



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:29 PM UTC

PDB ID : 5LMS / pdb_00005lms
EMDB ID : EMD-4078
Title : Structure of bacterial 30S-IF1-IF3-mRNA-tRNA translation pre-initiation complex(state-2C)
Authors : Hussain, T.; Llacer, J.L.; Wimberly, B.T.; Ramakrishnan, V.
Deposited on : 2016-08-01
Resolution : 5.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

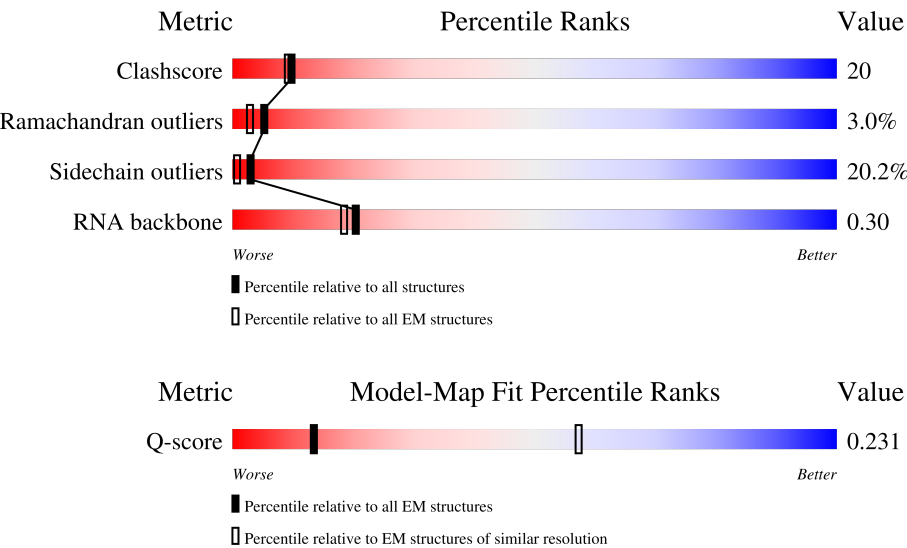
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 5.10 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.



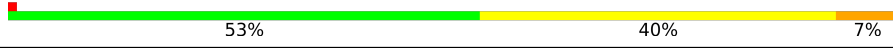
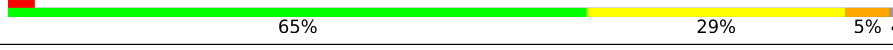
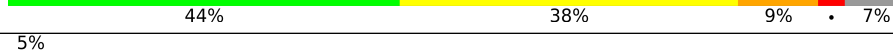
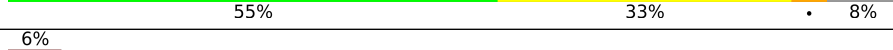
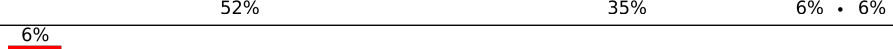
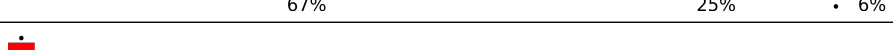
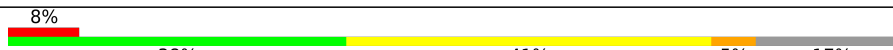
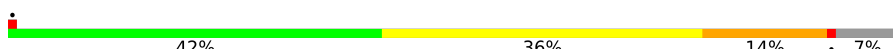
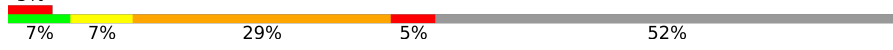
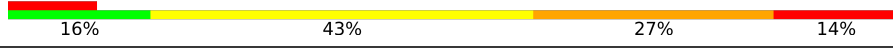
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	844 (4.60 - 5.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1522	 22% 57% 18% . .
2	B	256	 21% 49% 33% 8% . 9%
3	C	239	 52% 26% 8% 14%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	209	
5	E	162	
6	F	101	
7	G	156	
8	H	138	
9	I	128	
10	J	105	
11	K	129	
12	L	132	
13	M	126	
14	N	61	
15	O	89	
16	P	88	
17	Q	105	
18	R	88	
19	S	93	
20	T	106	
21	V	27	
22	W	72	
23	X	171	
24	Y	42	
25	Z	77	

