



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:29 PM GMT

PDB ID : 1TTT
Title : Phe-tRNA, elongation factor EF-TU:GDPNP ternary complex
Authors : Nissen, P.; Kjeldgaard, M.; Thirup, S.; Polekhina, G.; Reshetnikova, L.; Clark, B.F.C.; Nyborg, J.
Deposited on : 1995-11-16
Resolution : 2.70 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

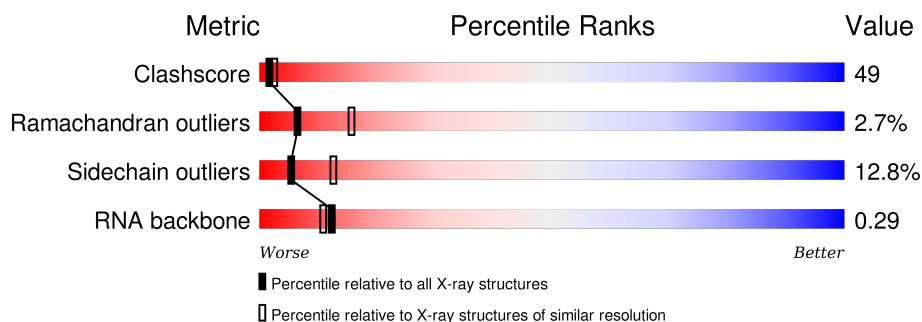
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RNA backbone	2183	1069 (3.10-2.30)

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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	D	76	
1	E	76	
1	F	76	
2	A	405	
2	B	405	
2	C	405	

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
1	M2G	D	26	-	-	X	-
1	2MG	E	10	-	-	X	-
1	M2G	E	26	-	-	X	-
1	2MG	F	10	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14573 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called TRANSFER RIBONUCLEIC ACID (YEAST, PHE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			
1	E	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			
1	F	76	Total	C	N	O	P	0	0	0
			1652	746	294	536	76			

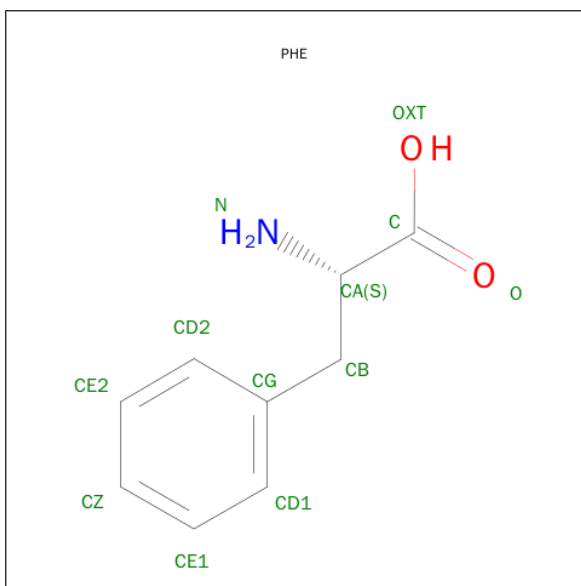
- Molecule 2 is a protein called OF ELONGATION FACTOR TU (EF-TU).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	405	Total	C	N	O	S	0	0	0
			3144	1986	548	598	12			
2	B	405	Total	C	N	O	S	0	0	0
			3144	1986	548	598	12			
2	C	405	Total	C	N	O	S	0	0	0
			3144	1986	548	598	12			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

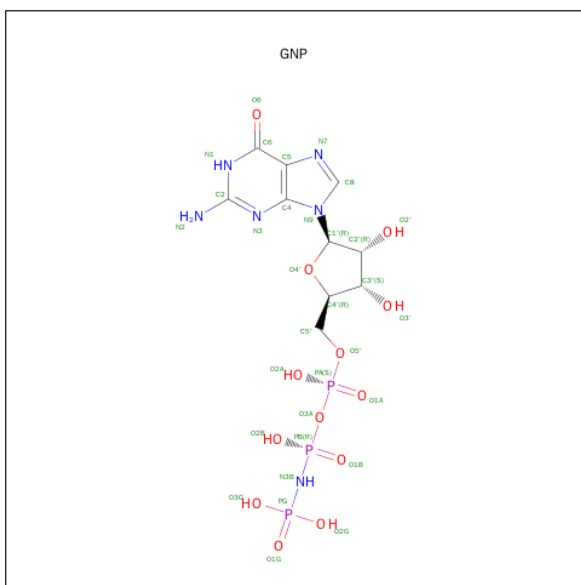
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: $\text{C}_9\text{H}_{11}\text{NO}_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total 11	C 9	N 1	O 1	0	0
4	E	1	Total 11	C 9	N 1	O 1	0	0
4	F	1	Total 11	C 9	N 1	O 1	0	0

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	B	1	Total	C	N	O	P	0	0
			32	10	6	13	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	6	13	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	21	Total	O	0	0
			21	21		
6	B	13	Total	O	0	0
			13	13		
6	C	7	Total	O	0	0
			7	7		
6	D	6	Total	O	0	0
			6	6		
6	E	2	Total	O	0	0
			2	2		
6	F	1	Total	O	0	0
			1	1		

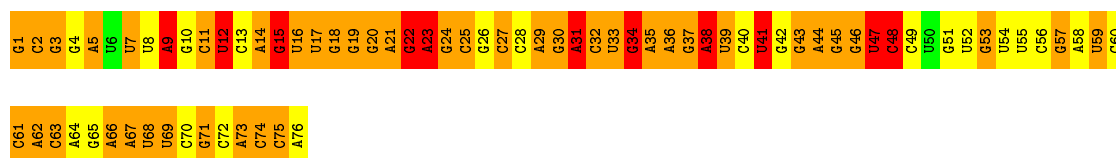
3 Residue-property plots

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.

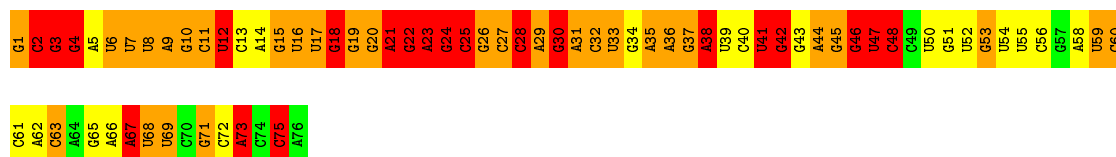
• Molecule 1: TRANSFER RIBONUCLEIC ACID (YEAST, PHE)

Chain D: 



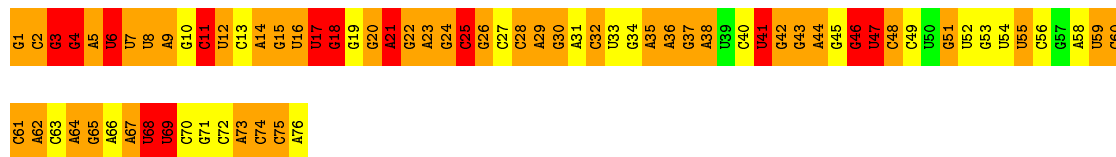
• Molecule 1: TRANSFER RIBONUCLEIC ACID (YEAST, PHE)

Chain E: 



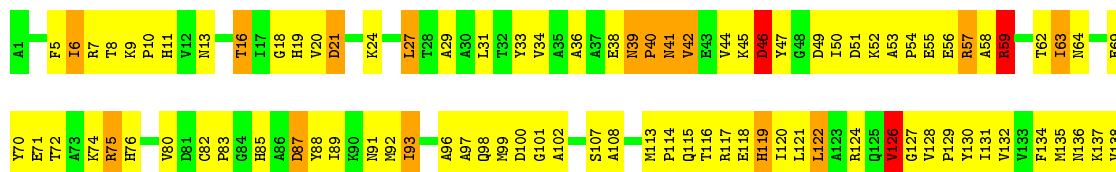
• Molecule 1: TRANSFER RIBONUCLEIC ACID (YEAST, PHE)

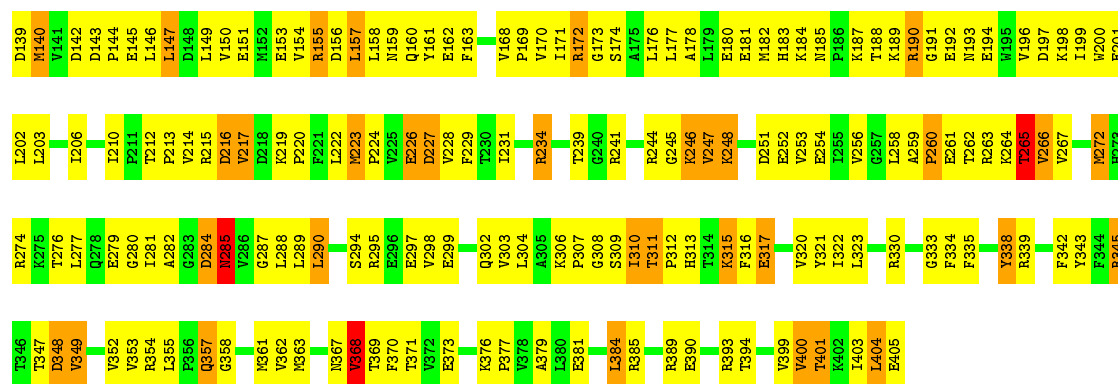
Chain F: 



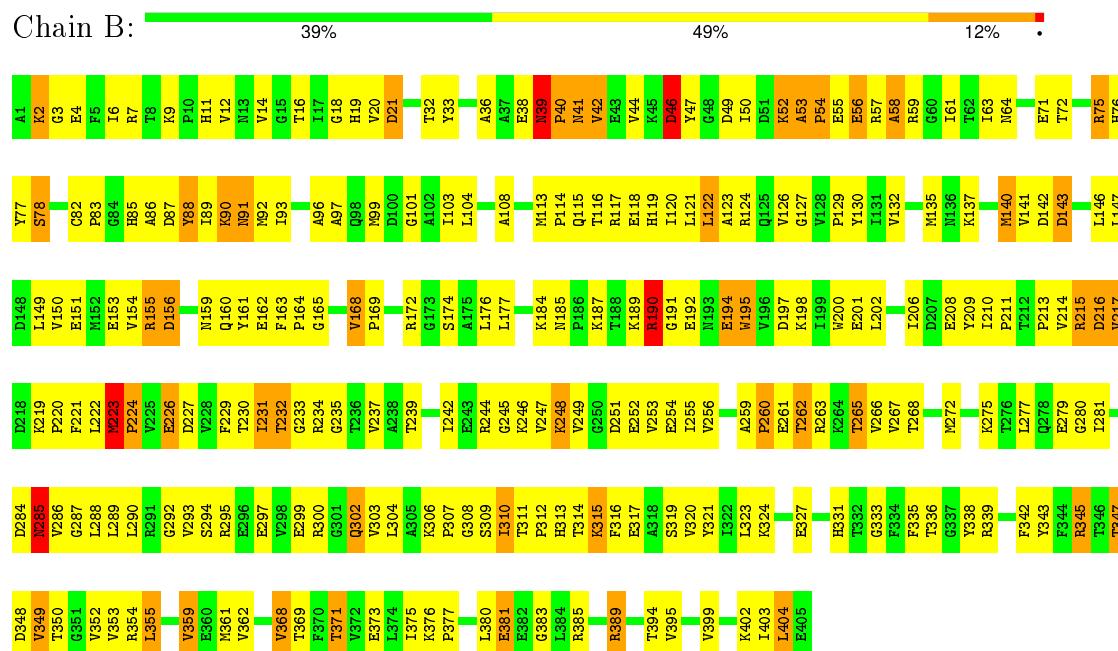
• Molecule 2: OF ELONGATION FACTOR TU (EF-TU)

Chain A: 

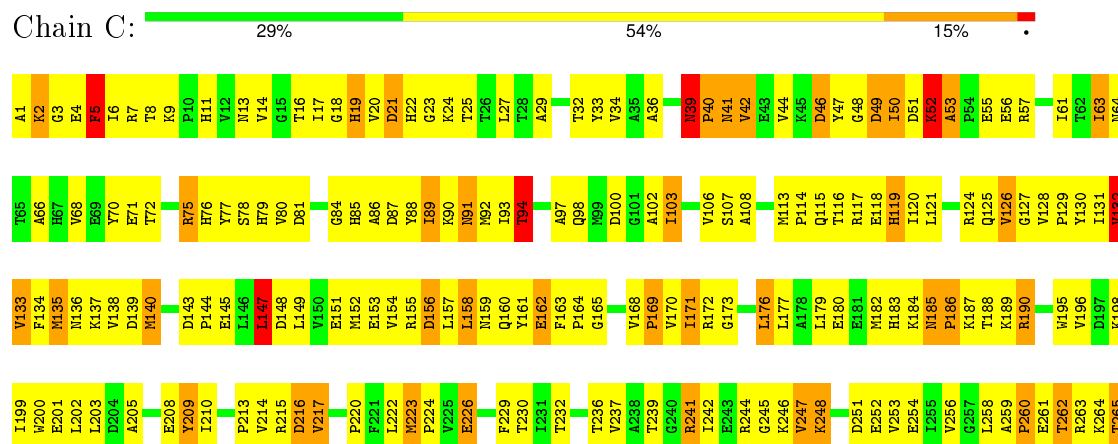




• Molecule 2: OF ELONGATION FACTOR TU (EF-TU)



• Molecule 2: OF ELONGATION FACTOR TU (EF-TU)



V266	E327	L404
V267	F335	E405
T268	T336	
G269	G337	
V270	Y338	
E271	R339	
H272	P340	
H273	Q341	
R274	F342	
I275	Y343	
T276	F344	
L277	R345	
Q278	T346	
E279	T347	
G280	D348	
I281	V349	
A282	T350	
G283	G351	
D284	V352	
V286	V353	
G287	R354	
L288	R355	
L289	P356	
L290	E360	
R291	M361	
G292	V362	
V293	M363	
S294	P364	
R295		
E296	V368	
E297	T369	
V298	F370	
E299	T371	
R300	V372	
G301	E373	
Q302	L374	
V303	I375	
L304	K376	
A305	P377	
K306	V378	
P307	A379	
G308	L380	
S309	E381	
I310		
T311	L384	
P312	R385	
H313		
T314	R389	
K315	E390	
F316	G391	
E317		
A318	T394	
S319		
V320	V399	
Y321	V400	
I322	T401	
L323	K402	
K324	I403	

4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	206.84Å 122.35Å 151.55Å 90.00° 126.30° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70	Depositor
% Data completeness (in resolution range)	91.1 (25.00-2.70)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.206 , 0.290	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	14573	wwPDB-VP
Average B, all atoms (Å ²)	52.0	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: OMC, 5MU, GNP, OMG, H2U, MG, YYG, 2MG, 5MC, 1MA, M2G, 7MG, PSU

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	D	0.46	1/1487 (0.1%)	2.28	87/2315 (3.8%)
1	E	0.47	1/1487 (0.1%)	2.25	92/2315 (4.0%)
1	F	0.45	0/1487	2.21	108/2315 (4.7%)
2	A	0.87	1/3204 (0.0%)	1.52	43/4345 (1.0%)
2	B	0.87	0/3204	1.47	27/4345 (0.6%)
2	C	0.86	0/3204	1.52	35/4345 (0.8%)
All	All	0.76	3/14073 (0.0%)	1.80	392/19980 (2.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	2	0
2	A	2	0
All	All	4	0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	1	G	OP3-P	-7.83	1.51	1.61
1	D	1	G	OP3-P	-5.69	1.54	1.61
2	A	400	VAL	CA-CB	-5.18	1.43	1.54

