:H:124:ARG:HG3	2.45	0.52
1:A:351:THR:HG22	1:A:352:VAL:N	2.25	0.52
1:A:1130:GLN:O	1:A:1134:ILE:HD12	2.10	0.52
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.45	0.52
1:A:711:ARG:NH1	7:I:97:MET:HE3	2.25	0.52
1:A:1150:SER:OG	7:I:46:HIS:HB2	2.10	0.52
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.43	0.52
4:E:48:ASP:C	4:E:50:MET:H	2.13	0.52
4:E:48:ASP:OD2	4:E:54:GLN:NE2	2.43	0.52
6:H:57:VAL:HG13	6:H:142:LEU:CD1	2.40	0.52
1:A:485:ASP:CG	13:R:9:G:O2'	2.48	0.51
1:A:534:LEU:O	1:A:574:GLY:HA3	2.10	0.51
4:E:156:LEU:HD11	4:E:195:VAL:HB	1.91	0.51
5:F:108:PHE:C	5:F:109:VAL:CG2	2.78	0.51
1:A:36:ARG:O	1:A:270:LEU:HD21	2.10	0.51
6:H:97:MET:HB2	6:H:118:PHE:CD2	2.45	0.51
12:N:13:DA:C5	12:N:14:DG:C6	2.98	0.51
1:A:185:TRP:HE3	1:A:199:LEU:HB2	1.74	0.51
1:A:483:ASP:O	2:B:979:LYS:HE2	2.10	0.51
1:A:966:ASN:O	1:A:970:THR:HG22	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.92	0.51
2:B:345:LYS:HG2	2:B:348:ARG:NH1	2.24	0.51
2:B:713:ALA:O	2:B:714:GLU:HB2	2.10	0.51
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.44	0.51
2:B:48:LEU:HD23	2:B:173:MET:SD	2.50	0.51
3:C:17:ASN:HD22	3:C:231:ASN:HD21	1.58	0.51
3:C:235:VAL:HG12	8:J:13:VAL:HG13	1.93	0.51
6:H:47:PHE:HB3	6:H:95:TYR:HD2	1.75	0.51
7:I:4:PHE:HD1	7:I:5:ARG:H	1.58	0.51
1:A:106:VAL:CG1	1:A:111:GLY:HA2	2.41	0.51
1:A:147:VAL:CG2	1:A:148:CYS:H	2.18	0.51
1:A:500:GLU:O	1:A:504:LEU:HB2	2.11	0.51
1:A:550:LEU:HG	1:A:556:TRP:CE2	2.45	0.51
1:A:1325:THR:OG1	4:E:146:HIS:O	2.29	0.51
2:B:788:ARG:HH11	2:B:788:ARG:CB	2.24	0.51
1:A:219:PHE:HB3	1:A:224:PHE:HB2	1.93	0.51
2:B:471:LYS:CB	2:B:473:MET:HB3	2.39	0.51
2:B:705:MET:HE3	2:B:742:GLU:HG2	1.91	0.51
2:B:987:LYS:H	2:B:987:LYS:HD2	1.75	0.51
2:B:1110:PRO:O	2:B:1119:VAL:HG13	2.11	0.51
1:A:317:LYS:N	1:A:318:SER:CA	2.73	0.51
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.40	0.51
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.93	0.51
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.93	0.51
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.44	0.51
6:H:4:THR:CG2	6:H:58:THR:HG22	2.40	0.51
1:A:1132:LYS:HG3	1:A:1135:ARG:NH1	2.21	0.51
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.10	0.51
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.08	0.51
6:H:103:LYS:HB3	6:H:115:TYR:CD2	2.46	0.51
7:I:78:CYS:C	7:I:80:SER:N	2.61	0.51
1:A:68:GLN:O	1:A:69:THR:HB	2.11	0.51
1:A:302:THR:O	1:A:324:SER:HB3	2.10	0.51
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.93	0.51
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.51
2:B:100:PRO:HD2	2:B:180:TYR:CE2	2.46	0.51
8:J:64:ASN:N	8:J:65:PRO:HD2	2.26	0.51
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.92	0.50
11:T:14:DG:H2"	11:T:15:DA:OP2	2.11	0.50
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.46	0.50
1:A:419:LYS:HG3	1:A:420:ARG:N	2.25	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:711:ARG:HH11	7:I:97:MET:CE	2.23	0.50
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.93	0.50
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	1.92	0.50
2:B:368:GLU:O	2:B:370:PHE:N	2.40	0.50
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.11	0.50
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.25	0.50
4:E:64:PRO:CG	4:E:76:GLY:HA2	2.42	0.50
6:H:129:TYR:CZ	6:H:130:ARG:NH2	2.66	0.50
9:K:91:CYS:O	9:K:95:ILE:HG13	2.11	0.50
1:A:57:ARG:HG2	1:A:68:GLN:HE21	1.75	0.50
1:A:896:ARG:HD2	1:A:897:TYR:CE2	2.46	0.50
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.94	0.50
1:A:114:LEU:HB2	1:A:142:CYS:SG	2.52	0.50
1:A:306:ASN:CG	1:A:313:GLN:HB3	2.31	0.50
1:A:600:PRO:HG2	1:A:601:LYS:H	1.76	0.50
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.12	0.50
1:A:41:MET:HA	1:A:49:LYS:HA	1.94	0.50
1:A:588:LEU:HD12	1:A:632:VAL:HG21	1.94	0.50
1:A:1264:GLU:OE2	7:I:46:HIS:HD2	1.95	0.50
2:B:487:THR:H	2:B:490:SER:HB3	1.76	0.50
3:C:44:LEU:HD12	3:C:160:LYS:C	2.32	0.50
8:J:48:ARG:O	8:J:52:THR:HB	2.11	0.50
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.93	0.50
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.47	0.50
1:A:317:LYS:CB	1:A:318:SER:HA	2.41	0.50
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.77	0.50
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.94	0.50
1:A:500:GLU:OE2	1:A:1438:THR:HG21	2.12	0.50
2:B:216:GLU:HG3	2:B:406:LEU:HD21	1.90	0.50
2:B:532:ALA:HB1	2:B:536:VAL:HG23	1.93	0.50
3:C:145:CYS:SG	3:C:146:LYS:N	2.85	0.50
11:T:8:DT:C2	11:T:9:DA:N7	2.80	0.50
1:A:185:TRP:HB2	1:A:199:LEU:HD13	1.93	0.50
3:C:46:ILE:HA	3:C:159:ALA:HA	1.94	0.50
10:L:34:CYS:SG	10:L:35:SER:N	2.84	0.50
1:A:508:PRO:O	1:A:511:ILE:HG13	2.12	0.49
1:A:946:VAL:HG22	4:E:201:LYS:HD3	1.94	0.49
2:B:211:VAL:O	2:B:480:SER:HA	2.11	0.49
2:B:667:GLN:O	2:B:667:GLN:HG3	2.10	0.49
2:B:796:LEU:O	2:B:799:PRO:HD3	2.12	0.49
3:C:51:VAL:O	10:L:64:LEU:HD22	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.32	0.49
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.94	0.49
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.76	0.49
6:H:129:TYR:OH	6:H:130:ARG:NE	2.45	0.49
6:H:145:ARG:O	6:H:145:ARG:HG3	2.11	0.49
11:T:2:DT:C4	11:T:3:DA:N6	2.80	0.49
1:A:1169:ILE:HD12	1:A:1169:ILE:H	1.76	0.49
2:B:886:LYS:HG2	2:B:940:PRO:HG3	1.93	0.49
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.94	0.49
1:A:469:ARG:HH11	1:A:469:ARG:CG	2.26	0.49
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.33	0.49
1:A:1391:ARG:O	1:A:1392:SER:C	2.51	0.49
3:C:3:GLU:HB3	9:K:104:ASN:OD1	2.12	0.49
12:N:8:DT:C5	12:N:9:DC:N4	2.80	0.49
1:A:12:ARG:HD3	2:B:1192:TYR:CD1	2.47	0.49
1:A:41:MET:CE	1:A:61:ILE:HD12	2.42	0.49
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.47	0.49
1:A:779:PHE:HA	2:B:699:GLU:OE1	2.12	0.49
1:A:855:THR:CG2	1:A:857:ARG:HE	2.26	0.49
1:A:1224:LEU:HD11	1:A:1240:CYS:HB3	1.94	0.49
2:B:365:THR:C	2:B:367:LEU:H	2.15	0.49
2:B:859:TYR:N	2:B:966:VAL:O	2.39	0.49
3:C:15:LYS:O	3:C:240:VAL:HG22	2.12	0.49
3:C:167:HIS:HD2	3:C:169:LYS:N	2.10	0.49
1:A:129:LYS:HA	1:A:134:ARG:NH2	2.27	0.49
2:B:899:ILE:HG22	2:B:900:ALA:N	2.28	0.49
2:B:1104:HIS:CB	2:B:1122:ARG:HG3	2.39	0.49
6:H:26:ILE:HG22	6:H:40:LEU:HB3	1.93	0.49
2:B:792:MET:HE3	2:B:857:ARG:HH12	1.77	0.49
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.95	0.49
1:A:770:VAL:HA	1:A:822:GLU:OE2	2.13	0.49
