



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 06:42 PM GMT

PDB ID : 2VQF
Title : MODIFIED URIDINES WITH C5-METHYLENE SUBSTITUENTS AT
THE FIRST POSITION OF THE TRNA ANTICODON STABILIZE U-G
WOBBLE PAIRING DURING DECODING
Authors : Kurata, S.; Weixlbaumer, A.; Ohtsuki, T.; Shimazaki, T.; Wada, T.; Kirino,
Y.; Takai, K.; Watanabe, K.; Ramakrishnan, V.; Suzuki, T.
Deposited on : 2008-03-14
Resolution : 2.90 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

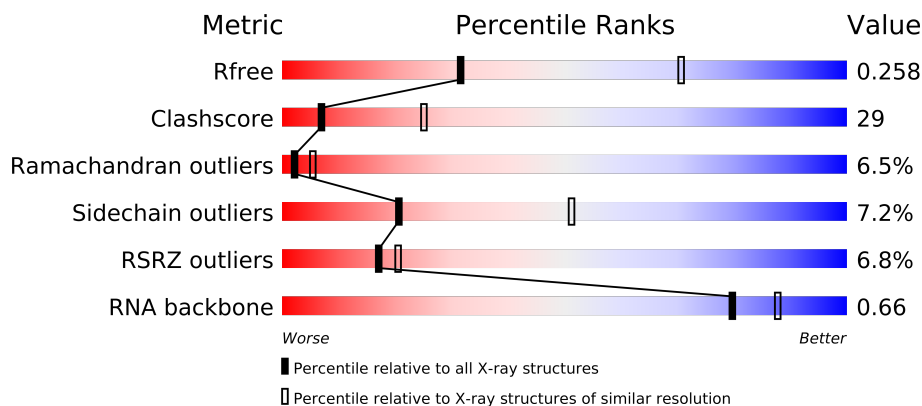
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 Å.

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



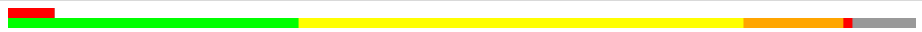
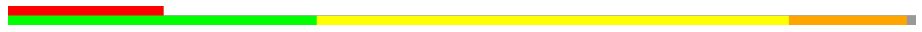




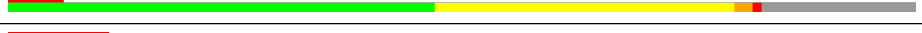


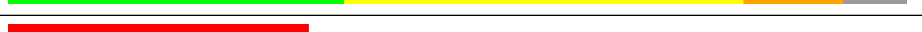

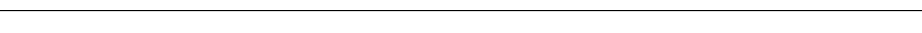
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1053 (2.90-2.90)
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)
RNA backbone	1838	1055 (3.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	L	135	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	U	27	
22	X	6	
23	Y	17	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 52314 atoms, of which 0 are hydrogen and 0 are deuterium.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1513	Total	C	N	O	P	0	0	0
			32511	14472	6016	10511	1512			

- Molecule 2 is a protein called 30S RIBOSOMAL PROTEIN S2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	0	1
			1901	1213	342	341	5			

- Molecule 3 is a protein called 30S RIBOSOMAL PROTEIN S3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	0	0	1
			1613	1016	315	281	1			

- Molecule 4 is a protein called 30S RIBOSOMAL PROTEIN S4.

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

- Molecule 5 is a protein called 30S RIBOSOMAL PROTEIN S5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	151	Total	C	N	O	S	0	0	1
			1147	724	218	201	4			

- Molecule 6 is a protein called 30S RIBOSOMAL PROTEIN S6.

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

- Molecule 7 is a protein called 30S RIBOSOMAL PROTEIN S7.

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

- Molecule 8 is a protein called 30S RIBOSOMAL PROTEIN S8.

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

- Molecule 9 is a protein called 30S RIBOSOMAL PROTEIN S9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	127	Total	C	N	O	S	0	0	0
			1011	639	198	174				

- Molecule 10 is a protein called 30S RIBOSOMAL PROTEIN S10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	99	Total	C	N	O	S	0	0	1
			793	498	157	137	1			

- Molecule 11 is a protein called 30S RIBOSOMAL PROTEIN S11.

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

- Molecule 12 is a protein called 30S RIBOSOMAL PROTEIN S12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	125	Total	C	N	O	S	0	0	1
			971	611	196	163	1			

- Molecule 13 is a protein called 30S RIBOSOMAL PROTEIN S13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	M	125	Total	C	N	O	S	0	0	0
			997	617	207	171	2			

- Molecule 14 is a protein called 30S RIBOSOMAL PROTEIN S14 TYPE Z.

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

- Molecule 15 is a protein called 30S RIBOSOMAL PROTEIN S15.

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

- Molecule 16 is a protein called 30S RIBOSOMAL PROTEIN S16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	P	84	Total	C	N	O	S	0	0	1
			701	443	140	117	1			

- Molecule 17 is a protein called 30S RIBOSOMAL PROTEIN S17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	Q	104	Total	C	N	O	S	0	0	0
			857	547	161	147	2			

- Molecule 18 is a protein called 30S RIBOSOMAL PROTEIN S18.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
18	R	73	Total	C	N	O	0	0	0
			597	380	118	99			

- Molecule 19 is a protein called 30S RIBOSOMAL PROTEIN S19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
19	S	81	Total	C	N	O	S	0	0	1
			648	414	120	112	2			

- Molecule 20 is a protein called 30S RIBOSOMAL PROTEIN S20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	T	99	Total	C	N	O	S	0	0	0
			762	469	162	129	2			

- Molecule 21 is a protein called 30S RIBOSOMAL PROTEIN THX.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
21	U	25	Total	C	N	O	0	0	1
			209	128	51	30			

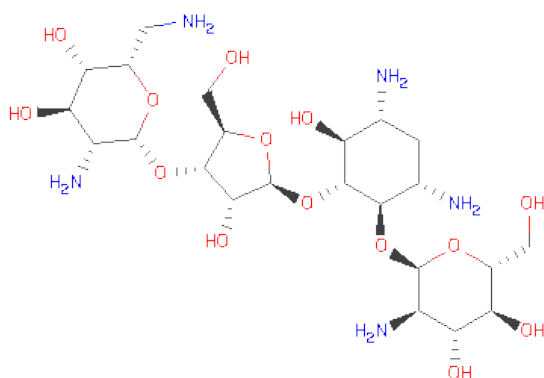
- Molecule 22 is a RNA chain called 5'-R(*UP*UP*GP*AP*AP*AP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	X	4	Total	C	N	O	P	0	0	0
			82	38	14	27	3			

- Molecule 23 is a RNA chain called 5'-R(*GP*CP*AP*UP*GP*CP*U*TM2P*AP*AP*AP*AP*CP*AP*UP*GP*C)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
23	Y	7	Total	C	N	O	P	S	0	0	0
			153	70	28	48	6	1			

- Molecule 24 is PAROMOMYCIN (three-letter code: PAR) (formula: C₂₃H₄₅N₅O₁₄).



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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
25	Z	214	Total	Mg	0	0
			214	214		

- Molecule 26 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
26	Z	2	Total 2	Zn 2	0	0

- Molecule 27 is POTASSIUM ION (three-letter code: K) (formula: K).

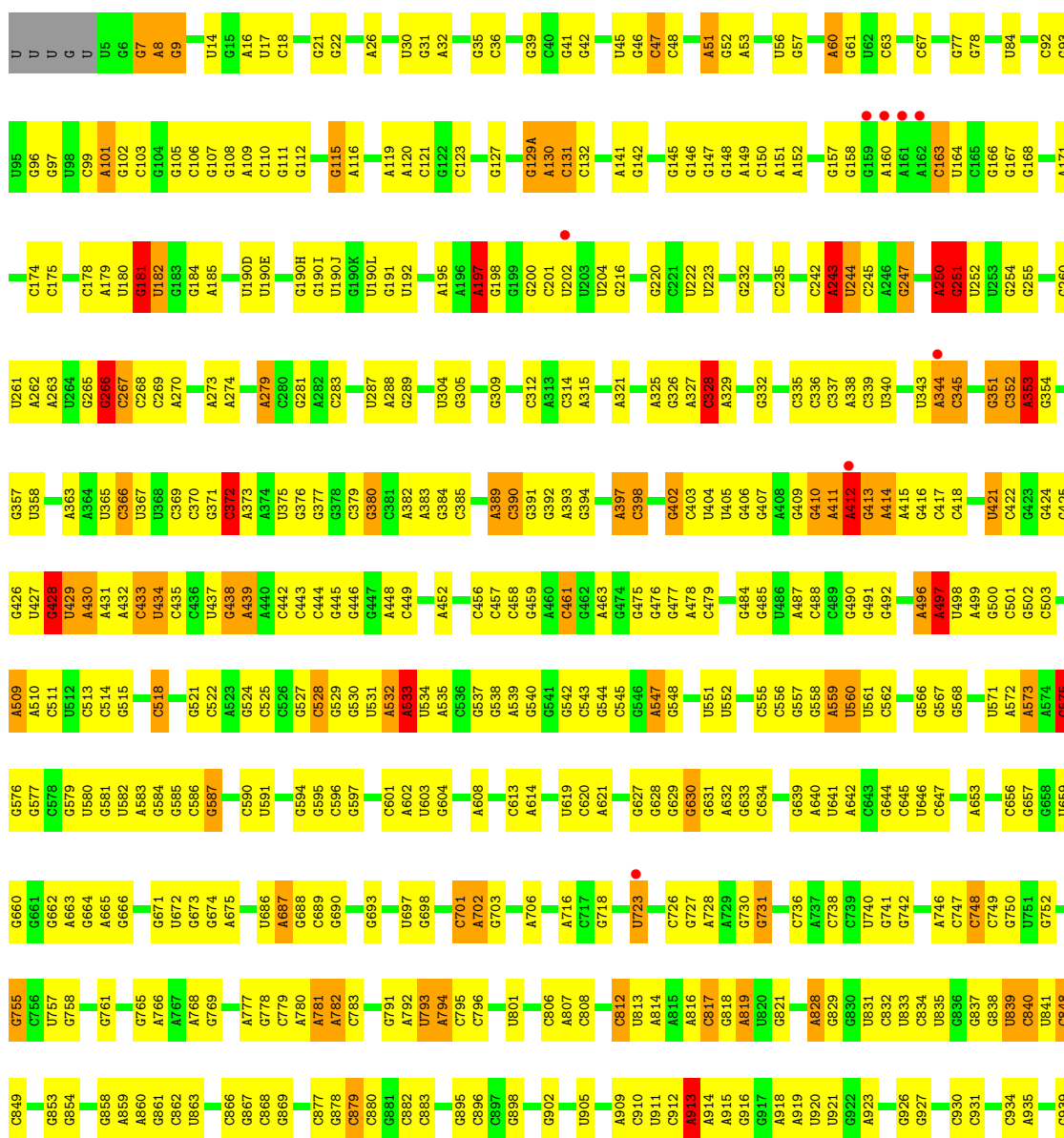
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
27	Z	73	Total 73	K 73	0	0

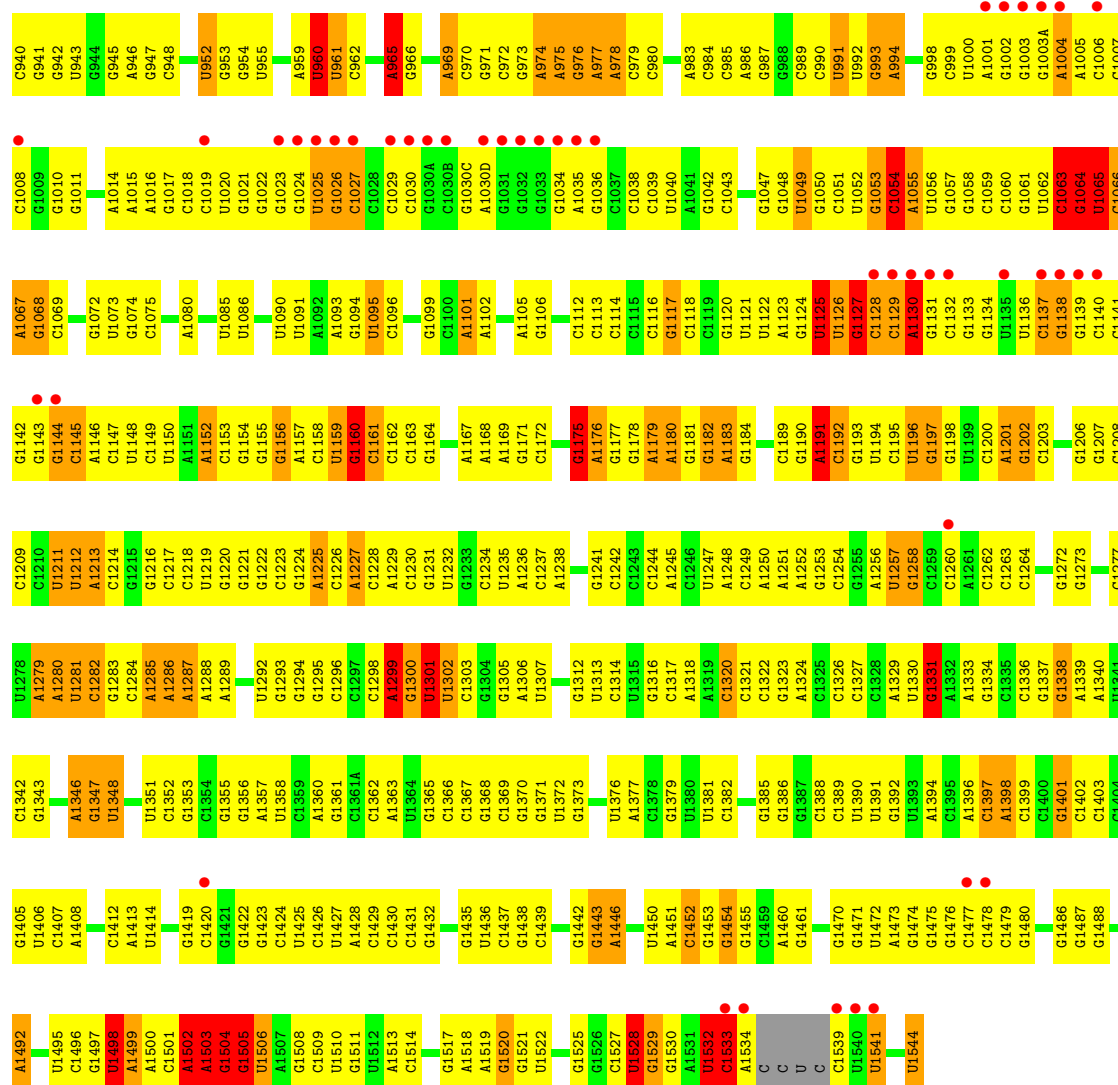
3 Residue-property plots

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

• Molecule 1: 16S RRNA

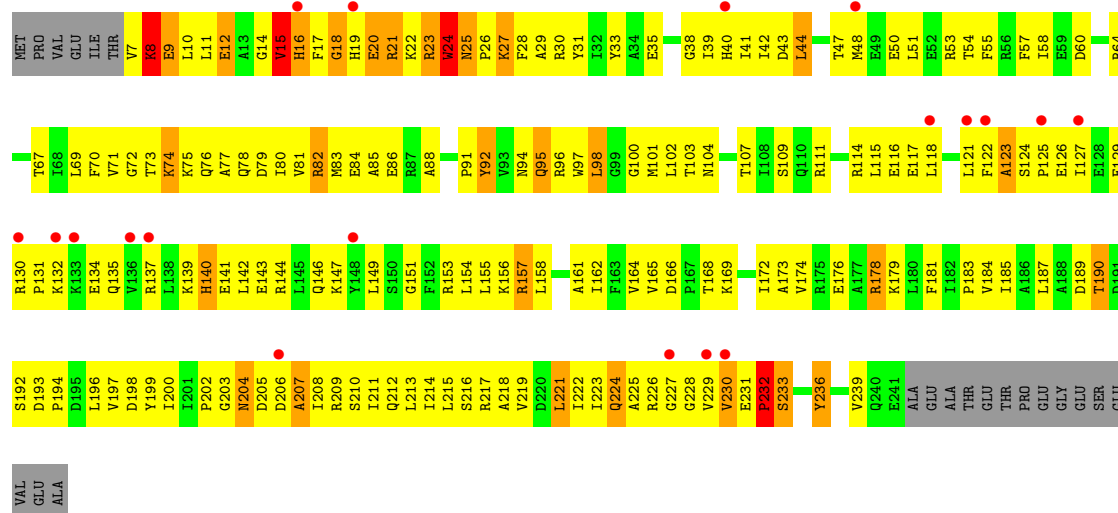
Chain A: 





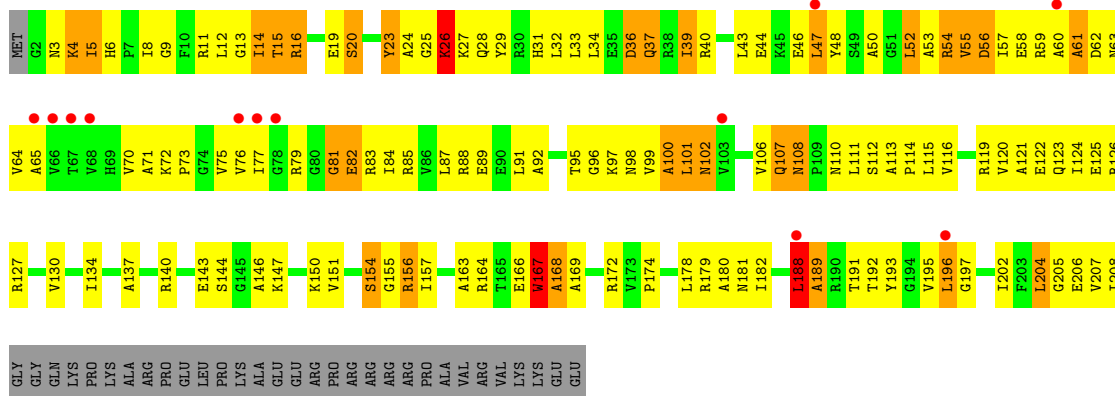
- Molecule 2: 30S RIBOSOMAL PROTEIN S2

Chain B:



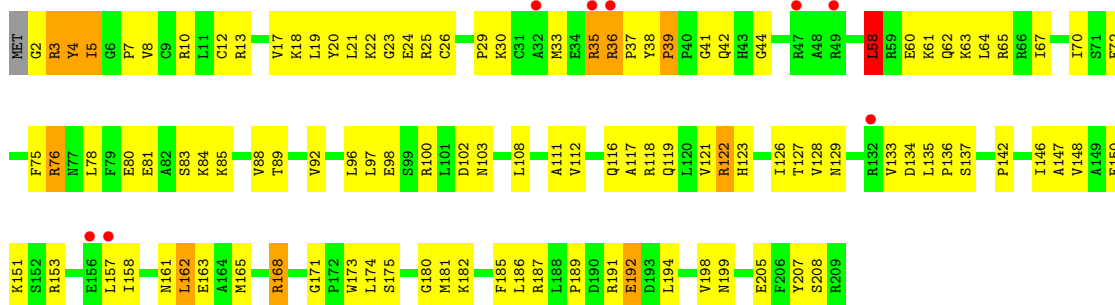
- Molecule 3: 30S RIBOSOMAL PROTEIN S3

Chain C:



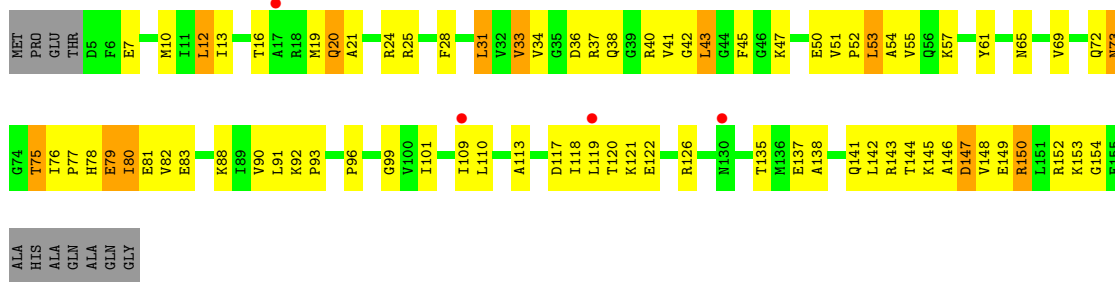
• Molecule 4: 30S RIBOSOMAL PROTEIN S4

Chain D:



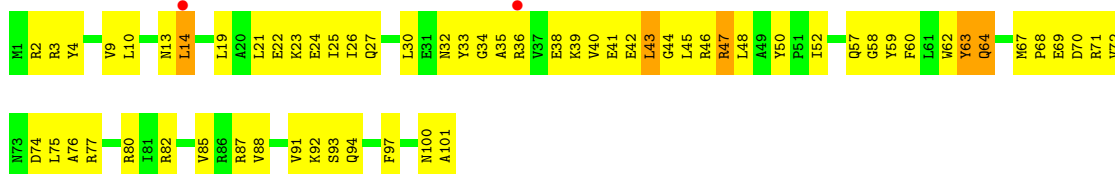
- Molecule 5: 30S RIBOSOMAL PROTEIN S5

Chain E:



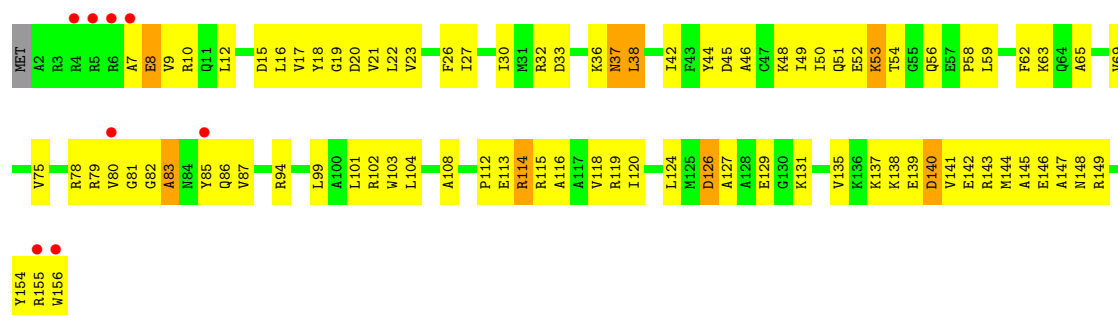
● Molecule 6: 30S RIBOSOMAL PROTEIN S6

Chain F:



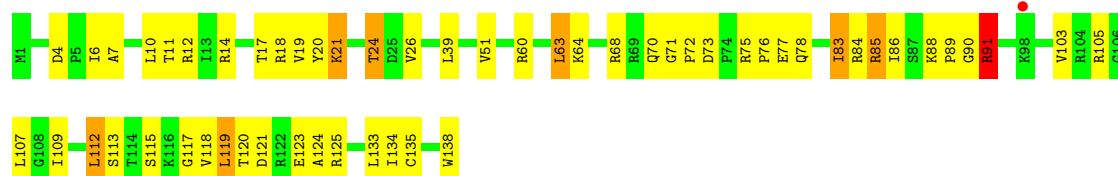
- Molecule 7: 30S RIBOSOMAL PROTEIN S7

Chain G:



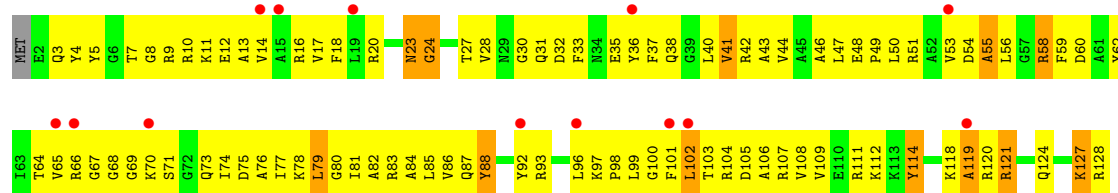
- Molecule 8: 30S RIBOSOMAL PROTEIN S8

Chain H:



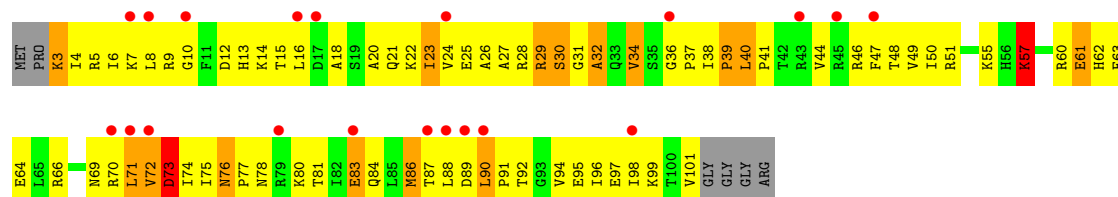
- Molecule 9: 30S RIBOSOMAL PROTEIN S9

Chain I:



- Molecule 10: 30S RIBOSOMAL PROTEIN S10

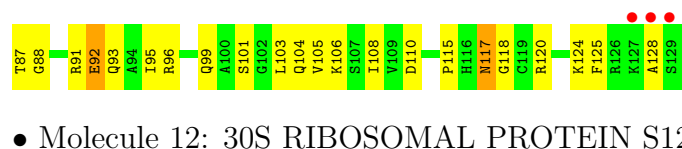
Chain J:



- Molecule 11: 30S RIBOSOMAL PROTEIN S11

Chain K:

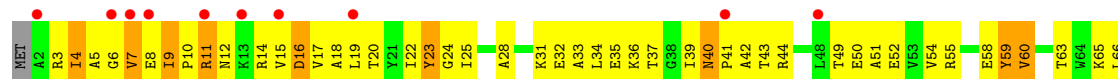




Chain L:



Chain M:



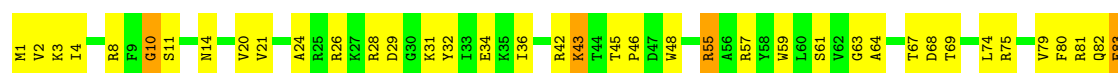
Chain N:



Chain O:

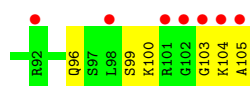


Chain P:



Chain Q:





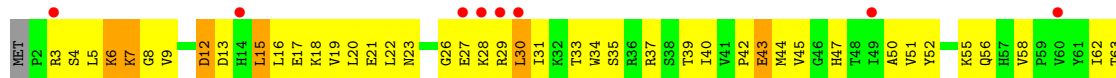
• Molecule 18: 30S RIBOSOMAL PROTEIN S18

Chain R:



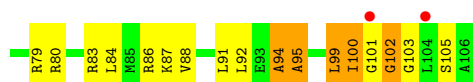
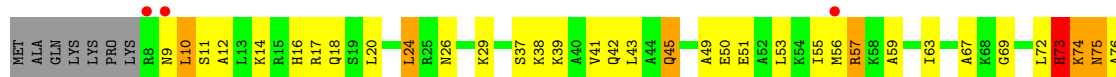
• Molecule 19: 30S RIBOSOMAL PROTEIN S19

Chain S:



• Molecule 20: 30S RIBOSOMAL PROTEIN S20

Chain T:



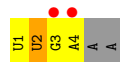
• Molecule 21: 30S RIBOSOMAL PROTEIN THX

Chain U:



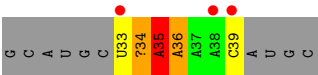
• Molecule 22: 5'-R(*UP*UP*GP*AP*AP*AP)-3'

Chain X:



• Molecule 23: 5'-R(*GP*CP*AP*UP*GP*CP*U*TM2P*AP*AP*AP*AP*CP*AP*UP*GP*C)-3'

Chain Y:



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	402.48 Å 402.48 Å 175.97 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.92 – 2.90 49.92 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.92-2.90) 97.4 (49.92-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.81 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.223 , 0.258 0.229 , 0.258	Depositor DCC
R_{free} test set	16936 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 55.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 341315 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	52314	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: K, ZN, PAR, MG, TM2

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.14	14/36390 (0.0%)	1.01	83/56793 (0.1%)
2	B	0.35	0/1936	0.61	0/2611
3	C	0.38	0/1637	0.61	0/2207
4	D	0.35	0/1733	0.57	0/2318
5	E	0.46	0/1163	0.71	0/1566
6	F	0.33	0/856	0.61	0/1154
7	G	0.35	0/1276	0.57	0/1709
8	H	0.44	0/1136	0.73	0/1527
9	I	0.35	0/1029	0.64	0/1378
10	J	0.37	0/806	0.63	0/1084
11	K	0.39	0/900	0.67	0/1213
12	L	0.45	0/987	0.77	1/1322 (0.1%)
13	M	0.34	0/1008	0.63	0/1347
14	N	0.40	0/501	0.68	0/664
15	O	0.36	0/745	0.61	0/992
16	P	0.48	0/717	0.73	0/965
17	Q	0.43	0/870	0.74	0/1159
18	R	0.37	0/603	0.61	0/799
19	S	0.35	0/662	0.61	0/892
20	T	0.38	0/764	0.73	0/1006
21	U	0.50	0/213	0.59	0/279
22	X	0.38	0/91	0.67	0/140
23	Y	2.01	3/140 (2.1%)	1.36	2/216 (0.9%)
All	All	0.95	17/56163 (0.0%)	0.91	86/83341 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	4	35

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1179	A	O3'-P	-77.75	0.67	1.61
1	A	1331	G	N3-C4	77.20	1.89	1.35
1	A	1063	C	O3'-P	-72.79	0.73	1.61
1	A	1175	G	O3'-P	-61.89	0.86	1.61
1	A	1192	C	O3'-P	-54.97	0.95	1.61
1	A	1191	A	O3'-P	-54.09	0.96	1.61
1	A	1144	G	O3'-P	-50.43	1.00	1.61
1	A	1532	U	O3'-P	-46.97	1.04	1.61
1	A	1156	G	O3'-P	-42.86	1.09	1.61
1	A	1064	G	O3'-P	31.21	1.98	1.61
1	A	1541	U	O3'-P	-25.77	1.30	1.61
1	A	1160	G	O3'-P	-23.93	1.32	1.61
23	Y	35	A	O3'-P	-20.26	1.36	1.61
23	Y	34	TM2	O3'-P	-9.96	1.49	1.61
1	A	1533	C	O3'-P	9.56	1.72	1.61
23	Y	36	A	O3'-P	-5.41	1.54	1.61
1	A	243	A	P-O5'	-5.00	1.54	1.59

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1144	G	P-O3'-C3'	-55.79	52.76	119.70
1	A	1331	G	C2-N3-C4	-52.06	85.87	111.90
1	A	1127	G	P-O3'-C3'	-42.98	68.12	119.70
1	A	1127	G	OP2-P-O3'	-39.59	18.11	105.20
1	A	1532	U	P-O3'-C3'	-38.65	73.31	119.70
1	A	1064	G	OP1-P-O3'	-35.66	26.76	105.20
1	A	1175	G	O3'-P-O5'	35.05	170.59	104.00
1	A	1160	G	O3'-P-O5'	34.22	169.02	104.00
1	A	1179	A	P-O3'-C3'	-33.26	79.79	119.70
1	A	1160	G	P-O3'-C3'	-32.21	81.05	119.70
1	A	1175	G	P-O3'-C3'	-31.24	82.22	119.70
1	A	1532	U	O3'-P-O5'	31.08	163.05	104.00
1	A	1144	G	O3'-P-O5'	-30.12	46.78	104.00
1	A	1331	G	N3-C4-C5	-30.02	113.59	128.60
1	A	1063	C	O3'-P-O5'	-27.82	51.13	104.00
1	A	1179	A	OP1-P-O3'	-25.08	50.03	105.20
1	A	1192	C	P-O3'-C3'	-22.94	92.17	119.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1533	C	P-O3'-C3'	-21.79	93.55	119.70
1	A	1192	C	OP2-P-O3'	-21.68	57.50	105.20
1	A	1532	U	OP2-P-O3'	-21.02	58.96	105.20
1	A	1331	G	N3-C2-N2	-20.96	105.23	119.90
1	A	1191	A	P-O3'-C3'	20.75	144.60	119.70
1	A	1160	G	OP1-P-O3'	-19.55	62.19	105.20
1	A	1179	A	O3'-P-O5'	18.15	138.49	104.00
1	A	1144	G	OP1-P-O3'	17.03	142.66	105.20
1	A	1063	C	OP1-P-O3'	15.96	140.30	105.20
1	A	1179	A	OP2-P-O3'	-14.91	72.41	105.20
1	A	1175	G	OP2-P-O3'	-13.80	74.84	105.20
23	Y	34	TM2	P-O3'-C3'	13.75	136.20	119.70
1	A	1175	G	OP1-P-O3'	-13.08	76.42	105.20
1	A	1533	C	O3'-P-O5'	12.94	128.58	104.00
1	A	1160	G	OP2-P-O3'	-12.46	77.78	105.20
1	A	1192	C	OP1-P-O3'	11.93	131.45	105.20
1	A	1541	U	OP2-P-O3'	11.17	129.76	105.20
1	A	1156	G	O3'-P-O5'	10.71	124.35	104.00
1	A	1064	G	O3'-P-O5'	-10.70	83.68	104.00
1	A	1498	U	C2'-C3'-O3'	10.31	132.19	109.50
1	A	115	G	C2'-C3'-O3'	9.92	131.33	109.50
1	A	1064	G	OP2-P-O3'	9.85	126.86	105.20
1	A	243	A	C2'-C3'-O3'	9.49	130.39	109.50
1	A	1301	U	C2'-C3'-O3'	9.17	129.68	109.50
1	A	1192	C	O3'-P-O5'	8.82	120.77	104.00
1	A	559	A	C2'-C3'-O3'	8.81	128.89	109.50
1	A	812	C	C2'-C3'-O3'	8.54	128.30	109.50
1	A	575	G	C2'-C3'-O3'	8.37	127.92	109.50
1	A	1331	G	N1-C2-N3	-8.36	118.88	123.90
1	A	1541	U	OP1-P-O3'	-8.22	87.12	105.20
1	A	412	A	N9-C1'-C2'	8.20	124.66	114.00
1	A	687	A	C2'-C3'-O3'	8.10	127.31	109.50
1	A	60	A	C2'-C3'-O3'	8.09	127.30	109.50
1	A	181	G	C2'-C3'-O3'	8.08	127.27	109.50
1	A	1528	U	C2'-C3'-O3'	8.02	127.15	109.50
1	A	410	G	C2'-C3'-O3'	7.95	126.99	109.50
1	A	1299	A	N9-C1'-C2'	7.84	124.19	114.00
1	A	328	C	C2'-C3'-O3'	7.81	126.68	109.50
23	Y	35	A	P-O3'-C3'	7.69	128.92	119.70
1	A	1503	A	C2'-C3'-O3'	7.67	126.38	109.50
1	A	913	A	C2'-C3'-O3'	7.31	125.58	109.50
1	A	533	A	C2'-C3'-O3'	7.11	125.14	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1065	U	C2'-C3'-O3'	7.04	124.99	109.50
1	A	1532	U	OP1-P-O3'	-6.99	89.83	105.20
1	A	1191	A	O3'-P-O5'	6.91	117.12	104.00
1	A	1331	G	N3-C4-N9	6.90	130.14	126.00
1	A	1064	G	P-O3'-C3'	6.88	127.95	119.70
1	A	366	C	C2'-C3'-O3'	6.78	124.54	113.70
1	A	1191	A	OP2-P-O3'	-6.66	90.56	105.20
1	A	509	A	C2'-C3'-O3'	6.58	124.22	113.70
1	A	1505	G	C2'-C3'-O3'	6.55	124.18	113.70
1	A	266	G	C2'-C3'-O3'	6.50	124.10	113.70
1	A	372	C	C2'-C3'-O3'	6.29	123.77	113.70
1	A	965	A	C2'-C3'-O3'	6.29	123.76	113.70
1	A	1156	G	P-O3'-C3'	5.98	126.88	119.70
1	A	960	U	C2'-C3'-O3'	5.70	122.82	113.70
1	A	428	G	C2'-C3'-O3'	5.63	122.71	113.70
12	L	119	LYS	N-CA-C	-5.58	95.92	111.00
1	A	1502	A	N9-C1'-C2'	5.58	121.25	114.00
1	A	686	U	N1-C1'-C2'	5.50	121.14	114.00
1	A	63	C	C5'-C4'-C3'	-5.41	107.35	116.00
1	A	1504	G	C2'-C3'-O3'	5.36	122.27	113.70
1	A	497	A	C2'-C3'-O3'	5.24	122.09	113.70
1	A	389	A	C5'-C4'-C3'	5.24	124.38	116.00
1	A	1533	C	OP1-P-O3'	-5.22	93.72	105.20
1	A	748	C	C2'-C3'-O3'	5.20	122.02	113.70
1	A	328	C	O4'-C1'-N1	-5.11	104.11	108.20
1	A	1279	A	N9-C1'-C2'	5.11	120.64	114.00
1	A	353	A	C5'-C4'-O4'	-5.06	103.03	109.10