All (392) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	22	G	O4'-C1'-N9	29.42	131.74	108.20
1	D	33	U	O4'-C1'-N1	20.76	124.81	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	G	O4'-C1'-N9	20.70	124.76	108.20
2	A	39	ASN	C-N-CD	-20.57	75.34	120.60
1	D	21	A	N9-C1'-C2'	-20.07	87.90	114.00
1	E	48	C	O5'-P-OP2	-19.66	87.11	110.70
1	E	15	G	O4'-C1'-N9	-18.97	93.02	108.20
1	D	22	G	N9-C1'-C2'	-18.94	89.38	114.00
2	C	39	ASN	C-N-CD	-18.86	79.10	120.60
1	F	13	C	O4'-C1'-N1	17.62	122.29	108.20
1	D	71	G	O4'-C1'-N9	-17.45	94.24	108.20
2	B	39	ASN	C-N-CD	-17.02	83.16	120.60
1	F	18	G	O4'-C1'-N9	16.54	121.43	108.20
1	D	45	G	O4'-C1'-N9	-16.07	95.34	108.20
1	D	28	C	O4'-C1'-N1	15.57	120.66	108.20
1	D	48	C	O4'-C1'-N1	15.13	120.31	108.20
1	E	21	A	N9-C1'-C2'	-14.93	94.59	114.00
1	F	1	G	O4'-C1'-N9	-14.87	96.30	108.20
1	F	51	G	O4'-C1'-N9	-14.85	96.32	108.20
1	F	21	A	N9-C1'-C2'	-14.69	94.90	114.00
1	E	25	C	O4'-C1'-N1	14.67	119.93	108.20
1	E	38	A	O5'-P-OP1	-14.45	92.69	105.70
1	E	71	G	O4'-C1'-N9	-14.35	96.72	108.20
1	D	18	G	O4'-C1'-N9	14.35	119.68	108.20
1	D	33	U	N1-C1'-C2'	-14.26	95.46	114.00
1	F	11	C	O4'-C1'-N1	14.13	119.50	108.20
1	F	71	G	O4'-C1'-N9	-14.10	96.92	108.20
1	F	68	U	O4'-C1'-N1	13.68	119.15	108.20
1	E	23	A	O4'-C1'-N9	13.38	118.91	108.20
1	F	5	A	O4'-C1'-N9	13.30	118.84	108.20
1	E	3	G	N9-C1'-C2'	-13.22	96.81	114.00
1	E	7	U	O4'-C1'-N1	13.22	118.78	108.20
1	D	47	U	N1-C1'-C2'	13.14	131.08	114.00
1	F	70	C	O4'-C1'-N1	12.76	118.41	108.20
1	D	19	G	O5'-P-OP1	-12.76	94.22	105.70
1	D	47	U	O4'-C1'-N1	12.75	118.40	108.20
1	E	6	U	O4'-C1'-N1	12.54	118.23	108.20
1	D	19	G	N9-C1'-C2'	-12.51	97.74	114.00
1	F	69	U	O4'-C1'-N1	12.37	118.09	108.20
1	E	53	G	O5'-P-OP2	-12.31	94.62	105.70
1	E	59	U	O4'-C1'-N1	12.31	118.05	108.20
1	F	42	G	O4'-C1'-N9	-12.21	98.43	108.20
1	D	38	A	N9-C1'-C2'	-12.15	98.21	114.00
1	E	30	G	O4'-C1'-N9	12.04	117.83	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	48	C	O4'-C1'-N1	12.03	117.82	108.20
1	E	36	A	N9-C1'-C2'	-12.00	98.40	114.00
1	D	42	G	O4'-C1'-N9	-11.98	98.62	108.20
1	E	41	U	O4'-C1'-N1	-11.96	98.63	108.20
1	D	41	U	O4'-C1'-N1	-11.70	98.84	108.20
1	E	47	U	N1-C1'-C2'	11.59	129.06	114.00
1	F	48	C	O4'-C1'-N1	11.51	117.41	108.20
1	F	28	C	O4'-C1'-N1	11.45	117.36	108.20
1	F	73	A	N9-C1'-C2'	-11.38	99.21	114.00
1	D	59	U	O4'-C1'-N1	11.35	117.28	108.20
1	F	9	A	O4'-C1'-N9	11.34	117.27	108.20
1	F	24	G	N9-C1'-C2'	-11.26	99.36	114.00
1	D	7	U	N1-C1'-C2'	-11.17	99.48	114.00
1	F	65	G	O4'-C1'-N9	-11.11	99.31	108.20
1	D	61	C	O4'-C1'-N1	11.11	117.08	108.20
1	E	4	G	O5'-P-OP2	-11.07	95.74	105.70
1	F	3	G	N9-C1'-C2'	-10.96	99.75	114.00
1	E	47	U	O5'-P-OP2	-10.90	95.89	105.70
1	D	3	G	N9-C1'-C2'	-10.66	100.14	114.00
1	D	23	A	O4'-C1'-N9	10.44	116.55	108.20
1	E	66	A	O4'-C1'-N9	-10.42	99.86	108.20
1	E	29	A	O4'-C1'-N9	10.41	116.53	108.20
1	F	66	A	O4'-C1'-N9	-10.40	99.88	108.20
1	F	18	G	N9-C1'-C2'	-10.13	100.83	114.00
1	F	48	C	O5'-P-OP2	-10.12	96.59	105.70
1	F	61	C	O4'-C1'-N1	10.11	116.29	108.20
1	F	25	C	O4'-C1'-N1	10.10	116.28	108.20
1	E	3	G	O4'-C1'-N9	10.08	116.26	108.20
1	D	27	C	O4'-C1'-N1	10.05	116.24	108.20
1	E	24	G	O4'-C1'-N9	-9.94	100.25	108.20
1	F	73	A	O4'-C1'-N9	-9.87	100.31	108.20
1	D	31	A	N9-C1'-C2'	-9.80	101.22	112.00
1	E	38	A	N9-C1'-C2'	-9.80	101.22	112.00
1	E	20	G	O4'-C1'-N9	-9.71	100.43	108.20
1	D	30	G	N9-C1'-C2'	-9.67	101.36	112.00
1	D	23	A	N9-C1'-C2'	9.67	126.57	114.00
1	E	44	A	O4'-C1'-N9	9.66	115.93	108.20
1	F	35	A	O4'-C1'-N9	-9.59	100.53	108.20
1	D	73	A	N9-C1'-C2'	-9.36	101.71	112.00
1	F	36	A	O4'-C1'-N9	9.32	115.66	108.20
1	D	25	C	N1-C1'-C2'	-9.29	101.78	112.00
1	D	66	A	O4'-C1'-N9	-9.29	100.77	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	U	O4'-C1'-N1	-9.27	100.78	108.20
1	E	2	C	OP2-P-O3'	9.24	125.54	105.20
1	F	47	U	N1-C1'-C2'	9.23	126.00	114.00
2	B	184	LYS	CD-CE-NZ	9.22	132.90	111.70
1	E	73	A	O4'-C1'-N9	-9.18	100.86	108.20
1	D	35	A	O4'-C1'-N9	-9.16	100.87	108.20
1	E	56	C	O4'-C1'-N1	-9.15	100.88	108.20
1	D	56	C	O4'-C1'-N1	-9.08	100.93	108.20
1	E	22	G	O5'-P-OP2	-9.08	97.53	105.70
1	E	28	C	N1-C1'-C2'	8.98	125.67	114.00
1	F	15	G	O4'-C1'-N9	-8.94	101.05	108.20
1	E	19	G	O5'-P-OP1	-8.86	97.72	105.70
1	D	18	G	N9-C1'-C2'	-8.82	102.30	112.00
1	F	25	C	N1-C1'-C2'	-8.82	102.30	112.00
1	F	38	A	O4'-C1'-N9	-8.79	101.16	108.20
1	F	43	G	O4'-C1'-N9	-8.77	101.18	108.20
1	F	33	U	O5'-P-OP2	-8.77	97.81	105.70
1	E	67	A	OP2-P-O3'	8.69	124.32	105.20
1	D	37	YYG	OP1-P-O3'	8.63	124.20	105.20
1	D	36	A	O4'-C1'-N9	8.59	115.07	108.20
1	E	6	U	O5'-P-OP1	8.58	120.99	110.70
1	F	24	G	O4'-C1'-N9	8.57	115.06	108.20
1	E	61	C	O4'-C1'-N1	8.42	114.94	108.20
1	E	31	A	O4'-C1'-N9	8.37	114.89	108.20
2	A	59	ARG	NE-CZ-NH1	-8.35	116.12	120.30
1	E	13	C	N1-C1'-C2'	8.34	124.85	114.00
1	D	43	G	O4'-C1'-N9	8.34	114.87	108.20
1	F	51	G	N9-C1'-C2'	8.34	124.84	114.00
1	D	74	C	O4'-C1'-N1	-8.24	101.61	108.20
1	F	47	U	O5'-P-OP2	-8.20	98.32	105.70
1	F	11	C	C2'-C3'-O3'	8.11	127.35	109.50
1	E	28	C	O4'-C1'-N1	8.06	114.65	108.20
1	E	41	U	O5'-P-OP1	8.05	120.36	110.70
1	E	65	G	O5'-P-OP1	-7.95	98.54	105.70
1	F	23	A	O4'-C1'-N9	7.95	114.56	108.20
1	E	60	C	N1-C1'-C2'	-7.94	103.26	112.00
1	D	21	A	C3'-C2'-O2'	-7.90	90.38	113.30
1	F	59	U	O4'-C1'-N1	7.89	114.51	108.20
1	F	44	A	O4'-C1'-N9	-7.87	101.90	108.20
1	F	29	A	O4'-C1'-N9	7.84	114.47	108.20
1	F	7	U	O4'-C1'-N1	-7.83	101.94	108.20
1	D	32	OMC	OP1-P-O3'	-7.80	88.04	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	135	MET	CG-SD-CE	7.79	112.66	100.20
2	B	223	MET	C-N-CD	-7.77	103.50	120.60
2	A	384	LEU	CB-CG-CD1	-7.77	97.79	111.00
1	E	32	OMC	OP1-P-O3'	-7.77	88.11	105.20
1	E	69	U	C2'-C3'-O3'	7.73	126.52	109.50
2	C	209	TYR	CZ-CE2-CD2	-7.71	112.86	119.80
2	A	163	PHE	N-CA-C	-7.67	90.28	111.00
1	E	52	U	O4'-C1'-N1	7.65	114.32	108.20
1	F	48	C	O5'-P-OP1	7.64	119.87	110.70
1	D	5	A	O4'-C1'-N9	7.64	114.31	108.20
1	D	3	G	O4'-C1'-N9	7.59	114.27	108.20
1	D	1	G	O4'-C1'-N9	-7.52	102.19	108.20
2	A	330	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	E	9	A	O4'-C1'-N9	7.46	114.17	108.20
1	E	18	G	N9-C1'-C2'	-7.45	103.80	112.00
1	F	20	G	O3'-P-O5'	-7.43	89.87	104.00
2	B	349	VAL	CB-CA-C	-7.41	97.32	111.40
1	E	12	U	O4'-C1'-N1	7.40	114.12	108.20
1	F	24	G	O5'-P-OP2	-7.39	99.05	105.70
1	E	21	A	O5'-P-OP2	7.38	119.56	110.70
1	E	68	U	N1-C1'-C2'	-7.37	103.89	112.00
2	C	266	VAL	CB-CA-C	-7.36	97.43	111.40
1	F	6	U	O4'-C1'-N1	7.34	114.07	108.20
2	C	185	ASN	C-N-CD	-7.27	104.60	120.60
1	D	7	U	O4'-C1'-N1	7.26	114.01	108.20
1	E	52	U	O5'-P-OP2	-7.24	99.18	105.70
1	F	11	C	N1-C1'-C2'	7.24	123.42	114.00
1	F	20	G	O5'-P-OP2	-7.24	99.19	105.70
1	E	73	A	N9-C1'-C2'	-7.21	104.07	112.00
1	F	55	PSU	OP2-P-O3'	7.21	121.05	105.20
1	D	53	G	O4'-C1'-N9	-7.17	102.46	108.20
1	F	35	A	O5'-P-OP2	7.15	119.28	110.70
1	E	22	G	O4'-C1'-N9	-7.12	102.50	108.20
1	D	63	C	OP1-P-O3'	-7.09	89.60	105.20
1	D	30	G	O4'-C1'-N9	7.09	113.87	108.20
2	B	42	VAL	N-CA-C	-7.08	91.89	111.00
2	C	132	VAL	N-CA-C	-7.07	91.91	111.00
1	F	22	G	O5'-P-OP2	-7.06	99.34	105.70
2	B	90	LYS	CD-CE-NZ	7.05	127.92	111.70
1	F	3	G	O4'-C1'-N9	7.03	113.83	108.20
1	F	76	A	O4'-C1'-N9	7.03	113.83	108.20
1	F	21	A	P-O5'-C5'	-7.03	109.66	120.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	62	A	O4'-C1'-N9	-7.00	102.60	108.20
1	D	9	A	O4'-C1'-N9	7.00	113.80	108.20
2	B	122	LEU	CA-CB-CG	-6.99	99.21	115.30
1	F	53	G	O5'-P-OP1	6.99	119.08	110.70
1	D	64	A	OP1-P-OP2	6.96	130.04	119.60
1	F	31	A	P-O5'-C5'	-6.96	109.77	120.90
1	F	23	A	N9-C1'-C2'	-6.93	104.38	112.00
1	E	47	U	OP2-P-O3'	6.89	120.36	105.20
1	F	43	G	N9-C1'-C2'	-6.87	104.44	112.00
1	D	65	G	O5'-P-OP2	-6.86	99.53	105.70
1	D	36	A	N9-C1'-C2'	-6.84	104.47	112.00
1	D	15	G	O4'-C1'-N9	-6.84	102.73	108.20
1	F	46	7MG	P-O3'-C3'	6.83	127.90	119.70
1	F	20	G	O5'-P-OP1	-6.81	99.57	105.70
1	F	41	U	O4'-C1'-N1	-6.80	102.76	108.20
1	D	22	G	C4'-C3'-O3'	6.80	126.60	113.00
1	E	35	A	O4'-C1'-N9	-6.79	102.77	108.20
1	E	24	G	N9-C1'-C2'	6.78	122.81	114.00
1	F	12	U	N1-C1'-C2'	6.77	122.81	114.00
1	D	68	U	O4'-C1'-N1	6.76	113.61	108.20
1	D	38	A	O5'-P-OP1	-6.75	99.63	105.70
1	D	69	U	C2'-C3'-O3'	6.74	124.48	113.70
2	A	349	VAL	CB-CA-C	-6.73	98.61	111.40
2	B	46	ASP	CB-CG-OD2	-6.73	112.25	118.30
1	E	69	U	O4'-C1'-N1	6.72	113.58	108.20
1	F	53	G	O4'-C1'-N9	-6.71	102.83	108.20
1	F	46	7MG	OP1-P-O3'	6.71	119.95	105.20
1	F	68	U	N1-C1'-C2'	-6.71	104.62	112.00
1	D	3	G	O3'-P-O5'	6.68	116.69	104.00
1	F	31	A	N9-C1'-C2'	-6.68	104.66	112.00
2	A	284	ASP	CB-CG-OD1	-6.64	112.33	118.30
1	D	15	G	N9-C1'-C2'	6.63	122.63	114.00
1	D	21	A	P-O5'-C5'	-6.63	110.28	120.90
2	C	281	ILE	CB-CA-C	-6.61	98.38	111.60
2	C	103	ILE	CB-CA-C	-6.59	98.41	111.60
2	A	367	ASN	N-CA-C	-6.56	93.28	111.00
1	D	62	A	OP2-P-O3'	6.55	119.61	105.20
2	A	59	ARG	NH1-CZ-NH2	6.53	126.59	119.40
2	A	274	ARG	NE-CZ-NH1	6.52	123.56	120.30
2	A	42	VAL	N-CA-C	-6.51	93.43	111.00
1	D	75	C	O5'-P-OP1	6.50	118.49	110.70
1	F	11	C	C3'-C2'-O2'	6.49	132.11	113.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	C	OP2-P-O3'	6.48	119.46	105.20
1	E	68	U	O4'-C1'-N1	6.48	113.38	108.20
2	B	285	ASN	N-CA-C	-6.47	93.52	111.00
1	E	1	G	OP1-P-O3'	6.43	119.34	105.20
1	F	23	A	OP2-P-O3'	6.42	119.32	105.20
1	E	35	A	C3'-C2'-O2'	-6.39	94.77	113.30
2	C	52	LYS	N-CA-C	6.38	128.23	111.00
2	C	354	ARG	NE-CZ-NH1	6.35	123.48	120.30
2	B	190	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	D	7	U	O5'-P-OP2	6.33	118.30	110.70
1	E	53	G	O4'-C1'-N9	-6.32	103.15	108.20
2	A	132	VAL	N-CA-C	-6.31	93.96	111.00
2	B	286	VAL	CB-CA-C	-6.31	99.41	111.40
1	D	18	G	OP1-P-O3'	6.29	119.03	105.20
1	F	30	G	O4'-C1'-N9	6.29	113.23	108.20
1	E	20	G	O5'-P-OP1	-6.27	100.06	105.70
1	E	46	7MG	OP2-P-O3'	6.26	118.98	105.20
1	F	8	U	O4'-C1'-N1	-6.26	103.19	108.20
2	A	51	ASP	N-CA-C	-6.25	94.14	111.00
1	D	20	G	N9-C1'-C2'	-6.24	105.14	112.00
1	F	44	A	N9-C1'-C2'	6.21	122.08	114.00
2	C	241	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	B	121	LEU	CA-CB-CG	-6.20	101.04	115.30
1	D	69	U	O5'-P-OP2	6.20	118.14	110.70
1	E	30	G	C2'-C3'-O3'	6.20	123.62	113.70
2	A	157	LEU	CB-CG-CD1	-6.18	100.50	111.00
2	A	227	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	D	63	C	N1-C1'-C2'	-6.13	105.26	112.00
1	D	64	A	OP2-P-O3'	6.12	118.67	105.20
2	C	127	GLY	N-CA-C	6.10	128.35	113.10
1	D	51	G	N9-C1'-C2'	6.09	121.92	114.00
1	F	20	G	OP2-P-O3'	6.09	118.61	105.20
1	F	21	A	C4'-C3'-O3'	6.09	125.17	113.00
2	A	247	VAL	CB-CA-C	-6.08	99.86	111.40
1	D	3	G	O5'-P-OP2	-6.07	100.24	105.70
2	C	304	LEU	CA-CB-CG	-6.06	101.37	115.30
1	D	24	G	N9-C1'-C2'	-6.04	105.36	112.00
2	A	59	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	C	290	LEU	CB-CG-CD1	-6.03	100.75	111.00
1	E	63	C	OP2-P-O3'	6.03	118.47	105.20
2	B	104	LEU	CB-CG-CD2	-6.03	100.75	111.00
1	E	48	C	O5'-P-OP1	6.02	117.92	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	28	C	C2'-C3'-O3'	6.00	123.31	113.70
1	E	75	C	N1-C1'-C2'	-5.98	105.42	112.00
1	E	38	A	O4'-C1'-N9	-5.97	103.42	108.20
2	C	2	LYS	N-CA-C	-5.97	94.88	111.00
1	E	63	C	O5'-P-OP1	5.96	117.86	110.70
1	F	38	A	N9-C1'-C2'	-5.96	105.44	112.00
2	C	203	LEU	CA-CB-CG	-5.95	101.61	115.30
1	F	11	C	O3'-P-O5'	-5.94	92.72	104.00
1	D	61	C	O5'-P-OP1	-5.93	100.36	105.70
1	F	62	A	O5'-P-OP2	-5.93	100.36	105.70
1	E	65	G	OP2-P-O3'	-5.91	92.19	105.20
1	D	29	A	O3'-P-O5'	-5.91	92.77	104.00
2	A	93	ILE	CG1-CB-CG2	-5.89	98.45	111.40
2	B	227	ASP	CB-CG-OD1	-5.87	113.01	118.30
1	E	8	U	N1-C1'-C2'	-5.87	105.55	112.00
1	E	73	A	O5'-P-OP1	5.85	117.72	110.70
1	E	22	G	OP1-P-O3'	5.84	118.05	105.20
1	F	28	C	N1-C1'-C2'	-5.81	105.61	112.00
2	B	355	LEU	CA-CB-CG	-5.81	101.94	115.30
1	E	30	G	N9-C1'-C2'	-5.80	105.62	112.00
1	E	15	G	C4'-C3'-O3'	-5.79	97.24	109.40
2	C	368	VAL	CB-CA-C	-5.79	100.40	111.40
1	E	24	G	OP2-P-O3'	5.77	117.90	105.20
1	D	11	C	N1-C1'-C2'	-5.77	105.66	112.00
1	F	30	G	N9-C1'-C2'	-5.76	105.66	112.00
1	F	67	A	OP2-P-O3'	5.76	117.88	105.20
2	A	310	ILE	N-CA-C	5.75	126.53	111.00
2	A	315	LYS	CD-CE-NZ	5.75	124.93	111.70
1	D	69	U	O3'-P-O5'	-5.75	93.08	104.00
1	E	42	G	C5'-C4'-O4'	-5.75	102.20	109.10
2	C	385	ARG	NE-CZ-NH2	-5.75	117.43	120.30
2	A	284	ASP	CB-CG-OD2	5.74	123.47	118.30
2	A	352	VAL	CB-CA-C	-5.74	100.49	111.40
1	F	31	A	O4'-C1'-N9	5.74	112.79	108.20
1	D	57	G	O4'-C1'-N9	-5.73	103.62	108.20
2	A	214	VAL	N-CA-C	-5.72	95.55	111.00
2	C	169	PRO	CA-N-CD	-5.72	103.49	111.50
2	C	323	LEU	CA-CB-CG	5.71	128.44	115.30
2	B	121	LEU	CB-CG-CD1	5.71	120.71	111.00
1	F	32	OMC	OP2-P-O3'	5.69	117.72	105.20
2	B	75	ARG	CB-CA-C	-5.68	99.03	110.40
1	D	22	G	O5'-P-OP2	-5.67	100.59	105.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	47	U	OP2-P-O3'	5.67	117.67	105.20
2	A	338	TYR	CB-CA-C	-5.66	99.08	110.40
1	F	36	A	O5'-P-OP2	-5.64	100.62	105.70
1	E	35	A	O5'-P-OP2	5.64	117.47	110.70
1	D	23	A	OP2-P-O3'	5.61	117.55	105.20
2	C	75	ARG	N-CA-C	5.60	126.12	111.00
1	F	4	G	O4'-C1'-N9	5.60	112.68	108.20
1	F	69	U	C2'-C3'-O3'	5.59	122.65	113.70
2	A	155	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	F	3	G	O3'-P-O5'	5.58	114.60	104.00
2	A	285	ASN	N-CA-C	-5.57	95.96	111.00
1	F	14	A	O4'-C1'-N9	5.56	112.65	108.20
1	E	3	G	O3'-P-O5'	5.55	114.56	104.00
2	B	389	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	B	143	ASP	N-CA-C	-5.55	96.03	111.00
1	E	43	G	N9-C1'-C2'	5.51	121.17	114.00
2	C	147	LEU	CB-CA-C	-5.51	99.73	110.20
1	F	31	A	O5'-P-OP2	5.50	117.30	110.70
1	F	72	C	O4'-C1'-N1	5.50	112.60	108.20
2	B	208	GLU	N-CA-C	5.50	125.84	111.00
1	D	71	G	C2'-C3'-O3'	5.48	122.47	113.70
2	C	5	PHE	N-CA-C	5.48	125.79	111.00
1	D	69	U	P-O3'-C3'	-5.47	113.13	119.70
1	D	52	U	O5'-P-OP2	-5.46	100.78	105.70
2	A	246	LYS	N-CA-C	5.45	125.72	111.00
1	D	70	C	N1-C1'-C2'	-5.45	106.01	112.00
1	E	42	G	O5'-C5'-C4'	-5.45	101.35	111.70
2	C	285	ASN	N-CA-C	-5.44	96.32	111.00
2	C	208	GLU	N-CA-C	5.42	125.65	111.00
1	D	12	U	O4'-C1'-N1	-5.41	103.87	108.20
1	E	69	U	O3'-P-O5'	-5.41	93.71	104.00
2	C	310	ILE	CB-CA-C	-5.40	100.79	111.60
2	A	265	THR	CB-CA-C	-5.40	97.02	111.60
2	A	345	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	E	29	A	O3'-P-O5'	-5.36	93.81	104.00
2	A	87	ASP	CB-CA-C	-5.36	99.67	110.40
1	F	47	U	O4'-C1'-N1	-5.36	103.91	108.20
2	C	298	VAL	CB-CA-C	-5.36	101.21	111.40
1	F	11	C	C4'-C3'-O3'	5.36	123.72	113.00
1	F	62	A	O5'-P-OP1	5.36	117.13	110.70
1	F	74	C	O4'-C1'-N1	-5.35	103.92	108.20
2	C	94	THR	N-CA-CB	5.35	120.46	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	17	H2U	OP2-P-O3'	5.35	116.97	105.20
1	F	12	U	O5'-P-OP2	5.35	117.12	110.70
2	A	75	ARG	CB-CA-C	-5.34	99.71	110.40
2	A	122	LEU	CB-CG-CD2	-5.34	101.92	111.00
2	A	368	VAL	CB-CA-C	-5.34	101.26	111.40
2	A	310	ILE	CB-CA-C	-5.33	100.94	111.60
2	C	304	LEU	CB-CG-CD2	-5.33	101.94	111.00
2	B	78	SER	N-CA-C	-5.32	96.65	111.00
1	D	23	A	O5'-P-OP2	-5.30	100.93	105.70
1	F	22	G	OP1-P-O3'	5.30	116.87	105.20
1	F	11	C	C1'-C2'-O2'	5.29	126.45	110.60
1	E	35	A	OP2-P-O3'	5.28	116.82	105.20
2	C	338	TYR	C-N-CA	-5.26	108.55	121.70
2	B	345	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	B	395	VAL	C-N-CA	-5.22	111.33	122.30
1	E	67	A	O4'-C1'-N9	5.22	112.38	108.20
1	F	60	C	N1-C1'-C2'	-5.21	106.27	112.00
1	F	68	U	O5'-P-OP2	-5.21	101.01	105.70
1	D	27	C	O5'-P-OP2	5.21	116.95	110.70
1	E	73	A	O5'-P-OP2	-5.20	101.02	105.70
1	F	11	C	P-O3'-C3'	-5.20	113.47	119.70
1	D	22	G	OP1-P-O3'	5.18	116.61	105.20
2	A	330	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	F	20	G	O4'-C1'-N9	-5.18	104.06	108.20
2	B	315	LYS	CB-CA-C	-5.17	100.05	110.40
1	F	70	C	N1-C1'-C2'	-5.16	106.33	112.00
2	B	56	GLU	N-CA-C	-5.15	97.09	111.00
1	E	1	G	C2'-C3'-O3'	5.15	121.94	113.70
2	C	42	VAL	N-CA-C	-5.14	97.11	111.00
2	A	272	MET	N-CA-C	-5.14	97.12	111.00
2	A	212	THR	N-CA-C	-5.14	97.12	111.00
2	B	162	GLU	N-CA-C	5.13	124.85	111.00
2	A	323	LEU	CA-CB-CG	5.12	127.08	115.30
2	A	400	VAL	CA-CB-CG1	-5.11	103.24	110.90
1	E	25	C	O5'-P-OP2	-5.10	101.11	105.70
1	F	41	U	O5'-P-OP1	5.10	116.82	110.70
2	C	49	ASP	CB-CG-OD1	-5.10	113.71	118.30
2	A	27	LEU	CA-CB-CG	-5.08	103.61	115.30
2	A	46	ASP	CB-CG-OD1	-5.08	113.72	118.30
2	C	53	ALA	N-CA-C	-5.08	97.27	111.00
1	F	64	A	P-O5'-C5'	-5.08	112.78	120.90
2	A	266	VAL	CB-CA-C	-5.08	101.76	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	2	C	OP2-P-O3'	5.07	116.36	105.20
1	F	12	U	O3'-P-O5'	5.07	113.62	104.00
2	C	133	VAL	CB-CA-C	-5.05	101.80	111.40
2	C	162	GLU	N-CA-C	5.04	124.61	111.00
2	B	195	TRP	N-CA-CB	-5.04	101.53	110.60
1	E	28	C	O5'-P-OP2	-5.03	101.17	105.70
1	F	56	C	O5'-P-OP1	-5.03	101.17	105.70
1	D	70	C	O5'-P-OP1	5.03	116.73	110.70
1	F	62	A	C1'-C2'-O2'	-5.03	95.52	110.60
1	D	34	OMG	OP1-P-O3'	5.02	116.24	105.20
2	A	126	VAL	CB-CA-C	5.01	120.92	111.40
1	E	31	A	N9-C1'-C2'	-5.01	106.49	112.00

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	11	C	C2',C3'
2	A	232	THR	CA
2	A	311	THR	CA

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	D	1652	0	856	116	0
1	E	1652	0	855	131	0
1	F	1652	0	856	108	0
2	A	3144	0	3161	282	0
2	B	3144	0	3160	302	0
2	C	3144	0	3162	362	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1	0	0	0	0
4	D	11	0	8	2	0
4	E	11	0	8	1	0
4	F	11	0	8	1	0
5	A	32	0	13	6	0
5	B	32	0	13	7	0
5	C	32	0	13	7	0
6	A	21	0	0	5	0
6	B	13	0	0	0	0
6	C	7	0	0	1	0
6	D	6	0	0	0	0
6	E	2	0	0	1	0
6	F	1	0	0	0	0
All	All	14573	0	12113	1273	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 49.