2:B:275:TYR:HE1	2:B:355:ILE:HG12	1.78	0.49
8:J:37:SER:OG	8:J:47:ARG:NH2	2.46	0.49
11:T:1:DC:C3'	11:T:2:DT:C5'	2.85	0.49
11:T:10:DA:C2	11:T:11:DG:C2	3.00	0.49
1:A:258:GLY:C	1:A:259:GLU:OE1	2.51	0.49
1:A:332:LYS:CG	1:A:333:GLU:N	2.74	0.49
1:A:1116:LEU:HD13	1:A:1329:THR:HG23	1.95	0.49
1:A:1215:ARG:HG2	1:A:1273:LEU:HA	1.95	0.49
1:A:259:GLU:HG3	1:A:264:PHE:CE1	2.48	0.49
1:A:494:SER:H	1:A:497:THR:HG22	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:814:PHE:HB2	2:B:519:TRP:HZ3	1.78	0.49
2:B:287:ARG:NH1	2:B:321:GLY:O	2.46	0.49
1:A:305:ASP:HB2	1:A:326:ARG:CB	2.43	0.48
1:A:567:LYS:HB2	6:H:96:VAL:HB	1.94	0.48
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.77	0.48
1:A:962:ARG:O	1:A:966:ASN:HB2	2.13	0.48
1:A:963:ILE:HD12	1:A:1049:ILE:HG12	1.95	0.48
4:E:59:SER:HB3	4:E:81:GLU:HA	1.94	0.48
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.95	0.48
1:A:552:TRP:NE1	1:A:655:PHE:CD2	2.81	0.48
1:A:839:ARG:HH21	1:A:839:ARG:CG	2.26	0.48
2:B:911:ILE:HG22	2:B:912:ILE:HG13	1.95	0.48
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.95	0.48
4:E:198:ILE:HD11	4:E:212:ARG:HG3	1.95	0.48
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.47	0.48
10:L:42:ARG:H	10:L:42:ARG:HG3	1.43	0.48
1:A:259:GLU:HG3	1:A:264:PHE:HZ	1.72	0.48
1:A:305:ASP:OD1	1:A:326:ARG:HD2	2.13	0.48
1:A:885:THR:HG22	1:A:893:PHE:HE1	1.77	0.48
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.13	0.48
2:B:169:ARG:N	2:B:454:THR:HG23	2.24	0.48
2:B:359:GLU:O	2:B:362:PRO:HD3	2.12	0.48
2:B:791:THR:O	2:B:858:SER:N	2.44	0.48
4:E:136:ASN:OD1	4:E:137:GLU:N	2.46	0.48
7:I:34:TYR:CE1	7:I:36:GLU:HB3	2.46	0.48
3:C:133:ILE:HD11	3:C:237:SER:HA	1.94	0.48
8:J:43:ARG:HD2	8:J:45:CYS:SG	2.53	0.48
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.46	0.48
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.95	0.48
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.95	0.48
11:T:2:DT:H1'	11:T:3:DA:H5'	1.96	0.48
1:A:115:LEU:HD22	1:A:119:ASN:HB2	1.94	0.48
1:A:260:ASP:OD1	1:A:261:ASP:N	2.47	0.48
1:A:469:ARG:HH11	1:A:469:ARG:CB	2.24	0.48
1:A:870:GLU:HB2	4:E:204:THR:CG2	2.41	0.48
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.29	0.48
2:B:357:GLN:HE21	2:B:368:GLU:HA	1.78	0.48
5:F:83:PRO:HG2	5:F:84:TYR:HD1	1.78	0.48
11:T:1:DC:H2'	11:T:2:DT:H6	1.76	0.48
1:A:24:PRO:HB3	1:A:237:THR:HB	1.96	0.48
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.47	0.48
2:B:107:GLY:O	2:B:108:VAL:HG22	2.14	0.48
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.95	0.48
2:B:376:PHE:CE1	2:B:569:TYR:HD2	2.32	0.48
2:B:1065:GLN:HE21	2:B:1069:PHE:HD2	1.62	0.48
6:H:108:SER:O	6:H:111:LEU:N	2.46	0.48
10:L:49:LYS:C	10:L:51:CYS:H	2.18	0.48
11:T:8:DT:C1'	11:T:9:DA:C8	2.96	0.48
1:A:31:SER:HA	1:A:81:PHE:O	2.13	0.48
1:A:305:ASP:CG	1:A:326:ARG:HD2	2.33	0.48
2:B:841:MET:HE3	2:B:990:ILE:HD11	1.94	0.48
2:B:1174:LYS:HB3	2:B:1179:GLN:HB2	1.95	0.48
8:J:43:ARG:HG3	8:J:45:CYS:SG	2.54	0.48
1:A:161:LEU:O	1:A:162:VAL:HG13	2.14	0.48
1:A:542:GLU:O	1:A:546:VAL:HG23	2.13	0.48
2:B:637:LEU:HD22	2:B:741:CYS:O	2.13	0.48
11:T:22:DT:H2'	11:T:23:DC:H5'	1.95	0.48
1:A:672:ASP:HB3	1:A:675:THR:H	1.79	0.47
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.44	0.47
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.95	0.47
11:T:21:DC:C4	11:T:22:DT:C5	3.02	0.47
1:A:161:LEU:C	1:A:162:VAL:HG13	2.34	0.47
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.14	0.47
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.14	0.47
2:B:857:ARG:HH11	2:B:857:ARG:CG	2.27	0.47
3:C:136:ASP:OD1	3:C:139:GLY:N	2.47	0.47
3:C:214:ASN:HB2	3:C:217:ASP:OD2	2.14	0.47
9:K:12:LEU:HD12	9:K:12:LEU:H	1.79	0.47
1:A:628:GLY:O	1:A:632:VAL:HG23	2.13	0.47
1:A:831:THR:HG23	1:A:832:ALA:N	2.29	0.47
2:B:106:ASP:OD2	10:L:47:ARG:NH1	2.47	0.47
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.96	0.47
2:B:203:PHE:HE2	2:B:212:LEU:HD12	1.79	0.47
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.95	0.47
6:H:135:LEU:O	6:H:136:LYS:C	2.52	0.47
9:K:51:LEU:HD13	9:K:59:ALA:HB3	1.95	0.47
1:A:107:CYS:N	1:A:114:LEU:HD21	2.29	0.47
1:A:254:GLU:HB2	2:B:916:THR:HG21	1.95	0.47
2:B:64:CYS:O	2:B:65:GLU:HB3	2.13	0.47
6:H:139:ASN:HB2	6:H:141:TYR:HE1	1.79	0.47
7:I:91:ARG:HA	7:I:91:ARG:HD3	1.66	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:27:LEU:HD13	10:L:58:LYS:HE3	1.97	0.47
1:A:148:CYS:SG	1:A:167:CYS:O	2.73	0.47
1:A:259:GLU:CG	1:A:264:PHE:HZ	2.25	0.47
1:A:495:GLU:O	1:A:498:ARG:HG3	2.14	0.47
1:A:789:LYS:N	7:I:67:THR:O	2.33	0.47
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.95	0.47
2:B:314:LEU:O	2:B:317:CYS:HB2	2.13	0.47
2:B:783:THR:HG21	8:J:59:LYS:HB3	1.95	0.47
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.97	0.47
6:H:113:ALA:HA	6:H:125:LEU:O	2.15	0.47
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.96	0.47
1:A:845:LEU:CD2	1:A:1374:VAL:HG11	2.45	0.47
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.78	0.47
1:A:1261:LYS:HE3	1:A:1261:LYS:HB2	1.76	0.47
2:B:43:LEU:HD11	2:B:811:TYR:O	2.14	0.47
2:B:487:THR:O	2:B:490:SER:HB3	2.15	0.47
2:B:844:SER:HB2	2:B:996:ARG:H	1.79	0.47
12:N:8:DT:C6	12:N:9:DC:N4	2.83	0.47
1:A:172:PRO:O	1:A:174:ILE:HG13	2.15	0.47
1:A:252:PHE:CD1	1:A:252:PHE:N	2.77	0.47
1:A:343:LYS:NZ	2:B:1155:SER:CB	2.77	0.47
1:A:463:ILE:HD13	1:A:469:ARG:HD2	1.97	0.47
1:A:707:GLY:O	1:A:1281:ARG:HD2	2.15	0.47
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.50	0.47
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.80	0.47
3:C:41:ILE:HD11	3:C:243:VAL:HG13	1.97	0.47
3:C:99:LEU:HD23	3:C:99:LEU:N	2.30	0.47
6:H:93:TYR:CD1	6:H:145:ARG:HB3	2.43	0.47
11:T:4:DC:N3	12:N:11:DG:O6	2.48	0.47
11:T:8:DT:N1	11:T:9:DA:N7	2.63	0.47
1:A:40:THR:C	1:A:41:MET:HG3	2.35	0.47
1:A:903:ASN:HD22	1:A:904:THR:H	1.63	0.47
1:A:975:HIS:HB3	1:A:1036:ARG:HH11	1.80	0.47
1:A:1342:GLU:HG2	4:E:212:ARG:NH1	2.29	0.47
2:B:598:GLU:O	2:B:598:GLU:HG3	2.13	0.47
2:B:1163:CYS:HA	2:B:1191:ILE:HD12	1.96	0.47
3:C:116:LYS:HG2	3:C:117:ASP:N	2.29	0.47
1:A:41:MET:HE3	1:A:61:ILE:HD12	1.97	0.47
1:A:403:LYS:O	1:A:415:LEU:HB2	2.15	0.47
1:A:698:GLN:CD	7:I:99:LEU:HD11	2.35	0.47
1:A:782:ARG:NH1	2:B:701:ILE:O	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:LEU:HD11	1:A:1033:GLN:HG3	1.97	0.47
1:A:980:ASP:OD2	1:A:1039:LYS:HB3	2.14	0.47
8:J:7:CYS:CB	8:J:49:MET:HE3	2.45	0.47