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 55648 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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					AltConf	Trace
1	A	1514	Total	C	N	O	P	0	0
			32522	14481	6019	10512	1510		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1900	1213	341	341	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1612	1016	314	281	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	150	Total	C	N	O	S	0	0
			1146	724	217	201	4		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	98	Total	C	N	O	S	0	0
			792	498	156	137	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	124	Total	C	N	O	S	0	0
			970	611	195	163	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	118	Total	C	N	O	S	0	0
			937	579	193	163	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	83	Total	C	N	O	S	0	0
			700	443	139	117	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	R	73	Total	C	N	O	0	0
			598	381	118	99		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	80	Total	C	N	O	S	0	0
			647	414	119	112	2		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	V	24	Total	C	N	O	0	0
			208	128	50	30		

- Molecule 22 is a protein called Translation initiation factor IF-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	71	Total	C	N	O	S	0	0
			565	359	102	102	2		

- Molecule 23 is a protein called Translation initiation factor IF-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	164	Total	C	N	O	S	0	0
			1336	841	245	241	9		

- Molecule 24 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	20	Total	C	N	O	P	0	0
			439	196	89	134	20		

- Molecule 25 is a RNA chain called tRNAi.

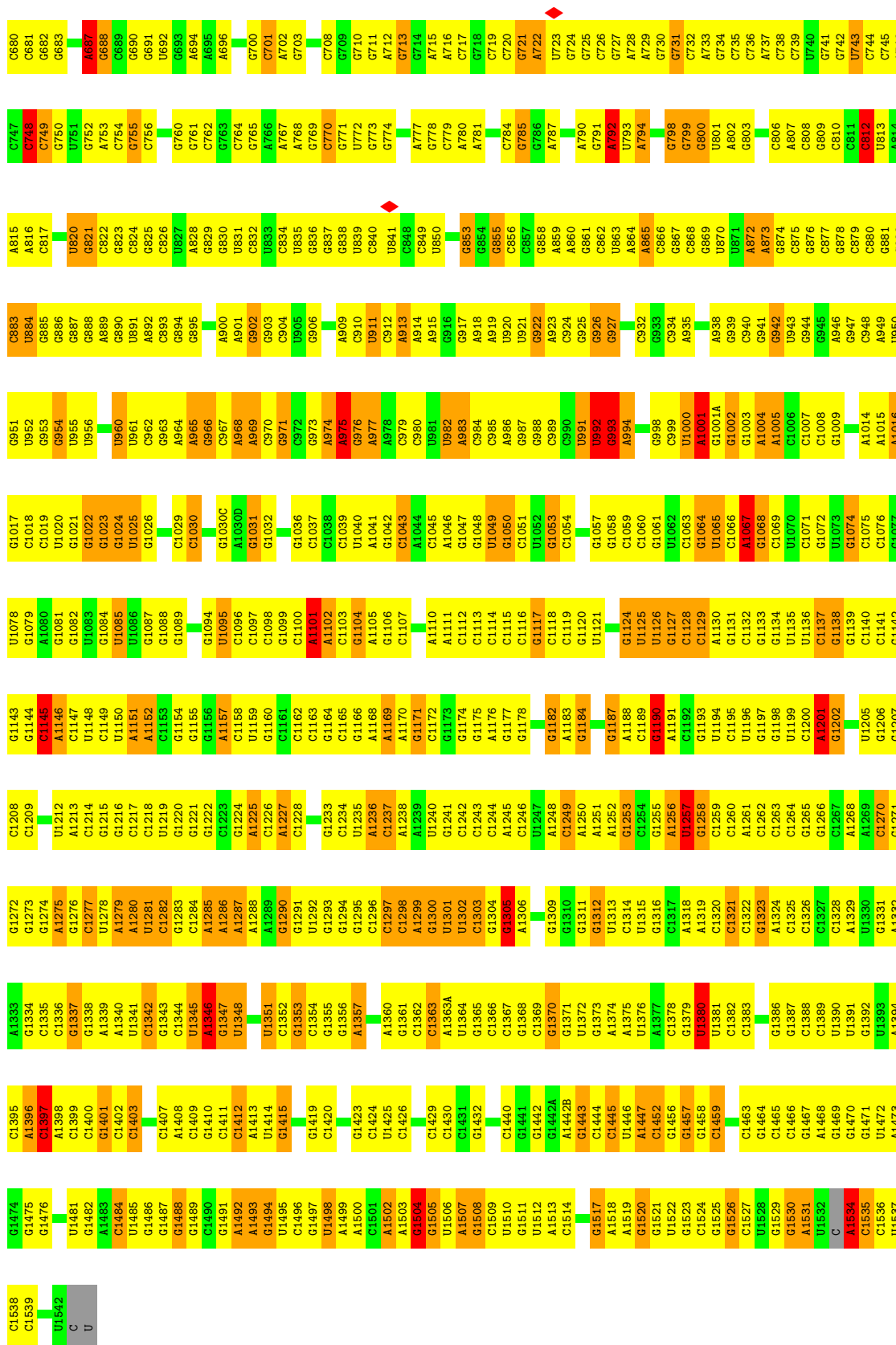
Mol	Chain	Residues	Atoms						AltConf	Trace
25	Z	77	Total	C	N	O	P	S	0	0
			1646	735	297	536	77	1		