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	115	G	C3'
1	A	243	A	C3'
1	A	410	G	C3'
1	A	412	A	C1'

All (35) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	C	Sidechain
1	A	1125	U	Sidechain
1	A	1130	A	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	1299	A	Sidechain
1	A	1331	G	Sidechain
1	A	14	U	Sidechain
1	A	1401	G	Sidechain
1	A	1414	U	Sidechain
1	A	1454	G	Sidechain
1	A	1492	A	Sidechain
1	A	1498	U	Sidechain
1	A	1544	U	Sidechain
1	A	197	A	Sidechain
1	A	250	A	Sidechain
1	A	251	G	Sidechain
1	A	265	G	Sidechain
1	A	274	A	Sidechain
1	A	279	A	Sidechain
1	A	380	G	Sidechain
1	A	402	G	Sidechain
1	A	528	C	Sidechain
1	A	529	G	Sidechain
1	A	571	U	Sidechain
1	A	573	A	Sidechain
1	A	575	G	Sidechain
1	A	587	G	Sidechain
1	A	641	U	Sidechain
1	A	656	C	Sidechain
1	A	727	G	Sidechain
1	A	752	G	Sidechain
1	A	84	U	Sidechain
1	A	879	C	Sidechain
1	A	898	G	Sidechain
1	A	905	U	Sidechain
1	A	952	U	Sidechain

5.2 Close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32511	0	16403	994	0
2	B	1901	0	1951	242	0
3	C	1613	0	1677	186	0
4	D	1703	0	1767	127	0
5	E	1147	0	1206	94	0
6	F	843	0	857	89	0
7	G	1257	0	1296	82	0
8	H	1116	0	1177	61	0
9	I	1011	0	1040	120	0
10	J	793	0	835	142	0
11	K	885	0	904	65	0
12	L	971	0	1057	110	0
13	M	997	0	1071	96	0
14	N	492	0	529	50	0
15	O	734	0	771	35	0
16	P	701	0	720	42	0
17	Q	857	0	930	58	0
18	R	597	0	668	43	0
19	S	648	0	673	71	0
20	T	762	0	859	51	0
21	U	209	0	221	21	0
22	X	82	0	44	18	0
23	Y	153	0	83	12	0
24	Z	42	0	45	1	0
25	Z	214	0	0	0	0
26	Z	2	0	0	0	0
27	Z	73	0	0	0	0
All	All	52314	0	36784	2558	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

All (2558) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1179:A:N6	1:A:1180:A:C2	1.81	1.49
1:A:1156:G:O3'	1:A:1157:A:P	1.09	1.47
1:A:1331:G:N3	1:A:1331:G:C4	1.89	1.40
1:A:1191:A:O3'	1:A:1192:C:P	0.96	1.36
1:A:1533:C:O2'	1:A:1534:A:H5'	1.25	1.31
1:A:1179:A:C6	1:A:1180:A:C2	2.21	1.28
1:A:1191:A:HO3'	1:A:1192:C:P	0.87	1.23
1:A:1156:G:C3'	1:A:1157:A:P	2.26	1.22
1:A:1331:G:C2	1:A:1331:G:C4	2.21	1.21