11:T:18:DA:H4'	11:T:19[B]:1CC:OP1	2.14	0.47
2:B:468:GLU:O	2:B:470:LYS:HA	2.15	0.47
3:C:167:HIS:CD2	3:C:169:LYS:H	2.31	0.47
4:E:64:PRO:HG2	4:E:76:GLY:HA2	1.97	0.47
1:A:74:MET:C	1:A:76:GLU:H	2.19	0.46
1:A:852:TYR:CZ	5:F:136:ARG:HG2	2.50	0.46
1:A:1397:LEU:HB2	1:A:1426:GLU:OE2	2.15	0.46
2:B:176:SER:O	2:B:182:SER:HB3	2.15	0.46
2:B:436:VAL:HG13	2:B:437:GLU:HG3	1.97	0.46
2:B:478:GLY:O	2:B:480:SER:N	2.48	0.46
3:C:57:VAL:HG11	8:J:57:ILE:HG13	1.97	0.46
1:A:321:PRO:HD3	2:B:473:MET:CE	2.44	0.46
1:A:494:SER:O	1:A:497:THR:HG22	2.15	0.46
1:A:845:LEU:HD21	1:A:1374:VAL:HG11	1.97	0.46
2:B:706:GLN:HG3	2:B:710:LEU:HD22	1.97	0.46
2:B:789:MET:CE	2:B:965:LYS:HB3	2.43	0.46
2:B:797:TYR:HB3	2:B:798:TYR:HD1	1.80	0.46
3:C:56:THR:HG23	3:C:58:LEU:N	2.25	0.46
4:E:19:VAL:O	4:E:23:VAL:HG23	2.15	0.46
11:T:21:DC:H3'	11:T:22:DT:H5"	1.97	0.46
1:A:550:LEU:HG	1:A:556:TRP:NE1	2.31	0.46
1:A:642:CYS:O	1:A:645:LEU:HB3	2.15	0.46
1:A:807:GLY:O	2:B:728:ARG:HD3	2.16	0.46
2:B:576:ASP:OD1	2:B:576:ASP:N	2.48	0.46
2:B:808:ALA:O	2:B:812:LEU:HG	2.16	0.46
2:B:864:LYS:HD2	2:B:866:TYR:N	2.24	0.46
2:B:1104:HIS:CG	2:B:1122:ARG:HG3	2.51	0.46
4:E:153:HIS:O	4:E:154:ILE:HD13	2.15	0.46
7:I:50:THR:HG22	7:I:52:ILE:HG22	1.97	0.46
1:A:492:PRO:CB	1:A:497:THR:HG23	2.44	0.46
1:A:577:ILE:HD12	1:A:578:LEU:N	2.29	0.46
1:A:701:LEU:HD21	7:I:114:GLN:HB2	1.96	0.46
1:A:908:LEU:HD11	1:A:983:ILE:HD11	1.96	0.46
2:B:619:ILE:HG13	7:I:65:ASP:HB2	1.96	0.46
2:B:711:GLU:N	2:B:712:PRO:HD2	2.31	0.46
6:H:83:GLN:O	6:H:87:ARG:N	2.48	0.46
6:H:137:GLN:O	6:H:139:ASN:N	2.48	0.46
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:VAL:HG12	1:A:111:GLY:HA2	1.98	0.46
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.97	0.46
1:A:882:SER:HA	1:A:953:ASN:HA	1.97	0.46
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.51	0.46
2:B:900:ALA:O	2:B:902:GLY:N	2.47	0.46
5:F:132:LEU:O	5:F:148:VAL:HG23	2.16	0.46
8:J:3:VAL:HG11	8:J:18:TRP:HB2	1.97	0.46
1:A:768:GLN:CG	1:A:816:HIS:HA	2.45	0.46
1:A:848:ILE:HD11	1:A:1374:VAL:HG21	1.97	0.46
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.56	0.46
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.15	0.46
3:C:54:ASN:OD1	3:C:56:THR:HG22	2.15	0.46
1:A:11:LEU:HA	2:B:1193:GLN:O	2.16	0.46
1:A:41:MET:CB	1:A:49:LYS:HG3	2.35	0.46
1:A:55:ASP:CB	1:A:56:PRO:CA	2.75	0.46
2:B:408:LEU:HB3	2:B:409:ALA:H	1.58	0.46
4:E:12:LEU:HD11	4:E:58:MET:HE1	1.97	0.46
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.97	0.46
7:I:24:ARG:HH11	7:I:24:ARG:HG3	1.79	0.46
12:N:11:DG:H2"	12:N:12:DT:H71	1.98	0.46
2:B:635:ARG:O	2:B:636:PRO:O	2.34	0.46
2:B:955:THR:HG22	2:B:956:THR:N	2.30	0.46
3:C:74:SER:O	3:C:77:ILE:HB	2.16	0.46
4:E:12:LEU:HD22	4:E:55:ARG:HH21	1.81	0.46
5:F:76:LYS:O	5:F:79:ARG:HD3	2.15	0.46
6:H:63:LEU:HD23	6:H:63:LEU:N	2.29	0.46
1:A:44:THR:HG22	1:A:44:THR:O	2.16	0.46
1:A:363:GLN:O	1:A:458:HIS:ND1	2.48	0.46
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.44	0.46
1:A:765:VAL:HG13	1:A:802:ASN:O	2.16	0.46
2:B:512:ARG:NH2	2:B:531:GLN:O	2.49	0.46
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.98	0.46
1:A:117:GLU:CD	1:A:117:GLU:H	2.19	0.46
1:A:401:GLY:O	1:A:435:HIS:HD2	1.99	0.46
1:A:469:ARG:HH21	2:B:976:ILE:HD13	1.81	0.46
1:A:1094:VAL:HA	1:A:1113:THR:HG21	1.97	0.46
2:B:800:GLN:CG	8:J:52:THR:HG22	2.45	0.46
4:E:164:LEU:HD13	4:E:211:TYR:CE2	2.51	0.46
11:T:24:DT:H2'	11:T:25:DC:O4'	2.16	0.46
1:A:571:LEU:CD1	6:H:46:LEU:HD11	2.47	0.45
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:ILE:HD12	2:B:651:LEU:HD12	1.97	0.45
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.98	0.45
10:L:38:LEU:HD23	10:L:40:LEU:HG	1.98	0.45
1:A:130:ASP:O	1:A:134:ARG:CB	2.64	0.45
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.51	0.45
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.98	0.45
1:A:598:LEU:HD23	1:A:598:LEU:HA	1.81	0.45
1:A:1022:LEU:HD11	1:A:1026:LEU:HD12	1.97	0.45
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.26	0.45
4:E:46:TYR:HE1	4:E:58:MET:HA	1.81	0.45
1:A:67:CYS:HB3	1:A:70:CYS:SG	2.56	0.45
1:A:148:CYS:HB3	1:A:167:CYS:O	2.17	0.45
1:A:306:ASN:OD1	1:A:313:GLN:HB3	2.16	0.45
1:A:375:THR:HG21	1:A:433:GLU:OE1	2.16	0.45
1:A:494:SER:O	1:A:498:ARG:HG2	2.15	0.45
6:H:89:LEU:H	6:H:89:LEU:HD13	1.81	0.45
1:A:209:ASN:HA	1:A:212:LYS:HB2	1.99	0.45
1:A:833:GLU:O	1:A:837:ILE:HG12	2.17	0.45
1:A:979:SER:OG	1:A:980:ASP:N	2.48	0.45
2:B:31:TRP:CE3	2:B:34:ILE:HD13	2.52	0.45
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.49	0.45
3:C:38:ILE:HG13	3:C:176:ILE:CD1	2.47	0.45
4:E:28:TYR:CE2	4:E:78:LEU:HD13	2.52	0.45
4:E:116:ILE:CG2	4:E:121:MET:HG3	2.46	0.45
4:E:204:THR:HG22	4:E:205:SER:N	2.31	0.45
10:L:42:ARG:NH2	10:L:43:THR:OG1	2.50	0.45
1:A:396:PRO:O	1:A:397:ASN:HB3	2.15	0.45
1:A:938:LYS:HB2	1:A:938:LYS:HE3	1.78	0.45
1:A:1109:LYS:HB3	1:A:1109:LYS:HE3	1.76	0.45
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.99	0.45
5:F:94:LEU:HD13	5:F:122:MET:HG2	1.98	0.45
7:I:7:CYS:HB2	7:I:14:LEU:HD23	1.98	0.45
8:J:1:MET:N	8:J:56:LEU:HD12	2.30	0.45
11:T:2:DT:C4	11:T:3:DA:C6	3.04	0.45
1:A:322:VAL:CG2	1:A:323:LYS:N	2.78	0.45
1:A:567:LYS:HA	1:A:567:LYS:HD3	1.61	0.45
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.16	0.45
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.99	0.45
2:B:468:GLU:CG	2:B:469:GLN:H	2.29	0.45
2:B:554:ILE:HD11	2:B:609:ILE:HG23	1.98	0.45
2:B:639:ILE:HD11	2:B:691:GLU:HG3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:72:LYS:HE2	5:F:73:ALA:N	2.31	0.45
1:A:369:SER:HB3	9:K:2:ASN:OD1	2.17	0.45
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.99	0.45
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.51	0.45
1:A:1224:LEU:CD1	1:A:1240:CYS:CB	2.93	0.45
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.98	0.45
3:C:67:LEU:HD23	3:C:144:ILE:HD11	1.99	0.45
4:E:117:THR:O	4:E:119:SER:N	2.50	0.45
1:A:92:HIS:NE2	1:A:304:MET:SD	2.90	0.45
1:A:1280:GLU:HB3	1:A:1281:ARG:H	1.69	0.45
1:A:1436:ILE:CD1	1:A:1436:ILE:N	2.78	0.45
2:B:475:SER:HA	2:B:476:ARG:HA	1.61	0.45
2:B:978:ASP:OD2	2:B:1098:MET:HG2	2.16	0.45
3:C:29:MET:HA	9:K:45:LEU:HD13	1.99	0.45
4:E:112:TYR:CD1	4:E:116:ILE:HD11	2.52	0.45
5:F:108:PHE:O	5:F:109:VAL:CG2	2.64	0.45
7:I:24:ARG:HH11	7:I:24:ARG:CB	2.30	0.45
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.47	0.45