All (1273) 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:E:9:A:H5'	1:E:46:7MG:H1'	1.22	1.15
2:A:217:VAL:HG12	2:A:246:LYS:HD3	1.28	1.11
2:A:54:PRO:HA	2:A:57:ARG:HG3	1.21	1.08
2:A:389:ARG:HG2	2:A:394:THR:HA	1.32	1.05
2:A:101:GLY:HA3	2:A:210:ILE:HD13	1.40	1.02
2:C:158:LEU:HD12	2:C:163:PHE:HB2	1.42	1.00
2:A:85:HIS:HD2	2:A:87:ASP:H	1.05	0.98
1:F:14:A:H2'	1:F:15:G:H5'	1.44	0.98
1:E:23:A:H2'	1:E:24:G:C8	1.98	0.98
2:C:68:VAL:HG22	2:C:79:HIS:HB3	1.47	0.97
2:B:18:GLY:H	2:B:119:HIS:HD2	1.04	0.97
1:F:10:2MG:HM23	1:F:11:C:H1'	1.46	0.97
2:C:18:GLY:H	2:C:119:HIS:HD2	1.06	0.96
1:E:10:2MG:HM23	1:E:11:C:H1'	1.46	0.96
2:C:354:ARG:HG3	2:C:354:ARG:HH11	1.31	0.95
1:E:14:A:H2'	1:E:15:G:H5'	1.49	0.95
2:A:311:THR:HG22	2:A:312:PRO:HD2	1.46	0.95
2:C:56:GLU:HG3	2:C:63:ILE:HG23	1.50	0.93
2:A:55:GLU:HG3	2:A:59:ARG:HG3	1.48	0.93
2:B:217:VAL:HG12	2:B:246:LYS:HD3	1.51	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:28:C:H42	1:E:42:G:H1	0.99	0.92
2:C:389:ARG:HG2	2:C:394:THR:HA	1.51	0.91
1:E:28:C:N4	1:E:42:G:H1	1.66	0.91
2:A:259:ALA:HB1	2:A:260:PRO:HD2	1.53	0.90
1:D:27:C:H42	1:D:43:G:H1	1.16	0.90
2:B:265:THR:HG21	2:B:290:LEU:HB3	1.53	0.90
2:B:19:HIS:HD2	2:B:115:GLN:H	1.14	0.90
2:C:263:ARG:HH21	2:C:297:GLU:HB3	1.37	0.89
2:B:335:PHE:CD1	2:B:361:MET:HB2	2.06	0.89
2:B:53:ALA:HB3	2:B:56:GLU:HB2	1.54	0.89
2:A:97:ALA:HA	2:A:126:VAL:HG13	1.53	0.89
1:D:11:C:H2'	1:D:12:U:H6	1.37	0.89
1:E:25:C:H2'	1:E:26:M2G:C8	2.08	0.88
2:C:169:PRO:HD2	2:C:209:TYR:CE2	2.08	0.88
2:C:316:PHE:HA	2:C:404:LEU:HD22	1.55	0.88
1:D:37:YYG:H31	1:D:37:YYG:H1'	1.55	0.88
2:B:213:PRO:HG2	2:B:215:ARG:CZ	2.03	0.88
1:E:11:C:H2'	1:E:12:U:H6	1.37	0.87
2:B:129:PRO:HB2	2:B:130:TYR:CD1	2.09	0.87
2:B:368:VAL:HG12	2:B:369:THR:H	1.37	0.87
2:A:54:PRO:CA	2:A:57:ARG:HG3	2.05	0.87
1:E:25:C:H2'	1:E:26:M2G:H8	1.37	0.87
1:E:15:G:H2'	1:E:16:H2U:H62	1.55	0.86
2:B:316:PHE:HA	2:B:404:LEU:HD22	1.57	0.86
2:B:354:ARG:HH11	2:B:354:ARG:HG3	1.40	0.86
2:C:132:VAL:HG23	2:C:209:TYR:HD2	1.41	0.86
1:D:11:C:H2'	1:D:12:U:C6	2.11	0.86
2:B:389:ARG:HG2	2:B:394:THR:HA	1.58	0.86
2:B:85:HIS:HD2	2:B:87:ASP:H	1.25	0.85
1:D:30:G:C2'	1:D:31:A:H5'	2.07	0.85
2:B:252:GLU:HA	2:B:266:VAL:HA	1.59	0.84
2:B:335:PHE:CE1	2:B:361:MET:HB2	2.13	0.84
2:C:19:HIS:HD2	2:C:115:GLN:H	1.24	0.84
2:B:259:ALA:HB1	2:B:260:PRO:HD2	1.60	0.84
1:D:15:G:C2'	1:D:16:H2U:H5'	2.08	0.84
2:C:272:MET:HE3	2:C:285:ASN:H	1.43	0.84
1:E:41:U:H2'	1:E:42:G:C8	2.11	0.84
2:B:82:CYS:HB3	2:B:83:PRO:HD2	1.58	0.84
2:C:259:ALA:HB1	2:C:260:PRO:HD2	1.58	0.84
1:F:40:5MC:C2'	1:F:41:U:H5'	2.08	0.84
1:E:14:A:C2'	1:E:15:G:H5'	2.08	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:A:H2'	1:D:24:G:H8	1.43	0.83
1:D:13:C:H2'	1:D:14:A:H8	1.43	0.83
1:E:23:A:H2'	1:E:24:G:H8	1.39	0.83
2:B:18:GLY:H	2:B:119:HIS:CD2	1.94	0.83
2:A:217:VAL:CG1	2:A:246:LYS:HD3	2.09	0.83
1:E:36:A:C2'	1:E:37:YYG:H5'	2.08	0.83
2:C:311:THR:HG22	2:C:312:PRO:HD2	1.61	0.82
2:B:129:PRO:HB2	2:B:130:TYR:CE1	2.14	0.82
1:F:16:H2U:H62	1:F:16:H2U:H5''	1.58	0.82
2:B:52:LYS:NZ	2:B:52:LYS:HB2	1.91	0.82
2:A:368:VAL:HG12	2:A:369:THR:H	1.42	0.82
2:B:217:VAL:CG1	2:B:246:LYS:HD3	2.09	0.81
2:B:313:HIS:CD2	2:B:403:ILE:HG21	2.14	0.81
2:C:97:ALA:HA	2:C:126:VAL:HG13	1.62	0.81
1:E:26:M2G:HM12	1:E:44:A:H2	1.45	0.81
1:E:24:G:C2'	1:E:25:C:H5'	2.10	0.81
1:D:23:A:H2'	1:D:24:G:C8	2.16	0.81
2:A:272:MET:HE3	2:A:285:ASN:H	1.45	0.81
2:A:264:LYS:HE2	2:A:307:PRO:HB3	1.62	0.81
2:B:63:ILE:HG13	2:B:64:ASN:N	1.95	0.81
1:F:36:A:C2'	1:F:37:YYG:H5'	2.10	0.81
2:A:63:ILE:HG13	2:A:64:ASN:N	1.95	0.80
1:E:24:G:H2'	1:E:25:C:O4'	1.79	0.80
2:B:19:HIS:CD2	2:B:115:GLN:H	2.00	0.80
1:E:10:2MG:HM23	1:E:11:C:C1'	2.11	0.80
1:E:11:C:H2'	1:E:12:U:C6	2.16	0.80
2:C:158:LEU:HD12	2:C:163:PHE:CB	2.11	0.80
1:F:14:A:C2'	1:F:15:G:H5'	2.11	0.80
1:D:10:2MG:N2	1:D:26:M2G:H1'	1.97	0.80
2:A:224:PRO:HA	2:A:303:VAL:HG22	1.64	0.79
2:A:252:GLU:HA	2:A:266:VAL:HA	1.64	0.79
1:F:9:A:H5'	1:F:46:7MG:H1'	1.63	0.79
1:E:9:A:C5'	1:E:46:7MG:H1'	2.09	0.79
2:C:18:GLY:H	2:C:119:HIS:CD2	1.97	0.79
2:A:55:GLU:HG3	2:A:59:ARG:CG	2.12	0.79
2:A:36:ALA:HA	2:A:42:VAL:HB	1.65	0.79
1:F:64:A:C4'	2:C:391:GLY:HA2	2.12	0.79
1:D:27:C:N4	1:D:43:G:H1	1.81	0.79
1:D:24:G:H2'	1:D:25:C:H6	1.47	0.78
2:B:113:MET:HB3	2:B:114:PRO:HD2	1.64	0.78
2:C:335:PHE:CE1	2:C:361:MET:HB2	2.19	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:19:HIS:HD2	2:A:115:GLN:H	1.30	0.78
1:E:39:PSU:H4'	2:C:360:GLU:CD	2.04	0.78
2:B:261:GLU:OE1	2:B:262:THR:HG23	1.84	0.78
2:B:299:GLU:O	2:B:302:GLN:HG3	1.84	0.78
2:C:19:HIS:CD2	2:C:115:GLN:H	2.02	0.77
2:A:313:HIS:CD2	2:A:403:ILE:HG21	2.18	0.77
2:A:92:MET:HE3	2:A:119:HIS:HA	1.66	0.77
2:C:149:LEU:O	2:C:153:GLU:HG3	1.84	0.77
2:C:356:PRO:HD3	2:C:370:PHE:HB3	1.66	0.77
2:B:315:LYS:HB3	2:B:404:LEU:HB2	1.65	0.77
2:B:92:MET:HG3	2:B:119:HIS:CE1	2.20	0.77
2:B:231:ILE:HG22	2:B:234:ARG:HB2	1.66	0.77
2:C:313:HIS:O	2:C:377:PRO:HA	1.86	0.76
1:E:37:YYG:H31	1:E:37:YYG:H1'	1.66	0.76
2:C:131:ILE:HD12	2:C:163:PHE:CD1	2.20	0.76
1:F:37:YYG:H1'	1:F:37:YYG:H31	1.67	0.76
2:B:53:ALA:HB3	2:B:56:GLU:CB	2.15	0.76
2:A:215:ARG:HG2	2:A:282:ALA:O	1.85	0.76
2:B:21:ASP:HA	5:B:406:GNP:HNB3	1.48	0.76
2:C:132:VAL:HG22	2:C:169:PRO:HG2	1.65	0.76
2:A:311:THR:CG2	2:A:312:PRO:HD2	2.16	0.76
1:D:47:U:O4	1:F:37:YYG:H5''	1.85	0.76
2:A:389:ARG:HG2	2:A:394:THR:CA	2.12	0.76
1:F:1:G:C2'	1:F:2:C:H5'	2.16	0.76
1:D:15:G:O2'	1:D:16:H2U:H5'	1.86	0.75
2:C:50:ILE:O	2:C:52:LYS:HG2	1.87	0.75
1:F:28:C:H2'	1:F:29:A:C8	2.21	0.75
1:E:36:A:O2'	1:E:37:YYG:H5'	1.85	0.75
2:C:195:TRP:CE3	2:C:195:TRP:HA	2.21	0.75
2:C:272:MET:CE	2:C:285:ASN:H	2.00	0.75
1:F:1:G:O2'	1:F:2:C:H5'	1.86	0.75
1:F:36:A:O2'	1:F:37:YYG:H5'	1.85	0.74
2:C:68:VAL:CG2	2:C:79:HIS:HB3	2.17	0.74
1:F:40:5MC:H2'	1:F:41:U:H5'	1.68	0.74
2:A:9:LYS:HE3	2:A:71:GLU:OE1	1.88	0.74
2:A:261:GLU:OE1	2:A:262:THR:HG23	1.86	0.74
2:A:139:ASP:OD1	2:A:140:MET:HG2	1.87	0.74
2:B:142:ASP:HA	2:B:147:LEU:HD11	1.70	0.74
1:F:28:C:H42	1:F:42:G:H1	1.36	0.73
2:C:33:TYR:CE1	2:C:44:VAL:HG21	2.23	0.73
2:B:33:TYR:CE2	2:B:44:VAL:HG21	2.23	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:97:ALA:HA	2:B:126:VAL:HG13	1.69	0.73
2:C:11:HIS:ND1	2:C:76:HIS:ND1	2.33	0.73
2:C:256:VAL:HG11	2:C:310:ILE:CG2	2.17	0.73
2:B:38:GLU:HG3	2:B:200:TRP:HZ2	1.53	0.73
2:B:315:LYS:CB	2:B:404:LEU:HB2	2.18	0.73
2:C:46:ASP:O	2:C:50:ILE:HG12	1.89	0.73
2:C:287:GLY:C	2:C:288:LEU:HD23	2.09	0.73
2:A:140:MET:HE3	2:A:140:MET:HA	1.71	0.72
1:F:10:2MG:H2'	1:F:11:C:H6	1.54	0.72
2:B:19:HIS:HD2	2:B:115:GLN:N	1.88	0.72
2:A:357:GLN:HG2	2:A:358:GLY:N	2.04	0.72
1:F:37:YYG:C1'	1:F:37:YYG:H31	2.20	0.72
2:C:252:GLU:HA	2:C:266:VAL:HA	1.72	0.72
1:F:64:A:O4'	2:C:391:GLY:HA2	1.89	0.72
1:F:40:5MC:O2'	1:F:41:U:H5'	1.88	0.72
2:C:261:GLU:OE1	2:C:262:THR:HG23	1.90	0.72
1:F:28:C:H2'	1:F:29:A:H8	1.55	0.72
2:B:389:ARG:CG	2:B:394:THR:HA	2.19	0.72
2:A:313:HIS:O	2:A:377:PRO:HA	1.90	0.71
2:C:335:PHE:CD1	2:C:361:MET:HB2	2.25	0.71
1:F:16:H2U:H62	1:F:16:H2U:C5'	2.20	0.71
1:E:30:G:H5''	1:E:31:A:OP2	1.89	0.71
2:A:188:THR:HG23	2:A:192:GLU:HB2	1.72	0.71
2:B:63:ILE:HB	2:B:88:TYR:CE2	2.26	0.71
2:C:338:TYR:O	2:C:353:VAL:HG23	1.90	0.71
2:C:164:PRO:O	2:C:168:VAL:HG23	1.90	0.71
2:A:91:ASN:HA	6:A:427:HOH:O	1.91	0.71
2:B:117:ARG:HD3	2:B:161:TYR:OH	1.91	0.70
2:B:187:LYS:O	2:B:189:LYS:HD3	1.91	0.70
2:A:19:HIS:CG	2:A:113:MET:HB2	2.25	0.70
1:D:26:M2G:N3	1:D:26:M2G:H2'	2.04	0.70
2:C:355:LEU:HD22	2:C:362:VAL:HG23	1.72	0.70
1:E:37:YYG:C1'	1:E:37:YYG:H31	2.21	0.70
2:B:52:LYS:HZ2	2:B:52:LYS:HB2	1.55	0.70
2:A:74:LYS:HG3	6:A:428:HOH:O	1.91	0.70
1:F:8:U:H5'	1:F:49:5MC:OP2	1.92	0.70
2:A:52:LYS:O	2:A:57:ARG:HD2	1.92	0.69
2:B:335:PHE:HD1	2:B:361:MET:HB2	1.57	0.69
2:C:272:MET:HE3	2:C:285:ASN:N	2.06	0.69
2:C:147:LEU:HD13	2:C:172:ARG:HD3	1.72	0.69
2:B:277:LEU:CD2	2:B:280:GLY:HA2	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:2MG:CM2	1:E:11:C:H1'	2.22	0.69
2:A:335:PHE:HA	2:A:355:LEU:HD11	1.73	0.69
2:B:272:MET:HE3	2:B:285:ASN:H	1.58	0.69
2:C:117:ARG:HD3	2:C:161:TYR:OH	1.93	0.69
1:E:23:A:O2'	1:E:24:G:H5'	1.93	0.69
2:C:85:HIS:CD2	2:C:87:ASP:H	2.11	0.69
2:C:132:VAL:CG2	2:C:209:TYR:HD2	2.05	0.69
2:B:354:ARG:NH1	2:B:354:ARG:HG3	2.07	0.69
1:E:1:G:C2'	1:E:2:C:H5'	2.23	0.69
1:D:17:H2U:H4'	1:D:18:G:H5''	1.75	0.69
2:B:103:ILE:HD11	2:B:206:ILE:HD11	1.74	0.68
1:D:37:YYG:C1'	1:D:37:YYG:H31	2.23	0.68
1:D:38:A:H2'	1:D:38:A:N3	2.07	0.68
2:C:306:LYS:HB3	2:C:309:SER:HB3	1.74	0.68
2:B:223:MET:HB2	2:B:242:ILE:HA	1.75	0.68
1:F:47:U:H5'	1:F:48:C:H5''	1.75	0.68
2:C:277:LEU:HD23	2:C:280:GLY:HA2	1.74	0.68
2:B:215:ARG:N	2:B:215:ARG:HD2	2.08	0.68
2:C:229:PHE:HE1	2:C:239:THR:HG21	1.59	0.68
1:D:1:G:C2'	1:D:2:C:H5'	2.23	0.68
1:F:10:2MG:HM23	1:F:11:C:C1'	2.23	0.68
2:A:222:LEU:HD11	2:A:303:VAL:HG11	1.74	0.68
2:B:389:ARG:HG2	2:B:394:THR:CA	2.23	0.68
2:A:18:GLY:H	2:A:119:HIS:HD2	1.42	0.68
1:F:19:G:H4'	1:F:20:G:C4	2.29	0.68
1:E:26:M2G:HM12	1:E:44:A:C2	2.27	0.68
2:A:53:ALA:O	2:A:56:GLU:HB2	1.93	0.68
2:B:256:VAL:O	2:B:302:GLN:HB3	1.94	0.68
1:F:1:G:OP3	2:C:300:ARG:NH1	2.27	0.67
2:A:338:TYR:O	2:A:353:VAL:HG23	1.94	0.67
2:A:147:LEU:HB3	2:A:172:ARG:NH1	2.09	0.67
2:C:263:ARG:NH2	2:C:297:GLU:HB3	2.09	0.67
2:B:313:HIS:O	2:B:377:PRO:HA	1.94	0.67
1:F:64:A:H4'	2:C:391:GLY:HA2	1.75	0.67
1:D:1:G:O2'	1:D:2:C:H5'	1.94	0.67
2:A:219:LYS:HB3	2:A:220:PRO:HD2	1.76	0.67
2:B:375:ILE:HG13	2:B:376:LYS:HG3	1.77	0.67
1:D:24:G:H2'	1:D:25:C:C6	2.29	0.67
1:E:38:A:N3	1:E:38:A:H2'	2.09	0.67
2:C:288:LEU:HD23	2:C:288:LEU:N	2.09	0.67
1:D:19:G:H4'	1:D:20:G:C4	2.30	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:YYG:C10	1:F:37:YYG:HN20	2.08	0.66
2:C:56:GLU:CG	2:C:63:ILE:HG23	2.25	0.66
2:B:40:PRO:CG	2:B:41:ASN:H	2.08	0.66
2:B:85:HIS:CD2	2:B:87:ASP:H	2.12	0.66
2:B:198:LYS:HE3	2:B:201:GLU:OE2	1.94	0.66
2:A:120:ILE:HD13	2:A:158:LEU:HD23	1.77	0.66
2:C:389:ARG:HG2	2:C:394:THR:CA	2.25	0.66
2:C:300:ARG:NH2	2:C:348:ASP:OD1	2.29	0.66
2:C:85:HIS:HD2	2:C:87:ASP:H	1.42	0.66
2:B:89:ILE:HG22	2:B:93:ILE:HD11	1.78	0.66
2:C:18:GLY:N	2:C:119:HIS:HD2	1.86	0.66
2:A:46:ASP:O	2:A:50:ILE:HG13	1.96	0.66
2:A:384:LEU:O	2:A:399:VAL:HG23	1.94	0.66
2:C:56:GLU:CG	2:C:63:ILE:H	2.09	0.66
2:B:229:PHE:HE1	2:B:239:THR:HG21	1.60	0.66
2:A:85:HIS:CD2	2:A:87:ASP:H	1.98	0.66
2:C:19:HIS:HD2	2:C:115:GLN:N	1.92	0.66
1:D:40:5MC:C2'	1:D:41:U:H5'	2.26	0.66
1:F:37:YYG:H103	2:A:335:PHE:CE2	2.31	0.65
2:B:248:LYS:HD3	2:B:248:LYS:N	2.11	0.65
2:B:18:GLY:N	2:B:119:HIS:HD2	1.87	0.65
1:D:30:G:O2'	1:D:31:A:H5'	1.96	0.65
1:D:39:PSU:O2'	1:D:40:5MC:H5'	1.96	0.65
1:D:74:C:OP1	2:A:52:LYS:NZ	2.30	0.65
2:C:132:VAL:HG23	2:C:209:TYR:CD2	2.30	0.65
1:D:40:5MC:H2'	1:D:41:U:H5'	1.77	0.65
2:A:33:TYR:CE1	2:A:44:VAL:HG21	2.31	0.65
2:A:306:LYS:HB3	2:A:309:SER:HB3	1.78	0.65
2:C:384:LEU:O	2:C:399:VAL:HG23	1.95	0.65
2:B:53:ALA:HB3	2:B:56:GLU:CG	2.26	0.65
2:B:354:ARG:HH12	2:B:373:GLU:CD	1.99	0.65
2:B:312:PRO:O	2:B:313:HIS:ND1	2.30	0.65
2:B:7:ARG:NH2	2:B:284:ASP:OD1	2.30	0.65
2:A:389:ARG:CG	2:A:394:THR:HA	2.19	0.65
1:F:41:U:H2'	1:F:42:G:O4'	1.95	0.65
2:C:118:GLU:OE2	2:C:389:ARG:NH1	2.30	0.65
2:A:248:LYS:HE3	2:A:251:ASP:OD2	1.97	0.65
2:B:19:HIS:CG	2:B:113:MET:HB2	2.31	0.65
2:C:91:ASN:OD1	2:C:91:ASN:N	2.28	0.65
1:E:24:G:H2'	1:E:25:C:H5'	1.77	0.65
1:E:26:M2G:HM23	1:E:27:C:O4'	1.95	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:261:GLU:OE1	2:C:262:THR:N	2.30	0.65
1:D:58:1MA:H5'	1:F:34:OMG:O6	1.98	0.64
2:B:316:PHE:CA	2:B:404:LEU:HD22	2.26	0.64
2:C:317:GLU:HB3	2:C:401:THR:HG22	1.78	0.64
2:C:155:ARG:NH2	2:C:170:VAL:HG23	2.12	0.64
1:E:36:A:H2'	1:E:37:YYG:H8	1.79	0.64
1:D:16:H2U:H4'	1:D:17:H2U:OP2	1.96	0.64
1:D:47:U:C4	1:F:37:YYG:H5''	2.32	0.64
2:C:253:VAL:N	2:C:265:THR:O	2.30	0.64
2:A:62:THR:HG22	2:A:83:PRO:HB3	1.78	0.64
2:A:155:ARG:NH1	2:A:168:VAL:O	2.30	0.64
1:D:7:U:H4'	1:D:8:U:OP2	1.97	0.64
2:A:55:GLU:OE2	2:A:59:ARG:HD3	1.98	0.64
2:C:33:TYR:HA	2:C:44:VAL:HG12	1.80	0.64
2:B:4:GLU:O	2:B:275:LYS:HB3	1.97	0.64
2:C:56:GLU:HG2	2:C:63:ILE:H	1.62	0.64
2:C:259:ALA:CB	2:C:260:PRO:HD2	2.23	0.64
2:C:33:TYR:HA	2:C:44:VAL:CG1	2.27	0.64
2:A:150:VAL:O	2:A:154:VAL:HG23	1.97	0.64
1:D:38:A:H5''	1:D:39:PSU:OP2	1.98	0.64
1:F:16:H2U:H5''	1:F:16:H2U:C6	2.28	0.63
2:B:9:LYS:NZ	2:B:72:THR:O	2.29	0.63
1:D:35:A:O2'	1:D:36:A:H5'	1.99	0.63
2:A:40:PRO:CG	2:A:41:ASN:H	2.11	0.63
1:E:28:C:H5''	1:E:29:A:OP2	1.98	0.63
1:E:35:A:O2'	1:E:36:A:H5'	1.98	0.63
2:A:317:GLU:HB3	2:A:401:THR:HG22	1.80	0.63
1:F:67:A:OP1	2:C:376:LYS:NZ	2.29	0.63
1:F:37:YYG:H103	2:A:335:PHE:CZ	2.33	0.63
2:C:223:MET:O	2:C:223:MET:HG3	1.98	0.63
2:A:6:ILE:O	2:A:8:THR:HG23	1.98	0.63
2:C:303:VAL:C	2:C:304:LEU:HD23	2.19	0.63
2:C:113:MET:HB3	2:C:114:PRO:HD2	1.81	0.63
2:A:256:VAL:HG11	2:A:310:ILE:HG22	1.79	0.63
2:A:97:ALA:HA	2:A:126:VAL:CG1	2.26	0.63
1:E:37:YYG:H141	1:E:37:YYG:H101	1.80	0.63
2:A:248:LYS:HD3	2:A:279:GLU:HG3	1.80	0.63
2:A:265:THR:HG21	2:A:290:LEU:HB3	1.81	0.63
2:A:294:SER:OG	2:A:297:GLU:HG3	1.99	0.63
2:B:124:ARG:HG2	2:B:124:ARG:HH11	1.64	0.63
2:B:118:GLU:HG2	2:B:122:LEU:HD11	1.81	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:335:PHE:CE1	2:A:361:MET:HB2	2.33	0.63
2:C:40:PRO:CG	2:C:41:ASN:H	2.10	0.63
2:C:303:VAL:O	2:C:304:LEU:HD23	1.98	0.63
2:C:6:ILE:O	2:C:8:THR:N	2.30	0.63
2:A:187:LYS:O	2:A:189:LYS:HD3	1.98	0.63
2:C:277:LEU:HD23	2:C:280:GLY:CA	2.29	0.62
2:C:36:ALA:HA	2:C:42:VAL:HB	1.80	0.62
2:B:209:TYR:O	2:B:211:PRO:HD3	1.99	0.62
2:C:342:PHE:O	2:C:348:ASP:HA	1.99	0.62
2:A:335:PHE:CD1	2:A:361:MET:HB2	2.33	0.62
2:C:217:VAL:O	2:C:245:GLY:HA2	1.99	0.62
2:A:315:LYS:HD3	2:A:405:GLU:OE2	2.00	0.62
2:B:97:ALA:HA	2:B:126:VAL:CG1	2.30	0.62
2:A:316:PHE:HA	2:A:404:LEU:HD22	1.81	0.62
2:B:287:GLY:O	2:B:288:LEU:HD23	2.00	0.62
1:D:67:A:OP1	2:A:376:LYS:NZ	2.28	0.62
2:C:121:LEU:HD13	2:C:161:TYR:CD1	2.35	0.62
2:C:25:THR:HG23	2:C:50:ILE:HG21	1.81	0.62
1:E:58:1MA:H4'	1:E:59:U:OP1	2.00	0.62
1:D:34:OMG:H5''	1:D:35:A:OP2	2.00	0.62
2:A:7:ARG:HH22	2:A:284:ASP:CG	2.03	0.61
2:B:56:GLU:HG3	2:B:63:ILE:HG12	1.80	0.61
2:C:195:TRP:HE3	2:C:195:TRP:HA	1.65	0.61
2:C:229:PHE:HE1	2:C:239:THR:CG2	2.13	0.61
1:D:30:G:H2'	1:D:31:A:H5'	1.81	0.61
2:A:55:GLU:HG3	2:A:59:ARG:CD	2.31	0.61
2:A:261:GLU:OE1	2:A:262:THR:N	2.30	0.61
2:C:256:VAL:HG11	2:C:310:ILE:HG22	1.79	0.61
2:C:27:LEU:HD21	2:C:202:LEU:CD2	2.31	0.61
2:B:96:ALA:HA	2:B:99:MET:HG3	1.83	0.61
2:B:38:GLU:HG3	2:B:200:TRP:CZ2	2.35	0.61
2:C:117:ARG:HH12	2:C:160:GLN:HE22	1.48	0.61
2:C:381:GLU:HG3	2:C:384:LEU:HB2	1.83	0.61
2:B:85:HIS:HD2	2:B:87:ASP:N	1.95	0.61
2:C:16:THR:OG1	2:C:81:ASP:HA	2.00	0.61
2:A:315:LYS:HG2	2:A:373:GLU:HG3	1.83	0.61
2:A:220:PRO:HB3	2:A:306:LYS:HD3	1.83	0.61
1:E:27:C:H5''	6:E:79:HOH:O	2.01	0.60
2:C:79:HIS:HE1	2:C:103:ILE:HD12	1.66	0.60
2:A:55:GLU:O	2:A:59:ARG:HG3	2.01	0.60
2:C:277:LEU:CD2	2:C:280:GLY:HA2	2.31	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:299:GLU:O	2:A:302:GLN:HG3	2.01	0.60
2:A:342:PHE:O	2:A:348:ASP:HA	2.00	0.60
2:A:85:HIS:CD2	2:A:87:ASP:HB2	2.35	0.60
2:C:19:HIS:CG	2:C:113:MET:HB2	2.36	0.60
2:C:336:THR:H	2:C:355:LEU:HD12	1.66	0.60
2:A:143:ASP:OD1	2:A:146:LEU:N	2.32	0.60
1:D:18:G:OP2	1:D:58:1MA:HM11	2.02	0.60
2:B:354:ARG:NH1	2:B:373:GLU:OE1	2.28	0.60
2:C:147:LEU:HD12	2:C:172:ARG:HH11	1.65	0.60
2:A:46:ASP:O	2:A:49:ASP:HB2	2.02	0.60
2:A:129:PRO:HB2	2:A:130:TYR:CD1	2.36	0.60
2:B:108:ALA:HB2	2:B:135:MET:HG2	1.82	0.60
2:B:92:MET:HE3	2:B:119:HIS:HA	1.82	0.60
2:B:189:LYS:HG2	2:B:192:GLU:OE2	2.02	0.60
1:F:8:U:O2	1:F:21:A:H2	1.84	0.60
2:B:55:GLU:HG2	2:B:59:ARG:HD3	1.84	0.60
1:E:9:A:HO2'	1:E:11:C:H5	1.49	0.60
2:C:354:ARG:CG	2:C:354:ARG:HH11	2.12	0.60
2:A:113:MET:HB3	2:A:114:PRO:HD2	1.82	0.60
2:A:19:HIS:CD2	2:A:115:GLN:H	2.15	0.60
2:C:156:ASP:O	2:C:159:ASN:HB2	2.02	0.60
1:D:33:U:H3	1:D:35:A:H3'	1.67	0.59
2:C:126:VAL:HG22	2:C:345:ARG:HA	1.84	0.59
1:D:16:H2U:O2'	1:D:16:H2U:H62	2.02	0.59
2:B:33:TYR:O	2:B:36:ALA:HB3	2.02	0.59
2:B:91:ASN:OD1	2:B:91:ASN:N	2.36	0.59
2:C:9:LYS:HE3	2:C:71:GLU:OE1	2.01	0.59
2:A:222:LEU:HD11	2:A:303:VAL:CG1	2.32	0.59
2:A:384:LEU:HD12	2:A:385:ARG:N	2.17	0.59
2:C:13:ASN:ND2	2:C:100:ASP:OD2	2.35	0.59
2:A:277:LEU:HD23	2:A:280:GLY:CA	2.32	0.59
2:C:180:GLU:O	2:C:183:HIS:HB2	2.03	0.59
2:B:231:ILE:CG2	2:B:234:ARG:HB2	2.31	0.59
2:C:46:ASP:O	2:C:49:ASP:HB2	2.02	0.59
2:C:27:LEU:HD13	2:C:134:PHE:CE2	2.38	0.59
2:B:277:LEU:HD23	2:B:280:GLY:HA2	1.84	0.59
2:A:216:ASP:N	2:A:216:ASP:OD1	2.30	0.59
2:B:202:LEU:O	2:B:202:LEU:HD12	2.02	0.59
2:C:56:GLU:HG2	2:C:63:ILE:N	2.17	0.59
2:C:40:PRO:HG2	2:C:41:ASN:H	1.66	0.59
1:E:41:U:H2'	1:E:42:G:H8	1.66	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:253:VAL:N	2:A:265:THR:O	2.30	0.59
2:C:108:ALA:HB2	2:C:135:MET:CG	2.33	0.59
2:C:315:LYS:HG2	2:C:373:GLU:HG3	1.83	0.59
1:F:28:C:N4	1:F:42:G:H1	1.99	0.59
2:B:355:LEU:HD22	2:B:362:VAL:HG23	1.85	0.59
2:C:5:PHE:CD2	2:C:275:LYS:HD2	2.38	0.59
2:B:311:THR:HG22	2:B:312:PRO:HD2	1.85	0.58
2:C:117:ARG:HH12	2:C:160:GLN:NE2	2.00	0.58
2:C:281:ILE:N	2:C:284:ASP:OD2	2.29	0.58
2:A:320:VAL:HG12	2:A:321:TYR:N	2.19	0.58
2:C:248:LYS:HD3	2:C:248:LYS:N	2.17	0.58
2:B:259:ALA:CB	2:B:260:PRO:HD2	2.21	0.58
2:C:98:GLN:OE1	2:C:226:GLU:HG3	2.03	0.58
2:B:217:VAL:HG12	2:B:246:LYS:CD	2.30	0.58
2:B:336:THR:N	2:B:355:LEU:HD12	2.18	0.58
2:C:92:MET:HE1	2:C:119:HIS:HA	1.85	0.58
2:C:29:ALA:O	2:C:33:TYR:HD2	1.85	0.58
1:D:10:2MG:C2	1:D:26:M2G:H1'	2.38	0.58
2:C:316:PHE:CA	2:C:404:LEU:HD22	2.29	0.58
2:C:311:THR:HG22	2:C:312:PRO:CD	2.33	0.58
2:C:138:VAL:HG21	2:C:172:ARG:HB3	1.86	0.58
2:A:31:LEU:HD13	2:A:70:TYR:OH	2.03	0.58
1:E:11:C:C2'	1:E:12:U:H6	2.14	0.58
1:D:2:C:H5''	2:A:88:TYR:CE1	2.39	0.58
2:A:259:ALA:CB	2:A:260:PRO:HD2	2.20	0.57
2:A:277:LEU:CD2	2:A:280:GLY:HA2	2.33	0.57
2:C:51:ASP:O	2:C:53:ALA:N	2.36	0.57
2:C:248:LYS:N	2:C:251:ASP:OD2	2.29	0.57
2:C:375:ILE:O	2:C:376:LYS:HG3	2.03	0.57
2:C:266:VAL:HG21	2:C:291:ARG:NH2	2.19	0.57
2:B:306:LYS:HB3	2:B:309:SER:HB3	1.86	0.57
1:D:38:A:C2'	1:D:39:PSU:H5''	2.34	0.57
2:C:48:GLY:O	2:C:52:LYS:HB3	2.05	0.57
2:B:150:VAL:O	2:B:154:VAL:HG23	2.03	0.57