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1191:A:C3'	1:A:1192:C:P	2.31	1.17
22:X:3:G:O2'	22:X:4:A:H5'	1.38	1.17
1:A:1156:G:H21	1:A:1179:A:N6	1.48	1.12
1:A:243:A:H4'	1:A:244:U:H5'	1.30	1.09
1:A:1305:G:H22	1:A:1331:G:H2'	1.17	1.06
3:C:64:VAL:HG23	3:C:99:VAL:HG11	1.39	1.05
3:C:14:ILE:HG22	3:C:15:THR:H	1.16	1.05
1:A:1190:G:H3'	3:C:3:ASN:ND2	1.72	1.04
1:A:266:G:H5''	1:A:268:C:H41	1.17	1.04
19:S:33:THR:HG22	19:S:35:SER:H	1.23	1.04
1:A:1250:A:H4'	9:I:68:GLY:H	1.19	1.03
2:B:60:ASP:HB3	2:B:64:ARG:HH12	1.22	1.03
1:A:1533:C:O2'	1:A:1534:A:C5'	2.07	1.03
1:A:991:U:H5	1:A:1212:U:H1'	1.21	1.02
2:B:208:ILE:HD12	2:B:208:ILE:H	1.22	1.02
1:A:1250:A:H4'	9:I:68:GLY:N	1.75	1.02
1:A:1130:A:C4	1:A:1146:A:C2	2.48	1.02
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.43	1.01
1:A:579:G:H5'	1:A:728:A:H1'	1.42	1.01
1:A:1305:G:N2	1:A:1331:G:H2'	1.77	1.00
1:A:1118:C:O2	1:A:1179:A:C5	2.15	0.99
2:B:77:ALA:HB2	2:B:211:ILE:HD13	1.42	0.99
4:D:168:ARG:HH11	4:D:168:ARG:HB3	1.25	0.98
1:A:1179:A:N6	1:A:1180:A:H2	1.55	0.97
3:C:58:GLU:HB3	10:J:92:THR:HG21	1.43	0.97
1:A:1116:C:H2'	1:A:1117:G:H5''	1.48	0.96
19:S:28:LYS:HG2	19:S:29:ARG:H	1.27	0.96
3:C:84:ILE:HD11	3:C:88:ARG:HH21	1.31	0.96
1:A:1118:C:O2	1:A:1179:A:C6	2.18	0.96
3:C:64:VAL:HB	3:C:99:VAL:HG21	1.43	0.96
11:K:110:ASP:HB2	18:R:88:LYS:HD2	1.47	0.96
1:A:432:A:H3'	1:A:433:C:H5''	1.48	0.95
1:A:1086:U:H3	1:A:1099:G:H22	1.06	0.95
13:M:49:THR:HG22	13:M:51:ALA:H	1.31	0.95
1:A:1175:G:N3	1:A:1176:A:C8	2.35	0.95
22:X:3:G:C2'	22:X:4:A:H5'	1.97	0.94
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.47	0.94
13:M:34:LEU:HD13	13:M:41:PRO:HA	1.50	0.93
1:A:1152:A:H5''	10:J:13:HIS:HD2	1.33	0.93
1:A:1175:G:C4	1:A:1176:A:C8	2.57	0.93
1:A:1063:C:H3'	1:A:1064:G:H2'	1.49	0.93
1:A:1156:G:N2	1:A:1179:A:N1	2.16	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:87:ILE:HG22	15:O:88:ARG:H	1.34	0.93
11:K:91:ARG:HD3	18:R:88:LYS:HE2	1.50	0.93
1:A:664:G:H22	1:A:741:G:H1	1.09	0.93
1:A:1281:U:H5'	1:A:1282:C:C5	2.03	0.92
1:A:1533:C:HO2'	1:A:1534:A:H5'	1.33	0.92
17:Q:67:LYS:HA	17:Q:70:ARG:HH12	1.34	0.92
1:A:1178:G:N2	1:A:1180:A:C8	2.38	0.92
12:L:47:LYS:HB3	12:L:48:PRO:CD	1.98	0.91
5:E:80:ILE:CD1	5:E:91:LEU:HB2	2.00	0.91
1:A:972:C:H4'	10:J:57:LYS:HG2	1.51	0.91
3:C:26:LYS:HD3	3:C:26:LYS:H	1.35	0.91
1:A:1356:G:H2'	1:A:1357:A:C8	2.06	0.90
1:A:1156:G:HO3'	1:A:1157:A:P	1.27	0.90
1:A:1179:A:C6	1:A:1180:A:N3	2.38	0.90
12:L:55:VAL:HG12	12:L:56:ALA:H	1.37	0.90
1:A:1178:G:N2	1:A:1180:A:H8	1.70	0.89
2:B:18:GLY:HA2	2:B:41:ILE:HA	1.54	0.89
3:C:91:LEU:HD21	3:C:99:VAL:H	1.36	0.89
1:A:1152:A:H5''	10:J:13:HIS:CD2	2.07	0.89
1:A:991:U:C5	1:A:1212:U:H1'	2.08	0.89
1:A:1238:A:H5'	1:A:1336:C:H41	1.38	0.89
7:G:75:VAL:HG21	7:G:86:GLN:HB3	1.54	0.89
1:A:1533:C:H2'	1:A:1534:A:O5'	1.73	0.89
1:A:1367:C:H5'	10:J:60:ARG:NH1	1.88	0.89
12:L:59:ARG:HH11	12:L:59:ARG:HB2	1.37	0.89
2:B:97:TRP:HZ2	2:B:102:LEU:HD13	1.38	0.89
13:M:59:TYR:O	13:M:63:THR:HG22	1.72	0.88
2:B:60:ASP:HB3	2:B:64:ARG:NH1	1.86	0.88
9:I:106:ALA:O	9:I:108:VAL:HG23	1.73	0.88
10:J:49:VAL:HG23	14:N:41:ARG:HB2	1.56	0.88
5:E:144:THR:HB	5:E:147:ASP:OD1	1.74	0.87
1:A:1116:C:C2'	1:A:1117:G:H5''	2.04	0.87
2:B:91:PRO:HG3	2:B:154:LEU:HB2	1.55	0.87
1:A:1179:A:N6	1:A:1180:A:N1	2.22	0.87
6:F:47:ARG:HE	6:F:47:ARG:H	1.22	0.87
1:A:1080:A:H5''	5:E:16:THR:HG21	1.54	0.87
1:A:243:A:C4'	1:A:244:U:H5'	2.04	0.86
4:D:150:GLU:CD	4:D:150:GLU:H	1.78	0.86
3:C:88:ARG:HG2	3:C:101:LEU:HD13	1.57	0.86
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.57	0.86
1:A:718:G:H5'	11:K:117:ASN:HD22	1.40	0.86
3:C:70:VAL:HG12	3:C:72:LYS:H	1.41	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1156:G:H21	1:A:1179:A:H61	1.19	0.85
7:G:69:VAL:HG21	7:G:104:LEU:HD21	1.58	0.85
19:S:20:LEU:HA	19:S:23:ASN:HD22	1.40	0.85
1:A:129(A):G:O2'	1:A:190(E):U:H2'	1.75	0.85
1:A:1137:C:H4'	1:A:1138:G:C2	2.12	0.85
18:R:47:THR:HA	18:R:83:GLU:HB2	1.58	0.85
10:J:30:SER:HB3	10:J:84:GLN:HE21	1.42	0.85
3:C:73:PRO:O	3:C:76:VAL:HG22	1.77	0.84
1:A:975:A:H5'	1:A:975:A:H8	1.40	0.84
1:A:1156:G:N2	1:A:1179:A:H61	1.75	0.84
6:F:47:ARG:NE	6:F:47:ARG:H	1.74	0.84
19:S:15:LEU:HA	19:S:18:LYS:HB3	1.58	0.84
1:A:1035:A:H2'	1:A:1036:G:H8	1.43	0.84
2:B:25:ASN:C	2:B:25:ASN:HD22	1.81	0.84
1:A:1190:G:OP1	3:C:4:LYS:HA	1.77	0.84
7:G:146:GLU:HG2	7:G:149:ARG:HH21	1.39	0.84
1:A:1062:U:H2'	1:A:1063:C:C5	2.13	0.84
4:D:23:GLY:HA3	4:D:112:VAL:HG22	1.60	0.84
14:N:3:ARG:HH21	14:N:6:LEU:HD11	1.43	0.84
9:I:104:ARG:HD3	9:I:105:ASP:H	1.42	0.83
2:B:8:LYS:HE2	2:B:9:GLU:H	1.42	0.83
7:G:114:ARG:H	7:G:114:ARG:HD2	1.42	0.83
2:B:19:HIS:NE2	2:B:206:ASP:HB3	1.93	0.83
1:A:1156:G:O3'	1:A:1157:A:OP2	1.93	0.82
9:I:53:VAL:HG21	9:I:85:LEU:HD21	1.59	0.82
3:C:15:THR:O	3:C:16:ARG:HB2	1.79	0.82
5:E:51:VAL:HB	5:E:52:PRO:HD3	1.61	0.82
1:A:1179:A:O2'	1:A:1180:A:H5'	1.78	0.82
22:X:3:G:H1	23:Y:34:TM2:H3	1.28	0.82
5:E:150:ARG:HH11	5:E:150:ARG:HG3	1.45	0.82
5:E:50:GLU:HG3	5:E:52:PRO:HD2	1.61	0.82
1:A:1156:G:N2	1:A:1179:A:N6	2.27	0.82
1:A:1179:A:H61	1:A:1180:A:H2	1.24	0.81
1:A:1502:A:H2	1:A:1505:G:H1	1.28	0.81
2:B:15:VAL:HG11	2:B:209:ARG:HB2	1.61	0.81
1:A:351:G:H4'	1:A:352:C:OP2	1.79	0.81
2:B:80:ILE:H	2:B:80:ILE:HD12	1.42	0.81
1:A:1369:C:H2'	1:A:1370:G:C8	2.15	0.81
1:A:432:A:C3'	1:A:433:C:H5''	2.11	0.81
1:A:975:A:H4'	1:A:976:G:H5''	1.62	0.80
11:K:57:THR:HG22	11:K:59:TYR:H	1.44	0.80
19:S:17:GLU:HA	19:S:20:LEU:HG	1.61	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.61	0.80
5:E:10:MET:SD	5:E:13:ILE:HD11	2.22	0.80
5:E:144:THR:HG22	5:E:146:ALA:H	1.45	0.80
13:M:37:THR:HG23	13:M:55:ARG:HD2	1.62	0.80
1:A:1305:G:H5'	21:U:4:GLY:HA3	1.62	0.80
1:A:1054:C:H3'	1:A:1054:C:O2	1.80	0.80
17:Q:96:GLN:HB3	17:Q:103:GLY:HA3	1.64	0.80
19:S:30:LEU:O	19:S:31:ILE:HD13	1.82	0.80
1:A:438:G:H4'	1:A:439:A:OP1	1.82	0.80
1:A:35:G:H2'	1:A:36:C:C6	2.17	0.80
1:A:1190:G:H3'	3:C:3:ASN:HD21	1.46	0.80
10:J:46:ARG:NH1	10:J:64:GLU:HB3	1.97	0.79
2:B:132:LYS:HA	2:B:135:GLN:HB2	1.64	0.79
1:A:1435:G:H2'	1:A:1436:U:C6	2.17	0.79
2:B:193:ASP:HB3	2:B:196:LEU:HD13	1.62	0.79
2:B:95:GLN:O	2:B:96:ARG:HD2	1.82	0.79
1:A:363:A:H62	12:L:28:LYS:HE3	1.46	0.79
21:U:5:ASP:O	21:U:11:GLY:HA3	1.83	0.79
19:S:7:LYS:HD2	19:S:7:LYS:O	1.83	0.79
23:Y:33:U:H2'	23:Y:34:TM2:H3'	1.63	0.79
1:A:1057:G:H5''	3:C:154:SER:HB2	1.64	0.79
1:A:235:C:H5'	17:Q:70:ARG:HG2	1.62	0.79
2:B:204:ASN:ND2	2:B:206:ASP:H	1.81	0.79
1:A:1238:A:H5'	1:A:1336:C:N4	1.98	0.79
7:G:79:ARG:HH12	7:G:82:GLY:H	1.31	0.79
19:S:13:ASP:HA	19:S:16:LEU:HB3	1.63	0.79
1:A:946:A:H2'	1:A:947:G:C8	2.18	0.79
10:J:10:GLY:N	10:J:16:LEU:HD11	1.98	0.79
10:J:84:GLN:O	10:J:88:LEU:HD12	1.83	0.78
1:A:250:A:H4'	1:A:251:G:O5'	1.82	0.78
2:B:215:LEU:O	2:B:219:VAL:HG23	1.83	0.78
2:B:178:ARG:NH2	8:H:68:ARG:HH22	1.82	0.78
2:B:42:ILE:HD12	2:B:42:ILE:H	1.48	0.78
1:A:1527:C:O2'	1:A:1528:U:H5'	1.84	0.78
13:M:54:VAL:O	13:M:58:GLU:HG2	1.84	0.78
9:I:93:ARG:HB3	9:I:93:ARG:NH1	1.99	0.78
1:A:433:C:C5'	1:A:433:C:H6	1.97	0.78
5:E:91:LEU:HD23	5:E:120:THR:HG22	1.66	0.78
1:A:1352:C:H2'	1:A:1353:G:C8	2.18	0.78
1:A:433:C:H6	1:A:433:C:H5'	1.48	0.77
12:L:47:LYS:HB3	12:L:48:PRO:HD3	1.64	0.77
1:A:1130:A:C2	1:A:1146:A:C4	2.71	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:G:50:ILE:O	7:G:54:THR:HB	1.83	0.77
2:B:139:LYS:O	2:B:139:LYS:HD3	1.85	0.77
14:N:22:THR:HB	14:N:33:VAL:HG21	1.65	0.77
15:O:78:TYR:CZ	15:O:82:ILE:HD11	2.19	0.77
9:I:114:TYR:CD2	10:J:60:ARG:HB2	2.20	0.77
13:M:36:LYS:HD2	13:M:59:TYR:OH	1.83	0.77
1:A:1003(A):G:H2'	1:A:1004:A:H4'	1.67	0.77
2:B:197:VAL:HB	2:B:200:ILE:HG12	1.66	0.77
1:A:1281:U:H5'	1:A:1282:C:H5	1.47	0.77
2:B:124:SER:O	2:B:127:ILE:HG13	1.84	0.77
1:A:1497:G:C2'	1:A:1498:U:H5'	2.15	0.77
1:A:1065:U:H5''	1:A:1190:G:N2	2.00	0.76
1:A:1123:A:H4'	10:J:37:PRO:HD2	1.66	0.76
3:C:102:ASN:N	3:C:102:ASN:HD22	1.82	0.76
1:A:1343:G:H1'	9:I:121:ARG:HH12	1.50	0.76
12:L:27:LEU:O	12:L:29:GLY:N	2.19	0.76
1:A:1156:G:O3'	1:A:1157:A:OP1	2.02	0.76
11:K:33:THR:HG22	11:K:39:PRO:HA	1.67	0.76
13:M:108:ARG:HE	13:M:108:ARG:HA	1.49	0.76
12:L:25:PRO:C	12:L:27:LEU:H	1.89	0.76
1:A:1497:G:O2'	1:A:1498:U:H5'	1.86	0.76
4:D:168:ARG:HB3	4:D:168:ARG:NH1	2.00	0.76
12:L:28:LYS:C	12:L:30:ALA:H	1.87	0.76
1:A:1356:G:H2'	1:A:1357:A:H8	1.48	0.76
14:N:58:LYS:HB3	14:N:58:LYS:HZ2	1.50	0.76
18:R:47:THR:HG22	18:R:48:GLY:H	1.51	0.76
2:B:48:MET:HA	2:B:51:LEU:HD12	1.68	0.75
20:T:67:ALA:HA	20:T:73:HIS:H	1.49	0.75
13:M:10:PRO:HB2	13:M:18:ALA:HB1	1.67	0.75
7:G:54:THR:HG22	7:G:56:GLN:H	1.50	0.75
12:L:41:ARG:HG2	12:L:42:THR:H	1.50	0.75
6:F:47:ARG:HE	6:F:47:ARG:N	1.84	0.75
1:A:1189:C:P	10:J:51:ARG:HH22	2.10	0.75
2:B:218:ALA:O	2:B:222:ILE:HG13	1.85	0.75
12:L:57:LYS:HD2	12:L:67:THR:HG22	1.67	0.75
5:E:82:VAL:HG21	5:E:138:ALA:HA	1.66	0.75
1:A:948:C:OP1	13:M:109:THR:HG22	1.87	0.75
7:G:140:ASP:O	7:G:144:MET:HB2	1.85	0.75
1:A:390:C:H2'	1:A:391:G:H8	1.50	0.75
22:X:2:U:O2'	22:X:3:G:H5'	1.87	0.75
12:L:46:LYS:HG2	12:L:92:ASP:O	1.87	0.75
5:E:80:ILE:HD11	5:E:91:LEU:HB2	1.66	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:718:G:C5'	11:K:117:ASN:HD22	1.99	0.74
2:B:95:GLN:C	2:B:96:ARG:HD2	2.07	0.74
1:A:953:G:H1'	13:M:125:ARG:HB2	1.69	0.74
1:A:1529:G:H3'	1:A:1529:G:OP2	1.87	0.74
8:H:90:GLY:O	8:H:91:ARG:HB2	1.85	0.74
1:A:975:A:H5'	1:A:975:A:C8	2.22	0.74
1:A:1161:C:H2'	1:A:1162:C:C5	2.23	0.74
21:U:6:ARG:HD2	21:U:15:ARG:HH12	1.52	0.74
16:P:67:THR:HG22	16:P:69:THR:H	1.53	0.74
6:F:2:ARG:HE	6:F:69:GLU:HG2	1.51	0.74
1:A:556:C:O2'	1:A:557:G:H5'	1.87	0.74
1:A:371:G:O2'	1:A:372:C:H5'	1.88	0.74
8:H:103:VAL:HG21	8:H:109:ILE:O	1.87	0.74
2:B:172:ILE:H	2:B:172:ILE:HD12	1.51	0.74
4:D:24:GLU:HG2	4:D:25:ARG:H	1.52	0.74
21:U:15:ARG:HH11	21:U:15:ARG:HG2	1.53	0.74
12:L:55:VAL:HG12	12:L:56:ALA:N	2.02	0.73
1:A:1479:C:H2'	1:A:1480:G:H8	1.51	0.73
6:F:101:ALA:HB2	18:R:28:GLU:HB2	1.70	0.73
1:A:262:A:H5'	20:T:74:LYS:HD3	1.70	0.73
3:C:44:GLU:HA	3:C:52:LEU:HD11	1.69	0.73
1:A:1533:C:C2'	1:A:1534:A:O5'	2.36	0.73
3:C:204:LEU:O	3:C:204:LEU:HD12	1.89	0.73
22:X:3:G:HO2'	22:X:4:A:H5'	1.53	0.73
10:J:6:ILE:HD13	10:J:73:ASP:H	1.54	0.73
9:I:48:GLU:HA	9:I:51:ARG:HH11	1.54	0.73
1:A:390:C:H2'	1:A:391:G:C8	2.24	0.73
15:O:39:LEU:HD12	15:O:56:LEU:HD13	1.71	0.73
1:A:1133:G:H2'	1:A:1134:G:H8	1.52	0.73
12:L:28:LYS:O	12:L:30:ALA:N	2.21	0.73
1:A:1095:U:H2'	1:A:1096:C:C6	2.23	0.73
13:M:5:ALA:HB3	13:M:8:GLU:HG3	1.70	0.73
2:B:51:LEU:HD22	2:B:55:PHE:HE1	1.53	0.73
12:L:7:ILE:O	12:L:11:VAL:HG23	1.87	0.73
1:A:1175:G:C2	1:A:1176:A:C4	2.77	0.73
2:B:25:ASN:ND2	2:B:27:LYS:H	1.87	0.72
3:C:107:GLN:H	3:C:107:GLN:CD	1.93	0.72
3:C:150:LYS:HG3	3:C:169:ALA:HB2	1.70	0.72
2:B:204:ASN:HD22	2:B:204:ASN:C	1.93	0.72
14:N:26:ARG:HH12	14:N:47:LEU:HD21	1.53	0.72
1:A:243:A:H4'	1:A:244:U:C5'	2.17	0.72
1:A:1373:G:H5''	7:G:36:LYS:HB2	1.70	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1247:U:O2'	1:A:1248:A:H5'	1.89	0.72
20:T:14:LYS:O	20:T:18:GLN:HG3	1.89	0.72
18:R:46:GLU:CD	18:R:46:GLU:H	1.92	0.72
5:E:144:THR:O	5:E:148:VAL:HG23	1.89	0.72
9:I:97:LYS:HB3	9:I:98:PRO:HD3	1.71	0.72
3:C:34:LEU:O	3:C:34:LEU:HD23	1.87	0.72
1:A:1152:A:H5'	10:J:70:ARG:HH22	1.55	0.72
13:M:50:GLU:O	13:M:54:VAL:HG23	1.90	0.72
16:P:74:LEU:O	16:P:79:VAL:HG23	1.90	0.72
1:A:1086:U:H3	1:A:1099:G:N2	1.85	0.72
1:A:1286:A:C8	1:A:1287:A:H4'	2.25	0.72
6:F:46:ARG:CB	6:F:47:ARG:HH21	2.03	0.71
1:A:382:A:H2'	1:A:383:A:C8	2.25	0.71
15:O:16:ALA:HB1	15:O:21:ASP:HB3	1.73	0.71
13:M:40:ASN:HB3	13:M:43:THR:HG23	1.71	0.71
14:N:26:ARG:NH1	14:N:47:LEU:HD21	2.05	0.71
13:M:11:ARG:HD3	13:M:12:ASN:HB2	1.71	0.71
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.73	0.71
9:I:118:LYS:O	9:I:119:ALA:HB3	1.91	0.71
1:A:1250:A:C4'	9:I:68:GLY:H	2.01	0.71
1:A:1175:G:C2	1:A:1176:A:C5	2.78	0.71
13:M:11:ARG:HG3	13:M:11:ARG:HH11	1.55	0.71
12:L:38:THR:O	12:L:79:GLU:HG3	1.89	0.71
3:C:110:ASN:ND2	3:C:140:ARG:HB3	2.06	0.71
1:A:1149:C:H2'	1:A:1150:U:C6	2.25	0.71
10:J:18:ALA:O	10:J:21:GLN:HB2	1.91	0.71
1:A:839:U:O2	1:A:839:U:H2'	1.90	0.71
3:C:6:HIS:HD2	3:C:8:ILE:H	1.38	0.70
1:A:657:G:H4'	15:O:28:GLN:HG2	1.72	0.70
1:A:254:G:H21	17:Q:16:GLN:NE2	1.89	0.70
15:O:87:ILE:HG22	15:O:88:ARG:N	2.05	0.70
1:A:664:G:OP1	18:R:64:ARG:HD2	1.90	0.70
6:F:46:ARG:HB3	6:F:46:ARG:NH1	2.06	0.70
1:A:629:G:H2'	1:A:630:G:H5''	1.72	0.70
1:A:266:G:C8	1:A:266:G:H5'	2.26	0.70
4:D:205:GLU:O	4:D:208:SER:HB3	1.91	0.70
20:T:43:LEU:HD13	20:T:51:GLU:HG3	1.74	0.70
1:A:1190:G:C3'	3:C:3:ASN:HD21	2.04	0.70
1:A:1229:A:H2'	1:A:1230:C:H6	1.57	0.70
6:F:44:GLY:HA2	6:F:59:TYR:CE1	2.27	0.70
6:F:100:ASN:HB2	18:R:23:LYS:HE3	1.72	0.70
1:A:1026:G:H3'	1:A:1027:C:H5''	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:14:ILE:HG22	3:C:15:THR:N	1.98	0.70
10:J:5:ARG:HA	10:J:73:ASP:OD1	1.91	0.70
1:A:1318:A:H1'	19:S:37:ARG:HH11	1.55	0.70
3:C:23:TYR:CD2	3:C:24:ALA:N	2.60	0.70
10:J:23:ILE:O	10:J:23:ILE:HG22	1.91	0.70
9:I:3:GLN:HE22	9:I:20:ARG:HH21	1.40	0.69
2:B:80:ILE:HD11	2:B:208:ILE:HG23	1.73	0.69
19:S:33:THR:HG22	19:S:35:SER:N	2.04	0.69
10:J:32:ALA:HB2	10:J:76:ASN:HB2	1.73	0.69
17:Q:27:PHE:CE1	17:Q:36:ILE:HD11	2.28	0.69
10:J:8:LEU:HB2	10:J:70:ARG:HB2	1.74	0.69
1:A:1167:A:H2'	1:A:1168:A:C8	2.28	0.69
10:J:6:ILE:H	10:J:6:ILE:HD12	1.56	0.69
1:A:1175:G:H2'	1:A:1176:A:H8	1.58	0.69
3:C:53:ALA:O	3:C:54:ARG:HB2	1.92	0.69
9:I:70:LYS:O	9:I:74:ILE:HG13	1.93	0.69
5:E:143:ARG:NH1	8:H:77:GLU:OE2	2.26	0.69
15:O:6:GLU:CD	15:O:6:GLU:H	1.96	0.69
17:Q:40:LYS:HG3	17:Q:41:LYS:N	2.07	0.69
6:F:62:TRP:C	6:F:63:TYR:HD2	1.97	0.69
19:S:4:SER:O	19:S:5:LEU:HD12	1.93	0.69
1:A:397:A:H5'	1:A:398:C:OP1	1.93	0.69
8:H:60:ARG:HG3	8:H:60:ARG:HH11	1.58	0.69
1:A:1190:G:C3'	3:C:3:ASN:ND2	2.54	0.69
1:A:1256:A:H2	1:A:1277:C:C4	2.11	0.69
10:J:30:SER:CB	10:J:84:GLN:HE21	2.05	0.69
2:B:196:LEU:H	2:B:196:LEU:HD12	1.57	0.69
15:O:17:ARG:HH11	15:O:17:ARG:HG3	1.57	0.69
3:C:26:LYS:CD	3:C:26:LYS:H	2.06	0.69
3:C:107:GLN:O	3:C:108:ASN:HB3	1.92	0.69
3:C:64:VAL:H	3:C:99:VAL:HB	1.58	0.68
1:A:254:G:OP1	17:Q:67:LYS:O	2.10	0.68
9:I:93:ARG:HB3	9:I:93:ARG:HH11	1.56	0.68
13:M:4:ILE:HG22	13:M:5:ALA:N	2.06	0.68
1:A:701:C:H5''	1:A:703:G:O4'	1.92	0.68
7:G:52:GLU:O	7:G:53:LYS:HB2	1.93	0.68
1:A:17:U:H2'	1:A:18:C:C6	2.29	0.68
7:G:120:ILE:H	7:G:120:ILE:HD12	1.58	0.68
1:A:370:C:O2'	1:A:371:G:H5'	1.94	0.68
1:A:1016:A:H2'	1:A:1017:G:O4'	1.93	0.68
12:L:126:LYS:HD2	12:L:126:LYS:O	1.94	0.68
1:A:328:C:O2	1:A:328:C:H2'	1.92	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1057:G:H5''	3:C:154:SER:CB	2.24	0.68
5:E:36:ASP:OD1	5:E:38:GLN:N	2.27	0.68
11:K:124:LYS:HD2	11:K:125:PHE:CE1	2.27	0.68
10:J:69:ASN:O	10:J:70:ARG:HD3	1.94	0.68
17:Q:65:ILE:N	17:Q:65:ILE:HD12	2.09	0.68
10:J:15:THR:HG22	10:J:94:VAL:HG23	1.76	0.68
1:A:1003(A):G:H2'	1:A:1004:A:C4'	2.23	0.68
1:A:1142:G:H2'	1:A:1143:G:O4'	1.93	0.68
3:C:121:ALA:O	3:C:125:GLU:HG3	1.94	0.68
3:C:50:ALA:HB1	3:C:70:VAL:HG11	1.76	0.67
1:A:1391:U:H2'	1:A:1392:G:C8	2.29	0.67
4:D:119:GLN:HG2	4:D:123:HIS:CD2	2.29	0.67
4:D:162:LEU:HD23	4:D:162:LEU:O	1.93	0.67
1:A:1367:C:H5'	10:J:60:ARG:HH12	1.57	0.67
1:A:266:G:H5''	1:A:268:C:N4	2.01	0.67
7:G:15:ASP:O	7:G:19:GLY:HA2	1.93	0.67
1:A:918:A:H2'	1:A:919:A:C8	2.29	0.67
9:I:55:ALA:O	9:I:56:LEU:HB3	1.94	0.67
1:A:1318:A:O2'	19:S:37:ARG:HD2	1.95	0.67
5:E:110:LEU:HD13	5:E:118:ILE:HG21	1.77	0.67
1:A:1479:C:H2'	1:A:1480:G:C8	2.29	0.67
3:C:123:GLN:O	3:C:126:ARG:HB3	1.94	0.67
19:S:52:TYR:HA	19:S:56:GLN:O	1.93	0.67
1:A:1347:G:N2	1:A:1373:G:H2'	2.09	0.67
21:U:6:ARG:HD2	21:U:15:ARG:NH1	2.09	0.67
15:O:4:THR:OG1	15:O:7:GLU:HG3	1.95	0.67
2:B:74:LYS:HZ1	2:B:206:ASP:HB2	1.59	0.67
6:F:2:ARG:NE	6:F:69:GLU:HG2	2.08	0.67
3:C:188:LEU:O	3:C:189:ALA:HB2	1.95	0.67
1:A:1130:A:N3	1:A:1146:A:C2	2.62	0.67
13:M:40:ASN:HD22	13:M:41:PRO:CD	2.07	0.67
1:A:1054:C:H2'	1:A:1055:A:H5''	1.77	0.67
2:B:161:ALA:HB1	2:B:185:ILE:HD11	1.77	0.67
10:J:39:PRO:O	10:J:40:LEU:HB2	1.94	0.67
17:Q:67:LYS:CA	17:Q:70:ARG:HH12	2.07	0.66
13:M:19:LEU:O	13:M:22:ILE:HD13	1.95	0.66
4:D:146:ILE:HD12	4:D:146:ILE:N	2.10	0.66
1:A:1156:G:N2	1:A:1179:A:C6	2.51	0.66
1:A:1193:G:O2'	1:A:1194:U:H5'	1.96	0.66
19:S:22:LEU:HD22	19:S:28:LYS:HB2	1.78	0.66
5:E:80:ILE:HD12	5:E:91:LEU:HB2	1.76	0.66
2:B:196:LEU:N	2:B:196:LEU:HD12	2.10	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:15:THR:HG22	10:J:94:VAL:CG2	2.25	0.66
6:F:19:LEU:O	6:F:23:LYS:HG3	1.95	0.66
1:A:939:G:H2'	1:A:940:C:C6	2.30	0.66
1:A:1175:G:C2	1:A:1176:A:C8	2.83	0.66
19:S:20:LEU:HA	19:S:23:ASN:ND2	2.09	0.66
10:J:32:ALA:H	10:J:78:ASN:HD21	1.42	0.66
12:L:46:LYS:HE2	12:L:47:LYS:HB2	1.76	0.66
1:A:838:G:H2'	1:A:839:U:H5''	1.76	0.66
19:S:5:LEU:O	19:S:6:LYS:HB2	1.95	0.66
6:F:48:LEU:HD13	6:F:52:ILE:HD12	1.77	0.66
1:A:818:G:C3'	1:A:819:A:H5''	2.25	0.66
1:A:1080:A:C5'	5:E:16:THR:HG21	2.25	0.66
1:A:1502:A:H2	1:A:1505:G:N1	1.92	0.66
19:S:4:SER:C	19:S:5:LEU:HD12	2.15	0.66
6:F:80:ARG:NH1	6:F:88:VAL:HB	2.10	0.66
17:Q:68:ARG:N	17:Q:70:ARG:NH1	2.44	0.66
12:L:28:LYS:C	12:L:30:ALA:N	2.49	0.66
4:D:162:LEU:HD13	4:D:181:MET:HE2	1.78	0.66
9:I:32:ASP:HB3	9:I:35:GLU:HB2	1.77	0.66
18:R:87:ARG:HG2	18:R:87:ARG:HH11	1.59	0.66
10:J:49:VAL:CG2	14:N:41:ARG:HB2	2.23	0.66
2:B:7:VAL:HG11	2:B:221:LEU:HD23	1.77	0.66
1:A:141:A:H1'	1:A:182:U:O2	1.95	0.66
20:T:53:LEU:HB2	20:T:100:ILE:CG2	2.26	0.66
12:L:43:VAL:HG12	12:L:44:THR:N	2.11	0.66
23:Y:34:TM2:H2'	23:Y:35:A:C8	2.31	0.66
13:M:15:VAL:HG23	13:M:43:THR:O	1.96	0.66
19:S:20:LEU:HD12	19:S:21:GLU:N	2.10	0.66
11:K:14:VAL:HG21	11:K:40:ILE:HD11	1.77	0.66
1:A:1127:G:H21	1:A:1146:A:N6	1.94	0.65
1:A:1075:C:H5'	2:B:103:THR:HG21	1.79	0.65
1:A:344:A:H4'	1:A:345:C:OP1	1.97	0.65
10:J:9:ARG:HB3	10:J:9:ARG:NH1	2.11	0.65
1:A:376:G:OP2	16:P:67:THR:HG21	1.97	0.65
5:E:137:GLU:O	5:E:141:GLN:HG3	1.97	0.65
6:F:100:ASN:HD22	18:R:23:LYS:HG2	1.61	0.65
6:F:39:LYS:HG3	6:F:40:VAL:H	1.61	0.65
1:A:983:A:H5'	1:A:984:C:OP2	1.96	0.65
3:C:82:GLU:O	3:C:85:ARG:HB3	1.96	0.65
11:K:11:LYS:O	11:K:11:LYS:HD2	1.96	0.65
2:B:16:HIS:CE1	2:B:214:ILE:HG12	2.31	0.65
4:D:64:LEU:HD23	4:D:64:LEU:C	2.17	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:26:A:N6	1:A:558:G:H1'	2.12	0.65
1:A:1277:C:HO2'	1:A:1279:A:H8	1.41	0.65
23:Y:34:TM2:H2'	23:Y:35:A:H8	1.62	0.65
1:A:1128:C:O2'	1:A:1130:A:C8	2.50	0.65
12:L:47:LYS:CB	12:L:48:PRO:HD3	2.25	0.65
1:A:1477:C:H2'	1:A:1478:C:H6	1.62	0.65
19:S:28:LYS:HG2	19:S:29:ARG:N	2.07	0.65
14:N:27:CYS:SG	14:N:29:ARG:HB2	2.36	0.65
17:Q:68:ARG:H	17:Q:70:ARG:NH1	1.95	0.65
1:A:1175:G:C4	1:A:1176:A:N7	2.64	0.65
6:F:39:LYS:HG3	6:F:40:VAL:N	2.11	0.65
1:A:1323:G:H2'	1:A:1324:A:C8	2.32	0.65
1:A:1066:C:O2'	1:A:1067:A:H5'	1.97	0.65
9:I:4:TYR:CE1	9:I:88:TYR:HA	2.32	0.65
19:S:62:ILE:HD12	19:S:66:MET:HG3	1.78	0.65
13:M:23:TYR:O	13:M:25:ILE:N	2.30	0.64
2:B:80:ILE:N	2:B:80:ILE:HD12	2.11	0.64
10:J:60:ARG:O	10:J:61:GLU:HB3	1.97	0.64
3:C:155:GLY:O	3:C:156:ARG:HB2	1.97	0.64
7:G:145:ALA:O	7:G:146:GLU:HB3	1.96	0.64
1:A:35:G:H2'	1:A:36:C:H6	1.61	0.64
12:L:24:VAL:HG12	12:L:26:ALA:HB2	1.79	0.64
9:I:128:ARG:HA	13:M:126:LYS:HE3	1.77	0.64
1:A:1021:G:O2'	1:A:1022:G:H5'	1.96	0.64
2:B:208:ILE:H	2:B:208:ILE:CD1	1.99	0.64
9:I:50:LEU:HD13	9:I:56:LEU:HA	1.79	0.64
2:B:172:ILE:HD12	2:B:172:ILE:N	2.12	0.64
1:A:109:A:H2'	1:A:326:G:N2	2.11	0.64
1:A:1156:G:H3'	1:A:1157:A:P	2.32	0.64
1:A:1347:G:C8	9:I:107:ARG:HB3	2.32	0.64
17:Q:104:LYS:HD3	17:Q:105:ALA:H	1.63	0.64
4:D:92:VAL:O	4:D:96:LEU:HD13	1.96	0.64
12:L:34:ARG:O	12:L:61:THR:HG23	1.96	0.64
1:A:1060:C:H2'	1:A:1061:G:H8	1.62	0.64
13:M:125:ARG:O	13:M:125:ARG:HD2	1.97	0.64
13:M:3:ARG:HA	13:M:8:GLU:O	1.97	0.64
1:A:415:A:H2'	1:A:416:G:H8	1.61	0.64
1:A:490:G:H2'	1:A:491:G:H8	1.62	0.64
2:B:231:GLU:H	2:B:231:GLU:CD	2.01	0.64
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.79	0.64
1:A:353:A:H5'	1:A:353:A:H8	1.61	0.64
13:M:49:THR:HG22	13:M:51:ALA:N	2.11	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:48:GLU:HA	9:I:51:ARG:NH1	2.12	0.64
5:E:53:LEU:H	5:E:53:LEU:HD23	1.63	0.64
2:B:15:VAL:HG11	2:B:209:ARG:CB	2.28	0.64
1:A:1497:G:H2'	1:A:1498:U:H5'	1.80	0.64
10:J:23:ILE:N	10:J:23:ILE:HD12	2.13	0.64
2:B:114:ARG:O	2:B:117:GLU:HB3	1.97	0.64
1:A:524:G:H2'	1:A:525:C:C6	2.33	0.64
1:A:393:A:O2'	1:A:394:G:H5'	1.96	0.64
14:N:32:SER:HB3	14:N:41:ARG:HB3	1.79	0.64
3:C:79:ARG:HG3	3:C:79:ARG:O	1.98	0.64
17:Q:45:HIS:HB3	17:Q:72:ARG:HG2	1.78	0.64
1:A:1152:A:H2'	1:A:1153:C:C6	2.33	0.64
3:C:52:LEU:H	3:C:52:LEU:CD2	2.10	0.64
1:A:1168:A:H2'	1:A:1169:A:C8	2.33	0.64
18:R:38:GLU:CD	18:R:38:GLU:H	2.01	0.64
10:J:89:ASP:HB2	10:J:91:PRO:HD2	1.78	0.64
12:L:89:ARG:HA	12:L:97:ARG:HA	1.78	0.64
14:N:24:CYS:HB2	14:N:40:CYS:HB3	1.80	0.63
7:G:75:VAL:CG2	7:G:86:GLN:HB3	2.26	0.63
4:D:24:GLU:HG2	4:D:25:ARG:N	2.13	0.63
1:A:731:G:OP1	1:A:766:A:H1'	1.98	0.63
1:A:1038:C:H2'	1:A:1039:C:H6	1.64	0.63
19:S:64:GLU:O	19:S:67:VAL:HG23	1.98	0.63
1:A:1208:C:H2'	1:A:1209:C:H6	1.63	0.63
10:J:6:ILE:N	10:J:6:ILE:HD12	2.13	0.63
1:A:954:G:H21	1:A:1227:A:H62	1.46	0.63
9:I:127:LYS:HD2	9:I:127:LYS:O	1.98	0.63
2:B:80:ILE:CD1	2:B:80:ILE:H	2.10	0.63
3:C:84:ILE:CD1	3:C:88:ARG:HH21	2.10	0.63
1:A:501:C:H2'	1:A:502:G:H8	1.63	0.63
1:A:1178:G:C2	1:A:1180:A:H8	2.17	0.63
20:T:53:LEU:O	20:T:57:ARG:HD2	1.99	0.63
9:I:17:VAL:HG21	9:I:80:GLY:HA3	1.80	0.63
1:A:107:G:C2'	1:A:108:G:H5'	2.29	0.63
1:A:1366:C:H2'	1:A:1367:C:C6	2.34	0.63
10:J:46:ARG:HG2	10:J:46:ARG:HH11	1.64	0.63
1:A:1477:C:H2'	1:A:1478:C:C6	2.33	0.63
1:A:1305:G:C5'	21:U:4:GLY:HA3	2.29	0.63
15:O:26:GLU:OE1	15:O:77:ARG:HD2	1.99	0.63
10:J:22:LYS:HZ2	10:J:22:LYS:HB2	1.62	0.63
1:A:807:A:H2'	1:A:808:C:C6	2.34	0.63
9:I:69:GLY:O	9:I:73:GLN:HG3	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:36:ASP:O	3:C:39:ILE:HB	1.98	0.63
1:A:421:U:H5'	1:A:422:C:C5	2.33	0.63
1:A:1533:C:C2'	1:A:1534:A:C5'	2.76	0.62
1:A:1141:C:H2'	1:A:1142:G:H8	1.64	0.62
8:H:19:VAL:HG23	8:H:21:LYS:HD3	1.80	0.62
1:A:1192:C:C5	1:A:1193:G:C8	2.87	0.62
17:Q:68:ARG:N	17:Q:70:ARG:HH11	1.96	0.62
12:L:47:LYS:CB	12:L:48:PRO:CD	2.75	0.62
3:C:28:GLN:HA	3:C:31:HIS:HD2	1.63	0.62
4:D:151:LYS:H	4:D:151:LYS:HD2	1.62	0.62
1:A:706:A:O4'	11:K:29:ILE:HD11	1.99	0.62
5:E:150:ARG:NH1	5:E:150:ARG:HG3	2.11	0.62
14:N:9:LYS:HD3	14:N:9:LYS:O	1.99	0.62
10:J:90:LEU:N	10:J:91:PRO:CD	2.62	0.62
5:E:12:LEU:HD13	5:E:31:LEU:HB2	1.81	0.62
16:P:11:SER:OG	16:P:14:ASN:HB3	1.99	0.62
1:A:1366:C:H2'	1:A:1367:C:H6	1.62	0.62
1:A:1132:C:H2'	1:A:1133:G:C8	2.34	0.62
17:Q:104:LYS:HD3	17:Q:105:ALA:N	2.14	0.62
1:A:1130:A:C5	1:A:1146:A:N1	2.67	0.62
1:A:1435:G:H2'	1:A:1436:U:H6	1.65	0.62
21:U:12:LYS:HB3	21:U:22:ARG:HD2	1.81	0.62
9:I:7:THR:O	9:I:83:ARG:HD2	2.00	0.62
1:A:1149:C:H2'	1:A:1150:U:H6	1.62	0.62
2:B:50:GLU:HB3	2:B:200:ILE:O	2.00	0.62
9:I:43:ALA:HA	9:I:74:ILE:HD13	1.82	0.62
4:D:64:LEU:HD12	4:D:198:VAL:HG11	1.82	0.62
1:A:405:U:H3'	1:A:406:G:H5'	1.82	0.62
7:G:18:TYR:CD2	7:G:59:LEU:HB2	2.35	0.62
6:F:67:MET:HB2	6:F:68:PRO:HD2	1.82	0.62
19:S:50:ALA:HA	19:S:58:VAL:O	1.99	0.62
1:A:1201:A:H4'	1:A:1202:G:O5'	1.99	0.62
13:M:59:TYR:C	13:M:63:THR:HG22	2.19	0.62
21:U:15:ARG:NH1	21:U:15:ARG:HG2	2.12	0.62
2:B:114:ARG:HD2	2:B:117:GLU:HG2	1.81	0.62
1:A:107:G:H2'	1:A:108:G:H5'	1.82	0.62
1:A:448:A:H2'	1:A:449:C:C6	2.35	0.62
6:F:3:ARG:HG2	6:F:93:SER:OG	1.99	0.62
8:H:119:LEU:HB2	8:H:123:GLU:HB2	1.82	0.62
1:A:1130:A:C6	1:A:1146:A:C6	2.88	0.61
13:M:37:THR:CG2	13:M:55:ARG:HD2	2.30	0.61
10:J:12:ASP:HB3	10:J:15:THR:HB	1.80	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:673:G:H2'	1:A:674:G:C8	2.34	0.61
1:A:1062:U:H2'	1:A:1063:C:C6	2.34	0.61
1:A:1326:C:OP1	21:U:12:LYS:NZ	2.32	0.61
7:G:59:LEU:HD11	7:G:63:LYS:HE3	1.81	0.61
20:T:45:GLN:HE21	20:T:45:GLN:C	2.04	0.61
1:A:522:C:H41	12:L:53:ARG:HH22	1.46	0.61
4:D:126:ILE:HG22	4:D:127:THR:N	2.14	0.61
10:J:98:ILE:HG22	10:J:99:LYS:N	2.15	0.61
2:B:77:ALA:CB	2:B:211:ILE:HG21	2.30	0.61
1:A:1121:U:H2'	1:A:1122:U:H6	1.66	0.61
1:A:1118:C:O2	1:A:1179:A:C4	2.52	0.61
10:J:6:ILE:HA	10:J:98:ILE:HG12	1.81	0.61
1:A:946:A:H2'	1:A:947:G:H8	1.64	0.61
3:C:23:TYR:OH	10:J:9:ARG:HD3	2.00	0.61
9:I:111:ARG:HG2	9:I:112:LYS:N	2.15	0.61
1:A:1251:A:H4'	9:I:12:GLU:OE2	2.00	0.61
10:J:5:ARG:O	10:J:98:ILE:HG23	2.00	0.61
2:B:189:ASP:HB2	2:B:205:ASP:OD2	2.01	0.61
21:U:24:ARG:O	21:U:25:LYS:HB2	2.00	0.61
1:A:1128:C:O2'	1:A:1130:A:H8	1.84	0.61
1:A:1125:U:H3	10:J:5:ARG:HH21	1.48	0.61
4:D:150:GLU:HG3	4:D:153:ARG:HH12	1.63	0.61
2:B:47:THR:HA	2:B:202:PRO:HG2	1.83	0.61
3:C:29:TYR:OH	14:N:54:PRO:HG2	2.00	0.61
19:S:17:GLU:O	19:S:21:GLU:HG3	2.00	0.61
9:I:53:VAL:O	9:I:54:ASP:HB2	2.01	0.61
6:F:4:TYR:HD1	6:F:92:LYS:HA	1.66	0.61
7:G:108:ALA:O	7:G:119:ARG:HD2	2.01	0.61
2:B:231:GLU:HB3	2:B:232:PRO:HD2	1.83	0.61
2:B:178:ARG:O	8:H:71:GLY:HA2	2.01	0.61
1:A:984:C:H2'	1:A:985:C:H6	1.66	0.61
4:D:189:PRO:HB2	4:D:194:LEU:HD21	1.83	0.61
1:A:1370:G:O2'	1:A:1371:G:H5'	2.01	0.61
1:A:579:G:H5'	1:A:728:A:C1'	2.27	0.61
2:B:204:ASN:HD22	2:B:205:ASP:N	1.99	0.61
1:A:1307:U:H5'	13:M:109:THR:HG21	1.82	0.61
6:F:69:GLU:CD	6:F:69:GLU:H	2.03	0.61
3:C:36:ASP:HA	3:C:39:ILE:HD12	1.82	0.61
13:M:40:ASN:HD22	13:M:41:PRO:N	1.99	0.61
3:C:70:VAL:HG12	3:C:71:ALA:N	2.16	0.61
1:A:1286:A:H2'	1:A:1287:A:H4'	1.83	0.61
2:B:114:ARG:HA	2:B:117:GLU:HB3	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:30:LYS:HA	4:D:35:ARG:HH12	1.66	0.61
1:A:575:G:OP1	1:A:575:G:H4'	2.01	0.61
9:I:9:ARG:HA	9:I:13:ALA:O	2.01	0.60
1:A:542:G:OP1	4:D:10:ARG:NH2	2.33	0.60
5:E:144:THR:HG22	5:E:146:ALA:N	2.14	0.60
5:E:53:LEU:N	5:E:53:LEU:HD23	2.15	0.60
1:A:818:G:O2'	1:A:819:A:H5''	2.01	0.60
2:B:141:GLU:O	2:B:144:ARG:HG2	2.01	0.60
1:A:1260:C:O5'	1:A:1284:C:H4'	2.01	0.60
5:E:80:ILE:H	5:E:80:ILE:HD12	1.66	0.60
6:F:46:ARG:HB3	6:F:47:ARG:HH21	1.67	0.60
1:A:1229:A:H2'	1:A:1230:C:C6	2.34	0.60
10:J:32:ALA:H	10:J:78:ASN:ND2	1.98	0.60
4:D:162:LEU:HD13	4:D:181:MET:CE	2.31	0.60
2:B:114:ARG:NH1	2:B:118:LEU:HD21	2.17	0.60
6:F:93:SER:O	6:F:94:GLN:HG3	2.01	0.60
3:C:60:ALA:O	3:C:61:ALA:HB2	2.01	0.60
4:D:10:ARG:HG3	4:D:10:ARG:HH11	1.66	0.60
2:B:97:TRP:HH2	2:B:176:GLU:CD	2.04	0.60
1:A:1286:A:H8	1:A:1287:A:H4'	1.66	0.60
1:A:1068:G:H8	1:A:1068:G:OP2	1.84	0.60
2:B:60:ASP:O	2:B:64:ARG:HG3	2.00	0.60
1:A:1127:G:N2	1:A:1146:A:N6	2.49	0.60
1:A:818:G:C2'	1:A:819:A:H5''	2.31	0.60
1:A:434:U:H2'	1:A:435:C:C6	2.36	0.60
2:B:10:LEU:HG	2:B:48:MET:CE	2.32	0.60
6:F:2:ARG:HE	6:F:69:GLU:CG	2.13	0.60
1:A:1026:G:H3'	1:A:1027:C:C5'	2.31	0.60
1:A:1234:C:O2'	1:A:1235:U:H5'	2.01	0.60
1:A:1438:G:H2'	1:A:1439:C:C6	2.37	0.60
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.84	0.60
6:F:47:ARG:O	6:F:47:ARG:HG2	2.00	0.60
4:D:150:GLU:N	4:D:150:GLU:CD	2.54	0.60
7:G:140:ASP:HA	7:G:143:ARG:HH21	1.67	0.60
14:N:58:LYS:HB3	14:N:58:LYS:NZ	2.17	0.60
1:A:1132:C:H2'	1:A:1133:G:H8	1.66	0.60
20:T:43:LEU:HD11	20:T:55:ILE:HD12	1.83	0.60
8:H:119:LEU:HD12	8:H:124:ALA:HA	1.82	0.60
1:A:190(L):U:O2	20:T:105:SER:HB2	2.02	0.60
1:A:1024:G:H3'	1:A:1025:U:H5''	1.82	0.60
18:R:86:VAL:O	18:R:87:ARG:HG2	2.02	0.60
18:R:47:THR:HG22	18:R:48:GLY:N	2.17	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
9:I:93:ARG:CB	9:I:93:ARG:HH11	2.14	0.60
1:A:1316:G:N2	1:A:1318:A:H3'	2.17	0.60
1:A:1022:G:H2'	1:A:1023:G:H8	1.67	0.60
1:A:1412:C:H2'	1:A:1413:A:C8	2.36	0.60
1:A:45:U:H2'	1:A:46:G:C8	2.37	0.60
1:A:1249:C:O2'	9:I:73:GLN:NE2	2.35	0.60
19:S:13:ASP:HA	19:S:16:LEU:CB	2.31	0.60
2:B:75:LYS:HE2	2:B:96:ARG:HH22	1.67	0.60
10:J:14:LYS:O	10:J:18:ALA:HB3	2.01	0.60
2:B:143:GLU:O	2:B:147:LYS:HG3	2.01	0.60
5:E:69:VAL:HG21	5:E:113:ALA:HB1	1.84	0.60
17:Q:67:LYS:O	17:Q:68:ARG:CB	2.49	0.60
9:I:30:GLY:O	9:I:31:GLN:HG3	2.02	0.60
18:R:42:ARG:HB3	18:R:42:ARG:NH1	2.16	0.60
1:A:1256:A:C2	1:A:1277:C:C4	2.89	0.60
2:B:12:GLU:C	2:B:14:GLY:H	2.05	0.60
5:E:82:VAL:HG21	5:E:138:ALA:CA	2.32	0.60
1:A:383:A:H2'	1:A:384:G:H5'	1.84	0.60
10:J:44:VAL:HG22	10:J:66:ARG:HB3	1.83	0.60
1:A:457:C:H2'	1:A:458:C:H6	1.67	0.60
13:M:34:LEU:HD13	13:M:41:PRO:CA	2.30	0.59
1:A:1347:G:O2'	1:A:1348:U:P	2.60	0.59
1:A:1054:C:C3'	1:A:1054:C:O2	2.49	0.59
16:P:28:ARG:HG3	16:P:29:ASP:OD2	2.03	0.59
4:D:24:GLU:O	4:D:25:ARG:HB3	2.01	0.59
3:C:116:VAL:HG21	3:C:202:ILE:HD11	1.83	0.59
1:A:853:G:O2'	1:A:854:G:H5'	2.01	0.59
2:B:84:GLU:OE1	2:B:216:SER:HA	2.02	0.59
10:J:27:ALA:HA	10:J:81:THR:HG23	1.83	0.59
1:A:112:G:H5'	1:A:389:A:H4'	1.83	0.59
10:J:24:VAL:O	10:J:28:ARG:HG3	2.02	0.59
2:B:213:LEU:O	2:B:217:ARG:HG2	2.02	0.59
22:X:3:G:C2'	22:X:4:A:C5'	2.77	0.59
2:B:23:ARG:NH1	2:B:24:TRP:HA	2.18	0.59
9:I:44:VAL:HG12	9:I:51:ARG:NH2	2.17	0.59
1:A:232:G:H1'	1:A:262:A:N1	2.17	0.59
10:J:76:ASN:O	10:J:78:ASN:N	2.35	0.59
3:C:79:ARG:HG2	3:C:82:GLU:HG2	1.83	0.59
1:A:746:A:O2'	1:A:747:C:H5'	2.02	0.59
2:B:102:LEU:HD12	2:B:102:LEU:N	2.17	0.59
9:I:17:VAL:CG2	9:I:80:GLY:HA3	2.33	0.59
2:B:168:THR:OG1	2:B:192:SER:HB3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1392:G:O2'	1:A:1502:A:H5''	2.01	0.59
9:I:118:LYS:O	9:I:119:ALA:CB	2.51	0.59
9:I:16:ARG:HB2	9:I:64:THR:HB	1.85	0.59
6:F:82:ARG:HB2	6:F:85:VAL:HG23	1.85	0.59
7:G:85:TYR:O	7:G:87:VAL:HG23	2.03	0.59
1:A:1130:A:N3	1:A:1146:A:N3	2.50	0.59
10:J:8:LEU:CD1	10:J:20:ALA:HB2	2.33	0.59
3:C:54:ARG:CG	3:C:55:VAL:H	2.15	0.59
1:A:1175:G:N2	1:A:1176:A:C4	2.71	0.59
5:E:90:VAL:O	5:E:120:THR:HA	2.03	0.59
9:I:103:THR:HG22	9:I:104:ARG:O	2.02	0.59
19:S:15:LEU:O	19:S:19:VAL:HG12	2.03	0.59
1:A:942:G:H2'	1:A:943:U:H6	1.66	0.59
12:L:54:LYS:N	12:L:54:LYS:HD2	2.18	0.59
1:A:1330:U:C4	1:A:1331:G:N3	2.71	0.59
1:A:1176:A:H2'	1:A:1177:G:C8	2.38	0.59
2:B:42:ILE:HG21	2:B:202:PRO:O	2.01	0.59
2:B:223:ILE:C	2:B:225:ALA:H	2.06	0.59
13:M:17:VAL:O	13:M:20:THR:HB	2.02	0.59
12:L:75:HIS:HD2	12:L:77:LEU:H	1.49	0.59
12:L:83:VAL:HG22	12:L:84:LEU:N	2.18	0.59
20:T:75:ASN:N	20:T:75:ASN:OD1	2.36	0.59
1:A:1130:A:C4	1:A:1146:A:N1	2.70	0.59
11:K:110:ASP:CB	18:R:88:LYS:HD2	2.27	0.59
19:S:17:GLU:HA	19:S:20:LEU:CG	2.31	0.59
1:A:522:C:H41	12:L:53:ARG:NH2	2.00	0.59
12:L:83:VAL:HG21	12:L:100:ILE:CG1	2.33	0.59
3:C:154:SER:OG	3:C:155:GLY:N	2.33	0.59
2:B:42:ILE:H	2:B:42:ILE:CD1	2.15	0.59
8:H:4:ASP:OD2	8:H:7:ALA:HB2	2.03	0.59
18:R:52:PRO:HB3	18:R:54:ARG:NH1	2.17	0.59
16:P:20:VAL:HG11	16:P:32:TYR:HB3	1.85	0.59
10:J:8:LEU:HD12	10:J:20:ALA:HB2	1.86	0.58
2:B:42:ILE:HD12	2:B:42:ILE:N	2.17	0.58
1:A:390:C:O3'	16:P:28:ARG:NH2	2.35	0.58
3:C:37:GLN:HE22	14:N:52:GLN:HE22	1.51	0.58
1:A:1085:U:H3'	1:A:1086:U:H5	1.67	0.58
2:B:122:PHE:HE2	2:B:139:LYS:HG2	1.68	0.58
1:A:1056:U:H5'	3:C:163:ALA:HB2	1.84	0.58
7:G:120:ILE:N	7:G:120:ILE:HD12	2.17	0.58
8:H:120:THR:OG1	8:H:123:GLU:HG3	2.03	0.58
8:H:119:LEU:HD12	8:H:124:ALA:N	2.18	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
12:L:83:VAL:HG21	12:L:100:ILE:HG13	1.83	0.58
7:G:46:ALA:O	7:G:50:ILE:HG12	2.02	0.58
1:A:940:C:H2'	1:A:941:G:H8	1.68	0.58
1:A:1006:C:H2'	1:A:1007:C:H6	1.65	0.58
4:D:3:ARG:HD2	4:D:118:ARG:HE	1.68	0.58
3:C:47:LEU:N	3:C:47:LEU:HD12	2.18	0.58
1:A:314:C:O2'	1:A:315:A:H5'	2.02	0.58
1:A:1366:C:C2	1:A:1367:C:C5	2.91	0.58
1:A:792:A:H4'	1:A:793:U:O5'	2.03	0.58
1:A:1428:A:H2'	1:A:1429:C:C6	2.39	0.58
1:A:426:G:O2'	1:A:427:U:H5'	2.04	0.58
4:D:191:ARG:O	4:D:191:ARG:HD2	2.03	0.58
22:X:3:G:H2'	22:X:4:A:H5'	1.82	0.58
2:B:97:TRP:CZ2	2:B:102:LEU:HD13	2.29	0.58
16:P:67:THR:HG22	16:P:68:ASP:N	2.19	0.58
6:F:23:LYS:O	6:F:27:GLN:HG2	2.02	0.58
2:B:232:PRO:O	2:B:233:SER:HB2	2.03	0.58
1:A:501:C:H2'	1:A:502:G:C8	2.38	0.58
1:A:833:U:H2'	1:A:834:C:C6	2.38	0.58
1:A:1101:A:H4'	1:A:1102:A:O5'	2.04	0.58
6:F:47:ARG:HA	6:F:57:GLN:HG2	1.84	0.58
20:T:83:ARG:HB3	20:T:87:LYS:NZ	2.18	0.58
12:L:41:ARG:CG	12:L:42:THR:H	2.15	0.58
10:J:3:LYS:N	10:J:3:LYS:HD3	2.19	0.58
10:J:32:ALA:HB2	10:J:76:ASN:CB	2.33	0.58
5:E:75:THR:HG23	5:E:76:ILE:N	2.18	0.58
1:A:427:U:OP1	4:D:13:ARG:NH2	2.36	0.58
1:A:1339:A:H2'	1:A:1340:A:O4'	2.04	0.58
9:I:82:ALA:O	9:I:86:VAL:HG23	2.04	0.58
20:T:37:SER:O	20:T:41:VAL:HG23	2.04	0.58
1:A:1342:C:O2'	1:A:1343:G:H5'	2.04	0.58
3:C:77:ILE:C	3:C:83:ARG:HB3	2.24	0.58
20:T:45:GLN:HB2	20:T:91:LEU:HD13	1.84	0.58
9:I:5:TYR:O	9:I:84:ALA:HA	2.04	0.58
1:A:179:A:H2'	1:A:180:U:C6	2.38	0.58
1:A:496:A:H4'	1:A:497:A:O5'	2.02	0.58
1:A:353:A:H5'	1:A:353:A:C8	2.39	0.58
10:J:47:PHE:CE2	14:N:37:PHE:HE1	2.21	0.58
1:A:273:A:H1'	17:Q:16:GLN:NE2	2.19	0.58
1:A:1250:A:H4'	9:I:68:GLY:CA	2.33	0.58
1:A:433:C:C6	1:A:433:C:H5'	2.36	0.58
1:A:1148:U:H2'	1:A:1149:C:O4'	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:166:ASP:OD2	2:B:169:LYS:HB2	2.04	0.58
19:S:80:TYR:O	19:S:82:GLY:N	2.37	0.58
1:A:939:G:H5''	7:G:102:ARG:NH2	2.18	0.58
1:A:1175:G:N1	1:A:1176:A:C5	2.72	0.57
1:A:1137:C:H4'	1:A:1138:G:N1	2.19	0.57
1:A:1218:C:H2'	1:A:1219:U:C6	2.38	0.57
1:A:706:A:C4'	11:K:29:ILE:HD11	2.33	0.57
1:A:47:C:H5''	1:A:365:U:C6	2.39	0.57
1:A:1117:G:N2	1:A:1180:A:H1'	2.18	0.57
1:A:1306:A:N6	1:A:1331:G:H1'	2.19	0.57
1:A:1085:U:H3'	1:A:1086:U:C5	2.39	0.57
20:T:59:ALA:O	20:T:63:ILE:HG13	2.05	0.57
1:A:780:A:O2'	1:A:781:A:H5''	2.04	0.57
2:B:178:ARG:NH1	8:H:71:GLY:O	2.37	0.57
3:C:54:ARG:CG	3:C:55:VAL:N	2.67	0.57
9:I:32:ASP:O	9:I:35:GLU:HB3	2.05	0.57
8:H:112:LEU:HD23	8:H:112:LEU:N	2.19	0.57
1:A:1129:C:OP1	9:I:62:TYR:OH	2.14	0.57
2:B:196:LEU:H	2:B:196:LEU:CD1	2.17	0.57
14:N:24:CYS:SG	14:N:40:CYS:N	2.77	0.57
1:A:269:C:H2'	1:A:270:A:C8	2.40	0.57
12:L:24:VAL:O	12:L:26:ALA:N	2.34	0.57
13:M:108:ARG:NE	13:M:108:ARG:HA	2.18	0.57
6:F:92:LYS:NZ	6:F:92:LYS:HB2	2.19	0.57
1:A:1178:G:C2	1:A:1180:A:C8	2.91	0.57
3:C:14:ILE:O	3:C:16:ARG:N	2.37	0.57
7:G:146:GLU:CG	7:G:149:ARG:HH21	2.14	0.57
13:M:5:ALA:HB3	13:M:8:GLU:CG	2.35	0.57
13:M:19:LEU:HA	13:M:22:ILE:HD13	1.87	0.57
4:D:173:TRP:CG	4:D:189:PRO:HG3	2.40	0.57
1:A:1443:G:C5'	1:A:1446:A:H3'	2.34	0.57
7:G:26:PHE:CE2	7:G:30:ILE:HD11	2.40	0.57
1:A:1397:C:H4'	1:A:1398:A:OP2	2.03	0.57
1:A:580:U:H2'	1:A:581:G:O4'	2.05	0.57
1:A:1179:A:C2'	1:A:1180:A:H5'	2.35	0.57
7:G:145:ALA:C	7:G:147:ALA:H	2.08	0.57
3:C:126:ARG:O	3:C:127:ARG:HB2	2.05	0.57
2:B:114:ARG:HH12	2:B:118:LEU:HD21	1.69	0.57
4:D:3:ARG:NE	4:D:5:ILE:HD11	2.20	0.57
1:A:247:G:OP2	17:Q:99:SER:HB2	2.04	0.57
15:O:78:TYR:CE1	15:O:82:ILE:HD11	2.39	0.57
1:A:834:C:H2'	1:A:835:U:H6	1.70	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
4:D:62:GLN:HE22	4:D:65:ARG:NH1	2.03	0.57
7:G:23:VAL:O	7:G:27:ILE:HG13	2.05	0.57
4:D:80:GLU:O	4:D:84:LYS:HG3	2.05	0.57
12:L:119:LYS:O	12:L:120:TYR:HB2	2.05	0.57
2:B:30:ARG:HD2	2:B:31:TYR:CE2	2.39	0.57
1:A:1190:G:H3'	3:C:3:ASN:HD22	1.69	0.57
1:A:1251:A:H5'	9:I:12:GLU:OE1	2.04	0.57
18:R:88:LYS:HG2	18:R:88:LYS:OXT	2.03	0.57
6:F:45:LEU:O	6:F:45:LEU:HD12	2.05	0.57
1:A:1373:G:H5''	7:G:36:LYS:CB	2.35	0.57
4:D:70:ILE:HG22	4:D:75:PHE:HB2	1.84	0.57
1:A:1124:G:H2'	1:A:1145:C:H5	1.69	0.57
8:H:83:ILE:O	8:H:83:ILE:HG23	2.05	0.57
1:A:254:G:O2'	1:A:255:G:H5'	2.04	0.56
10:J:57:LYS:HD2	10:J:60:ARG:NH2	2.19	0.56
2:B:69:LEU:HD22	2:B:155:LEU:HD11	1.87	0.56
2:B:25:ASN:ND2	2:B:25:ASN:C	2.53	0.56
1:A:491:G:H2'	1:A:492:G:H8	1.70	0.56
1:A:877:C:O2'	1:A:878:G:H5'	2.05	0.56
1:A:1178:G:N3	1:A:1180:A:C8	2.73	0.56
5:E:91:LEU:CD2	5:E:120:THR:HG22	2.34	0.56
9:I:108:VAL:HG12	9:I:109:VAL:N	2.20	0.56
6:F:43:LEU:HD12	6:F:46:ARG:HD2	1.85	0.56
1:A:190(D):U:O2'	1:A:190(E):U:H5'	2.05	0.56
10:J:32:ALA:HB2	10:J:76:ASN:CG	2.25	0.56
15:O:4:THR:HG1	15:O:7:GLU:HG3	1.69	0.56
1:A:1326:C:H2'	1:A:1327:C:C6	2.40	0.56
1:A:757:U:H2'	1:A:758:G:O4'	2.05	0.56
19:S:51:VAL:HG21	19:S:71:LEU:HB3	1.87	0.56
1:A:1250:A:H2'	1:A:1251:A:C8	2.39	0.56
13:M:40:ASN:ND2	13:M:42:ALA:H	2.03	0.56
3:C:130:VAL:HG21	3:C:157:ILE:HG23	1.87	0.56
13:M:9:ILE:N	13:M:9:ILE:HD12	2.19	0.56
4:D:173:TRP:HB2	4:D:187:ARG:O	2.04	0.56
8:H:121:ASP:O	8:H:125:ARG:HB2	2.05	0.56
17:Q:4:LYS:HE3	17:Q:6:LEU:HD21	1.86	0.56
17:Q:63:ARG:HG2	17:Q:64:PRO:HD2	1.88	0.56
5:E:78:HIS:HD2	8:H:107:LEU:HD12	1.68	0.56
1:A:1024:G:H2'	1:A:1025:U:O4'	2.05	0.56
3:C:95:THR:C	3:C:97:LYS:H	2.08	0.56
20:T:76:ALA:O	20:T:80:ARG:HG3	2.06	0.56
17:Q:67:LYS:HA	17:Q:70:ARG:NH1	2.13	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:91:PRO:HG2	2:B:155:LEU:HG	1.86	0.56
1:A:953:G:H1'	13:M:125:ARG:CB	2.34	0.56
13:M:11:ARG:HG3	13:M:11:ARG:NH1	2.20	0.56
5:E:20:GLN:NE2	5:E:21:ALA:O	2.38	0.56
3:C:172:ARG:HB3	3:C:172:ARG:HH11	1.71	0.56
3:C:58:GLU:HB2	3:C:65:ALA:HB2	1.86	0.56
1:A:973:G:H3'	1:A:974:A:H5''	1.88	0.56
19:S:19:VAL:HG13	19:S:20:LEU:N	2.20	0.56
2:B:75:LYS:HA	2:B:78:GLN:HB2	1.86	0.56
1:A:1392:G:H21	1:A:1502:A:H8	1.53	0.56
1:A:1161:C:O2	1:A:1161:C:H2'	2.05	0.56
21:U:14:TRP:CZ3	21:U:15:ARG:HD2	2.41	0.56
1:A:818:G:H3'	1:A:819:A:C5'	2.36	0.56
1:A:547:A:H4'	1:A:548:G:O5'	2.05	0.56
2:B:14:GLY:C	2:B:15:VAL:HG22	2.26	0.56
6:F:13:ASN:O	6:F:14:LEU:HD12	2.05	0.56
1:A:977:A:H2'	1:A:978:A:H5'	1.87	0.56
1:A:99:C:H2'	1:A:101:A:C8	2.41	0.56
5:E:79:GLU:HG3	5:E:93:PRO:CD	2.26	0.56
1:A:1347:G:H22	1:A:1373:G:H2'	1.69	0.56
1:A:1034:G:N2	1:A:1035:A:H62	2.03	0.56
2:B:51:LEU:HD22	2:B:55:PHE:CE1	2.39	0.56
20:T:99:LEU:O	20:T:101:GLY:N	2.39	0.56
8:H:119:LEU:HD12	8:H:124:ALA:CA	2.35	0.56
4:D:8:VAL:HB	4:D:21:LEU:HD13	1.88	0.56
4:D:128:VAL:HG12	4:D:129:ASN:ND2	2.21	0.56
1:A:1228:C:OP1	13:M:115:LYS:HE3	2.05	0.56
2:B:77:ALA:HB2	2:B:211:ILE:HG21	1.86	0.56
2:B:54:THR:O	2:B:57:PHE:HB3	2.06	0.56
14:N:22:THR:HB	14:N:33:VAL:CG2	2.34	0.56
20:T:72:LEU:O	20:T:73:HIS:O	2.23	0.56
9:I:111:ARG:HD2	14:N:61:TRP:OXT	2.05	0.56
11:K:32:ILE:CD1	11:K:68:ALA:HB1	2.36	0.56
12:L:55:VAL:CG1	12:L:56:ALA:H	2.13	0.56
3:C:102:ASN:N	3:C:102:ASN:ND2	2.52	0.56
1:A:328:C:O2	1:A:328:C:C2'	2.54	0.56
4:D:189:PRO:CB	4:D:194:LEU:HD21	2.35	0.56
7:G:65:ALA:O	7:G:69:VAL:HG23	2.07	0.55
3:C:52:LEU:H	3:C:52:LEU:HD23	1.69	0.55
10:J:3:LYS:O	10:J:101:VAL:N	2.39	0.55
1:A:1156:G:C3'	1:A:1157:A:OP2	2.49	0.55
3:C:3:ASN:O	3:C:4:LYS:HB2	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
14:N:8:GLU:O	14:N:11:LYS:HB2	2.07	0.55
1:A:1053:G:C3'	1:A:1054:C:H5'	2.35	0.55
1:A:1288:A:H2'	1:A:1289:A:C8	2.42	0.55
3:C:34:LEU:HG	14:N:25:VAL:HG21	1.89	0.55
10:J:34:VAL:HG13	10:J:74:ILE:HG12	1.88	0.55
6:F:39:LYS:HB3	6:F:64:GLN:HB3	1.87	0.55
1:A:1020:U:H2'	1:A:1021:G:H8	1.70	0.55
3:C:70:VAL:O	3:C:106:VAL:HG23	2.05	0.55
2:B:187:LEU:HD21	2:B:204:ASN:H	1.71	0.55
5:E:51:VAL:O	5:E:54:ALA:HB3	2.06	0.55
1:A:1498:U:H4'	1:A:1519:A:C2	2.41	0.55
1:A:371:G:C2'	1:A:372:C:H5'	2.35	0.55
4:D:20:TYR:HD2	4:D:26:CYS:HB3	1.71	0.55
1:A:983:A:HO2'	1:A:1049:U:HO2'	1.54	0.55
1:A:1499:A:H1'	1:A:1520:G:H5'	1.88	0.55
11:K:104:GLN:OE1	11:K:106:LYS:HD3	2.06	0.55
1:A:730:G:N2	1:A:765:G:H5"	2.21	0.55
1:A:1125:U:H5'	1:A:1126:U:H5	1.72	0.55
1:A:629:G:H2'	1:A:630:G:C4'	2.36	0.55
11:K:40:ILE:HG22	11:K:41:THR:HG23	1.88	0.55
18:R:53:ARG:HA	18:R:56:THR:OG1	2.07	0.55
7:G:38:LEU:HD12	7:G:38:LEU:O	2.06	0.55
7:G:80:VAL:HG21	7:G:154:TYR:CE1	2.42	0.55
10:J:7:LYS:HB3	10:J:97:GLU:HB2	1.88	0.55
1:A:1053:G:H3'	1:A:1054:C:H5'	1.88	0.55
12:L:27:LEU:HG	12:L:28:LYS:H	1.70	0.55
1:A:1208:C:H2'	1:A:1209:C:C6	2.42	0.55
12:L:77:LEU:HD21	12:L:107:ALA:HA	1.89	0.55
3:C:147:LYS:HD3	3:C:205:GLY:H	1.72	0.55
8:H:20:TYR:CE1	8:H:76:PRO:HG2	2.41	0.55
1:A:974:A:OP2	14:N:41:ARG:NH1	2.39	0.55
2:B:204:ASN:C	2:B:204:ASN:ND2	2.58	0.55
1:A:1318:A:H1'	19:S:37:ARG:NH1	2.22	0.55
4:D:2:GLY:O	4:D:3:ARG:O	2.25	0.55
1:A:190(L):U:C2	20:T:105:SER:HB2	2.41	0.55
1:A:1333:A:H2'	1:A:1334:G:O4'	2.06	0.55
1:A:287:U:O2'	1:A:288:A:H5'	2.05	0.55
2:B:224:GLN:O	2:B:224:GLN:HG2	2.06	0.55
11:K:87:THR:HA	11:K:91:ARG:HH21	1.72	0.55
5:E:147:ASP:OD1	5:E:147:ASP:N	2.33	0.55
2:B:8:LYS:N	2:B:8:LYS:HD3	2.21	0.55
1:A:337:C:H2'	1:A:338:A:C8	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
21:U:14:TRP:HZ3	21:U:15:ARG:HD2	1.72	0.55
1:A:629:G:H2'	1:A:630:G:C5'	2.35	0.55
1:A:969:A:H61	13:M:126:LYS:HB2	1.72	0.55
18:R:52:PRO:O	18:R:56:THR:HG23	2.06	0.55
16:P:20:VAL:HG11	16:P:32:TYR:CB	2.37	0.55
1:A:620:C:N1	4:D:135:LEU:HD13	2.22	0.55
1:A:828:A:H2'	1:A:829:G:O4'	2.07	0.55
1:A:750:G:N3	15:O:23:GLY:HA3	2.21	0.55
3:C:39:ILE:HG22	3:C:40:ARG:N	2.22	0.55
15:O:77:ARG:O	15:O:80:ALA:HB3	2.07	0.55
1:A:915:A:H2'	1:A:916:G:H5'	1.89	0.55
2:B:122:PHE:O	2:B:123:ALA:HB2	2.07	0.55
10:J:94:VAL:HG12	10:J:95:GLU:N	2.22	0.55
1:A:940:C:H2'	1:A:941:G:C8	2.42	0.55
20:T:53:LEU:HB2	20:T:100:ILE:HG21	1.88	0.55
1:A:457:C:H2'	1:A:458:C:C6	2.41	0.55
12:L:83:VAL:CG2	12:L:100:ILE:HG23	2.36	0.55
3:C:8:ILE:HG23	3:C:16:ARG:HG2	1.88	0.55
2:B:21:ARG:O	2:B:39:ILE:HA	2.07	0.55
2:B:139:LYS:C	2:B:139:LYS:HD3	2.27	0.55
1:A:1015:A:H2'	1:A:1016:A:C8	2.42	0.55
1:A:411:A:O2'	1:A:412:A:H5'	2.07	0.55
2:B:85:ALA:HB3	2:B:92:TYR:HD2	1.72	0.55
16:P:26:ARG:NH2	16:P:31:LYS:NZ	2.55	0.55
1:A:1152:A:H2'	1:A:1153:C:H6	1.72	0.54
2:B:14:GLY:O	2:B:15:VAL:HG13	2.07	0.54
13:M:37:THR:HG23	13:M:55:ARG:CD	2.34	0.54
13:M:11:ARG:HD3	13:M:12:ASN:N	2.22	0.54
6:F:19:LEU:C	6:F:19:LEU:HD23	2.28	0.54
1:A:1007:C:H42	1:A:1022:G:H1	1.56	0.54
5:E:12:LEU:CD1	5:E:31:LEU:HB2	2.37	0.54
1:A:404:U:H5'	4:D:122:ARG:HD2	1.87	0.54
3:C:20:SER:O	14:N:54:PRO:HB3	2.06	0.54
16:P:43:LYS:HB3	16:P:48:TRP:CG	2.42	0.54
7:G:82:GLY:O	7:G:83:ALA:HB2	2.07	0.54
12:L:41:ARG:NH2	12:L:57:LYS:NZ	2.56	0.54
6:F:100:ASN:HD22	18:R:23:LYS:CG	2.20	0.54
1:A:415:A:H2'	1:A:416:G:C8	2.42	0.54
1:A:411:A:O2'	1:A:413:G:H5'	2.06	0.54
1:A:1443:G:H5''	1:A:1446:A:H3'	1.88	0.54
1:A:528:C:H5'	1:A:535:A:C6	2.43	0.54
19:S:33:THR:HG22	19:S:34:TRP:N	2.22	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1123:A:H2	10:J:39:PRO:HG2	1.72	0.54
2:B:162:ILE:HG22	2:B:164:VAL:HG23	1.88	0.54
7:G:20:ASP:OD2	7:G:22:LEU:HB3	2.07	0.54
1:A:1232:U:P	9:I:124:GLN:HE21	2.30	0.54
1:A:357:G:O2'	1:A:358:U:H5'	2.07	0.54
2:B:22:LYS:HG3	2:B:35:GLU:OE2	2.08	0.54
2:B:73:THR:HG23	2:B:95:GLN:O	2.07	0.54
2:B:55:PHE:HE2	2:B:218:ALA:HA	1.72	0.54
1:A:1230:C:O2'	1:A:1231:G:H5'	2.08	0.54
1:A:629:G:C2'	1:A:630:G:H5''	2.36	0.54
4:D:127:THR:CG2	4:D:147:ALA:HB3	2.37	0.54
12:L:115:LYS:O	12:L:117:ARG:N	2.38	0.54
1:A:959:A:C2	1:A:1222:G:O4'	2.60	0.54
17:Q:75:ARG:HG3	17:Q:75:ARG:HH11	1.72	0.54
1:A:1175:G:C5	1:A:1176:A:N7	2.76	0.54
5:E:80:ILE:HD11	5:E:91:LEU:HD12	1.89	0.54
5:E:148:VAL:O	5:E:152:ARG:HG3	2.07	0.54
13:M:37:THR:O	13:M:37:THR:HG22	2.08	0.54
12:L:27:LEU:C	12:L:29:GLY:N	2.60	0.54
1:A:840:C:H4'	1:A:848:C:O2	2.08	0.54
10:J:22:LYS:HB2	10:J:22:LYS:NZ	2.22	0.54
1:A:755:G:OP2	15:O:65:ARG:HD2	2.08	0.54
6:F:36:ARG:NH2	6:F:38:GLU:HG2	2.22	0.54
1:A:1112:C:C4	3:C:178:LEU:HD23	2.43	0.54
2:B:82:ARG:O	2:B:86:GLU:HG3	2.08	0.54
6:F:33:TYR:HA	6:F:71:ARG:CZ	2.37	0.54
1:A:149:A:H2'	1:A:150:C:C6	2.42	0.54
2:B:229:VAL:O	2:B:229:VAL:HG12	2.08	0.54
1:A:1532:U:O2'	1:A:1533:C:H6	1.90	0.54
3:C:25:GLY:O	3:C:27:LYS:N	2.40	0.54
7:G:143:ARG:O	7:G:147:ALA:HB2	2.08	0.54
2:B:74:LYS:NZ	2:B:206:ASP:HB2	2.21	0.54
1:A:738:C:H5''	6:F:69:GLU:HB3	1.90	0.54
17:Q:40:LYS:HG2	17:Q:42:TYR:CE1	2.43	0.54
6:F:23:LYS:NZ	6:F:42:GLU:OE2	2.39	0.54
10:J:90:LEU:N	10:J:91:PRO:HD2	2.23	0.54
1:A:666:G:H5'	1:A:726:C:H1'	1.90	0.54
5:E:121:LYS:HD2	5:E:122:GLU:H	1.71	0.54
20:T:86:ARG:HH11	20:T:86:ARG:HG3	1.72	0.54
17:Q:67:LYS:O	17:Q:68:ARG:HB3	2.08	0.54
11:K:57:THR:HG22	11:K:59:TYR:N	2.18	0.54
1:A:421:U:H5'	1:A:422:C:H5	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1419:G:O2'	1:A:1420:C:H5'	2.08	0.54
1:A:1179:A:N1	1:A:1180:A:C2	2.74	0.54
1:A:1123:A:C2	10:J:39:PRO:HG2	2.42	0.54
1:A:1060:C:O2	1:A:1198:G:C2	2.60	0.54
1:A:1277:C:O2'	1:A:1279:A:H8	1.91	0.54
1:A:1035:A:H2'	1:A:1036:G:C8	2.33	0.54
1:A:1498:U:H4'	1:A:1519:A:H2	1.73	0.54
1:A:1001:A:H2'	1:A:1002:G:H8	1.72	0.54
16:P:20:VAL:CG1	16:P:21:VAL:N	2.70	0.54
8:H:6:ILE:O	8:H:10:LEU:HG	2.08	0.54
1:A:245:C:O2	1:A:283:C:N3	2.40	0.54
1:A:539:A:H2'	1:A:540:G:C8	2.42	0.54
1:A:1179:A:C2'	1:A:1180:A:C5'	2.86	0.54
1:A:1211:U:H5'	1:A:1212:U:OP1	2.08	0.54
3:C:88:ARG:HG2	3:C:101:LEU:CD1	2.34	0.54
5:E:10:MET:O	5:E:10:MET:HG3	2.08	0.54
19:S:80:TYR:CZ	19:S:81:ARG:HB3	2.43	0.54
3:C:188:LEU:O	3:C:189:ALA:CB	2.56	0.54
1:A:392:G:H2'	1:A:393:A:C8	2.43	0.54
1:A:1002:G:H2'	1:A:1003:G:C8	2.43	0.54
1:A:1346:A:C4	7:G:10:ARG:NH2	2.76	0.54
1:A:1091:U:O2	1:A:1093:A:H8	1.90	0.54
3:C:11:ARG:O	3:C:14:ILE:O	2.26	0.53
9:I:10:ARG:HG2	9:I:75:ASP:HB2	1.90	0.53
2:B:75:LYS:HD3	2:B:78:GLN:OE1	2.08	0.53
19:S:80:TYR:CG	19:S:81:ARG:N	2.76	0.53
4:D:173:TRP:CD2	4:D:189:PRO:HG3	2.42	0.53
1:A:1005:A:H2'	1:A:1006:C:H5'	1.90	0.53
1:A:1091:U:O2	1:A:1093:A:C8	2.61	0.53
1:A:911:U:H2'	1:A:912:C:C6	2.43	0.53
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.43	0.53
16:P:8:ARG:HG2	16:P:8:ARG:HH11	1.72	0.53
1:A:433:C:C5'	1:A:433:C:C6	2.87	0.53
6:F:92:LYS:HZ2	6:F:92:LYS:HB2	1.73	0.53
2:B:172:ILE:H	2:B:172:ILE:CD1	2.19	0.53
1:A:984:C:H2'	1:A:985:C:C6	2.42	0.53
1:A:1001:A:H2'	1:A:1002:G:C8	2.44	0.53
18:R:37:VAL:O	18:R:41:LYS:HB2	2.08	0.53
6:F:60:PHE:CE2	18:R:78:LEU:HD21	2.44	0.53
15:O:33:THR:HG23	15:O:63:ARG:NH1	2.23	0.53
1:A:235:C:C5'	17:Q:70:ARG:HG2	2.35	0.53
19:S:39:THR:HG22	19:S:40:ILE:N	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:22:LYS:C	10:J:24:VAL:H	2.12	0.53
1:A:1001:A:H2	1:A:1040:U:H3	1.54	0.53
11:K:99:GLN:HG2	11:K:105:VAL:HG21	1.90	0.53
1:A:432:A:H3'	1:A:433:C:C5'	2.31	0.53
1:A:1373:G:C5'	7:G:36:LYS:HB2	2.37	0.53
1:A:1229:A:O2'	13:M:125:ARG:NE	2.41	0.53
3:C:110:ASN:HD22	3:C:140:ARG:HB3	1.74	0.53
6:F:27:GLN:NE2	6:F:27:GLN:HA	2.23	0.53
16:P:10:GLY:HA3	16:P:14:ASN:O	2.09	0.53
1:A:1024:G:C3'	1:A:1025:U:H5''	2.38	0.53
11:K:47:VAL:HG12	11:K:48:ILE:HD13	1.90	0.53
14:N:14:PRO:O	14:N:15:LYS:CB	2.56	0.53
10:J:39:PRO:O	10:J:69:ASN:O	2.25	0.53
4:D:165:MET:HA	4:D:168:ARG:HG3	1.90	0.53
2:B:122:PHE:CE2	2:B:139:LYS:HG2	2.43	0.53
2:B:178:ARG:HH21	8:H:68:ARG:HH22	1.54	0.53
11:K:33:THR:HG22	11:K:39:PRO:CA	2.37	0.53
9:I:17:VAL:HG11	9:I:81:ILE:N	2.24	0.53
1:A:413:G:O6	4:D:35:ARG:HG3	2.08	0.53
1:A:1262:C:O2'	1:A:1263:C:H5'	2.09	0.53
5:E:99:GLY:O	5:E:117:ASP:HA	2.08	0.53
1:A:192:U:C1'	20:T:103:GLY:HA2	2.38	0.53
9:I:14:VAL:HG22	9:I:66:ARG:O	2.09	0.53
2:B:25:ASN:HD22	2:B:26:PRO:N	2.06	0.53
4:D:18:LYS:HD3	4:D:20:TYR:CE2	2.44	0.53
1:A:1121:U:H2'	1:A:1122:U:C6	2.42	0.53
14:N:37:PHE:CE2	14:N:53:LEU:HD13	2.44	0.53
1:A:192:U:H1'	20:T:103:GLY:HA2	1.91	0.53
1:A:56:U:H2'	1:A:57:G:C8	2.44	0.53
15:O:36:ILE:HA	15:O:59:MET:HE3	1.91	0.53
13:M:73:GLU:O	13:M:76:ALA:HB3	2.09	0.53
14:N:36:PHE:O	14:N:36:PHE:CD1	2.61	0.53
1:A:1330:U:OP1	13:M:23:TYR:O	2.26	0.53
2:B:178:ARG:NH2	8:H:68:ARG:NH2	2.54	0.53
17:Q:27:PHE:HB2	17:Q:28:PRO:HD2	1.90	0.53
1:A:1232:U:OP1	9:I:124:GLN:HG2	2.08	0.53
16:P:34:GLU:OE2	16:P:55:ARG:HD3	2.08	0.53
1:A:1179:A:H2'	1:A:1180:A:C5'	2.39	0.53
13:M:40:ASN:HD22	13:M:41:PRO:HD2	1.72	0.53
10:J:49:VAL:HG21	14:N:41:ARG:O	2.08	0.53
1:A:1347:G:C2'	1:A:1348:U:OP2	2.56	0.53
10:J:46:ARG:HH11	10:J:64:GLU:HB3	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
17:Q:75:ARG:HG3	17:Q:75:ARG:NH1	2.23	0.53
1:A:1347:G:O2'	1:A:1348:U:OP2	2.27	0.53
2:B:91:PRO:HG3	2:B:154:LEU:CB	2.35	0.53
1:A:761:G:O2'	17:Q:105:ALA:HB2	2.09	0.53
4:D:151:LYS:H	4:D:151:LYS:CD	2.22	0.53
1:A:730:G:H21	1:A:765:G:H5''	1.74	0.53
1:A:1130:A:N9	1:A:1146:A:C2	2.76	0.52
6:F:46:ARG:CA	6:F:47:ARG:HH21	2.22	0.52
2:B:209:ARG:HG2	2:B:239:VAL:HG13	1.91	0.52
3:C:155:GLY:CA	3:C:164:ARG:H	2.21	0.52
11:K:15:ALA:HA	11:K:77:MET:HA	1.90	0.52
10:J:90:LEU:H	10:J:91:PRO:CD	2.20	0.52
8:H:113:SER:HB2	8:H:134:ILE:HD11	1.90	0.52
1:A:475:G:H2'	1:A:476:G:H8	1.74	0.52
22:X:3:G:H22	23:Y:34:TM2:C2	2.21	0.52
3:C:107:GLN:NE2	3:C:107:GLN:H	2.06	0.52
6:F:94:GLN:NE2	18:R:32:ARG:HD3	2.24	0.52
16:P:20:VAL:HG13	16:P:32:TYR:HB2	1.92	0.52
1:A:269:C:H2'	1:A:270:A:H8	1.75	0.52
1:A:166:G:H2'	1:A:167:G:H8	1.74	0.52
15:O:5:LYS:HD2	15:O:5:LYS:H	1.73	0.52
1:A:1179:A:N1	1:A:1180:A:N3	2.57	0.52
1:A:976:G:H5'	1:A:1358:U:O2'	2.09	0.52
2:B:78:GLN:O	2:B:94:ASN:OD1	2.28	0.52
1:A:1390:U:H2'	1:A:1391:U:C6	2.44	0.52
3:C:108:ASN:ND2	3:C:111:LEU:HG	2.24	0.52
17:Q:40:LYS:HE3	17:Q:42:TYR:OH	2.09	0.52
5:E:96:PRO:HA	5:E:117:ASP:OD2	2.10	0.52
13:M:49:THR:HB	13:M:52:GLU:HG3	1.90	0.52
2:B:8:LYS:HE2	2:B:9:GLU:N	2.20	0.52
3:C:134:ILE:HG22	3:C:168:ALA:HB3	1.90	0.52
12:L:24:VAL:HG12	12:L:26:ALA:CB	2.39	0.52
20:T:67:ALA:HA	20:T:73:HIS:N	2.23	0.52
5:E:92:LYS:HB3	5:E:119:LEU:HB2	1.90	0.52
6:F:27:GLN:HE21	6:F:27:GLN:HA	1.74	0.52
1:A:942:G:O2'	1:A:943:U:H5'	2.10	0.52
5:E:121:LYS:HD2	5:E:122:GLU:N	2.24	0.52
11:K:95:ILE:CG2	11:K:108:ILE:HD13	2.40	0.52
5:E:126:ARG:HG3	5:E:126:ARG:HH11	1.74	0.52
9:I:9:ARG:HG2	9:I:14:VAL:HG12	1.91	0.52
14:N:29:ARG:HH11	14:N:29:ARG:HG2	1.75	0.52
12:L:55:VAL:CG1	12:L:56:ALA:N	2.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:30:SER:OG	10:J:81:THR:HA	2.09	0.52
1:A:1048:G:H5''	14:N:3:ARG:HG3	1.92	0.52
12:L:41:ARG:HH22	12:L:57:LYS:NZ	2.08	0.52
1:A:1216:G:H5''	14:N:5:ALA:CB	2.40	0.52
3:C:127:ARG:HH11	3:C:127:ARG:HG3	1.73	0.52
1:A:490:G:H2'	1:A:491:G:C8	2.44	0.52
6:F:22:GLU:HA	6:F:22:GLU:OE2	2.09	0.52
1:A:1056:U:O2'	1:A:1057:G:H5'	2.10	0.52
1:A:382:A:H2'	1:A:383:A:H8	1.71	0.52
3:C:137:ALA:HA	3:C:140:ARG:HE	1.75	0.52
13:M:22:ILE:N	13:M:22:ILE:HD12	2.24	0.52
1:A:157:G:O2'	1:A:158:G:H5'	2.08	0.52
2:B:33:TYR:HB2	2:B:43:ASP:HA	1.90	0.52
1:A:1130:A:C5	1:A:1146:A:C6	2.97	0.52
1:A:370:C:C2'	1:A:371:G:H5'	2.39	0.52
3:C:79:ARG:HG2	3:C:82:GLU:CG	2.40	0.52
10:J:28:ARG:HH11	10:J:28:ARG:HG2	1.74	0.52
4:D:117:ALA:O	4:D:121:VAL:HG23	2.09	0.52
4:D:148:VAL:HG11	4:D:158:ILE:HD13	1.92	0.52
1:A:1069:C:O2'	1:A:1192:C:H1'	2.10	0.52
2:B:97:TRP:CH2	2:B:176:GLU:CD	2.82	0.52
9:I:102:LEU:HD12	9:I:103:THR:H	1.74	0.52
3:C:157:ILE:HG21	3:C:164:ARG:NH2	2.24	0.52
11:K:13:GLN:HA	11:K:75:TYR:O	2.09	0.52
4:D:127:THR:HG23	4:D:147:ALA:HB3	1.92	0.52
2:B:22:LYS:HE3	2:B:35:GLU:OE2	2.10	0.52
8:H:84:ARG:O	8:H:135:CYS:HB2	2.10	0.52
16:P:75:ARG:HH11	16:P:75:ARG:HG3	1.74	0.52
2:B:156:LYS:O	2:B:156:LYS:HG2	2.10	0.52
1:A:961:U:C2'	1:A:962:C:H5'	2.40	0.52
1:A:1042:G:O2'	1:A:1043:C:H5'	2.09	0.52
5:E:81:GLU:HG2	5:E:88:LYS:HE2	1.92	0.52
2:B:103:THR:OG1	2:B:176:GLU:HB2	2.10	0.52
1:A:1161:C:H2'	1:A:1162:C:H5	1.71	0.52
1:A:818:G:C3'	1:A:819:A:C5'	2.88	0.52
4:D:70:ILE:HD11	4:D:100:ARG:CZ	2.40	0.52
1:A:26:A:H61	1:A:558:G:H1'	1.75	0.52
10:J:30:SER:HA	10:J:80:LYS:HG3	1.91	0.52
1:A:1390:U:H2'	1:A:1391:U:H6	1.75	0.52
7:G:79:ARG:NH1	7:G:82:GLY:H	2.05	0.52
15:O:25:THR:HG21	15:O:70:LEU:HG	1.92	0.52
1:A:1003(A):G:C2'	1:A:1004:A:H4'	2.37	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
6:F:45:LEU:HA	6:F:58:GLY:O	2.10	0.52
1:A:1124:G:H2'	1:A:1145:C:C5	2.45	0.52
1:A:1124:G:HO2'	1:A:1145:C:N4	2.08	0.52
1:A:417:C:O2'	1:A:418:C:H5'	2.10	0.52
10:J:46:ARG:HH12	10:J:64:GLU:HB3	1.71	0.51
1:A:791:G:C6	1:A:792:A:N7	2.77	0.51
5:E:33:VAL:HG11	5:E:109:ILE:HA	1.93	0.51
13:M:102:ARG:HH11	13:M:102:ARG:HB2	1.75	0.51
22:X:2:U:H2'	22:X:3:G:C8	2.45	0.51
23:Y:34:TM2:O2'	23:Y:35:A:P	2.68	0.51
1:A:267:C:OP2	17:Q:67:LYS:HD2	2.11	0.51
9:I:107:ARG:HH11	9:I:107:ARG:HG2	1.75	0.51
1:A:1392:G:N2	1:A:1502:A:H8	2.09	0.51
1:A:1160:G:C6	1:A:1181:G:O6	2.63	0.51
19:S:3:ARG:O	19:S:4:SER:HB3	2.10	0.51
20:T:50:GLU:HB2	20:T:99:LEU:HD12	1.92	0.51
1:A:46:G:O2'	1:A:365:U:H1'	2.10	0.51
15:O:10:LYS:HD2	15:O:10:LYS:O	2.10	0.51
1:A:662:G:H2'	1:A:663:A:C8	2.45	0.51
1:A:1372:U:H2'	1:A:1373:G:O4'	2.11	0.51
1:A:1300:G:O2'	1:A:1301:U:P	2.68	0.51
5:E:101:ILE:HD12	5:E:119:LEU:HD23	1.92	0.51
16:P:43:LYS:HA	16:P:48:TRP:CB	2.40	0.51
1:A:131:C:H2'	1:A:132:C:C6	2.45	0.51
2:B:60:ASP:CB	2:B:64:ARG:HH12	2.10	0.51
3:C:100:ALA:O	3:C:101:LEU:HB2	2.10	0.51
1:A:1221:G:O2'	1:A:1222:G:H5'	2.09	0.51
5:E:126:ARG:HG3	5:E:126:ARG:NH1	2.26	0.51
1:A:1113:C:O2'	1:A:1114:C:H5'	2.08	0.51
2:B:111:ARG:HB3	2:B:149:LEU:HD11	1.91	0.51
7:G:135:VAL:O	7:G:139:GLU:HG3	2.10	0.51
1:A:1060:C:O2'	1:A:1061:G:H5'	2.10	0.51
1:A:1343:G:H1'	9:I:121:ARG:NH1	2.23	0.51
19:S:40:ILE:HG21	19:S:62:ILE:CD1	2.40	0.51
2:B:92:TYR:C	2:B:92:TYR:CD1	2.84	0.51
1:A:860:A:H2'	1:A:861:G:O4'	2.11	0.51
1:A:532:A:O2'	1:A:533:A:P	2.69	0.51
1:A:736:C:OP2	18:R:68:LYS:HE2	2.11	0.51
1:A:432:A:C2'	1:A:433:C:H5''	2.40	0.51
9:I:99:LEU:HB3	9:I:101:PHE:CE1	2.45	0.51
2:B:98:LEU:O	2:B:101:MET:HG3	2.11	0.51
2:B:178:ARG:HB3	2:B:178:ARG:NH1	2.25	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
15:O:4:THR:HB	15:O:6:GLU:OE2	2.10	0.51
1:A:818:G:H3'	1:A:819:A:H5''	1.93	0.51
1:A:1020:U:H2'	1:A:1021:G:C8	2.45	0.51
1:A:1381:U:O2'	1:A:1382:C:H5'	2.11	0.51
1:A:250:A:O5'	1:A:250:A:H8	1.92	0.51
20:T:83:ARG:O	20:T:87:LYS:HG3	2.11	0.51
7:G:15:ASP:HB3	7:G:19:GLY:N	2.26	0.51
1:A:392:G:H2'	1:A:393:A:H8	1.76	0.51
13:M:84:ILE:O	13:M:85:GLY:C	2.49	0.51
13:M:31:LYS:O	13:M:35:GLU:HG3	2.10	0.51
1:A:619:U:O2	4:D:133:VAL:HA	2.11	0.51
1:A:560:U:H5'	1:A:566:G:N2	2.25	0.51
1:A:1505:G:H3'	1:A:1505:G:C8	2.46	0.51
10:J:75:ILE:HG22	10:J:76:ASN:N	2.26	0.51
4:D:121:VAL:O	4:D:134:ASP:HA	2.11	0.51
1:A:407:G:O2'	4:D:116:GLN:HG3	2.10	0.51
22:X:1:U:H2'	22:X:2:U:H5'	1.93	0.51
23:Y:34:TM2:O2'	23:Y:35:A:O5'	2.23	0.51
1:A:1249:C:H6	1:A:1249:C:H5''	1.76	0.51
10:J:6:ILE:HG23	10:J:98:ILE:HD11	1.92	0.51
1:A:1355:G:O2'	1:A:1356:G:H5'	2.10	0.51
9:I:78:LYS:HD3	9:I:101:PHE:HD2	1.76	0.51
1:A:629:G:C3'	1:A:630:G:H5''	2.41	0.51
6:F:62:TRP:C	6:F:63:TYR:CD2	2.83	0.51
1:A:1427:U:H2'	1:A:1428:A:C8	2.45	0.51
4:D:61:LYS:HE3	4:D:207:TYR:OH	2.10	0.51
4:D:36:ARG:HB2	4:D:38:TYR:CZ	2.45	0.51
9:I:58:ARG:HD2	9:I:59:PHE:CE1	2.46	0.51
3:C:91:LEU:HD21	3:C:99:VAL:N	2.17	0.51
11:K:87:THR:HG22	11:K:88:GLY:N	2.26	0.51
12:L:47:LYS:HG2	12:L:48:PRO:HD3	1.92	0.51
1:A:1347:G:OP2	9:I:107:ARG:HG2	2.10	0.51
8:H:103:VAL:HG21	8:H:109:ILE:C	2.31	0.51
1:A:629:G:H2'	1:A:630:G:O4'	2.11	0.51
1:A:397:A:N3	1:A:397:A:H3'	2.25	0.51
6:F:82:ARG:HB2	6:F:85:VAL:CG2	2.41	0.51
12:L:75:HIS:CD2	12:L:77:LEU:H	2.27	0.51
1:A:178:C:O2'	1:A:179:A:H5'	2.11	0.51
1:A:1160:G:O6	1:A:1181:G:O6	2.28	0.50
20:T:43:LEU:CD1	20:T:55:ILE:HD12	2.40	0.50
1:A:1026:G:C3'	1:A:1027:C:H5''	2.40	0.50
1:A:1510:U:H2'	1:A:1511:G:C8	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:697:U:H2'	1:A:698:G:H5'	1.93	0.50
5:E:78:HIS:CE1	5:E:142:LEU:HD23	2.46	0.50
15:O:17:ARG:NH1	15:O:77:ARG:NH1	2.59	0.50
9:I:128:ARG:HA	13:M:126:LYS:CE	2.41	0.50
1:A:582:U:OP1	15:O:64:ARG:NH2	2.41	0.50
11:K:24:SER:HB3	11:K:27:ASN:O	2.11	0.50
2:B:211:ILE:O	2:B:215:LEU:HB2	2.11	0.50
1:A:1063:C:H2'	1:A:1064:G:C8	2.47	0.50
12:L:27:LEU:C	12:L:29:GLY:H	2.15	0.50
20:T:69:GLY:O	20:T:73:HIS:CD2	2.64	0.50
3:C:54:ARG:HG2	3:C:55:VAL:N	2.27	0.50
1:A:1014:A:C2	1:A:1219:U:H1'	2.47	0.50
3:C:47:LEU:CD1	3:C:47:LEU:H	2.24	0.50
1:A:1159:U:C4	1:A:1182:G:C6	2.98	0.50
8:H:24:THR:HG22	8:H:63:LEU:HD21	1.92	0.50
12:L:86:ARG:HG3	12:L:86:ARG:HH11	1.77	0.50
22:X:3:G:H22	23:Y:34:TM2:H3	1.59	0.50
1:A:1112:C:O2	3:C:179:ARG:HG2	2.11	0.50
19:S:28:LYS:CG	19:S:29:ARG:H	2.04	0.50
2:B:123:ALA:H	2:B:127:ILE:HG12	1.76	0.50
3:C:167:TRP:O	3:C:168:ALA:HB3	2.10	0.50