1:A:849:MET:SD	1:A:1061:GLY:HA2	2.56	0.45
8:J:48:ARG:NE	8:J:49:MET:HE2	2.32	0.45
1:A:91:PHE:HA	1:A:235:ILE:HG22	1.99	0.45
1:A:305:ASP:HB2	1:A:326:ARG:HB2	1.99	0.45
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.45
1:A:481:ASP:O	1:A:485:ASP:CG	2.56	0.45
1:A:1301:GLU:HA	1:A:1302:PRO:HD3	1.83	0.45
2:B:987:LYS:H	2:B:987:LYS:CD	2.29	0.45
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.52	0.45
2:B:1174:LYS:HE3	2:B:1174:LYS:HB2	1.73	0.45
10:L:38:LEU:HD23	10:L:40:LEU:CD1	2.47	0.45
1:A:258:GLY:O	1:A:259:GLU:OE1	2.35	0.44
1:A:298:PHE:O	1:A:302:THR:HG22	2.17	0.44
1:A:919:ILE:HG21	1:A:925:LEU:CD1	2.47	0.44
1:A:1138:ILE:HD11	1:A:1319:VAL:HG11	1.97	0.44
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.98	0.44
7:I:22:ASN:HB3	7:I:24:ARG:HD3	1.98	0.44
1:A:35:ILE:CD1	1:A:241:VAL:HG11	2.40	0.44
1:A:495:GLU:HB2	5:F:99:LEU:HD23	2.00	0.44
2:B:275:TYR:CE1	2:B:355:ILE:HG12	2.52	0.44
3:C:235:VAL:HG12	8:J:13:VAL:CG1	2.47	0.44
8:J:7:CYS:SG	8:J:9:SER:HB2	2.57	0.44
1:A:591:PHE:N	1:A:591:PHE:HD1	2.15	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:743:VAL:O	1:A:747:VAL:HG23	2.17	0.44
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.51	0.44
2:B:105:SER:C	2:B:107:GLY:N	2.70	0.44
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.97	0.44
3:C:27:LEU:HD12	3:C:228:PHE:CE1	2.52	0.44
3:C:99:LEU:HB3	3:C:120:ILE:HA	1.99	0.44
1:A:901:LEU:HD22	1:A:919:ILE:O	2.18	0.44
2:B:1002:THR:HG23	2:B:1004:GLU:HG3	1.99	0.44
3:C:242:GLN:HB3	3:C:246:ARG:HD2	1.99	0.44
4:E:167:ARG:HD3	4:E:167:ARG:HA	1.69	0.44
6:H:3:ASN:HD22	6:H:3:ASN:HA	1.63	0.44
10:L:31:CYS:HB3	10:L:34:CYS:O	2.18	0.44
1:A:388:LEU:HD23	1:A:391:LEU:HD12	1.99	0.44
1:A:451:HIS:H	1:A:451:HIS:CD2	2.36	0.44
1:A:780:VAL:HG22	2:B:699:GLU:OE2	2.18	0.44
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.18	0.44
2:B:1063:GLY:O	3:C:202:PRO:HG2	2.18	0.44
10:L:47:ARG:O	10:L:56:LEU:HD11	2.18	0.44
13:R:7:A:O2'	13:R:8:G:H5'	2.18	0.44
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.00	0.44
2:B:369:GLY:O	2:B:370:PHE:CG	2.71	0.44
2:B:973:ILE:HG22	2:B:974:PRO:HD2	2.00	0.44
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.77	0.44
7:I:87:GLN:HE22	7:I:97:MET:HG2	1.82	0.44
1:A:57:ARG:HA	1:A:68:GLN:CG	2.48	0.44
1:A:98:LYS:O	1:A:102:VAL:HG23	2.18	0.44
1:A:485:ASP:CB	13:R:9:G:O2'	2.66	0.44
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	2.00	0.44
2:B:387:LEU:HD22	2:B:387:LEU:HA	1.85	0.44
2:B:800:GLN:CB	8:J:52:THR:HG22	2.47	0.44
3:C:40:GLU:OE1	3:C:254:LYS:NZ	2.44	0.44
1:A:242:PRO:HA	1:A:243:PRO:HD3	1.81	0.44
1:A:588:LEU:O	1:A:607:ILE:N	2.42	0.44
1:A:1153:TYR:CE1	7:I:42:LEU:HD13	2.53	0.44
2:B:107:GLY:C	2:B:108:VAL:CG2	2.85	0.44
2:B:254:LEU:HD23	2:B:361:LEU:HD21	2.00	0.44
2:B:600:LEU:HD22	2:B:615:MET:SD	2.58	0.44
2:B:1060:ARG:HD2	2:B:1060:ARG:HA	1.72	0.44
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.57	0.44
12:N:6:DT:OP2	12:N:6:DT:C6	2.70	0.44
1:A:54:ASN:HD22	1:A:61:ILE:HD13	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:GLU:O	1:A:78:PRO:HD3	2.18	0.43
2:B:188:ASP:O	2:B:192:LEU:HD12	2.18	0.43
8:J:1:MET:H1	8:J:56:LEU:HD12	1.83	0.43
1:A:518:LYS:HB2	1:A:519:PRO:HD2	2.00	0.43
1:A:597:LEU:HB3	6:H:115:TYR:CZ	2.53	0.43
3:C:51:VAL:O	10:L:64:LEU:HD13	2.17	0.43
6:H:129:TYR:CE2	6:H:130:ARG:NH2	2.81	0.43
8:J:21:TYR:CZ	8:J:25:LEU:HD11	2.53	0.43
1:A:365:GLY:O	1:A:468:PHE:HA	2.19	0.43
1:A:722:LEU:HD11	1:A:794:PRO:HB3	2.01	0.43
1:A:793:SER:HB2	1:A:794:PRO:HD2	2.00	0.43
1:A:802:ASN:OD1	2:B:729:ILE:N	2.28	0.43
1:A:899:VAL:O	1:A:929:LEU:HG	2.18	0.43
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.18	0.43
2:B:118:ARG:HA	2:B:207:GLY:HA2	2.01	0.43
2:B:471:LYS:HB2	2:B:473:MET:CA	2.47	0.43
2:B:563:MET:HA	2:B:589:VAL:O	2.18	0.43
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.53	0.43
3:C:167:HIS:HE1	10:L:70:ARG:O	2.00	0.43
5:F:83:PRO:HG2	5:F:84:TYR:CD1	2.53	0.43
6:H:62:SER:N	6:H:63:LEU:HA	2.33	0.43
7:I:24:ARG:NH1	7:I:37:GLU:OE2	2.48	0.43
7:I:74:GLU:HG2	7:I:79:HIS:HA	2.00	0.43
1:A:12:ARG:HB3	2:B:1218:THR:HB	1.99	0.43
1:A:602:ASP:OD1	1:A:616:VAL:HG23	2.18	0.43
1:A:662:PHE:O	2:B:828:ALA:HA	2.18	0.43
1:A:994:GLN:HG2	1:A:1019:CYS:SG	2.58	0.43
3:C:252:GLN:CG	9:K:95:ILE:HG23	2.48	0.43
4:E:77:SER:CB	4:E:105:PHE:CD1	3.01	0.43
7:I:53:GLY:O	7:I:89:GLN:HB2	2.17	0.43
1:A:289:ILE:O	1:A:293:GLU:HG3	2.18	0.43
1:A:314:ALA:O	1:A:320:ARG:HB3	2.18	0.43
1:A:497:THR:OG1	2:B:1146:PHE:HA	2.18	0.43
1:A:545:GLN:O	1:A:549:MET:HG3	2.17	0.43
1:A:606:LEU:HD11	1:A:608:ILE:HD11	1.99	0.43
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.99	0.43
2:B:851:PHE:O	2:B:974:PRO:HD3	2.18	0.43
2:B:1065:GLN:NE2	2:B:1069:PHE:HD2	2.15	0.43
6:H:104:PHE:CE1	6:H:114:VAL:HG12	2.53	0.43
6:H:109:LYS:HD2	6:H:109:LYS:HA	1.62	0.43
1:A:224:PHE:HB3	1:A:229:SER:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:GLY:HA3	2:B:516:ASN:HB2	2.00	0.43
1:A:814:PHE:HB2	2:B:519:TRP:CZ3	2.53	0.43
1:A:1021:LEU:HD11	1:A:1025:ARG:NH1	2.34	0.43
2:B:120:ARG:HG2	2:B:955:THR:HG21	2.01	0.43
2:B:222:ILE:HD11	2:B:627:PHE:CE1	2.54	0.43
2:B:254:LEU:CD2	2:B:361:LEU:HD21	2.49	0.43
2:B:639:ILE:HD11	2:B:691:GLU:CD	2.39	0.43
3:C:9:LYS:HB2	3:C:9:LYS:HE2	1.79	0.43
4:E:21:GLU:HG3	4:E:35:VAL:HG11	2.01	0.43
6:H:107:VAL:CG1	6:H:108:SER:H	2.10	0.43
7:I:75:CYS:O	7:I:79:HIS:HA	2.18	0.43
11:T:5:DC:H2"	11:T:6:DG:OP2	2.19	0.43
1:A:987:VAL:HG23	1:A:1028:THR:OG1	2.18	0.43
2:B:605:ARG:CG	2:B:691:GLU:OE2	2.66	0.43
7:I:54:GLU:O	7:I:89:GLN:HB2	2.18	0.43
8:J:7:CYS:HA	8:J:49:MET:HG2	2.00	0.43
1:A:151:ASP:O	1:A:152:VAL:C	2.56	0.43
1:A:272:ALA:O	1:A:296:LEU:HB2	2.19	0.43
1:A:399:HIS:HA	1:A:400:PRO:HA	1.62	0.43
1:A:595:THR:HG21	1:A:604:GLY:HA3	2.01	0.43
1:A:698:GLN:HG2	7:I:99:LEU:HG	2.00	0.43
1:A:896:ARG:HB3	1:A:897:TYR:CD2	2.53	0.43
2:B:90:ILE:HA	2:B:133:LYS:O	2.18	0.43
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.49	0.43
3:C:69:LEU:O	8:J:6:ARG:NH1	2.52	0.43
3:C:268:ASP:OD1	3:C:268:ASP:N	2.52	0.43
4:E:116:ILE:HG21	4:E:121:MET:HG3	2.00	0.43
11:T:3:DA:H1'	11:T:4:DC:O4'	2.19	0.43
1:A:84:ILE:HD11	1:A:270:LEU:HG	2.00	0.43
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.78	0.43
2:B:706:GLN:HG3	2:B:710:LEU:CD2	2.49	0.43
3:C:248:ILE:HG23	9:K:98:LEU:HD22	2.00	0.43
1:A:67:CYS:O	1:A:70:CYS:SG	2.77	0.43