2:B:14:VAL:HA	2:B:101:GLY:O	2.04	0.57
1:E:26:M2G:CM1	1:E:44:A:H2	2.17	0.57
1:E:75:C:OP1	2:B:52:LYS:HD3	2.03	0.57
2:B:216:ASP:N	2:B:216:ASP:OD1	2.35	0.57
2:A:138:VAL:HG21	2:A:173:GLY:N	2.19	0.57
2:B:63:ILE:HB	2:B:88:TYR:HE2	1.69	0.57
1:F:44:A:O2'	1:F:45:G:H5'	2.05	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:LEU:HB2	5:C:406:GNP:C5	2.35	0.57
2:C:213:PRO:HG2	2:C:215:ARG:CZ	2.35	0.57
2:A:19:HIS:HD2	2:A:115:GLN:N	2.02	0.56
2:A:343:TYR:CE2	2:A:348:ASP:HB2	2.40	0.56
2:C:113:MET:HB3	2:C:114:PRO:CD	2.35	0.56
2:A:21:ASP:HA	5:A:406:GNP:HNB3	1.68	0.56
2:B:219:LYS:HB3	2:B:220:PRO:HD2	1.87	0.56
2:A:75:ARG:NH2	2:A:210:ILE:O	2.30	0.56
2:C:169:PRO:HG2	2:C:209:TYR:CD2	2.41	0.56
1:E:32:OMC:H2'	1:E:33:U:H6	1.70	0.56
2:B:231:ILE:N	2:B:231:ILE:HD13	2.20	0.56
2:C:108:ALA:HB2	2:C:135:MET:HG2	1.86	0.56
2:C:117:ARG:HG3	2:C:161:TYR:HE2	1.68	0.56
2:B:103:ILE:CD1	2:B:206:ILE:HD11	2.35	0.56
2:B:248:LYS:HD2	2:B:279:GLU:OE2	2.06	0.56
2:B:339:ARG:HD2	2:B:352:VAL:HG22	1.86	0.56
2:A:287:GLY:O	2:A:288:LEU:HD23	2.04	0.56
2:A:313:HIS:HD2	2:A:403:ILE:CD1	2.18	0.56
4:D:77:PHE:N	2:A:272:MET:HA	2.21	0.56
2:C:281:ILE:HG13	2:C:284:ASP:OD2	2.05	0.56
2:C:258:LEU:N	2:C:258:LEU:HD23	2.20	0.56
2:C:75:ARG:NH2	2:C:210:ILE:O	2.29	0.56
2:B:54:PRO:O	2:B:58:ALA:N	2.36	0.56
2:B:247:VAL:C	2:B:248:LYS:HD3	2.26	0.56
2:A:343:TYR:HA	2:A:347:THR:O	2.05	0.56
2:B:140:MET:HA	2:B:140:MET:CE	2.36	0.56
1:E:18:G:O6	1:E:55:PSU:H1'	2.06	0.56
2:B:127:GLY:O	2:B:129:PRO:HD3	2.06	0.56
2:C:107:SER:HB2	2:C:137:LYS:HD2	1.88	0.56
2:C:368:VAL:HG12	2:C:369:THR:H	1.71	0.56
2:B:229:PHE:O	2:B:237:VAL:N	2.29	0.56
2:A:118:GLU:OE2	2:A:389:ARG:NH1	2.38	0.56
2:C:79:HIS:HE1	2:C:103:ILE:CD1	2.18	0.56
2:B:40:PRO:HG2	2:B:41:ASN:H	1.70	0.55
1:E:15:G:H2'	1:E:16:H2U:C6	2.32	0.55
1:F:34:OMG:H2'	1:F:35:A:O4'	2.06	0.55
1:F:3:G:O2'	1:F:4:G:H5'	2.07	0.55
2:A:55:GLU:CG	2:A:59:ARG:HG3	2.29	0.55
2:A:143:ASP:O	2:A:147:LEU:HD22	2.07	0.55
2:A:202:LEU:O	2:A:202:LEU:HD12	2.06	0.55
2:B:320:VAL:HG12	2:B:321:TYR:N	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:17:H2U:H4'	1:E:18:G:OP2	2.06	0.55
2:B:118:GLU:HG2	2:B:122:LEU:CD1	2.35	0.55
1:F:47:U:H5'	1:F:48:C:C5'	2.36	0.55
2:C:135:MET:CE	2:C:151:GLU:HB2	2.36	0.55
2:C:136:ASN:HA	2:C:173:GLY:O	2.07	0.55
1:D:29:A:H2	1:D:41:U:O2	1.89	0.55
2:C:336:THR:N	2:C:355:LEU:HD12	2.21	0.55
2:C:299:GLU:O	2:C:302:GLN:HG3	2.06	0.55
1:E:1:G:C3'	1:E:2:C:H5'	2.37	0.55
2:B:63:ILE:HB	2:B:88:TYR:CD2	2.41	0.55
2:B:87:ASP:C	2:B:88:TYR:HD1	2.10	0.55
2:A:143:ASP:OD1	2:A:145:GLU:N	2.39	0.55
2:B:338:TYR:O	2:B:353:VAL:HG23	2.06	0.55
2:B:177:LEU:N	2:B:177:LEU:HD12	2.21	0.55
2:C:1:ALA:HB2	2:C:271:GLU:OE2	2.06	0.55
1:E:34:OMG:O5'	1:E:34:OMG:H8	1.90	0.55
2:B:21:ASP:HA	5:B:406:GNP:N3B	2.19	0.55
2:A:9:LYS:NZ	2:A:72:THR:O	2.29	0.55
2:C:315:LYS:HB2	2:C:404:LEU:HB2	1.88	0.55
2:C:177:LEU:HB3	2:C:195:TRP:CD1	2.41	0.55
1:F:36:A:H2'	1:F:37:YYG:H5'	1.89	0.55
2:A:46:ASP:HB2	2:A:49:ASP:OD2	2.07	0.55
2:C:368:VAL:CG1	2:C:369:THR:H	2.20	0.54
1:F:36:A:H2'	1:F:37:YYG:H8	1.89	0.54
2:B:103:ILE:HA	2:B:132:VAL:O	2.07	0.54
2:C:9:LYS:NZ	2:C:72:THR:O	2.31	0.54
2:C:14:VAL:O	2:C:79:HIS:HA	2.06	0.54
2:B:248:LYS:HE3	2:B:251:ASP:OD2	2.07	0.54
2:A:227:ASP:OD1	2:A:228:VAL:N	2.40	0.54
1:F:9:A:C5'	1:F:46:7MG:H1'	2.36	0.54
2:C:19:HIS:NE2	2:C:114:PRO:HD2	2.21	0.54
2:B:256:VAL:HG11	2:B:310:ILE:HG22	1.90	0.54
2:A:334:PHE:O	2:A:361:MET:HA	2.08	0.54
1:D:2:C:H4'	2:A:88:TYR:HE1	1.72	0.54
1:D:45:G:O5'	1:D:45:G:H8	1.91	0.54
2:B:53:ALA:HB1	2:B:54:PRO:CD	2.37	0.54
1:E:16:H2U:H4'	1:E:17:H2U:OP2	1.95	0.54
2:C:63:ILE:HG13	2:C:64:ASN:N	2.22	0.54
2:C:263:ARG:HG3	2:C:264:LYS:H	1.73	0.54
2:A:18:GLY:H	2:A:119:HIS:CD2	2.24	0.54
2:A:315:LYS:HE2	2:A:404:LEU:HB3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:248:LYS:HE3	2:C:251:ASP:OD2	2.07	0.54
2:C:89:ILE:O	2:C:93:ILE:HD12	2.07	0.54
2:B:294:SER:OG	2:B:297:GLU:HG3	2.06	0.54
2:C:140:MET:CE	2:C:140:MET:HA	2.37	0.54
2:A:108:ALA:HB2	2:A:135:MET:HG2	1.88	0.54
1:E:25:C:C2	1:E:26:M2G:C8	2.96	0.54
2:C:315:LYS:CB	2:C:404:LEU:HB2	2.38	0.54
2:C:117:ARG:HG3	2:C:157:LEU:HD11	1.90	0.54
2:B:385:ARG:HA	2:B:399:VAL:HA	1.89	0.54
2:A:38:GLU:OE2	2:A:190:ARG:HG3	2.07	0.54
2:A:38:GLU:HG3	2:A:200:TRP:CZ2	2.43	0.54
2:A:27:LEU:HG	2:A:27:LEU:O	2.06	0.54
1:E:8:U:O2	1:E:21:A:H2	1.91	0.54
1:D:46:7MG:H4'	1:D:47:U:OP2	2.07	0.54
2:C:237:VAL:HG22	2:C:289:LEU:HD13	1.88	0.54
2:C:169:PRO:CG	2:C:209:TYR:CD2	2.91	0.53
1:F:10:2MG:H2'	1:F:11:C:C6	2.40	0.53
1:F:26:M2G:H2'	1:F:26:M2G:N3	2.23	0.53
2:B:277:LEU:HD23	2:B:280:GLY:CA	2.38	0.53
2:B:59:ARG:NH1	2:B:88:TYR:OH	2.41	0.53
1:F:19:G:OP1	1:F:60:C:N4	2.41	0.53
1:F:19:G:H4'	1:F:20:G:N3	2.23	0.53
2:C:216:ASP:N	2:C:216:ASP:OD1	2.41	0.53
2:C:263:ARG:HG3	2:C:264:LYS:N	2.22	0.53
2:A:400:VAL:HG12	2:A:401:THR:N	2.24	0.53
1:F:25:C:C4	1:F:26:M2G:N7	2.77	0.53
1:F:6:U:H2'	1:F:7:U:C6	2.44	0.53
2:B:176:LEU:HB2	5:B:406:GNP:C5	2.39	0.53
1:E:11:C:C2	1:E:12:U:C5	2.97	0.53
2:B:11:HIS:HE1	2:B:78:SER:OG	1.89	0.53
2:A:24:LYS:HE3	2:A:82:CYS:O	2.09	0.53
1:E:10:2MG:H2'	1:E:11:C:C6	2.43	0.53
2:C:356:PRO:CD	2:C:370:PHE:HB3	2.38	0.53
1:E:3:G:C8	1:E:3:G:H3'	2.43	0.53
2:A:312:PRO:O	2:A:313:HIS:ND1	2.41	0.53
1:D:2:C:H5''	2:A:88:TYR:HE1	1.74	0.53
1:F:10:2MG:C4	1:F:11:C:C5	2.97	0.53
2:C:335:PHE:HA	2:C:355:LEU:HD11	1.91	0.53
2:B:230:THR:HA	2:B:235:GLY:O	2.09	0.53
2:B:151:GLU:O	2:B:155:ARG:HG3	2.08	0.53
2:A:101:GLY:HA3	2:A:210:ILE:CD1	2.26	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:3:G:H3'	1:F:3:G:C8	2.44	0.53
1:D:24:G:O2'	1:D:25:C:H5'	2.09	0.53
1:D:34:OMG:HM22	1:D:35:A:H5'	1.91	0.53
1:E:35:A:C2'	1:E:36:A:H5'	2.39	0.53
2:C:399:VAL:HG22	2:C:400:VAL:N	2.23	0.53
2:C:17:ILE:HD12	2:C:119:HIS:HB3	1.90	0.52
2:B:190:ARG:HG2	2:B:200:TRP:CE2	2.44	0.52
2:A:384:LEU:HD12	2:A:385:ARG:H	1.74	0.52
2:A:117:ARG:HH12	2:A:160:GLN:HE22	1.57	0.52
2:C:106:VAL:HG21	2:C:154:VAL:HG21	1.91	0.52
2:C:169:PRO:HD2	2:C:209:TYR:CD2	2.44	0.52
1:D:36:A:O2'	1:D:37:YYG:H5'	2.09	0.52
2:B:313:HIS:HD2	2:B:403:ILE:HD13	1.74	0.52
1:F:26:M2G:C5	1:F:27:C:C5	2.98	0.52
2:A:313:HIS:HD2	2:A:403:ILE:HD13	1.74	0.52
2:A:222:LEU:HD12	2:A:223:MET:N	2.24	0.52
2:C:161:TYR:O	2:C:162:GLU:HB2	2.10	0.52
2:B:174:SER:OG	2:B:177:LEU:HD13	2.09	0.52
1:D:25:C:N3	1:D:26:M2G:C8	2.78	0.52
2:B:88:TYR:N	2:B:88:TYR:HD1	2.07	0.52
2:C:241:ARG:HD2	6:C:412:HOH:O	2.09	0.52
1:D:11:C:C6	1:D:12:U:H5	2.27	0.52
2:C:315:LYS:HD3	2:C:405:GLU:HG3	1.90	0.52
1:E:36:A:H2'	1:E:37:YYG:H5'	1.89	0.52
1:D:9:A:H5'	1:D:46:7MG:H1'	1.90	0.52
1:F:37:YYG:C10	1:F:37:YYG:N20	2.72	0.52
4:F:77:PHE:N	2:C:273:HIS:H	2.07	0.52
1:F:11:C:C2	1:F:12:U:C5	2.98	0.52
2:C:19:HIS:HA	2:C:115:GLN:HB2	1.92	0.52
1:D:35:A:C2'	1:D:36:A:H5'	2.40	0.52
2:B:55:GLU:OE2	2:B:59:ARG:NH1	2.40	0.52
2:A:62:THR:HB	5:A:406:GNP:O3G	2.10	0.52
2:C:222:LEU:HD12	2:C:303:VAL:HG13	1.92	0.52
2:A:85:HIS:HD2	2:A:87:ASP:N	1.90	0.52
1:F:10:2MG:CM2	1:F:11:C:H1'	2.32	0.52
1:D:10:2MG:HN2	1:D:26:M2G:H1'	1.71	0.52
2:A:54:PRO:O	2:A:58:ALA:N	2.33	0.52
2:C:102:ALA:O	2:C:131:ILE:HA	2.10	0.52
1:D:14:A:C2'	1:D:15:G:H5'	2.40	0.52
1:D:11:C:O5'	1:D:11:C:H6	1.93	0.52
1:D:26:M2G:HM12	1:D:44:A:H2	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:ILE:O	2:B:61:ILE:HG13	2.10	0.52
1:D:29:A:H2'	1:D:30:G:C8	2.45	0.52
2:A:354:ARG:NH1	2:A:373:GLU:OE1	2.30	0.52
2:C:380:LEU:C	2:C:381:GLU:HG2	2.26	0.52
2:B:7:ARG:HH22	2:B:284:ASP:CG	2.12	0.52
2:B:221:PHE:HA	2:B:244:ARG:O	2.10	0.52
2:C:318:ALA:HA	2:C:401:THR:HB	1.91	0.51
1:E:19:G:H4'	1:E:20:G:C4	2.46	0.51
1:E:24:G:C8	1:E:25:C:C5	2.98	0.51
1:E:34:OMG:H2'	1:E:35:A:O4'	2.10	0.51
2:B:117:ARG:HH12	2:B:160:GLN:HE22	1.59	0.51
2:C:140:MET:HA	2:C:140:MET:HE3	1.92	0.51
2:B:254:GLU:OE1	2:B:308:GLY:N	2.36	0.51
2:B:217:VAL:HG12	2:B:246:LYS:NZ	2.25	0.51
2:B:362:VAL:CG2	2:B:368:VAL:HG21	2.41	0.51
2:A:47:TYR:O	2:A:50:ILE:N	2.40	0.51
1:D:25:C:C2	1:D:26:M2G:C8	2.98	0.51
2:B:368:VAL:HG12	2:B:369:THR:N	2.18	0.51
2:C:237:VAL:HA	2:C:288:LEU:O	2.10	0.51
1:E:24:G:C6	1:E:25:C:N3	2.79	0.51
2:C:354:ARG:NH1	2:C:354:ARG:HG3	2.09	0.51
1:D:14:A:C5	1:D:22:G:C2	2.98	0.51
1:D:13:C:C2	1:D:14:A:C8	2.98	0.51
1:E:1:G:P	2:B:300:ARG:HH11	2.34	0.51
2:B:190:ARG:HG2	2:B:200:TRP:NE1	2.26	0.51
2:C:70:TYR:O	2:C:77:TYR:HB2	2.10	0.51
2:A:149:LEU:O	2:A:153:GLU:HG3	2.10	0.51
1:D:37:YYG:H103	2:B:335:PHE:HE2	1.76	0.51
2:A:333:GLY:HA3	2:A:363:MET:SD	2.50	0.51
2:A:317:GLU:N	2:A:404:LEU:HD22	2.25	0.51
1:D:66:A:O2'	1:D:67:A:H5'	2.11	0.51
1:F:24:G:C6	1:F:25:C:C4	2.99	0.51
1:D:10:2MG:C6	1:D:11:C:C4	2.99	0.51
1:D:15:G:H2'	1:D:16:H2U:H5'	1.92	0.51
2:B:253:VAL:N	2:B:265:THR:O	2.35	0.51
2:C:355:LEU:CD2	2:C:362:VAL:HG23	2.40	0.51
2:C:147:LEU:HB3	2:C:172:ARG:NH1	2.26	0.51
2:C:320:VAL:HG12	2:C:321:TYR:N	2.26	0.51
2:B:55:GLU:HG2	2:B:59:ARG:CD	2.41	0.51
2:C:11:HIS:HD1	2:C:76:HIS:CE1	2.24	0.51
1:F:64:A:H4'	2:C:391:GLY:CA	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:ARG:HB2	2:B:163:PHE:CZ	2.45	0.51
2:B:254:GLU:O	2:B:304:LEU:HA	2.11	0.51
2:B:214:VAL:O	2:B:214:VAL:HG12	2.11	0.51
1:E:10:2MG:N2	1:E:11:C:C2	2.79	0.51
1:D:48:C:N4	1:D:59:U:C5	2.79	0.51
2:A:188:THR:HG23	2:A:192:GLU:CB	2.41	0.51
1:E:10:2MG:C4	1:E:11:C:C5	2.99	0.50
1:F:27:C:H2'	1:F:28:C:H6	1.75	0.50
2:C:19:HIS:CD2	2:C:113:MET:HB3	2.46	0.50
1:D:44:A:C6	1:D:45:G:C6	2.99	0.50
2:A:333:GLY:HA2	2:A:362:VAL:O	2.12	0.50
2:B:254:GLU:CD	2:B:308:GLY:H	2.14	0.50
1:E:24:G:C5	1:E:25:C:C2	3.00	0.50
1:F:24:G:H2'	1:F:25:C:C6	2.46	0.50
1:F:24:G:C5	1:F:25:C:C4	2.99	0.50
2:A:55:GLU:CG	2:A:59:ARG:HD3	2.41	0.50
1:D:25:C:C4	1:D:26:M2G:N7	2.79	0.50
1:F:59:U:C5	1:F:60:C:N4	2.79	0.50
1:E:24:G:N7	1:E:25:C:C4	2.80	0.50
1:F:26:M2G:C6	1:F:27:C:C4	2.99	0.50
2:B:113:MET:HB3	2:B:114:PRO:CD	2.40	0.50
2:B:231:ILE:HG22	2:B:234:ARG:HG3	1.92	0.50
2:C:179:LEU:HG	2:C:183:HIS:CE1	2.45	0.50
2:A:69:GLU:O	2:A:70:TYR:HB3	2.10	0.50
1:D:14:A:C6	1:D:22:G:C2	2.99	0.50
2:B:88:TYR:CD1	2:B:88:TYR:N	2.79	0.50
1:E:1:G:C2	1:E:73:A:N3	2.79	0.50
2:A:151:GLU:HG3	2:A:170:VAL:HG11	1.94	0.50
1:D:11:C:C2	1:D:12:U:C5	3.00	0.50
1:E:59:U:C5	1:E:60:C:N4	2.78	0.50
5:C:406:GNP:O3G	5:C:406:GNP:O2B	2.29	0.50
1:F:74:C:C4	1:F:75:C:C4	2.98	0.50
1:E:26:M2G:C4	1:E:27:C:C5	2.99	0.50
2:B:190:ARG:HA	2:B:197:ASP:OD1	2.12	0.50
1:F:24:G:C5	1:F:25:C:C5	3.00	0.50
1:D:24:G:C5	1:D:25:C:C5	3.00	0.50
2:B:46:ASP:O	2:B:50:ILE:HG13	2.11	0.50
1:E:25:C:C4	1:E:26:M2G:N7	2.79	0.50
2:C:131:ILE:HD12	2:C:163:PHE:CE1	2.47	0.50
1:F:24:G:N7	1:F:25:C:C5	2.79	0.50
1:D:48:C:N4	1:D:59:U:C4	2.80	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:140:MET:HA	2:A:140:MET:CE	2.41	0.50
2:B:229:PHE:HE1	2:B:239:THR:CG2	2.25	0.50
2:A:40:PRO:HG2	2:A:41:ASN:OD1	2.11	0.50
2:A:7:ARG:NH2	2:A:284:ASP:OD1	2.44	0.50
1:E:10:2MG:H2'	1:E:11:C:H6	1.76	0.50
1:E:30:G:OP2	1:E:30:G:H8	1.95	0.50
2:C:21:ASP:HA	5:C:406:GNP:HNB3	1.77	0.50
1:F:74:C:C5	1:F:75:C:C4	3.00	0.50
2:A:198:LYS:O	2:A:201:GLU:HB2	2.11	0.50
2:C:34:VAL:CG1	2:C:200:TRP:CE2	2.95	0.50
2:B:217:VAL:O	2:B:245:GLY:HA2	2.12	0.49
2:C:177:LEU:HD23	2:C:195:TRP:NE1	2.27	0.49
2:A:139:ASP:OD2	2:A:174:SER:HB2	2.11	0.49
2:A:188:THR:CG2	2:A:192:GLU:HB2	2.40	0.49
2:C:134:PHE:CD1	2:C:171:ILE:HG22	2.46	0.49
2:C:56:GLU:CD	2:C:63:ILE:H	2.15	0.49
2:B:217:VAL:CG1	2:B:246:LYS:NZ	2.75	0.49
2:C:312:PRO:O	2:C:313:HIS:ND1	2.46	0.49
2:B:231:ILE:HG22	2:B:234:ARG:CB	2.38	0.49
2:A:315:LYS:HD3	2:A:405:GLU:CD	2.31	0.49
1:F:44:A:H8	1:F:44:A:O5'	1.94	0.49
2:A:98:GLN:OE1	2:A:226:GLU:HG3	2.11	0.49
2:C:236:THR:HG21	2:C:293:VAL:HG23	1.93	0.49
2:B:49:ASP:N	2:B:49:ASP:OD1	2.42	0.49
1:F:12:U:C2	1:F:24:G:N2	2.80	0.49
2:C:389:ARG:HA	2:C:394:THR:HA	1.94	0.49
1:F:10:2MG:C6	1:F:26:M2G:C2	3.01	0.49
1:D:24:G:C4	1:D:25:C:C6	3.01	0.49
1:D:37:YYG:H103	2:B:335:PHE:CE2	2.46	0.49
2:B:404:LEU:N	2:B:404:LEU:HD13	2.27	0.49
1:D:38:A:C3'	1:D:39:PSU:H5''	2.41	0.49
1:F:68:U:C4	1:F:69:U:C5	3.00	0.49
2:B:33:TYR:CZ	2:B:44:VAL:HG21	2.46	0.49
2:B:143:ASP:HB3	2:B:146:LEU:HB2	1.94	0.49
1:E:10:2MG:C6	1:E:11:C:C4	3.00	0.49
2:B:85:HIS:CD2	2:B:86:ALA:N	2.80	0.49
2:C:342:PHE:CD1	2:C:342:PHE:N	2.80	0.49
2:A:213:PRO:HG2	2:A:215:ARG:CZ	2.43	0.49
2:C:281:ILE:O	2:C:284:ASP:OD2	2.30	0.49
1:D:14:A:H2'	1:D:15:G:H5'	1.95	0.49
2:B:36:ALA:HA	2:B:42:VAL:HB	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:90:LYS:HB3	2:B:91:ASN:OD1	2.12	0.49
2:C:94:THR:CG2	2:C:346:THR:HG22	2.43	0.49
2:B:120:ILE:O	2:B:123:ALA:HB3	2.12	0.49
1:E:29:A:H2'	1:E:30:G:C8	2.48	0.49
2:B:59:ARG:O	2:B:61:ILE:HG23	2.12	0.49
2:C:33:TYR:CE1	2:C:44:VAL:CG2	2.95	0.49
2:A:281:ILE:O	2:A:281:ILE:HG13	2.12	0.49
2:A:322:ILE:HD12	2:A:334:PHE:HE1	1.78	0.49
2:A:121:LEU:HD13	2:A:161:TYR:CD2	2.48	0.49
1:E:7:U:H4'	1:E:8:U:OP2	2.13	0.49
2:A:72:THR:HB	6:A:428:HOH:O	2.12	0.49
2:A:188:THR:HG22	2:A:189:LYS:N	2.28	0.49
2:C:147:LEU:CD1	2:C:172:ARG:HH11	2.26	0.49
2:A:316:PHE:CA	2:A:404:LEU:HD22	2.42	0.49
2:C:145:GLU:HA	2:C:145:GLU:OE1	2.13	0.49
1:E:28:C:N3	1:E:42:G:N2	2.53	0.49
1:D:23:A:C2	1:D:24:G:C5	3.00	0.49
2:C:88:TYR:N	2:C:88:TYR:CD1	2.77	0.49
1:E:2:C:P	2:B:90:LYS:HE3	2.53	0.48
2:C:217:VAL:HG12	2:C:281:ILE:HG22	1.95	0.48
1:E:54:5MU:OP1	2:B:331:HIS:HE1	1.96	0.48
2:B:156:ASP:O	2:B:159:ASN:N	2.46	0.48
2:B:343:TYR:CD1	2:B:343:TYR:N	2.80	0.48
1:E:47:U:O2	1:E:50:U:OP1	2.30	0.48
2:C:362:VAL:HG21	2:C:368:VAL:HG21	1.95	0.48
2:A:142:ASP:O	2:A:144:PRO:HD3	2.13	0.48
2:C:399:VAL:O	2:C:399:VAL:HG13	2.12	0.48
2:C:40:PRO:HG2	2:C:41:ASN:OD1	2.13	0.48
2:C:47:TYR:OH	5:C:406:GNP:O1A	2.28	0.48
2:A:38:GLU:HG3	2:A:200:TRP:HZ2	1.78	0.48
1:F:74:C:C5	1:F:75:C:N4	2.81	0.48
1:F:25:C:H2'	1:F:26:M2G:C8	2.48	0.48
2:B:82:CYS:HB3	2:B:83:PRO:CD	2.37	0.48
2:A:276:THR:HG22	2:A:277:LEU:N	2.28	0.48
2:C:124:ARG:HG2	2:C:125:GLN:OE1	2.13	0.48
1:E:24:G:C6	1:E:25:C:C2	3.00	0.48
1:E:14:A:C3'	1:E:15:G:H5'	2.44	0.48
1:D:22:G:C6	1:D:23:A:N7	2.81	0.48
2:B:335:PHE:HE1	2:B:361:MET:HB2	1.73	0.48
2:C:270:VAL:HG12	2:C:277:LEU:HB3	1.94	0.48
1:F:59:U:O2'	1:F:60:C:H5'	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:7:ARG:NH2	2:A:281:ILE:HG12	2.28	0.48
1:E:23:A:HO2'	1:E:24:G:H5'	1.79	0.48
1:D:14:A:N6	1:D:22:G:C6	2.82	0.48
2:C:368:VAL:HB	2:C:370:PHE:CD2	2.49	0.48
2:C:247:VAL:O	2:C:279:GLU:HA	2.12	0.48
2:B:263:ARG:NH1	2:B:297:GLU:HB3	2.28	0.48
1:E:24:G:C5	1:E:25:C:C4	3.02	0.48
1:D:14:A:C4	1:D:22:G:N2	2.81	0.48
1:F:37:YYG:HN20	1:F:37:YYG:C11	2.27	0.48
1:E:1:G:H2'	1:E:2:C:H5'	1.95	0.48
2:C:306:LYS:HB3	2:C:309:SER:CB	2.41	0.48
2:C:90:LYS:O	2:C:93:ILE:HB	2.13	0.48
2:A:89:ILE:HG22	2:A:93:ILE:HD12	1.95	0.48
2:C:205:ALA:O	2:C:209:TYR:N	2.38	0.48
1:E:67:A:OP1	2:B:376:LYS:NZ	2.30	0.48
2:A:24:LYS:HB2	2:A:24:LYS:HE2	1.50	0.48
2:C:94:THR:HG23	2:C:346:THR:HG22	1.96	0.48
1:F:17:H2U:O2'	1:F:18:G:OP1	2.30	0.48
2:C:220:PRO:O	2:C:244:ARG:HG3	2.14	0.48
1:F:65:G:O2'	2:C:350:THR:OG1	2.29	0.48
1:E:10:2MG:C2	1:E:11:C:C2	3.02	0.48
2:C:56:GLU:HG2	2:C:61:ILE:O	2.13	0.48
1:D:37:YYG:O5'	1:D:37:YYG:H8	2.14	0.48
2:C:353:VAL:HG13	2:C:370:PHE:CD1	2.49	0.48
2:C:384:LEU:HD12	2:C:385:ARG:N	2.28	0.48
2:A:13:ASN:HB2	2:A:100:ASP:OD2	2.13	0.48
2:C:362:VAL:HG11	2:C:368:VAL:CG2	2.43	0.48
2:C:213:PRO:O	2:C:215:ARG:HD2	2.13	0.48
1:F:24:G:O2'	1:F:25:C:H5'	2.14	0.48
2:A:180:GLU:O	2:A:183:HIS:HB2	2.14	0.48
1:D:14:A:H2'	1:D:14:A:N3	2.28	0.47
1:D:59:U:C5	1:D:60:C:N4	2.82	0.47
2:B:113:MET:O	2:B:116:THR:HB	2.14	0.47
2:A:168:VAL:HA	2:A:169:PRO:HD3	1.71	0.47
2:C:247:VAL:C	2:C:248:LYS:HD3	2.33	0.47
2:A:256:VAL:HG11	2:A:310:ILE:CG2	2.43	0.47
2:B:130:TYR:CD1	2:B:130:TYR:N	2.81	0.47
2:A:362:VAL:HG11	2:A:368:VAL:HG21	1.96	0.47
2:B:281:ILE:HG12	2:B:284:ASP:OD2	2.14	0.47
2:C:100:ASP:O	2:C:129:PRO:HD2	2.13	0.47
2:C:363:MET:HE3	2:C:364:PRO:HD2	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:71:GLU:HB2	2:B:75:ARG:O	2.13	0.47
1:D:26:M2G:C6	1:D:27:C:C5	3.02	0.47
2:B:87:ASP:HB2	2:B:88:TYR:CD1	2.49	0.47
2:B:355:LEU:HB3	2:B:359:VAL:HG12	1.96	0.47
2:C:224:PRO:HA	2:C:303:VAL:HG22	1.97	0.47
2:A:277:LEU:HD23	2:A:280:GLY:HA2	1.92	0.47
2:B:219:LYS:HB3	2:B:220:PRO:CD	2.44	0.47
2:B:155:ARG:HD3	2:B:165:GLY:O	2.13	0.47
1:E:10:2MG:H3'	1:E:10:2MG:OP2	2.14	0.47
2:B:19:HIS:CD2	2:B:113:MET:HB2	2.50	0.47
1:E:3:G:O2'	1:E:4:G:H5'	2.15	0.47
2:A:171:ILE:N	2:A:171:ILE:HD12	2.29	0.47
2:B:226:GLU:O	2:B:226:GLU:HG2	2.14	0.47
1:F:47:U:O2	1:F:47:U:H3'	2.15	0.47
2:A:226:GLU:OE2	2:A:227:ASP:HB2	2.15	0.47
1:E:10:2MG:C6	1:E:11:C:N4	2.83	0.47
2:C:368:VAL:CG2	2:C:370:PHE:HE2	2.28	0.47
1:E:75:C:OP2	2:B:52:LYS:HE2	2.15	0.47
2:A:46:ASP:H	2:A:49:ASP:CG	2.16	0.47
1:E:25:C:O2'	1:E:26:M2G:O4'	2.30	0.47
2:C:335:PHE:HA	2:C:355:LEU:CD1	2.44	0.47
2:A:19:HIS:CE1	2:A:20:VAL:HG12	2.49	0.47
2:B:231:ILE:HG22	2:B:234:ARG:CG	2.44	0.47
2:C:50:ILE:HG12	2:C:50:ILE:H	1.42	0.47
2:B:75:ARG:NH2	2:B:210:ILE:O	2.38	0.47
2:A:234:ARG:HB3	2:A:289:LEU:CD2	2.43	0.47
2:C:20:VAL:HA	2:C:84:GLY:HA3	1.97	0.47
1:D:32:OMC:H6	1:D:32:OMC:O5'	1.97	0.47
1:F:25:C:C4	1:F:26:M2G:C5	3.03	0.47
2:C:266:VAL:HG21	2:C:291:ARG:HH21	1.80	0.47
2:B:40:PRO:HD2	2:B:41:ASN:OD1	2.15	0.47
2:A:277:LEU:HD21	2:A:280:GLY:HA2	1.96	0.47
2:B:141:VAL:HG23	2:B:141:VAL:O	2.15	0.47
2:B:38:GLU:OE2	2:B:190:ARG:HG3	2.15	0.47
2:A:128:VAL:HA	2:A:129:PRO:HD3	1.65	0.47
2:B:118:GLU:O	2:B:122:LEU:HG	2.15	0.47
1:D:39:PSU:O4	1:D:39:PSU:O4'	2.29	0.47
1:F:37:YYG:HN20	1:F:37:YYG:H102	1.79	0.47
2:C:34:VAL:HG12	2:C:200:TRP:CZ2	2.50	0.47
1:E:53:G:H3'	1:E:54:5MU:H71	1.96	0.47
2:C:66:ALA:O	2:C:80:VAL:HA	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:C:H2'	1:D:60:C:H6	1.51	0.46
2:B:336:THR:H	2:B:355:LEU:HD12	1.80	0.46
2:C:259:ALA:HB1	2:C:260:PRO:CD	2.39	0.46
2:B:90:LYS:HA	2:B:93:ILE:HD12	1.97	0.46
2:B:345:ARG:HH22	2:B:381:GLU:CD	2.18	0.46
1:E:30:G:C6	1:E:31:A:C5	3.04	0.46
2:A:53:ALA:O	2:A:57:ARG:HG2	2.15	0.46
2:C:404:LEU:N	2:C:404:LEU:HD13	2.25	0.46
2:B:52:LYS:HA	2:B:57:ARG:HE	1.79	0.46
4:D:77:PHE:N	2:A:285:ASN:O	2.49	0.46
2:A:113:MET:O	2:A:116:THR:HB	2.16	0.46
1:F:51:G:H2'	1:F:52:U:O4'	2.15	0.46
2:C:214:VAL:HG12	2:C:214:VAL:O	2.14	0.46
2:A:229:PHE:HE1	2:A:239:THR:HG21	1.80	0.46
1:E:30:G:C6	1:E:31:A:C6	3.03	0.46