12:L:26:ALA:O	12:L:27:LEU:O	2.30	0.50
1:A:1133:G:H2'	1:A:1134:G:C8	2.41	0.50
20:T:39:LYS:HD3	20:T:55:ILE:HD13	1.93	0.50
6:F:45:LEU:HB3	6:F:59:TYR:HD1	1.77	0.50
1:A:1143:G:H2'	1:A:1144:G:C8	2.46	0.50
1:A:521:G:OP1	12:L:73:GLU:O	2.27	0.50
16:P:45:THR:HB	16:P:46:PRO:HD2	1.92	0.50
4:D:150:GLU:HG3	4:D:153:ARG:NH1	2.26	0.50
1:A:337:C:H2'	1:A:338:A:H8	1.76	0.50
20:T:39:LYS:CD	20:T:55:ILE:HD13	2.41	0.50
1:A:942:G:H2'	1:A:943:U:C6	2.45	0.50
9:I:87:GLN:O	9:I:88:TYR:C	2.49	0.50
1:A:1201:A:O2'	1:A:1202:G:OP2	2.26	0.50
1:A:1425:U:H2'	1:A:1426:C:C6	2.46	0.50
5:E:146:ALA:O	5:E:150:ARG:HB2	2.12	0.50
9:I:53:VAL:HG23	9:I:55:ALA:H	1.77	0.50
2:B:51:LEU:CD2	2:B:55:PHE:HE1	2.22	0.50
3:C:119:ARG:O	3:C:122:GLU:HB3	2.12	0.50
1:A:1513:A:H2'	1:A:1514:C:C6	2.46	0.50
2:B:116:GLU:HG2	2:B:153:ARG:HH11	1.77	0.50
12:L:8:ASN:O	12:L:12:ARG:HG3	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:91:LEU:HD23	3:C:92:ALA:N	2.27	0.50
9:I:97:LYS:HA	9:I:102:LEU:HD21	1.93	0.50
2:B:25:ASN:HD22	2:B:27:LYS:H	1.57	0.50
1:A:438:G:C4'	1:A:439:A:OP1	2.57	0.50
21:U:5:ASP:HB3	21:U:8:THR:OG1	2.12	0.50
10:J:15:THR:O	10:J:15:THR:HG22	2.12	0.50
15:O:17:ARG:HG3	15:O:17:ARG:NH1	2.25	0.50
7:G:62:PHE:HD1	7:G:124:LEU:HD21	1.76	0.50
1:A:539:A:H2'	1:A:540:G:H8	1.75	0.50
1:A:895:G:H2'	1:A:896:C:C6	2.46	0.50
17:Q:10:VAL:HG13	17:Q:19:VAL:HB	1.94	0.50
1:A:537:G:OP1	12:L:113:ARG:NH2	2.45	0.50
2:B:102:LEU:CD1	2:B:102:LEU:N	2.75	0.50
9:I:105:ASP:OD2	9:I:107:ARG:HD3	2.11	0.50
1:A:1054:C:H5	1:A:1196:U:C5	2.30	0.50
9:I:33:PHE:C	9:I:35:GLU:H	2.15	0.50
1:A:978:A:O2'	1:A:1322:C:N3	2.44	0.50
1:A:538:G:OP2	12:L:115:LYS:HD2	2.11	0.50
1:A:1223:C:P	19:S:78:ARG:NH1	2.85	0.50
1:A:861:G:O2'	1:A:862:C:H5'	2.11	0.50
4:D:83:SER:HA	4:D:89:THR:HG23	1.94	0.50
2:B:72:GLY:HA3	2:B:165:VAL:HG21	1.93	0.50
10:J:80:LYS:O	10:J:80:LYS:HD3	2.12	0.50
1:A:1399:C:C2	1:A:1502:A:N6	2.80	0.50
17:Q:96:GLN:HB3	17:Q:103:GLY:CA	2.38	0.50
1:A:1227:A:OP2	13:M:96:LEU:HD21	2.11	0.50
6:F:33:TYR:HA	6:F:71:ARG:NH1	2.27	0.50
17:Q:10:VAL:HG23	17:Q:55:ASP:O	2.12	0.50
1:A:543:C:O2'	1:A:544:G:H5'	2.12	0.50
17:Q:68:ARG:H	17:Q:70:ARG:HH11	1.56	0.49
1:A:1123:A:O3'	10:J:36:GLY:HA3	2.12	0.49
1:A:1365:G:O2'	1:A:1366:C:H5'	2.11	0.49
2:B:24:TRP:HB3	2:B:40:HIS:NE2	2.27	0.49
15:O:21:ASP:OD2	15:O:24:SER:HB3	2.11	0.49
16:P:4:ILE:HG13	16:P:64:ALA:HB1	1.93	0.49
3:C:87:LEU:C	3:C:89:GLU:H	2.16	0.49
1:A:633:G:H2'	1:A:634:C:C6	2.46	0.49
1:A:1360:A:O2'	1:A:1361:G:H5'	2.12	0.49
1:A:110:C:H2'	1:A:111:G:O4'	2.12	0.49
1:A:1154:G:O2'	1:A:1155:G:H5'	2.12	0.49
18:R:87:ARG:HG2	18:R:87:ARG:NH1	2.26	0.49
10:J:30:SER:HB2	10:J:80:LYS:O	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:192:SER:O	2:B:194:PRO:HD3	2.12	0.49
3:C:23:TYR:CD2	3:C:23:TYR:C	2.86	0.49
10:J:9:ARG:HH11	10:J:9:ARG:CB	2.24	0.49
1:A:738:C:OP2	6:F:92:LYS:NZ	2.40	0.49
1:A:141:A:O2'	1:A:142:G:H5'	2.12	0.49
2:B:16:HIS:HE1	2:B:214:ILE:HG12	1.76	0.49
1:A:478:A:O2'	1:A:479:C:H5'	2.12	0.49
3:C:62:ASP:O	3:C:99:VAL:HG12	2.13	0.49
14:N:9:LYS:HD3	14:N:9:LYS:C	2.33	0.49
1:A:947:G:H2'	1:A:948:C:O4'	2.13	0.49
9:I:36:TYR:HD2	9:I:37:PHE:CE2	2.30	0.49
4:D:64:LEU:HD23	4:D:64:LEU:O	2.12	0.49
2:B:223:ILE:HG22	2:B:226:ARG:HH21	1.78	0.49
3:C:172:ARG:HH12	3:C:174:PRO:HG3	1.77	0.49
1:A:631:G:H5'	1:A:632:A:OP1	2.12	0.49
1:A:644:G:O2'	1:A:645:C:H5'	2.12	0.49
5:E:149:GLU:O	5:E:153:LYS:HG2	2.12	0.49
1:A:1127:G:N2	1:A:1146:A:H62	2.10	0.49
1:A:1152:A:H5'	10:J:70:ARG:NH2	2.25	0.49
3:C:155:GLY:HA3	3:C:164:ARG:H	1.78	0.49
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.95	0.49
12:L:50:SER:O	12:L:51:ALA:HB2	2.13	0.49
2:B:181:PHE:CD2	8:H:70:GLN:HB3	2.48	0.49
12:L:47:LYS:CG	12:L:48:PRO:HD3	2.43	0.49
12:L:92:ASP:O	12:L:94:PRO:HD3	2.12	0.49
1:A:129(A):G:O2'	1:A:130:A:OP2	2.31	0.49
2:B:121:LEU:HA	2:B:124:SER:OG	2.13	0.49
1:A:556:C:C2'	1:A:557:G:H5'	2.41	0.49
16:P:57:ARG:NH1	16:P:79:VAL:O	2.46	0.49
1:A:919:A:O2'	1:A:920:U:H5'	2.12	0.49
1:A:1006:C:H2'	1:A:1007:C:C6	2.45	0.49
12:L:45:PRO:HD3	12:L:51:ALA:O	2.12	0.49
1:A:639:G:O2'	1:A:640:A:H5'	2.13	0.49
4:D:180:GLY:O	4:D:182:LYS:HG2	2.11	0.49
3:C:64:VAL:CG2	3:C:99:VAL:HG11	2.28	0.49
2:B:69:LEU:HB3	2:B:162:ILE:HD13	1.94	0.49
1:A:1054:C:C5	1:A:1196:U:C6	3.00	0.49
2:B:184:VAL:O	2:B:184:VAL:HG12	2.12	0.49
1:A:1313:U:H5	19:S:4:SER:HB2	1.78	0.49
8:H:51:VAL:HG11	8:H:60:ARG:NH1	2.28	0.49
3:C:83:ARG:C	3:C:85:ARG:H	2.15	0.49
1:A:1503:A:HO2'	1:A:1504:G:P	2.36	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:206:GLU:O	3:C:208:ILE:N	2.46	0.49
1:A:689:C:P	11:K:46:GLY:HA3	2.53	0.49
1:A:972:C:P	10:J:57:LYS:HE2	2.53	0.49
1:A:338:A:H2	1:A:351:G:H22	1.58	0.49
2:B:178:ARG:HB3	2:B:178:ARG:HH11	1.76	0.49
3:C:53:ALA:O	3:C:54:ARG:CB	2.60	0.49
12:L:43:VAL:HG12	12:L:44:THR:H	1.77	0.49
1:A:1424:C:O2'	1:A:1425:U:H5'	2.13	0.49
4:D:102:ASP:HB3	4:D:136:PRO:HB3	1.95	0.49
6:F:74:ASP:O	6:F:77:ARG:HB3	2.13	0.49
1:A:77:G:O2'	1:A:78:G:H5'	2.13	0.49
9:I:104:ARG:CD	9:I:105:ASP:H	2.17	0.49
1:A:130:A:C8	17:Q:63:ARG:HG3	2.48	0.49
14:N:6:LEU:C	14:N:8:GLU:H	2.16	0.49
6:F:14:LEU:HD13	6:F:19:LEU:HB2	1.95	0.49
1:A:1381:U:H2'	1:A:1382:C:H6	1.77	0.49
17:Q:59:ILE:HG23	17:Q:71:PHE:CD1	2.48	0.49
7:G:115:ARG:HB2	7:G:118:VAL:HG23	1.95	0.49
14:N:23:ARG:HH11	14:N:23:ARG:HG2	1.77	0.49
4:D:33:MET:CE	4:D:37:PRO:HA	2.43	0.49
22:X:1:U:C2'	22:X:2:U:H5'	2.43	0.49
2:B:51:LEU:O	2:B:55:PHE:HD1	1.95	0.49
1:A:1051:C:H2'	1:A:1052:U:C6	2.48	0.49
15:O:8:LYS:O	15:O:11:VAL:HB	2.13	0.49
9:I:31:GLN:HE21	9:I:35:GLU:HG3	1.77	0.49
2:B:118:LEU:HB2	2:B:142:LEU:HD13	1.95	0.49
10:J:22:LYS:HZ1	10:J:89:ASP:HA	1.78	0.49
4:D:3:ARG:HD2	4:D:118:ARG:NE	2.28	0.49
1:A:180:U:H2'	1:A:181:G:H5'	1.94	0.49
1:A:1106:G:OP1	3:C:172:ARG:HD3	2.13	0.49
6:F:36:ARG:HH21	6:F:38:GLU:HG2	1.78	0.49
1:A:92:C:O2'	1:A:93:G:H5'	2.13	0.49
1:A:1454:G:H2'	1:A:1455:G:H8	1.78	0.49
13:M:23:TYR:HB2	13:M:67:GLU:OE2	2.12	0.49
3:C:91:LEU:HD11	3:C:99:VAL:O	2.13	0.49
11:K:91:ARG:NH1	18:R:88:LYS:HE3	2.27	0.49
1:A:431:A:O2'	1:A:432:A:H5'	2.13	0.49
1:A:1052:U:H2'	1:A:1055:A:OP1	2.13	0.49
1:A:1288:A:H2'	1:A:1289:A:H8	1.77	0.49
12:L:43:VAL:CG1	12:L:44:THR:N	2.76	0.49
1:A:601:C:O2'	1:A:602:A:H5'	2.13	0.49
3:C:46:GLU:C	3:C:48:TYR:H	2.16	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:867:G:O2'	1:A:868:C:H5'	2.12	0.49
3:C:43:LEU:HD23	3:C:43:LEU:C	2.33	0.49
4:D:173:TRP:CD1	4:D:189:PRO:HG3	2.49	0.48
20:T:94:ALA:O	20:T:95:ALA:HB2	2.13	0.48
11:K:101:SER:O	11:K:103:LEU:N	2.38	0.48
1:A:127:G:HO2'	17:Q:2:PRO:N	2.11	0.48
12:L:19:ARG:HH11	12:L:19:ARG:HG3	1.78	0.48
2:B:86:GLU:C	2:B:88:ALA:H	2.17	0.48
19:S:22:LEU:HD21	19:S:28:LYS:HD2	1.94	0.48
2:B:204:ASN:HD22	2:B:206:ASP:H	1.61	0.48
2:B:230:VAL:HG12	2:B:231:GLU:N	2.28	0.48
2:B:118:LEU:HD11	2:B:141:GLU:OE2	2.12	0.48
3:C:60:ALA:O	3:C:61:ALA:CB	2.61	0.48
1:A:977:A:C2'	1:A:978:A:H5'	2.43	0.48
8:H:20:TYR:CE2	8:H:75:ARG:HD2	2.47	0.48
13:M:14:ARG:NH1	13:M:16:ASP:OD2	2.46	0.48
3:C:58:GLU:HB3	10:J:92:THR:CG2	2.29	0.48
3:C:15:THR:O	3:C:16:ARG:CB	2.58	0.48
1:A:1175:G:C2	1:A:1176:A:N9	2.81	0.48
16:P:20:VAL:CG1	16:P:32:TYR:HB2	2.44	0.48
16:P:42:ARG:O	16:P:43:LYS:C	2.52	0.48
3:C:195:VAL:O	3:C:196:LEU:HD22	2.13	0.48
14:N:46:GLU:O	14:N:49:HIS:HB2	2.13	0.48
3:C:58:GLU:O	3:C:64:VAL:HA	2.13	0.48
1:A:740:U:O2'	1:A:741:G:H5'	2.13	0.48
12:L:59:ARG:NH1	12:L:59:ARG:HB2	2.18	0.48
6:F:46:ARG:HA	6:F:47:ARG:HH21	1.79	0.48
2:B:7:VAL:CG1	2:B:221:LEU:HD23	2.40	0.48
2:B:161:ALA:HB1	2:B:185:ILE:CD1	2.42	0.48
3:C:28:GLN:O	3:C:31:HIS:HB2	2.13	0.48
1:A:633:G:H2'	1:A:634:C:H6	1.78	0.48
7:G:129:GLU:OE2	7:G:131:LYS:HE2	2.14	0.48
2:B:130:ARG:HB3	2:B:131:PRO:HD2	1.95	0.48
19:S:44:MET:O	19:S:47:HIS:HB2	2.13	0.48
12:L:60:LEU:HD21	12:L:66:VAL:HG22	1.95	0.48
18:R:73:ALA:HB3	18:R:79:LEU:HD12	1.95	0.48
18:R:74:ARG:HB3	18:R:81:PHE:CE1	2.48	0.48
17:Q:68:ARG:HH11	17:Q:68:ARG:HG2	1.79	0.48
1:A:1129:C:OP1	9:I:62:TYR:CE2	2.66	0.48
1:A:409:G:H1	1:A:433:C:N4	2.11	0.48
13:M:40:ASN:HB3	13:M:43:THR:CG2	2.41	0.48
12:L:37:CYS:O	12:L:79:GLU:O	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:954:G:H2'	1:A:955:U:C6	2.49	0.48
4:D:17:VAL:CG1	4:D:18:LYS:N	2.76	0.48
6:F:101:ALA:CB	18:R:28:GLU:HB2	2.41	0.48
1:A:1168:A:C6	1:A:1169:A:C6	3.01	0.48
1:A:1014:A:H2'	1:A:1015:A:C8	2.48	0.48
1:A:923:A:OP1	5:E:21:ALA:HB2	2.12	0.48
16:P:26:ARG:CD	16:P:31:LYS:O	2.62	0.48
16:P:81:ARG:HB2	16:P:81:ARG:NH1	2.29	0.48
1:A:1191:A:C3'	1:A:1192:C:OP2	2.51	0.48
1:A:1127:G:H2'	1:A:1128:C:C6	2.48	0.48
10:J:38:ILE:HB	10:J:71:LEU:CB	2.43	0.48
2:B:98:LEU:N	2:B:98:LEU:HD23	2.29	0.48
10:J:9:ARG:CB	10:J:9:ARG:NH1	2.77	0.48
1:A:1216:G:H5''	14:N:5:ALA:HB2	1.96	0.48
4:D:8:VAL:HB	4:D:21:LEU:CD1	2.43	0.48
2:B:116:GLU:HG2	2:B:153:ARG:NH1	2.28	0.48
24:Z:1:PAR:H43	24:Z:1:PAR:H642	1.95	0.48
3:C:63:ASN:HA	3:C:99:VAL:HG12	1.94	0.48
1:A:1371:G:OP1	9:I:11:LYS:O	2.32	0.48
1:A:975:A:H4'	1:A:976:G:C5'	2.37	0.48
1:A:1056:U:H5'	3:C:163:ALA:CB	2.44	0.48
3:C:134:ILE:CG2	3:C:168:ALA:HB3	2.44	0.48
1:A:1343:G:C1'	9:I:121:ARG:HH12	2.22	0.48
1:A:8:A:N6	4:D:205:GLU:O	2.47	0.48
6:F:45:LEU:HA	6:F:59:TYR:HA	1.96	0.48
1:A:325:A:H2'	1:A:326:G:O4'	2.14	0.48
11:K:99:GLN:CG	11:K:105:VAL:HG21	2.43	0.48
18:R:68:LYS:O	18:R:72:ARG:HG3	2.14	0.48
1:A:866:C:H2'	1:A:867:G:O4'	2.13	0.48
5:E:24:ARG:HH11	5:E:24:ARG:HG2	1.78	0.48
1:A:1251:A:H1'	1:A:1369:C:HO2'	1.78	0.48
10:J:50:ILE:HA	10:J:60:ARG:HA	1.94	0.48
9:I:53:VAL:CG1	9:I:96:LEU:HD11	2.44	0.48
1:A:1227:A:H3'	1:A:1227:A:H8	1.78	0.48
1:A:16:A:C2'	1:A:17:U:H5'	2.44	0.48
1:A:1216:G:O2'	1:A:1217:C:H5'	2.13	0.48
3:C:95:THR:O	3:C:97:LYS:N	2.46	0.48
20:T:86:ARG:NH1	20:T:86:ARG:HG3	2.28	0.48
1:A:1272:G:O2'	1:A:1273:G:H5'	2.14	0.48
1:A:1521:G:H2'	1:A:1522:U:C6	2.49	0.48
1:A:123:C:OP1	1:A:312:C:H5'	2.14	0.48
1:A:1532:U:O2'	1:A:1533:C:C6	2.66	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
22:X:3:G:H2'	22:X:4:A:C5'	2.43	0.48
10:J:7:LYS:HD2	10:J:71:LEU:CD2	2.44	0.48
1:A:409:G:H1	1:A:433:C:H42	1.62	0.48
2:B:97:TRP:CH2	2:B:176:GLU:OE2	2.66	0.48
1:A:1054:C:C2'	1:A:1055:A:H5''	2.44	0.48
1:A:343:U:H2'	1:A:345:C:C5	2.49	0.48
4:D:70:ILE:HD11	4:D:100:ARG:NH2	2.29	0.48
6:F:67:MET:SD	6:F:75:LEU:HD12	2.54	0.48
1:A:1376:U:H2'	1:A:1377:A:C8	2.49	0.48
1:A:723:U:H2'	1:A:723:U:O2	2.12	0.48
1:A:1306:A:H61	1:A:1331:G:H1'	1.79	0.48
1:A:1127:G:H21	1:A:1146:A:H61	1.59	0.48
9:I:9:ARG:CG	9:I:14:VAL:HG12	2.43	0.48
2:B:18:GLY:CA	2:B:41:ILE:HA	2.35	0.48
1:A:513:C:H2'	1:A:514:C:C6	2.49	0.48
1:A:1244:C:O2'	1:A:1245:A:H5'	2.14	0.48
3:C:56:ASP:O	3:C:57:ILE:HG13	2.14	0.48
5:E:81:GLU:HG3	5:E:90:VAL:HG22	1.96	0.47
1:A:974:A:P	14:N:41:ARG:HH12	2.35	0.47
3:C:154:SER:HB3	3:C:197:GLY:H	1.79	0.47
8:H:88:LYS:O	8:H:89:PRO:C	2.52	0.47
7:G:15:ASP:HB2	7:G:20:ASP:O	2.14	0.47
19:S:55:LYS:HG2	19:S:56:GLN:HG3	1.96	0.47
4:D:63:LYS:HD2	4:D:198:VAL:HG22	1.96	0.47
1:A:1007:C:O2'	1:A:1008:C:H5'	2.14	0.47
8:H:119:LEU:CD1	8:H:124:ALA:HA	2.44	0.47
1:A:961:U:O2'	1:A:962:C:H5'	2.14	0.47
1:A:145:G:O2'	1:A:146:G:H5'	2.14	0.47
9:I:65:VAL:HG11	9:I:77:ILE:HD11	1.96	0.47
10:J:63:PHE:HE1	14:N:45:ARG:HG3	1.79	0.47
1:A:1407:C:O2'	1:A:1408:A:H5'	2.14	0.47
1:A:432:A:H2'	1:A:433:C:H5''	1.96	0.47
10:J:49:VAL:O	10:J:60:ARG:O	2.32	0.47
10:J:48:THR:HG1	10:J:62:HIS:CD2	2.31	0.47
2:B:55:PHE:CE2	2:B:218:ALA:HA	2.49	0.47
12:L:83:VAL:HG23	12:L:100:ILE:HG23	1.95	0.47
16:P:3:LYS:O	16:P:21:VAL:HA	2.14	0.47
1:A:1228:C:H4'	13:M:116:THR:HA	1.96	0.47
1:A:1113:C:O5'	1:A:1113:C:H6	1.97	0.47
13:M:85:GLY:O	13:M:86:CYS:O	2.33	0.47
5:E:57:LYS:HG2	5:E:61:TYR:CE2	2.49	0.47
1:A:1470:G:O2'	1:A:1471:G:H5'	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
11:K:115:PRO:C	11:K:117:ASN:H	2.18	0.47
10:J:30:SER:CB	10:J:80:LYS:HG3	2.44	0.47
10:J:80:LYS:O	10:J:83:GLU:HB2	2.13	0.47
2:B:15:VAL:HB	2:B:210:SER:HB2	1.96	0.47
4:D:20:TYR:CD2	4:D:26:CYS:HB3	2.49	0.47
1:A:848:C:H2'	1:A:849:C:H6	1.79	0.47
3:C:31:HIS:C	3:C:33:LEU:H	2.17	0.47
1:A:101:A:O2'	1:A:102:G:H5'	2.14	0.47
1:A:879:C:O2'	1:A:880:C:H5'	2.14	0.47
3:C:6:HIS:NE2	3:C:8:ILE:HD12	2.30	0.47
1:A:1347:G:C6	9:I:107:ARG:NH2	2.82	0.47
3:C:52:LEU:HD23	3:C:52:LEU:N	2.29	0.47
3:C:54:ARG:O	3:C:55:VAL:HG23	2.14	0.47
8:H:60:ARG:NH1	8:H:60:ARG:HG3	2.28	0.47
3:C:47:LEU:N	3:C:47:LEU:CD1	2.77	0.47
13:M:102:ARG:NH1	13:M:102:ARG:HB2	2.30	0.47
12:L:19:ARG:NH1	12:L:19:ARG:HG3	2.30	0.47
7:G:137:LYS:O	7:G:141:VAL:HG12	2.14	0.47
14:N:44:LEU:C	14:N:44:LEU:HD12	2.34	0.47
1:A:1250:A:O3'	9:I:67:GLY:HA2	2.15	0.47
5:E:82:VAL:HG11	5:E:137:GLU:HB3	1.96	0.47
1:A:586:C:H5''	8:H:90:GLY:CA	2.45	0.47
1:A:1161:C:H2'	1:A:1162:C:C6	2.50	0.47
3:C:112:SER:OG	3:C:115:LEU:HD12	2.15	0.47
4:D:62:GLN:HA	4:D:62:GLN:NE2	2.29	0.47
1:A:167:G:O2'	1:A:168:G:H5'	2.14	0.47
3:C:120:VAL:O	3:C:124:ILE:HG13	2.14	0.47
1:A:545:C:H5''	4:D:72:GLU:HG2	1.97	0.47
20:T:16:HIS:CE1	20:T:20:LEU:HD11	2.50	0.47
1:A:1116:C:H2'	1:A:1117:G:C5'	2.33	0.47
10:J:71:LEU:O	10:J:72:VAL:HB	2.14	0.47
1:A:1149:C:O2'	1:A:1280:A:N1	2.45	0.47
7:G:145:ALA:O	7:G:147:ALA:N	2.45	0.47
1:A:1505:G:H2'	1:A:1541:U:OP2	2.14	0.47
1:A:1095:U:H2'	1:A:1096:C:H6	1.73	0.47
1:A:327:A:O3'	1:A:328:C:H4'	2.15	0.47
5:E:7:GLU:OE2	5:E:37:ARG:NE	2.45	0.47
1:A:1005:A:C2'	1:A:1006:C:H5'	2.44	0.47
1:A:1038:C:H2'	1:A:1039:C:C6	2.46	0.47
1:A:96:G:O2'	1:A:97:G:H5'	2.15	0.47
7:G:45:ASP:O	7:G:49:ILE:HG13	2.15	0.47
1:A:1112:C:N3	3:C:178:LEU:HD23	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1249:C:H2'	1:A:1250:A:H5'	1.95	0.47
1:A:1063:C:H2'	1:A:1064:G:H8	1.77	0.47
15:O:87:ILE:CG2	15:O:88:ARG:H	2.15	0.47
2:B:27:LYS:HD2	2:B:193:ASP:OD2	2.15	0.47
6:F:2:ARG:NE	6:F:69:GLU:CG	2.74	0.47
15:O:39:LEU:CD1	15:O:56:LEU:HB2	2.45	0.47
10:J:31:GLY:HA3	10:J:78:ASN:ND2	2.30	0.47
20:T:57:ARG:HE	20:T:102:GLY:HA3	1.79	0.47
12:L:89:ARG:NH2	12:L:91:LYS:HG2	2.28	0.47
12:L:77:LEU:HD21	12:L:107:ALA:HB2	1.97	0.47
1:A:780:A:C2	1:A:801:U:C5	3.03	0.47
8:H:10:LEU:HD22	8:H:83:ILE:HD11	1.97	0.47
11:K:48:ILE:HD13	11:K:48:ILE:N	2.30	0.47
2:B:115:LEU:HD21	2:B:153:ARG:NH2	2.30	0.47
1:A:279:A:H5''	1:A:281:G:O4'	2.15	0.47
4:D:157:LEU:HD11	4:D:161:ASN:HD21	1.80	0.47
16:P:1:MET:O	16:P:24:ALA:HB2	2.14	0.47
1:A:309:G:H1'	1:A:608:A:C2	2.49	0.47
4:D:19:LEU:HD22	4:D:67:ILE:HG12	1.97	0.47
17:Q:67:LYS:CA	17:Q:70:ARG:NH1	2.75	0.47
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.97	0.47
10:J:57:LYS:HD2	10:J:60:ARG:HH21	1.80	0.47
10:J:30:SER:HB2	10:J:80:LYS:HG3	1.97	0.47
2:B:10:LEU:O	2:B:12:GLU:N	2.46	0.47
3:C:155:GLY:O	3:C:156:ARG:CB	2.63	0.47
7:G:32:ARG:O	7:G:33:ASP:HB2	2.15	0.47
6:F:62:TRP:CG	18:R:35:ARG:NH1	2.82	0.47
1:A:1038:C:C6	1:A:1039:C:H5	2.33	0.47
12:L:77:LEU:HD21	12:L:107:ALA:CB	2.44	0.47
1:A:1429:C:O2'	1:A:1430:C:H5'	2.15	0.47
7:G:80:VAL:O	7:G:80:VAL:HG12	2.15	0.47
16:P:81:ARG:HG3	16:P:83:GLU:HG2	1.97	0.47
1:A:463:A:H4'	16:P:80:PHE:O	2.15	0.47
17:Q:81:ARG:O	17:Q:81:ARG:HG3	2.15	0.47
5:E:79:GLU:CD	5:E:79:GLU:H	2.19	0.47
19:S:15:LEU:HD12	19:S:16:LEU:N	2.30	0.47
1:A:458:C:H2'	1:A:459:G:H8	1.80	0.47
12:L:52:LEU:O	12:L:54:LYS:HD2	2.15	0.47
8:H:20:TYR:HE2	8:H:75:ARG:HD2	1.78	0.47
14:N:44:LEU:O	14:N:44:LEU:HD12	2.15	0.47
5:E:45:PHE:CE2	5:E:47:LYS:HD2	2.50	0.47
20:T:10:LEU:O	20:T:12:ALA:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:105:G:H2'	1:A:106:C:C6	2.49	0.47
1:A:1320:C:O2'	1:A:1321:C:H5'	2.15	0.47
10:J:6:ILE:HD13	10:J:73:ASP:N	2.28	0.47
9:I:100:GLY:HA2	9:I:102:LEU:HD11	1.97	0.47
9:I:97:LYS:N	9:I:98:PRO:CD	2.77	0.47
19:S:15:LEU:HD12	19:S:16:LEU:H	1.80	0.47
3:C:19:GLU:O	3:C:40:ARG:NH2	2.48	0.47
9:I:46:ALA:HB2	9:I:74:ILE:HG23	1.97	0.47
1:A:921:U:O2	5:E:19:MET:HB2	2.15	0.47
9:I:127:LYS:O	9:I:128:ARG:CB	2.63	0.47
8:H:4:ASP:OD1	8:H:85:ARG:NH1	2.48	0.47
14:N:53:LEU:HB3	14:N:56:VAL:HG21	1.96	0.47
1:A:1157:A:H4'	1:A:1158:C:O5'	2.15	0.46
12:L:46:LYS:O	12:L:47:LYS:C	2.54	0.46
6:F:46:ARG:HH11	6:F:46:ARG:CB	2.27	0.46
3:C:113:ALA:N	3:C:114:PRO:CD	2.78	0.46
1:A:16:A:H2'	1:A:17:U:H5'	1.97	0.46
7:G:16:LEU:HD22	7:G:16:LEU:N	2.30	0.46
11:K:12:ARG:O	11:K:12:ARG:HD2	2.14	0.46
18:R:36:ASN:ND2	18:R:38:GLU:HG2	2.30	0.46
1:A:406:G:H5''	4:D:5:ILE:HG23	1.96	0.46
7:G:58:PRO:HG2	7:G:59:LEU:H	1.80	0.46
1:A:1182:G:O2'	1:A:1183:A:P	2.72	0.46
8:H:11:THR:HA	8:H:14:ARG:NH1	2.30	0.46
3:C:64:VAL:HB	3:C:99:VAL:CG2	2.30	0.46
10:J:40:LEU:HD11	10:J:71:LEU:HD23	1.97	0.46
2:B:77:ALA:HB1	2:B:211:ILE:HG21	1.97	0.46
1:A:1060:C:H2'	1:A:1061:G:C8	2.47	0.46
2:B:196:LEU:N	2:B:196:LEU:CD1	2.77	0.46
14:N:9:LYS:HE3	14:N:21:TYR:O	2.16	0.46
1:A:1300:G:O2'	1:A:1301:U:H6	1.98	0.46
1:A:1498:U:C4'	1:A:1519:A:H2	2.29	0.46
12:L:38:THR:HB	12:L:57:LYS:HB3	1.96	0.46
7:G:120:ILE:H	7:G:120:ILE:CD1	2.26	0.46
7:G:62:PHE:HA	7:G:124:LEU:HD22	1.96	0.46
19:S:40:ILE:HG21	19:S:62:ILE:HD13	1.96	0.46
18:R:42:ARG:HH11	18:R:42:ARG:HB3	1.79	0.46
2:B:223:ILE:CG2	2:B:226:ARG:HH21	2.28	0.46
1:A:814:A:H2'	1:A:816:A:H5''	1.96	0.46
8:H:138:TRP:OXT	8:H:138:TRP:HE3	1.98	0.46
1:A:1116:C:C3'	1:A:1117:G:H5''	2.45	0.46
1:A:1129:C:O2'	1:A:1130:A:P	2.74	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:38:ILE:HB	10:J:71:LEU:HB3	1.96	0.46
4:D:168:ARG:CB	4:D:168:ARG:HH11	2.13	0.46
10:J:57:LYS:O	10:J:57:LYS:HD2	2.14	0.46
9:I:50:LEU:O	9:I:53:VAL:HG22	2.15	0.46
1:A:339:C:H2'	1:A:340:U:C6	2.49	0.46
20:T:100:ILE:O	20:T:101:GLY:C	2.54	0.46
1:A:965:A:C2	1:A:969:A:C2	3.04	0.46
4:D:5:ILE:HG22	4:D:5:ILE:O	2.13	0.46
8:H:119:LEU:HD23	8:H:119:LEU:N	2.31	0.46
15:O:5:LYS:N	15:O:5:LYS:HD2	2.30	0.46
13:M:84:ILE:O	13:M:84:ILE:HG13	2.15	0.46
16:P:63:GLY:O	16:P:64:ALA:C	2.54	0.46
1:A:1065:U:H5''	1:A:1190:G:H21	1.77	0.46
22:X:2:U:H2'	22:X:3:G:H8	1.78	0.46
1:A:1370:G:C2	1:A:1371:G:C8	3.04	0.46
1:A:1075:C:OP1	2:B:179:LYS:NZ	2.49	0.46
13:M:37:THR:HG22	13:M:39:ILE:HG13	1.96	0.46
3:C:119:ARG:NE	3:C:140:ARG:HH12	2.12	0.46
10:J:3:LYS:HB3	10:J:75:ILE:HA	1.96	0.46
1:A:1120:G:O2'	1:A:1121:U:H5'	2.15	0.46
1:A:912:C:O2'	1:A:913:A:H5'	2.14	0.46
2:B:181:PHE:HD2	8:H:70:GLN:HB3	1.81	0.46
1:A:147:G:O2'	1:A:148:G:H5'	2.15	0.46
1:A:52:G:O2'	1:A:53:A:H5'	2.15	0.46
7:G:138:LYS:C	7:G:138:LYS:HD3	2.36	0.46
1:A:1074:G:O3'	2:B:103:THR:CG2	2.63	0.46
9:I:100:GLY:HA2	9:I:102:LEU:CD1	2.46	0.46
2:B:19:HIS:O	2:B:20:GLU:O	2.34	0.46
9:I:92:TYR:O	9:I:96:LEU:HD13	2.15	0.46
12:L:24:VAL:CG1	12:L:26:ALA:HB2	2.43	0.46
1:A:1227:A:H3'	1:A:1227:A:C8	2.51	0.46
11:K:32:ILE:HD13	11:K:68:ALA:HB1	1.96	0.46
8:H:86:ILE:HG12	8:H:135:CYS:HA	1.97	0.46
17:Q:51:TYR:C	17:Q:52:LYS:HD2	2.36	0.46
9:I:42:ARG:NH2	9:I:71:SER:O	2.49	0.46
1:A:1286:A:C2	21:U:18:TYR:OH	2.69	0.46
1:A:414:A:H2'	1:A:415:A:C8	2.51	0.46
1:A:1504:G:H3'	1:A:1504:G:OP2	2.15	0.46
7:G:115:ARG:HB2	7:G:118:VAL:CG2	2.45	0.46
1:A:986:A:H2'	1:A:987:G:O4'	2.16	0.46
12:L:85:ILE:HG23	12:L:98:TYR:HB3	1.96	0.46
1:A:945:G:H2'	1:A:945:G:N3	2.30	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:64:VAL:N	3:C:99:VAL:HB	2.29	0.46
1:A:1130:A:C2	1:A:1146:A:N3	2.83	0.46
4:D:163:GLU:C	4:D:165:MET:H	2.19	0.46
2:B:76:GLN:HG3	2:B:206:ASP:OD1	2.16	0.46
9:I:48:GLU:N	9:I:49:PRO:CD	2.79	0.46
1:A:1505:G:H8	1:A:1505:G:H3'	1.81	0.46
1:A:261:U:OP1	20:T:79:ARG:NH2	2.49	0.46
5:E:82:VAL:CG2	5:E:138:ALA:HA	2.41	0.46
4:D:17:VAL:HG12	4:D:18:LYS:N	2.30	0.46
6:F:13:ASN:O	6:F:14:LEU:O	2.33	0.46
6:F:21:LEU:O	6:F:24:GLU:HB3	2.16	0.46
1:A:834:C:H2'	1:A:835:U:C6	2.50	0.46
1:A:1321:C:H5''	13:M:87:TYR:CE2	2.51	0.46
1:A:882:C:O2'	1:A:883:C:H5'	2.16	0.46
1:A:200:G:H2'	1:A:201:C:O4'	2.16	0.46
3:C:5:ILE:H	3:C:5:ILE:HD12	1.80	0.46
1:A:1127:G:H4'	9:I:66:ARG:NH1	2.30	0.46
10:J:6:ILE:HG23	10:J:98:ILE:CD1	2.46	0.46
10:J:98:ILE:CG2	10:J:99:LYS:N	2.78	0.46
19:S:12:ASP:O	19:S:15:LEU:HD12	2.15	0.46
5:E:51:VAL:HB	5:E:52:PRO:CD	2.41	0.46
1:A:954:G:H5''	13:M:120:LYS:HD3	1.97	0.46
1:A:369:C:O2'	1:A:370:C:H5'	2.16	0.46
3:C:36:ASP:OD2	3:C:36:ASP:N	2.42	0.46
1:A:994:A:H2'	1:A:994:A:N3	2.31	0.46
1:A:627:G:H2'	1:A:628:G:H8	1.81	0.46
1:A:1130:A:OP2	1:A:1130:A:H3'	2.16	0.46
2:B:24:TRP:HZ3	2:B:29:ALA:HB2	1.81	0.46
2:B:132:LYS:C	2:B:134:GLU:N	2.67	0.46
10:J:75:ILE:O	10:J:76:ASN:HB2	2.16	0.46
1:A:701:C:O2'	1:A:702:A:OP2	2.27	0.46
12:L:68:ALA:HB3	12:L:100:ILE:HD11	1.98	0.46
16:P:20:VAL:CG1	16:P:32:TYR:CB	2.93	0.46
1:A:961:U:H2'	1:A:962:C:H5'	1.98	0.46
1:A:551:U:H2'	1:A:552:U:C6	2.51	0.46
3:C:3:ASN:O	3:C:4:LYS:CB	2.64	0.46
1:A:1154:G:H2'	1:A:1155:G:H8	1.81	0.46
12:L:46:LYS:HG3	12:L:47:LYS:N	2.31	0.46
10:J:60:ARG:HD3	10:J:60:ARG:HA	1.89	0.46
14:N:9:LYS:C	14:N:11:LYS:H	2.20	0.46
1:A:1053:G:C3'	1:A:1054:C:C5'	2.94	0.46
2:B:178:ARG:HH22	8:H:68:ARG:HH22	1.61	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1227:A:C4	19:S:81:ARG:NH1	2.83	0.46
12:L:11:VAL:HG13	17:Q:29:HIS:CD2	2.50	0.46
11:K:124:LYS:HD2	11:K:125:PHE:CZ	2.50	0.46
19:S:67:VAL:HG12	19:S:68:GLY:N	2.30	0.46
1:A:459:G:C6	1:A:461:C:H5''	2.50	0.46
4:D:192:GLU:HA	4:D:192:GLU:OE1	2.15	0.46
2:B:38:GLY:C	2:B:39:ILE:HG13	2.36	0.45
10:J:16:LEU:HD21	10:J:94:VAL:HG13	1.97	0.45
21:U:6:ARG:CD	21:U:15:ARG:NH1	2.79	0.45
4:D:151:LYS:N	4:D:151:LYS:HD2	2.31	0.45
1:A:1423:G:O2'	1:A:1424:C:H5'	2.16	0.45
1:A:1427:U:H2'	1:A:1428:A:H8	1.81	0.45
3:C:87:LEU:C	3:C:89:GLU:N	2.69	0.45
1:A:1405:G:O2'	1:A:1406:U:H5'	2.16	0.45
8:H:14:ARG:O	8:H:18:ARG:HD3	2.16	0.45
1:A:103:C:P	20:T:17:ARG:HH11	2.40	0.45
1:A:999:C:H2'	1:A:1000:U:C6	2.50	0.45
1:A:1018:C:H6	1:A:1018:C:O5'	1.99	0.45
1:A:1533:C:H2'	1:A:1534:A:C5'	2.42	0.45
2:B:208:ILE:HD12	2:B:208:ILE:N	2.06	0.45
8:H:91:ARG:HG3	12:L:7:ILE:HG13	1.99	0.45
1:A:383:A:C2'	1:A:384:G:H5'	2.46	0.45
1:A:1313:U:C5	19:S:4:SER:HB2	2.52	0.45
6:F:48:LEU:HD13	6:F:52:ILE:CD1	2.44	0.45
11:K:43:SER:O	11:K:44:SER:HB3	2.16	0.45
1:A:831:U:H2'	1:A:832:C:C6	2.51	0.45
11:K:32:ILE:HD12	11:K:32:ILE:N	2.31	0.45
3:C:32:LEU:HD22	3:C:59:ARG:NH1	2.31	0.45
2:B:83:MET:HA	2:B:83:MET:HE2	1.97	0.45
10:J:30:SER:CA	10:J:80:LYS:HG3	2.46	0.45
14:N:25:VAL:HG12	14:N:38:GLY:O	2.15	0.45
10:J:23:ILE:CD1	10:J:23:ILE:N	2.78	0.45
5:E:76:ILE:HG13	5:E:142:LEU:HD13	1.98	0.45
3:C:83:ARG:C	3:C:85:ARG:N	2.70	0.45
11:K:29:ILE:HG22	11:K:44:SER:HB2	1.98	0.45
12:L:119:LYS:O	12:L:120:TYR:CB	2.64	0.45
1:A:7:G:H21	5:E:121:LYS:HG2	1.81	0.45
1:A:1152:A:C5'	10:J:13:HIS:HD2	2.16	0.45
5:E:51:VAL:O	5:E:55:VAL:HG23	2.16	0.45
1:A:1288:A:H1'	1:A:1352:C:O2'	2.17	0.45
5:E:143:ARG:HA	5:E:143:ARG:HD3	1.57	0.45
1:A:1313:U:OP2	19:S:6:LYS:HA	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1141:C:O2'	1:A:1142:G:H5'	2.16	0.45
1:A:1486:G:H2'	1:A:1487:G:O4'	2.16	0.45
1:A:1090:U:H2'	1:A:1091:U:H6	1.81	0.45
2:B:157:ARG:HH11	2:B:157:ARG:HG3	1.80	0.45
1:A:443:C:H2'	1:A:444:C:H6	1.82	0.45
1:A:1544:U:O3'	22:X:1:U:C5'	2.65	0.45
4:D:10:ARG:CG	4:D:10:ARG:HH11	2.30	0.45
1:A:630:G:H8	1:A:630:G:H5'	1.82	0.45
15:O:7:GLU:O	15:O:11:VAL:HG23	2.16	0.45
5:E:40:ARG:HH11	5:E:40:ARG:HG2	1.82	0.45
1:A:792:A:H1'	1:A:794:A:N7	2.32	0.45
1:A:979:C:H2'	1:A:980:C:H5'	1.98	0.45
1:A:1030(C):G:H2'	1:A:1030(D):A:C8	2.52	0.45
1:A:67:C:O2'	1:A:171:A:H1'	2.16	0.45
1:A:1125:U:H5'	1:A:1126:U:C5	2.51	0.45
1:A:1060:C:H5''	10:J:51:ARG:HB3	1.98	0.45
1:A:718:G:H5'	11:K:117:ASN:ND2	2.20	0.45
2:B:184:VAL:N	2:B:198:ASP:OD2	2.50	0.45
1:A:1226:C:N4	13:M:104:ARG:HG3	2.32	0.45
5:E:77:PRO:HG2	5:E:142:LEU:HD22	1.98	0.45
4:D:64:LEU:HD22	4:D:75:PHE:CZ	2.51	0.45
1:A:1437:C:H2'	1:A:1438:G:H8	1.82	0.45
16:P:20:VAL:HG13	16:P:21:VAL:N	2.32	0.45
2:B:92:TYR:C	2:B:92:TYR:HD1	2.19	0.45
1:A:106:C:O2	1:A:379:C:H4'	2.17	0.45
3:C:5:ILE:N	3:C:5:ILE:HD12	2.32	0.45
1:A:1296:C:H4'	1:A:1302:U:C5	2.52	0.45
7:G:99:LEU:HD22	7:G:103:TRP:CZ2	2.52	0.45
1:A:1394:A:C5	1:A:1501:C:H4'	2.51	0.45
1:A:960:U:O2	1:A:960:U:H2'	2.16	0.45
9:I:79:LEU:HD21	9:I:102:LEU:O	2.17	0.45
5:E:144:THR:CG2	5:E:145:LYS:N	2.79	0.45
1:A:129(A):G:O2'	1:A:190(E):U:C6	2.70	0.45
13:M:33:ALA:O	13:M:37:THR:HB	2.17	0.45
20:T:45:GLN:NE2	20:T:45:GLN:O	2.50	0.45
16:P:43:LYS:HB3	16:P:48:TRP:CD2	2.51	0.45
16:P:4:ILE:HG23	16:P:36:ILE:HD11	1.99	0.45
4:D:102:ASP:HB3	4:D:136:PRO:HA	1.99	0.45
1:A:627:G:H2'	1:A:628:G:C8	2.51	0.45
17:Q:17:LYS:HA	17:Q:46:ASP:O	2.17	0.45
1:A:1431:C:C2'	1:A:1432:G:H5'	2.47	0.45
1:A:1251:A:H2'	1:A:1252:A:C8	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:579:G:C5'	1:A:728:A:H1'	2.30	0.45
5:E:83:GLU:HG3	5:E:88:LYS:HG3	1.99	0.45
2:B:69:LEU:HD22	2:B:155:LEU:CD1	2.45	0.45
2:B:48:MET:O	2:B:51:LEU:HB2	2.16	0.45
20:T:49:ALA:O	20:T:53:LEU:HD13	2.17	0.45
11:K:14:VAL:O	11:K:15:ALA:HB3	2.17	0.45
1:A:1202:G:O2'	1:A:1203:C:H5'	2.17	0.45
5:E:28:PHE:O	5:E:47:LYS:HA	2.17	0.45
6:F:30:LEU:HB3	6:F:35:ALA:HB3	1.98	0.45
19:S:43:GLU:CD	19:S:43:GLU:H	2.20	0.45
4:D:108:LEU:HD21	4:D:174:LEU:HD13	1.99	0.45
1:A:1191:A:H3'	1:A:1192:C:OP2	2.17	0.45
3:C:14:ILE:O	3:C:15:THR:C	2.55	0.45
1:A:266:G:O2'	1:A:267:C:OP2	2.32	0.45
2:B:60:ASP:C	2:B:64:ARG:NH1	2.70	0.45
10:J:46:ARG:HG2	10:J:46:ARG:NH1	2.29	0.45
2:B:132:LYS:C	2:B:134:GLU:H	2.19	0.45
1:A:250:A:O4'	1:A:252:U:C6	2.70	0.45
1:A:953:G:H2'	1:A:954:G:O4'	2.17	0.45
17:Q:40:LYS:HE3	17:Q:42:TYR:CZ	2.51	0.45
4:D:146:ILE:N	4:D:146:ILE:CD1	2.78	0.45
1:A:491:G:H2'	1:A:492:G:C8	2.50	0.45
1:A:1147:C:H4'	9:I:5:TYR:CE2	2.52	0.45
4:D:58:LEU:CD2	4:D:62:GLN:HG2	2.47	0.45
11:K:21:ILE:HD12	11:K:95:ILE:HD13	1.99	0.45
6:F:91:VAL:HG11	18:R:72:ARG:NH1	2.32	0.45
3:C:195:VAL:C	3:C:196:LEU:HD22	2.37	0.45
1:A:335:C:H2'	1:A:336:C:C6	2.51	0.45
1:A:445:G:O2'	1:A:446:G:H5'	2.17	0.45
1:A:594:G:O2'	1:A:595:G:H5'	2.17	0.45
1:A:659:U:O2'	1:A:660:G:H5'	2.17	0.45
15:O:2:PRO:O	15:O:3:ILE:HG13	2.16	0.45
5:E:43:LEU:HD23	5:E:43:LEU:HA	1.83	0.45
7:G:12:LEU:H	7:G:12:LEU:HD12	1.82	0.45
2:B:24:TRP:CG	2:B:25:ASN:N	2.85	0.45
1:A:1055:A:C2	1:A:1056:U:H1'	2.52	0.45
10:J:3:LYS:CB	10:J:75:ILE:HA	2.46	0.45
6:F:26:ILE:HG21	6:F:63:TYR:OH	2.16	0.45
11:K:15:ALA:CA	11:K:77:MET:HA	2.47	0.45
5:E:31:LEU:HD23	5:E:31:LEU:HA	1.78	0.45
1:A:1232:U:H5''	9:I:124:GLN:O	2.17	0.45
8:H:17:THR:HG22	8:H:63:LEU:HG	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1179:A:H2'	1:A:1180:A:O4'	2.16	0.44
3:C:9:GLY:HA2	3:C:12:LEU:HG	1.99	0.44
1:A:1129:C:OP1	9:I:62:TYR:CZ	2.69	0.44
1:A:1061:G:H2'	1:A:1062:U:C6	2.53	0.44
2:B:69:LEU:HD12	2:B:70:PHE:N	2.32	0.44
19:S:23:ASN:HA	19:S:26:GLY:O	2.17	0.44
2:B:7:VAL:HG11	2:B:221:LEU:CD2	2.44	0.44
13:M:6:GLY:O	13:M:8:GLU:HG2	2.16	0.44
12:L:77:LEU:HD21	12:L:107:ALA:CA	2.46	0.44
17:Q:59:ILE:CG2	17:Q:71:PHE:CD1	3.00	0.44
1:A:1178:G:N3	1:A:1180:A:N7	2.65	0.44
1:A:1129:C:O2'	1:A:1130:A:OP2	2.34	0.44
1:A:974:A:P	14:N:29:ARG:HH22	2.39	0.44
3:C:70:VAL:HG12	3:C:71:ALA:H	1.82	0.44
2:B:126:GLU:HG2	2:B:129:GLU:OE1	2.17	0.44
1:A:1181:G:O2'	1:A:1184:G:H5'	2.16	0.44
9:I:37:PHE:CD1	9:I:43:ALA:HB1	2.52	0.44
6:F:63:TYR:CD2	6:F:63:TYR:N	2.85	0.44
8:H:60:ARG:CG	8:H:60:ARG:NH1	2.80	0.44
13:M:19:LEU:C	13:M:22:ILE:HD13	2.36	0.44
1:A:45:U:H2'	1:A:46:G:H8	1.80	0.44
2:B:92:TYR:CD1	2:B:151:GLY:HA3	2.52	0.44
15:O:5:LYS:CD	15:O:5:LYS:H	2.30	0.44
1:A:693:G:C8	1:A:1539:C:H1'	2.52	0.44
1:A:1472:U:O2'	1:A:1473:A:H5'	2.17	0.44
13:M:106:ASN:O	13:M:107:ALA:HB3	2.18	0.44
2:B:44:LEU:HG	2:B:44:LEU:H	1.45	0.44
1:A:402:G:O2'	1:A:403:C:H5'	2.17	0.44
3:C:15:THR:HG21	3:C:179:ARG:HA	2.00	0.44
17:Q:63:ARG:HG2	17:Q:64:PRO:CD	2.46	0.44
1:A:1051:C:H2'	1:A:1052:U:H6	1.82	0.44
1:A:384:G:O2'	1:A:385:C:H5'	2.17	0.44
1:A:969:A:C2'	1:A:970:C:H5'	2.48	0.44
8:H:118:VAL:C	8:H:119:LEU:HD23	2.37	0.44
4:D:35:ARG:HH11	4:D:35:ARG:HG2	1.83	0.44
16:P:43:LYS:HA	16:P:48:TRP:HB3	1.98	0.44
1:A:862:C:O2'	1:A:863:U:H5'	2.18	0.44
11:K:27:ASN:OD1	11:K:28:THR:N	2.50	0.44
1:A:499:A:H4'	1:A:500:G:OP1	2.17	0.44
1:A:304:U:H2'	1:A:305:G:C8	2.53	0.44
1:A:930:C:C2'	1:A:931:C:H5'	2.47	0.44
11:K:110:ASP:OD2	18:R:88:LYS:NZ	2.42	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:70:VAL:C	3:C:106:VAL:HG23	2.37	0.44
1:A:262:A:C6	1:A:263:A:C6	3.05	0.44
9:I:33:PHE:CE2	9:I:47:LEU:HD11	2.53	0.44
1:A:1487:G:O2'	1:A:1488:G:H5'	2.17	0.44
1:A:1474:G:O2'	1:A:1475:G:H5'	2.18	0.44
1:A:1220:G:H2'	1:A:1221:G:C8	2.53	0.44
11:K:48:ILE:HG22	11:K:49:GLY:H	1.82	0.44
1:A:644:G:C5	1:A:645:C:C5	3.05	0.44
13:M:14:ARG:N	13:M:44:ARG:HH12	2.15	0.44
1:A:596:C:O2'	1:A:597:G:H5'	2.17	0.44
7:G:8:GLU:H	7:G:8:GLU:HG3	1.59	0.44
18:R:87:ARG:O	18:R:88:LYS:HB3	2.18	0.44
13:M:40:ASN:HD22	13:M:40:ASN:C	2.18	0.44
19:S:20:LEU:HD12	19:S:21:GLU:HG3	2.00	0.44
10:J:26:ALA:HB1	10:J:84:GLN:HB3	1.99	0.44
1:A:1054:C:H5	1:A:1196:U:C6	2.36	0.44
6:F:69:GLU:O	6:F:71:ARG:N	2.50	0.44
3:C:40:ARG:HB3	3:C:44:GLU:HG3	1.99	0.44
4:D:173:TRP:O	4:D:186:LEU:HB2	2.17	0.44
4:D:60:GLU:O	4:D:63:LYS:HB3	2.17	0.44
5:E:20:GLN:HB3	5:E:20:GLN:HE21	1.60	0.44
16:P:26:ARG:HD2	16:P:31:LYS:O	2.17	0.44
4:D:111:ALA:HB3	4:D:117:ALA:HB2	2.00	0.44
12:L:73:GLU:CD	12:L:74:GLY:N	2.71	0.44
1:A:190(H):G:O2'	1:A:190(I):G:H5'	2.17	0.44
1:A:858:G:O6	1:A:869:G:H3'	2.18	0.44
4:D:142:PRO:HA	4:D:185:PHE:HD2	1.83	0.44
4:D:76:ARG:HH11	4:D:76:ARG:HG3	1.83	0.44
12:L:48:PRO:C	12:L:49:ASN:HD22	2.20	0.44
5:E:53:LEU:H	5:E:53:LEU:CD2	2.23	0.44
19:S:40:ILE:HD13	19:S:62:ILE:HD13	1.98	0.44
10:J:28:ARG:NH1	10:J:28:ARG:HG2	2.32	0.44
1:A:1222:G:C2'	1:A:1223:C:H5'	2.47	0.44
11:K:26:ASN:O	11:K:27:ASN:HB2	2.18	0.44
7:G:126:ASP:HA	7:G:131:LYS:HE3	2.00	0.44
2:B:54:THR:O	2:B:58:ILE:HG13	2.18	0.44
7:G:120:ILE:HG22	7:G:124:LEU:HD12	1.98	0.44
4:D:100:ARG:O	4:D:103:ASN:HB3	2.18	0.44
4:D:78:LEU:HD22	4:D:96:LEU:HB3	2.00	0.44
1:A:1120:G:H2'	1:A:1121:U:C6	2.52	0.44
3:C:29:TYR:CD2	3:C:29:TYR:C	2.90	0.44
1:A:458:C:H2'	1:A:459:G:C8	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1443:G:H5'	1:A:1446:A:H3'	1.98	0.44
1:A:620:C:C2	4:D:135:LEU:HD13	2.53	0.44
1:A:528:C:H5'	1:A:535:A:N6	2.33	0.44
1:A:1263:C:H2'	1:A:1264:C:C6	2.53	0.44
3:C:193:TYR:HE1	3:C:196:LEU:HD21	1.83	0.44
1:A:1406:U:O2'	1:A:1407:C:H5'	2.18	0.44
4:D:163:GLU:C	4:D:165:MET:N	2.71	0.44
5:E:93:PRO:HG2	8:H:105:ARG:NH2	2.33	0.44
10:J:29:ARG:O	10:J:84:GLN:NE2	2.50	0.44
5:E:76:ILE:HG22	5:E:78:HIS:O	2.18	0.44
6:F:40:VAL:HG22	6:F:41:GLU:N	2.32	0.44
12:L:126:LYS:HD2	12:L:126:LYS:C	2.38	0.44
1:A:437:U:O2'	4:D:123:HIS:CD2	2.71	0.44
1:A:160:A:H1'	1:A:344:A:N7	2.33	0.44
4:D:4:TYR:O	4:D:5:ILE:HB	2.18	0.44
1:A:689:C:H2'	1:A:690:G:O4'	2.18	0.44
11:K:93:GLN:HE21	11:K:96:ARG:HH21	1.65	0.44
1:A:542:G:H5'	4:D:41:GLY:HA3	1.99	0.44
1:A:1367:C:H5'	10:J:60:ARG:HH11	1.75	0.44
1:A:1367:C:H4'	10:J:48:THR:HG21	2.00	0.44
2:B:75:LYS:HE2	2:B:96:ARG:NH2	2.32	0.44
12:L:25:PRO:C	12:L:27:LEU:N	2.61	0.44
20:T:74:LYS:HB3	20:T:74:LYS:HE3	1.77	0.44
1:A:112:G:H4'	1:A:389:A:H5''	1.99	0.44
10:J:23:ILE:O	10:J:23:ILE:CG2	2.63	0.44
10:J:3:LYS:HA	10:J:74:ILE:O	2.18	0.44
7:G:38:LEU:HD11	7:G:42:ILE:HD11	1.99	0.44
2:B:71:VAL:O	2:B:165:VAL:HG23	2.17	0.44
16:P:82:GLN:O	16:P:83:GLU:C	2.56	0.44
4:D:81:GLU:O	4:D:85:LYS:HG3	2.17	0.44
1:A:1450:U:H2'	1:A:1452:C:C5	2.53	0.44
1:A:1194:U:O2'	1:A:1195:C:H5'	2.17	0.43
3:C:3:ASN:N	3:C:3:ASN:OD1	2.51	0.43
5:E:80:ILE:CD1	5:E:91:LEU:HD12	2.48	0.43
1:A:1238:A:N7	1:A:1303:C:H1'	2.33	0.43
7:G:145:ALA:C	7:G:147:ALA:N	2.71	0.43
1:A:1047:G:O2'	1:A:1048:G:H5'	2.17	0.43
1:A:1298:C:H4'	1:A:1299:A:O4'	2.18	0.43
11:K:11:LYS:O	11:K:12:ARG:HB2	2.18	0.43
1:A:9:G:N7	1:A:558:G:O2'	2.48	0.43
10:J:89:ASP:CB	10:J:91:PRO:HD2	2.46	0.43
18:R:54:ARG:H	18:R:54:ARG:HD3	1.82	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:47:LEU:HD12	3:C:47:LEU:H	1.82	0.43
1:A:1425:U:H3	1:A:1475:G:H1	1.65	0.43
1:A:51:A:H4'	1:A:52:G:C5'	2.47	0.43
12:L:104:VAL:O	12:L:105:TYR:HB2	2.18	0.43
5:E:72:GLN:O	5:E:73:ASN:HB3	2.18	0.43
3:C:91:LEU:C	3:C:91:LEU:HD23	2.38	0.43
2:B:74:LYS:O	2:B:76:GLN:N	2.43	0.43
1:A:1505:G:H4'	1:A:1506:U:O5'	2.18	0.43
3:C:150:LYS:CG	3:C:169:ALA:HB2	2.45	0.43
3:C:112:SER:C	3:C:114:PRO:HD2	2.37	0.43
1:A:1222:G:O2'	1:A:1223:C:H5'	2.18	0.43
1:A:603:U:H2'	1:A:604:G:C8	2.53	0.43
12:L:40:VAL:HG21	12:L:78:GLN:O	2.18	0.43
1:A:1010:G:H2'	1:A:1011:G:H8	1.83	0.43
1:A:1156:G:H3'	1:A:1157:A:OP2	2.17	0.43
12:L:47:LYS:HB3	12:L:48:PRO:HD2	1.91	0.43
17:Q:63:ARG:O	17:Q:65:ILE:HD12	2.18	0.43
3:C:157:ILE:CG2	3:C:164:ARG:HH21	2.31	0.43
16:P:67:THR:CG2	16:P:68:ASP:N	2.81	0.43
1:A:983:A:H2	1:A:984:C:C6	2.36	0.43
9:I:4:TYR:O	9:I:18:PHE:HA	2.17	0.43
9:I:81:ILE:HG22	9:I:81:ILE:O	2.17	0.43
4:D:58:LEU:HD22	4:D:62:GLN:HG2	1.99	0.43
17:Q:52:LYS:O	17:Q:55:ASP:HB2	2.18	0.43
2:B:157:ARG:HG2	2:B:158:LEU:N	2.31	0.43
1:A:613:C:O2'	1:A:614:A:H5'	2.18	0.43
12:L:58:VAL:O	12:L:65:GLU:HA	2.17	0.43
9:I:9:ARG:HD3	9:I:14:VAL:HG12	2.01	0.43
5:E:93:PRO:HG2	8:H:105:ARG:CZ	2.48	0.43
1:A:718:G:C4'	11:K:117:ASN:HD22	2.30	0.43
1:A:976:G:N7	1:A:1358:U:C2	2.87	0.43
2:B:187:LEU:HD21	2:B:203:GLY:HA3	1.99	0.43
3:C:164:ARG:NH1	3:C:166:GLU:OE1	2.52	0.43
3:C:108:ASN:ND2	3:C:144:SER:HB3	2.33	0.43
1:A:382:A:C2	1:A:383:A:C4	3.07	0.43
5:E:142:LEU:O	5:E:143:ARG:HD3	2.19	0.43
1:A:1003:G:N2	1:A:1039:C:N3	2.66	0.43
6:F:21:LEU:O	6:F:25:ILE:HG13	2.18	0.43
1:A:620:C:C1'	4:D:135:LEU:HD13	2.49	0.43
1:A:149:A:H2'	1:A:150:C:H6	1.82	0.43
12:L:60:LEU:N	12:L:64:TYR:O	2.48	0.43
1:A:993:G:O2'	1:A:994:A:P	2.76	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:107:THR:C	2:B:109:SER:N	2.71	0.43
1:A:424:G:H2'	1:A:425:G:H8	1.83	0.43
1:A:1171:G:H2'	1:A:1172:C:C6	2.54	0.43
17:Q:82:MET:O	17:Q:86:GLU:HG2	2.18	0.43
1:A:487:A:H2'	1:A:488:C:O4'	2.19	0.43
1:A:1495:U:H2'	1:A:1496:C:C6	2.53	0.43
4:D:42:GLN:CG	4:D:42:GLN:O	2.65	0.43
1:A:1193:G:HO2'	1:A:1194:U:H5'	1.83	0.43
11:K:91:ARG:HD2	11:K:92:GLU:OE1	2.18	0.43
1:A:1059:C:O2'	1:A:1060:C:H5'	2.18	0.43
2:B:74:LYS:HD3	2:B:205:ASP:O	2.18	0.43
12:L:41:ARG:NH2	12:L:57:LYS:HZ3	2.15	0.43
1:A:952:U:O2'	1:A:953:G:H5'	2.18	0.43
3:C:54:ARG:HG3	3:C:55:VAL:H	1.82	0.43
1:A:1217:C:O2'	1:A:1218:C:H5'	2.18	0.43
2:B:185:ILE:H	2:B:185:ILE:HD12	1.83	0.43
11:K:14:VAL:HG21	11:K:40:ILE:CD1	2.48	0.43
4:D:64:LEU:HD21	4:D:97:LEU:CD1	2.48	0.43
19:S:63:THR:OG1	19:S:66:MET:HG2	2.19	0.43
1:A:475:G:H2'	1:A:476:G:C8	2.53	0.43
9:I:8:GLY:HA3	9:I:76:ALA:O	2.18	0.43
1:A:646:U:H2'	1:A:647:C:C6	2.53	0.43
17:Q:79:SER:O	17:Q:80:GLY:O	2.36	0.43
1:A:1191:A:H5''	3:C:4:LYS:NZ	2.33	0.43
3:C:11:ARG:O	3:C:13:GLY:N	2.52	0.43
10:J:6:ILE:CD1	10:J:73:ASP:H	2.26	0.43
2:B:10:LEU:HD23	2:B:10:LEU:C	2.39	0.43
21:U:15:ARG:CG	21:U:15:ARG:HH11	2.26	0.43
3:C:53:ALA:HB2	3:C:115:LEU:HG	2.00	0.43
4:D:3:ARG:CZ	4:D:5:ILE:HD11	2.48	0.43
6:F:25:ILE:HD13	6:F:82:ARG:HD3	2.01	0.43
1:A:476:G:O2'	1:A:477:G:H5'	2.19	0.43
2:B:157:ARG:HG3	2:B:157:ARG:NH1	2.33	0.43
13:M:121:LYS:C	13:M:123:ALA:H	2.22	0.43
1:A:1112:C:C2	3:C:178:LEU:HB2	2.54	0.43
3:C:14:ILE:CG2	3:C:15:THR:H	1.98	0.43
1:A:1236:A:H2'	1:A:1237:C:C6	2.54	0.43
9:I:75:ASP:O	9:I:78:LYS:HB3	2.19	0.43
5:E:152:ARG:HA	8:H:64:LYS:NZ	2.33	0.43
2:B:24:TRP:HB3	2:B:40:HIS:CD2	2.53	0.43
1:A:1351:U:O2'	1:A:1352:C:H5'	2.19	0.43
1:A:1518:A:H2'	1:A:1519:A:C8	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:73:HIS:O	20:T:74:LYS:CB	2.67	0.43
1:A:1226:C:H5'	19:S:80:TYR:CE1	2.54	0.43
6:F:71:ARG:O	6:F:72:VAL:C	2.57	0.43
1:A:838:G:N2	1:A:849:C:C2	2.87	0.43
1:A:1312:G:N7	19:S:3:ARG:O	2.52	0.43
1:A:941:G:C2	1:A:942:G:C8	3.07	0.43
1:A:404:U:H2'	1:A:405:U:H6	1.83	0.43
4:D:126:ILE:HG22	4:D:127:THR:H	1.81	0.43
1:A:1223:C:OP2	1:A:1224:G:H2'	2.18	0.43
4:D:121:VAL:HG12	4:D:134:ASP:HA	1.99	0.43
1:A:895:G:H2'	1:A:896:C:H6	1.82	0.43
1:A:518:C:H2'	1:A:530:G:N3	2.33	0.43
1:A:1337:G:H5''	1:A:1338:G:OP2	2.19	0.43
1:A:1072:G:H2'	1:A:1073:U:C6	2.54	0.43
1:A:163:C:O2'	1:A:164:U:H5'	2.18	0.43
20:T:26:ASN:O	20:T:29:LYS:N	2.51	0.43
2:B:74:LYS:HD2	2:B:166:ASP:HB2	2.00	0.43
2:B:74:LYS:O	2:B:75:LYS:HB2	2.18	0.43
21:U:23:PRO:C	21:U:25:LYS:H	2.22	0.43
1:A:832:C:O2'	1:A:833:U:H5'	2.19	0.43
3:C:95:THR:C	3:C:97:LYS:N	2.72	0.43
3:C:5:ILE:H	3:C:5:ILE:CD1	2.32	0.43
1:A:184:G:O2'	1:A:185:A:H5'	2.19	0.43
19:S:42:PRO:O	19:S:45:VAL:HG23	2.19	0.43
2:B:53:ARG:NH1	2:B:199:TYR:CD2	2.87	0.43
1:A:242:C:H2'	1:A:243:A:H5'	2.01	0.43
19:S:33:THR:CG2	19:S:34:TRP:N	2.82	0.43
2:B:82:ARG:HD3	2:B:83:MET:HE2	2.01	0.43
6:F:43:LEU:HD13	6:F:43:LEU:O	2.18	0.43
10:J:81:THR:C	10:J:83:GLU:N	2.72	0.43
7:G:146:GLU:C	7:G:148:ASN:H	2.20	0.43
1:A:1505:G:C2'	1:A:1541:U:OP2	2.67	0.43
13:M:37:THR:HG23	13:M:55:ARG:CG	2.49	0.43
13:M:19:LEU:CA	13:M:22:ILE:HD13	2.49	0.43
1:A:915:A:C2'	1:A:916:G:H5'	2.49	0.43
4:D:33:MET:O	4:D:37:PRO:HB3	2.18	0.43
5:E:24:ARG:O	5:E:25:ARG:HG2	2.19	0.43
12:L:6:THR:OG1	12:L:9:GLN:HG3	2.18	0.43
1:A:909:A:H2'	1:A:910:C:O4'	2.19	0.43
1:A:41:G:H2'	1:A:42:G:C8	2.53	0.43
12:L:93:LEU:HD23	12:L:93:LEU:N	2.34	0.43
23:Y:34:TM2:H6	23:Y:34:TM2:O5'	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1237:C:H2'	1:A:1336:C:H5	1.84	0.43
1:A:1138:G:N1	1:A:1140:C:C2	2.87	0.43
6:F:101:ALA:HB2	18:R:28:GLU:CB	2.42	0.43
1:A:706:A:H4'	11:K:29:ILE:HD11	2.00	0.43
8:H:4:ASP:OD2	8:H:7:ALA:CB	2.66	0.43
17:Q:57:VAL:HG23	17:Q:59:ILE:HD13	2.00	0.43
1:A:1453:G:H2'	1:A:1454:G:O4'	2.19	0.43
1:A:339:C:H2'	1:A:340:U:H6	1.84	0.42
1:A:384:G:H2'	1:A:385:C:C6	2.54	0.42
6:F:41:GLU:HB2	6:F:62:TRP:HB3	2.00	0.42
10:J:47:PHE:CZ	14:N:37:PHE:HE1	2.36	0.42
1:A:1320:C:O2	19:S:72:GLY:HA3	2.18	0.42
1:A:1251:A:H1'	1:A:1369:C:O2'	2.18	0.42
10:J:8:LEU:CD2	10:J:96:ILE:HG12	2.48	0.42
1:A:1281:U:H4'	1:A:1282:C:OP2	2.20	0.42
12:L:46:LYS:CG	12:L:47:LYS:N	2.82	0.42
9:I:96:LEU:N	9:I:96:LEU:HD12	2.33	0.42
1:A:1056:U:C5'	3:C:163:ALA:HB2	2.49	0.42
1:A:586:C:O3'	8:H:89:PRO:HB2	2.20	0.42
13:M:9:ILE:H	13:M:9:ILE:HD12	1.84	0.42
9:I:3:GLN:HE22	9:I:20:ARG:NH2	2.12	0.42
3:C:79:ARG:C	3:C:81:GLY:H	2.22	0.42
4:D:98:GLU:HG2	4:D:189:PRO:HG2	2.01	0.42
7:G:18:TYR:CE2	7:G:59:LEU:HB2	2.54	0.42
1:A:1221:G:C2'	1:A:1222:G:H5'	2.49	0.42
12:L:113:ARG:NH1	12:L:116:SER:H	2.16	0.42
2:B:107:THR:C	2:B:109:SER:H	2.22	0.42
1:A:151:A:H2'	1:A:152:A:O4'	2.18	0.42
1:A:1329:A:P	13:M:28:ALA:HB3	2.59	0.42
19:S:74:PHE:CD1	19:S:74:PHE:N	2.86	0.42
1:A:1305:G:O2'	1:A:1331:G:N2	2.53	0.42
1:A:1330:U:H5''	1:A:1331:G:OP2	2.18	0.42
10:J:6:ILE:O	10:J:71:LEU:HD13	2.19	0.42
1:A:1175:G:C2	1:A:1176:A:N7	2.86	0.42
2:B:124:SER:CB	2:B:125:PRO:HD2	2.41	0.42
1:A:1351:U:H4'	7:G:33:ASP:OD2	2.18	0.42
15:O:70:LEU:HD13	15:O:78:TYR:HA	2.01	0.42
4:D:24:GLU:C	4:D:26:CYS:H	2.23	0.42
13:M:3:ARG:CZ	13:M:7:VAL:HA	2.48	0.42
13:M:11:ARG:HD3	13:M:11:ARG:C	2.40	0.42
1:A:393:A:C2'	1:A:394:G:H5'	2.50	0.42
4:D:126:ILE:CG2	4:D:127:THR:N	2.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:456:C:O2'	1:A:457:C:H5'	2.19	0.42
12:L:54:LYS:CD	12:L:54:LYS:N	2.81	0.42
1:A:792:A:C4	1:A:794:A:C6	3.07	0.42
4:D:61:LYS:NZ	4:D:62:GLN:NE2	2.67	0.42
1:A:335:C:H2'	1:A:336:C:H6	1.83	0.42
2:B:79:ASP:C	2:B:81:VAL:N	2.71	0.42
1:A:778:G:O2'	1:A:779:C:H5'	2.19	0.42
1:A:1385:G:O2'	1:A:1386:G:H5'	2.20	0.42
9:I:10:ARG:CD	9:I:105:ASP:HB3	2.49	0.42
17:Q:65:ILE:N	17:Q:65:ILE:CD1	2.79	0.42
13:M:4:ILE:HG22	13:M:5:ALA:H	1.80	0.42
1:A:840:C:H4'	1:A:848:C:C2	2.55	0.42
1:A:939:G:H2'	1:A:940:C:H6	1.78	0.42
1:A:413:G:H1'	1:A:428:G:H21	1.83	0.42
1:A:247:G:OP1	17:Q:100:LYS:HE3	2.19	0.42
1:A:998:G:O2'	1:A:999:C:H5'	2.19	0.42
1:A:594:G:C2'	1:A:595:G:H5'	2.49	0.42
12:L:10:LEU:HD21	12:L:15:ARG:NE	2.34	0.42
1:A:1388:C:H2'	1:A:1389:C:C6	2.55	0.42
1:A:1212:U:H4'	1:A:1213:A:C8	2.55	0.42
1:A:1256:A:H2	1:A:1277:C:C5	2.38	0.42
10:J:49:VAL:HG22	14:N:41:ARG:HD2	2.00	0.42
2:B:135:GLN:C	2:B:137:ARG:H	2.23	0.42
1:A:490:G:O2'	1:A:491:G:H5'	2.20	0.42
8:H:117:GLY:O	8:H:119:LEU:HD23	2.19	0.42
2:B:85:ALA:CB	2:B:92:TYR:HD2	2.32	0.42
1:A:1508:G:O2'	1:A:1509:C:H5'	2.19	0.42
1:A:197:A:N1	1:A:220:G:O2'	2.46	0.42
8:H:72:PRO:O	8:H:73:ASP:HB3	2.20	0.42
2:B:216:SER:O	2:B:219:VAL:N	2.50	0.42
1:A:1058:G:C6	1:A:1059:C:N3	2.88	0.42
10:J:30:SER:HB2	10:J:80:LYS:C	2.39	0.42
2:B:204:ASN:HD21	2:B:206:ASP:H	1.62	0.42
2:B:123:ALA:N	2:B:127:ILE:HG12	2.34	0.42
13:M:108:ARG:CA	13:M:108:ARG:HE	2.21	0.42
13:M:6:GLY:O	13:M:7:VAL:HG22	2.20	0.42
1:A:794:A:H2'	1:A:795:C:C6	2.54	0.42
1:A:833:U:H2'	1:A:834:C:H6	1.81	0.42
5:E:20:GLN:O	5:E:21:ALA:C	2.58	0.42
2:B:85:ALA:HB3	2:B:92:TYR:CD2	2.53	0.42
9:I:40:LEU:O	9:I:42:ARG:N	2.53	0.42
12:L:111:LYS:O	12:L:112:ASP:HB2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:56:MET:CE	20:T:88:VAL:HG11	2.50	0.42
23:Y:35:A:H2'	23:Y:36:A:O4'	2.20	0.42
1:A:1279:A:H5''	1:A:1280:A:OP1	2.19	0.42
9:I:102:LEU:CD1	9:I:102:LEU:H	2.33	0.42
1:A:1034:G:N2	1:A:1035:A:N6	2.66	0.42
1:A:838:G:C2'	1:A:839:U:H5''	2.47	0.42
5:E:101:ILE:HD12	5:E:119:LEU:CD2	2.50	0.42
9:I:37:PHE:HD1	9:I:43:ALA:HB1	1.84	0.42
6:F:63:TYR:N	6:F:63:TYR:HD2	2.16	0.42
1:A:1314:C:OP2	19:S:6:LYS:CD	2.68	0.42
4:D:64:LEU:CD2	4:D:64:LEU:C	2.87	0.42
1:A:1422:G:O2'	1:A:1423:G:H5'	2.19	0.42
4:D:12:CYS:SG	4:D:19:LEU:HB2	2.59	0.42
13:M:60:VAL:HG12	13:M:66:LEU:HD11	2.01	0.42
13:M:94:ARG:NH1	13:M:94:ARG:HG3	2.34	0.42
2:B:80:ILE:HD11	2:B:208:ILE:CG2	2.47	0.42
1:A:1130:A:H1'	1:A:1146:A:H2	1.83	0.42
10:J:4:ILE:O	10:J:73:ASP:HA	2.19	0.42
2:B:96:ARG:O	2:B:98:LEU:HD23	2.19	0.42
3:C:130:VAL:O	3:C:134:ILE:HG13	2.20	0.42
10:J:94:VAL:CG1	10:J:95:GLU:N	2.82	0.42
12:L:41:ARG:HH22	12:L:57:LYS:HZ3	1.68	0.42
1:A:1285:A:H4'	1:A:1286:A:O5'	2.20	0.42
10:J:21:GLN:O	10:J:25:GLU:HG3	2.20	0.42
1:A:1167:A:H2'	1:A:1168:A:H8	1.83	0.42
2:B:185:ILE:HD12	2:B:185:ILE:N	2.34	0.42
4:D:98:GLU:OE2	4:D:103:ASN:ND2	2.42	0.42
12:L:61:THR:C	12:L:63:GLY:H	2.23	0.42
2:B:144:ARG:C	2:B:146:GLN:H	2.23	0.42
12:L:83:VAL:CG2	12:L:84:LEU:N	2.83	0.42
16:P:75:ARG:HG3	16:P:75:ARG:NH1	2.35	0.42
9:I:24:GLY:HA2	9:I:59:PHE:O	2.19	0.42
1:A:1503:A:O2'	1:A:1504:G:O5'	2.37	0.42
4:D:33:MET:HE3	4:D:37:PRO:HA	2.01	0.42
1:A:21:G:H2'	1:A:22:G:C8	2.55	0.42
1:A:1305:G:OP1	21:U:2:GLY:N	2.53	0.42
22:X:3:G:O2'	22:X:4:A:C5'	2.33	0.42
3:C:11:ARG:O	3:C:12:LEU:C	2.58	0.42
18:R:87:ARG:HB3	18:R:88:LYS:H	1.45	0.42
1:A:741:G:H2'	1:A:742:G:O4'	2.20	0.42
2:B:20:GLU:HB2	2:B:190:THR:HB	2.02	0.42
15:O:70:LEU:HB3	15:O:78:TYR:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1225:A:N3	1:A:1225:A:H2'	2.35	0.42
6:F:34:GLY:N	6:F:71:ARG:NH2	2.68	0.42
1:A:8:A:H5'	5:E:101:ILE:HG22	2.02	0.42
7:G:51:GLN:O	7:G:53:LYS:N	2.44	0.42
1:A:817:C:C2	1:A:819:A:O4'	2.72	0.42
1:A:109:A:C6	1:A:326:G:C6	3.07	0.42
12:L:53:ARG:HH11	12:L:53:ARG:HG2	1.84	0.42
13:M:32:GLU:O	13:M:35:GLU:HB2	2.19	0.42
8:H:11:THR:O	8:H:12:ARG:C	2.57	0.42
1:A:1010:G:H2'	1:A:1011:G:C8	2.55	0.42
17:Q:66:SER:OG	17:Q:69:LYS:HB2	2.20	0.42
11:K:69:ALA:O	11:K:73:MET:HG2	2.20	0.42
1:A:782:A:H2'	1:A:783:C:O4'	2.20	0.42
1:A:1175:G:N3	1:A:1176:A:N9	2.67	0.42
9:I:114:TYR:HD2	10:J:60:ARG:HB2	1.76	0.42
7:G:149:ARG:HD2	11:K:59:TYR:CE1	2.54	0.42
11:K:59:TYR:O	11:K:62:GLN:N	2.53	0.42
2:B:20:GLU:O	2:B:21:ARG:O	2.38	0.42
9:I:55:ALA:O	9:I:56:LEU:CB	2.65	0.42
1:A:338:A:H2'	1:A:339:C:O4'	2.20	0.42
10:J:15:THR:CG2	10:J:94:VAL:HG23	2.48	0.42
6:F:69:GLU:C	6:F:71:ARG:H	2.24	0.42
20:T:57:ARG:NE	20:T:102:GLY:HA3	2.34	0.42
1:A:1475:G:H2'	1:A:1476:G:C8	2.55	0.42
1:A:513:C:H2'	1:A:514:C:H6	1.83	0.42
1:A:930:C:H2'	1:A:931:C:H5'	2.02	0.42
17:Q:82:MET:HA	17:Q:85:VAL:HG23	2.02	0.42
1:A:184:G:H2'	1:A:185:A:H8	1.84	0.42
1:A:197:A:H4'	1:A:198:G:O5'	2.19	0.42
2:B:100:GLY:O	2:B:104:ASN:N	2.46	0.42
1:A:1279:A:O2'	1:A:1282:C:N4	2.53	0.41
2:B:73:THR:O	2:B:75:LYS:N	2.53	0.41
2:B:184:VAL:HG12	2:B:197:VAL:HA	2.02	0.41
5:E:36:ASP:O	5:E:37:ARG:HB2	2.20	0.41
1:A:920:U:H2'	1:A:921:U:C6	2.55	0.41
4:D:60:GLU:OE2	4:D:198:VAL:HA	2.20	0.41
1:A:107:G:H2'	1:A:108:G:C5'	2.50	0.41
1:A:806:C:O2'	1:A:807:A:H5'	2.20	0.41
14:N:35:ARG:C	14:N:37:PHE:H	2.24	0.41
1:A:1499:A:C1'	1:A:1520:G:H5'	2.49	0.41
2:B:236:TYR:O	2:B:236:TYR:CD2	2.73	0.41
1:A:1153:C:C2	1:A:1154:G:C8	3.09	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:88:ALA:HB2	2:B:219:VAL:CG1	2.45	0.41
12:L:46:LYS:CG	12:L:47:LYS:H	2.32	0.41
1:A:1363:A:H1'	1:A:1365:G:N7	2.35	0.41
3:C:25:GLY:HA3	3:C:26:LYS:NZ	2.36	0.41
6:F:46:ARG:HB3	6:F:46:ARG:HH11	1.78	0.41
1:A:1299:A:C5	1:A:1301:U:C2	3.08	0.41
2:B:197:VAL:CB	2:B:200:ILE:HG12	2.43	0.41
13:M:96:LEU:O	13:M:97:PRO:C	2.56	0.41
8:H:77:GLU:CG	8:H:78:GLN:N	2.83	0.41
7:G:15:ASP:OD2	7:G:44:TYR:OH	2.37	0.41
9:I:128:ARG:HG2	13:M:126:LYS:HD3	2.03	0.41
16:P:81:ARG:CG	16:P:83:GLU:HG2	2.50	0.41
1:A:1029:C:H2'	1:A:1030:C:C6	2.55	0.41
5:E:42:GLY:HA2	5:E:65:ASN:O	2.20	0.41
13:M:67:GLU:O	13:M:69:GLU:N	2.53	0.41
1:A:1347:G:H3'	9:I:108:VAL:O	2.19	0.41
1:A:1298:C:H2'	7:G:114:ARG:NH2	2.36	0.41
2:B:209:ARG:HG2	2:B:239:VAL:CG1	2.50	0.41
3:C:157:ILE:HG21	3:C:164:ARG:HH21	1.85	0.41
1:A:1527:C:C2'	1:A:1528:U:H5'	2.50	0.41
6:F:40:VAL:HA	6:F:63:TYR:HA	2.01	0.41
1:A:1396:A:H2	5:E:19:MET:HG3	1.85	0.41
6:F:14:LEU:HD12	6:F:14:LEU:O	2.20	0.41
4:D:175:SER:HB3	4:D:186:LEU:HD11	2.00	0.41
1:A:448:A:H2'	1:A:449:C:H6	1.82	0.41
1:A:190(I):G:O2'	1:A:190(J):U:H5'	2.20	0.41
2:B:173:ALA:O	2:B:174:VAL:C	2.58	0.41
1:A:1294:G:O2'	1:A:1295:G:H5'	2.21	0.41
3:C:180:ALA:HB1	3:C:182:ILE:HG13	2.01	0.41
20:T:24:LEU:O	20:T:24:LEU:HD12	2.19	0.41
1:A:1305:G:H5''	21:U:4:GLY:C	2.41	0.41
1:A:1189:C:OP1	10:J:51:ARG:NH2	2.44	0.41
10:J:48:THR:OG1	10:J:62:HIS:CD2	2.74	0.41
3:C:70:VAL:CG1	3:C:71:ALA:N	2.82	0.41
2:B:27:LYS:O	2:B:194:PRO:HG2	2.20	0.41
9:I:50:LEU:O	9:I:51:ARG:C	2.57	0.41
2:B:124:SER:C	2:B:126:GLU:H	2.23	0.41
8:H:68:ARG:HH11	8:H:68:ARG:HG2	1.86	0.41
2:B:184:VAL:HB	2:B:198:ASP:OD2	2.21	0.41
19:S:5:LEU:O	19:S:6:LYS:CB	2.64	0.41
15:O:74:ASP:CG	15:O:77:ARG:HG3	2.41	0.41
7:G:15:ASP:OD2	7:G:16:LEU:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
20:T:100:ILE:HG13	20:T:100:ILE:O	2.20	0.41
2:B:140:HIS:HA	2:B:143:GLU:OE1	2.20	0.41
16:P:21:VAL:HG21	16:P:59:TRP:CD1	2.55	0.41
7:G:26:PHE:HD1	7:G:101:LEU:HD22	1.85	0.41
1:A:1262:C:H42	1:A:1273:G:H1	1.68	0.41
1:A:1360:A:H8	1:A:1360:A:OP2	2.04	0.41
7:G:78:ARG:NH1	7:G:156:TRP:HB2	2.35	0.41
13:M:65:LYS:HG3	13:M:69:GLU:HG2	2.03	0.41
1:A:1197:G:O2'	1:A:1198:G:H5'	2.21	0.41
9:I:102:LEU:HD12	9:I:102:LEU:H	1.85	0.41
19:S:20:LEU:O	19:S:23:ASN:HB2	2.20	0.41
1:A:976:G:C8	1:A:1358:U:O2	2.73	0.41
1:A:375:U:C2	1:A:376:G:C8	3.09	0.41
3:C:111:LEU:HD23	3:C:111:LEU:HA	1.93	0.41
1:A:377:G:OP1	16:P:3:LYS:HD3	2.21	0.41
7:G:141:VAL:HG13	7:G:142:GLU:N	2.36	0.41
1:A:429:U:H1'	1:A:430:A:H5''	2.01	0.41
1:A:222:U:H2'	1:A:223:U:C6	2.55	0.41
1:A:1157:A:C6	1:A:1180:A:N7	2.89	0.41
13:M:23:TYR:HB2	13:M:67:GLU:CD	2.41	0.41
1:A:1194:U:H2'	1:A:1195:C:C6	2.55	0.41
22:X:2:U:C2'	22:X:3:G:H5'	2.50	0.41
22:X:3:G:N2	23:Y:34:TM2:O2	2.50	0.41
9:I:11:LYS:O	9:I:12:GLU:HB3	2.20	0.41
2:B:60:ASP:HB3	2:B:64:ARG:CZ	2.46	0.41
19:S:17:GLU:CA	19:S:20:LEU:HG	2.40	0.41
14:N:9:LYS:C	14:N:11:LYS:N	2.74	0.41
2:B:51:LEU:O	2:B:54:THR:HB	2.21	0.41
1:A:260:G:H2'	1:A:261:U:C6	2.56	0.41
1:A:263:A:OP2	20:T:79:ARG:NH1	2.53	0.41
20:T:79:ARG:O	20:T:83:ARG:HG3	2.21	0.41
7:G:116:ALA:O	7:G:120:ILE:CD1	2.69	0.41
1:A:1207:G:O2'	1:A:1208:C:H5'	2.20	0.41
11:K:22:HIS:HB3	11:K:29:ILE:HG12	2.02	0.41
1:A:1283:G:O2'	1:A:1284:C:H5'	2.20	0.41
2:B:223:ILE:C	2:B:225:ALA:N	2.73	0.41
1:A:795:C:H5''	1:A:796:C:OP2	2.21	0.41
1:A:620:C:H2'	1:A:621:A:O4'	2.21	0.41
1:A:585:G:H4'	12:L:8:ASN:OD1	2.21	0.41
3:C:180:ALA:O	3:C:181:ASN:HB3	2.21	0.41
4:D:39:PRO:O	4:D:44:GLY:HA3	2.20	0.41
1:A:1253:G:H2'	1:A:1254:C:C6	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
10:J:86:MET:HE3	10:J:86:MET:O	2.21	0.41
9:I:11:LYS:O	9:I:12:GLU:CB	2.67	0.41
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.51	0.41
2:B:207:ALA:HB3	2:B:210:SER:HB3	2.02	0.41
3:C:134:ILE:HG22	3:C:168:ALA:CB	2.51	0.41
1:A:587:G:OP1	8:H:89:PRO:HB3	2.21	0.41
12:L:43:VAL:CG1	12:L:44:THR:H	2.34	0.41
7:G:18:TYR:OH	7:G:58:PRO:HG3	2.20	0.41
4:D:29:PRO:O	4:D:35:ARG:NH1	2.53	0.41
3:C:46:GLU:O	3:C:48:TYR:N	2.52	0.41
13:M:14:ARG:HB3	13:M:16:ASP:OD1	2.20	0.41
17:Q:79:SER:OG	17:Q:80:GLY:N	2.53	0.41
1:A:989:C:O2'	1:A:990:C:H5'	2.21	0.41
9:I:27:THR:HG22	9:I:28:VAL:N	2.35	0.41
12:L:20:LYS:HA	12:L:20:LYS:HD3	1.85	0.41
11:K:92:GLU:OE2	18:R:88:LYS:OXT	2.38	0.41
1:A:1003(A):G:C6	1:A:1004:A:N3	2.89	0.41
12:L:41:ARG:HG2	12:L:42:THR:N	2.27	0.41
21:U:6:ARG:CG	21:U:15:ARG:NH1	2.84	0.41
1:A:555:C:H2'	1:A:556:C:C6	2.56	0.41
3:C:52:LEU:N	3:C:52:LEU:CD2	2.79	0.41
3:C:108:ASN:HD21	3:C:144:SER:CB	2.33	0.41
7:G:21:VAL:HG23	7:G:22:LEU:N	2.35	0.41
1:A:1206:G:H4'	3:C:192:THR:O	2.21	0.41
2:B:22:LYS:HE3	2:B:35:GLU:CD	2.41	0.41
13:M:77:ASN:O	13:M:80:ARG:HB3	2.21	0.41
13:M:81:LEU:HD11	13:M:88:ARG:HH21	1.86	0.41
1:A:1525:G:P	11:K:120:ARG:HH22	2.44	0.41
1:A:768:A:H2'	1:A:769:G:O4'	2.21	0.41
1:A:254:G:H21	17:Q:16:GLN:HE22	1.65	0.41
1:A:1369:C:H2'	1:A:1370:G:H8	1.73	0.41
19:S:22:LEU:CD2	19:S:28:LYS:HD2	2.51	0.41
11:K:87:THR:HG22	11:K:88:GLY:H	1.85	0.41
1:A:1347:G:H2'	1:A:1373:G:H1	1.85	0.41
10:J:30:SER:CB	10:J:81:THR:HA	2.50	0.41
2:B:26:PRO:C	2:B:28:PHE:H	2.25	0.41
2:B:7:VAL:C	2:B:8:LYS:HG3	2.41	0.41
1:A:1399:C:C2	1:A:1401:G:C5	3.08	0.41
2:B:12:GLU:C	2:B:14:GLY:N	2.71	0.41
2:B:209:ARG:NH1	2:B:239:VAL:HG11	2.35	0.41
1:A:363:A:N6	12:L:28:LYS:HE3	2.25	0.41
1:A:1227:A:C8	1:A:1227:A:C3'	3.04	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:97:PRO:HB3	13:M:101:GLN:OE1	2.21	0.41
4:D:22:LYS:HB2	4:D:26:CYS:SG	2.61	0.41
13:M:8:GLU:C	13:M:9:ILE:HG13	2.40	0.41
1:A:380:G:C2	1:A:384:G:C6	3.09	0.41
1:A:837:G:O2'	1:A:838:G:H5'	2.21	0.41
7:G:116:ALA:HA	7:G:119:ARG:NH2	2.36	0.41
11:K:40:ILE:HG23	11:K:75:TYR:CD2	2.56	0.41
3:C:79:ARG:NE	3:C:82:GLU:HG2	2.36	0.41
4:D:173:TRP:CE2	4:D:189:PRO:HG3	2.55	0.41
19:S:62:ILE:HA	19:S:66:MET:HE2	2.02	0.41
9:I:16:ARG:HG3	9:I:16:ARG:HH11	1.86	0.41
6:F:10:LEU:HD23	6:F:85:VAL:HA	2.02	0.41
1:A:1426:C:H2'	1:A:1427:U:C6	2.56	0.41
1:A:828:A:H5''	1:A:859:A:C2	2.55	0.41
1:A:1223:C:P	19:S:78:ARG:HH12	2.43	0.41
20:T:92:LEU:O	20:T:94:ALA:N	2.44	0.41
12:L:60:LEU:CD2	12:L:66:VAL:HG22	2.51	0.41
1:A:567:G:H2'	1:A:568:G:O4'	2.21	0.41
7:G:9:VAL:HG11	7:G:94:ARG:NH1	2.36	0.41
1:A:1402:C:H2'	1:A:1403:C:O4'	2.21	0.41
1:A:1163:C:O2'	1:A:1164:G:H5'	2.20	0.41
11:K:67:ASP:OD1	11:K:71:LYS:HE3	2.21	0.41
21:U:9:ARG:HH11	21:U:9:ARG:HG3	1.86	0.41
10:J:98:ILE:HG22	10:J:99:LYS:H	1.86	0.41
19:S:27:GLU:HB3	19:S:28:LYS:H	1.76	0.41
11:K:91:ARG:CD	18:R:88:LYS:HE2	2.34	0.41
9:I:56:LEU:HD23	9:I:56:LEU:C	2.41	0.41
2:B:124:SER:HB2	2:B:125:PRO:CD	2.43	0.41
1:A:701:C:O2'	1:A:702:A:P	2.79	0.41
6:F:76:ALA:O	6:F:80:ARG:HG3	2.20	0.41
4:D:100:ARG:NH1	4:D:137:SER:HA	2.37	0.41
4:D:64:LEU:HD22	4:D:75:PHE:CE1	2.56	0.41
8:H:19:VAL:CG2	8:H:21:LYS:HD3	2.48	0.41
11:K:29:ILE:HG21	11:K:29:ILE:HD13	1.82	0.41
1:A:674:G:O2'	1:A:675:A:H5'	2.21	0.41
1:A:412:A:H4'	1:A:413:G:H8	1.86	0.41
1:A:191:G:C4	20:T:105:SER:HB3	2.55	0.41
1:A:1105:A:H2'	1:A:1106:G:H8	1.85	0.41
11:K:26:ASN:O	11:K:27:ASN:CB	2.68	0.41
1:A:514:C:O2'	1:A:515:G:H5'	2.21	0.41
1:A:671:G:H2'	1:A:672:U:O4'	2.20	0.41
10:J:87:THR:O	10:J:87:THR:HG22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
13:M:23:TYR:CB	13:M:67:GLU:HA	2.52	0.40
6:F:46:ARG:HB3	6:F:46:ARG:CZ	2.51	0.40
10:J:81:THR:C	10:J:83:GLU:H	2.23	0.40
1:A:1047:G:O5'	1:A:1047:G:H8	2.04	0.40
2:B:189:ASP:CB	2:B:205:ASP:OD2	2.68	0.40
5:E:50:GLU:HB3	5:E:53:LEU:HG	2.03	0.40
1:A:1392:G:N2	1:A:1502:A:C8	2.88	0.40
1:A:1053:G:H3'	1:A:1054:C:C5'	2.51	0.40
1:A:1288:A:O4'	1:A:1353:G:H4'	2.21	0.40
8:H:51:VAL:HG21	8:H:60:ARG:HG2	2.03	0.40
9:I:127:LYS:O	9:I:127:LYS:CD	2.69	0.40
1:A:1257:U:H5''	1:A:1258:G:OP2	2.21	0.40
1:A:642:A:C8	8:H:115:SER:HA	2.55	0.40
23:Y:34:TM2:O3S	23:Y:36:A:N6	2.54	0.40
1:A:1126:U:H2'	1:A:1127:G:C8	2.56	0.40
7:G:48:LYS:O	7:G:51:GLN:HB2	2.21	0.40
5:E:36:ASP:OD2	5:E:40:ARG:HB2	2.21	0.40
3:C:188:LEU:HB3	3:C:189:ALA:H	1.59	0.40
6:F:97:PHE:HB2	18:R:32:ARG:NH2	2.36	0.40
4:D:61:LYS:HD3	4:D:62:GLN:HE21	1.86	0.40
1:A:603:U:H2'	1:A:604:G:H8	1.85	0.40
7:G:37:ASN:ND2	9:I:41:VAL:HG12	2.36	0.40
1:A:1460:A:H2'	1:A:1461:G:O4'	2.21	0.40
1:A:583:A:H2'	1:A:584:G:O4'	2.21	0.40
1:A:1368:G:O2'	1:A:1369:C:H5'	2.22	0.40
1:A:1058:G:O2'	1:A:1059:C:H5'	2.21	0.40
1:A:1237:C:H3'	1:A:1336:C:H41	1.86	0.40
9:I:108:VAL:CG1	9:I:109:VAL:N	2.83	0.40
1:A:718:G:C5'	11:K:117:ASN:ND2	2.76	0.40
19:S:19:VAL:CG1	19:S:20:LEU:N	2.84	0.40
7:G:114:ARG:N	7:G:114:ARG:HD2	2.24	0.40
9:I:120:ARG:O	9:I:121:ARG:C	2.58	0.40
1:A:389:A:H2'	1:A:390:C:C5'	2.52	0.40
5:E:76:ILE:CG2	5:E:78:HIS:O	2.69	0.40
1:A:397:A:H5'	1:A:398:C:P	2.62	0.40
1:A:1019:C:O2'	1:A:1020:U:H5'	2.22	0.40
1:A:502:G:H2'	1:A:503:C:O4'	2.21	0.40
1:A:1202:G:C2'	1:A:1203:C:H5'	2.51	0.40
1:A:1439:C:P	20:T:38:LYS:HZ3	2.44	0.40
17:Q:52:LYS:HD2	17:Q:52:LYS:N	2.36	0.40
4:D:102:ASP:HB3	4:D:136:PRO:CA	2.51	0.40
2:B:130:ARG:CB	2:B:131:PRO:HD2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:C:H2'	1:A:175:C:H6	1.85	0.40
1:A:1292:U:H2'	1:A:1293:G:C8	2.56	0.40
1:A:267:C:H2'	1:A:268:C:C6	2.56	0.40
3:C:134:ILE:HG23	3:C:151:VAL:HB	2.02	0.40
12:L:26:ALA:C	12:L:27:LEU:O	2.59	0.40
13:M:108:ARG:NH1	13:M:114:ARG:HG2	2.37	0.40
5:E:135:THR:O	5:E:138:ALA:N	2.55	0.40
3:C:113:ALA:N	3:C:202:ILE:HD12	2.36	0.40
3:C:127:ARG:NH1	3:C:127:ARG:HG3	2.35	0.40
1:A:1202:G:C2	14:N:42:ILE:HG21	2.56	0.40
1:A:1474:G:H2'	1:A:1475:G:H8	1.86	0.40
1:A:1241:G:H2'	1:A:1242:C:C6	2.56	0.40
1:A:716:A:H1'	11:K:118:GLY:HA2	2.03	0.40
1:A:663:A:O2'	1:A:664:G:H5'	2.21	0.40
1:A:1299:A:C5	1:A:1301:U:O2	2.75	0.40
12:L:29:GLY:O	12:L:30:ALA:C	2.60	0.40
10:J:9:ARG:C	10:J:16:LEU:HD11	2.41	0.40
14:N:33:VAL:HG23	14:N:33:VAL:O	2.21	0.40
12:L:41:ARG:NH2	12:L:57:LYS:HZ2	2.18	0.40
1:A:1226:C:C4	13:M:104:ARG:HG3	2.57	0.40
1:A:1317:C:H2'	1:A:1318:A:O4'	2.22	0.40
1:A:1206:G:C6	1:A:1207:G:C5	3.10	0.40
1:A:807:A:H2'	1:A:808:C:H6	1.82	0.40
7:G:18:TYR:HD2	7:G:59:LEU:HD22	1.87	0.40
1:A:1413:A:C2	1:A:1488:G:C2	3.09	0.40
1:A:1499:A:O2'	1:A:1500:A:H5'	2.22	0.40
1:A:1263:C:H2'	1:A:1264:C:H6	1.85	0.40
10:J:63:PHE:CE1	14:N:45:ARG:HG3	2.56	0.40
1:A:590:C:O2'	1:A:591:U:H5'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	233/256 (91%)	147 (63%)	65 (28%)	21 (9%)	1	2
3	C	205/239 (86%)	135 (66%)	44 (22%)	26 (13%)	0	1
4	D	206/209 (99%)	169 (82%)	29 (14%)	8 (4%)	5	18
5	E	149/162 (92%)	132 (89%)	16 (11%)	1 (1%)	30	72
6	F	99/101 (98%)	73 (74%)	22 (22%)	4 (4%)	5	17
7	G	153/156 (98%)	120 (78%)	25 (16%)	8 (5%)	3	10
8	H	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	15	50
9	I	125/128 (98%)	95 (76%)	22 (18%)	8 (6%)	2	6
10	J	97/105 (92%)	62 (64%)	19 (20%)	16 (16%)	0	0
11	K	117/129 (91%)	94 (80%)	18 (15%)	5 (4%)	4	15
12	L	123/135 (91%)	90 (73%)	21 (17%)	12 (10%)	1	2
13	M	123/126 (98%)	97 (79%)	14 (11%)	12 (10%)	1	2
14	N	58/61 (95%)	44 (76%)	10 (17%)	4 (7%)	2	4
15	O	86/89 (97%)	73 (85%)	10 (12%)	3 (4%)	6	23
16	P	82/88 (93%)	71 (87%)	9 (11%)	2 (2%)	9	35
17	Q	102/105 (97%)	88 (86%)	12 (12%)	2 (2%)	11	40
18	R	71/88 (81%)	55 (78%)	13 (18%)	3 (4%)	4	16
19	S	79/93 (85%)	60 (76%)	13 (16%)	6 (8%)	2	4
20	T	97/106 (92%)	73 (75%)	15 (16%)	9 (9%)	1	2
21	U	23/27 (85%)	16 (70%)	6 (26%)	1 (4%)	4	15
All	All	2364/2541 (93%)	1817 (77%)	394 (17%)	153 (6%)	2	5

