



# Full wwPDB X-ray Structure Validation Report

Sep 15, 2014 – 11:35 AM EDT

PDB ID : 1VXI  
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-U on the Ribosome  
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.  
Deposited on : 2013-07-12  
Resolution : 2.94 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

---

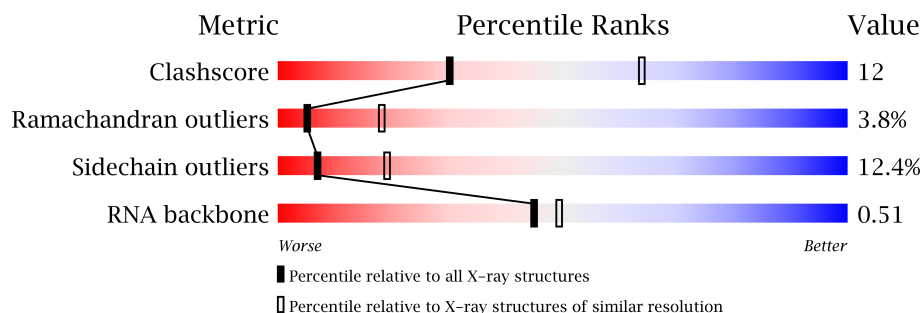
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23489

# 1 Overall quality at a glance

The reported resolution of this entry is 2.94 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))
Clashscore	79885	1761 (2.98-2.90)
Ramachandran outliers	78287	1708 (2.98-2.90)
Sidechain outliers	78261	1710 (2.98-2.90)
RNA backbone	1838	1002 (3.44-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	1522	
2	B	256	
3	C	239	
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	V	77	
23	X	25	
24	Y	17	

## 2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 53733 atoms, of which 0 are hydrogen and 0 are deuterium.

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

- Molecule 1 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1500	Total	C	N	O	P	0	0	0
			32249	14354	5984	10412	1499			

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	237	Total	C	N	O	S	0	0	0
			1924	1228	344	347	5			

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	205	Total	C	N	O	S	0	0	0
			1605	1011	313	280	1			

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	208	Total	C	N	O	S	0	0	0
			1703	1066	339	291	7			

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	0
			1155	729	218	204	4			

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	101	Total	C	N	O	S	0	0	0
			843	531	155	154	3			

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	155	Total	C	N	O	S	0	0	0
			1257	781	252	218	6			

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	138	Total	C	N	O	S	0	0	0
			1116	705	215	193	3			

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1010	639	197	174				

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	0
			801	504	157	139	1			

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	119	Total	C	N	O	S	0	0	0
			885	549	168	165	3			

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	0
			975	614	196	164	1			

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	121	Total	C	N	O	S	0	0	0
			964	597	199	166	2			

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	60	Total	C	N	O	S	0	0	0
			492	312	104	72	4			

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	O	88	Total	C	N	O	S	0	0	0
			734	459	147	126	2			

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	0
			705	446	140	118	1			

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	100	Total	C	N	O	S	0	0	0
			834	534	155	143	2			

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	70	Total	C	N	O	0	0	0
			574	367	112	95			

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	84	Total	C	N	O	S	0	0	0
			674	430	126	116	2			

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			763	470	162	129	2			

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	0
			217	134	52	31			

- Molecule 22 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	V	77	Total	C	N	O	P	0	0	0
			1644	732	297	538	77			

- Molecule 23 is a RNA chain called A-site ASL SufA6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	X	8	Total	C	N	O	P	0	0	0
			167	75	28	56	8			

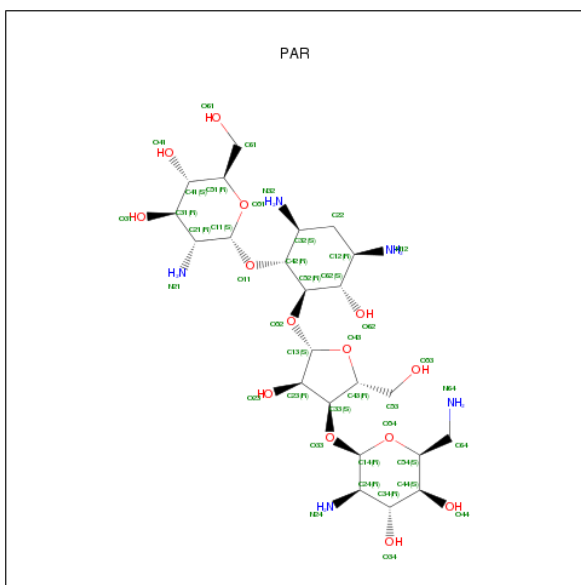
- Molecule 24 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	Y	15	Total	C	N	O	P	0	0	0
			323	144	58	106	15			

- Molecule 25 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	X	1	Total	Mg	0	0
			1	1		
25	A	72	Total	Mg	0	0
			72	72		
25	V	1	Total	Mg	0	0
			1	1		
25	M	1	Total	Mg	0	0
			1	1		

- Molecule 26 is PAROMOMYCIN (three-letter code: PAR) (formula: C<sub>23</sub>H<sub>45</sub>N<sub>5</sub>O<sub>14</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
26	A	1	Total	C	N	O	0	0
			42	23	5	14		

- Molecule 27 is ZINC ION (three-letter code: ZN) (formula:  $\text{Zn}$ ).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
27	D	1	Total Zn 1 1	0	0
27	N	1	Total Zn 1 1	0	0

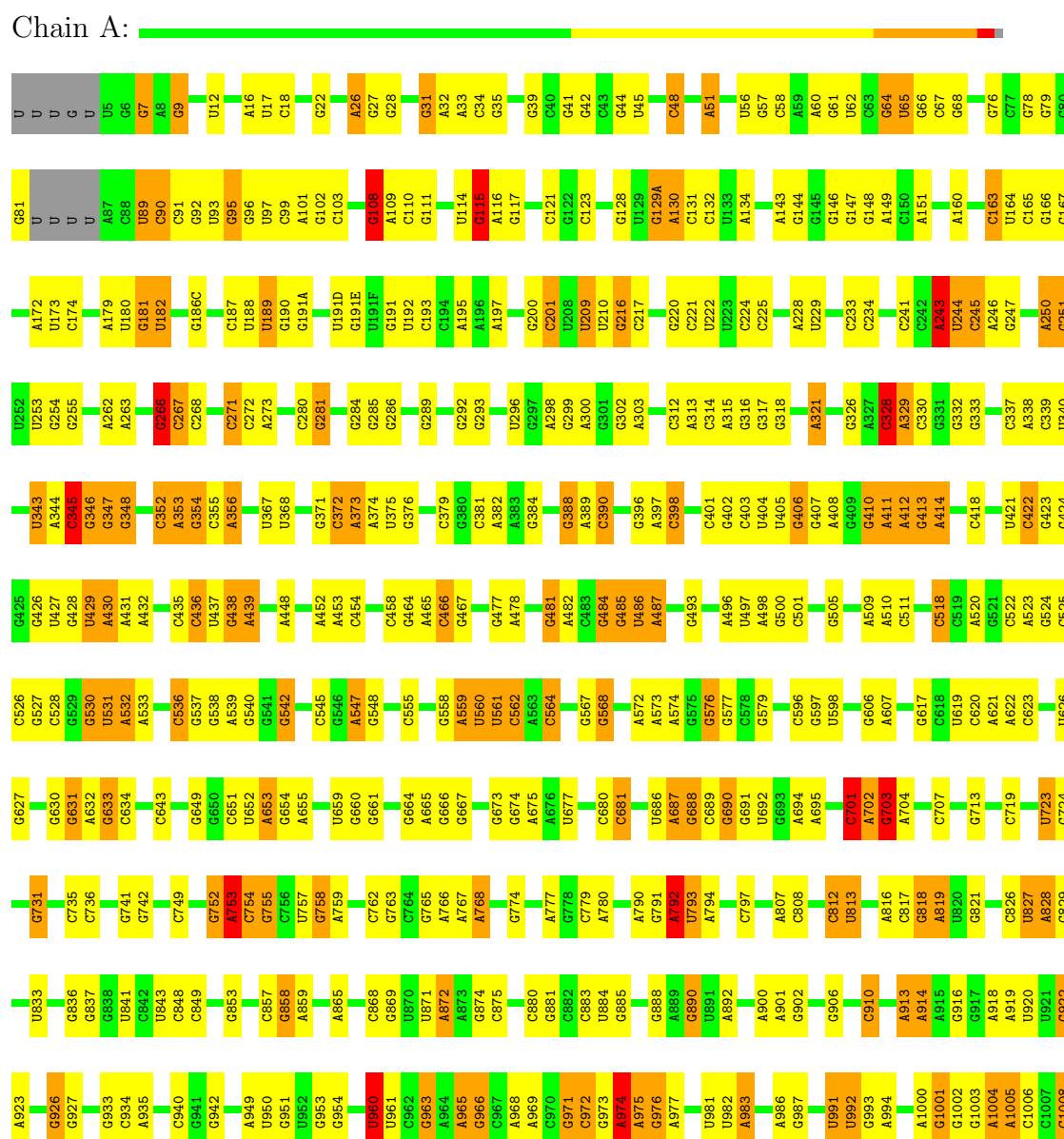


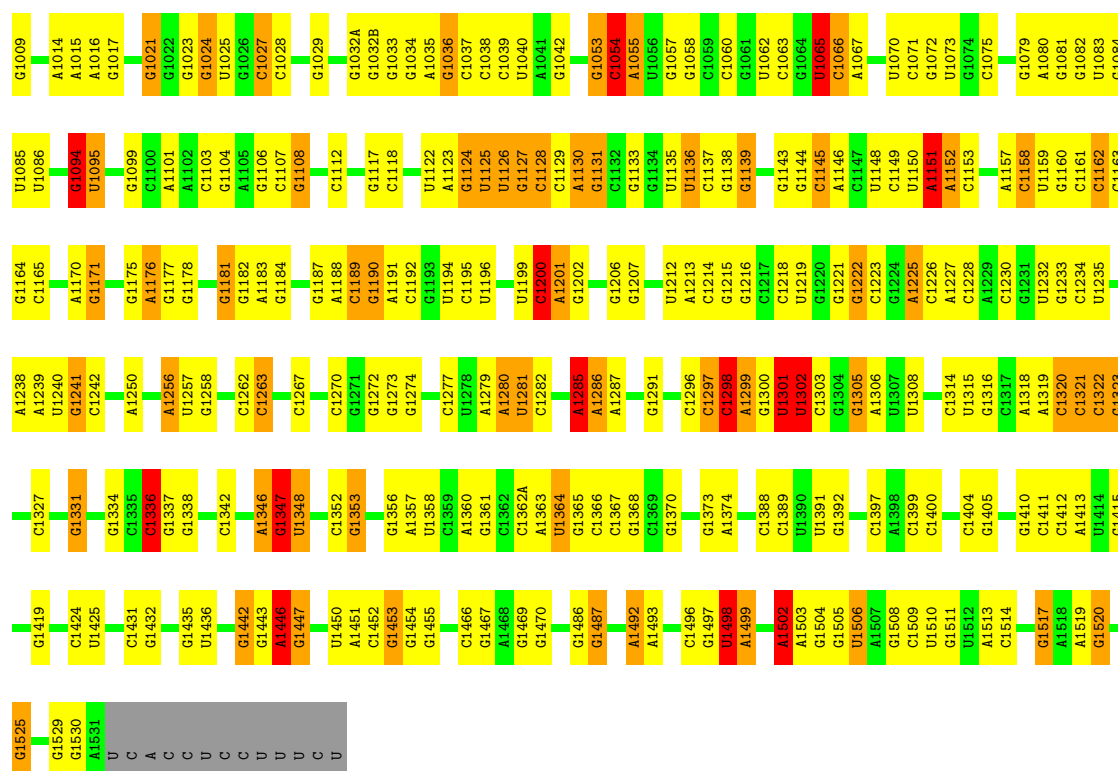
### 3 Residue-property plots

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

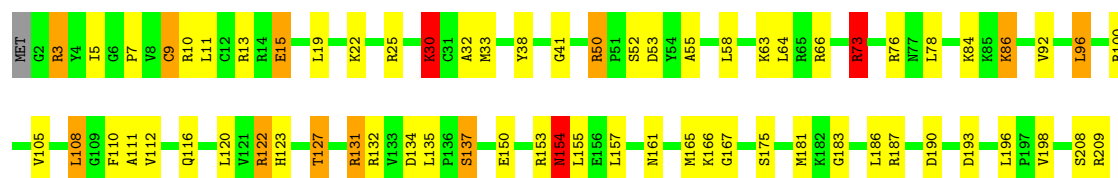
Note EDS was not executed.

#### • Molecule 1: 16S rRNA



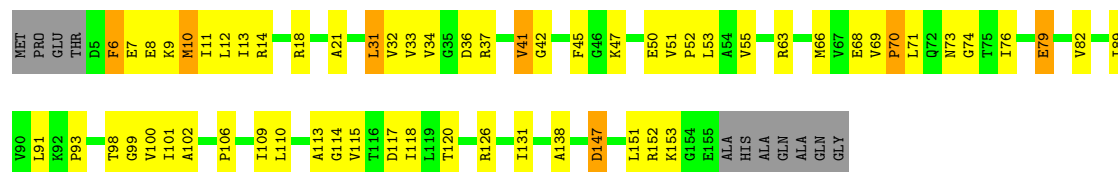


Chain D: 



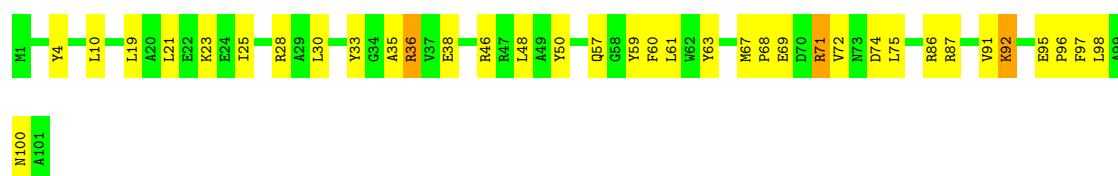
- Molecule 5: 30S ribosomal protein S5

Chain E: 



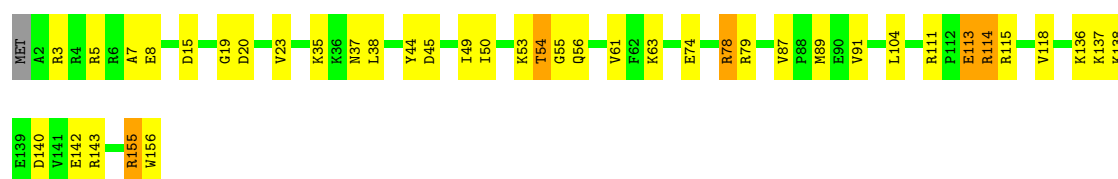
- Molecule 6: 30S ribosomal protein S6

Chain F: 



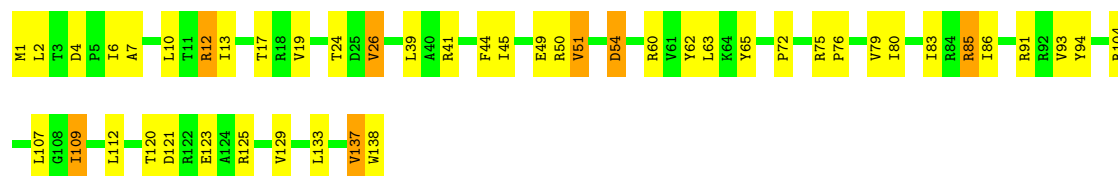
- Molecule 7: 30S ribosomal protein S7

Chain G: 



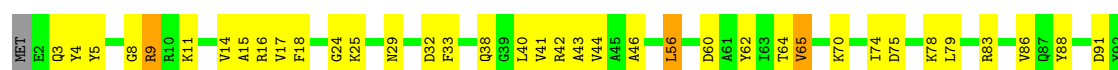
- Molecule 8: 30S ribosomal protein S8

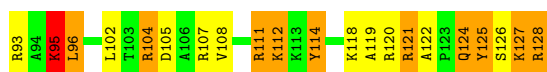
Chain H: 



- Molecule 9: 30S ribosomal protein S9

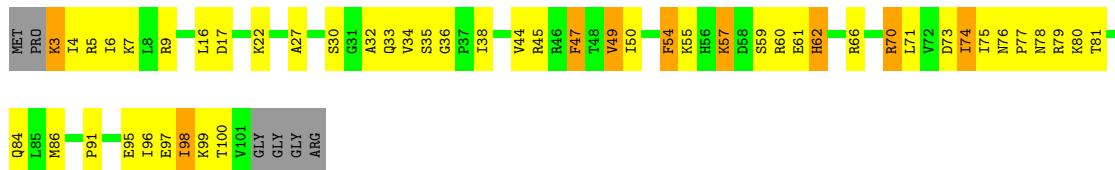
Chain I: 





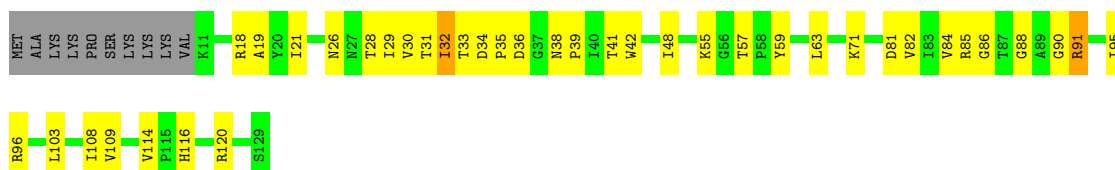
- Molecule 10: 30S ribosomal protein S10

Chain J:



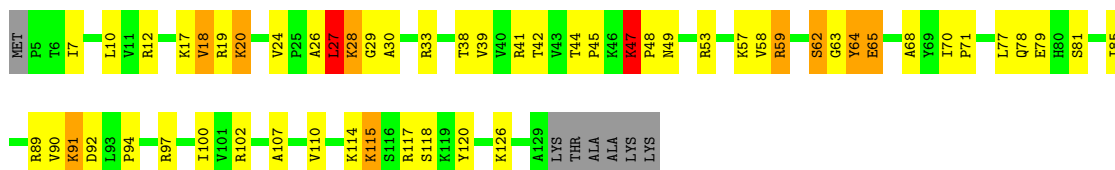
- Molecule 11: 30S ribosomal protein S11

Chain K:



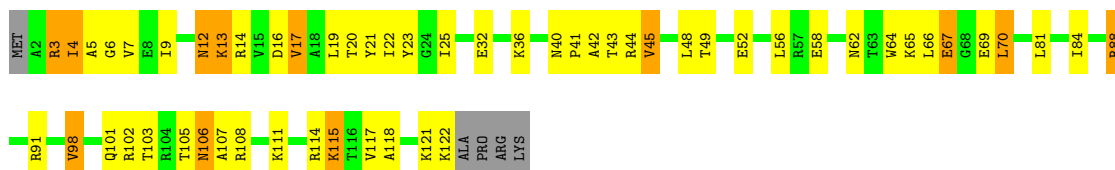
- Molecule 12: 30S ribosomal protein S12

Chain L:



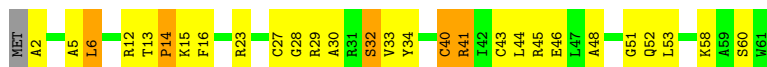
- Molecule 13: 30S ribosomal protein S13

Chain M:



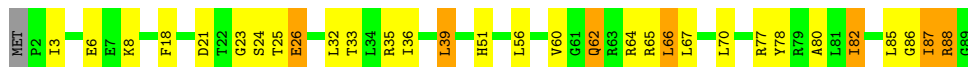
- Molecule 14: 30S ribosomal protein S14

Chain N:



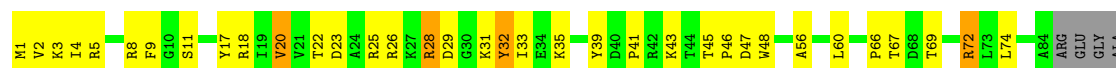
- Molecule 15: 30S ribosomal protein S15

Chain O:



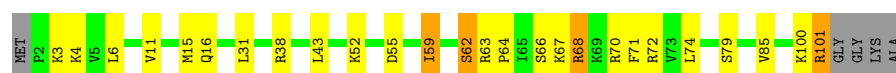
- Molecule 16: 30S ribosomal protein S16

Chain P: 



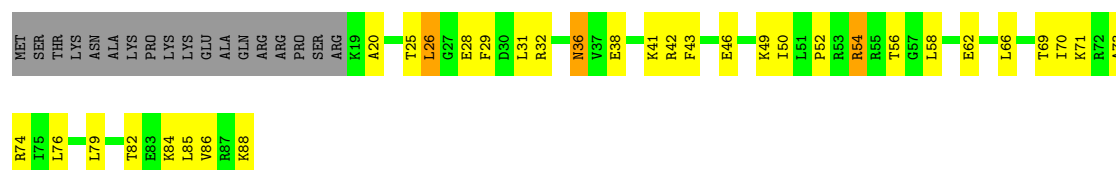
- Molecule 17: 30S ribosomal protein S17

Chain Q: 



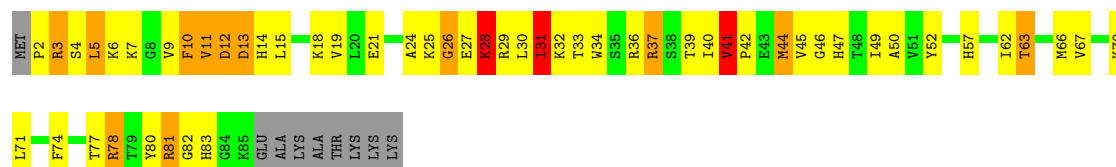
- Molecule 18: 30S ribosomal protein S18

Chain R: 



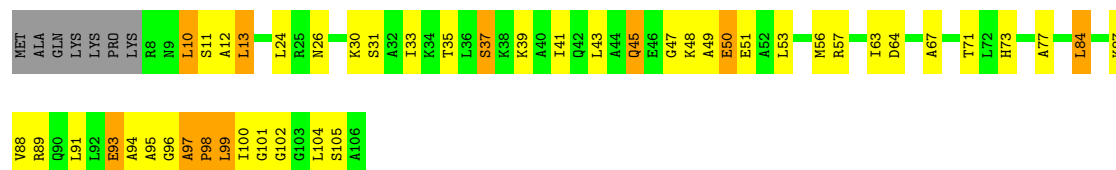
- Molecule 19: 30S ribosomal protein S19

Chain S: 



- Molecule 20: 30S ribosomal protein S20

Chain T: 



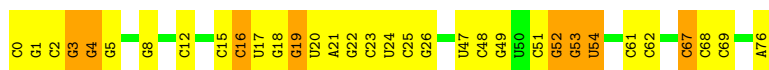
- Molecule 21: 30S ribosomal protein S21

Chain U: 



- Molecule 22: P-site tRNA fMet

Chain V: 



- Molecule 23: A-site ASL SufA6

Chain X: 



- Molecule 24: messenger RNA

Chain Y: 



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	209.81Å 449.41Å 620.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.22 – 2.94	Depositor
% Data completeness (in resolution range)	98.6 (155.22-2.94)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.219 , 0.265	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	53733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.54	0/36101	1.09	114/56346 (0.2%)
2	B	0.32	0/1959	0.54	0/2642
3	C	0.36	0/1629	0.56	0/2195
4	D	0.40	0/1733	0.60	0/2318
5	E	0.39	0/1171	0.59	0/1576
6	F	0.38	0/856	0.58	0/1154
7	G	0.34	0/1276	0.50	0/1709
8	H	0.38	0/1136	0.58	0/1527
9	I	0.33	0/1029	0.57	0/1379
10	J	0.35	0/814	0.59	0/1095
11	K	0.38	0/900	0.58	0/1213
12	L	0.45	0/991	0.74	1/1327 (0.1%)
13	M	0.36	0/974	0.63	0/1303
14	N	0.42	0/501	0.66	0/664
15	O	0.39	0/745	0.54	0/992
16	P	0.35	0/721	0.57	0/970
17	Q	0.35	0/847	0.54	0/1131
18	R	0.37	0/579	0.59	0/768
19	S	0.37	0/689	0.69	1/926 (0.1%)
20	T	0.31	0/765	0.59	0/1007
21	U	0.31	0/221	0.61	0/288
22	V	0.59	1/1836 (0.1%)	1.06	4/2859 (0.1%)
23	X	0.67	0/185	1.08	0/285
24	Y	0.40	0/333	0.94	0/517
All	All	0.49	1/57991 (0.0%)	0.97	120/86191 (0.1%)

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



Mol	Chain	#Chirality outliers	#Planarity outliers
12	L	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	0	C	OP3-P	-10.49	1.48	1.61

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1336	C	C2-N1-C1'	8.34	127.98	118.80
1	A	792	A	O4'-C1'-N9	8.34	114.87	108.20
1	A	518	C	C2-N3-C4	-8.27	115.76	119.90
1	A	963	G	N3-C4-C5	-8.09	124.55	128.60
1	A	1301	U	C2-N1-C1'	8.03	127.34	117.70
1	A	792	A	N1-C6-N6	7.87	123.32	118.60
1	A	1054	C	C2-N1-C1'	7.82	127.41	118.80
1	A	328	C	C2-N1-C1'	7.77	127.34	118.80
1	A	812	C	P-O3'-C3'	7.68	128.92	119.70
1	A	1302	U	C2-N1-C1'	7.42	126.61	117.70
1	A	1158	C	C2-N1-C1'	7.38	126.92	118.80
1	A	1498	U	C2-N1-C1'	7.35	126.52	117.70
1	A	792	A	C4-C5-N7	7.34	114.37	110.70
1	A	753	A	P-O3'-C3'	7.33	128.49	119.70
1	A	1151	A	O4'-C1'-N9	7.18	113.94	108.20
12	L	47	LYS	C-N-CD	-7.14	104.90	120.60
1	A	328	C	C6-N1-C2	-6.97	117.51	120.30
1	A	1336	C	C6-N1-C2	-6.91	117.54	120.30
1	A	1054	C	C6-N1-C1'	-6.84	112.59	120.80
1	A	328	C	N1-C2-O2	6.82	122.99	118.90
1	A	1065	U	P-O3'-C3'	6.81	127.88	119.70
1	A	1128	C	C6-N1-C2	-6.80	117.58	120.30
1	A	1200	C	P-O3'-C3'	6.79	127.85	119.70
1	A	1108	G	C5-C6-N1	-6.74	108.13	111.50
1	A	963	G	N3-C4-N9	6.74	130.04	126.00
1	A	1298	C	P-O3'-C3'	6.67	127.71	119.70
22	V	16	C	C2-N1-C1'	6.61	126.07	118.80
1	A	1200	C	OP2-P-O3'	6.58	119.67	105.20
1	A	703	G	N3-C4-C5	-6.55	125.32	128.60
22	V	16	C	N1-C2-O2	6.55	122.83	118.90
1	A	1336	C	N1-C2-O2	6.51	122.81	118.90
1	A	117	G	N1-C6-O6	6.48	123.79	119.90
1	A	690	G	O4'-C1'-N9	6.48	113.38	108.20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	410	G	P-O3'-C3'	6.46	127.45	119.70
1	A	1297	C	P-O3'-C3'	6.45	127.44	119.70
1	A	108	G	C4-C5-N7	6.42	113.37	110.80
1	A	792	A	N9-C4-C5	-6.41	103.23	105.80
1	A	1053	G	C4-N9-C1'	-6.41	118.17	126.50
1	A	827	U	N3-C2-O2	-6.41	117.72	122.20
1	A	914	A	O5'-P-OP1	-6.37	99.97	105.70
1	A	576	G	O5'-P-OP2	-6.32	100.01	105.70
1	A	960	U	N3-C2-O2	-6.26	117.82	122.20
1	A	1158	C	C6-N1-C2	-6.20	117.82	120.30
1	A	913	A	P-O3'-C3'	6.18	127.11	119.70
1	A	1302	U	N1-C2-O2	6.18	127.12	122.80
1	A	115	G	P-O3'-C3'	6.14	127.06	119.70
1	A	1301	U	N1-C2-O2	6.13	127.09	122.80
1	A	703	G	N3-C4-N9	6.11	129.66	126.00
1	A	703	G	C4-N9-C1'	5.99	134.28	126.50
1	A	328	C	N3-C2-O2	-5.89	117.78	121.90
1	A	1094	G	OP2-P-O3'	5.89	118.16	105.20
1	A	974	A	O4'-C1'-N9	5.88	112.91	108.20
1	A	1347	G	C4-N9-C1'	-5.81	118.95	126.50
1	A	792	A	C5-N7-C8	-5.80	101.00	103.90
1	A	243	A	P-O3'-C3'	5.76	126.61	119.70
1	A	1065	U	OP2-P-O3'	5.75	117.85	105.20
1	A	687	A	P-O3'-C3'	5.75	126.60	119.70
1	A	246	A	C8-N9-C4	5.69	108.07	105.80
1	A	768	A	C8-N9-C4	5.67	108.07	105.80
1	A	1302	U	C6-N1-C1'	-5.66	113.27	121.20
1	A	558	G	N1-C6-O6	5.66	123.29	119.90
1	A	328	C	C5-C6-N1	5.61	123.80	121.00
1	A	1347	G	OP2-P-O3'	5.60	117.52	105.20
1	A	910	C	C6-N1-C2	5.60	122.54	120.30
1	A	1094	G	P-O3'-C3'	5.59	126.41	119.70
1	A	1301	U	C6-N1-C1'	-5.57	113.41	121.20
1	A	1336	C	N3-C2-O2	-5.53	118.03	121.90
1	A	681	C	N3-C2-O2	-5.53	118.03	121.90
1	A	1301	U	C5-C6-N1	5.52	125.46	122.70
1	A	792	A	C3'-C2'-C1'	-5.52	97.09	101.50
1	A	1108	G	C5-C6-O6	5.51	131.90	128.60
1	A	345	C	P-O3'-C3'	5.50	126.30	119.70
1	A	1336	C	C5-C6-N1	5.49	123.74	121.00
1	A	1446	A	P-O3'-C3'	5.48	126.27	119.70
1	A	1370	G	N1-C6-O6	5.44	123.16	119.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	435	C	C6-N1-C2	-5.43	118.13	120.30
1	A	1336	C	C6-N1-C1'	-5.42	114.29	120.80
1	A	1053	G	C8-N9-C4	5.41	108.56	106.40
1	A	1496	C	C6-N1-C2	5.39	122.46	120.30
1	A	701	C	P-O3'-C3'	5.37	126.14	119.70
1	A	518	C	N1-C2-N3	5.36	122.95	119.20
1	A	1517	G	O5'-P-OP2	-5.36	100.88	105.70
1	A	115	G	N3-C4-C5	-5.35	125.93	128.60
1	A	1108	G	C4-C5-N7	-5.33	108.67	110.80
1	A	703	G	P-O3'-C3'	5.32	126.08	119.70
1	A	1502	A	C5-N7-C8	-5.30	101.25	103.90
1	A	1222	G	N3-C2-N2	-5.27	116.21	119.90
1	A	266	G	P-O3'-C3'	5.26	126.01	119.70
1	A	792	A	C6-C5-N7	-5.26	128.62	132.30
1	A	792	A	N9-C1'-C2'	5.25	120.83	114.00
1	A	723	U	N1-C2-O2	5.25	126.47	122.80
1	A	1498	U	P-O3'-C3'	5.24	125.99	119.70
1	A	328	C	P-O3'-C3'	5.23	125.98	119.70
1	A	681	C	C6-N1-C2	-5.23	118.21	120.30
1	A	888	G	C5-C6-O6	-5.22	125.47	128.60
19	S	41	VAL	C-N-CD	-5.20	109.15	120.60
1	A	108	G	N9-C4-C5	-5.18	103.33	105.40
1	A	690	G	N3-C2-N2	-5.18	116.27	119.90
1	A	1506	U	N1-C2-O2	-5.17	119.18	122.80
1	A	1347	G	O4'-C1'-N9	5.17	112.33	108.20
1	A	318	G	N1-C6-O6	5.16	123.00	119.90
1	A	858	G	N7-C8-N9	5.16	115.68	113.10
1	A	1285	A	P-O3'-C3'	5.16	125.89	119.70
1	A	1346	A	P-O3'-C3'	5.15	125.88	119.70
22	V	16	C	C6-N1-C2	-5.14	118.24	120.30
1	A	690	G	C2-N3-C4	-5.12	109.34	111.90
1	A	812	C	OP2-P-O3'	5.12	116.45	105.20
1	A	1502	A	C2-N3-C4	-5.10	108.05	110.60
1	A	1027	C	OP1-P-O3'	5.09	116.40	105.20
22	V	16	C	N3-C2-O2	-5.09	118.34	121.90
1	A	890	G	O4'-C1'-N9	5.09	112.27	108.20
1	A	1498	U	N3-C2-O2	-5.06	118.66	122.20
1	A	1054	C	P-O3'-C3'	5.05	125.76	119.70
1	A	542	G	O5'-P-OP1	-5.05	101.16	105.70
1	A	971	G	O4'-C1'-N9	5.05	112.24	108.20
1	A	410	G	OP1-P-O3'	5.04	116.29	105.20
1	A	330	C	N1-C2-O2	5.04	121.92	118.90

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	960	U	C2-N1-C1'	5.02	123.73	117.70
1	A	481	G	P-O3'-C3'	5.01	125.71	119.70
1	A	1347	G	C8-N9-C1'	5.01	133.51	127.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
12	L	47	LYS	Peptide

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32249	0	16279	523	0
2	B	1924	0	1975	80	0
3	C	1605	0	1668	63	0
4	D	1703	0	1764	47	0
5	E	1155	0	1213	42	0
6	F	843	0	857	21	0
7	G	1257	0	1296	24	0
8	H	1116	0	1177	25	0
9	I	1010	0	1037	50	0
10	J	801	0	849	42	0
11	K	885	0	904	28	0
12	L	975	0	1062	46	0
13	M	964	0	1034	37	0
14	N	492	0	529	17	0
15	O	734	0	771	19	0
16	P	705	0	725	26	0
17	Q	834	0	904	19	0
18	R	574	0	644	21	0
19	S	674	0	699	41	0
20	T	763	0	861	36	0
21	U	217	0	234	4	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	V	1644	0	836	17	0
23	X	167	0	87	0	0
24	Y	323	0	165	4	0
25	A	72	0	0	0	0
25	M	1	0	0	0	0
25	V	1	0	0	0	0
25	X	1	0	0	0	0
26	A	42	0	45	1	0
27	D	1	0	0	0	0
27	N	1	0	0	0	0
All	All	53733	0	37615	1079	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (1079) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:963:G:N3	10:J:55:LYS:NZ	2.11	0.97
1:A:1502:A:H2	1:A:1505:G:H1	1.22	0.87
1:A:971:G:HO2'	1:A:1365:G:HO2'	1.19	0.87
1:A:664:G:H22	1:A:741:G:H1	1.22	0.86
4:D:157:LEU:O	4:D:161:ASN:ND2	2.07	0.86
1:A:501:C:OP1	12:L:117:ARG:NH2	2.10	0.84
1:A:448:A:OP2	1:A:485:G:N2	2.10	0.83
1:A:1298:C:OP2	7:G:114:ARG:NH2	2.10	0.83
2:B:69:LEU:HB3	2:B:162:ILE:HG22	1.61	0.81
1:A:1305:G:N2	1:A:1331:G:H2'	1.96	0.80
1:A:1086:U:H3	1:A:1099:G:H22	1.29	0.80
13:M:65:LYS:HD3	13:M:69:GLU:HG3	1.63	0.79
3:C:32:LEU:HD13	3:C:59:ARG:HD3	1.64	0.79
1:A:1002:G:H1	1:A:1038:C:H42	1.28	0.79
20:T:33:ILE:O	20:T:37:SER:OG	2.01	0.79
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.64	0.79
3:C:59:ARG:HH12	3:C:97:LYS:HE3	1.48	0.78
4:D:9:CYS:SG	4:D:22:LYS:NZ	2.52	0.78
1:A:1053:G:H5'	1:A:1054:C:H5'	1.65	0.78
13:M:14:ARG:H	13:M:44:ARG:HD3	1.49	0.77
1:A:1128:C:H5'	9:I:16:ARG:HH22	1.50	0.77
3:C:20:SER:HB2	3:C:40:ARG:HH22	1.50	0.77
1:A:880:C:OP1	12:L:12:ARG:NH1	2.18	0.77
1:A:1139:G:N2	1:A:1143:G:O6	2.18	0.77
1:A:58:C:O2'	1:A:388:G:N7	2.17	0.76