2:B:63:ILE:HA	2:B:88:TYR:CD2	2.51	0.46
2:A:33:TYR:HB3	2:A:182:MET:HG3	1.98	0.46
2:C:265:THR:HG23	2:C:291:ARG:O	2.15	0.46
2:C:120:ILE:HD12	2:C:157:LEU:HG	1.97	0.46
2:B:11:HIS:HD1	2:B:76:HIS:CE1	2.33	0.46
1:D:18:G:O6	1:D:55:PSU:H1'	2.15	0.46
2:B:335:PHE:HE1	2:B:361:MET:SD	2.38	0.46
2:A:46:ASP:HB2	2:A:49:ASP:CG	2.36	0.46
2:C:380:LEU:HB2	2:C:403:ILE:HD13	1.97	0.46
2:C:399:VAL:CG2	2:C:400:VAL:N	2.79	0.46
2:C:90:LYS:O	2:C:93:ILE:N	2.47	0.46
2:A:177:LEU:CD1	2:A:177:LEU:N	2.79	0.46
1:E:24:G:H3'	1:E:25:C:H6	1.81	0.46
2:B:246:LYS:HB2	2:B:280:GLY:O	2.16	0.46
1:D:11:C:H2'	1:D:12:U:C5	2.50	0.46
2:B:361:MET:O	2:B:361:MET:HG2	2.15	0.46
2:B:53:ALA:CB	2:B:56:GLU:HB2	2.36	0.46
2:B:362:VAL:HG21	2:B:368:VAL:HG21	1.97	0.46
2:B:36:ALA:CB	2:B:44:VAL:HG12	2.45	0.46
2:B:89:ILE:HG22	2:B:93:ILE:CD1	2.45	0.46
2:A:399:VAL:HG22	2:A:400:VAL:N	2.29	0.46
2:C:324:LYS:O	2:C:327:GLU:N	2.48	0.46
2:B:268:THR:OG1	2:B:289:LEU:HD23	2.15	0.46
2:A:389:ARG:HA	2:A:393:ARG:O	2.16	0.46
2:A:311:THR:HG22	2:A:312:PRO:CD	2.34	0.46
1:D:24:G:C6	1:D:25:C:C4	3.04	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:ALA:HB1	2:B:54:PRO:HD3	1.96	0.46
2:A:19:HIS:CD2	2:A:113:MET:HB2	2.50	0.46
2:C:133:VAL:HG12	2:C:134:PHE:N	2.31	0.46
2:C:85:HIS:CD2	2:C:86:ALA:N	2.84	0.46
2:C:217:VAL:HG12	2:C:246:LYS:HD3	1.97	0.46
2:B:75:ARG:HD3	2:B:77:TYR:OH	2.15	0.46
2:C:131:ILE:CD1	2:C:163:PHE:CE1	2.99	0.46
1:D:30:G:C3'	1:D:31:A:H5'	2.42	0.46
1:E:33:U:H4'	1:E:37:YYG:H191	1.97	0.46
2:C:256:VAL:HG11	2:C:310:ILE:HG21	1.94	0.46
2:B:177:LEU:N	2:B:177:LEU:CD1	2.79	0.46
2:B:156:ASP:O	2:B:159:ASN:HB2	2.15	0.46
2:A:178:ALA:O	2:A:181:GLU:HB3	2.16	0.46
2:C:139:ASP:OD1	2:C:139:ASP:N	2.49	0.46
1:E:17:H2U:H3'	1:E:18:G:H5''	1.98	0.46
1:D:59:U:O2'	1:D:60:C:H5'	2.16	0.46
2:A:368:VAL:CG1	2:A:369:THR:H	2.08	0.46
2:A:20:VAL:HG13	2:A:20:VAL:O	2.15	0.46
2:C:199:ILE:HD13	2:C:199:ILE:N	2.30	0.46
2:C:134:PHE:CD1	2:C:171:ILE:CG2	2.99	0.46
1:E:62:A:H2'	1:E:63:C:O4'	2.15	0.46
1:F:18:G:O6	1:F:55:PSU:H1'	2.15	0.46
2:A:102:ALA:O	2:A:131:ILE:HA	2.14	0.46
1:E:24:G:O2'	1:E:25:C:H5'	2.16	0.46
2:C:131:ILE:O	2:C:209:TYR:HE2	1.99	0.46
2:C:19:HIS:CD2	2:C:113:MET:CB	2.99	0.46
1:E:38:A:H5'	2:C:336:THR:HG22	1.98	0.46
2:A:353:VAL:HG13	2:A:370:PHE:CD1	2.51	0.46
2:B:117:ARG:HH12	2:B:160:GLN:NE2	2.14	0.46
2:B:335:PHE:CE1	2:B:361:MET:CE	2.99	0.45
2:C:11:HIS:CE1	2:C:272:MET:HE2	2.51	0.45
2:C:310:ILE:HD13	2:C:310:ILE:HG21	1.65	0.45
4:E:77:PHE:N	2:B:272:MET:HA	2.31	0.45
2:A:400:VAL:CG1	2:A:401:THR:N	2.79	0.45
2:C:23:GLY:HA2	5:C:406:GNP:PA	2.56	0.45
2:A:193:ASN:HB3	2:A:196:VAL:HB	1.98	0.45
2:C:182:MET:SD	2:C:188:THR:HB	2.56	0.45
1:F:11:C:HO2'	1:F:12:U:H6	1.63	0.45
1:D:25:C:C4	1:D:26:M2G:C8	3.04	0.45
2:B:118:GLU:OE2	2:B:389:ARG:NH1	2.49	0.45
2:C:265:THR:HG22	2:C:291:ARG:N	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:315:LYS:HD3	2:A:405:GLU:HG3	1.98	0.45
2:C:39:ASN:HA	2:C:40:PRO:HD3	1.47	0.45
2:A:177:LEU:HD12	2:A:177:LEU:N	2.30	0.45
1:D:22:G:N1	1:D:23:A:N7	2.64	0.45
1:D:26:M2G:CM1	1:D:44:A:H2	2.29	0.45
2:A:36:ALA:CB	2:A:44:VAL:HG12	2.47	0.45
2:B:47:TYR:OH	5:B:406:GNP:O1A	2.30	0.45
2:C:33:TYR:HA	2:C:44:VAL:HG11	1.98	0.45
2:B:163:PHE:HA	2:B:164:PRO:HD2	1.67	0.45
2:B:55:GLU:CG	2:B:59:ARG:HD2	2.47	0.45
2:A:334:PHE:CD2	2:A:338:TYR:CD2	3.05	0.45
2:A:199:ILE:HG22	2:A:203:LEU:HD12	1.98	0.45
2:B:137:LYS:HB3	2:B:140:MET:HG3	1.97	0.45
2:A:202:LEU:HD12	2:A:202:LEU:C	2.35	0.45
2:C:4:GLU:O	2:C:4:GLU:HG2	2.17	0.45
2:B:149:LEU:O	2:B:153:GLU:HG3	2.16	0.45
2:A:85:HIS:CD2	2:A:87:ASP:CB	3.00	0.45
2:C:63:ILE:CG1	2:C:64:ASN:N	2.80	0.45
1:D:58:1MA:HM12	1:D:61:C:H1'	1.97	0.45
2:C:266:VAL:O	2:C:268:THR:HG23	2.17	0.45
2:C:85:HIS:HD2	2:C:86:ALA:N	2.15	0.45
2:C:217:VAL:CG1	2:C:281:ILE:HG22	2.46	0.45
2:A:276:THR:CG2	2:A:277:LEU:N	2.79	0.45
1:D:36:A:C2	1:D:37:YYG:C4	2.99	0.45
2:B:63:ILE:HA	2:B:88:TYR:HD2	1.81	0.45
2:B:38:GLU:OE2	2:B:189:LYS:HB3	2.17	0.45
2:C:27:LEU:HD21	2:C:202:LEU:HD21	1.98	0.45
2:A:399:VAL:CG2	2:A:400:VAL:N	2.79	0.45
2:A:134:PHE:CD1	2:A:171:ILE:CG2	3.00	0.45
2:A:140:MET:SD	5:A:406:GNP:N2	2.89	0.45
2:A:320:VAL:CG1	2:A:321:TYR:N	2.80	0.45
2:C:90:LYS:HA	2:C:93:ILE:HD12	1.99	0.45
2:A:289:LEU:HD12	2:A:289:LEU:HA	1.76	0.45
1:E:44:A:C2'	1:E:45:G:H5'	2.47	0.45
1:F:46:7MG:H81	1:F:46:7MG:H2'	1.65	0.45
2:C:56:GLU:OE2	2:C:63:ILE:N	2.42	0.45
2:B:63:ILE:CG2	2:B:88:TYR:HE2	2.30	0.45
2:C:342:PHE:CE2	2:C:372:VAL:HG21	2.52	0.45
2:B:336:THR:N	2:B:355:LEU:CD1	2.80	0.45
2:C:11:HIS:CE1	2:C:272:MET:CE	3.00	0.45
2:B:33:TYR:CZ	2:B:44:VAL:CG2	3.00	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:266:VAL:HG12	2:C:267:VAL:O	2.15	0.45
2:A:248:LYS:HD2	2:A:279:GLU:OE2	2.17	0.45
2:B:122:LEU:HA	2:B:122:LEU:HD23	1.50	0.45
2:A:176:LEU:HB2	5:A:406:GNP:C5	2.47	0.45
2:C:33:TYR:CD1	2:C:44:VAL:HG11	2.52	0.45
2:B:285:ASN:C	2:B:285:ASN:HD22	2.20	0.45
2:B:124:ARG:HH11	2:B:124:ARG:CG	2.27	0.45
1:E:37:YYG:C4	1:E:38:A:C8	3.00	0.45
2:B:261:GLU:OE1	2:B:262:THR:N	2.44	0.45
2:C:155:ARG:NH2	2:C:170:VAL:CG2	2.79	0.45
2:A:6:ILE:HG22	2:A:6:ILE:O	2.17	0.45
2:C:254:GLU:O	2:C:304:LEU:HA	2.17	0.45
2:A:16:THR:O	2:A:82:CYS:HB2	2.17	0.45
1:E:53:G:C8	1:E:54:5MU:H72	2.51	0.45
2:C:24:LYS:HE2	2:C:24:LYS:HB2	1.56	0.45
2:A:368:VAL:HG12	2:A:369:THR:N	2.22	0.44
2:A:304:LEU:HA	2:A:304:LEU:HD23	1.67	0.44
2:C:75:ARG:HD2	2:C:77:TYR:OH	2.17	0.44
2:C:113:MET:O	2:C:116:THR:HB	2.17	0.44
2:A:313:HIS:CD2	2:A:403:ILE:CD1	2.99	0.44
2:B:19:HIS:CD2	2:B:113:MET:CB	2.99	0.44
2:C:336:THR:N	2:C:355:LEU:CD1	2.79	0.44
2:A:322:ILE:HD12	2:A:334:PHE:CE1	2.51	0.44
2:C:40:PRO:CG	2:C:41:ASN:N	2.79	0.44
1:D:32:OMC:O3'	1:D:32:OMC:HM23	2.17	0.44
2:B:249:VAL:HG13	2:B:268:THR:C	2.37	0.44
2:C:187:LYS:O	2:C:189:LYS:HD3	2.16	0.44
2:A:217:VAL:O	2:A:245:GLY:HA2	2.16	0.44
1:D:14:A:C6	1:D:22:G:N1	2.85	0.44
2:A:223:MET:O	2:A:223:MET:HG3	2.12	0.44
2:A:171:ILE:N	2:A:171:ILE:CD1	2.79	0.44
1:D:59:U:C2'	1:D:60:C:H5'	2.47	0.44
2:A:144:PRO:HA	2:A:147:LEU:HD23	1.99	0.44
2:B:320:VAL:CG1	2:B:321:TYR:N	2.79	0.44
2:A:159:ASN:O	2:A:162:GLU:N	2.47	0.44
2:A:258:LEU:HD23	2:A:258:LEU:HA	1.63	0.44
1:F:32:OMC:HM23	1:F:32:OMC:H1'	1.63	0.44
1:D:62:A:C2'	1:D:63:C:H5'	2.47	0.44
2:C:19:HIS:CG	2:C:113:MET:CB	3.00	0.44
2:A:115:GLN:O	2:A:119:HIS:HB2	2.18	0.44
2:C:384:LEU:HD12	2:C:385:ARG:H	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:159:ASN:O	2:A:162:GLU:HA	2.17	0.44
2:C:145:GLU:O	2:C:148:ASP:HB2	2.18	0.44
2:C:339:ARG:HD2	2:C:352:VAL:CG2	2.48	0.44
2:A:53:ALA:HB1	2:A:54:PRO:CD	2.48	0.44
2:A:313:HIS:CD2	2:A:403:ILE:HD13	2.53	0.44
2:A:19:HIS:CG	2:A:113:MET:CB	3.00	0.44
2:A:315:LYS:HE2	2:A:404:LEU:CB	2.48	0.44
1:E:21:A:O2'	1:E:22:G:O4'	2.35	0.44
2:C:33:TYR:CZ	2:C:44:VAL:HB	2.52	0.44
2:C:147:LEU:HD12	2:C:172:ARG:NH1	2.29	0.44
1:E:1:G:C4	1:E:73:A:C2	3.05	0.44
2:C:270:VAL:CG1	2:C:277:LEU:HB3	2.48	0.44
2:B:342:PHE:O	2:B:348:ASP:HA	2.18	0.44
1:D:17:H2U:C4'	1:D:18:G:H5''	2.43	0.44
2:B:315:LYS:HB2	2:B:404:LEU:HB2	1.94	0.44
2:C:272:MET:O	2:C:275:LYS:HB2	2.18	0.44
2:C:356:PRO:HG3	2:C:369:THR:O	2.18	0.44
2:C:265:THR:CG2	2:C:291:ARG:N	2.80	0.44
2:B:124:ARG:NH1	2:B:124:ARG:CG	2.79	0.44
2:A:202:LEU:O	2:A:206:ILE:HG13	2.18	0.44
2:B:20:VAL:O	2:B:20:VAL:HG13	2.17	0.44
2:C:343:TYR:N	2:C:343:TYR:CD1	2.86	0.44
1:D:8:U:O2	1:D:15:G:O6	2.36	0.44
2:A:303:VAL:CG1	2:A:304:LEU:N	2.79	0.44
2:C:177:LEU:HD12	2:C:177:LEU:N	2.33	0.44
2:B:126:VAL:O	2:B:126:VAL:HG13	2.18	0.44
1:D:71:G:C2'	1:D:72:C:H5'	2.47	0.44
2:C:223:MET:HB2	2:C:242:ILE:HA	1.99	0.44
2:C:89:ILE:HD13	2:C:89:ILE:HG23	1.84	0.44
2:C:155:ARG:NH1	2:C:165:GLY:O	2.46	0.43
2:B:304:LEU:HA	2:B:304:LEU:HD23	1.59	0.43
2:B:2:LYS:HB3	2:B:3:GLY:H	1.58	0.43
1:E:26:M2G:CM1	1:E:44:A:C2	2.96	0.43
2:B:213:PRO:HG2	2:B:215:ARG:NH2	2.31	0.43
2:A:303:VAL:HG13	2:A:304:LEU:N	2.33	0.43
2:C:52:LYS:HA	2:C:57:ARG:CZ	2.48	0.43
2:C:171:ILE:CG2	2:C:172:ARG:N	2.80	0.43
2:A:181:GLU:OE1	2:A:181:GLU:HA	2.18	0.43
2:A:52:LYS:HG3	2:A:53:ALA:N	2.33	0.43
2:B:83:PRO:O	2:B:83:PRO:HG2	2.18	0.43
1:E:32:OMC:O2	1:E:32:OMC:HM22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:36:ALA:HB2	2:A:44:VAL:HG12	1.99	0.43
5:A:406:GNP:H2'	5:A:406:GNP:H8	1.24	0.43
2:B:32:THR:OG1	2:B:33:TYR:N	2.51	0.43
2:C:144:PRO:O	2:C:147:LEU:HB2	2.19	0.43
2:A:354:ARG:HH11	2:A:354:ARG:HG3	1.83	0.43
2:B:222:LEU:HB3	2:B:244:ARG:HG2	2.00	0.43
2:C:363:MET:HE2	2:C:363:MET:HB3	1.85	0.43
2:A:345:ARG:HB2	6:A:414:HOH:O	2.18	0.43
2:A:335:PHE:CD1	2:A:361:MET:CB	3.00	0.43
2:C:126:VAL:HG13	2:C:126:VAL:O	2.18	0.43
2:A:40:PRO:HD2	2:A:41:ASN:OD1	2.18	0.43
2:C:135:MET:HE3	2:C:151:GLU:HB2	2.01	0.43
2:A:96:ALA:HA	2:A:99:MET:HG3	2.00	0.43
1:E:23:A:C6	1:E:24:G:C6	3.05	0.43
1:D:13:C:C2	1:D:14:A:N7	2.86	0.43
2:C:315:LYS:HE2	2:C:315:LYS:HB3	1.79	0.43
2:C:248:LYS:HE3	2:C:251:ASP:CG	2.39	0.43
2:C:324:LYS:H	2:C:327:GLU:HB2	1.83	0.43
1:D:62:A:H2'	1:D:63:C:O4'	2.18	0.43
1:F:21:A:C5	1:F:46:7MG:C6	3.06	0.43
1:F:3:G:C3'	1:F:3:G:C8	3.01	0.43
2:C:289:LEU:HA	2:C:289:LEU:HD12	1.68	0.43
2:A:146:LEU:O	2:A:146:LEU:HD12	2.18	0.43
1:D:19:G:H2'	1:D:19:G:H8	1.37	0.43
1:E:24:G:H3'	1:E:25:C:C6	2.53	0.43
2:A:368:VAL:CG1	2:A:369:THR:N	2.79	0.43
1:F:37:YYG:C2'	1:F:37:YYG:H31	2.49	0.43
2:B:347:THR:HG22	2:B:348:ASP:N	2.34	0.43
2:A:191:GLY:H	2:A:197:ASP:CG	2.21	0.43
2:A:118:GLU:O	2:A:122:LEU:HG	2.19	0.43
2:C:53:ALA:HB3	2:C:56:GLU:OE1	2.17	0.43
2:C:316:PHE:CZ	2:C:372:VAL:HB	2.54	0.43
2:B:316:PHE:HB2	2:B:402:LYS:O	2.18	0.43
2:A:72:THR:CG2	2:A:203:LEU:HD22	2.49	0.43
2:B:11:HIS:O	2:B:12:VAL:HG23	2.18	0.43
2:A:29:ALA:HB1	2:A:45:LYS:O	2.18	0.43
2:A:124:ARG:HH11	2:A:124:ARG:HG2	1.83	0.43
2:B:63:ILE:CB	2:B:88:TYR:CE2	2.99	0.43
2:C:117:ARG:HG3	2:C:161:TYR:CE2	2.50	0.43
2:B:132:VAL:HG22	2:B:169:PRO:HG2	2.01	0.43
2:C:215:ARG:HG2	2:C:282:ALA:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:34:OMG:C2'	1:F:35:A:H5'	2.49	0.43
2:A:113:MET:HB3	2:A:114:PRO:CD	2.46	0.43
2:B:117:ARG:NH1	2:B:160:GLN:HE22	2.17	0.43
2:B:350:THR:O	2:B:375:ILE:HG23	2.19	0.43
2:B:124:ARG:NH2	2:B:385:ARG:NH2	2.67	0.43
2:C:248:LYS:CD	2:C:248:LYS:N	2.80	0.43
2:C:21:ASP:O	2:C:23:GLY:N	2.52	0.43
2:B:342:PHE:N	2:B:342:PHE:CD1	2.87	0.43
1:E:21:A:H8	1:E:21:A:O5'	2.01	0.42
1:F:37:YYG:C11	1:F:37:YYG:N20	2.82	0.42
2:A:254:GLU:OE1	2:A:308:GLY:N	2.46	0.42
2:B:21:ASP:CA	5:B:406:GNP:HNB3	2.24	0.42
2:A:140:MET:CG	5:A:406:GNP:N2	2.82	0.42
2:B:103:ILE:HD11	2:B:206:ILE:CD1	2.46	0.42
2:B:140:MET:HA	2:B:140:MET:HE2	2.00	0.42
1:E:3:G:C3'	1:E:3:G:C8	3.00	0.42
2:A:34:VAL:HG13	6:A:426:HOH:O	2.18	0.42
2:A:122:LEU:HA	2:A:122:LEU:HD23	1.81	0.42
2:B:333:GLY:HA2	2:B:362:VAL:O	2.19	0.42
2:B:232:THR:O	2:B:234:ARG:N	2.53	0.42
2:A:306:LYS:HB3	2:A:309:SER:CB	2.47	0.42
2:B:247:VAL:O	2:B:279:GLU:HA	2.18	0.42
2:B:339:ARG:HB3	2:B:352:VAL:HG22	2.01	0.42
2:A:160:GLN:HE21	2:A:160:GLN:HB3	1.50	0.42
1:F:62:A:H2'	1:F:63:C:O4'	2.20	0.42
2:A:184:LYS:O	2:A:185:ASN:HB3	2.19	0.42
1:D:36:A:C2	1:D:37:YYG:N9	2.87	0.42
2:C:315:LYS:HA	2:C:372:VAL:O	2.20	0.42
2:B:176:LEU:O	2:B:176:LEU:HD12	2.19	0.42
2:C:177:LEU:CD1	2:C:177:LEU:N	2.82	0.42
2:A:263:ARG:HH21	2:A:297:GLU:HB3	1.85	0.42
1:E:44:A:O2'	1:E:45:G:H5'	2.20	0.42
1:D:8:U:H5'	1:D:49:5MC:OP2	2.20	0.42
1:E:39:PSU:H4'	2:C:360:GLU:OE2	2.19	0.42
2:A:71:GLU:HB3	2:A:76:HIS:HA	2.01	0.42
1:F:48:C:OP2	1:F:48:C:H6	2.02	0.42
2:C:21:ASP:O	5:C:406:GNP:H5'2	2.19	0.42
1:D:29:A:O2'	1:D:30:G:H5'	2.19	0.42
2:B:223:MET:HA	2:B:224:PRO:HD2	1.61	0.42
2:B:39:ASN:HA	2:B:40:PRO:HD3	1.44	0.42
2:A:5:PHE:N	2:A:276:THR:O	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:ASP:O	2:B:146:LEU:HB3	2.19	0.42
1:E:9:A:O2'	1:E:11:C:H5	2.03	0.42
1:F:10:2MG:C5	1:F:11:C:C5	3.07	0.42
1:F:11:C:H2'	1:F:12:U:C6	2.55	0.42
2:B:404:LEU:HD12	2:B:404:LEU:HA	1.73	0.42
2:C:311:THR:HA	2:C:312:PRO:HD3	1.88	0.42
2:C:198:LYS:O	2:C:201:GLU:N	2.53	0.42
2:C:128:VAL:HA	2:C:129:PRO:HD3	1.95	0.42
1:E:51:G:H4'	2:B:339:ARG:HG2	2.01	0.42
2:C:184:LYS:O	2:C:185:ASN:HB3	2.19	0.42
1:F:10:2MG:N3	1:F:11:C:C6	2.87	0.42
1:E:14:A:C3'	1:E:15:G:C5'	2.98	0.42
2:B:19:HIS:CD2	2:B:115:GLN:NE2	2.87	0.42
2:C:335:PHE:CD1	2:C:361:MET:CB	2.99	0.42
1:E:34:OMG:HM23	1:E:34:OMG:H1'	1.06	0.42
2:B:194:GLU:O	2:B:197:ASP:N	2.52	0.42
2:B:226:GLU:O	2:B:300:ARG:HG3	2.20	0.42
1:F:54:5MU:H2'	1:F:55:PSU:O4'	2.20	0.42
2:C:185:ASN:HA	2:C:186:PRO:HD3	1.11	0.42
1:E:10:2MG:N1	1:E:11:C:C4	2.88	0.42
2:C:154:VAL:O	2:C:158:LEU:HB2	2.20	0.42
2:C:338:TYR:C	2:C:340:PRO:HD3	2.40	0.42
1:E:37:YYG:H132	1:E:37:YYG:O6	2.20	0.42
1:D:2:C:H4'	2:A:88:TYR:CE1	2.52	0.42
2:B:248:LYS:CD	2:B:248:LYS:N	2.79	0.42
2:C:6:ILE:HD13	2:C:6:ILE:HA	1.81	0.42
2:B:293:VAL:O	2:B:293:VAL:HG23	2.18	0.42
2:A:136:ASN:CG	2:A:137:LYS:H	2.23	0.42
2:B:215:ARG:N	2:B:215:ARG:CD	2.80	0.42
2:C:143:ASP:HA	2:C:144:PRO:HD2	1.53	0.42
2:C:21:ASP:CG	5:C:406:GNP:H5'2	2.40	0.42
2:B:140:MET:HA	2:B:140:MET:HE3	2.01	0.42
2:A:234:ARG:HB3	2:A:289:LEU:HD22	2.02	0.42
2:C:169:PRO:CD	2:C:209:TYR:CD2	3.03	0.42
2:B:262:THR:HG23	2:B:262:THR:H	1.47	0.42
2:C:248:LYS:O	2:C:251:ASP:OD2	2.38	0.42
2:B:222:LEU:HD11	2:B:303:VAL:HG11	2.01	0.42
2:B:380:LEU:HA	2:B:380:LEU:HD23	1.80	0.42
1:E:24:G:C5	1:E:25:C:N3	2.88	0.41
2:C:13:ASN:N	2:C:100:ASP:OD2	2.44	0.41
1:F:55:PSU:C3'	1:F:55:PSU:C6	3.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:115:GLN:O	2:C:119:HIS:N	2.42	0.41
2:A:310:ILE:HG23	2:A:311:THR:N	2.34	0.41
1:E:36:A:H2'	1:E:37:YYG:C8	2.49	0.41
2:C:32:THR:HB	2:C:44:VAL:HA	2.01	0.41
2:C:304:LEU:HD23	2:C:304:LEU:N	2.12	0.41
1:E:71:G:C2'	1:E:72:C:H5'	2.50	0.41
2:A:313:HIS:CD2	2:A:403:ILE:CG2	2.99	0.41
2:C:389:ARG:CG	2:C:394:THR:HA	2.36	0.41
2:A:322:ILE:HG13	2:A:362:VAL:HG11	2.02	0.41
2:B:124:ARG:HG2	2:B:124:ARG:NH1	2.33	0.41
1:E:71:G:H5''	1:E:71:G:H8	1.85	0.41
1:E:27:C:O2'	1:E:28:C:OP1	2.29	0.41
2:B:191:GLY:H	2:B:197:ASP:CG	2.23	0.41
2:A:147:LEU:HA	2:A:147:LEU:HD13	1.69	0.41
2:A:316:PHE:C	2:A:404:LEU:HD22	2.39	0.41
2:A:127:GLY:O	2:A:129:PRO:HD3	2.20	0.41
2:C:213:PRO:HG2	2:C:215:ARG:NE	2.35	0.41
2:B:146:LEU:HA	2:B:146:LEU:HD12	1.72	0.41
1:F:15:G:H2'	1:F:16:H2U:H62	2.02	0.41
1:E:37:YYG:H101	1:E:37:YYG:C14	2.48	0.41
2:C:252:GLU:HA	2:C:265:THR:O	2.20	0.41
1:E:1:G:C2	1:E:73:A:C2	3.09	0.41
2:C:21:ASP:C	2:C:23:GLY:H	2.23	0.41
2:C:350:THR:HG22	2:C:351:GLY:N	2.34	0.41
2:A:229:PHE:N	2:A:229:PHE:CD1	2.89	0.41
2:C:316:PHE:CE1	2:C:372:VAL:HB	2.55	0.41
2:C:355:LEU:CD2	2:C:362:VAL:CG2	2.98	0.41
1:F:37:YYG:H141	1:F:37:YYG:O22	2.20	0.41
2:B:310:ILE:HD12	2:B:310:ILE:HG21	1.61	0.41
2:B:230:THR:C	2:B:231:ILE:HD13	2.41	0.41
2:B:176:LEU:C	2:B:176:LEU:HD12	2.40	0.41
2:B:176:LEU:CB	5:B:406:GNP:C6	2.99	0.41
1:F:27:C:H2'	1:F:28:C:C6	2.55	0.41
2:C:376:LYS:HA	2:C:377:PRO:HD3	1.77	0.41
2:A:370:PHE:HB2	2:A:371:THR:H	1.69	0.41
2:A:6:ILE:HG21	2:A:6:ILE:HD12	1.80	0.41
2:C:190:ARG:H	2:C:190:ARG:HG3	1.72	0.41
2:A:157:LEU:HA	2:A:157:LEU:HD12	1.32	0.41
1:E:48:C:H6	1:E:48:C:OP2	2.04	0.41
2:B:255:ILE:HG21	2:B:255:ILE:HD13	1.83	0.41
2:B:217:VAL:HG23	2:B:217:VAL:H	1.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:312:PRO:HB2	2:C:377:PRO:HB2	2.02	0.41
2:B:299:GLU:N	2:B:302:GLN:OE1	2.51	0.41
2:B:176:LEU:HB3	5:B:406:GNP:C6	2.51	0.41
2:C:248:LYS:HE3	2:C:251:ASP:OD1	2.21	0.41
1:E:16:H2U:H61	1:E:16:H2U:H2'	0.80	0.41
1:D:14:A:C5	1:D:22:G:N2	2.89	0.41
1:D:53:G:H2'	1:D:54:5MU:O4'	2.20	0.41
2:B:54:PRO:O	2:B:58:ALA:HB2	2.21	0.41
2:B:362:VAL:CG1	2:B:368:VAL:HG21	2.51	0.41
1:D:31:A:C2	1:D:40:5MC:C2	3.09	0.41
1:F:67:A:C5	1:F:68:U:C5	3.08	0.41
2:A:362:VAL:HG13	2:A:368:VAL:HG22	2.03	0.41
2:A:254:GLU:CD	2:A:307:PRO:HA	2.41	0.41
2:A:11:HIS:O	2:A:215:ARG:NH1	2.42	0.41
2:C:33:TYR:HE1	2:C:44:VAL:HG21	1.83	0.41
2:A:219:LYS:HB2	2:A:244:ARG:HD3	2.03	0.41
2:C:284:ASP:HB3	2:C:286:VAL:HG12	2.03	0.41
2:C:128:VAL:HG12	2:C:130:TYR:H	1.85	0.41
2:C:136:ASN:CG	2:C:137:LYS:H	2.23	0.41
2:B:155:ARG:HB3	2:B:165:GLY:O	2.20	0.41
2:C:321:TYR:OH	2:C:327:GLU:OE1	2.28	0.41
1:F:74:C:N4	1:F:75:C:N4	2.69	0.41
2:C:199:ILE:HG22	2:C:199:ILE:O	2.21	0.41
2:B:324:LYS:O	2:B:327:GLU:N	2.53	0.41
2:A:390:GLU:O	2:A:393:ARG:HG2	2.21	0.41
1:F:9:A:HO2'	1:F:11:C:H5	1.65	0.41
1:D:12:U:O2	1:D:13:C:N1	2.54	0.41
1:F:34:OMG:HM23	1:F:34:OMG:H1'	1.18	0.41
2:A:9:LYS:CB	2:A:10:PRO:CD	2.99	0.41
2:C:265:THR:HG21	2:C:290:LEU:HB3	2.02	0.41
2:C:134:PHE:CE1	2:C:171:ILE:HG22	2.56	0.41
2:C:284:ASP:CB	2:C:286:VAL:CG1	2.99	0.41
1:E:59:U:C4	1:E:60:C:N3	2.89	0.41
2:C:136:ASN:OD1	2:C:137:LYS:N	2.49	0.41
2:C:349:VAL:CG2	2:C:374:LEU:HD22	2.51	0.41
2:A:254:GLU:O	2:A:304:LEU:HA	2.21	0.40
2:B:36:ALA:HB2	2:B:44:VAL:HG12	2.03	0.40
2:B:168:VAL:HA	2:B:169:PRO:HD2	1.65	0.40
2:C:222:LEU:CD1	2:C:303:VAL:CG1	2.99	0.40
2:C:217:VAL:CG1	2:C:281:ILE:CG2	3.00	0.40
2:B:220:PRO:O	2:B:244:ARG:HG3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:LEU:CD1	2:B:303:VAL:CG1	2.99	0.40
2:A:160:GLN:C	2:A:162:GLU:H	2.25	0.40
2:C:182:MET:SD	2:C:196:VAL:CG2	3.09	0.40
2:C:2:LYS:HB2	2:C:3:GLY:H	1.50	0.40
2:C:106:VAL:HG21	2:C:154:VAL:CG2	2.51	0.40
2:A:310:ILE:HG21	2:A:310:ILE:HD13	1.87	0.40
2:B:299:GLU:HG2	2:B:302:GLN:OE1	2.21	0.40
2:C:172:ARG:O	2:C:198:LYS:HE2	2.21	0.40
2:B:87:ASP:HB2	2:B:88:TYR:CE1	2.56	0.40
2:C:259:ALA:CB	2:C:260:PRO:CD	2.98	0.40
2:A:223:MET:HA	2:A:224:PRO:HD2	1.65	0.40
2:B:194:GLU:HB3	2:B:195:TRP:H	1.66	0.40
2:B:172:ARG:O	2:B:198:LYS:HE2	2.21	0.40
2:A:40:PRO:HG2	2:A:41:ASN:H	1.82	0.40
1:E:28:C:H2'	1:E:28:C:O2	2.21	0.40
1:F:16:H2U:H61	1:F:16:H2U:H2'	1.53	0.40
1:E:32:OMC:H1'	1:E:32:OMC:HM23	1.27	0.40
1:F:61:C:H2'	1:F:62:A:C8	2.57	0.40
2:B:371:THR:HG22	2:B:371:THR:O	2.17	0.40
2:A:310:ILE:CG2	2:A:311:THR:N	2.79	0.40
2:C:133:VAL:HG23	2:C:168:VAL:CG1	2.51	0.40
2:B:383:GLY:HA2	2:B:399:VAL:CG2	2.52	0.40
2:C:66:ALA:O	2:C:80:VAL:HG13	2.22	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	
2	A	403/405 (100%)	362 (90%)	35 (9%)	6 (2%)	13	32
2	B	403/405 (100%)	359 (89%)	31 (8%)	13 (3%)	5	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	403/405 (100%)	353 (88%)	36 (9%)	14 (4%)	4	10
All	All	1209/1215 (100%)	1074 (89%)	102 (8%)	33 (3%)	6	16