1:A:368:LYS:HG2	1:A:372:LYS:HE3	2.00	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.54	0.43
1:A:447:GLN:OE1	11:T:21:DC:H2"	2.19	0.43
1:A:968:GLN:HB3	1:A:973:ILE:HD11	2.01	0.43
1:A:1017:LEU:HB2	4:E:205:SER:C	2.39	0.43
2:B:332:ASP:C	2:B:334:ILE:H	2.22	0.43
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.54	0.43
4:E:177:ARG:HD3	4:E:215:MET:SD	2.59	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:1:DC:H3'	11:T:1:DC:H6	1.84	0.43
1:A:1001:ARG:HB2	5:F:80:ALA:O	2.19	0.42
2:B:851:PHE:HB3	2:B:1094:ARG:HD2	2.01	0.42
2:B:981:ALA:HB2	2:B:1095:LEU:HD11	2.01	0.42
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.47	0.42
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.19	0.42
4:E:176:PRO:O	4:E:212:ARG:HA	2.20	0.42
6:H:89:LEU:HD22	6:H:91:ASP:H	1.84	0.42
1:A:74:MET:C	1:A:76:GLU:N	2.72	0.42
1:A:469:ARG:CG	1:A:469:ARG:NH1	2.82	0.42
2:B:364:ILE:HG21	2:B:374:LYS:CD	2.49	0.42
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.00	0.42
2:B:664:THR:HG1	2:B:678:GLU:N	2.17	0.42
2:B:702:LEU:HD12	2:B:702:LEU:HA	1.88	0.42
2:B:711:GLU:N	2:B:712:PRO:CD	2.82	0.42
2:B:722:ASP:OD1	2:B:722:ASP:N	2.53	0.42
3:C:8:VAL:HG11	9:K:105:PHE:CD1	2.54	0.42
1:A:34:LYS:H	1:A:34:LYS:HG2	1.60	0.42
1:A:254:GLU:HB3	2:B:916:THR:HG21	2.00	0.42
1:A:912:LEU:CD1	1:A:1033:GLN:HG3	2.49	0.42
2:B:277:LYS:HD2	2:B:335:GLY:O	2.19	0.42
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.24	0.42
2:B:424:LEU:HD11	2:B:448:ILE:HG23	2.02	0.42
2:B:779:GLY:HA2	2:B:796:LEU:HB2	2.01	0.42
4:E:144:ILE:HG13	4:E:145:THR:N	2.34	0.42
5:F:73:ALA:HA	5:F:143:PHE:CZ	2.54	0.42
8:J:23:ASN:O	8:J:27:GLU:HB3	2.18	0.42
1:A:41:MET:HG2	1:A:61:ILE:HD11	2.01	0.42
1:A:111:GLY:O	1:A:214:ILE:HA	2.19	0.42
1:A:355:GLY:HA3	1:A:482:PHE:CE2	2.54	0.42
1:A:567:LYS:HA	1:A:568:PRO:HA	1.68	0.42
1:A:602:ASP:CG	1:A:616:VAL:HG23	2.40	0.42
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.34	0.42
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.54	0.42
2:B:475:SER:OG	2:B:476:ARG:HG3	2.15	0.42
2:B:637:LEU:CD2	2:B:741:CYS:O	2.67	0.42
2:B:654:ARG:HA	2:B:654:ARG:HD3	1.79	0.42
2:B:727:LYS:HD3	2:B:1049:ASP:CG	2.40	0.42
5:F:108:PHE:C	5:F:109:VAL:HG23	2.39	0.42
11:T:8:DT:O4	12:N:7:DA:N1	2.52	0.42
1:A:1224:LEU:HD11	1:A:1240:CYS:CB	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:ILE:HD12	2:B:418:LYS:CG	2.48	0.42
4:E:48:ASP:C	4:E:50:MET:N	2.73	0.42
6:H:4:THR:HG21	6:H:58:THR:HG23	1.98	0.42
9:K:20:LYS:O	9:K:33:ILE:HA	2.19	0.42
1:A:353:ILE:HD13	1:A:487:MET:CE	2.49	0.42
1:A:355:GLY:N	1:A:482:PHE:CZ	2.88	0.42
1:A:533:LYS:HA	1:A:533:LYS:HD2	1.84	0.42
2:B:104:GLU:OE2	10:L:54:ARG:CZ	2.68	0.42
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.50	0.42
2:B:855:PHE:HZ	2:B:857:ARG:HH11	1.62	0.42
3:C:5:GLY:O	3:C:7:GLN:HG2	2.20	0.42
3:C:249:ASP:O	3:C:253:LYS:HB2	2.20	0.42
4:E:54:GLN:HE21	4:E:54:GLN:HB2	1.53	0.42
5:F:74:ILE:HG13	5:F:75:PRO:HD2	2.02	0.42
6:H:108:SER:C	6:H:110:ASP:N	2.73	0.42
7:I:30:ARG:HE	7:I:30:ARG:HB3	1.78	0.42
7:I:60:GLN:OE1	7:I:107:SER:OG	2.35	0.42
7:I:88:SER:HA	7:I:100:PHE:HE2	1.85	0.42
1:A:356:ASP:C	1:A:358:ASN:H	2.23	0.42
1:A:1044:TRP:O	1:A:1047:SER:N	2.53	0.42
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	2.01	0.42
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.35	0.42
2:B:831:SER:HG	2:B:994:TYR:HE2	1.66	0.42
2:B:1017:ILE:HA	2:B:1017:ILE:HD13	1.79	0.42
3:C:129:ILE:HD12	3:C:129:ILE:HA	1.79	0.42
5:F:111:LEU:C	5:F:113:GLY:H	2.23	0.42
6:H:80:ARG:HG2	9:K:57:LEU:HD22	2.02	0.42
11:T:20:DC:H5'	11:T:20:DC:H6	1.85	0.42
2:B:28:GLU:C	2:B:30:SER:H	2.23	0.42
2:B:261:ARG:HD3	2:B:261:ARG:HA	1.82	0.42
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.87	0.42
8:J:3:VAL:HG21	8:J:18:TRP:HB2	2.02	0.42
1:A:57:ARG:HG2	1:A:68:GLN:NE2	2.33	0.42
1:A:179:LEU:HD22	1:A:297:GLN:HG3	2.02	0.42
1:A:475:THR:HG22	1:A:476:SER:N	2.35	0.42
1:A:606:LEU:HD11	1:A:608:ILE:CD1	2.49	0.42
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.53	0.42
2:B:365:THR:C	2:B:367:LEU:N	2.73	0.42
2:B:839:MET:HE2	2:B:1010:LEU:HD21	2.01	0.42
2:B:1152:MET:HE2	2:B:1197:PRO:HD3	2.02	0.42
8:J:12:LYS:O	8:J:14:VAL:HG22	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:47:ARG:N	10:L:47:ARG:HD3	2.35	0.42
11:T:9:DA:C2'	11:T:10:DA:N7	2.81	0.42
1:A:315:LEU:CB	1:A:316:GLN:HB2	2.33	0.42
1:A:818:MET:HE3	2:B:514:LEU:O	2.20	0.42
1:A:922:ASP:C	1:A:924:LYS:N	2.73	0.42
2:B:295:GLY:H	2:B:298:LEU:HG	1.85	0.42
2:B:857:ARG:O	2:B:967:ARG:HA	2.20	0.42
4:E:90:VAL:CG1	12:N:12:DT:H3'	2.50	0.42
6:H:46:LEU:HD23	6:H:46:LEU:HA	1.77	0.42
7:I:75:CYS:C	7:I:77:LYS:H	2.23	0.42
8:J:42:LYS:HG3	8:J:43:ARG:N	2.32	0.42
10:L:26:THR:HA	10:L:27:LEU:HA	1.71	0.42
12:N:13:DA:C6	12:N:14:DG:O6	2.72	0.42
1:A:86:LEU:HA	1:A:273:ASN:OD1	2.20	0.41
1:A:403:LYS:HB3	1:A:404:TYR:HD1	1.84	0.41
1:A:815:PHE:O	1:A:818:MET:N	2.52	0.41
1:A:1392:SER:O	1:A:1399:ARG:HD3	2.19	0.41
2:B:423:LYS:O	2:B:427:ASP:HB2	2.19	0.41
2:B:431:TYR:CZ	2:B:447:ALA:HB3	2.55	0.41
3:C:36:VAL:HG23	9:K:41:THR:HG21	2.02	0.41
3:C:39:ALA:HA	3:C:164:ALA:HB3	2.02	0.41
4:E:9:ILE:HD11	4:E:53:PRO:HD3	2.02	0.41
4:E:119:SER:CB	12:N:12:DT:H4'	2.50	0.41
8:J:8:PHE:CD2	8:J:49:MET:SD	3.13	0.41
1:A:180:LYS:HE3	1:A:294:SER:HB3	2.01	0.41
1:A:839:ARG:CG	1:A:839:ARG:NH2	2.82	0.41
1:A:918:GLU:HG3	1:A:919:ILE:HG12	2.02	0.41
1:A:1151:GLU:OE2	7:I:45:ARG:NH1	2.53	0.41
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.02	0.41
2:B:174:LEU:HD21	2:B:204:ILE:HD11	2.01	0.41
2:B:500:THR:HA	2:B:501:PRO:HD3	1.84	0.41
2:B:1096:ARG:O	2:B:1097:HIS:HB2	2.20	0.41
4:E:90:VAL:HG12	12:N:12:DT:H5"	2.02	0.41
6:H:16:ASP:HA	6:H:17:PRO:HD2	1.95	0.41
1:A:903:ASN:HD22	1:A:904:THR:N	2.19	0.41
2:B:96:TYR:HB2	2:B:129:PHE:HB2	2.01	0.41
2:B:492:LEU:HA	2:B:492:LEU:HD23	1.74	0.41
2:B:705:MET:CE	2:B:742:GLU:HG2	2.49	0.41
6:H:108:SER:O	6:H:110:ASP:N	2.53	0.41
10:L:47:ARG:HD3	10:L:47:ARG:H	1.85	0.41
1:A:401:GLY:C	1:A:435:HIS:CD2	2.94	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:828:ALA:O	1:A:831:THR:CG2	2.52	0.41
1:A:954:TRP:HA	1:A:955:PRO:HD2	1.85	0.41
1:A:1392:SER:C	1:A:1394:THR:H	2.23	0.41
2:B:467:GLY:O	2:B:469:GLN:N	2.53	0.41
2:B:558:LEU:HD13	2:B:580:VAL:HG11	2.02	0.41
2:B:710:LEU:HD12	2:B:710:LEU:HA	1.87	0.41
2:B:906:SER:HB3	2:B:946:ASN:HB2	2.01	0.41
2:B:1081:LEU:HD23	2:B:1081:LEU:HA	1.71	0.41