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
16:P:45:THR:HG22	16:P:47:ASP:H	1.51	0.76
1:A:1178:G:N2	1:A:1181:G:N7	2.33	0.75
1:A:1002:G:H2'	1:A:1003:G:H8	1.52	0.75
1:A:532:A:H2	1:A:1206:G:H21	1.34	0.75
1:A:356:A:N3	1:A:368:U:O2'	2.19	0.75
17:Q:66:SER:O	17:Q:70:ARG:NH1	2.21	0.74
1:A:971:G:N2	1:A:1363:A:OP2	2.20	0.74
1:A:619:U:H3	4:D:135:LEU:HD23	1.52	0.74
1:A:1321:C:H3'	1:A:1322:C:H5''	1.69	0.74
1:A:1305:G:H22	1:A:1331:G:H2'	1.52	0.74
1:A:1314:C:N4	19:S:3:ARG:O	2.18	0.73
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.69	0.73
5:E:10:MET:HB3	5:E:32:VAL:HG22	1.70	0.71
9:I:114:TYR:HE1	10:J:60:ARG:H	1.38	0.71
6:F:50:TYR:OH	18:R:74:ARG:O	2.06	0.71
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.72	0.71
1:A:974:A:OP2	14:N:29:ARG:NH2	2.23	0.71
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.73	0.71
1:A:1129:C:N4	1:A:1133:G:O6	2.24	0.70
1:A:1298:C:HO2'	1:A:1299:A:P	2.13	0.70
1:A:1129:C:H4'	1:A:1130:A:H5'	1.73	0.70
10:J:50:ILE:HA	10:J:60:ARG:HG2	1.72	0.70
10:J:61:GLU:OE2	14:N:45:ARG:NH1	2.25	0.70
18:R:58:LEU:HD23	18:R:62:GLU:HB3	1.74	0.70
14:N:48:ALA:HB2	14:N:53:LEU:HD12	1.73	0.70
2:B:185:ILE:HG22	2:B:199:TYR:HB2	1.74	0.70
1:A:1200:C:O2'	1:A:1201:A:OP2	2.09	0.69
4:D:105:VAL:HG13	4:D:110:PHE:HB2	1.74	0.69
19:S:10:PHE:HB2	19:S:39:THR:H	1.54	0.69
6:F:68:PRO:HG2	6:F:71:ARG:HG3	1.74	0.69
20:T:100:ILE:HG13	20:T:102:GLY:H	1.56	0.69
1:A:130:A:N3	1:A:263:A:O2'	2.24	0.69
1:A:963:G:N2	1:A:972:C:N3	2.34	0.69
14:N:13:THR:N	14:N:14:PRO:HD2	2.09	0.68
2:B:235:SER:OG	2:B:236:TYR:N	2.25	0.68
19:S:40:ILE:HG12	19:S:41:VAL:HG13	1.76	0.67
5:E:31:LEU:HD23	5:E:45:PHE:CD1	2.30	0.67
8:H:120:THR:H	8:H:123:GLU:HB2	1.59	0.67
1:A:396:G:O2'	1:A:398:C:OP1	2.09	0.67
2:B:174:VAL:HG13	2:B:184:VAL:HG11	1.75	0.67
5:E:37:ARG:HA	5:E:114:GLY:H	1.58	0.67
1:A:826:C:H2'	1:A:827:U:O2	1.94	0.67

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:168:THR:HB	2:B:192:SER:HB2	1.77	0.67
1:A:266:G:H5''	1:A:267:C:C5	2.30	0.66
1:A:1218:C:H2'	1:A:1219:U:C6	2.30	0.66
1:A:561:U:O2'	1:A:562:C:OP2	2.11	0.66
10:J:7:LYS:HB2	10:J:97:GLU:HB2	1.76	0.66
13:M:105:THR:O	13:M:107:ALA:N	2.29	0.66
1:A:390:C:O3'	16:P:28:ARG:NH2	2.28	0.66
1:A:564:C:O2'	8:H:91:ARG:NH2	2.29	0.66
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.77	0.66
1:A:547:A:OP1	4:D:73:ARG:NH2	2.30	0.65
1:A:1342:C:H4'	9:I:125:TYR:HB3	1.78	0.65
1:A:559:A:OP1	5:E:126:ARG:NH2	2.30	0.65
1:A:674:G:H2'	1:A:675:A:H8	1.60	0.65
1:A:67:C:H2'	1:A:68:G:C8	2.31	0.65
1:A:1126:U:H5	1:A:1127:G:C4	2.14	0.65
1:A:243:A:H4'	1:A:244:U:O5'	1.97	0.65
2:B:178:ARG:NH1	2:B:196:LEU:O	2.29	0.65
5:E:152:ARG:NH2	8:H:107:LEU:O	2.28	0.65
11:K:21:ILE:HB	11:K:84:VAL:HG12	1.78	0.65
20:T:97:ALA:O	20:T:99:LEU:N	2.30	0.65
1:A:1286:A:H5''	21:U:26:LYS:HD2	1.78	0.65
3:C:122:GLU:OE1	3:C:126:ARG:NH2	2.29	0.64
15:O:26:GLU:OE2	15:O:77:ARG:NH1	2.31	0.64
1:A:1226:C:O2'	13:M:111:LYS:NZ	2.30	0.64
1:A:664:G:N2	1:A:741:G:H1	1.93	0.64
1:A:963:G:H1	1:A:972:C:H42	1.45	0.64
1:A:1095:U:P	1:A:1108:G:H1	2.21	0.64
3:C:11:ARG:O	3:C:13:GLY:N	2.30	0.64
3:C:19:GLU:O	3:C:40:ARG:NH2	2.30	0.64
8:H:7:ALA:HB2	8:H:85:ARG:HD3	1.80	0.64
1:A:701:C:O2'	1:A:702:A:OP2	2.14	0.63
2:B:187:LEU:HA	2:B:201:ILE:HB	1.79	0.63
2:B:79:ASP:HA	2:B:82:ARG:HB2	1.80	0.63
5:E:98:THR:HB	5:E:117:ASP:HB3	1.79	0.63
13:M:91:ARG:HB2	13:M:98:VAL:HG13	1.80	0.63
1:A:427:U:OP1	4:D:13:ARG:NH2	2.31	0.63
5:E:147:ASP:O	5:E:151:LEU:HG	1.97	0.63
1:A:299:G:H2'	1:A:300:A:C8	2.34	0.63
13:M:23:TYR:HB3	13:M:67:GLU:HA	1.81	0.63
1:A:975:A:H5'	1:A:975:A:H8	1.64	0.63
10:J:32:ALA:HB3	10:J:76:ASN:HB2	1.79	0.62
9:I:24:GLY:N	9:I:60:ASP:OD1	2.29	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1125:U:OP2	1:A:1145:C:N4	2.33	0.62
2:B:92:TYR:CE1	2:B:151:GLY:HA3	2.34	0.62
1:A:62:U:O2'	1:A:379:C:O2	2.14	0.62
2:B:212:GLN:NE2	2:B:235:SER:HB2	2.15	0.62
1:A:1298:C:O2'	1:A:1299:A:OP2	2.12	0.62
2:B:12:GLU:O	2:B:16:HIS:ND1	2.22	0.62
10:J:5:ARG:HH21	10:J:99:LYS:HD2	1.63	0.62
19:S:13:ASP:OD1	19:S:13:ASP:N	2.32	0.62
2:B:54:THR:HG21	2:B:201:ILE:HD11	1.82	0.62
1:A:1130:A:O2'	9:I:3:GLN:NE2	2.28	0.62
1:A:976:G:H5''	1:A:1358:U:O2'	1.98	0.62
7:G:111:ARG:NH1	7:G:113:GLU:OE2	2.32	0.62
1:A:1023:G:H3'	1:A:1024:G:H5''	1.82	0.62
4:D:111:ALA:HB2	4:D:120:LEU:HD12	1.82	0.62
5:E:42:GLY:HA3	5:E:66:MET:HG2	1.82	0.62
9:I:29:ASN:OD1	9:I:65:VAL:N	2.29	0.62
1:A:677:U:H3	1:A:713:G:H22	1.47	0.61
20:T:100:ILE:HG13	20:T:102:GLY:N	2.15	0.61
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.61
1:A:1347:G:HO2'	1:A:1373:G:H1	1.46	0.61
1:A:250:A:H4'	1:A:251:G:O5'	2.00	0.61
1:A:973:G:H3'	1:A:974:A:H5''	1.81	0.61
2:B:67:THR:HG21	2:B:155:LEU:HG	1.81	0.61
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.33	0.61
15:O:87:ILE:HG22	15:O:88:ARG:H	1.64	0.61
1:A:686:U:O4	1:A:703:G:H1'	1.99	0.61
1:A:64:G:N2	1:A:68:G:O6	2.34	0.60
1:A:438:G:H4'	4:D:123:HIS:CD2	2.35	0.60
17:Q:11:VAL:HG12	17:Q:85:VAL:HG13	1.83	0.60
1:A:328:C:H4'	1:A:329:A:H5'	1.83	0.60
1:A:991:U:O2'	1:A:992:U:O5'	2.18	0.60
1:A:1280:A:O2'	1:A:1281:U:OP1	2.20	0.60
1:A:1446:A:O2'	1:A:1447:G:O5'	2.20	0.60
1:A:828:A:H2'	1:A:829:G:O4'	2.02	0.60
1:A:963:G:H21	10:J:55:LYS:HE2	1.67	0.60
1:A:1435:G:H2'	1:A:1436:U:C6	2.37	0.60
2:B:235:SER:O	2:B:237:ALA:N	2.35	0.60
1:A:963:G:H21	10:J:55:LYS:CE	2.14	0.60
1:A:1262:C:H2'	1:A:1263:C:C6	2.37	0.59
1:A:690:G:H22	11:K:55:LYS:NZ	2.00	0.59
13:M:3:ARG:HA	13:M:9:ILE:HG21	1.83	0.59
6:F:61:LEU:HB3	6:F:63:TYR:HE2	1.66	0.59