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	40	PRO
2	B	2	LYS
2	B	53	ALA
2	B	54	PRO
2	C	5	PHE
2	C	50	ILE
2	C	52	LYS
2	A	41	ASN
2	A	194	GLU
2	B	58	ALA
2	C	19	HIS
2	C	40	PRO
2	A	260	PRO
2	B	40	PRO
2	B	41	ASN
2	B	194	GLU
2	C	7	ARG
2	C	41	ASN
2	C	260	PRO
2	A	379	ALA
2	C	22	HIS
2	C	291	ARG
2	C	55	GLU
2	C	379	ALA
2	B	292	GLY
2	B	224	PRO
2	B	260	PRO
2	B	368	VAL
2	C	368	VAL
2	C	186	PRO
2	B	233	GLY
2	A	368	VAL
2	B	359	VAL

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	A	338/338 (100%)	297 (88%)	41 (12%)	6	14
2	B	338/338 (100%)	299 (88%)	39 (12%)	7	16
2	C	338/338 (100%)	288 (85%)	50 (15%)	4	9
All	All	1014/1014 (100%)	884 (87%)	130 (13%)	5	12

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	6	ILE
2	A	16	THR
2	A	21	ASP
2	A	39	ASN
2	A	46	ASP
2	A	57	ARG
2	A	59	ARG
2	A	63	ILE
2	A	80	VAL
2	A	107	SER
2	A	119	HIS
2	A	126	VAL
2	A	140	MET
2	A	147	LEU
2	A	156	ASP
2	A	172	ARG
2	A	190	ARG
2	A	216	ASP
2	A	217	VAL
2	A	223	MET
2	A	226	GLU
2	A	231	ILE
2	A	234	ARG
2	A	241	ARG
2	A	247	VAL
2	A	248	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	265	THR
2	A	267	VAL
2	A	285	ASN
2	A	290	LEU
2	A	295	ARG
2	A	298	VAL
2	A	311	THR
2	A	317	GLU
2	A	339	ARG
2	A	348	ASP
2	A	349	VAL
2	A	357	GLN
2	A	381	GLU
2	A	401	THR
2	A	404	LEU
2	B	6	ILE
2	B	16	THR
2	B	21	ASP
2	B	39	ASN
2	B	46	ASP
2	B	52	LYS
2	B	88	TYR
2	B	91	ASN
2	B	140	MET
2	B	155	ARG
2	B	156	ASP
2	B	168	VAL
2	B	185	ASN
2	B	190	ARG
2	B	215	ARG
2	B	216	ASP
2	B	217	VAL
2	B	223	MET
2	B	226	GLU
2	B	231	ILE
2	B	232	THR
2	B	248	LYS
2	B	262	THR
2	B	265	THR
2	B	267	VAL
2	B	285	ASN
2	B	295	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	302	GLN
2	B	307	PRO
2	B	310	ILE
2	B	314	THR
2	B	317	GLU
2	B	319	SER
2	B	323	LEU
2	B	347	THR
2	B	349	VAL
2	B	371	THR
2	B	381	GLU
2	B	404	LEU
2	C	5	PHE
2	C	21	ASP
2	C	39	ASN
2	C	46	ASP
2	C	52	LYS
2	C	63	ILE
2	C	78	SER
2	C	89	ILE
2	C	91	ASN
2	C	94	THR
2	C	119	HIS
2	C	126	VAL
2	C	132	VAL
2	C	140	MET
2	C	147	LEU
2	C	152	MET
2	C	156	ASP
2	C	158	LEU
2	C	171	ILE
2	C	176	LEU
2	C	190	ARG
2	C	216	ASP
2	C	217	VAL
2	C	223	MET
2	C	226	GLU
2	C	230	THR
2	C	232	THR
2	C	247	VAL
2	C	248	LYS
2	C	262	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	265	THR
2	C	267	VAL
2	C	285	ASN
2	C	295	ARG
2	C	297	GLU
2	C	298	VAL
2	C	302	GLN
2	C	303	VAL
2	C	307	PRO
2	C	311	THR
2	C	319	SER
2	C	335	PHE
2	C	342	PHE
2	C	347	THR
2	C	349	VAL
2	C	354	ARG
2	C	368	VAL
2	C	381	GLU
2	C	401	THR
2	C	404	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	19	HIS
2	A	64	ASN
2	A	67	HIS
2	A	85	HIS
2	A	98	GLN
2	A	115	GLN
2	A	119	HIS
2	A	160	GLN
2	A	183	HIS
2	A	285	ASN
2	A	313	HIS
2	A	341	GLN
2	B	19	HIS
2	B	64	ASN
2	B	85	HIS
2	B	115	GLN
2	B	119	HIS
2	B	160	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	185	ASN
2	B	331	HIS
2	B	341	GLN
2	B	367	ASN
2	C	19	HIS
2	C	67	HIS
2	C	85	HIS
2	C	119	HIS
2	C	160	GLN
2	C	183	HIS
2	C	285	ASN
2	C	341	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	D	75/76 (98%)	27 (36%)	5 (6%)
1	E	75/76 (98%)	32 (42%)	11 (14%)
1	F	75/76 (98%)	24 (32%)	6 (8%)
All	All	225/228 (98%)	83 (36%)	22 (9%)