6:H:84:ALA:HB1	6:H:89:LEU:HB3	2.01	0.41
1:A:294:SER:HA	1:A:297:GLN:HB3	2.01	0.41
1:A:362:ASP:OD1	1:A:362:ASP:N	2.46	0.41
1:A:597:LEU:HB3	6:H:115:TYR:OH	2.20	0.41
1:A:1154:TYR:CE1	1:A:1156:PRO:HG3	2.55	0.41
2:B:46:GLN:H	2:B:46:GLN:HG3	1.49	0.41
3:C:164:ALA:HA	3:C:167:HIS:O	2.21	0.41
4:E:3:GLN:HB2	4:E:4:GLU:H	1.45	0.41
6:H:62:SER:HB2	6:H:63:LEU:C	2.41	0.41
6:H:89:LEU:HB2	6:H:91:ASP:OD2	2.20	0.41
11:T:3:DA:C2'	11:T:4:DC:C5'	2.75	0.41
11:T:9:DA:C2	11:T:10:DA:C2	3.08	0.41
11:T:16:DC:H1'	11:T:17:DG:C5'	2.30	0.41
1:A:351:THR:HG23	2:B:1103:ILE:HG12	2.02	0.41
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.38	0.41
1:A:469:ARG:NH2	2:B:976:ILE:HD13	2.36	0.41
1:A:1399:ARG:NH1	1:A:1408:ILE:HD12	2.36	0.41
2:B:217:ARG:HD3	2:B:407:ASP:OD2	2.21	0.41
2:B:1182:CYS:SG	2:B:1182:CYS:O	2.79	0.41
2:B:1183:LYS:NZ	2:B:1183:LYS:CB	2.81	0.41
4:E:7:ARG:O	4:E:10:SER:N	2.53	0.41
8:J:25:LEU:HA	8:J:25:LEU:HD23	1.78	0.41
9:K:12:LEU:HD12	9:K:12:LEU:N	2.34	0.41
9:K:87:LEU:O	9:K:90:ALA:HB3	2.20	0.41
11:T:27:DA:N1	13:R:2:U:O4	2.53	0.41
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.84	0.41
1:A:709:THR:OG1	1:A:712:GLU:HB2	2.21	0.41
2:B:96:TYR:N	2:B:129:PHE:O	2.52	0.41
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.56	0.41
3:C:123:ASN:OD1	3:C:125:MET:HB3	2.20	0.41
4:E:135:PHE:CD2	4:E:140:LEU:HD21	2.48	0.41
5:F:101:ILE:HG21	5:F:120:ILE:HD12	2.03	0.41
1:A:44:THR:O	1:A:45:GLN:HB2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:MET:O	1:A:76:GLU:N	2.53	0.41
1:A:330:LYS:HD2	1:A:331:GLY:O	2.21	0.41
1:A:483:ASP:OD1	1:A:485:ASP:OD1	2.39	0.41
1:A:567:LYS:H	6:H:96:VAL:HB	1.85	0.41
1:A:577:ILE:HD12	1:A:578:LEU:H	1.85	0.41
2:B:315:LYS:N	2:B:316:PRO:HD2	2.36	0.41
2:B:711:GLU:HB3	2:B:738:PHE:CE2	2.56	0.41
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.94	0.41
3:C:44:LEU:HD12	3:C:160:LYS:O	2.21	0.41
4:E:20:LYS:HB3	4:E:35:VAL:HG22	2.03	0.41
7:I:55:THR:O	7:I:55:THR:HG23	2.21	0.41
8:J:7:CYS:O	8:J:11:GLY:N	2.53	0.41
11:T:3:DA:N1	12:N:12:DT:O4	2.54	0.41
1:A:265:LYS:HA	1:A:265:LYS:HD2	1.86	0.41
1:A:337:ARG:HD2	1:A:839:ARG:NH1	2.35	0.41
1:A:569:LYS:HE3	3:C:221:TYR:O	2.21	0.41
1:A:599:SER:O	6:H:25:ARG:NH2	2.54	0.41
1:A:625:SER:HB2	1:A:626:ASN:H	1.76	0.41
1:A:831:THR:CG2	1:A:832:ALA:N	2.84	0.41
1:A:855:THR:HG22	1:A:857:ARG:HG2	2.03	0.41
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.36	0.41
1:A:1209:MET:SD	1:A:1236:LEU:HD13	2.61	0.41
2:B:413:LEU:HD23	2:B:413:LEU:HA	1.94	0.41
2:B:798:TYR:CE2	8:J:4:PRO:HA	2.56	0.41
3:C:227:THR:HG22	3:C:229:TYR:CE1	2.56	0.41
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.90	0.41
7:I:87:GLN:NE2	7:I:97:MET:HG2	2.35	0.41
8:J:13:VAL:O	8:J:17:LYS:NZ	2.52	0.41
1:A:1291:VAL:HA	1:A:1292:PRO:HD3	1.93	0.41
2:B:412:LEU:HA	2:B:412:LEU:HD23	1.82	0.41
2:B:1107:ALA:O	2:B:1108:ARG:HB3	2.21	0.41
3:C:18:VAL:HG22	3:C:240:VAL:HB	2.03	0.41
3:C:252:GLN:HG3	9:K:95:ILE:HG23	2.03	0.41
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.56	0.41
7:I:111:THR:HG22	7:I:112:SER:N	2.35	0.41
12:N:13:DA:C5	12:N:14:DG:C5	3.09	0.41
1:A:130:ASP:O	1:A:134:ARG:HB2	2.21	0.40
1:A:341:MET:HB3	2:B:1132:GLU:HG2	2.03	0.40
1:A:403:LYS:CB	1:A:404:TYR:HD1	2.34	0.40
1:A:419:LYS:C	1:A:421:ALA:H	2.24	0.40
1:A:452:LYS:HG3	1:A:453:MET:N	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:MET:HG3	2:B:1021:MET:CG	2.49	0.40
1:A:1059:HIS:ND1	5:F:86:THR:HA	2.35	0.40
1:A:1349:TYR:CD1	1:A:1349:TYR:C	2.94	0.40
2:B:37:PHE:O	2:B:39:ARG:N	2.53	0.40
2:B:780:VAL:HG11	8:J:56:LEU:HD22	2.02	0.40
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.55	0.40
6:H:98:TYR:CE1	6:H:141:TYR:CZ	3.08	0.40
9:K:47:ARG:HH11	9:K:47:ARG:HB3	1.86	0.40
1:A:102:VAL:C	1:A:104:GLU:H	2.25	0.40
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.84	0.40
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.56	0.40
1:A:1280:GLU:OE2	1:A:1280:GLU:N	2.54	0.40
2:B:325:GLN:HE21	2:B:325:GLN:HB2	1.73	0.40
2:B:855:PHE:HZ	2:B:857:ARG:HH12	1.65	0.40
3:C:33:LEU:HG	3:C:37:MET:CE	2.51	0.40
9:K:61:TYR:HA	9:K:72:LYS:O	2.21	0.40
1:A:106:VAL:HA	1:A:114:LEU:HD23	2.02	0.40
1:A:343:LYS:NZ	2:B:1156:ASP:OD1	2.54	0.40
1:A:1116:LEU:HD13	1:A:1116:LEU:HA	1.97	0.40
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.21	0.40
2:B:125:SER:HB3	2:B:171:PRO:HA	2.02	0.40
2:B:241:ARG:HA	2:B:253:THR:HG22	2.01	0.40
2:B:599:THR:O	2:B:603:LEU:HG	2.22	0.40
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.55	0.40
2:B:916:THR:HG23	2:B:935:ARG:HB2	2.03	0.40
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.51	0.40
6:H:101:ALA:HB2	6:H:116:TYR:CE1	2.57	0.40
11:T:6:DG:H2"	11:T:7:DA:OP2	2.21	0.40
12:N:11:DG:H2"	12:N:12:DT:C7	2.52	0.40
1:A:118:HIS:CE1	1:A:162:VAL:O	2.75	0.40
1:A:132:LYS:NZ	1:A:132:LYS:HB2	2.36	0.40
1:A:344:ARG:HA	2:B:1129:ARG:HA	2.03	0.40
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.55	0.40
1:A:1153:TYR:CE2	1:A:1163:ILE:HD11	2.56	0.40
2:B:267:ARG:O	2:B:316:PRO:CG	2.69	0.40
2:B:639:ILE:HD11	2:B:691:GLU:HB2	2.03	0.40
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.57	0.40
2:B:843:GLN:O	2:B:843:GLN:NE2	2.55	0.40
2:B:997:GLU:H	2:B:997:GLU:HG3	1.34	0.40
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.87	0.40
3:C:127:ARG:HE	3:C:127:ARG:HB2	1.73	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:14:ARG:NH1	4:E:141:VAL:HG12	2.37	0.40
5:F:98:ALA:O	5:F:102:SER:HB3	2.22	0.40
1:A:64:ASN:O	1:A:66:LYS:N	2.55	0.40
1:A:840:ARG:NE	1:A:1384:VAL:O	2.37	0.40
1:A:873:MET:HB2	1:A:878:ILE:HD11	2.02	0.40
1:A:1105:LEU:HD23	1:A:1384:VAL:HG21	2.04	0.40
2:B:846:ILE:HD13	2:B:974:PRO:HG2	2.04	0.40
2:B:1189:ILE:HD12	2:B:1190:ASP:H	1.86	0.40
4:E:165:LEU:HD22	4:E:165:LEU:HA	1.88	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	1379/1733 (80%)	1166 (85%)	182 (13%)	31 (2%)	6 37
2	B	1085/1224 (89%)	932 (86%)	125 (12%)	28 (3%)	5 33
3	C	264/318 (83%)	228 (86%)	35 (13%)	1 (0%)	34 72
4	E	212/215 (99%)	184 (87%)	25 (12%)	3 (1%)	11 46
5	F	82/155 (53%)	74 (90%)	7 (8%)	1 (1%)	13 50
6	H	129/146 (88%)	98 (76%)	27 (21%)	4 (3%)	4 30
7	I	117/122 (96%)	97 (83%)	17 (14%)	3 (3%)	5 33
8	J	63/70 (90%)	56 (89%)	6 (10%)	1 (2%)	9 43
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100 100
10	L	43/70 (61%)	25 (58%)	14 (33%)	4 (9%)	0 8
All	All	3486/4173 (84%)	2966 (85%)	444 (13%)	76 (2%)	6 37