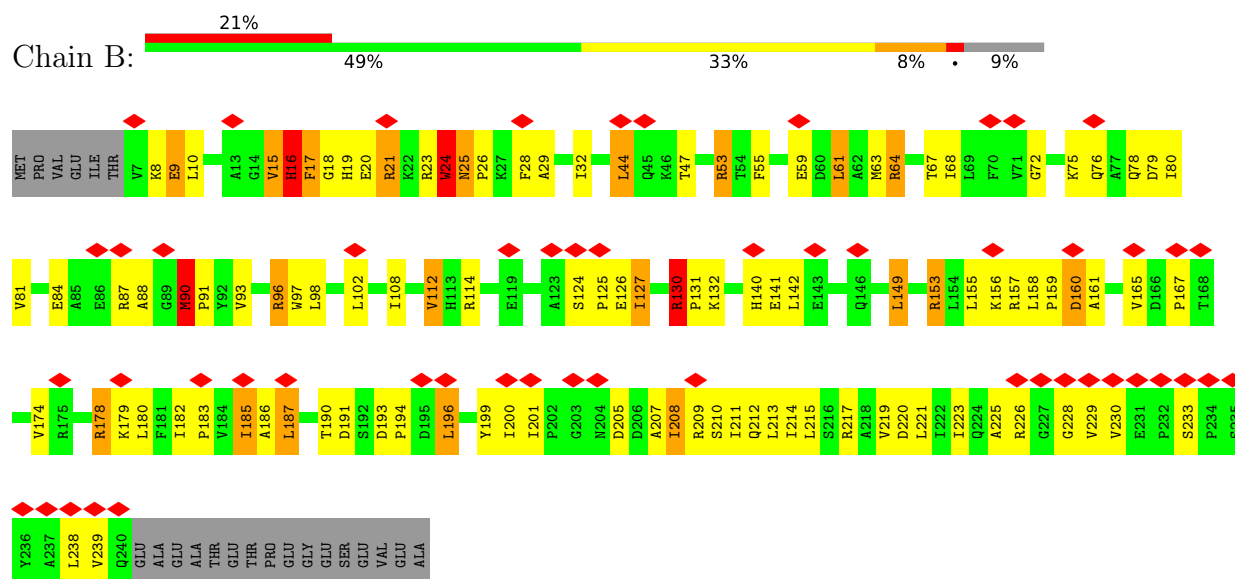
- Molecule 26 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
26	D	1	Total	Zn	0
			1	1	
26	N	1	Total	Zn	0
			1	1	