All (83) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	4	G
1	D	5	A
1	D	9	A
1	D	12	U
1	D	14	A
1	D	15	G
1	D	16	H2U
1	D	17	H2U
1	D	21	A
1	D	22	G
1	D	23	A
1	D	31	A
1	D	34	OMG
1	D	38	A
1	D	39	PSU
1	D	41	U
1	D	44	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	46	7MG
1	D	47	U
1	D	48	C
1	D	57	G
1	D	67	A
1	D	68	U
1	D	69	U
1	D	73	A
1	D	75	C
1	D	76	A
1	E	2	C
1	E	3	G
1	E	4	G
1	E	5	A
1	E	6	U
1	E	10	2MG
1	E	11	C
1	E	12	U
1	E	16	H2U
1	E	17	H2U
1	E	18	G
1	E	22	G
1	E	23	A
1	E	24	G
1	E	25	C
1	E	26	M2G
1	E	28	C
1	E	30	G
1	E	33	U
1	E	37	YYG
1	E	38	A
1	E	40	5MC
1	E	41	U
1	E	42	G
1	E	45	G
1	E	47	U
1	E	48	C
1	E	67	A
1	E	68	U
1	E	69	U
1	E	73	A
1	E	75	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	3	G
1	F	4	G
1	F	5	A
1	F	6	U
1	F	11	C
1	F	17	H2U
1	F	18	G
1	F	21	A
1	F	22	G
1	F	23	A
1	F	25	C
1	F	26	M2G
1	F	30	G
1	F	37	YYG
1	F	38	A
1	F	41	U
1	F	43	G
1	F	46	7MG
1	F	47	U
1	F	58	1MA
1	F	68	U
1	F	69	U
1	F	73	A
1	F	75	C

All (22) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	3	G
1	D	16	H2U
1	D	21	A
1	D	22	G
1	D	46	7MG
1	E	3	G
1	E	16	H2U
1	E	17	H2U
1	E	21	A
1	E	22	G
1	E	25	C
1	E	27	C
1	E	30	G
1	E	46	7MG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	47	U
1	E	69	U
1	F	3	G
1	F	11	C
1	F	16	H2U
1	F	21	A
1	F	22	G
1	F	46	7MG

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

42 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$
1	2MG	D	10	1	17,26,27	1.06	1 (5%)	21,38,41	2.94	6 (28%)
1	H2U	D	16	1	17,21,22	0.89	0	23,30,33	2.65	7 (30%)
1	H2U	D	17	1	17,21,22	0.74	1 (5%)	23,30,33	2.06	6 (26%)
1	M2G	D	26	1	17,27,28	1.12	1 (5%)	22,40,43	3.38	7 (31%)
1	OMC	D	32	1	13,22,23	0.79	0	20,31,34	1.31	3 (15%)
1	OMG	D	34	1	17,26,27	1.13	1 (5%)	21,38,41	2.68	5 (23%)
1	YYG	D	37	1	27,42,43	1.99	6 (22%)	29,62,65	3.65	11 (37%)
1	PSU	D	39	1	13,21,22	1.36	2 (15%)	18,30,33	6.16	6 (33%)
1	5MC	D	40	1	13,22,23	2.92	2 (15%)	15,32,35	1.77	3 (20%)
1	7MG	D	46	1	19,26,27	2.33	4 (21%)	24,39,42	2.37	5 (20%)
1	5MC	D	49	1	13,22,23	1.10	2 (15%)	15,32,35	2.05	3 (20%)
1	5MU	D	54	1	12,22,23	7.17	4 (33%)	14,32,35	5.60	6 (42%)
1	PSU	D	55	1	13,21,22	1.78	3 (23%)	18,30,33	6.21	7 (38%)
1	1MA	D	58	1	14,25,26	1.07	1 (7%)	15,37,40	1.56	2 (13%)
1	2MG	E	10	1	17,26,27	1.08	1 (5%)	21,38,41	2.85	6 (28%)
1	H2U	E	16	1	17,21,22	0.68	0	23,30,33	3.39	10 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	H2U	E	17	1	17,21,22	1.15	2 (11%)	23,30,33	2.19	6 (26%)
1	M2G	E	26	1	17,27,28	1.22	2 (11%)	22,40,43	5.48	8 (36%)
1	OMC	E	32	1	13,22,23	0.75	0	20,31,34	1.35	3 (15%)
1	OMG	E	34	1	17,26,27	1.10	1 (5%)	21,38,41	2.91	5 (23%)
1	YYG	E	37	1	27,42,43	1.82	6 (22%)	29,62,65	2.68	12 (41%)
1	PSU	E	39	1	13,21,22	1.98	4 (30%)	18,30,33	6.45	7 (38%)
1	5MC	E	40	1	13,22,23	3.83	2 (15%)	15,32,35	0.68	0
1	7MG	E	46	1	19,26,27	1.67	3 (15%)	24,39,42	2.57	5 (20%)
1	5MC	E	49	1	13,22,23	0.93	1 (7%)	15,32,35	1.14	2 (13%)
1	5MU	E	54	1	12,22,23	3.22	3 (25%)	14,32,35	4.44	3 (21%)
1	PSU	E	55	1	13,21,22	1.53	3 (23%)	18,30,33	6.19	6 (33%)
1	1MA	E	58	1	14,25,26	1.01	1 (7%)	15,37,40	1.38	2 (13%)
1	2MG	F	10	1	17,26,27	1.05	1 (5%)	21,38,41	2.91	6 (28%)
1	H2U	F	16	1	17,21,22	1.09	2 (11%)	23,30,33	3.13	12 (52%)
1	H2U	F	17	1	17,21,22	1.12	2 (11%)	23,30,33	1.89	8 (34%)
1	M2G	F	26	1	17,27,28	1.17	1 (5%)	22,40,43	2.29	4 (18%)
1	OMC	F	32	1	13,22,23	0.74	0	20,31,34	1.29	2 (10%)
1	OMG	F	34	1	17,26,27	1.11	1 (5%)	21,38,41	2.78	4 (19%)
1	YYG	F	37	1	27,42,43	1.75	3 (11%)	29,62,65	2.78	11 (37%)
1	PSU	F	39	1	13,21,22	1.85	3 (23%)	18,30,33	6.34	7 (38%)
1	5MC	F	40	1	13,22,23	4.36	2 (15%)	15,32,35	2.11	2 (13%)
1	7MG	F	46	1	19,26,27	1.70	3 (15%)	24,39,42	2.49	5 (20%)
1	5MC	F	49	1	13,22,23	1.54	2 (15%)	15,32,35	1.18	1 (6%)
1	5MU	F	54	1	12,22,23	2.63	3 (25%)	14,32,35	4.41	2 (14%)
1	PSU	F	55	1	13,21,22	2.12	3 (23%)	18,30,33	6.29	5 (27%)
1	1MA	F	58	1	14,25,26	1.04	1 (7%)	15,37,40	1.16	1 (6%)

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
1	2MG	D	10	1	-	0/5/27/28	0/3/3/3
1	H2U	D	16	1	-	0/7/38/39	0/2/2/2
1	H2U	D	17	1	-	0/7/38/39	0/2/2/2
1	M2G	D	26	1	-	0/7/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMC	D	32	1	-	0/5/27/28	0/2/2/2
1	OMG	D	34	1	-	0/5/27/28	0/3/3/3
1	YYG	D	37	1	-	0/20/42/43	0/4/4/4
1	PSU	D	39	1	-	0/7/25/26	0/2/2/2
1	5MC	D	40	1	-	0/3/25/26	0/2/2/2
1	7MG	D	46	1	-	0/7/37/38	0/3/3/3
1	5MC	D	49	1	-	0/3/25/26	0/2/2/2
1	5MU	D	54	1	-	0/3/25/26	0/2/2/2
1	PSU	D	55	1	-	0/7/25/26	0/2/2/2
1	1MA	D	58	1	-	0/3/25/26	0/3/3/3
1	2MG	E	10	1	-	0/5/27/28	0/3/3/3
1	H2U	E	16	1	-	0/7/38/39	0/2/2/2
1	H2U	E	17	1	-	0/7/38/39	0/2/2/2
1	M2G	E	26	1	-	0/7/29/30	0/3/3/3
1	OMC	E	32	1	-	0/5/27/28	0/2/2/2
1	OMG	E	34	1	-	0/5/27/28	0/3/3/3
1	YYG	E	37	1	-	0/20/42/43	0/4/4/4
1	PSU	E	39	1	-	0/7/25/26	0/2/2/2
1	5MC	E	40	1	-	0/3/25/26	0/2/2/2
1	7MG	E	46	1	-	0/7/37/38	0/3/3/3
1	5MC	E	49	1	-	0/3/25/26	0/2/2/2
1	5MU	E	54	1	-	0/3/25/26	0/2/2/2
1	PSU	E	55	1	-	0/7/25/26	0/2/2/2
1	1MA	E	58	1	-	0/3/25/26	0/3/3/3
1	2MG	F	10	1	-	0/5/27/28	0/3/3/3
1	H2U	F	16	1	-	0/7/38/39	0/2/2/2
1	H2U	F	17	1	-	0/7/38/39	0/2/2/2
1	M2G	F	26	1	-	0/7/29/30	0/3/3/3
1	OMC	F	32	1	-	0/5/27/28	0/2/2/2
1	OMG	F	34	1	-	0/5/27/28	0/3/3/3
1	YYG	F	37	1	-	0/20/42/43	0/4/4/4
1	PSU	F	39	1	-	0/7/25/26	0/2/2/2
1	5MC	F	40	1	-	0/3/25/26	0/2/2/2
1	7MG	F	46	1	-	0/7/37/38	0/3/3/3
1	5MC	F	49	1	-	0/3/25/26	0/2/2/2
1	5MU	F	54	1	-	0/3/25/26	0/2/2/2
1	PSU	F	55	1	-	0/7/25/26	0/2/2/2
1	1MA	F	58	1	-	0/3/25/26	0/3/3/3

All (84) bond length outliers are listed below:

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	54	5MU	C5M-C5	-24.46	1.02	1.51
1	F	40	5MC	CM5-C5	-15.37	1.19	1.51
1	E	40	5MC	CM5-C5	-13.42	1.23	1.51
1	E	54	5MU	C5M-C5	-10.30	1.30	1.51
1	D	40	5MC	CM5-C5	-10.06	1.30	1.51
1	F	54	5MU	C5M-C5	-8.05	1.35	1.51
1	D	37	YYG	O23-C21	-6.18	1.25	1.34
1	F	37	YYG	O23-C21	-5.90	1.26	1.34
1	D	46	7MG	C8-N9	-5.66	1.37	1.45
1	F	55	PSU	C5-C1'	-5.56	1.47	1.52
1	E	37	YYG	O23-C21	-5.45	1.26	1.34
1	F	46	7MG	C8-N9	-5.21	1.37	1.45
1	E	46	7MG	C8-N9	-5.20	1.37	1.45
1	E	39	PSU	C5-C1'	-4.74	1.48	1.52
1	D	55	PSU	C5-C1'	-4.21	1.48	1.52
1	F	39	PSU	C5-C1'	-4.12	1.48	1.52
1	F	37	YYG	O18-C16	-3.52	1.24	1.33
1	E	37	YYG	O18-C16	-3.48	1.24	1.33
1	F	37	YYG	C4-N3	-3.38	1.35	1.39
1	F	55	PSU	C6-C5	-3.33	1.33	1.38
1	D	37	YYG	C4-N3	-3.26	1.35	1.39
1	E	55	PSU	C6-C5	-3.26	1.33	1.38
1	E	37	YYG	C4-N3	-3.18	1.35	1.39
1	E	39	PSU	C6-C5	-3.12	1.34	1.38
1	F	39	PSU	C6-C5	-3.09	1.34	1.38
1	D	55	PSU	C6-C5	-3.08	1.34	1.38
1	D	39	PSU	C6-C5	-2.90	1.34	1.38
1	D	46	7MG	C8-N7	-2.81	1.30	1.43
1	E	46	7MG	C8-N7	-2.73	1.31	1.43
1	F	46	7MG	C8-N7	-2.73	1.31	1.43
1	D	37	YYG	C3-N3	-2.69	1.45	1.49
1	D	49	5MC	CM5-C5	-2.62	1.45	1.51
1	F	54	5MU	C6-C5	-2.39	1.33	1.40
1	E	55	PSU	C5-C1'	-2.32	1.50	1.52
1	E	39	PSU	O4'-C1'	-2.30	1.40	1.44
1	E	54	5MU	C6-C5	-2.27	1.33	1.40
1	D	54	5MU	C6-C5	-2.21	1.34	1.40
1	E	49	5MC	C6-C5	-2.20	1.34	1.40
1	F	40	5MC	C6-C5	-2.17	1.34	1.40
1	F	49	5MC	C6-C5	-2.14	1.34	1.40
1	E	40	5MC	C6-C5	-2.14	1.34	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	40	5MC	C6-C5	-2.10	1.34	1.40
1	D	49	5MC	C6-C5	-2.09	1.34	1.40
1	E	37	YYG	C8-N7	-2.01	1.30	1.34
1	E	26	M2G	C2-N1	2.06	1.38	1.34
1	E	17	H2U	O2-C2	2.07	1.27	1.23
1	F	16	H2U	C1'-N1	2.09	1.50	1.45
1	D	17	H2U	C2-N1	2.12	1.38	1.35
1	D	54	5MU	C6-N1	2.17	1.38	1.35
1	F	17	H2U	C1'-N1	2.18	1.50	1.45
1	D	37	YYG	C15-N20	2.49	1.51	1.45
1	E	37	YYG	O22-C21	2.58	1.26	1.21
1	F	58	1MA	C6-N6	2.63	1.33	1.29
1	D	55	PSU	C4-N3	2.64	1.38	1.33
1	D	39	PSU	C4-N3	2.65	1.38	1.33
1	E	58	1MA	C6-N6	2.66	1.34	1.29
1	D	46	7MG	C6-N1	2.72	1.38	1.33
1	E	39	PSU	C4-N3	2.75	1.38	1.33
1	F	39	PSU	C4-N3	2.80	1.38	1.33
1	E	37	YYG	C15-N20	2.82	1.52	1.45
1	D	54	5MU	C4-N3	2.83	1.38	1.33
1	F	54	5MU	C4-N3	2.86	1.38	1.33
1	E	55	PSU	C4-N3	2.88	1.38	1.33
1	E	54	5MU	C4-N3	2.89	1.38	1.33
1	D	58	1MA	C6-N6	2.92	1.34	1.29
1	F	55	PSU	C4-N3	3.10	1.38	1.33
1	D	26	M2G	C6-N1	3.13	1.38	1.33
1	E	17	H2U	C2-N1	3.26	1.40	1.35
1	F	17	H2U	C2-N1	3.27	1.40	1.35
1	D	37	YYG	O22-C21	3.27	1.28	1.21
1	D	34	OMG	C6-N1	3.34	1.39	1.33
1	D	10	2MG	C6-N1	3.37	1.39	1.33
1	F	26	M2G	C6-N1	3.38	1.39	1.33
1	F	34	OMG	C6-N1	3.40	1.39	1.33
1	F	10	2MG	C6-N1	3.41	1.39	1.33
1	E	10	2MG	C6-N1	3.42	1.39	1.33
1	E	34	OMG	C6-N1	3.45	1.39	1.33
1	F	16	H2U	C2-N1	3.46	1.40	1.35
1	F	46	7MG	C6-N1	3.47	1.39	1.33
1	E	46	7MG	C6-N1	3.49	1.39	1.33
1	E	26	M2G	C6-N1	3.63	1.39	1.33
1	D	37	YYG	O17-C16	3.76	1.30	1.21
1	F	49	5MC	CM5-C5	4.68	1.60	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	46	7MG	CM7-N7	7.06	1.58	1.46