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	PRO
1	A	286	HIS
1	A	315	LEU
1	A	600	PRO
1	A	1174	PHE
2	B	230	ALA
2	B	636	PRO
2	B	711	GLU
2	B	884	ARG
2	B	1046	PRO
6	H	107	VAL
10	L	28	LYS
1	A	142	CYS
1	A	986	ILE
1	A	1234	GLU
2	B	65	GLU
2	B	275	TYR
2	B	479	VAL
2	B	637	LEU
2	B	714	GLU
2	B	780	VAL
2	B	864	LYS
2	B	881	ASN
2	B	1220	ARG
5	F	73	ALA
6	H	129	TYR
7	I	33	SER
7	I	79	HIS
1	A	214	ILE
1	A	609	ASP
1	A	922	ASP
1	A	1123	GLY
2	B	468	GLU
2	B	865	LYS
3	C	142	VAL
4	E	86	PRO
6	H	138	GLU
1	A	107	CYS
1	A	109	HIS
1	A	397	ASN
1	A	923	LEU
1	A	1036	ARG
1	A	1281	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1437	GLY
2	B	246	LYS
2	B	648	HIS
2	B	901	PRO
7	I	9	ASP
10	L	32	ALA
10	L	54	ARG
1	A	55	ASP
1	A	75	ASN
1	A	224	PHE
1	A	453	MET
1	A	958	VAL
1	A	1280	GLU
2	B	251	ILE
2	B	408	LEU
2	B	707	PRO
2	B	1108	ARG
4	E	125	PRO
6	H	109	LYS
1	A	35	ILE
1	A	65	LEU
1	A	252	PHE
1	A	1156	PRO
2	B	462	ALA
4	E	118	PRO
10	L	55	ILE
1	A	162	VAL
1	A	89	PRO
2	B	1103	ILE
2	B	369	GLY
2	B	167	ILE
2	B	593	PRO
8	J	13	VAL

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	1216/1520 (80%)	1014 (83%)	202 (17%)	2 13
2	B	957/1061 (90%)	820 (86%)	137 (14%)	3 19
3	C	234/274 (85%)	195 (83%)	39 (17%)	2 12
4	E	196/197 (100%)	169 (86%)	27 (14%)	3 20
5	F	74/137 (54%)	61 (82%)	13 (18%)	2 10
6	H	117/128 (91%)	99 (85%)	18 (15%)	2 16
7	I	113/116 (97%)	88 (78%)	25 (22%)	1 5
8	J	60/65 (92%)	47 (78%)	13 (22%)	1 5
9	K	99/102 (97%)	89 (90%)	10 (10%)	7 32
10	L	40/57 (70%)	33 (82%)	7 (18%)	2 10
All	All	3106/3657 (85%)	2615 (84%)	491 (16%)	2 15

All (491) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	34	LYS
1	A	35	ILE
1	A	41	MET
1	A	49	LYS
1	A	53	LEU
1	A	54	ASN
1	A	55	ASP
1	A	65	LEU
1	A	66	LYS
1	A	71	GLN
1	A	76	GLU
1	A	107	CYS
1	A	109	HIS
1	A	114	LEU
1	A	126	LEU
1	A	129	LYS
1	A	131	SER
1	A	132	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	148	CYS
1	A	151	ASP
1	A	163	SER
1	A	164	ARG
1	A	169	ASN
1	A	179	LEU
1	A	185	TRP
1	A	208	LEU
1	A	211	PHE
1	A	222	LEU
1	A	226	GLU
1	A	227	VAL
1	A	249	SER
1	A	251	SER
1	A	252	PHE
1	A	254	GLU
1	A	255	SER
1	A	256	GLN
1	A	257	ARG
1	A	259	GLU
1	A	287	HIS
1	A	289	ILE
1	A	297	GLN
1	A	307	ASP
1	A	311	GLN
1	A	313	GLN
1	A	316	GLN
1	A	317	LYS
1	A	320	ARG
1	A	323	LYS
1	A	330	LYS
1	A	332	LYS
1	A	335	ARG
1	A	343	LYS
1	A	359	LEU
1	A	372	LYS
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	393	ARG
1	A	398	GLU
1	A	416	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	419	LYS
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	485	ASP
1	A	496	GLU
1	A	504	LEU
1	A	509	LEU
1	A	512	VAL
1	A	513	SER
1	A	517	ASN
1	A	532	ARG
1	A	544	ASP
1	A	550	LEU
1	A	567	LYS
1	A	590	ARG
1	A	591	PHE
1	A	596	THR
1	A	599	SER
1	A	601	LYS
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	621	THR
1	A	625	SER
1	A	629	LEU
1	A	635	ARG
1	A	666	ILE
1	A	672	ASP
1	A	702	LEU
1	A	710	LEU
1	A	732	LEU
1	A	740	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	752	LYS
1	A	764	CYS
1	A	768	GLN
1	A	774	ARG
1	A	783	THR
1	A	788	SER
1	A	801	GLU
1	A	821	ARG
1	A	826	ASP
1	A	829	VAL
1	A	838	GLN
1	A	839	ARG
1	A	879	GLU
1	A	881	GLN
1	A	885	THR
1	A	886	ILE
1	A	896	ARG
1	A	902	LEU
1	A	903	ASN
1	A	911	SER
1	A	917	SER
1	A	920	LEU
1	A	923	LEU
1	A	926	GLN
1	A	929	LEU
1	A	941	LYS
1	A	961	ARG
1	A	970	THR
1	A	976	THR
1	A	977	LYS
1	A	995	GLU
1	A	996	ASN
1	A	1000	LEU
1	A	1001	ARG
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1034	GLU
1	A	1035	TYR
1	A	1062	GLU
1	A	1064	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1067	LEU
1	A	1081	LEU
1	A	1093	LYS
1	A	1095	THR
1	A	1128	GLN
1	A	1135	ARG
1	A	1142	THR
1	A	1146	VAL
1	A	1165	GLU
1	A	1172	LEU
1	A	1187	GLN
1	A	1205	LYS
1	A	1206	ASP
1	A	1208	THR
1	A	1219	THR
1	A	1221	LYS
1	A	1223	ASP
1	A	1224	LEU
1	A	1237	ILE
1	A	1240	CYS
1	A	1257	ASP
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1280	GLU
1	A	1281	ARG
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1300	LYS
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1351	GLU
1	A	1354	ASN
1	A	1359	ASP
1	A	1366	ARG
1	A	1374	VAL
1	A	1376	THR
1	A	1383	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1386	ARG
1	A	1391	ARG
1	A	1392	SER
1	A	1393	ASN
1	A	1407	GLU
1	A	1425	SER
1	A	1426	GLU
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE
2	B	28	GLU
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	97	VAL
2	B	98	THR
2	B	103	ASN
2	B	105	SER
2	B	106	ASP
2	B	109	THR
2	B	128	LEU
2	B	134	LYS
2	B	165	VAL
2	B	167	ILE
2	B	175	ARG
2	B	176	SER
2	B	183	GLU
2	B	194	GLU
2	B	217	ARG
2	B	225	VAL
2	B	242	SER
2	B	244	LEU
2	B	246	LYS
2	B	248	SER
2	B	249	ARG
2	B	267	ARG
2	B	268	THR
2	B	275	TYR
2	B	315	LYS
2	B	319	GLU
2	B	328	GLU
2	B	345	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	346	GLU
2	B	351	TYR
2	B	371	GLU
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG
2	B	415	GLN
2	B	425	THR
2	B	426	LYS
2	B	427	ASP
2	B	428	ILE
2	B	432	MET
2	B	448	ILE
2	B	454	THR
2	B	461	LEU
2	B	466	TRP
2	B	468	GLU
2	B	473	MET
2	B	474	SER
2	B	476	ARG
2	B	480	SER
2	B	482	VAL
2	B	483	LEU
2	B	487	THR
2	B	510	LYS
2	B	513	GLN
2	B	527	THR
2	B	542	MET
2	B	549	THR
2	B	552	MET
2	B	556	THR
2	B	563	MET
2	B	570	VAL
2	B	598	GLU
2	B	617	ARG
2	B	635	ARG
2	B	651	LEU
2	B	653	VAL
2	B	655	LYS
2	B	667	GLN
2	B	680	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	708	GLU
2	B	710	LEU
2	B	711	GLU
2	B	714	GLU
2	B	730	ARG
2	B	737	THR
2	B	751	VAL
2	B	755	ILE
2	B	762	ASN
2	B	780	VAL
2	B	786	ASN
2	B	788	ARG
2	B	790	ASP
2	B	791	THR
2	B	810	GLU
2	B	822	ASN
2	B	827	ILE
2	B	844	SER
2	B	857	ARG
2	B	866	TYR
2	B	879	ARG
2	B	883	LEU
2	B	884	ARG
2	B	943	SER
2	B	946	ASN
2	B	953	LEU
2	B	957	ASN
2	B	963	PHE
2	B	970	THR
2	B	983	ARG
2	B	987	LYS
2	B	992	ILE
2	B	997	GLU
2	B	999	MET
2	B	1004	GLU
2	B	1007	VAL
2	B	1019	SER
2	B	1021	MET
2	B	1028	GLU
2	B	1055	ILE
2	B	1065	GLN
2	B	1066	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1072	MET
2	B	1077	THR
2	B	1082	MET
2	B	1092	TYR
2	B	1095	LEU
2	B	1098	MET
2	B	1103	ILE
2	B	1113	VAL
2	B	1124	ARG
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1174	LYS
2	B	1176	ASN
2	B	1183	LYS
2	B	1186	ASP
2	B	1188	LYS
2	B	1194	ILE
2	B	1202	LEU
2	B	1220	ARG
3	C	4	GLU
3	C	11	ARG
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	41	ILE
3	C	53	THR