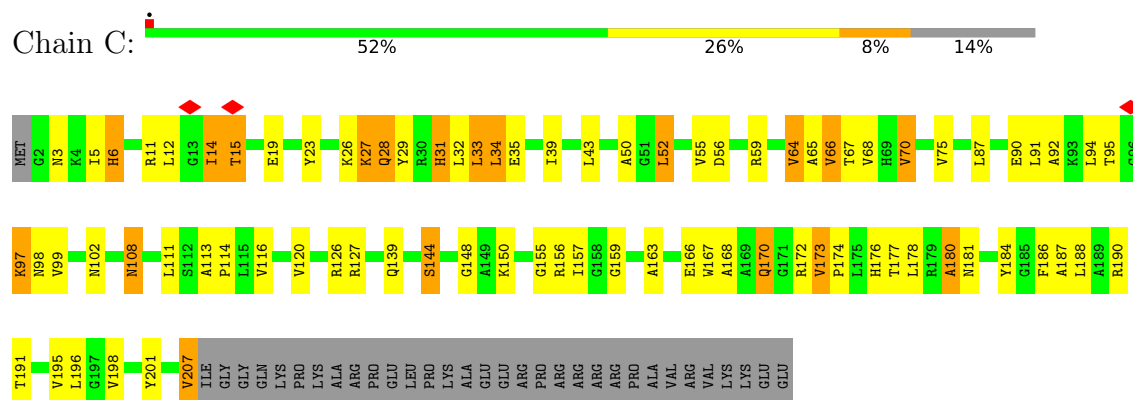
- Molecule 27 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
27	W	1	Total	Mg	0
			1	1	
27	Z	1	Total	Mg	0
			1	1	