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	15	VAL
2	B	16	HIS
2	B	20	GLU
2	B	21	ARG
2	B	24	TRP
2	B	74	LYS
2	B	123	ALA
2	B	230	VAL
2	B	232	PRO
3	C	15	THR
3	C	16	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	26	LYS
3	C	61	ALA
3	C	101	LEU
3	C	154	SER
3	C	156	ARG
3	C	189	ALA
3	C	207	VAL
4	D	3	ARG
6	F	14	LEU
6	F	64	GLN
7	G	17	VAL
7	G	53	LYS
8	H	91	ARG
9	I	23	ASN
9	I	55	ALA
9	I	88	TYR
10	J	30	SER
10	J	32	ALA
10	J	34	VAL
11	K	12	ARG
12	L	27	LEU
12	L	28	LYS
12	L	47	LYS
12	L	48	PRO
13	M	23	TYR
13	M	24	GLY
13	M	67	GLU
13	M	86	CYS
17	Q	80	GLY
17	Q	81	ARG
18	R	87	ARG
19	S	6	LYS
19	S	81	ARG
20	T	11	SER
20	T	73	HIS
20	T	95	ALA
20	T	99	LEU
20	T	100	ILE
2	B	8	LYS
2	B	95	GLN
2	B	190	THR
2	B	207	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	224	GLN
3	C	47	LEU
3	C	54	ARG
3	C	100	ALA
3	C	146	ALA
3	C	188	LEU
4	D	171	GLY
6	F	70	ASP
7	G	7	ALA
7	G	81	GLY
7	G	155	ARG
8	H	83	ILE
9	I	41	VAL
10	J	39	PRO
10	J	57	LYS
12	L	29	GLY
12	L	91	LYS
12	L	128	ALA
13	M	59	TYR
13	M	68	GLY
13	M	85	GLY
14	N	15	LYS
14	N	23	ARG
15	O	85	LEU
16	P	10	GLY
16	P	83	GLU
19	S	9	VAL
19	S	30	LEU
20	T	74	LYS
20	T	94	ALA
20	T	102	GLY
2	B	18	GLY
3	C	55	VAL
3	C	81	GLY
3	C	96	GLY
3	C	168	ALA
4	D	4	TYR
4	D	35	ARG
4	D	39	PRO
7	G	83	ALA
9	I	38	GLN
9	I	119	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	J	61	GLU
12	L	41	ARG
12	L	116	SER
13	M	7	VAL
14	N	17	LYS
20	T	9	ASN
2	B	228	GLY
3	C	20	SER
3	C	98	ASN
3	C	108	ASN
4	D	88	VAL
6	F	32	ASN
9	I	24	GLY
10	J	40	LEU
10	J	72	VAL
11	K	50	TYR
11	K	117	ASN
13	M	60	VAL
14	N	22	THR
18	R	20	ALA
18	R	25	THR
19	S	8	GLY
21	U	25	LYS
2	B	11	LEU
3	C	4	LYS
3	C	167	TRP
4	D	58	LEU
7	G	37	ASN
9	I	58	ARG
10	J	23	ILE
10	J	73	ASP
10	J	77	PRO
10	J	86	MET
11	K	13	GLN
11	K	128	ALA
12	L	51	ALA
2	B	27	LYS
3	C	39	ILE
10	J	55	LYS
10	J	90	LEU
12	L	62	SER
13	M	4	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	M	124	PRO
15	O	86	GLY
19	S	43	GLU
4	D	5	ILE
7	G	112	PRO
13	M	117	VAL
2	B	227	GLY
3	C	14	ILE
3	C	75	VAL
12	L	121	GLY
2	B	183	PRO
5	E	154	GLY
10	J	41	PRO
10	J	76	ASN
2	B	233	SER
15	O	3	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	202/220 (92%)	182 (90%)	20 (10%)	11	34
3	C	160/188 (85%)	144 (90%)	16 (10%)	11	32
4	D	180/181 (99%)	172 (96%)	8 (4%)	39	77
5	E	115/123 (94%)	101 (88%)	14 (12%)	7	20
6	F	90/90 (100%)	87 (97%)	3 (3%)	50	87
7	G	126/127 (99%)	121 (96%)	5 (4%)	42	81
8	H	119/119 (100%)	109 (92%)	10 (8%)	16	42
9	I	98/99 (99%)	91 (93%)	7 (7%)	21	52
10	J	87/92 (95%)	81 (93%)	6 (7%)	22	54
11	K	90/99 (91%)	88 (98%)	2 (2%)	64	92
12	L	104/111 (94%)	96 (92%)	8 (8%)	18	47
13	M	100/101 (99%)	90 (90%)	10 (10%)	11	32
14	N	49/50 (98%)	47 (96%)	2 (4%)	41	80