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:V:2:C:H2'	22:V:3:G:H5'	1.83	0.59
1:A:347:G:O2'	1:A:348:G:OP2	2.19	0.59
1:A:411:A:C4	1:A:413:G:H1'	2.37	0.59
2:B:92:TYR:HE1	2:B:151:GLY:HA3	1.65	0.59
1:A:271:C:H2'	1:A:272:C:H6	1.67	0.59
1:A:973:G:OP1	10:J:57:LYS:NZ	2.34	0.59
1:A:166:G:H2'	1:A:167:G:H8	1.67	0.59
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.38	0.59
1:A:1062:U:H2'	1:A:1063:C:C6	2.38	0.59
4:D:9:CYS:SG	4:D:22:LYS:HE2	2.39	0.59
10:J:76:ASN:O	10:J:78:ASN:ND2	2.36	0.59
14:N:23:ARG:HD2	14:N:28:GLY:O	2.03	0.59
20:T:10:LEU:HG	20:T:12:ALA:H	1.67	0.59
1:A:243:A:H4'	1:A:244:U:H3'	1.84	0.58
1:A:7:G:H5'	1:A:298:A:O4'	2.03	0.58
12:L:38:THR:HG23	12:L:57:LYS:HB3	1.84	0.58
1:A:1175:G:H2'	1:A:1176:A:C8	2.38	0.58
3:C:14:ILE:HG12	3:C:15:THR:H	1.67	0.58
13:M:13:LYS:HA	13:M:44:ARG:HD2	1.83	0.58
1:A:1291:G:OP1	7:G:37:ASN:ND2	2.36	0.58
20:T:56:MET:HG3	20:T:88:VAL:HG21	1.85	0.58
20:T:63:ILE:HG22	20:T:77:ALA:HB1	1.86	0.58
2:B:15:VAL:H	2:B:16:HIS:CE1	2.22	0.58
2:B:72:GLY:HA2	2:B:165:VAL:HG22	1.86	0.58
2:B:96:ARG:H	2:B:96:ARG:HD2	1.67	0.58
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.85	0.58
6:F:36:ARG:NH1	6:F:38:GLU:OE2	2.37	0.58
8:H:39:LEU:HB3	8:H:45:ILE:HG12	1.86	0.58
1:A:1065:U:O2'	1:A:1066:C:OP2	2.16	0.58
1:A:680:C:H2'	1:A:681:C:H6	1.69	0.58
3:C:95:THR:HG22	3:C:97:LYS:HG3	1.84	0.58
2:B:93:VAL:HG11	2:B:97:TRP:HD1	1.68	0.58
19:S:80:TYR:O	19:S:82:GLY:N	2.36	0.58
5:E:91:LEU:HD12	5:E:120:THR:HG22	1.85	0.58
7:G:89:MET:HE1	7:G:156:TRP:H	1.69	0.57
1:A:522:C:H41	12:L:53:ARG:HH22	1.50	0.57
4:D:9:CYS:HB3	4:D:32:ALA:HB2	1.86	0.57
1:A:539:A:OP1	12:L:114:LYS:NZ	2.22	0.57
1:A:753:A:H4'	1:A:754:C:O5'	2.03	0.57
17:Q:55:ASP:HA	17:Q:79:SER:HA	1.85	0.57
3:C:70:VAL:HG21	3:C:76:VAL:HG11	1.85	0.57
11:K:21:ILE:HG13	11:K:30:VAL:HG12	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:673:G:H2'	1:A:674:G:C8	2.39	0.57
1:A:1453:G:H2'	20:T:39:LYS:HE2	1.84	0.57
1:A:701:C:H1'	1:A:703:G:C6	2.39	0.57
2:B:96:ARG:HD3	2:B:148:TYR:HE1	1.70	0.57
4:D:154:ASN:OD1	4:D:154:ASN:N	2.37	0.57
1:A:1016:A:H2'	1:A:1017:G:O4'	2.04	0.57
16:P:20:VAL:HG23	16:P:35:LYS:HA	1.86	0.57
19:S:32:LYS:HA	19:S:50:ALA:HB3	1.86	0.57
22:V:51:C:H2'	22:V:52:G:O4'	2.05	0.57
1:A:96:G:H2'	1:A:97:U:O4'	2.03	0.57
1:A:1443:G:H5''	1:A:1446:A:H2	1.69	0.57
9:I:15:ALA:HB2	9:I:65:VAL:HG23	1.86	0.57
1:A:1347:G:C8	9:I:107:ARG:HB3	2.40	0.56
1:A:128:G:O2'	17:Q:3:LYS:NZ	2.33	0.56
10:J:50:ILE:HD11	10:J:57:LYS:HD3	1.85	0.56
1:A:27:G:H4'	4:D:209:ARG:HG3	1.86	0.56
1:A:1232:U:OP1	9:I:124:GLN:NE2	2.38	0.56
22:V:68:C:H2'	22:V:69:C:C6	2.41	0.56
2:B:178:ARG:HG3	8:H:72:PRO:HA	1.86	0.56
1:A:343:U:HO2'	1:A:344:A:H8	1.53	0.56
1:A:1392:G:H21	1:A:1502:A:H8	1.52	0.56
3:C:174:PRO:HD2	3:C:182:ILE:HD11	1.88	0.56
7:G:54:THR:O	7:G:56:GLN:N	2.39	0.56
16:P:20:VAL:HG21	16:P:32:TYR:CD1	2.40	0.56
1:A:1368:G:OP1	9:I:111:ARG:NH2	2.34	0.56
1:A:437:U:H2'	1:A:438:G:O4'	2.04	0.56
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.86	0.56
2:B:21:ARG:O	2:B:23:ARG:HD3	2.05	0.56
1:A:191:G:O2'	20:T:101:GLY:O	2.23	0.56
22:V:61:C:H2'	22:V:62:C:H6	1.71	0.56
1:A:1060:C:C4	3:C:2:GLY:HA2	2.41	0.56
22:V:3:G:O2'	22:V:4:G:H8	1.88	0.56
1:A:890:G:O2'	1:A:906:G:O6	2.22	0.56
1:A:522:C:H41	12:L:53:ARG:NH2	2.04	0.56
3:C:130:VAL:O	3:C:134:ILE:HG12	2.06	0.56
3:C:9:GLY:HA2	3:C:12:LEU:HD23	1.88	0.56
4:D:122:ARG:NH1	4:D:134:ASP:O	2.39	0.56
4:D:11:LEU:HD13	4:D:66:ARG:HG2	1.87	0.56
1:A:266:G:H5''	1:A:267:C:H5	1.70	0.55
1:A:674:G:H2'	1:A:675:A:C8	2.41	0.55
1:A:953:G:H5'	1:A:965:A:H61	1.71	0.55
1:A:1450:U:O2'	1:A:1451:A:N7	2.35	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:188:U:H2'	1:A:189:U:H5''	1.88	0.55
10:J:34:VAL:HG22	10:J:74:ILE:HG22	1.89	0.55
2:B:158:LEU:HD13	2:B:182:ILE:HD11	1.89	0.55
5:E:37:ARG:HA	5:E:114:GLY:N	2.21	0.55
5:E:50:GLU:HB3	5:E:53:LEU:HD13	1.88	0.55
15:O:18:PHE:CE1	15:O:21:ASP:HB2	2.41	0.55
6:F:97:PHE:HD2	18:R:31:LEU:HD21	1.70	0.55
1:A:404:U:H2'	1:A:405:U:H6	1.71	0.55
20:T:49:ALA:HB1	20:T:99:LEU:HB2	1.89	0.55
1:A:200:G:H1	1:A:217:C:H42	1.54	0.55
1:A:619:U:N3	4:D:135:LEU:HD23	2.21	0.55
2:B:82:ARG:NH1	2:B:86:GLU:OE2	2.40	0.55
24:Y:30:C:H2'	24:Y:31:G:H8	1.71	0.55
1:A:1298:C:H4'	1:A:1299:A:C4	2.41	0.55
1:A:266:G:O2'	1:A:267:C:OP2	2.23	0.55
8:H:86:ILE:HG22	8:H:93:VAL:HG21	1.89	0.55
11:K:34:ASP:OD1	11:K:38:ASN:N	2.39	0.55
1:A:606:G:N2	1:A:631:G:H8	2.04	0.55
9:I:16:ARG:HB2	9:I:64:THR:HB	1.89	0.55
1:A:1356:G:H2'	1:A:1357:A:C8	2.42	0.55
1:A:339:C:H2'	1:A:340:U:H6	1.71	0.55
1:A:1223:C:P	19:S:78:ARG:HH12	2.30	0.55
1:A:1129:C:H5'	1:A:1130:A:OP1	2.08	0.54
4:D:92:VAL:O	4:D:96:LEU:HD22	2.07	0.54
8:H:54:ASP:OD1	8:H:54:ASP:N	2.39	0.54
12:L:70:ILE:HG12	12:L:100:ILE:HD12	1.88	0.54
1:A:1453:G:H8	20:T:39:LYS:HE2	1.72	0.54
3:C:150:LYS:HE2	3:C:152:ILE:HD11	1.88	0.54
10:J:33:GLN:HB2	10:J:75:ILE:HD11	1.89	0.54
1:A:1455:G:H5''	20:T:31:SER:HB2	1.88	0.54
5:E:100:VAL:HG22	5:E:118:ILE:HG22	1.90	0.54
1:A:1525:G:P	11:K:120:ARG:HH22	2.29	0.54
13:M:22:ILE:HD12	13:M:25:ILE:HD12	1.89	0.54
18:R:31:LEU:HD23	18:R:31:LEU:H	1.73	0.54
5:E:12:LEU:HD21	5:E:14:ARG:HD3	1.89	0.54
1:A:339:C:H2'	1:A:340:U:C6	2.42	0.54
1:A:598:U:H4'	8:H:94:TYR:CD2	2.43	0.54
1:A:807:A:H2'	1:A:808:C:C6	2.42	0.54
12:L:115:LYS:O	12:L:117:ARG:N	2.35	0.54
1:A:1008:C:H42	1:A:1021:G:H1	1.55	0.54
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.90	0.54
7:G:20:ASP:HB3	7:G:23:VAL:HG23	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:49:ILE:O	7:G:53:LYS:HB3	2.08	0.54
10:J:9:ARG:HB2	10:J:95:GLU:HB3	1.88	0.54
1:A:1189:C:H5''	1:A:1190:G:OP2	2.08	0.54
1:A:35:G:O2'	12:L:118:SER:O	2.20	0.54
22:V:23:C:H2'	22:V:24:U:C6	2.43	0.54
1:A:1510:U:H2'	1:A:1511:G:C8	2.42	0.54
3:C:15:THR:HG23	3:C:181:ASN:HD22	1.73	0.54
1:A:707:C:OP1	11:K:85:ARG:NH1	2.41	0.54
13:M:3:ARG:HA	13:M:9:ILE:CG2	2.37	0.54
16:P:43:LYS:HG2	16:P:48:TRP:CE3	2.42	0.54
10:J:32:ALA:H	10:J:78:ASN:HD21	1.55	0.54
1:A:1234:C:O2'	1:A:1235:U:H5'	2.08	0.53
2:B:162:ILE:O	2:B:185:ILE:HG12	2.08	0.53
2:B:82:ARG:HA	2:B:92:TYR:CE2	2.43	0.53
3:C:14:ILE:O	3:C:16:ARG:N	2.35	0.53
1:A:1314:C:N4	19:S:2:PRO:O	2.40	0.53
1:A:1305:G:O2'	1:A:1306:A:C8	2.61	0.53
1:A:346:G:H1'	1:A:347:G:H5'	1.90	0.53
1:A:691:G:H2'	1:A:692:U:C6	2.44	0.53
10:J:4:ILE:HG12	10:J:100:THR:HG22	1.89	0.53
1:A:1301:U:H3'	1:A:1302:U:H5'	1.91	0.53
1:A:1399:C:C2	1:A:1502:A:N6	2.77	0.53
1:A:64:G:H5'	1:A:65:U:H5'	1.90	0.53
17:Q:4:LYS:HE3	17:Q:6:LEU:HD21	1.90	0.53
19:S:36:ARG:NH1	19:S:52:TYR:O	2.42	0.53
1:A:881:G:P	12:L:12:ARG:HH22	2.32	0.53
1:A:949:A:N7	13:M:106:ASN:ND2	2.56	0.53
2:B:60:ASP:O	2:B:64:ARG:HG2	2.09	0.53
1:A:933:G:O6	7:G:3:ARG:NH2	2.41	0.53
9:I:111:ARG:NE	9:I:112:LYS:O	2.38	0.53
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.90	0.53
1:A:130:A:N6	1:A:233:C:O2	2.42	0.53
1:A:1002:G:H2'	1:A:1003:G:C8	2.40	0.53
1:A:966:G:O2'	9:I:127:LYS:O	2.27	0.53
8:H:121:ASP:HB2	8:H:125:ARG:NH2	2.24	0.53
20:T:95:ALA:O	20:T:97:ALA:N	2.42	0.53
1:A:1277:C:O2'	1:A:1279:A:H1'	2.09	0.53
1:A:1318:A:H4'	19:S:11:VAL:CG1	2.39	0.53
1:A:633:G:H5'	1:A:634:C:OP2	2.08	0.53
18:R:25:THR:HB	18:R:26:LEU:HD23	1.91	0.53
19:S:31:ILE:HG23	19:S:49:ILE:HA	1.91	0.53
1:A:1191:A:H5''	3:C:4:LYS:HZ2	1.74	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:818:G:O2'	1:A:819:A:H5'	2.09	0.53
12:L:7:ILE:HD13	12:L:10:LEU:HD12	1.90	0.53
1:A:1014:A:H4'	19:S:14:HIS:CD2	2.43	0.53
1:A:1221:G:O3'	19:S:77:THR:HG21	2.08	0.52
2:B:44:LEU:H	2:B:44:LEU:HD12	1.74	0.52
7:G:15:ASP:HB3	7:G:19:GLY:H	1.74	0.52
20:T:47:GLY:O	20:T:49:ALA:N	2.41	0.52
1:A:1129:C:O2'	1:A:1131:G:N7	2.41	0.52
1:A:1321:C:H5''	1:A:1322:C:C5'	2.39	0.52
1:A:524:G:H2'	1:A:525:C:C6	2.45	0.52
3:C:40:ARG:O	3:C:44:GLU:HB2	2.09	0.52
1:A:1299:A:H2'	1:A:1301:U:H1'	1.91	0.52
1:A:404:U:H2'	1:A:405:U:C6	2.44	0.52
1:A:439:A:OP2	1:A:493:G:N1	2.39	0.52
16:P:8:ARG:O	16:P:9:PHE:HD2	1.93	0.52
20:T:53:LEU:O	20:T:57:ARG:NH1	2.42	0.52
3:C:189:ALA:HB3	3:C:196:LEU:HB2	1.91	0.52
1:A:1123:A:H4'	10:J:36:GLY:HA3	1.92	0.52
10:J:78:ASN:O	10:J:81:THR:OG1	2.25	0.52
14:N:43:CYS:HA	14:N:46:GLU:HG3	1.92	0.52
1:A:1005:A:HO2'	1:A:1037:C:HO2'	1.55	0.52
2:B:35:GLU:O	2:B:36:ARG:HD3	2.10	0.52
19:S:19:VAL:HG11	19:S:44:MET:HG2	1.91	0.52
1:A:1034:G:H2'	1:A:1035:A:H8	1.75	0.52
1:A:561:U:HO2'	1:A:562:C:P	2.30	0.52
2:B:29:ALA:O	2:B:32:ILE:HG22	2.10	0.52
4:D:13:ARG:HD2	4:D:38:TYR:O	2.10	0.52
7:G:78:ARG:HG3	7:G:79:ARG:N	2.25	0.52
1:A:555:C:OP2	12:L:20:LYS:NZ	2.42	0.52
1:A:991:U:HO2'	1:A:992:U:P	2.32	0.52
4:D:108:LEU:HB3	4:D:110:PHE:CE1	2.45	0.52
1:A:719:C:O2'	18:R:50:ILE:O	2.16	0.52
2:B:170:GLU:O	2:B:174:VAL:HG23	2.10	0.51
3:C:47:LEU:HD11	3:C:76:VAL:HB	1.91	0.51
12:L:77:LEU:HD21	12:L:107:ALA:HA	1.92	0.51
20:T:26:ASN:HB2	20:T:71:THR:HG23	1.92	0.51
1:A:143:A:H2	1:A:220:G:H1	1.57	0.51
1:A:148:G:H2'	1:A:149:A:H8	1.75	0.51
1:A:321:A:H62	1:A:328:C:H1'	1.74	0.51
1:A:405:U:OP2	4:D:3:ARG:NH2	2.44	0.51
1:A:1327:C:OP2	21:U:12:LYS:NZ	2.35	0.51
1:A:165:C:H2'	1:A:166:G:H8	1.74	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
5:E:102:ALA:HB1	5:E:106:PRO:HG2	1.93	0.51
5:E:13:ILE:HD11	5:E:55:VAL:HG22	1.91	0.51
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.76	0.51
9:I:70:LYS:O	9:I:74:ILE:HG13	2.10	0.51
13:M:14:ARG:N	13:M:44:ARG:HD3	2.21	0.51
1:A:1318:A:H4'	19:S:11:VAL:HG11	1.93	0.51
9:I:11:LYS:H	9:I:104:ARG:HH21	1.58	0.51
20:T:89:ARG:HH21	20:T:104:LEU:HD11	1.76	0.51
1:A:1424:C:H2'	1:A:1425:U:O4'	2.11	0.51
2:B:21:ARG:HB2	2:B:39:ILE:HA	1.91	0.51
7:G:155:ARG:NH2	7:G:155:ARG:O	2.43	0.51
17:Q:100:LYS:O	17:Q:101:ARG:NE	2.42	0.51
1:A:266:G:H5'	1:A:268:C:H41	1.75	0.51
1:A:1106:G:H5''	3:C:172:ARG:HG2	1.92	0.51
19:S:15:LEU:O	19:S:19:VAL:N	2.36	0.51
20:T:10:LEU:O	20:T:13:LEU:HG	2.11	0.51
1:A:1200:C:H4'	1:A:1201:A:H5'	1.93	0.51
1:A:486:U:H2'	1:A:487:A:C8	2.45	0.51
1:A:757:U:H2'	1:A:758:G:O4'	2.11	0.51
4:D:78:LEU:HD22	4:D:96:LEU:HB3	1.92	0.51
6:F:97:PHE:CD2	18:R:31:LEU:HD21	2.46	0.51
1:A:1228:C:OP1	13:M:115:LYS:HE3	2.11	0.51
1:A:201:C:H42	1:A:216:G:H1	1.59	0.51
15:O:33:THR:HG21	15:O:85:LEU:HD22	1.93	0.51
19:S:26:GLY:O	19:S:28:LYS:N	2.43	0.51
1:A:1391:U:H2'	1:A:1392:G:C8	2.46	0.51
1:A:201:C:N4	1:A:209:U:O2	2.43	0.51
1:A:538:G:H5''	12:L:114:LYS:HB2	1.93	0.51
1:A:953:G:H2'	1:A:954:G:O4'	2.10	0.51
1:A:412:A:H4'	1:A:413:G:O5'	2.11	0.50
3:C:138:VAL:HG22	3:C:151:VAL:HG23	1.93	0.50
1:A:1060:C:C5	3:C:2:GLY:HA2	2.46	0.50
11:K:41:THR:HG21	11:K:71:LYS:HB3	1.93	0.50
1:A:93:U:H2'	1:A:95:G:O4'	2.11	0.50
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.93	0.50
6:F:86:ARG:O	6:F:87:ARG:HG2	2.11	0.50
1:A:1346:A:H1'	1:A:1348:U:C6	2.46	0.50
1:A:89:U:O2'	1:A:90:C:OP1	2.28	0.50
2:B:9:GLU:HB3	2:B:48:MET:SD	2.50	0.50
3:C:54:ARG:HD3	3:C:56:ASP:OD1	2.10	0.50
1:A:1347:G:O2'	1:A:1348:U:OP2	2.25	0.50
1:A:568:G:O2'	1:A:574:A:N1	2.38	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:G:H2'	1:A:58:C:C6	2.46	0.50
1:A:686:U:H1'	11:K:42:TRP:HE1	1.77	0.50
1:A:67:C:H2'	1:A:68:G:H8	1.74	0.50
2:B:114:ARG:O	2:B:117:GLU:HB2	2.10	0.50
2:B:189:ASP:HB3	2:B:203:GLY:O	2.12	0.50
19:S:4:SER:O	19:S:5:LEU:HD13	2.11	0.50
19:S:40:ILE:HG23	19:S:67:VAL:O	2.12	0.50
1:A:987:G:H1	1:A:1218:C:H42	1.60	0.50
1:A:1513:A:H2'	1:A:1514:C:C6	2.47	0.50
2:B:111:ARG:HH21	2:B:114:ARG:HG2	1.76	0.50
2:B:21:ARG:O	2:B:23:ARG:N	2.44	0.50
4:D:108:LEU:HD21	4:D:183:GLY:HA3	1.93	0.50
1:A:130:A:C8	17:Q:63:ARG:HG3	2.46	0.50
1:A:1321:C:H5''	1:A:1322:C:H5''	1.93	0.50
1:A:1347:G:H22	1:A:1373:G:H2'	1.76	0.50
1:A:353:A:H5'	1:A:353:A:H8	1.77	0.50
22:V:68:C:H2'	22:V:69:C:H6	1.76	0.50
1:A:1525:G:OP1	11:K:120:ARG:NH2	2.45	0.50
15:O:67:LEU:HB3	15:O:78:TYR:HE1	1.76	0.50
1:A:1015:A:H2'	1:A:1016:A:C8	2.46	0.50
2:B:32:ILE:HD11	2:B:40:HIS:HB3	1.94	0.50
4:D:112:VAL:HG12	4:D:116:GLN:OE1	2.12	0.50
5:E:76:ILE:HG13	5:E:93:PRO:HB3	1.94	0.50
11:K:86:GLY:O	11:K:91:ARG:HD3	2.11	0.50
13:M:49:THR:HB	13:M:52:GLU:H	1.77	0.50
1:A:371:G:H2'	1:A:372:C:O4'	2.12	0.50
2:B:162:ILE:HD11	2:B:184:VAL:HG22	1.94	0.50
1:A:973:G:C4	10:J:55:LYS:HE2	2.47	0.50
1:A:1314:C:OP1	19:S:6:LYS:HE3	2.12	0.49
1:A:17:U:H2'	1:A:18:C:C6	2.47	0.49
20:T:64:ASP:HA	20:T:67:ALA:HB3	1.93	0.49
6:F:97:PHE:HB2	18:R:32:ARG:CZ	2.41	0.49
1:A:523:A:H61	12:L:92:ASP:HB2	1.77	0.49
14:N:23:ARG:NH1	14:N:30:ALA:HB2	2.27	0.49
16:P:28:ARG:NH1	16:P:29:ASP:OD1	2.45	0.49
1:A:452:A:H4'	16:P:72:ARG:NH2	2.28	0.49
1:A:160:A:H1'	1:A:344:A:C5	2.47	0.49
1:A:620:C:H2'	1:A:621:A:O4'	2.13	0.49
9:I:40:LEU:C	9:I:42:ARG:H	2.15	0.49
11:K:82:VAL:HB	11:K:108:ILE:HG12	1.94	0.49
12:L:71:PRO:O	12:L:102:ARG:HD3	2.12	0.49
13:M:20:THR:C	13:M:22:ILE:H	2.15	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
19:S:41:VAL:HB	19:S:42:PRO:CA	2.42	0.49
1:A:108:G:H5'	1:A:109:A:H5'	1.94	0.49
1:A:165:C:H2'	1:A:166:G:C8	2.47	0.49
1:A:426:G:OP1	4:D:38:TYR:OH	2.24	0.49
10:J:49:VAL:HG22	14:N:41:ARG:HB2	1.94	0.49
13:M:81:LEU:HD13	13:M:88:ARG:HD2	1.94	0.49
1:A:163:C:H2'	1:A:164:U:C6	2.48	0.49
22:V:25:C:H2'	22:V:26:G:O4'	2.12	0.49
1:A:1075:C:OP1	2:B:179:LYS:HE2	2.13	0.49
1:A:520:A:N1	1:A:536:C:H1'	2.28	0.49
2:B:24:TRP:CZ3	2:B:26:PRO:HA	2.48	0.49
12:L:62:SER:HB2	12:L:64:TYR:HD1	1.76	0.49
24:Y:30:C:H2'	24:Y:31:G:C8	2.48	0.49
1:A:833:U:H3	1:A:853:G:H1	1.61	0.49
3:C:148:GLY:HA3	3:C:172:ARG:O	2.12	0.49
11:K:59:TYR:CZ	11:K:63:LEU:HD11	2.47	0.49
13:M:14:ARG:HG2	13:M:17:VAL:HG23	1.95	0.49
20:T:89:ARG:NH2	20:T:104:LEU:HD11	2.27	0.49
1:A:632:A:C8	1:A:633:G:C8	3.00	0.49
1:A:762:C:H2'	1:A:763:G:H8	1.78	0.49
2:B:47:THR:HA	2:B:202:PRO:HG2	1.95	0.49
5:E:10:MET:SD	5:E:13:ILE:HD13	2.53	0.49
10:J:35:SER:OG	10:J:73:ASP:HB2	2.13	0.49
1:A:686:U:O2'	11:K:42:TRP:NE1	2.45	0.49
6:F:19:LEU:HD21	6:F:59:TYR:CE2	2.47	0.49
1:A:690:G:H2'	1:A:691:G:O4'	2.12	0.48
1:A:883:C:C2'	1:A:884:U:H5'	2.43	0.48
3:C:134:ILE:HG23	3:C:151:VAL:HB	1.94	0.48
3:C:79:ARG:HH12	3:C:82:GLU:HG3	1.77	0.48
5:E:31:LEU:HD23	5:E:45:PHE:HD1	1.78	0.48
6:F:35:ALA:HA	6:F:67:MET:HB3	1.94	0.48
1:A:1135:U:H4'	1:A:1136:U:H5	1.77	0.48
1:A:413:G:HO2'	1:A:414:A:P	2.35	0.48
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.95	0.48
16:P:26:ARG:HH21	16:P:31:LYS:HB3	1.77	0.48
24:Y:29:U:H2'	24:Y:30:C:C6	2.48	0.48
1:A:1128:C:N3	1:A:1144:G:N2	2.37	0.48
1:A:1486:G:H2'	1:A:1487:G:O4'	2.14	0.48
1:A:1499:A:H1'	1:A:1520:G:H5'	1.94	0.48
1:A:406:G:H5'	4:D:5:ILE:HD13	1.95	0.48
3:C:7:PRO:O	3:C:11:ARG:HG2	2.13	0.48
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.94	0.48