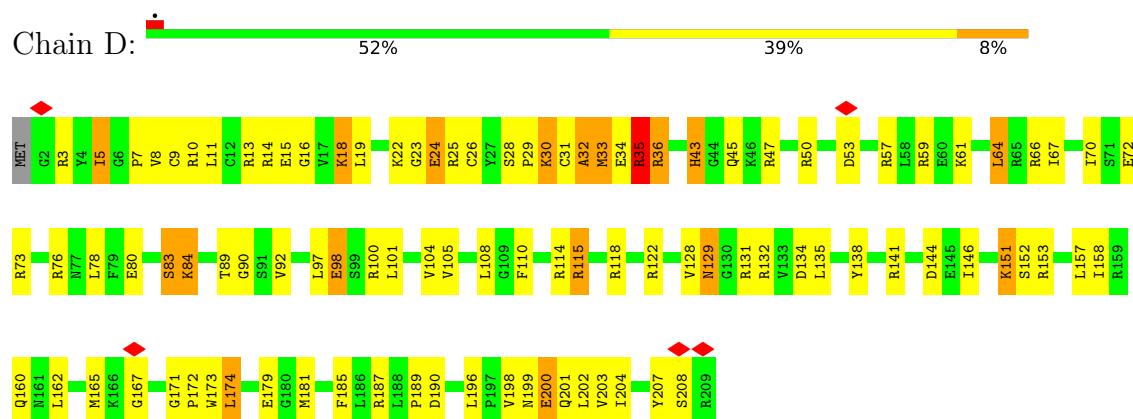




• Molecule 3: 30S ribosomal protein S3

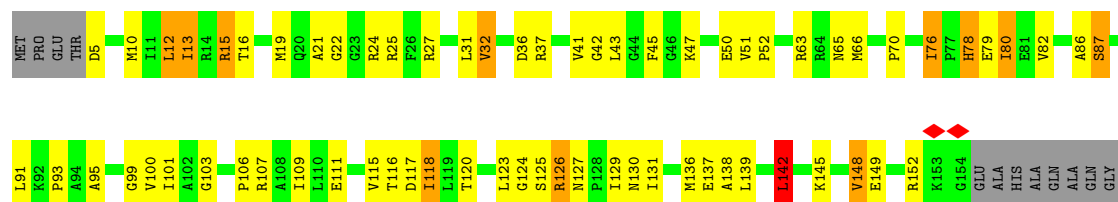


• Molecule 4: 30S ribosomal protein S4

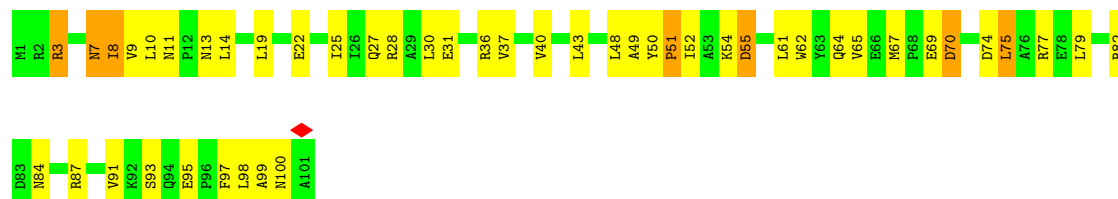


• Molecule 5: 30S ribosomal protein S5

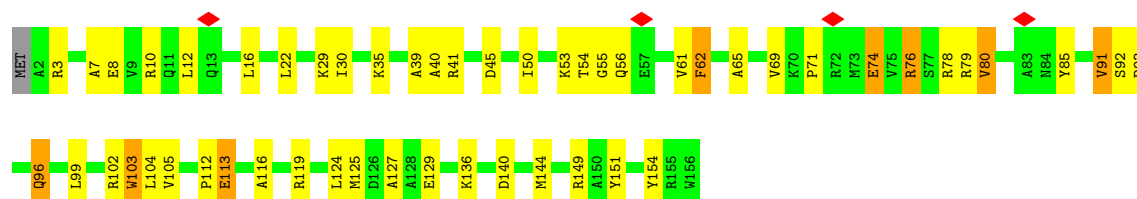




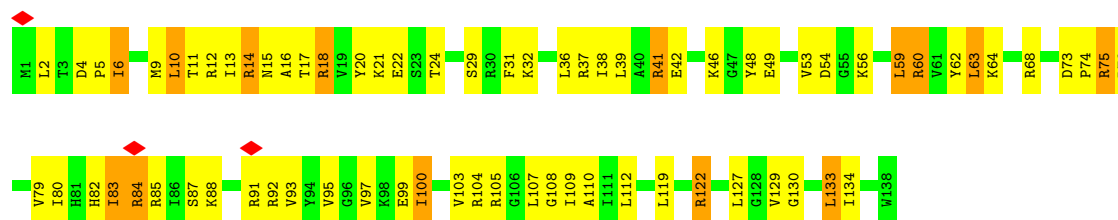
• Molecule 6: 30S ribosomal protein S6