3	C	56	THR
3	C	57	VAL
3	C	66	ARG
3	C	77	ILE
3	C	79	GLN
3	C	80	LEU
3	C	89	GLU
3	C	96	SER
3	C	99	LEU
3	C	100	THR
3	C	102	GLN
3	C	106	GLU
3	C	116	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	120	ILE
3	C	129	ILE
3	C	137	LYS
3	C	140	ASN
3	C	149	LYS
3	C	151	GLN
3	C	189	THR
3	C	197	SER
3	C	222	LYS
3	C	226	ASP
3	C	235	VAL
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	253	LYS
3	C	259	LEU
3	C	267	GLN
3	C	268	ASP
4	E	3	GLN
4	E	11	ARG
4	E	14	ARG
4	E	31	THR
4	E	37	LEU
4	E	40	GLU
4	E	54	GLN
4	E	78	LEU
4	E	90	VAL
4	E	92	THR
4	E	94	LYS
4	E	98	ILE
4	E	103	LYS
4	E	110	PHE
4	E	123	LEU
4	E	127	ILE
4	E	131	THR
4	E	134	THR
4	E	150	VAL
4	E	153	HIS
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	179	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	196	VAL
4	E	201	LYS
4	E	204	THR
5	F	72	LYS
5	F	79	ARG
5	F	82	THR
5	F	93	ILE
5	F	97	ARG
5	F	102	SER
5	F	110	ASP
5	F	112	GLU
5	F	114	GLU
5	F	123	LYS
5	F	133	VAL
5	F	149	GLU
5	F	155	LEU
6	H	2	SER
6	H	3	ASN
6	H	19	ARG
6	H	21	ASN
6	H	34	ASP
6	H	62	SER
6	H	78	SER
6	H	89	LEU
6	H	97	MET
6	H	109	LYS
6	H	124	ARG
6	H	130	ARG
6	H	135	LEU
6	H	139	ASN
6	H	142	LEU
6	H	143	LEU
6	H	145	ARG
6	H	146	ARG
7	I	2	THR
7	I	3	THR
7	I	4	PHE
7	I	7	CYS
7	I	8	ARG
7	I	9	ASP
7	I	10	CYS
7	I	14	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	I	24	ARG
7	I	28	GLU
7	I	29	CYS
7	I	30	ARG
7	I	37	GLU
7	I	50	THR
7	I	55	THR
7	I	70	ARG
7	I	71	SER
7	I	77	LYS
7	I	84	VAL
7	I	88	SER
7	I	89	GLN
7	I	90	GLN
7	I	95	THR
7	I	107	SER
7	I	116	ASN
8	J	2	ILE
8	J	5	VAL
8	J	6	ARG
8	J	7	CYS
8	J	14	VAL
8	J	28	ASP
8	J	29	GLU
8	J	31	ASP
8	J	43	ARG
8	J	46	CYS
8	J	48	ARG
8	J	59	LYS
8	J	64	ASN
9	K	1	MET
9	K	6	ARG
9	K	26	LYS
9	K	47	ARG
9	K	51	LEU
9	K	77	THR
9	K	101	LEU
9	K	103	THR
9	K	106	GLU
9	K	107	THR
10	L	34	CYS
10	L	42	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	L	47	ARG
10	L	50	ASP
10	L	51	CYS
10	L	54	ARG
10	L	63	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	64	ASN
1	A	68	GLN
1	A	80	HIS
1	A	435	HIS
1	A	700	ASN
1	A	903	ASN
1	A	1222	ASN
1	A	1393	ASN
2	B	110	HIS
2	B	357	GLN
2	B	590	HIS
2	B	706	GLN
2	B	762	ASN
2	B	843	GLN
2	B	1025	HIS
2	B	1084	GLN
2	B	1093	GLN
2	B	1141	HIS
2	B	1193	GLN
3	C	167	HIS
3	C	195	GLN
3	C	231	ASN
4	E	54	GLN
6	H	3	ASN
7	I	46	HIS
7	I	89	GLN
7	I	108	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	2	U
13	R	9	G

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
11	1CC	T	19[A]	11	20,23,24	1.10	2 (10%)	26,33,36	1.24	2 (7%)
11	1CC	T	19[B]	11	20,23,24	1.53	4 (20%)	26,33,36	1.77	8 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	1CC	T	19[A]	11	-	3/11/25/26	0/2/2/2
11	1CC	T	19[B]	11	-	4/11/25/26	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	19[B]	1CC	C2'-C1'	-3.61	1.42	1.52
11	T	19[B]	1CC	O4'-C1'	2.45	1.47	1.42
11	T	19[A]	1CC	C2-N1	-2.22	1.35	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	19[B]	1CC	C2-N1	-2.22	1.35	1.40
11	T	19[B]	1CC	C5-C4	2.22	1.47	1.43
11	T	19[A]	1CC	C5-C4	2.20	1.47	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	T	19[B]	1CC	O4'-C1'-C2'	-3.81	99.05	106.25
11	T	19[A]	1CC	C5-C6-N1	-2.89	119.25	123.10
11	T	19[B]	1CC	C5-C6-N1	-2.89	119.26	123.10
11	T	19[B]	1CC	C3'-C2'-C1'	2.72	109.34	102.54
11	T	19[B]	1CC	O2-C2-N3	-2.60	118.11	122.33
11	T	19[A]	1CC	O2-C2-N3	-2.58	118.14	122.33
11	T	19[B]	1CC	C4'-O4'-C1'	2.53	115.57	109.45
11	T	19[B]	1CC	O4'-C4'-C3'	-2.36	100.17	105.67
11	T	19[B]	1CC	O3'-C3'-C2'	2.19	118.72	110.90
11	T	19[B]	1CC	O3'-C3'-C4'	-2.14	101.90	110.10

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	T	19[B]	1CC	C3'-C4'-C5'-O5'
11	T	19[A]	1CC	C3'-C4'-C5'-O5'
11	T	19[A]	1CC	O4'-C4'-C5'-O5'
11	T	19[B]	1CC	O4'-C4'-C5'-O5'
11	T	19[B]	1CC	C2'-C1'-N1-C2
11	T	19[B]	1CC	C2'-C1'-N1-C6
11	T	19[A]	1CC	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	19[A]	1CC	7	0
11	T	19[B]	1CC	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	1393/1733 (80%)	-0.22	26 (1%) 66 61	24, 80, 185, 300	0
2	B	1103/1224 (90%)	-0.35	8 (0%) 87 83	28, 70, 149, 285	0
3	C	266/318 (83%)	-0.59	0 100 100	33, 70, 111, 170	0
4	E	214/215 (99%)	-0.18	2 (0%) 84 79	43, 108, 202, 264	0
5	F	84/155 (54%)	-0.58	0 100 100	54, 83, 139, 196	0
6	H	133/146 (91%)	0.08	3 (2%) 60 54	52, 105, 179, 286	0
7	I	119/122 (97%)	-0.49	0 100 100	43, 85, 133, 169	0
8	J	65/70 (92%)	-0.55	0 100 100	34, 64, 108, 142	0
9	K	114/120 (95%)	-0.39	0 100 100	36, 73, 110, 158	0
10	L	45/70 (64%)	0.21	3 (6%) 17 16	61, 137, 242, 287	0
11	T	28/29 (96%)	0.68	7 (25%) 0 0	54, 278, 349, 351	0
12	N	14/14 (100%)	1.09	2 (14%) 2 3	244, 289, 323, 331	0
13	R	9/9 (100%)	-0.49	0 100 100	56, 68, 129, 140	0
All	All	3587/4225 (84%)	-0.29	51 (1%) 75 69	24, 78, 183, 351	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	254	GLU	7.3
1	A	1176	LEU	6.8
1	A	153	PRO	4.6
6	H	84	ALA	4.5
2	B	1221	SER	4.3
1	A	151	ASP	4.2
1	A	44	THR	4.0
6	H	139	ASN	3.8
2	B	250	PHE	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	709	ASP	3.7
1	A	141	LEU	3.7
4	E	83	CYS	3.6
1	A	255	SER	3.6
1	A	147	VAL	3.5
1	A	256	GLN	3.5
1	A	146	MET	3.4
2	B	869	SER	3.4
11	T	12	DC	3.3
11	T	11	DG	3.3
2	B	643	ASP	3.2
1	A	597	LEU	3.1
1	A	69	THR	3.1
11	T	3	DA	3.1
4	E	93	MET	2.9
2	B	865	LYS	2.9
10	L	50	ASP	2.9
6	H	85	GLY	2.9
1	A	45	GLN	2.7
1	A	174	ILE	2.7
2	B	69	LEU	2.6
1	A	144	THR	2.6
1	A	162	VAL	2.6
11	T	1	DC	2.6
11	T	4	DC	2.5
1	A	163	SER	2.5
1	A	259	GLU	2.4
2	B	866	TYR	2.3
10	L	46	VAL	2.2
1	A	108	MET	2.2
12	N	1	DC	2.2
1	A	49	LYS	2.2
12	N	14	DG	2.2
11	T	2	DT	2.1
1	A	598	LEU	2.1
1	A	286	HIS	2.1
1	A	59	GLY	2.1
10	L	43	THR	2.1
11	T	5	DC	2.1
1	A	145	LYS	2.0
1	A	183	GLY	2.0
1	A	253	ASN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
11	1CC	T	19[A]	22/23	0.87	0.22	37,75,128,168	22
11	1CC	T	19[B]	22/23	0.87	0.22	63,101,153,155	22

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
15	MG	A	1803	1/1	0.75	0.19	78,78,78,78	0
14	ZN	A	1802	1/1	0.77	0.10	117,117,117,117	0
14	ZN	B	1301	1/1	0.84	0.20	197,197,197,197	0
14	ZN	I	202	1/1	0.87	0.16	96,96,96,96	0
14	ZN	L	101	1/1	0.91	0.12	211,211,211,211	0
14	ZN	A	1801	1/1	0.93	0.13	247,247,247,247	0
14	ZN	C	401	1/1	0.97	0.10	96,96,96,96	0
14	ZN	I	201	1/1	0.98	0.09	100,100,100,100	0
14	ZN	J	101	1/1	0.99	0.20	76,76,76,76	0

6.5 Other polymers (i)

There are no such residues in this entry.