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1256:A:OP2	3:C:26:LYS:NZ	2.34	0.48
2:B:101:MET:HA	2:B:108:ILE:HG13	1.95	0.48
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.95	0.48
6:F:36:ARG:CZ	6:F:38:GLU:HG2	2.44	0.48
1:A:1319:A:H2'	1:A:1323:G:N7	2.29	0.48
1:A:56:U:H2'	1:A:57:G:C8	2.48	0.48
1:A:868:C:H2'	1:A:869:G:O4'	2.12	0.48
2:B:73:THR:OG1	2:B:170:GLU:OE2	2.23	0.48
11:K:18:ARG:NH2	11:K:35:PRO:O	2.45	0.48
20:T:93:GLU:OE1	20:T:94:ALA:N	2.46	0.48
1:A:1347:G:N2	1:A:1373:G:H2'	2.28	0.48
1:A:701:C:HO2'	1:A:702:A:P	2.35	0.48
2:B:204:ASN:ND2	2:B:206:ASP:H	2.11	0.48
9:I:9:ARG:HB2	9:I:14:VAL:HA	1.96	0.48
15:O:70:LEU:HD11	15:O:77:ARG:HG3	1.96	0.48
24:Y:29:U:H2'	24:Y:30:C:H6	1.78	0.48
1:A:1122:U:O4	1:A:1123:A:N6	2.47	0.48
1:A:403:C:OP1	4:D:137:SER:OG	2.32	0.48
1:A:95:G:C6	1:A:96:G:C6	3.02	0.48
6:F:10:LEU:HD22	6:F:61:LEU:HD11	1.94	0.48
19:S:39:THR:HG22	19:S:40:ILE:H	1.78	0.48
1:A:1094:G:O2'	1:A:1095:U:OP2	2.22	0.48
1:A:892:A:O2'	1:A:1415:G:H4'	2.13	0.48
1:A:688:G:H2'	1:A:689:C:H6	1.79	0.48
1:A:692:U:H5'	1:A:797:C:H5'	1.95	0.48
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.94	0.48
9:I:114:TYR:CD2	9:I:114:TYR:N	2.81	0.48
1:A:1151:A:O2'	1:A:1152:A:O5'	2.23	0.48
1:A:407:G:H2'	1:A:408:A:H8	1.77	0.48
1:A:564:C:C6	17:Q:31:LEU:HD11	2.49	0.48
1:A:110:C:O2'	16:P:25:ARG:O	2.22	0.48
16:P:22:THR:HA	16:P:33:ILE:HG12	1.96	0.48
1:A:33:A:H2'	1:A:34:C:C6	2.49	0.48
1:A:407:G:H2'	1:A:408:A:C8	2.48	0.48
1:A:659:U:H2'	1:A:660:G:H8	1.79	0.48
3:C:70:VAL:HG12	3:C:72:LYS:H	1.79	0.48
5:E:6:PHE:CE2	5:E:36:ASP:HB3	2.48	0.48
8:H:49:GLU:HG2	8:H:62:TYR:HE2	1.78	0.48
1:A:1149:C:OP1	9:I:9:ARG:NH2	2.41	0.47
1:A:1241:G:H2'	1:A:1242:C:C6	2.48	0.47
1:A:1319:A:H5'	1:A:1320:C:OP1	2.14	0.47
1:A:28:G:O2'	1:A:296:U:OP1	2.30	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:38:ILE:HD11	10:J:71:LEU:HD23	1.96	0.47
1:A:31:G:O2'	1:A:48:C:N4	2.46	0.47
2:B:84:GLU:OE1	2:B:87:ARG:NH2	2.43	0.47
18:R:36:ASN:ND2	18:R:36:ASN:O	2.41	0.47
1:A:1412:C:H2'	1:A:1413:A:C8	2.49	0.47
1:A:179:A:H2'	1:A:180:U:C6	2.50	0.47
1:A:109:A:H2'	1:A:326:G:N2	2.29	0.47
3:C:34:LEU:HD23	3:C:38:ARG:HG3	1.95	0.47
3:C:79:ARG:NH1	3:C:82:GLU:HG3	2.29	0.47
4:D:15:GLU:HG2	4:D:63:LYS:HB2	1.97	0.47
1:A:1298:C:C4	7:G:114:ARG:HD2	2.50	0.47
9:I:121:ARG:NH1	9:I:122:ALA:O	2.47	0.47
9:I:126:SER:O	9:I:128:ARG:N	2.43	0.47
18:R:66:LEU:O	18:R:70:ILE:HG13	2.14	0.47
1:A:1004:A:H1'	1:A:1036:G:N2	2.30	0.47
3:C:22:TRP:CD1	3:C:59:ARG:HD2	2.49	0.47
3:C:81:GLY:O	3:C:85:ARG:HB2	2.14	0.47
12:L:24:VAL:HG12	12:L:24:VAL:O	2.14	0.47
12:L:7:ILE:HA	12:L:7:ILE:HD13	1.82	0.47
20:T:98:PRO:O	20:T:100:ILE:N	2.46	0.47
5:E:8:GLU:OE2	5:E:63:ARG:NH2	2.46	0.47
6:F:69:GLU:O	6:F:72:VAL:HG12	2.14	0.47
9:I:4:TYR:CZ	9:I:88:TYR:HB2	2.49	0.47
12:L:27:LEU:O	12:L:29:GLY:N	2.46	0.47
15:O:66:LEU:HA	15:O:66:LEU:HD12	1.66	0.47
20:T:35:THR:O	20:T:39:LYS:HG3	2.14	0.47
1:A:1000:A:H2'	1:A:1001:G:H8	1.79	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.47
1:A:429:U:H1'	1:A:430:A:H5''	1.97	0.47
1:A:1070:U:H2'	1:A:1071:C:H6	1.79	0.47
1:A:328:C:H4'	1:A:329:A:C5'	2.45	0.47
2:B:93:VAL:HG11	2:B:97:TRP:CD1	2.50	0.47
9:I:114:TYR:HD1	10:J:60:ARG:HB2	1.79	0.47
11:K:48:ILE:HG13	11:K:63:LEU:HB2	1.97	0.47
1:A:35:G:N3	12:L:118:SER:OG	2.46	0.47
10:J:47:PHE:HB3	14:N:34:TYR:CE2	2.50	0.47
1:A:1192:C:OP2	3:C:4:LYS:NZ	2.41	0.47
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.15	0.47
1:A:1315:U:H2'	1:A:1316:G:O4'	2.14	0.47
1:A:1348:U:H3	1:A:1374:A:H2	1.57	0.47
2:B:18:GLY:H	2:B:42:ILE:HG22	1.80	0.47
5:E:89:ILE:HG12	5:E:91:LEU:HD13	1.97	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1118:C:P	9:I:104:ARG:HH11	2.37	0.47
1:A:1057:G:H2'	1:A:1058:G:O4'	2.15	0.47
1:A:1152:A:H2'	1:A:1153:C:H6	1.79	0.47
1:A:1225:A:N3	1:A:1225:A:H2'	2.29	0.47
1:A:1227:A:OP2	13:M:111:LYS:HE3	2.15	0.47
1:A:1366:C:H2'	1:A:1367:C:H6	1.80	0.47
1:A:767:A:H2'	1:A:768:A:O4'	2.15	0.47
1:A:791:G:C6	1:A:792:A:C2	3.03	0.47
1:A:910:C:P	12:L:97:ARG:HH22	2.38	0.47
1:A:1126:U:H1'	1:A:1280:A:C5	2.50	0.46
1:A:244:U:H4'	1:A:245:C:O5'	2.15	0.46
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.97	0.46
19:S:33:THR:OG1	19:S:34:TRP:N	2.49	0.46
19:S:41:VAL:HA	19:S:44:MET:HG3	1.97	0.46
22:V:3:G:O2'	22:V:4:G:P	2.72	0.46
1:A:1262:C:H2'	1:A:1263:C:H6	1.77	0.46
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.95	0.46
13:M:12:ASN:HD22	13:M:12:ASN:N	2.13	0.46
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.97	0.46
19:S:41:VAL:HG23	19:S:67:VAL:HG13	1.98	0.46
3:C:14:ILE:HG12	3:C:15:THR:N	2.30	0.46
7:G:74:GLU:HG2	7:G:91:VAL:HG22	1.98	0.46
9:I:18:PHE:HB2	9:I:62:TYR:HB3	1.97	0.46
9:I:83:ARG:O	9:I:86:VAL:HG12	2.15	0.46
1:A:1306:A:H61	1:A:1331:G:H1'	1.80	0.46
1:A:134:A:H61	16:P:25:ARG:NH1	2.14	0.46
1:A:1443:G:H5'	1:A:1446:A:OP2	2.15	0.46
1:A:191(D):U:H2'	1:A:191(E):G:H8	1.80	0.46
1:A:791:G:C2'	1:A:792:A:H5'	2.45	0.46
4:D:30:LYS:C	4:D:32:ALA:H	2.18	0.46
7:G:115:ARG:HB2	7:G:118:VAL:HG22	1.97	0.46
2:B:163:PHE:CD2	2:B:185:ILE:HG13	2.50	0.46
3:C:178:LEU:HD13	3:C:178:LEU:HA	1.84	0.46
10:J:62:HIS:H	10:J:62:HIS:CD2	2.33	0.46
19:S:41:VAL:HB	19:S:42:PRO:HA	1.96	0.46
1:A:485:G:O2'	1:A:486:U:O5'	2.31	0.46
1:A:981:U:H5	1:A:982:U:HO2'	1.61	0.46
3:C:78:GLY:HA3	3:C:83:ARG:HB3	1.98	0.46
12:L:62:SER:O	12:L:64:TYR:N	2.48	0.46
1:A:1285:A:H4'	1:A:1286:A:O5'	2.16	0.46
1:A:221:C:H2'	1:A:222:U:C6	2.51	0.46
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:36:LYS:HD3	13:M:36:LYS:C	2.36	0.46
15:O:56:LEU:O	15:O:60:VAL:HG23	2.16	0.46
16:P:1:MET:O	16:P:3:LYS:HG3	2.16	0.46
20:T:87:LYS:HA	20:T:87:LYS:HD2	1.74	0.46
1:A:272:C:H2'	1:A:273:A:C8	2.51	0.46
2:B:204:ASN:HD22	2:B:205:ASP:N	2.13	0.46
2:B:70:PHE:O	2:B:93:VAL:N	2.34	0.46
1:A:1055:A:O2'	3:C:161:GLU:OE2	2.25	0.46
18:R:32:ARG:HA	18:R:69:THR:HG21	1.97	0.46
20:T:26:ASN:O	20:T:30:LYS:HB2	2.16	0.46
2:B:114:ARG:O	2:B:118:LEU:HG	2.16	0.46
7:G:50:ILE:HG21	7:G:61:VAL:HG21	1.98	0.46
12:L:92:ASP:O	12:L:94:PRO:HD3	2.16	0.46
15:O:6:GLU:CD	15:O:6:GLU:H	2.15	0.46
22:V:2:C:C2'	22:V:3:G:H5'	2.46	0.46
5:E:41:VAL:HG13	5:E:113:ALA:HB2	1.97	0.46
6:F:48:LEU:HG	6:F:57:GLN:HA	1.98	0.46
9:I:18:PHE:HD1	9:I:62:TYR:HD2	1.62	0.46
2:B:217:ARG:HB2	2:B:217:ARG:HE	1.54	0.45
2:B:55:PHE:HD1	2:B:58:ILE:HG13	1.81	0.45
5:E:99:GLY:N	5:E:117:ASP:OD2	2.47	0.45
1:A:1226:C:O2'	13:M:103:THR:O	2.28	0.45
1:A:498:A:H4'	1:A:500:G:OP1	2.17	0.45
13:M:58:GLU:O	13:M:62:ASN:ND2	2.33	0.45
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.98	0.45
1:A:1360:A:H2'	1:A:1361:G:C8	2.51	0.45
1:A:486:U:H2'	1:A:487:A:H8	1.79	0.45
1:A:792:A:H4'	1:A:793:U:O5'	2.16	0.45
1:A:960:U:O2	1:A:960:U:H2'	2.16	0.45
2:B:140:HIS:HA	2:B:143:GLU:OE1	2.17	0.45
9:I:114:TYR:N	9:I:114:TYR:HD2	2.14	0.45
19:S:47:HIS:O	19:S:62:ILE:HG12	2.17	0.45
1:A:1024:G:H4'	1:A:1024:G:OP1	2.16	0.45
1:A:525:C:H2'	1:A:526:C:C6	2.51	0.45
1:A:539:A:H2'	1:A:540:G:C8	2.51	0.45
1:A:686:U:HO2'	11:K:42:TRP:HE1	1.61	0.45
6:F:100:ASN:O	18:R:28:GLU:HG2	2.17	0.45
19:S:63:THR:HG23	19:S:66:MET:HG2	1.99	0.45
1:A:1067:A:N1	1:A:1108:G:O2'	2.43	0.45
1:A:1082:G:H2'	1:A:1083:U:O4'	2.15	0.45
1:A:1161:C:O2'	1:A:1162:C:H5'	2.17	0.45
1:A:129(A):G:O2'	1:A:189:U:H3'	2.15	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:C:H2'	1:A:273:A:H8	1.81	0.45
1:A:597:G:H1	1:A:643:C:H42	1.64	0.45
1:A:857:C:H2'	1:A:858:G:O4'	2.17	0.45
7:G:45:ASP:O	7:G:49:ILE:HG12	2.17	0.45
8:H:86:ILE:HG13	8:H:133:LEU:HD22	1.98	0.45
15:O:32:LEU:HD11	15:O:62:GLN:HG2	1.99	0.45
1:A:191:G:C4	20:T:105:SER:HB3	2.51	0.45
1:A:1034:G:H2'	1:A:1035:A:C8	2.51	0.45
1:A:1149:C:H2'	1:A:1150:U:C6	2.51	0.45
1:A:1306:A:N6	1:A:1331:G:H1'	2.31	0.45
1:A:51:A:N7	1:A:114:U:O2'	2.45	0.45
3:C:48:TYR:OH	3:C:122:GLU:OE2	2.22	0.45
16:P:17:TYR:CE1	16:P:41:PRO:HG3	2.52	0.45
1:A:179:A:H2'	1:A:180:U:H6	1.82	0.45
1:A:321:A:C2	1:A:333:G:C2	3.05	0.45
1:A:626:U:C2	1:A:627:G:C8	3.04	0.45
1:A:922:G:C6	1:A:923:A:C6	3.05	0.45
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.35	0.45
8:H:75:ARG:HA	8:H:76:PRO:HD2	1.71	0.45
13:M:65:LYS:O	13:M:70:LEU:HD23	2.17	0.45
1:A:1191:A:H2'	1:A:1192:C:C6	2.52	0.45
1:A:1346:A:OP1	9:I:120:ARG:NH1	2.40	0.45
1:A:1493:A:OP1	26:A:1673:PAR:H51	2.17	0.45
3:C:153:VAL:HG22	3:C:198:VAL:HG22	1.98	0.45
4:D:86:LYS:HD2	4:D:86:LYS:H	1.82	0.45
17:Q:43:LEU:HD12	17:Q:68:ARG:HG2	1.97	0.45
20:T:33:ILE:HG23	20:T:63:ILE:HG12	1.99	0.45
1:A:1015:A:H2'	1:A:1016:A:H8	1.81	0.45
1:A:485:G:O2'	1:A:486:U:P	2.75	0.45
1:A:926:G:C6	1:A:1505:G:C6	3.05	0.45
1:A:986:A:H2'	1:A:987:G:O4'	2.16	0.45
2:B:115:LEU:HD13	2:B:145:LEU:HB3	1.98	0.45
4:D:50:ARG:H	4:D:50:ARG:HG3	1.63	0.45
1:A:102:G:C6	1:A:103:C:C4	3.05	0.45
1:A:1225:A:H5''	1:A:1226:C:OP2	2.17	0.45