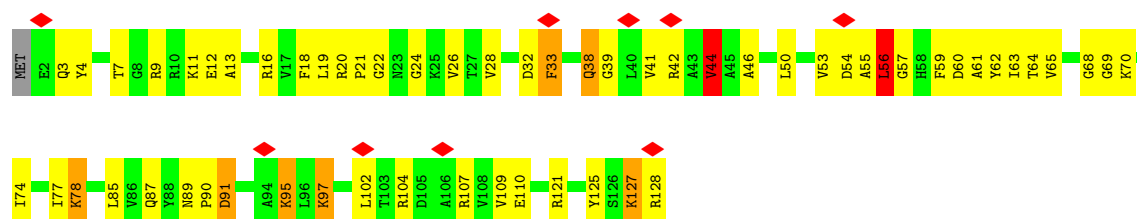
• Molecule 7: 30S ribosomal protein S7



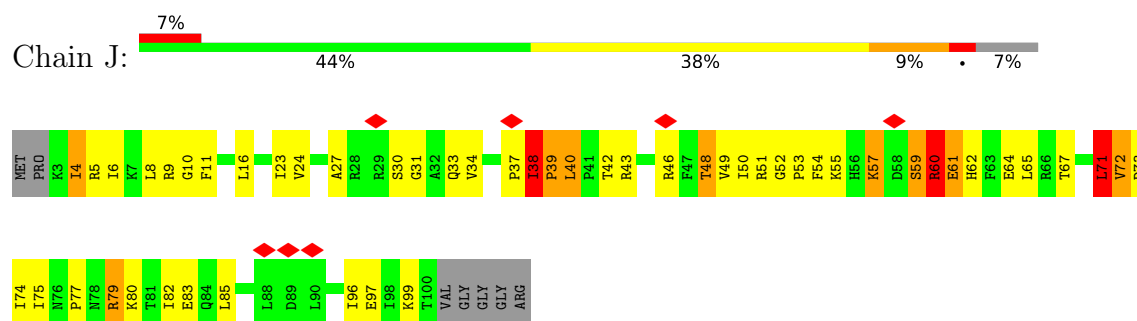
• Molecule 8: 30S ribosomal protein S8



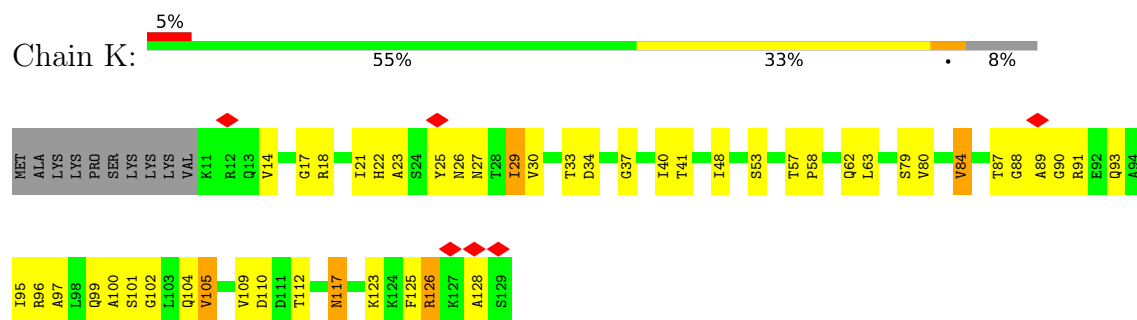
• Molecule 9: 30S ribosomal protein S9



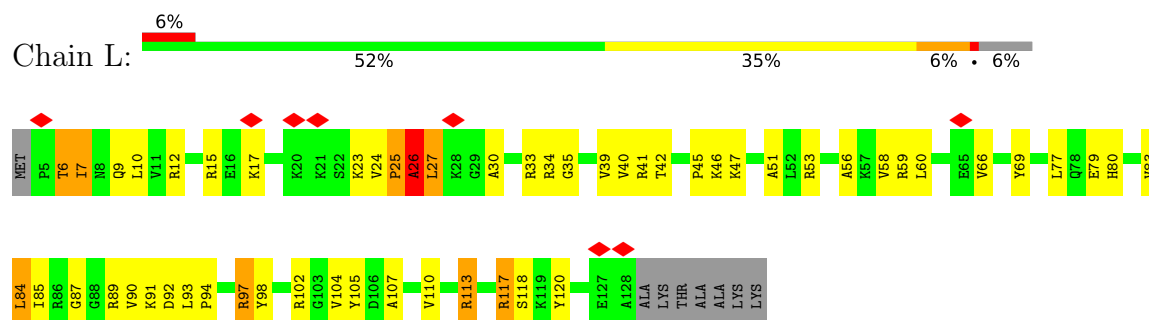
- Molecule 10: 30S ribosomal protein S10



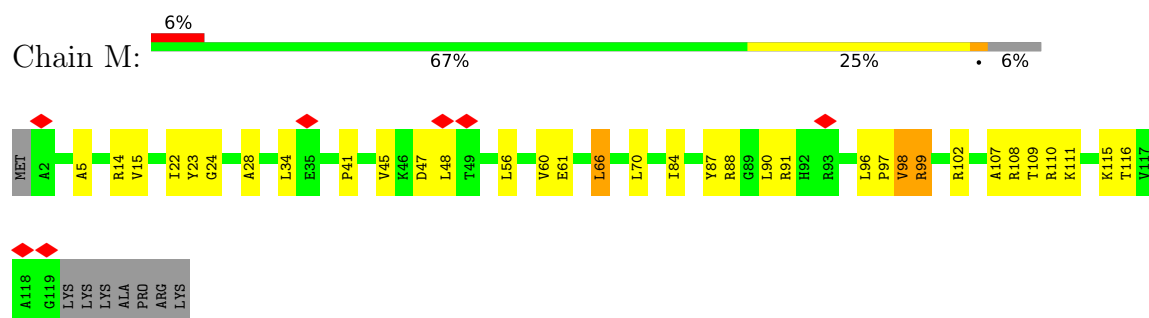
- Molecule 11: 30S ribosomal protein S11



- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13

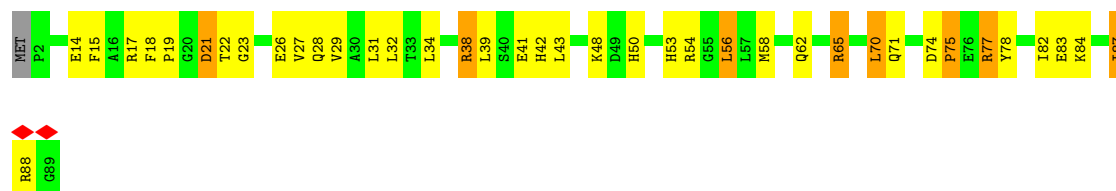


- Molecule 14: 30S ribosomal protein S14 type Z

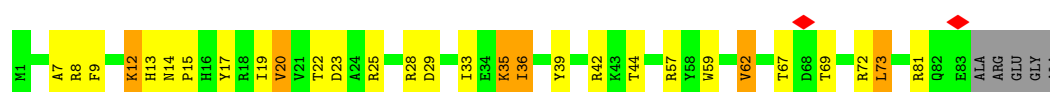




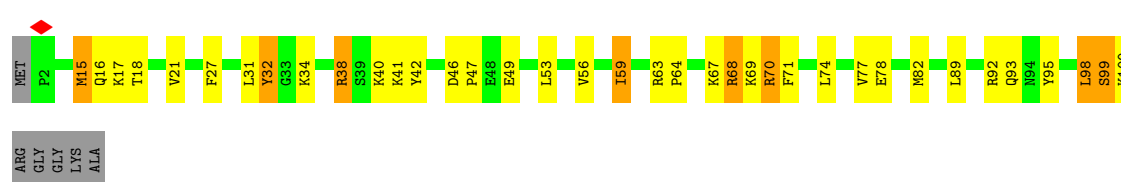
- Molecule 15: 30S ribosomal protein S15



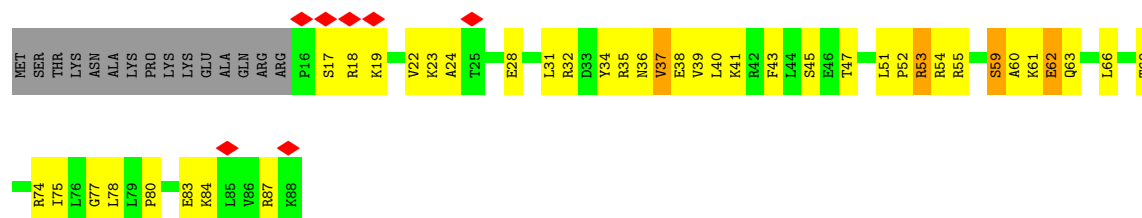
- Molecule 16: 30S ribosomal protein S16



- Molecule 17: 30S ribosomal protein S17



- Molecule 18: 30S ribosomal protein S18



- Molecule 19: 30S ribosomal protein S19



GLY
LYS
GLU
ALA
LYS
LYS
ALA
THR
LYS
LYS

- Molecule 20: 30S ribosomal protein S20

Chain T: 

MET ALA GLN LYS LYS PRO LYS LYS R8 R9 S10 S11 A12 L13 K14 R15 Q18 S19 L24 L20 R23 R25 A28 K29 I33 I41 Q42 L43 A44 Q45 A49 E50 E51 A52 L53 K54 I55 M56 R57 E60 S61 L62 K65 K68 G69 S70 T71 L72 H73 K74 N75 A76

A77 A78 R79 R80 R81 S82 R83 L84 M85 R86 K87 V88 R89 Q90 L91 L92 E93 A94 A95 G96 A97 I100 L104 S105 A106

- Molecule 21: 30S ribosomal protein Thx

Chain V: 

MET G2 K3 G4 K12 I13 Y21 K25 LYS LYS

- Molecule 22: Translation initiation factor IF-1

Chain W: 