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	O	79/80 (99%)	73 (92%)	6 (8%)	19	48
16	P	72/74 (97%)	68 (94%)	4 (6%)	30	66
17	Q	96/97 (99%)	90 (94%)	6 (6%)	25	60
18	R	64/77 (83%)	60 (94%)	4 (6%)	25	60
19	S	71/80 (89%)	68 (96%)	3 (4%)	40	79
20	T	76/82 (93%)	68 (90%)	8 (10%)	10	29
21	U	19/22 (86%)	17 (90%)	2 (10%)	10	29
All	All	1997/2112 (95%)	1853 (93%)	144 (7%)	21	51

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	8	LYS
2	B	9	GLU
2	B	12	GLU
2	B	15	VAL
2	B	17	PHE
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	44	LEU
2	B	67	THR
2	B	82	ARG
2	B	92	TYR
2	B	98	LEU
2	B	140	HIS
2	B	157	ARG
2	B	178	ARG
2	B	204	ASN
2	B	221	LEU
2	B	232	PRO
2	B	236	TYR
3	C	5	ILE
3	C	23	TYR
3	C	26	LYS
3	C	36	ASP
3	C	37	GLN
3	C	52	LEU
3	C	56	ASP
3	C	82	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	102	ASN
3	C	107	GLN
3	C	143	GLU
3	C	167	TRP
3	C	188	LEU
3	C	191	THR
3	C	196	LEU
3	C	204	LEU
4	D	36	ARG
4	D	58	LEU
4	D	76	ARG
4	D	122	ARG
4	D	162	LEU
4	D	168	ARG
4	D	192	GLU
4	D	199	ASN
5	E	12	LEU
5	E	20	GLN
5	E	31	LEU
5	E	33	VAL
5	E	34	VAL
5	E	41	VAL
5	E	43	LEU
5	E	53	LEU
5	E	73	ASN
5	E	75	THR
5	E	79	GLU
5	E	80	ILE
5	E	147	ASP
5	E	150	ARG
6	F	43	LEU
6	F	47	ARG
6	F	63	TYR
7	G	8	GLU
7	G	38	LEU
7	G	114	ARG
7	G	126	ASP
7	G	140	ASP
8	H	21	LYS
8	H	24	THR
8	H	26	VAL
8	H	39	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	H	63	LEU
8	H	85	ARG
8	H	91	ARG
8	H	112	LEU
8	H	119	LEU
8	H	133	LEU
9	I	23	ASN
9	I	60	ASP
9	I	79	LEU
9	I	102	LEU
9	I	114	TYR
9	I	121	ARG
9	I	127	LYS
10	J	3	LYS
10	J	29	ARG
10	J	57	LYS
10	J	71	LEU
10	J	73	ASP
10	J	83	GLU
11	K	11	LYS
11	K	92	GLU
12	L	33	ARG
12	L	48	PRO
12	L	53	ARG
12	L	59	ARG
12	L	73	GLU
12	L	93	LEU
12	L	113	ARG
12	L	126	LYS
13	M	9	ILE
13	M	11	ARG
13	M	16	ASP
13	M	40	ASN
13	M	70	LEU
13	M	102	ARG
13	M	108	ARG
13	M	110	ARG
13	M	115	LYS
13	M	125	ARG
14	N	41	ARG
14	N	44	LEU
15	O	5	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	10	LYS
15	O	31	LEU
15	O	34	LEU
15	O	64	ARG
15	O	81	LEU
16	P	2	VAL
16	P	43	LYS
16	P	55	ARG
16	P	61	SER
17	Q	9	VAL
17	Q	38	ARG
17	Q	52	LYS
17	Q	59	ILE
17	Q	68	ARG
17	Q	74	LEU
18	R	36	ASN
18	R	54	ARG
18	R	84	LYS
18	R	87	ARG
19	S	7	LYS
19	S	12	ASP
19	S	15	LEU
20	T	10	LEU
20	T	24	LEU
20	T	42	GLN
20	T	45	GLN
20	T	57	ARG
20	T	73	HIS
20	T	75	ASN
20	T	84	LEU
21	U	6	ARG
21	U	15	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	25	ASN
2	B	204	ASN
3	C	3	ASN
3	C	31	HIS
3	C	63	ASN
3	C	102	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	107	GLN
3	C	110	ASN
4	D	42	GLN
4	D	62	GLN
4	D	123	HIS
4	D	161	ASN
4	D	199	ASN
5	E	20	GLN
5	E	73	ASN
5	E	78	HIS
6	F	13	ASN
6	F	18	GLN
6	F	27	GLN
6	F	32	ASN
6	F	57	GLN
6	F	94	GLN
6	F	100	ASN
7	G	37	ASN
7	G	68	ASN
7	G	96	GLN
9	I	23	ASN
9	I	31	GLN
9	I	73	GLN
9	I	89	ASN
10	J	78	ASN
10	J	84	GLN
11	K	38	ASN
11	K	93	GLN
11	K	117	ASN
12	L	49	ASN
12	L	75	HIS
13	M	12	ASN
13	M	40	ASN
13	M	62	ASN
14	N	52	GLN
15	O	13	GLN
15	O	37	ASN
15	O	46	HIS
16	P	16	HIS
16	P	65	GLN
16	P	76	GLN
17	Q	16	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	96	GLN
19	S	23	ASN
19	S	56	GLN
20	T	45	GLN
20	T	73	HIS
20	T	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1511/1522 (99%)	202 (13%)	68 (4%)
22	X	3/6 (50%)	1 (33%)	0
23	Y	6/17 (35%)	2 (33%)	0
All	All	1520/1545 (98%)	205 (13%)	68 (4%)