1:A:827:U:C5	1:A:872:A:N1	2.85	0.45
1:A:950:U:H2'	1:A:951:G:H8	1.82	0.45
9:I:25:LYS:HB2	9:I:25:LYS:HE3	1.72	0.45
9:I:111:ARG:HH22	10:J:62:HIS:CE1	2.35	0.45
11:K:28:THR:OG1	11:K:90:GLY:HA3	2.17	0.45
19:S:24:ALA:O	19:S:25:LYS:HB3	2.17	0.45
19:S:66:MET:HB2	19:S:74:PHE:CZ	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:U:H2'	1:A:254:G:C8	2.52	0.44
1:A:484:G:H4'	1:A:485:G:O5'	2.16	0.44
1:A:606:G:H1	1:A:631:G:H5''	1.81	0.44
4:D:25:ARG:NH1	4:D:30:LYS:HG3	2.32	0.44
8:H:51:VAL:HG11	8:H:60:ARG:HG3	1.99	0.44
10:J:16:LEU:HD11	10:J:70:ARG:HB2	1.99	0.44
1:A:1322:C:OP1	1:A:1322:C:H6	2.00	0.44
1:A:1363:A:H4'	1:A:1364:U:H2'	1.98	0.44
2:B:12:GLU:C	2:B:14:GLY:H	2.21	0.44
2:B:33:TYR:HB2	2:B:43:ASP:HB2	1.99	0.44
5:E:110:LEU:HD13	5:E:118:ILE:HD13	1.98	0.44
1:A:1128:C:H5'	9:I:16:ARG:NH2	2.27	0.44
1:A:741:G:H2'	1:A:742:G:O4'	2.17	0.44
7:G:138:LYS:HE2	7:G:142:GLU:OE2	2.17	0.44
8:H:65:TYR:HA	8:H:79:VAL:HG23	1.98	0.44
8:H:83:ILE:HB	8:H:137:VAL:HG13	1.99	0.44
9:I:95:LYS:HZ3	9:I:96:LEU:HD13	1.83	0.44
10:J:61:GLU:OE1	14:N:58:LYS:HE2	2.17	0.44
12:L:45:PRO:HG3	12:L:53:ARG:HD3	1.98	0.44
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.17	0.44
1:A:109:A:C6	1:A:326:G:C6	3.05	0.44
1:A:1117:G:H5''	9:I:104:ARG:NH1	2.32	0.44
1:A:1239:A:H62	1:A:1299:A:H62	1.65	0.44
1:A:337:C:H2'	1:A:338:A:C8	2.52	0.44
1:A:735:C:H5'	18:R:71:LYS:HD3	2.00	0.44
1:A:542:G:H5'	4:D:41:GLY:HA3	1.98	0.44
7:G:87:VAL:HG11	7:G:155:ARG:HA	1.99	0.44
13:M:115:LYS:HB2	13:M:115:LYS:HE3	1.75	0.44
18:R:52:PRO:HB2	18:R:54:ARG:HG2	2.00	0.44
19:S:81:ARG:HE	19:S:81:ARG:HB2	1.36	0.44
20:T:87:LYS:O	20:T:91:LEU:HG	2.18	0.44
1:A:148:G:H2'	1:A:149:A:C8	2.51	0.44
1:A:765:G:N2	1:A:813:U:OP2	2.50	0.44
1:A:421:U:H3	3:C:127:ARG:HH21	1.63	0.44
1:A:376:G:H5''	16:P:5:ARG:HB2	1.99	0.44
22:V:19:G:H5'	22:V:20:U:C5	2.52	0.44
1:A:1388:C:H2'	1:A:1389:C:C6	2.52	0.44
1:A:458:C:H2'	1:A:464:G:H8	1.83	0.44
1:A:690:G:H22	11:K:55:LYS:HZ2	1.65	0.44
15:O:32:LEU:O	15:O:36:ILE:HG13	2.18	0.44
15:O:82:ILE:O	15:O:86:GLY:N	2.51	0.44
22:V:61:C:H2'	22:V:62:C:C6	2.51	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1103:C:H2'	1:A:1104:G:O4'	2.17	0.44
1:A:680:C:H2'	1:A:681:C:C6	2.51	0.44
3:C:47:LEU:HA	3:C:47:LEU:HD12	1.83	0.44
12:L:42:THR:HA	12:L:53:ARG:O	2.18	0.44
15:O:77:ARG:HA	15:O:80:ALA:HB3	1.99	0.44
16:P:18:ARG:NH1	16:P:32:TYR:OH	2.50	0.44
1:A:110:C:H2'	1:A:111:G:O4'	2.18	0.44
1:A:1129:C:C4'	1:A:1130:A:H5'	2.44	0.44
1:A:865:A:H2	1:A:918:A:H4'	1.82	0.44
1:A:883:C:O2'	1:A:884:U:H5'	2.18	0.44
1:A:974:A:OP2	14:N:41:ARG:NH1	2.51	0.44
3:C:82:GLU:O	3:C:86:VAL:HG13	2.17	0.44
5:E:9:LYS:HB2	5:E:9:LYS:HE3	1.89	0.44
6:F:33:TYR:HB2	6:F:75:LEU:HD12	1.99	0.44
11:K:19:ALA:HB2	11:K:32:ILE:HG22	2.00	0.44
13:M:23:TYR:HE1	13:M:70:LEU:HD12	1.83	0.44
15:O:26:GLU:HG2	15:O:26:GLU:H	1.54	0.44
15:O:39:LEU:HD13	15:O:56:LEU:HB2	2.00	0.44
1:A:1320:C:OP1	19:S:70:LYS:HE3	2.17	0.44
22:V:23:C:H2'	22:V:24:U:H6	1.83	0.44
1:A:292:G:N7	1:A:293:G:H1'	2.33	0.44
1:A:975:A:H5'	1:A:975:A:C8	2.48	0.44
3:C:72:LYS:HB3	3:C:75:VAL:HG23	2.00	0.44
12:L:39:VAL:HG12	12:L:41:ARG:HG3	2.00	0.44
1:A:755:G:OP2	15:O:65:ARG:HG2	2.18	0.44
16:P:39:TYR:CZ	16:P:41:PRO:HB3	2.53	0.44
1:A:667:G:H4'	15:O:51:HIS:ND1	2.33	0.43
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.99	0.43
3:C:108:ASN:HB3	3:C:111:LEU:HD12	2.00	0.43
12:L:24:VAL:O	12:L:26:ALA:N	2.47	0.43
12:L:78:GLN:HB3	12:L:79:GLU:H	1.67	0.43
16:P:4:ILE:HB	16:P:66:PRO:HB3	2.00	0.43
1:A:1239:A:O2'	1:A:1298:C:N4	2.51	0.43
1:A:210:U:O2'	1:A:216:G:N7	2.43	0.43
1:A:719:C:H1'	18:R:49:LYS:HB3	1.99	0.43
4:D:100:ARG:NH1	4:D:137:SER:HB3	2.33	0.43
4:D:153:ARG:NH1	4:D:181:MET:HB2	2.32	0.43
1:A:1079:G:C6	1:A:1080:A:N6	2.86	0.43
1:A:1222:G:H5''	19:S:78:ARG:NH1	2.33	0.43
1:A:1497:G:C2'	1:A:1498:U:H5'	2.49	0.43
1:A:352:C:O2'	1:A:354:G:OP1	2.26	0.43
1:A:421:U:H5''	1:A:422:C:OP2	2.19	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:118:LYS:O	9:I:119:ALA:HB3	2.18	0.43
10:J:32:ALA:H	10:J:78:ASN:ND2	2.16	0.43
1:A:267:C:OP2	17:Q:67:LYS:HD2	2.18	0.43
1:A:1451:A:N3	1:A:1451:A:H2'	2.33	0.43
1:A:181:G:O2'	1:A:182:U:H6	2.01	0.43
1:A:191:G:C2	1:A:192:U:C2	3.07	0.43
1:A:381:C:H2'	1:A:382:A:O4'	2.19	0.43
1:A:865:A:C2	1:A:918:A:H4'	2.53	0.43
1:A:874:G:C6	1:A:875:C:C4	3.07	0.43
10:J:54:PHE:CZ	10:J:55:LYS:HE3	2.54	0.43
12:L:62:SER:C	12:L:64:TYR:H	2.21	0.43
12:L:58:VAL:O	12:L:65:GLU:HA	2.18	0.43
15:O:25:THR:HG21	15:O:70:LEU:HB2	2.00	0.43
16:P:45:THR:HG22	16:P:47:ASP:N	2.26	0.43
17:Q:62:SER:HB3	17:Q:72:ARG:HE	1.84	0.43
20:T:98:PRO:C	20:T:100:ILE:H	2.21	0.43
1:A:975:A:N6	1:A:1367:C:O4'	2.52	0.43
1:A:1446:A:O2'	1:A:1447:G:P	2.76	0.43
1:A:464:G:C6	1:A:466:C:H5'	2.53	0.43
1:A:9:G:H5''	5:E:126:ARG:HE	1.84	0.43
2:B:100:GLY:N	2:B:176:GLU:OE2	2.47	0.43
2:B:215:LEU:HA	2:B:215:LEU:HD22	1.73	0.43
1:A:923:A:OP1	5:E:21:ALA:HB2	2.18	0.43
12:L:110:VAL:CG2	12:L:120:TYR:HB3	2.48	0.43
13:M:14:ARG:H	13:M:44:ARG:CD	2.25	0.43
14:N:29:ARG:HD3	14:N:40:CYS:HB2	1.99	0.43
2:B:37:ASN:C	2:B:39:ILE:H	2.20	0.43
10:J:44:VAL:HG13	10:J:66:ARG:HG2	1.99	0.43
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.58	0.43
1:A:254:G:OP1	17:Q:67:LYS:O	2.37	0.43
1:A:1072:G:H2'	1:A:1073:U:C6	2.54	0.43
1:A:1124:G:H3'	1:A:1145:C:H41	1.84	0.43
1:A:1273:G:H3'	1:A:1274:G:H8	1.82	0.43
1:A:536:C:H2'	1:A:537:G:C8	2.54	0.43
9:I:8:GLY:HA2	9:I:79:LEU:HD12	2.01	0.43
1:A:960:U:H1'	1:A:1223:C:H5'	2.00	0.43
1:A:1318:A:O2'	19:S:37:ARG:HD3	2.18	0.43
1:A:131:C:H2'	1:A:132:C:C6	2.53	0.43
1:A:731:G:H5'	1:A:766:A:H4'	2.00	0.43
2:B:172:ILE:O	2:B:175:ARG:HB3	2.18	0.43
2:B:7:VAL:HG21	2:B:217:ARG:NH1	2.34	0.43
7:G:140:ASP:HA	7:G:143:ARG:NH1	2.34	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:59:ARG:NH1	12:L:65:GLU:OE2	2.51	0.43
13:M:4:ILE:HG22	13:M:5:ALA:N	2.34	0.43
14:N:6:LEU:HD23	14:N:23:ARG:HH22	1.83	0.43
1:A:1000:A:H2'	1:A:1001:G:C8	2.54	0.43
1:A:1314:C:H2'	1:A:1315:U:C6	2.54	0.43
1:A:1404:C:H2'	1:A:1405:G:C8	2.54	0.43
1:A:191(D):U:H2'	1:A:191(E):G:C8	2.54	0.43
1:A:347:G:H1'	1:A:348:G:H5''	2.00	0.43
1:A:837:G:H1	1:A:849:C:H42	1.66	0.43
1:A:872:A:C5	1:A:874:G:C8	3.06	0.43
1:A:900:A:H2'	1:A:901:A:C8	2.53	0.43
2:B:212:GLN:NE2	2:B:216:SER:HB2	2.34	0.43
3:C:149:ALA:HA	3:C:201:TYR:O	2.18	0.43
1:A:1118:C:OP1	9:I:9:ARG:HD3	2.18	0.43
1:A:1346:A:H1'	1:A:1348:U:C5	2.54	0.43
1:A:1466:C:H2'	1:A:1467:G:O4'	2.19	0.43
1:A:224:C:H2'	1:A:225:C:C6	2.53	0.43
1:A:228:A:H2'	1:A:229:U:O4'	2.19	0.43
4:D:196:LEU:O	4:D:198:VAL:N	2.51	0.43
5:E:42:GLY:CA	5:E:66:MET:HG2	2.48	0.43
5:E:69:VAL:O	5:E:71:LEU:N	2.51	0.43
8:H:13:ILE:O	8:H:17:THR:HG23	2.18	0.43
12:L:28:LYS:HB3	12:L:30:ALA:HB2	2.01	0.43
1:A:1352:C:OP1	21:U:3:LYS:NZ	2.37	0.42
1:A:1392:G:N2	1:A:1502:A:H8	2.16	0.42
1:A:411:A:C6	1:A:429:U:C4	3.07	0.42
1:A:652:U:C4	1:A:752:G:N3	2.87	0.42
1:A:791:G:H2'	1:A:792:A:H5'	2.01	0.42
5:E:131:ILE:HD13	5:E:131:ILE:HA	1.84	0.42
6:F:30:LEU:HB3	6:F:35:ALA:HB3	2.01	0.42
10:J:6:ILE:HG22	10:J:98:ILE:HG23	2.01	0.42
1:A:1095:U:OP1	1:A:1108:G:N2	2.49	0.42
1:A:436:C:H2'	1:A:437:U:O4'	2.19	0.42
2:B:68:ILE:HB	2:B:70:PHE:HE1	1.84	0.42
4:D:112:VAL:N	4:D:116:GLN:OE1	2.38	0.42
8:H:104:ARG:HD2	8:H:138:TRP:CD2	2.53	0.42
1:A:255:G:H1'	17:Q:16:GLN:OE1	2.19	0.42
1:A:254:G:O2'	17:Q:15:MET:HB3	2.19	0.42
1:A:530:G:H4'	1:A:531:U:OP2	2.20	0.42
1:A:742:G:OP2	15:O:35:ARG:NH2	2.44	0.42
5:E:79:GLU:H	5:E:79:GLU:HG3	1.45	0.42
7:G:38:LEU:HD12	7:G:38:LEU:O	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:44:THR:HA	12:L:45:PRO:HD3	1.69	0.42
13:M:7:VAL:O	13:M:9:ILE:HG23	2.19	0.42
1:A:280:C:O2	17:Q:38:ARG:HG3	2.19	0.42
18:R:56:THR:HB	18:R:58:LEU:HD12	2.02	0.42
1:A:313:A:H2'	1:A:314:C:C6	2.54	0.42
7:G:89:MET:CE	7:G:156:TRP:H	2.32	0.42
1:A:1108:G:H5'	3:C:176:HIS:ND1	2.34	0.42
1:A:1233:G:H2'	1:A:1234:C:H6	1.84	0.42
1:A:1250:A:N1	1:A:1353:G:N2	2.64	0.42
1:A:1453:G:H8	20:T:39:LYS:CE	2.31	0.42
1:A:1112:C:N3	3:C:178:LEU:HB2	2.35	0.42
4:D:120:LEU:HD23	4:D:120:LEU:HA	1.89	0.42
9:I:32:ASP:OD1	9:I:33:PHE:N	2.53	0.42
18:R:43:PHE:CE2	18:R:58:LEU:HD11	2.54	0.42
20:T:50:GLU:HG3	20:T:51:GLU:N	2.33	0.42
1:A:1347:G:O2'	1:A:1348:U:P	2.77	0.42
1:A:16:A:N1	1:A:919:A:H2	2.18	0.42
1:A:560:U:O2'	1:A:561:U:OP2	2.30	0.42
1:A:918:A:H2'	1:A:919:A:C8	2.55	0.42
1:A:950:U:H2'	1:A:951:G:C8	2.55	0.42
1:A:963:G:N2	1:A:972:C:C2	2.83	0.42
2:B:113:HIS:O	2:B:116:GLU:HB2	2.20	0.42
2:B:7:VAL:HG11	2:B:217:ARG:CZ	2.49	0.42
3:C:85:ARG:HA	3:C:85:ARG:HD2	1.83	0.42
6:F:95:GLU:HA	6:F:96:PRO:HD3	1.87	0.42
9:I:91:ASP:C	9:I:93:ARG:H	2.21	0.42
1:A:501:C:P	12:L:117:ARG:HH22	2.42	0.42
13:M:121:LYS:HA	13:M:121:LYS:HD3	1.90	0.42
1:A:376:G:H5''	16:P:5:ARG:HD2	2.01	0.42
1:A:1148:U:H2'	1:A:1149:C:O4'	2.19	0.42