All (222) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	PSU	N1-C2-N3	-20.92	114.99	128.33
1	F	55	PSU	N1-C2-N3	-20.91	114.99	128.33
1	E	55	PSU	N1-C2-N3	-20.90	115.00	128.33
1	E	39	PSU	N1-C2-N3	-20.89	115.00	128.33
1	D	55	PSU	N1-C2-N3	-20.86	115.03	128.33
1	F	39	PSU	N1-C2-N3	-20.76	115.09	128.33
1	D	37	YYG	C2'-C1'-N9	-11.59	96.58	114.29
1	E	26	M2G	CM2-N2-C2	-10.97	110.06	121.34
1	D	26	M2G	C2'-C1'-N9	-9.59	99.64	114.29
1	D	54	5MU	C5-C4-N3	-9.51	114.54	125.14
1	F	54	5MU	C5-C4-N3	-9.40	114.67	125.14
1	E	54	5MU	C5-C4-N3	-9.40	114.68	125.14
1	E	39	PSU	C4-C5-C1'	-9.05	104.70	121.23
1	D	10	2MG	C5-C6-N1	-8.87	111.46	123.59
1	E	10	2MG	C5-C6-N1	-8.87	111.47	123.59
1	F	34	OMG	C5-C6-N1	-8.83	111.52	123.59
1	D	34	OMG	C5-C6-N1	-8.82	111.53	123.59
1	F	26	M2G	C5-C6-N1	-8.82	111.53	123.59
1	E	34	OMG	C5-C6-N1	-8.82	111.53	123.59
1	E	26	M2G	C5-C6-N1	-8.81	111.54	123.59
1	F	10	2MG	C5-C6-N1	-8.79	111.57	123.59
1	D	26	M2G	C5-C6-N1	-8.73	111.65	123.59
1	F	55	PSU	C5-C1'-C2'	-8.26	100.86	115.52
1	E	46	7MG	C5-C6-N1	-7.79	111.49	123.46
1	F	46	7MG	C5-C6-N1	-7.76	111.53	123.46
1	D	46	7MG	C5-C6-N1	-7.51	111.92	123.46
1	D	16	H2U	C6-N1-C2	-7.49	110.92	122.23
1	F	40	5MC	CM5-C5-C6	-7.46	103.59	118.62
1	E	16	H2U	O2-C2-N1	-7.40	113.62	123.30
1	E	16	H2U	C4-N3-C2	-7.30	119.76	125.79
1	D	17	H2U	C4-N3-C2	-6.92	120.08	125.79
1	E	37	YYG	C2'-C1'-N9	-6.88	103.78	114.29
1	F	39	PSU	C4-C5-C1'	-6.78	108.84	121.23
1	F	16	H2U	C4-N3-C2	-6.66	120.29	125.79
1	F	37	YYG	C14-C15-C16	-6.65	91.39	110.23
1	D	37	YYG	C14-C15-C16	-6.16	92.79	110.23
1	D	55	PSU	C5-C1'-C2'	-6.15	104.60	115.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	37	YYG	C2'-C1'-N9	-5.91	105.25	114.29
1	D	26	M2G	CM2-N2-C2	-5.81	115.37	121.34
1	E	55	PSU	C5-C1'-C2'	-5.72	105.37	115.52
1	D	54	5MU	O2'-C2'-C3'	-5.66	93.43	111.83
1	E	17	H2U	O3'-C3'-C2'	-5.66	93.43	111.83
1	E	16	H2U	C1'-N1-C2	-5.42	110.77	118.27
1	D	54	5MU	C5M-C5-C6	-5.41	107.72	118.62
1	D	39	PSU	C4-C5-C1'	-5.28	111.60	121.23
1	F	39	PSU	O2'-C2'-C3'	-5.27	94.70	111.83
1	D	16	H2U	C5-C6-N1	-5.11	105.16	110.70
1	F	16	H2U	O2-C2-N3	-5.11	111.49	121.48
1	F	16	H2U	O2-C2-N1	-5.03	116.73	123.30
1	F	16	H2U	C6-N1-C2	-4.91	114.82	122.23
1	E	37	YYG	O18-C16-O17	-4.89	113.69	123.79
1	E	16	H2U	C6-N1-C2	-4.63	115.24	122.23
1	E	34	OMG	O4'-C1'-N9	-4.61	98.44	108.10
1	D	16	H2U	O2-C2-N1	-4.55	117.36	123.30
1	F	34	OMG	CM2-O2'-C2'	-4.53	101.80	114.59
1	D	16	H2U	C4-N3-C2	-4.48	122.09	125.79
1	E	46	7MG	O3'-C3'-C4'	-4.43	97.75	111.05
1	D	37	YYG	O23-C21-O22	-4.35	119.03	124.70
1	E	39	PSU	C5-C1'-C2'	-4.09	108.26	115.52
1	D	10	2MG	CM2-N2-C2	-4.08	118.46	123.07
1	F	37	YYG	C14-C15-N20	-4.04	103.18	110.87
1	D	37	YYG	C13-C12-C11	-3.96	123.85	130.59
1	F	32	OMC	O2'-C2'-C3'	-3.88	101.53	111.21
1	D	10	2MG	C2'-C1'-N9	-3.85	108.41	114.29
1	E	16	H2U	O4-C4-C5	-3.83	113.76	122.34
1	E	58	1MA	C2-N3-C4	-3.81	110.50	116.40
1	E	34	OMG	CM2-O2'-C2'	-3.79	103.88	114.59
1	F	17	H2U	C6-N1-C2	-3.75	116.57	122.23
1	E	55	PSU	O2'-C2'-C1'	-3.70	103.68	111.83
1	F	58	1MA	C2-N3-C4	-3.66	110.74	116.40
1	D	58	1MA	C2-N3-C4	-3.63	110.78	116.40
1	E	32	OMC	CM2-O2'-C2'	-3.56	104.54	114.59
1	E	17	H2U	C4-N3-C2	-3.55	122.86	125.79
1	E	37	YYG	O4'-C1'-N9	-3.42	100.94	108.10
1	F	37	YYG	C13-C12-C11	-3.23	125.09	130.59
1	D	40	5MC	O2'-C2'-C3'	-3.18	101.48	111.83
1	F	17	H2U	C4-N3-C2	-3.17	123.17	125.79
1	E	37	YYG	C14-C15-C16	-3.17	101.26	110.23
1	D	54	5MU	O4'-C1'-N1	-3.15	101.44	108.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	17	H2U	O2-C2-N1	-3.03	119.33	123.30
1	E	16	H2U	O3'-C3'-C2'	-2.95	102.23	111.83
1	E	10	2MG	C2-N3-C4	-2.69	111.85	115.09
1	F	26	M2G	C2-N3-C4	-2.67	111.87	115.09
1	F	16	H2U	O4-C4-N3	-2.66	116.31	120.45
1	D	26	M2G	C2-N3-C4	-2.64	111.90	115.09
1	D	10	2MG	C2-N3-C4	-2.64	111.90	115.09
1	D	34	OMG	CM2-O2'-C2'	-2.63	107.16	114.59
1	D	55	PSU	C4-C5-C1'	-2.63	116.44	121.23
1	D	26	M2G	C1'-N9-C4	-2.57	123.06	126.94
1	F	10	2MG	C2-N3-C4	-2.56	112.01	115.09
1	E	17	H2U	N3-C2-N1	-2.56	114.05	116.60
1	D	16	H2U	O4-C4-C5	-2.54	116.64	122.34
1	E	54	5MU	O3'-C3'-C4'	-2.51	103.53	111.05
1	E	37	YYG	O23-C21-O22	-2.50	121.44	124.70
1	E	16	H2U	O3'-C3'-C4'	-2.50	103.55	111.05
1	D	17	H2U	O3'-C3'-C4'	-2.50	103.56	111.05
1	F	17	H2U	O2-C2-N1	-2.48	120.06	123.30
1	D	46	7MG	O3'-C3'-C2'	-2.46	103.83	111.83
1	F	17	H2U	O2-C2-N3	-2.45	116.70	121.48
1	E	26	M2G	C2-N3-C4	-2.42	112.18	115.09
1	F	37	YYG	O22-C21-N20	-2.41	120.66	124.86
1	F	16	H2U	O4-C4-C5	-2.39	116.98	122.34
1	E	34	OMG	N3-C2-N1	-2.38	123.82	127.44
1	F	37	YYG	O23-C21-O22	-2.34	121.65	124.70
1	D	16	H2U	C6-C5-C4	-2.33	103.86	116.24
1	D	39	PSU	O2'-C2'-C3'	-2.33	104.25	111.83
1	F	34	OMG	N3-C2-N1	-2.30	123.95	127.44
1	E	17	H2U	O2-C2-N3	-2.30	116.99	121.48
1	D	34	OMG	N3-C2-N1	-2.28	123.97	127.44
1	E	16	H2U	O2-C2-N3	-2.27	117.05	121.48
1	E	32	OMC	C2'-C1'-N1	-2.23	107.12	113.53
1	D	32	OMC	O3'-C3'-C2'	-2.12	105.03	111.16
1	E	39	PSU	O2'-C2'-C1'	-2.10	107.21	111.83
1	F	26	M2G	C2'-C1'-N9	-2.09	111.09	114.29
1	D	17	H2U	O4-C4-C5	-2.08	117.67	122.34
1	E	58	1MA	O2'-C2'-C3'	-2.05	105.18	111.83
1	D	55	PSU	O2'-C2'-C1'	-2.02	107.38	111.83
1	D	17	H2U	C5-C6-N1	2.02	112.89	110.70
1	D	49	5MC	O2'-C2'-C3'	2.03	118.42	111.83
1	D	49	5MC	O3'-C3'-C4'	2.06	117.23	111.05
1	F	40	5MC	O3'-C3'-C4'	2.06	117.25	111.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	46	7MG	CM7-N7-C8	2.07	126.38	120.52
1	F	46	7MG	O3'-C3'-C4'	2.08	117.28	111.05
1	F	37	YYG	C19-O18-C16	2.11	120.94	115.99
1	E	37	YYG	C13-C14-C15	2.13	119.62	113.12
1	D	40	5MC	CM5-C5-C6	2.18	123.02	118.62
1	E	37	YYG	O23-C21-N20	2.20	114.76	110.64
1	E	49	5MC	CM5-C5-C6	2.25	123.14	118.62
1	D	34	OMG	O3'-C3'-C2'	2.26	117.70	111.16
1	F	10	2MG	O2'-C2'-C3'	2.28	119.24	111.83
1	F	39	PSU	O4'-C1'-C2'	2.32	107.09	104.73
1	D	46	7MG	O2'-C2'-C1'	2.34	118.12	109.94
1	E	46	7MG	O5'-C5'-C4'	2.39	117.86	109.12
1	E	46	7MG	CM7-N7-C8	2.49	127.59	120.52
1	D	39	PSU	O4'-C1'-C2'	2.52	107.30	104.73
1	E	55	PSU	O4'-C1'-C2'	2.53	107.31	104.73
1	D	37	YYG	O4'-C1'-N9	2.54	113.41	108.10
1	E	26	M2G	C2'-C1'-N9	2.57	118.21	114.29
1	E	37	YYG	C24-O23-C21	2.59	118.84	115.63
1	F	17	H2U	C5-C4-N3	2.60	119.15	116.71
1	D	46	7MG	O3'-C3'-C4'	2.62	118.92	111.05
1	F	16	H2U	C5-C4-N3	2.63	119.19	116.71
1	D	37	YYG	O23-C21-N20	2.63	115.58	110.64
1	F	26	M2G	N3-C2-N2	2.64	120.15	117.16
1	D	10	2MG	N2-C2-N3	2.66	120.03	116.94
1	F	16	H2U	O2'-C2'-C3'	2.67	120.53	111.83
1	D	26	M2G	CM2-N2-CM1	2.68	124.79	115.96
1	F	37	YYG	O3'-C3'-C2'	2.68	120.55	111.83
1	F	39	PSU	C5-C1'-C2'	2.69	120.29	115.52
1	E	39	PSU	O4'-C1'-C2'	2.70	107.48	104.73
1	E	49	5MC	O2'-C2'-C3'	2.71	120.63	111.83
1	E	37	YYG	C16-C15-N20	2.73	117.04	110.75
1	E	10	2MG	N2-C2-N3	2.78	120.17	116.94
1	F	10	2MG	N2-C2-N3	2.78	120.17	116.94
1	F	16	H2U	O3'-C3'-C2'	2.83	121.02	111.83
1	D	32	OMC	O2'-C2'-C3'	2.85	118.34	111.21
1	E	10	2MG	O3'-C3'-C4'	2.86	119.62	111.05
1	F	55	PSU	O4'-C1'-C2'	2.91	107.70	104.73
1	E	10	2MG	O4'-C1'-N9	2.92	114.22	108.10
1	F	16	H2U	O3'-C3'-C4'	2.95	119.90	111.05
1	E	37	YYG	C15-N20-C21	2.99	129.21	121.12
1	D	32	OMC	C2-N3-C4	3.06	119.92	115.61
1	D	55	PSU	O4'-C1'-C2'	3.08	107.86	104.73

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	37	YYG	C13-C14-C15	3.08	122.53	113.12
1	E	32	OMC	C2-N3-C4	3.08	119.96	115.61
1	F	17	H2U	C1'-N1-C2	3.12	122.59	118.27
1	E	16	H2U	N3-C2-N1	3.14	119.73	116.60
1	F	32	OMC	C2-N3-C4	3.17	120.09	115.61
1	F	49	5MC	O3'-C3'-C4'	3.25	120.80	111.05
1	D	55	PSU	C6-N1-C2	3.31	120.80	115.47
1	D	39	PSU	C6-N1-C2	3.34	120.84	115.47
1	F	16	H2U	C5-C6-N1	3.36	114.34	110.70
1	F	39	PSU	C6-N1-C2	3.38	120.91	115.47
1	F	17	H2U	N3-C2-N1	3.41	120.00	116.60
1	E	39	PSU	C6-N1-C2	3.44	121.00	115.47
1	D	26	M2G	O4'-C1'-N9	3.45	115.33	108.10
1	F	55	PSU	C6-N1-C2	3.46	121.03	115.47
1	F	17	H2U	C5-C6-N1	3.48	114.47	110.70
1	E	55	PSU	C6-N1-C2	3.49	121.08	115.47
1	F	46	7MG	O3'-C3'-C2'	3.52	123.28	111.83
1	D	17	H2U	N3-C2-N1	3.65	120.25	116.60
1	E	37	YYG	O18-C16-C15	3.71	121.14	111.52
1	D	16	H2U	C1'-N1-C2	3.71	123.40	118.27
1	F	37	YYG	O23-C21-N20	3.76	117.69	110.64
1	E	26	M2G	O2'-C2'-C3'	3.81	124.20	111.83
1	E	17	H2U	C1'-N1-C2	3.86	123.61	118.27
1	D	37	YYG	C15-N20-C21	4.12	132.27	121.12
1	D	58	1MA	C2'-C1'-N9	4.47	121.12	114.29
1	F	10	2MG	C2'-C1'-N9	4.61	121.33	114.29
1	E	26	M2G	O3'-C3'-C4'	4.86	125.63	111.05
1	E	17	H2U	C5-C4-N3	5.00	121.41	116.71
1	D	37	YYG	C19-O18-C16	5.06	127.85	115.99
1	D	40	5MC	O4'-C1'-N1	5.07	118.77	108.08
1	F	37	YYG	C16-C15-N20	5.60	123.65	110.75
1	F	37	YYG	C3-N3-C4	5.73	126.97	118.39
1	D	37	YYG	C16-C15-N20	5.97	124.52	110.75
1	F	16	H2U	N3-C2-N1	6.39	122.98	116.60
1	D	46	7MG	C6-N1-C2	6.41	124.84	115.94
1	E	37	YYG	C3-N3-C4	6.46	128.07	118.39
1	E	46	7MG	C6-N1-C2	6.49	124.94	115.94
1	F	34	OMG	C6-N1-C2	6.53	125.01	115.94
1	F	46	7MG	C6-N1-C2	6.57	125.06	115.94
1	D	34	OMG	C6-N1-C2	6.60	125.10	115.94
1	E	34	OMG	C6-N1-C2	6.65	125.17	115.94
1	F	10	2MG	C6-N1-C2	6.74	125.11	115.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	10	2MG	C6-N1-C2	6.75	125.12	115.31
1	E	10	2MG	C6-N1-C2	6.81	125.22	115.31
1	D	49	5MC	CM5-C5-C6	6.82	132.35	118.62
1	E	16	H2U	C5-C6-N1	6.93	118.21	110.70
1	D	37	YYG	C3-N3-C4	7.71	129.95	118.39
1	E	26	M2G	O4'-C1'-N9	8.43	125.74	108.10
1	D	54	5MU	C5M-C5-C4	9.65	132.50	120.05
1	F	55	PSU	C4-N3-C2	13.37	126.80	115.25
1	F	39	PSU	C4-N3-C2	13.37	126.80	115.25
1	E	54	5MU	C4-N3-C2	13.37	126.81	115.25
1	F	54	5MU	C4-N3-C2	13.38	126.81	115.25
1	E	39	PSU	C4-N3-C2	13.42	126.84	115.25
1	D	54	5MU	C4-N3-C2	13.45	126.88	115.25
1	E	55	PSU	C4-N3-C2	13.46	126.88	115.25
1	D	55	PSU	C4-N3-C2	13.61	127.01	115.25
1	D	39	PSU	C4-N3-C2	13.75	127.13	115.25
1	E	26	M2G	CM1-N2-C2	17.87	139.72	121.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

38 monomers are involved in 156 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	10	2MG	4	0
1	D	16	H2U	5	0
1	D	17	H2U	3	0
1	D	26	M2G	11	0
1	D	32	OMC	2	0
1	D	34	OMG	2	0
1	D	37	YYG	8	0
1	D	39	PSU	5	0
1	D	40	5MC	4	0
1	D	46	7MG	2	0
1	D	49	5MC	1	0
1	D	54	5MU	1	0
1	D	55	PSU	1	0
1	D	58	1MA	3	0
1	E	10	2MG	12	0
1	E	16	H2U	4	0
1	E	17	H2U	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	26	M2G	11	0
1	E	32	OMC	3	0
1	E	34	OMG	3	0
1	E	37	YYG	12	0
1	E	39	PSU	2	0
1	E	46	7MG	2	0
1	E	54	5MU	3	0
1	E	55	PSU	1	0
1	E	58	1MA	1	0
1	F	10	2MG	9	0
1	F	16	H2U	5	0
1	F	17	H2U	1	0
1	F	26	M2G	7	0
1	F	32	OMC	1	0
1	F	34	OMG	4	0
1	F	37	YYG	17	0
1	F	40	5MC	3	0
1	F	46	7MG	4	0
1	F	49	5MC	1	0
1	F	54	5MU	1	0
1	F	55	PSU	3	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\# Z > 2$
5	GNP	A	406	3	28,34,34	1.85	7 (25%)	33,54,54	4.48	16 (48%)
5	GNP	B	406	3	28,34,34	1.66	3 (10%)	33,54,54	2.76	8 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GNP	C	406	3	28,34,34	2.38	5 (17%)	33,54,54	5.11	13 (39%)
4	PHE	D	77	1	10,11,12	1.02	1 (10%)	10,13,15	2.15	2 (20%)
4	PHE	E	77	1	10,11,12	0.93	1 (10%)	10,13,15	1.51	2 (20%)
4	PHE	F	77	1	10,11,12	1.15	1 (10%)	10,13,15	2.01	2 (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
5	GNP	A	406	3	-	1/12/38/38	0/3/3/3
5	GNP	B	406	3	-	1/12/38/38	0/3/3/3
5	GNP	C	406	3	-	1/12/38/38	0/3/3/3
4	PHE	D	77	1	-	0/4/6/8	0/1/1/1
4	PHE	E	77	1	-	0/4/6/8	0/1/1/1
4	PHE	F	77	1	-	0/4/6/8	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	406	GNP	PB-O3A	-7.99	1.49	1.59
5	B	406	GNP	PB-O3A	-6.26	1.51	1.59
5	A	406	GNP	PB-O3A	-4.79	1.53	1.59
5	A	406	GNP	PB-O2B	-3.50	1.46	1.56
5	C	406	GNP	PG-O2G	-3.34	1.47	1.56
5	B	406	GNP	PG-O2G	-2.95	1.48	1.56
5	A	406	GNP	PG-O2G	-2.82	1.48	1.56
4	D	77	PHE	CA-N	-2.73	1.39	1.47
4	F	77	PHE	CA-N	-2.59	1.39	1.47
4	E	77	PHE	CA-N	-2.26	1.40	1.47
5	A	406	GNP	PB-N3B	-2.14	1.57	1.63
5	A	406	GNP	PG-O3G	-2.03	1.51	1.56
5	C	406	GNP	C2-N1	2.07	1.39	1.35
5	C	406	GNP	C6-N1	2.88	1.38	1.33
5	A	406	GNP	PG-O1G	3.20	1.49	1.46
5	B	406	GNP	C6-N1	3.21	1.39	1.33
5	A	406	GNP	C6-N1	3.44	1.39	1.33
5	C	406	GNP	PG-O1G	6.99	1.54	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	406	GNP	C1'-N9-C4	-17.24	100.94	126.94
5	C	406	GNP	C2'-C1'-N9	-11.76	96.32	114.29
5	C	406	GNP	O3A-PA-O5'	-10.70	74.56	102.94
5	A	406	GNP	C5-C6-N1	-9.38	110.76	123.59
5	B	406	GNP	C5-C6-N1	-9.22	110.99	123.59
5	C	406	GNP	C5-C6-N1	-7.65	113.13	123.59
4	F	77	PHE	CG-CB-CA	-5.74	101.24	114.21
5	B	406	GNP	C2'-C1'-N9	-5.25	106.26	114.29
4	D	77	PHE	CG-CB-CA	-5.01	102.88	114.21
5	B	406	GNP	C1'-N9-C4	-4.84	119.64	126.94
4	D	77	PHE	O-C-CA	-4.47	113.85	125.49
5	B	406	GNP	O1G-PG-N3B	-4.38	105.17	111.90
5	C	406	GNP	O1B-PB-N3B	-4.29	105.31	111.90
4	E	77	PHE	O-C-CA	-3.76	115.70	125.49
5	B	406	GNP	O1B-PB-N3B	-3.21	106.97	111.90
5	A	406	GNP	O3'-C3'-C4'	-3.17	101.55	111.05
5	A	406	GNP	O5'-C5'-C4'	-3.10	97.68	109.12
5	A	406	GNP	O2A-PA-O5'	-2.73	94.72	108.46
4	F	77	PHE	O-C-CA	-2.65	118.59	125.49
5	A	406	GNP	O3G-PG-O1G	-2.58	106.64	113.49
4	E	77	PHE	CG-CB-CA	-2.50	108.57	114.21
5	A	406	GNP	N3-C2-N1	-2.39	123.80	127.44
5	A	406	GNP	O3'-C3'-C2'	-2.09	105.02	111.83
5	A	406	GNP	O2A-PA-O1A	2.04	123.59	112.53
5	A	406	GNP	O4'-C4'-C5'	2.15	117.01	109.32
5	C	406	GNP	O2A-PA-O1A	2.23	124.62	112.53
5	B	406	GNP	C4'-O4'-C1'	2.30	112.25	109.72
5	C	406	GNP	C4-C5-N7	2.37	111.66	109.48
5	C	406	GNP	O5'-PA-O1A	2.64	119.86	109.62
5	C	406	GNP	O5'-C5'-C4'	2.72	119.14	109.12
5	C	406	GNP	O2'-C2'-C3'	2.78	120.88	111.83
5	A	406	GNP	PA-O3A-PB	2.89	142.34	132.67
5	B	406	GNP	O2A-PA-O3A	3.29	120.03	105.09
5	A	406	GNP	C4-C5-N7	3.79	112.97	109.48
5	A	406	GNP	O3G-PG-O2G	4.39	120.58	107.58
5	C	406	GNP	C6-N1-C2	4.67	122.42	115.94
5	C	406	GNP	O3A-PB-N3B	5.28	120.97	106.44
5	A	406	GNP	O3A-PA-O5'	5.81	118.36	102.94
5	B	406	GNP	C6-N1-C2	6.12	124.43	115.94
5	A	406	GNP	O2B-PB-O1B	6.12	122.77	110.00
5	A	406	GNP	C6-N1-C2	7.46	126.29	115.94
5	C	406	GNP	O2B-PB-O1B	11.13	133.22	110.00
5	A	406	GNP	C1'-N9-C4	18.33	154.59	126.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	406	GNP	O1B-PB-N3B-PG
5	C	406	GNP	O1B-PB-N3B-PG
5	B	406	GNP	O1B-PB-N3B-PG

There are no ring outliers.

6 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	406	GNP	6	0
5	B	406	GNP	7	0
5	C	406	GNP	7	0
4	D	77	PHE	2	0
4	E	77	PHE	1	0
4	F	77	PHE	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.