All (205) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	9	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	61	G
1	A	101	A
1	A	116	A
1	A	120	A
1	A	121	C
1	A	130	A
1	A	131	C
1	A	163	C
1	A	182	U
1	A	195	A
1	A	197	A
1	A	202	U
1	A	204	U
1	A	216	G
1	A	244	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	289	G
1	A	321	A
1	A	328	C
1	A	329	A
1	A	332	G
1	A	344	A
1	A	345	C
1	A	352	C
1	A	353	A
1	A	354	G
1	A	366	C
1	A	367	U
1	A	373	A
1	A	390	C
1	A	397	A
1	A	398	C
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	414	A
1	A	421	U
1	A	428	G
1	A	429	U
1	A	430	A
1	A	433	C
1	A	434	U
1	A	439	A
1	A	442	C
1	A	452	A
1	A	461	C
1	A	484	G
1	A	485	G
1	A	497	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	518	C
1	A	527	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	572	A
1	A	573	A
1	A	575	G
1	A	576	G
1	A	577	G
1	A	630	G
1	A	653	A
1	A	665	A
1	A	688	G
1	A	701	C
1	A	702	A
1	A	723	U
1	A	731	G
1	A	749	C
1	A	755	G
1	A	777	A
1	A	781	A
1	A	782	A
1	A	793	U
1	A	794	A
1	A	813	U
1	A	817	C
1	A	819	A
1	A	821	G
1	A	828	A
1	A	839	U
1	A	840	C
1	A	841	U
1	A	848	C
1	A	902	G
1	A	914	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	926	G
1	A	927	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	961	U
1	A	966	G
1	A	969	A
1	A	971	G
1	A	974	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	978	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1004	A
1	A	1025	U
1	A	1026	G
1	A	1027	C
1	A	1050	G
1	A	1053	G
1	A	1054	C
1	A	1055	A
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1068	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1117	G
1	A	1125	U
1	A	1126	U
1	A	1127	G
1	A	1128	C
1	A	1129	C
1	A	1130	A
1	A	1131	G
1	A	1136	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1145	C
1	A	1152	A
1	A	1159	U
1	A	1161	C
1	A	1176	A
1	A	1180	A
1	A	1183	A
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1257	U
1	A	1258	G
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1286	A
1	A	1287	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1320	C
1	A	1331	G
1	A	1338	G
1	A	1346	A
1	A	1348	U
1	A	1362	C
1	A	1379	G
1	A	1398	A
1	A	1442	G
1	A	1446	A
1	A	1452	C
1	A	1492	A
1	A	1499	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1517	G
1	A	1520	G
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1533	C
22	X	2	U
23	Y	35	A
23	Y	39	C