1:A:1206:G:C6	1:A:1207:G:C5	3.07	0.42
1:A:1223:C:P	19:S:78:ARG:NH1	2.92	0.42
1:A:123:C:OP1	1:A:312:C:H5'	2.19	0.42
1:A:1296:C:OP1	13:M:44:ARG:NH2	2.53	0.42
1:A:1302:U:H2'	1:A:1302:U:O2	2.19	0.42
1:A:942:G:C2	1:A:1342:C:C2	3.07	0.42
1:A:1431:C:H2'	1:A:1432:G:O4'	2.20	0.42
1:A:431:A:H2'	1:A:432:A:O4'	2.20	0.42
1:A:735:C:H2'	1:A:736:C:H6	1.83	0.42
2:B:19:HIS:CE1	2:B:206:ASP:HB2	2.54	0.42
3:C:91:LEU:O	3:C:95:THR:OG1	2.19	0.42
8:H:121:ASP:OD1	8:H:121:ASP:N	2.46	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:963:G:N2	10:J:55:LYS:HE2	2.34	0.42
13:M:40:ASN:ND2	13:M:43:THR:HG23	2.34	0.42
1:A:1084:G:C5	1:A:1085:U:C4	3.08	0.42
1:A:1410:G:H2'	1:A:1411:C:H6	1.85	0.42
1:A:1492:A:OP1	12:L:47:LYS:N	2.53	0.42
1:A:1497:G:H2'	1:A:1498:U:H5'	2.02	0.42
1:A:102:G:O2'	1:A:151:A:N3	2.45	0.42
1:A:187:C:H2'	1:A:188:U:O4'	2.20	0.42
1:A:654:G:H2'	1:A:655:A:O4'	2.20	0.42
2:B:223:ILE:HA	2:B:226:ARG:HB3	2.02	0.42
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.34	0.42
7:G:15:ASP:O	7:G:19:GLY:HA2	2.20	0.42
9:I:125:TYR:HD2	9:I:126:SER:H	1.68	0.42
19:S:78:ARG:H	19:S:78:ARG:HG2	1.56	0.42
1:A:1002:G:H1	1:A:1038:C:N4	2.07	0.42
1:A:1127:G:N1	1:A:1145:C:C2	2.87	0.42
1:A:1233:G:C4	1:A:1234:C:C5	3.08	0.42
1:A:1442:G:C5	1:A:1446:A:C6	3.08	0.42
1:A:284:G:H2'	1:A:285:G:C8	2.55	0.42
1:A:401:C:H2'	1:A:402:G:C8	2.54	0.42
9:I:4:TYR:CE1	9:I:88:TYR:HB2	2.55	0.42
11:K:109:VAL:HG11	18:R:84:LYS:HD3	2.02	0.42
20:T:39:LYS:H	20:T:39:LYS:HG3	1.63	0.42
1:A:1170:A:H2'	1:A:1171:G:O4'	2.20	0.42
1:A:1241:G:H2'	1:A:1242:C:H6	1.85	0.42
1:A:345:C:H1'	1:A:346:G:OP2	2.19	0.42
1:A:9:G:C6	1:A:26:A:N6	2.88	0.42
13:M:16:ASP:HB3	13:M:41:PRO:HB3	2.01	0.42
13:M:3:ARG:HG3	13:M:9:ILE:HG21	2.02	0.42
22:V:16:C:O2	22:V:16:C:H2'	2.19	0.42
1:A:1000:A:O5'	1:A:1000:A:H8	2.03	0.41
1:A:1469:G:H2'	1:A:1470:G:C8	2.55	0.41
1:A:164:U:H2'	1:A:165:C:C6	2.54	0.41
1:A:280:C:H4'	1:A:281:G:OP2	2.20	0.41
1:A:818:G:C3'	1:A:819:A:H5'	2.50	0.41
10:J:3:LYS:HB2	10:J:75:ILE:O	2.19	0.41
1:A:539:A:OP2	12:L:115:LYS:HE3	2.20	0.41
13:M:20:THR:O	13:M:22:ILE:N	2.51	0.41
1:A:1194:U:H2'	1:A:1195:C:C6	2.55	0.41
1:A:477:G:H2'	1:A:478:A:C8	2.55	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.19	0.41
4:D:127:THR:HA	4:D:132:ARG:HA	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:104:ARG:HD2	8:H:138:TRP:CG	2.56	0.41
9:I:40:LEU:O	9:I:42:ARG:N	2.48	0.41
20:T:53:LEU:HD12	20:T:100:ILE:HG23	2.02	0.41
9:I:46:ALA:HB2	9:I:74:ILE:HG23	2.02	0.41
11:K:88:GLY:C	11:K:90:GLY:H	2.23	0.41
16:P:60:LEU:HD23	16:P:60:LEU:HA	1.80	0.41
16:P:56:ALA:HB1	16:P:74:LEU:HD13	2.02	0.41
18:R:38:GLU:O	18:R:42:ARG:NH1	2.54	0.41
19:S:40:ILE:CG1	19:S:41:VAL:HG13	2.47	0.41
22:V:5:G:H1	22:V:67:C:H42	1.67	0.41
1:A:1190:G:OP1	3:C:4:LYS:HA	2.20	0.41
1:A:1492:A:OP1	12:L:47:LYS:HB3	2.20	0.41
1:A:790:A:N1	1:A:1497:G:H5''	2.35	0.41
1:A:373:A:H2'	1:A:374:A:H8	1.86	0.41
1:A:376:G:OP1	16:P:5:ARG:HB2	2.20	0.41
1:A:453:A:C6	1:A:454:C:C4	3.09	0.41
1:A:690:G:H22	11:K:55:LYS:HZ1	1.66	0.41
9:I:125:TYR:HD2	9:I:126:SER:N	2.18	0.41
11:K:18:ARG:HA	11:K:81:ASP:H	1.86	0.41
12:L:102:ARG:HE	12:L:102:ARG:HB3	1.71	0.41
13:M:12:ASN:N	13:M:45:VAL:HG13	2.35	0.41
1:A:1216:G:H5''	14:N:5:ALA:HB2	2.02	0.41
16:P:17:TYR:HE1	16:P:41:PRO:HG3	1.85	0.41
16:P:23:ASP:O	16:P:26:ARG:HB2	2.20	0.41
1:A:1446:A:HO2'	1:A:1447:G:P	2.44	0.41
3:C:150:LYS:HE3	3:C:167:TRP:HE1	1.84	0.41
12:L:62:SER:HB2	12:L:64:TYR:CD1	2.56	0.41
17:Q:59:ILE:HB	17:Q:71:PHE:HB3	2.03	0.41
2:B:80:ILE:HD11	2:B:208:ILE:HG12	2.02	0.41
6:F:46:ARG:HB3	6:F:60:PHE:CE1	2.55	0.41
10:J:3:LYS:HD2	10:J:77:PRO:HD3	2.01	0.41
16:P:8:ARG:C	16:P:9:PHE:HD2	2.24	0.41
18:R:85:LEU:HD23	18:R:88:LYS:HD2	2.03	0.41
1:A:1226:C:H4'	1:A:1227:A:OP1	2.20	0.41
1:A:1308:U:OP1	13:M:98:VAL:HG23	2.21	0.41
1:A:186(C):G:C6	1:A:191(E):G:C6	3.09	0.41
1:A:221:C:H2'	1:A:222:U:H6	1.84	0.41
1:A:241:C:C2	1:A:286:G:C2	3.09	0.41
1:A:528:C:H41	12:L:49:ASN:CG	2.24	0.41
1:A:694:A:H2'	1:A:695:A:O4'	2.21	0.41
1:A:779:C:H2'	1:A:780:A:O4'	2.20	0.41
1:A:963:G:H21	10:J:55:LYS:HD3	1.84	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
8:H:44:PHE:HE2	8:H:109:ILE:CG2	2.34	0.41
11:K:48:ILE:HA	11:K:48:ILE:HD13	1.83	0.41
1:A:1152:A:H2'	1:A:1153:C:C6	2.55	0.41
1:A:1199:U:H4'	10:J:54:PHE:CZ	2.56	0.41
1:A:192:U:H2'	1:A:193:C:C6	2.56	0.41
1:A:44:G:C2	1:A:45:U:H1'	2.56	0.41
1:A:651:C:H2'	1:A:652:U:C6	2.56	0.41
2:B:118:LEU:CB	2:B:142:LEU:HD12	2.50	0.41
3:C:119:ARG:HH21	3:C:140:ARG:CZ	2.34	0.41
10:J:76:ASN:HA	10:J:77:PRO:HD2	1.96	0.41
12:L:68:ALA:HB2	12:L:85:ILE:HD11	2.03	0.41
12:L:70:ILE:HA	12:L:71:PRO:HD3	1.81	0.41
14:N:51:GLY:O	14:N:53:LEU:N	2.53	0.41
17:Q:62:SER:CB	17:Q:72:ARG:HE	2.33	0.41
22:V:1:G:H2'	22:V:2:C:H6	1.86	0.41
1:A:1112:C:C2	3:C:178:LEU:HB2	2.55	0.41
1:A:1128:C:H42	1:A:1144:G:H1	1.69	0.41
1:A:1213:A:C5	1:A:1215:G:C4	3.09	0.41
1:A:1336:C:O2	1:A:1336:C:H2'	2.20	0.41
1:A:302:G:C6	1:A:303:A:C5	3.09	0.41
1:A:375:U:C2	1:A:376:G:C8	3.09	0.41
1:A:418:C:H1'	1:A:540:G:O2'	2.21	0.41
1:A:622:A:C8	1:A:623:C:C6	3.09	0.41
1:A:626:U:N3	1:A:627:G:N7	2.69	0.41
1:A:438:G:H4'	4:D:123:HIS:NE2	2.36	0.41
4:D:52:SER:O	4:D:55:ALA:HB3	2.21	0.41
5:E:68:GLU:HG3	5:E:68:GLU:O	2.21	0.41
9:I:79:LEU:O	9:I:83:ARG:HG2	2.19	0.41
10:J:54:PHE:CD2	10:J:55:LYS:HG3	2.56	0.41
20:T:11:SER:HA	20:T:13:LEU:HD12	2.01	0.41
1:A:1004:A:H1'	1:A:1036:G:H22	1.86	0.41
1:A:652:U:H1'	1:A:653:A:C2	2.56	0.41
1:A:659:U:H2'	1:A:660:G:C8	2.55	0.41
2:B:126:GLU:O	2:B:129:GLU:HB2	2.20	0.41
3:C:138:VAL:HG13	3:C:149:ALA:HB3	2.02	0.41
4:D:131:ARG:H	4:D:131:ARG:HG2	1.67	0.41
4:D:186:LEU:HD23	4:D:186:LEU:HA	1.95	0.41
5:E:82:VAL:HB	5:E:138:ALA:HB2	2.03	0.41
5:E:69:VAL:HA	5:E:70:PRO:HD2	1.76	0.41
8:H:12:ARG:HD3	8:H:26:VAL:HB	2.03	0.41
19:S:36:ARG:HA	19:S:71:LEU:HB2	2.02	0.41
1:A:1107:C:C4	1:A:1108:G:C8	3.09	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:166:ASP:HB3	2:B:169:LYS:HB2	2.02	0.41
3:C:42:LEU:HA	3:C:42:LEU:HD12	1.87	0.41
4:D:64:LEU:HD13	4:D:198:VAL:HG11	2.02	0.41
6:F:25:ILE:HD13	6:F:28:ARG:NH1	2.35	0.41
10:J:6:ILE:O	10:J:71:LEU:HD12	2.21	0.41
11:K:19:ALA:CB	11:K:32:ILE:HG22	2.50	0.41
22:V:53:G:O2'	22:V:54:U:O5'	2.39	0.41
1:A:1363:A:H1'	1:A:1365:G:N7	2.36	0.40
1:A:22:G:H4'	1:A:885:G:C8	2.56	0.40
1:A:965:A:H4'	1:A:966:G:OP1	2.20	0.40
5:E:51:VAL:HB	5:E:52:PRO:HD3	2.03	0.40
7:G:89:MET:HE3	7:G:155:ARG:HB2	2.03	0.40
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.36	0.40
9:I:95:LYS:NZ	9:I:96:LEU:HD13	2.36	0.40
20:T:43:LEU:HA	20:T:43:LEU:HD23	1.88	0.40
1:A:1164:G:H2'	1:A:1165:C:H6	1.87	0.40
1:A:652:U:H1'	1:A:653:A:H2	1.86	0.40
1:A:982:U:H4'	1:A:983:A:O5'	2.21	0.40
2:B:120:ALA:C	2:B:122:PHE:H	2.25	0.40
2:B:19:HIS:NE2	2:B:206:ASP:HB2	2.36	0.40
3:C:188:LEU:HA	3:C:188:LEU:HD13	1.90	0.40
4:D:165:MET:O	4:D:167:GLY:N	2.54	0.40
5:E:34:VAL:HG11	5:E:63:ARG:HG2	2.02	0.40
11:K:38:ASN:HA	11:K:39:PRO:HD3	1.75	0.40
1:A:1216:G:OP1	14:N:2:ALA:HA	2.21	0.40
1:A:1032(B):G:H2'	1:A:1033:G:H8	1.86	0.40
1:A:1314:C:OP2	19:S:4:SER:OG	2.37	0.40
1:A:1508:G:H2'	1:A:1509:C:C6	2.56	0.40
1:A:97:U:H2'	1:A:99:C:C6	2.56	0.40
9:I:75:ASP:HA	9:I:78:LYS:HB3	2.04	0.40
11:K:18:ARG:HB3	11:K:33:THR:OG1	2.21	0.40
12:L:38:THR:CG2	12:L:57:LYS:HB3	2.49	0.40
12:L:90:VAL:O	12:L:92:ASP:N	2.54	0.40
1:A:114:U:H2'	1:A:115:G:C8	2.57	0.40
1:A:41:G:H2'	1:A:42:G:H8	1.86	0.40
1:A:951:G:OP2	13:M:102:ARG:NH2	2.54	0.40
3:C:20:SER:HB2	3:C:40:ARG:NH2	2.29	0.40
4:D:108:LEU:HB3	4:D:110:PHE:CD1	2.57	0.40
5:E:89:ILE:HG12	5:E:91:LEU:CD1	2.52	0.40
19:S:15:LEU:HA	19:S:18:LYS:HB3	2.04	0.40
1:A:1239:A:H62	1:A:1299:A:N6	2.19	0.40
1:A:233:C:H2'	1:A:234:C:H6	1.86	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:56:ASP:HB2	3:C:67:THR:HB	2.03	0.40
5:E:12:LEU:HB3	5:E:31:LEU:CB	2.52	0.40
9:I:5:TYR:HA	9:I:17:VAL:O	2.21	0.40
10:J:77:PRO:O	10:J:79:ARG:NH1	2.54	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	235/256 (92%)	178 (76%)	42 (18%)	15 (6%)	2	5
3	C	203/239 (85%)	171 (84%)	29 (14%)	3 (2%)	15	50
4	D	206/209 (99%)	177 (86%)	24 (12%)	5 (2%)	9	34
5	E	149/162 (92%)	133 (89%)	13 (9%)	3 (2%)	11	40
6	F	99/101 (98%)	94 (95%)	5 (5%)	0	100	100
7	G	153/156 (98%)	138 (90%)	13 (8%)	2 (1%)	18	54
8	H	136/138 (99%)	120 (88%)	12 (9%)	4 (3%)	7	27
9	I	125/128 (98%)	97 (78%)	24 (19%)	4 (3%)	6	24
10	J	97/105 (92%)	78 (80%)	14 (14%)	5 (5%)	3	9
11	K	117/129 (91%)	100 (86%)	15 (13%)	2 (2%)	14	45
12	L	123/132 (93%)	98 (80%)	15 (12%)	10 (8%)	1	3
13	M	119/126 (94%)	94 (79%)	16 (13%)	9 (8%)	2	3
14	N	58/61 (95%)	46 (79%)	6 (10%)	6 (10%)	1	2
15	O	86/89 (97%)	80 (93%)	4 (5%)	2 (2%)	10	35
16	P	82/88 (93%)	71 (87%)	10 (12%)	1 (1%)	19	57
17	Q	98/105 (93%)	88 (90%)	10 (10%)	0	100	100
18	R	68/88 (77%)	61 (90%)	6 (9%)	1 (2%)	15	50