All (68) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	60	A
1	A	115	G
1	A	119	A
1	A	129(A)	G
1	A	181	G
1	A	243	A
1	A	250	A
1	A	266	G
1	A	328	C
1	A	344	A
1	A	351	G
1	A	353	A
1	A	366	C
1	A	372	C
1	A	410	G
1	A	412	A
1	A	428	G
1	A	429	U
1	A	433	C
1	A	438	G
1	A	484	G
1	A	496	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	497	A
1	A	509	A
1	A	532	A
1	A	533	A
1	A	559	A
1	A	560	U
1	A	575	G
1	A	687	A
1	A	701	C
1	A	748	C
1	A	793	U
1	A	812	C
1	A	913	A
1	A	960	U
1	A	965	A
1	A	992	U
1	A	993	G
1	A	1049	U
1	A	1063	C
1	A	1065	U
1	A	1067	A
1	A	1127	G
1	A	1129	C
1	A	1160	G
1	A	1175	G
1	A	1182	G
1	A	1191	A
1	A	1201	A
1	A	1211	U
1	A	1225	A
1	A	1281	U
1	A	1285	A
1	A	1300	G
1	A	1301	U
1	A	1347	G
1	A	1397	C
1	A	1443	G
1	A	1451	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1505	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1528	U
1	A	1532	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
23	TM2	Y	34	23	27,29,30	1.34	2 (7%)	35,42,45	2.28	10 (28%)

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
23	TM2	Y	34	23	-	1/14/33/34	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Y	34	TM2	C11-S12	4.98	1.85	1.77
23	Y	34	TM2	C7-N8	2.60	1.59	1.45

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	34	TM2	O2S-S12-C11	6.13	112.06	106.81
23	Y	34	TM2	C7-C5-C4	-5.46	111.49	120.18
23	Y	34	TM2	O1S-S12-C11	4.98	111.08	106.81
23	Y	34	TM2	C11-C9-N8	-4.89	96.71	111.21
23	Y	34	TM2	C6-N1-C2	-3.81	121.33	122.41
23	Y	34	TM2	C5-C7-N8	3.70	134.09	114.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Y	34	TM2	C7-C5-C6	2.96	129.34	121.78
23	Y	34	TM2	O3S-S12-C11	2.64	109.27	105.93
23	Y	34	TM2	O2S-S12-O1S	-2.04	105.98	113.26
23	Y	34	TM2	C7-N8-C9	-2.01	106.08	113.47

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
23	Y	34	TM2	O2P-P-O5'-C5'

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 290 ligands modelled in this entry, 289 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
24	PAR	Z	1	-	45,45,45	1.64	9 (20%)	67,67,67	1.41	6 (8%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	PAR	Z	1	-	-	0/18/94/94	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Z	1	PAR	C22-C32	4.47	1.55	1.52
24	Z	1	PAR	C22-C12	4.38	1.55	1.52
24	Z	1	PAR	C42-C32	2.94	1.57	1.52
24	Z	1	PAR	O54-C14	2.82	1.49	1.41
24	Z	1	PAR	C52-C42	2.72	1.57	1.52
24	Z	1	PAR	C11-C21	2.53	1.57	1.52
24	Z	1	PAR	C31-C21	2.40	1.56	1.53
24	Z	1	PAR	C14-C24	2.34	1.57	1.52
24	Z	1	PAR	O51-C11	2.20	1.47	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Z	1	PAR	O54-C54-C64	5.01	113.13	106.97
24	Z	1	PAR	O33-C14-C24	4.25	116.49	108.09
24	Z	1	PAR	O52-C13-C23	4.16	114.92	107.50
24	Z	1	PAR	C14-O54-C54	3.64	120.80	113.73
24	Z	1	PAR	O52-C13-O43	-3.14	108.50	111.51
24	Z	1	PAR	C22-C32-C42	2.89	114.96	109.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1513/1522 (99%)	0.33	53 (3%) 42 50	44, 78, 143, 201	0
2	B	235/256 (91%)	0.40	19 (8%) 12 15	67, 107, 151, 161	0
3	C	207/239 (86%)	0.32	12 (5%) 22 26	75, 100, 145, 149	0
4	D	208/209 (99%)	0.21	8 (3%) 38 45	62, 87, 111, 119	0
5	E	151/162 (93%)	-0.07	4 (2%) 53 63	55, 70, 97, 114	0
6	F	101/101 (100%)	-0.05	2 (1%) 62 71	73, 105, 120, 124	0
7	G	155/156 (99%)	0.10	8 (5%) 26 32	72, 98, 130, 148	0
8	H	138/138 (100%)	-0.09	1 (0%) 84 90	51, 69, 83, 94	0
9	I	127/128 (99%)	0.55	13 (10%) 7 9	66, 110, 126, 132	0
10	J	99/105 (94%)	1.05	20 (20%) 2 2	72, 138, 174, 177	0
11	K	119/129 (92%)	0.14	3 (2%) 54 64	54, 81, 109, 134	0
12	L	125/135 (92%)	0.30	7 (5%) 24 28	43, 83, 104, 127	0
13	M	125/126 (99%)	1.21	21 (16%) 2 3	76, 97, 145, 188	0
14	N	60/61 (98%)	0.77	6 (10%) 8 10	78, 98, 125, 131	0
15	O	88/89 (98%)	0.21	4 (4%) 32 39	64, 83, 113, 137	0
16	P	84/88 (95%)	-0.01	0 100 100	56, 70, 84, 108	0
17	Q	104/105 (99%)	0.40	7 (6%) 17 21	52, 71, 113, 156	0
18	R	73/88 (82%)	0.40	5 (6%) 17 20	76, 90, 136, 161	0
19	S	81/93 (87%)	0.58	10 (12%) 5 6	83, 121, 144, 149	0
20	T	99/106 (93%)	0.38	5 (5%) 27 33	57, 75, 105, 112	0
21	U	25/27 (92%)	0.51	2 (8%) 12 15	74, 86, 116, 120	0
22	X	4/6 (66%)	1.82	2 (50%) 0 0	77, 107, 116, 120	0
23	Y	7/17 (41%)	3.28	3 (42%) 1 0	101, 121, 154, 161	0
All	All	3928/4086 (96%)	0.34	215 (5%) 17 29	43, 86, 142, 201	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
13	M	121	LYS	19.1
13	M	124	PRO	16.0
1	A	1534	A	13.7
13	M	123	ALA	11.9
13	M	125	ARG	11.5
13	M	120	LYS	11.4
23	Y	33	U	10.7
17	Q	105	ALA	10.3
11	K	129	SER	10.1
17	Q	104	LYS	9.6
19	S	3	ARG	9.6
1	A	1540	U	9.3
13	M	126	LYS	9.1
1	A	1129	C	8.7
11	K	128	ALA	7.9
1	A	1541	U	7.3
17	Q	103	GLY	7.0
1	A	1539	C	7.0
2	B	16	HIS	6.6
10	J	70	ARG	6.6
7	G	5	ARG	6.5
17	Q	102	GLY	6.5
10	J	17	ASP	6.4
10	J	90	LEU	6.3
18	R	17	SER	6.1
13	M	122	LYS	6.0
10	J	10	GLY	5.7
23	Y	39	C	5.6
15	O	89	GLY	5.5
20	T	9	ASN	5.4
9	I	66	ARG	5.3
18	R	16	PRO	5.2
1	A	1533	C	5.1
13	M	7	VAL	5.0
3	C	76	VAL	4.9
10	J	24	VAL	4.8
19	S	49	ILE	4.7
2	B	136	VAL	4.6
1	A	1002	G	4.5
22	X	4	A	4.4
1	A	1024	G	4.4
4	D	32	ALA	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	118	ALA	4.3
3	C	68	VAL	4.2
15	O	23	GLY	4.2
1	A	1034	G	4.2
1	A	1027	C	4.1
20	T	8	ARG	4.1
4	D	156	GLU	4.0
1	A	1132	C	3.9
14	N	6	LEU	3.8
1	A	1001	A	3.8
1	A	1003	G	3.8
2	B	133	LYS	3.7
9	I	19	LEU	3.6
9	I	15	ALA	3.5
1	A	1131	G	3.5
4	D	35	ARG	3.5
18	R	18	ARG	3.5
1	A	1478	C	3.5
1	A	160	A	3.5
1	A	1006	C	3.4
1	A	1138	G	3.4
10	J	87	THR	3.4
17	Q	101	ARG	3.4
1	A	202	U	3.3
23	Y	38	A	3.3
2	B	229	VAL	3.3
10	J	16	LEU	3.3
1	A	1144	G	3.2
7	G	156	TRP	3.2
9	I	65	VAL	3.2
2	B	19	HIS	3.2
1	A	1004	A	3.2
9	I	92	TYR	3.2
10	J	43	ARG	3.2
21	U	24	ARG	3.2
1	A	1003(A)	G	3.2
13	M	11	ARG	3.1
4	D	157	LEU	3.1
14	N	17	LYS	3.1
1	A	1033	G	3.1
9	I	102	LEU	3.1
1	A	723	U	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
19	S	71	LEU	3.1
10	J	88	LEU	3.1
20	T	104	LEU	3.0
19	S	60	VAL	3.0
10	J	71	LEU	3.0
1	A	1128	C	3.0
1	A	161	A	3.0
3	C	65	ALA	3.0
1	A	1029	C	3.0
1	A	1477	C	3.0
13	M	13	LYS	3.0
1	A	1130	A	2.9
9	I	101	PHE	2.9
3	C	196	LEU	2.9
14	N	2	ALA	2.9
4	D	36	ARG	2.9
19	S	28	LYS	2.9
3	C	77	ILE	2.9
4	D	49	ARG	2.9
1	A	1143	G	2.8
7	G	155	ARG	2.8
15	O	22	THR	2.8
9	I	70	LYS	2.8
10	J	72	VAL	2.8
1	A	1031	G	2.8
1	A	1025	U	2.8
7	G	4	ARG	2.8
1	A	1026	G	2.8
7	G	80	VAL	2.8
14	N	3	ARG	2.8
18	R	88	LYS	2.7
3	C	60	ALA	2.7
1	A	1036	G	2.7
2	B	206	ASP	2.7
7	G	6	ARG	2.7
1	A	1137	C	2.7
2	B	125	PRO	2.7
13	M	119	GLY	2.7
6	F	14	LEU	2.7
9	I	96	LEU	2.7
3	C	78	GLY	2.7
1	A	159	G	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	8	GLU	2.7
3	C	188	LEU	2.7
9	I	36	TYR	2.7
3	C	103	VAL	2.7
5	E	119	LEU	2.6
1	A	1030(D)	A	2.6
4	D	132	ARG	2.6
17	Q	92	ARG	2.6
2	B	127	ILE	2.6
13	M	117	VAL	2.6
1	A	1135	U	2.6
1	A	1030(A)	G	2.6
2	B	137	ARG	2.6
14	N	35	ARG	2.6
1	A	1260	C	2.6
2	B	118	LEU	2.6
10	J	83	GLU	2.5
19	S	14	HIS	2.5
7	G	85	TYR	2.5
1	A	1030	C	2.5
3	C	66	VAL	2.5
10	J	8	LEU	2.5
4	D	47	ARG	2.5
10	J	79	ARG	2.5
13	M	48	LEU	2.5
1	A	1019	C	2.5
1	A	412	A	2.5
21	U	10	ARG	2.5
5	E	17	ALA	2.5
1	A	1139	G	2.5
12	L	28	LYS	2.5
10	J	47	PHE	2.4
1	A	344	A	2.4
10	J	45	ARG	2.4
1	A	1032	G	2.4
1	A	162	A	2.4
1	A	1035	A	2.4
2	B	40	HIS	2.4
2	B	48	MET	2.4
19	S	27	GLU	2.4
22	X	3	G	2.4
15	O	88	ARG	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
13	M	15	VAL	2.3
20	T	56	MET	2.3
9	I	119	ALA	2.3
1	A	1030(B)	C	2.3
7	G	7	ALA	2.3
2	B	148	TYR	2.3
20	T	101	GLY	2.3
17	Q	98	LEU	2.2
19	S	29	ARG	2.2
1	A	1023	G	2.2
10	J	36	GLY	2.2
13	M	6	GLY	2.2
2	B	130	ARG	2.2
2	B	227	GLY	2.2
2	B	122	PHE	2.2
13	M	2	ALA	2.2
3	C	67	THR	2.2
12	L	115	LYS	2.2
2	B	230	VAL	2.2
10	J	98	ILE	2.2
12	L	60	LEU	2.1
2	B	132	LYS	2.1
8	H	98	LYS	2.1
13	M	41	PRO	2.1
18	R	19	LYS	2.1
10	J	89	ASP	2.1
5	E	109	ILE	2.1
5	E	130	ASN	2.1
1	A	1420	C	2.1
12	L	33	ARG	2.1
12	L	113	ARG	2.1
19	S	69	HIS	2.1
1	A	1008	C	2.1
2	B	121	LEU	2.1
19	S	30	LEU	2.1
3	C	47	LEU	2.0
9	I	14	VAL	2.0
9	I	53	VAL	2.0
10	J	7	LYS	2.0
13	M	88	ARG	2.0
12	L	120	TYR	2.0
6	F	36	ARG	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
14	N	34	TYR	2.0
13	M	19	LEU	2.0
11	K	127	LYS	2.0
12	L	34	ARG	2.0
1	A	1140	C	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
23	TM2	Y	34	28/29	0.40	-	108,113,122,123	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
27	K	Z	229	1/1	0.22	-	157,157,157,157	0
25	MG	Z	214	1/1	0.70	-	80,80,80,80	0
25	MG	Z	81	1/1	0.28	-	95,95,95,95	0
25	MG	Z	110	1/1	1.84	-	130,130,130,130	0
25	MG	Z	60	1/1	0.94	-	105,105,105,105	0
25	MG	Z	16	1/1	0.17	-	69,69,69,69	0
25	MG	Z	113	1/1	0.74	-	114,114,114,114	0
27	K	Z	266	1/1	0.50	-	123,123,123,123	0
25	MG	Z	128	1/1	1.62	-	125,125,125,125	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	201	1/1	0.07	-	58,58,58,58	0
25	MG	Z	3	1/1	1.93	-	152,152,152,152	0
27	K	Z	286	1/1	0.42	-	161,161,161,161	0
25	MG	Z	216	1/1	0.07	-	106,106,106,106	0
25	MG	Z	67	1/1	0.26	-	98,98,98,98	0
25	MG	Z	172	1/1	0.17	-	111,111,111,111	0
25	MG	Z	130	1/1	0.64	-	104,104,104,104	0
27	K	Z	265	1/1	0.38	-	145,145,145,145	0
25	MG	Z	168	1/1	0.25	-	111,111,111,111	0
27	K	Z	259	1/1	0.25	-	146,146,146,146	0
27	K	Z	231	1/1	0.33	-	125,125,125,125	0
25	MG	Z	44	1/1	0.93	-	109,109,109,109	0
25	MG	Z	114	1/1	2.69	-	171,171,171,171	0
25	MG	Z	152	1/1	0.67	-	76,76,76,76	0
27	K	Z	221	1/1	0.45	-	150,150,150,150	0
27	K	Z	282	1/1	0.23	-	129,129,129,129	0
25	MG	Z	192	1/1	0.81	-	65,65,65,65	0
25	MG	Z	88	1/1	0.52	-	114,114,114,114	0
25	MG	Z	129	1/1	0.16	-	84,84,84,84	0
25	MG	Z	142	1/1	0.72	-	99,99,99,99	0
25	MG	Z	104	1/1	0.32	-	71,71,71,71	0
27	K	Z	219	1/1	0.15	-	101,101,101,101	0
25	MG	Z	28	1/1	1.13	-	94,94,94,94	0
27	K	Z	237	1/1	0.37	-	117,117,117,117	0
25	MG	Z	22	1/1	0.38	-	65,65,65,65	0
25	MG	Z	33	1/1	0.43	-	119,119,119,119	0
25	MG	Z	118	1/1	0.22	-	115,115,115,115	0
25	MG	Z	186	1/1	1.02	-	118,118,118,118	0
25	MG	Z	162	1/1	0.88	-	69,69,69,69	0
25	MG	Z	125	1/1	0.94	-	132,132,132,132	0
25	MG	Z	77	1/1	0.58	-	132,132,132,132	0
27	K	Z	235	1/1	0.26	-	128,128,128,128	0
25	MG	Z	106	1/1	0.34	-	65,65,65,65	0
27	K	Z	233	1/1	0.14	-	136,136,136,136	0
25	MG	Z	68	1/1	1.26	-	153,153,153,153	0
25	MG	Z	34	1/1	0.44	-	125,125,125,125	0
27	K	Z	225	1/1	0.17	-	129,129,129,129	0
25	MG	Z	8	1/1	1.03	-	95,95,95,95	0
25	MG	Z	160	1/1	0.29	-	88,88,88,88	0
27	K	Z	287	1/1	1.02	-	117,117,117,117	0
25	MG	Z	146	1/1	0.40	-	94,94,94,94	0
27	K	Z	285	1/1	0.61	-	116,116,116,116	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	K	Z	258	1/1	0.68	-	168,168,168,168	0
25	MG	Z	109	1/1	0.88	-	124,124,124,124	0
27	K	Z	246	1/1	0.91	-	159,159,159,159	0
25	MG	Z	209	1/1	0.17	-	68,68,68,68	0
25	MG	Z	164	1/1	0.81	-	154,154,154,154	0
27	K	Z	284	1/1	0.55	-	88,88,88,88	0
25	MG	Z	54	1/1	1.23	-	119,119,119,119	0
25	MG	Z	137	1/1	0.17	-	75,75,75,75	0
25	MG	Z	187	1/1	0.34	-	102,102,102,102	0
25	MG	Z	182	1/1	0.36	-	73,73,73,73	0
25	MG	Z	211	1/1	0.82	-	136,136,136,136	0
25	MG	Z	57	1/1	0.84	-	88,88,88,88	0
25	MG	Z	121	1/1	1.28	-	106,106,106,106	0
27	K	Z	236	1/1	0.51	-	98,98,98,98	0
25	MG	Z	7	1/1	1.15	-	117,117,117,117	0
25	MG	Z	199	1/1	0.49	-	96,96,96,96	0
25	MG	Z	30	1/1	1.44	-	117,117,117,117	0
25	MG	Z	24	1/1	0.34	-	105,105,105,105	0
25	MG	Z	6	1/1	0.07	-	82,82,82,82	0
25	MG	Z	80	1/1	0.24	-	101,101,101,101	0
25	MG	Z	150	1/1	0.49	-	102,102,102,102	0
25	MG	Z	37	1/1	0.68	-	98,98,98,98	0
27	K	Z	224	1/1	0.18	-	106,106,106,106	0
27	K	Z	218	1/1	0.35	-	106,106,106,106	0
25	MG	Z	46	1/1	0.83	-	107,107,107,107	0
27	K	Z	245	1/1	0.59	-	108,108,108,108	0
27	K	Z	249	1/1	0.33	-	155,155,155,155	0
25	MG	Z	174	1/1	0.16	-	71,71,71,71	0
25	MG	Z	65	1/1	1.14	-	130,130,130,130	0
25	MG	Z	86	1/1	1.03	-	124,124,124,124	0
25	MG	Z	66	1/1	1.17	-	125,125,125,125	0
27	K	Z	240	1/1	0.26	-	108,108,108,108	0
25	MG	Z	102	1/1	0.80	-	110,110,110,110	0
25	MG	Z	41	1/1	1.10	-	104,104,104,104	0
25	MG	Z	180	1/1	0.18	-	118,118,118,118	0
25	MG	Z	59	1/1	0.78	-	128,128,128,128	0
27	K	Z	228	1/1	1.30	-	200,200,200,200	0
25	MG	Z	143	1/1	0.48	-	76,76,76,76	0
25	MG	Z	161	1/1	0.79	-	48,48,48,48	0
25	MG	Z	89	1/1	1.17	-	133,133,133,133	0
25	MG	Z	159	1/1	0.69	-	95,95,95,95	0
25	MG	Z	105	1/1	1.08	-	106,106,106,106	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	73	1/1	0.56	-	114,114,114,114	0
25	MG	Z	200	1/1	0.91	-	125,125,125,125	0
25	MG	Z	61	1/1	0.94	-	92,92,92,92	0
25	MG	Z	215	1/1	0.44	-	95,95,95,95	0
25	MG	Z	9	1/1	0.47	-	67,67,67,67	0
25	MG	Z	62	1/1	2.16	-	111,111,111,111	0
25	MG	Z	103	1/1	0.25	-	80,80,80,80	0
25	MG	Z	45	1/1	0.52	-	138,138,138,138	0
25	MG	Z	97	1/1	0.54	-	139,139,139,139	0
26	ZN	Z	141	1/1	0.25	-	102,102,102,102	0
27	K	Z	255	1/1	0.67	-	94,94,94,94	0
27	K	Z	288	1/1	0.35	-	113,113,113,113	0
25	MG	Z	19	1/1	0.23	-	92,92,92,92	0
27	K	Z	289	1/1	0.14	-	122,122,122,122	0
25	MG	Z	194	1/1	0.16	-	143,143,143,143	0
25	MG	Z	5	1/1	1.26	-	110,110,110,110	0
25	MG	Z	101	1/1	0.46	-	74,74,74,74	0
25	MG	Z	148	1/1	0.46	-	80,80,80,80	0
25	MG	Z	163	1/1	1.15	-	152,152,152,152	0
25	MG	Z	120	1/1	0.29	-	85,85,85,85	0
25	MG	Z	49	1/1	0.37	-	89,89,89,89	0
25	MG	Z	197	1/1	0.75	-	66,66,66,66	0
25	MG	Z	176	1/1	0.27	-	71,71,71,71	0
25	MG	Z	95	1/1	0.57	-	107,107,107,107	0
25	MG	Z	71	1/1	1.63	-	126,126,126,126	0
27	K	Z	239	1/1	0.14	-	130,130,130,130	0
25	MG	Z	154	1/1	0.54	-	116,116,116,116	0
27	K	Z	234	1/1	0.23	-	128,128,128,128	0
25	MG	Z	191	1/1	0.05	-	103,103,103,103	0
25	MG	Z	32	1/1	0.92	-	186,186,186,186	0
25	MG	Z	111	1/1	1.24	-	139,139,139,139	0
27	K	Z	260	1/1	0.66	-	136,136,136,136	0
27	K	Z	248	1/1	0.72	-	138,138,138,138	0
25	MG	Z	31	1/1	1.27	-	122,122,122,122	0
27	K	Z	280	1/1	0.21	-	151,151,151,151	0
27	K	Z	274	1/1	1.15	-	161,161,161,161	0
25	MG	Z	184	1/1	0.75	-	66,66,66,66	0
25	MG	Z	107	1/1	0.76	-	90,90,90,90	0
25	MG	Z	149	1/1	0.49	-	99,99,99,99	0
25	MG	Z	75	1/1	0.64	-	114,114,114,114	0
25	MG	Z	83	1/1	1.49	-	123,123,123,123	0
25	MG	Z	14	1/1	0.28	-	84,84,84,84	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	K	Z	281	1/1	0.20	-	143,143,143,143	0
25	MG	Z	175	1/1	0.12	-	67,67,67,67	0
27	K	Z	283	1/1	0.40	-	173,173,173,173	0
25	MG	Z	17	1/1	0.16	-	68,68,68,68	0
27	K	Z	270	1/1	0.41	-	81,81,81,81	0
27	K	Z	277	1/1	0.80	-	151,151,151,151	0
27	K	Z	223	1/1	0.48	-	120,120,120,120	0
25	MG	Z	193	1/1	1.21	-	86,86,86,86	0
27	K	Z	268	1/1	0.79	-	94,94,94,94	0
25	MG	Z	133	1/1	0.31	-	104,104,104,104	0
25	MG	Z	183	1/1	0.89	-	127,127,127,127	0
25	MG	Z	173	1/1	0.51	-	100,100,100,100	0
25	MG	Z	27	1/1	0.28	-	148,148,148,148	0
25	MG	Z	91	1/1	0.51	-	104,104,104,104	0
27	K	Z	278	1/1	0.11	-	164,164,164,164	0
27	K	Z	222	1/1	0.29	-	129,129,129,129	0
27	K	Z	243	1/1	0.21	-	146,146,146,146	0
25	MG	Z	181	1/1	0.54	-	60,60,60,60	0
27	K	Z	227	1/1	0.31	-	142,142,142,142	0
25	MG	Z	134	1/1	0.39	-	87,87,87,87	0
27	K	Z	261	1/1	0.38	-	111,111,111,111	0
25	MG	Z	10	1/1	5.15	-	181,181,181,181	0
25	MG	Z	63	1/1	1.36	-	115,115,115,115	0
25	MG	Z	207	1/1	0.12	-	68,68,68,68	0
25	MG	Z	43	1/1	0.56	-	118,118,118,118	0
25	MG	Z	96	1/1	0.66	-	103,103,103,103	0
25	MG	Z	39	1/1	0.26	-	100,100,100,100	0
25	MG	Z	47	1/1	0.83	-	104,104,104,104	0
25	MG	Z	124	1/1	0.97	-	119,119,119,119	0
25	MG	Z	53	1/1	0.78	-	65,65,65,65	0
27	K	Z	267	1/1	0.67	-	150,150,150,150	0
25	MG	Z	117	1/1	0.11	-	107,107,107,107	0
25	MG	Z	87	1/1	0.30	-	97,97,97,97	0
25	MG	Z	90	1/1	2.10	-	149,149,149,149	0
25	MG	Z	210	1/1	0.33	-	80,80,80,80	0
25	MG	Z	79	1/1	0.56	-	28,28,28,28	0
25	MG	Z	21	1/1	0.71	-	51,51,51,51	0
25	MG	Z	11	1/1	0.32	-	111,111,111,111	0
25	MG	Z	205	1/1	0.24	-	44,44,44,44	0
25	MG	Z	100	1/1	0.57	-	88,88,88,88	0
25	MG	Z	147	1/1	0.70	-	101,101,101,101	0
26	ZN	Z	140	1/1	0.75	-	174,174,174,174	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
27	K	Z	264	1/1	0.56	-	94,94,94,94	0
25	MG	Z	144	1/1	0.59	-	73,73,73,73	0
27	K	Z	226	1/1	0.23	-	140,140,140,140	0
25	MG	Z	178	1/1	0.38	-	142,142,142,142	0
25	MG	Z	92	1/1	1.30	-	126,126,126,126	0
25	MG	Z	169	1/1	0.28	-	94,94,94,94	0
25	MG	Z	23	1/1	0.84	-	113,113,113,113	0
27	K	Z	279	1/1	0.59	-	121,121,121,121	0
25	MG	Z	38	1/1	0.50	-	124,124,124,124	0
25	MG	Z	126	1/1	3.49	-	135,135,135,135	0
25	MG	Z	166	1/1	0.09	-	61,61,61,61	0
27	K	Z	269	1/1	0.66	-	84,84,84,84	0
25	MG	Z	179	1/1	0.54	-	58,58,58,58	0
27	K	Z	276	1/1	0.73	-	184,184,184,184	0
25	MG	Z	213	1/1	0.27	-	131,131,131,131	0
25	MG	Z	70	1/1	1.34	-	99,99,99,99	0
25	MG	Z	188	1/1	0.30	-	91,91,91,91	0
25	MG	Z	25	1/1	0.88	-	119,119,119,119	0
25	MG	Z	165	1/1	0.09	-	112,112,112,112	0
25	MG	Z	74	1/1	0.12	-	86,86,86,86	0
25	MG	Z	157	1/1	0.26	-	145,145,145,145	0
25	MG	Z	50	1/1	0.30	-	96,96,96,96	0
25	MG	Z	300	1/1	0.08	-	68,68,68,68	0
25	MG	Z	18	1/1	0.48	-	81,81,81,81	0
25	MG	Z	64	1/1	0.93	-	141,141,141,141	0
25	MG	Z	189	1/1	0.13	-	104,104,104,104	0
25	MG	Z	4	1/1	0.28	-	47,47,47,47	0
25	MG	Z	98	1/1	0.68	-	117,117,117,117	0
27	K	Z	254	1/1	0.55	-	98,98,98,98	0
25	MG	Z	94	1/1	0.35	-	75,75,75,75	0
27	K	Z	256	1/1	0.30	-	145,145,145,145	0
25	MG	Z	122	1/1	0.95	-	123,123,123,123	0
25	MG	Z	69	1/1	0.62	-	104,104,104,104	0
25	MG	Z	155	1/1	0.25	-	80,80,80,80	0
25	MG	Z	84	1/1	0.73	-	85,85,85,85	0
27	K	Z	220	1/1	0.29	-	127,127,127,127	0
25	MG	Z	2	1/1	0.12	-	148,148,148,148	0
25	MG	Z	185	1/1	0.21	-	63,63,63,63	0
27	K	Z	263	1/1	1.11	-	78,78,78,78	0
25	MG	Z	119	1/1	0.19	-	75,75,75,75	0
25	MG	Z	208	1/1	0.70	-	90,90,90,90	0
25	MG	Z	138	1/1	0.69	-	100,100,100,100	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	136	1/1	1.08	-	66,66,66,66	0
25	MG	Z	115	1/1	1.13	-	132,132,132,132	0
25	MG	Z	204	1/1	0.17	-	108,108,108,108	0
25	MG	Z	203	1/1	0.18	-	200,200,200,200	0
25	MG	Z	135	1/1	0.83	-	99,99,99,99	0
25	MG	Z	202	1/1	0.51	-	56,56,56,56	0
27	K	Z	250	1/1	0.31	-	168,168,168,168	0
27	K	Z	271	1/1	0.43	-	155,155,155,155	0
25	MG	Z	15	1/1	1.17	-	169,169,169,169	0
25	MG	Z	167	1/1	0.24	-	174,174,174,174	0
25	MG	Z	151	1/1	0.91	-	109,109,109,109	0
25	MG	Z	112	1/1	1.01	-	113,113,113,113	0
27	K	Z	247	1/1	0.77	-	152,152,152,152	0
25	MG	Z	29	1/1	0.69	-	89,89,89,89	0
25	MG	Z	195	1/1	0.37	-	76,76,76,76	0
25	MG	Z	78	1/1	2.12	-	137,137,137,137	0
25	MG	Z	13	1/1	0.21	-	62,62,62,62	0
27	K	Z	273	1/1	0.34	-	157,157,157,157	0
25	MG	Z	35	1/1	2.40	-	134,134,134,134	0
27	K	Z	257	1/1	0.21	-	111,111,111,111	0
25	MG	Z	132	1/1	0.62	-	96,96,96,96	0
27	K	Z	241	1/1	1.24	-	167,167,167,167	0
25	MG	Z	116	1/1	0.51	-	112,112,112,112	0
24	PAR	Z	1	42/42	0.21	-	66,72,84,88	0
25	MG	Z	131	1/1	0.68	-	106,106,106,106	0
27	K	Z	217	1/1	0.07	-	81,81,81,81	0
27	K	Z	252	1/1	0.46	-	85,85,85,85	0
25	MG	Z	206	1/1	0.48	-	69,69,69,69	0
25	MG	Z	93	1/1	0.38	-	70,70,70,70	0
25	MG	Z	42	1/1	0.90	-	113,113,113,113	0
27	K	Z	251	1/1	0.37	-	120,120,120,120	0
25	MG	Z	48	1/1	1.57	-	130,130,130,130	0
25	MG	Z	190	1/1	0.20	-	96,96,96,96	0
25	MG	Z	55	1/1	0.80	-	141,141,141,141	0
27	K	Z	242	1/1	0.18	-	119,119,119,119	0
25	MG	Z	158	1/1	0.90	-	102,102,102,102	0
27	K	Z	230	1/1	1.46	-	188,188,188,188	0
25	MG	Z	72	1/1	0.24	-	159,159,159,159	0
25	MG	Z	99	1/1	0.17	-	52,52,52,52	0
27	K	Z	253	1/1	0.21	-	72,72,72,72	0
25	MG	Z	12	1/1	0.61	-	88,88,88,88	0
27	K	Z	275	1/1	0.48	-	132,132,132,132	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
25	MG	Z	82	1/1	0.42	-	96,96,96,96	0
25	MG	Z	52	1/1	0.25	-	74,74,74,74	0
27	K	Z	262	1/1	0.67	-	149,149,149,149	0
25	MG	Z	20	1/1	0.65	-	85,85,85,85	0
25	MG	Z	196	1/1	0.20	-	92,92,92,92	0
25	MG	Z	198	1/1	0.10	-	123,123,123,123	0
25	MG	Z	177	1/1	0.11	-	124,124,124,124	0
25	MG	Z	127	1/1	0.30	-	88,88,88,88	0
27	K	Z	272	1/1	0.33	-	132,132,132,132	0
25	MG	Z	123	1/1	0.26	-	79,79,79,79	0
25	MG	Z	153	1/1	0.60	-	104,104,104,104	0
25	MG	Z	36	1/1	0.34	-	96,96,96,96	0
25	MG	Z	85	1/1	0.49	-	124,124,124,124	0
25	MG	Z	26	1/1	1.99	-	130,130,130,130	0
25	MG	Z	40	1/1	1.57	-	131,131,131,131	0
25	MG	Z	170	1/1	0.12	-	131,131,131,131	0
25	MG	Z	156	1/1	0.88	-	120,120,120,120	0
25	MG	Z	76	1/1	0.52	-	130,130,130,130	0
27	K	Z	238	1/1	0.35	-	146,146,146,146	0
25	MG	Z	145	1/1	0.16	-	54,54,54,54	0
27	K	Z	232	1/1	1.16	-	156,156,156,156	0
25	MG	Z	108	1/1	0.33	-	73,73,73,73	0
27	K	Z	244	1/1	0.33	-	140,140,140,140	0
25	MG	Z	212	1/1	0.31	-	81,81,81,81	0
25	MG	Z	56	1/1	0.38	-	142,142,142,142	0
25	MG	Z	171	1/1	0.23	-	117,117,117,117	0
25	MG	Z	58	1/1	0.72	-	98,98,98,98	0
25	MG	Z	139	1/1	0.10	-	83,83,83,83	0
25	MG	Z	51	1/1	1.41	-	109,109,109,109	0

6.5 Other polymers ⓘ

There are no such residues in this entry.