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	82/93 (88%)	54 (66%)	17 (21%)	11 (13%)	0	1
20	T	97/106 (92%)	75 (77%)	16 (16%)	6 (6%)	2	6
21	U	23/27 (85%)	18 (78%)	4 (17%)	1 (4%)	4	14
All	All	2356/2538 (93%)	1971 (84%)	295 (12%)	90 (4%)	5	18

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	230	VAL
2	B	236	TYR
3	C	12	LEU
3	C	79	ARG
4	D	154	ASN
11	K	91	ARG
12	L	48	PRO
12	L	64	TYR
13	M	67	GLU
13	M	106	ASN
13	M	118	ALA
14	N	14	PRO
14	N	16	PHE
14	N	52	GLN
19	S	3	ARG
19	S	12	ASP
20	T	48	LYS
20	T	96	GLY
2	B	15	VAL
4	D	30	LYS
4	D	166	LYS
5	E	115	VAL
7	G	55	GLY
8	H	50	ARG
9	I	41	VAL
9	I	127	LYS
10	J	30	SER
10	J	86	MET
12	L	63	GLY
12	L	91	LYS
12	L	115	LYS
13	M	6	GLY
13	M	21	TYR

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
19	S	41	VAL
19	S	45	VAL
20	T	99	LEU
2	B	13	ALA
2	B	22	LYS
2	B	24	TRP
2	B	135	GLN
2	B	207	ALA
4	D	73	ARG
4	D	155	LEU
7	G	7	ALA
8	H	2	LEU
9	I	56	LEU
9	I	95	LYS
10	J	59	SER
11	K	103	LEU
13	M	4	ILE
13	M	12	ASN
13	M	42	ALA
19	S	27	GLU
19	S	28	LYS
2	B	19	HIS
2	B	101	MET
2	B	155	LEU
5	E	70	PRO
8	H	129	VAL
12	L	19	ARG
12	L	28	LYS
14	N	15	LYS
14	N	32	SER
15	O	88	ARG
18	R	20	ALA
19	S	9	VAL
20	T	84	LEU
20	T	98	PRO
21	U	9	ARG
2	B	121	LEU
3	C	181	ASN
10	J	27	ALA
12	L	27	LEU
12	L	65	GLU
13	M	101	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	O	23	GLY
20	T	97	ALA
2	B	26	PRO
2	B	126	GLU
2	B	237	ALA
10	J	91	PRO
14	N	60	SER
19	S	7	LYS
5	E	74	GLY
12	L	18	VAL
19	S	26	GLY
19	S	46	GLY
8	H	51	VAL
16	P	46	PRO
19	S	31	ILE

### 5.3.2 Protein sidechains ⓘ

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	
2	B	205/220 (93%)	180 (88%)	25 (12%)	7	20
3	C	159/188 (85%)	146 (92%)	13 (8%)	17	43
4	D	180/181 (99%)	154 (86%)	26 (14%)	5	13
5	E	116/123 (94%)	104 (90%)	12 (10%)	10	30
6	F	90/90 (100%)	82 (91%)	8 (9%)	14	39
7	G	126/127 (99%)	114 (90%)	12 (10%)	12	35
8	H	119/119 (100%)	106 (89%)	13 (11%)	9	26
9	I	98/99 (99%)	80 (82%)	18 (18%)	2	6
10	J	89/92 (97%)	74 (83%)	15 (17%)	3	8
11	K	90/99 (91%)	81 (90%)	9 (10%)	11	32
12	L	104/109 (95%)	93 (89%)	11 (11%)	10	28
13	M	97/101 (96%)	78 (80%)	19 (20%)	2	5
14	N	49/50 (98%)	42 (86%)	7 (14%)	5	13

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	79/80 (99%)	69 (87%)	10 (13%)	6	18
16	P	72/74 (97%)	64 (89%)	8 (11%)	9	25
17	Q	95/97 (98%)	89 (94%)	6 (6%)	25	60
18	R	61/77 (79%)	52 (85%)	9 (15%)	4	12
19	S	73/80 (91%)	57 (78%)	16 (22%)	1	4
20	T	76/82 (93%)	66 (87%)	10 (13%)	6	16
21	U	20/22 (91%)	19 (95%)	1 (5%)	34	72
All	All	1998/2110 (95%)	1750 (88%)	248 (12%)	7	19

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	5	ILE
2	B	7	VAL
2	B	8	LYS
2	B	15	VAL
2	B	23	ARG
2	B	24	TRP
2	B	33	TYR
2	B	36	ARG
2	B	67	THR
2	B	71	VAL
2	B	82	ARG
2	B	92	TYR
2	B	113	HIS
2	B	145	LEU
2	B	155	LEU
2	B	163	PHE
2	B	172	ILE
2	B	175	ARG
2	B	178	ARG
2	B	187	LEU
2	B	195	ASP
2	B	196	LEU
2	B	204	ASN
2	B	215	LEU
2	B	235	SER
3	C	3	ASN
3	C	5	ILE
3	C	12	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	C	21	ARG
3	C	45	LYS
3	C	47	LEU
3	C	56	ASP
3	C	94	LEU
3	C	95	THR
3	C	131	ARG
3	C	178	LEU
3	C	184	TYR
3	C	192	THR
4	D	3	ARG
4	D	9	CYS
4	D	15	GLU
4	D	19	LEU
4	D	30	LYS
4	D	33	MET
4	D	50	ARG
4	D	53	ASP
4	D	58	LEU
4	D	73	ARG
4	D	76	ARG
4	D	84	LYS
4	D	86	LYS
4	D	96	LEU
4	D	108	LEU
4	D	122	ARG
4	D	127	THR
4	D	131	ARG
4	D	137	SER
4	D	150	GLU
4	D	154	ASN
4	D	175	SER
4	D	187	ARG
4	D	190	ASP
4	D	193	ASP
4	D	208	SER
5	E	6	PHE
5	E	7	GLU
5	E	10	MET
5	E	11	ILE
5	E	18	ARG
5	E	31	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	E	41	VAL
5	E	73	ASN
5	E	79	GLU
5	E	101	ILE
5	E	147	ASP
5	E	153	LYS
6	F	21	LEU
6	F	23	LYS
6	F	36	ARG
6	F	71	ARG
6	F	74	ASP
6	F	91	VAL
6	F	92	LYS
6	F	98	LEU
7	G	5	ARG
7	G	8	GLU
7	G	35	LYS
7	G	54	THR
7	G	63	LYS
7	G	78	ARG
7	G	104	LEU
7	G	113	GLU
7	G	114	ARG
7	G	136	LYS
7	G	137	LYS
7	G	155	ARG
8	H	1	MET
8	H	12	ARG
8	H	19	VAL
8	H	24	THR
8	H	26	VAL
8	H	41	ARG
8	H	54	ASP
8	H	63	LEU
8	H	80	ILE
8	H	85	ARG
8	H	109	ILE
8	H	112	LEU
8	H	137	VAL
9	I	9	ARG
9	I	38	GLN
9	I	44	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
9	I	56	LEU
9	I	65	VAL
9	I	95	LYS
9	I	96	LEU
9	I	102	LEU
9	I	104	ARG
9	I	105	ASP
9	I	108	VAL
9	I	111	ARG
9	I	112	LYS
9	I	114	TYR
9	I	121	ARG
9	I	124	GLN
9	I	125	TYR
9	I	128	ARG
10	J	3	LYS
10	J	17	ASP
10	J	22	LYS
10	J	45	ARG
10	J	47	PHE
10	J	49	VAL
10	J	54	PHE
10	J	57	LYS
10	J	62	HIS
10	J	70	ARG
10	J	74	ILE
10	J	80	LYS
10	J	84	GLN
10	J	96	ILE
10	J	98	ILE
11	K	26	ASN
11	K	29	ILE
11	K	31	THR
11	K	32	ILE
11	K	36	ASP
11	K	57	THR
11	K	96	ARG
11	K	114	VAL
11	K	116	HIS
12	L	17	LYS
12	L	18	VAL
12	L	20	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
12	L	27	LEU
12	L	33	ARG
12	L	59	ARG
12	L	62	SER
12	L	81	SER
12	L	89	ARG
12	L	91	LYS
12	L	126	LYS
13	M	3	ARG
13	M	13	LYS
13	M	17	VAL
13	M	19	LEU
13	M	32	GLU
13	M	45	VAL
13	M	48	LEU
13	M	56	LEU
13	M	64	TRP
13	M	66	LEU
13	M	70	LEU
13	M	84	ILE
13	M	88	ARG
13	M	98	VAL
13	M	108	ARG
13	M	114	ARG
13	M	115	LYS
13	M	117	VAL
13	M	122	LYS
14	N	6	LEU
14	N	12	ARG
14	N	32	SER
14	N	33	VAL
14	N	40	CYS
14	N	41	ARG
14	N	44	LEU
15	O	3	ILE
15	O	8	LYS
15	O	24	SER
15	O	26	GLU
15	O	39	LEU
15	O	62	GLN
15	O	64	ARG
15	O	66	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
15	O	82	ILE
15	O	87	ILE
16	P	2	VAL
16	P	11	SER
16	P	20	VAL
16	P	28	ARG
16	P	32	TYR
16	P	67	THR
16	P	69	THR
16	P	72	ARG
17	Q	52	LYS
17	Q	59	ILE
17	Q	62	SER
17	Q	68	ARG
17	Q	74	LEU
17	Q	101	ARG
18	R	26	LEU
18	R	29	PHE
18	R	36	ASN
18	R	41	LYS
18	R	46	GLU
18	R	54	ARG
18	R	76	LEU
18	R	82	THR
18	R	86	VAL
19	S	5	LEU
19	S	10	PHE
19	S	11	VAL
19	S	12	ASP
19	S	13	ASP
19	S	21	GLU
19	S	28	LYS
19	S	29	ARG
19	S	30	LEU
19	S	31	ILE
19	S	37	ARG
19	S	44	MET
19	S	63	THR
19	S	78	ARG
19	S	81	ARG
19	S	83	HIS
20	T	10	LEU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
20	T	13	LEU
20	T	24	LEU
20	T	37	SER
20	T	41	ILE
20	T	45	GLN
20	T	50	GLU
20	T	73	HIS
20	T	84	LEU
20	T	93	GLU
21	U	6	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	204	ASN
2	B	212	GLN
10	J	78	ASN
11	K	26	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1498/1522 (98%)	311 (20%)	50 (3%)
22	V	76/77 (98%)	17 (22%)	1 (1%)
23	X	7/25 (28%)	1 (14%)	0
24	Y	14/17 (82%)	6 (42%)	1 (7%)
All	All	1595/1641 (97%)	335 (21%)	52 (3%)

All (335) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	9	G
1	A	12	U
1	A	26	A
1	A	32	A
1	A	39	G
1	A	48	C
1	A	51	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	61	G
1	A	64	G
1	A	65	U
1	A	66	G
1	A	76	G
1	A	78	G
1	A	79	G
1	A	81	G
1	A	89	U
1	A	90	C
1	A	91	C
1	A	92	G
1	A	95	G
1	A	101	A
1	A	108	G
1	A	116	A
1	A	121	C
1	A	129(A)	G
1	A	130	A
1	A	144	G
1	A	146	G
1	A	147	G
1	A	163	C
1	A	172	A
1	A	173	U
1	A	174	C
1	A	182	U
1	A	189	U
1	A	190	G
1	A	191(A)	G
1	A	195	A
1	A	197	A
1	A	201	C
1	A	209	U
1	A	216	G
1	A	243	A
1	A	244	U
1	A	245	C
1	A	247	G
1	A	251	G
1	A	262	A
1	A	267	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	271	C
1	A	281	G
1	A	289	G
1	A	316	G
1	A	317	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	343	U
1	A	345	C
1	A	346	G
1	A	347	G
1	A	348	G
1	A	352	C
1	A	353	A
1	A	354	G
1	A	355	C
1	A	356	A
1	A	367	U
1	A	372	C
1	A	373	A
1	A	384	G
1	A	388	G
1	A	389	A
1	A	390	C
1	A	397	A
1	A	398	C
1	A	406	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	422	C
1	A	423	G
1	A	424	G
1	A	429	U
1	A	430	A
1	A	436	C
1	A	438	G
1	A	439	A
1	A	465	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	466	C
1	A	467	G
1	A	482	A
1	A	485	G
1	A	486	U
1	A	487	A
1	A	496	A
1	A	497	U
1	A	505	G
1	A	509	A
1	A	510	A
1	A	511	C
1	A	518	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	536	C
1	A	545	C
1	A	547	A
1	A	548	G
1	A	559	A
1	A	561	U
1	A	562	C
1	A	564	C
1	A	568	G
1	A	572	A
1	A	573	A
1	A	576	G
1	A	577	G
1	A	579	G
1	A	596	C
1	A	607	A
1	A	617	G
1	A	630	G
1	A	631	G
1	A	633	G
1	A	649	G
1	A	653	A
1	A	661	G
1	A	665	A
1	A	666	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	688	G
1	A	701	C
1	A	702	A
1	A	704	A
1	A	723	U
1	A	724	G
1	A	731	G
1	A	749	C
1	A	752	G
1	A	753	A
1	A	754	C
1	A	755	G
1	A	759	A
1	A	774	G
1	A	777	A
1	A	792	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	816	A
1	A	817	C
1	A	818	G
1	A	819	A
1	A	821	G
1	A	828	A
1	A	836	G
1	A	841	U
1	A	843	U
1	A	848	C
1	A	859	A
1	A	871	U
1	A	872	A
1	A	902	G
1	A	914	A
1	A	916	G
1	A	920	U
1	A	922	G
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	940	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	960	U
1	A	961	U
1	A	966	G
1	A	968	A
1	A	969	A
1	A	972	C
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	983	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1001	G
1	A	1004	A
1	A	1005	A
1	A	1006	C
1	A	1008	C
1	A	1009	G
1	A	1021	G
1	A	1024	G
1	A	1025	U
1	A	1028	C
1	A	1029	G
1	A	1032(A)	G
1	A	1036	G
1	A	1039	C
1	A	1040	U
1	A	1042	G
1	A	1054	C
1	A	1055	A
1	A	1066	C
1	A	1081	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1124	G
1	A	1125	U
1	A	1126	U
1	A	1127	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1130	A
1	A	1131	G
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1146	A
1	A	1151	A
1	A	1152	A
1	A	1157	A
1	A	1158	C
1	A	1159	U
1	A	1160	G
1	A	1162	C
1	A	1163	C
1	A	1171	G
1	A	1176	A
1	A	1177	G
1	A	1181	G
1	A	1182	G
1	A	1183	A
1	A	1184	G
1	A	1187	G
1	A	1188	A
1	A	1189	C
1	A	1190	G
1	A	1196	U
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1214	C
1	A	1225	A
1	A	1230	C
1	A	1238	A
1	A	1240	U
1	A	1241	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1263	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1267	C
1	A	1270	C
1	A	1272	G
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1305	G
1	A	1320	C
1	A	1321	C
1	A	1322	C
1	A	1323	G
1	A	1331	G
1	A	1334	G
1	A	1336	C
1	A	1337	G
1	A	1338	G
1	A	1347	G
1	A	1348	U
1	A	1353	G
1	A	1362(A)	C
1	A	1364	U
1	A	1397	C
1	A	1400	C
1	A	1419	G
1	A	1442	G
1	A	1446	A
1	A	1447	G
1	A	1452	C
1	A	1453	G
1	A	1454	G
1	A	1487	G
1	A	1492	A
1	A	1499	A
1	A	1502	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1503	A
1	A	1504	G
1	A	1506	U
1	A	1517	G
1	A	1519	A
1	A	1520	G
1	A	1525	G
1	A	1529	G
1	A	1530	G
22	V	3	G
22	V	4	G
22	V	8	G
22	V	12	C
22	V	15	C
22	V	17	U
22	V	18	G
22	V	19	G
22	V	21	A
22	V	22	G
22	V	47	U
22	V	48	C
22	V	49	G
22	V	52	G
22	V	54	U
22	V	67	C
22	V	76	A
23	X	7	U
24	Y	31	G
24	Y	32	U
24	Y	33	U
24	Y	34	C
24	Y	40	G
24	Y	42	G

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	31	G
1	A	60	A
1	A	64	G
1	A	78	G
1	A	89	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	115	G
1	A	181	G
1	A	243	A
1	A	244	U
1	A	250	A
1	A	266	G
1	A	315	A
1	A	328	C
1	A	345	C
1	A	388	G
1	A	410	G
1	A	412	A
1	A	428	G
1	A	429	U
1	A	481	G
1	A	484	G
1	A	485	G
1	A	509	A
1	A	530	G
1	A	560	U
1	A	687	A
1	A	701	C
1	A	703	G
1	A	753	A
1	A	758	G
1	A	793	U
1	A	812	C
1	A	819	A
1	A	913	A
1	A	960	U
1	A	965	A
1	A	991	U
1	A	992	U
1	A	1027	C
1	A	1065	U
1	A	1094	G
1	A	1200	C
1	A	1285	A
1	A	1297	C
1	A	1298	C
1	A	1336	C
1	A	1347	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1446	A
1	A	1498	U
1	A	1503	A
22	V	53	G
24	Y	30	C

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

1 non-standard protein/DNA/RNA residue is 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
24	1MG	Y	37	24	24,26,27	2.77	6 (25%)	34,39,42	4.58	7 (20%)

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
24	1MG	Y	37	24	-	0/8/25/26	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	37	1MG	C4-N3	7.80	1.48	1.35
24	Y	37	1MG	C2-N2	6.61	1.48	1.33
24	Y	37	1MG	C2-N1	5.70	1.45	1.37
24	Y	37	1MG	P-OP1	4.83	1.52	1.46
24	Y	37	1MG	C5-N7	-3.39	1.34	1.38
24	Y	37	1MG	O5'-C5'	-2.14	1.41	1.44

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	37	1MG	C6-C5-N7	-21.95	133.07	134.24
24	Y	37	1MG	C6-N1-C2	11.39	123.83	120.71
24	Y	37	1MG	C2-N3-C4	4.47	120.66	115.30
24	Y	37	1MG	N3-C4-N9	4.44	133.42	126.91
24	Y	37	1MG	C5-C4-N3	-4.41	120.99	126.07
24	Y	37	1MG	N2-C2-N1	3.70	123.47	118.45
24	Y	37	1MG	N3-C2-N1	-3.56	117.42	123.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 78 ligands modelled in this entry, 77 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z  > 2$
26	PAR	A	1673	-	45,45,45	1.36	6 (13%)	67,67,67	1.33	5 (7%)

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
26	PAR	A	1673	-	-	0/18/94/94	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	1673	PAR	C52-C42	3.08	1.58	1.52
26	A	1673	PAR	O54-C14	2.89	1.49	1.41
26	A	1673	PAR	C11-C21	2.78	1.57	1.52
26	A	1673	PAR	C64-C54	2.77	1.58	1.51
26	A	1673	PAR	O51-C11	2.65	1.48	1.41
26	A	1673	PAR	C14-C24	2.24	1.56	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1673	PAR	C14-O54-C54	4.35	122.16	113.73
26	A	1673	PAR	O52-C13-C23	4.24	115.07	107.50
26	A	1673	PAR	O33-C14-C24	4.17	116.32	108.08
26	A	1673	PAR	O54-C54-C64	2.81	111.32	105.97
26	A	1673	PAR	C11-O51-C51	2.60	118.76	113.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.