MET A1 K2 E3 K4 D5 T6 I7 R8 T9 E10 G11 V12 V13 T14 E15 A16 L17 P18 N19 A20 T21 F22 R23 V24 D27 S28 G29 P30 E31 I32 L33 S37 M40 R46 P49 G50 D51 R52 V53 V54 V55 E56 R64 G65 R66 I67 V68 V69 R70 K71

- Molecule 23: Translation initiation factor IF-3

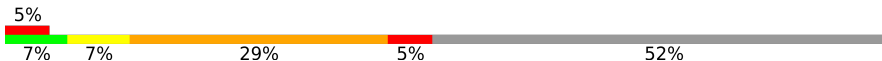
Chain X: 

MET K3 E4 Y5 T7 N8 R9 R10 I11 A12 R13 K14 K15 V16 V17 V18 V19 G20 P21 D22 G23 K24 Q25 L26 G27 I28 M29 D30 T31 R32 E33 A34 L35 R36 L37 A38 Q39 E40 M41 D42 L43 D44 L45 V46 L47 V48 G49 P50 N51 A52 D53 P54 P55 V56 A57 R58 I59 M60 D61

Y62 S63 K64 W65 Y67 E68 Q69 Q70 M71 A72 E73 K74 E75 A76 R77 R78 LYS ALA LYS ARG T83 T84 E85 V85 K86 S87 I88 K89 F90 R91 V92 K93 I94 D95 E96 Y99 L103 I106 Q111 V116 K117 V118 T119 I120 M121 F122 R123 G124 R125 E126 V127 A128 E131

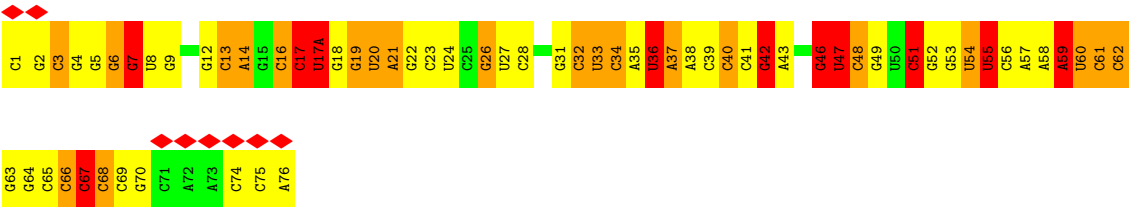
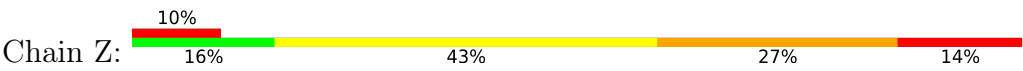
R135 I136 L137 V140 D143 V150 P154 E155 M156 L157 G158 R159 N162 M163 L164 P167 V168 K169 V170 SER ALA

- Molecule 24: mRNA

Chain Y: 

G C U C U U U U A A C A A U U U A U C A20 G21 G22 C23 A24 A25 G26 G27 A28 G29 G30 U31 A32 A33 A34 A35 A36 U37 G38 U39 C A

- Molecule 25: tRNAi



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	7898	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	104478	Depositor
Image detector	OTHER	Depositor
Maximum map value	0.356	Depositor
Minimum map value	-0.108	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.055	Depositor
Map size ($\text{\AA}$)	348.4, 348.4, 348.4	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.34, 1.34, 1.34	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, G7M, 4SU, OMC, 5MU, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.45	0/36394	0.86	84/56779 (0.1%)
2	B	0.81	1/1935 (0.1%)	1.18	7/2609 (0.3%)
3	C	0.65	0/1636	1.23	13/2205 (0.6%)
4	D	0.65	0/1733	1.26	10/2318 (0.4%)
5	E	0.65	0/1162	1.37	8/1564 (0.5%)
6	F	0.64	0/856	1.14	5/1154 (0.4%)
7	G	0.70	0/1276	1.18	3/1709 (0.2%)
8	H	0.62	0/1136	1.16	3/1527 (0.2%)
9	I	0.69	0/1029	1.20	2/1379 (0.1%)
10	J	0.84	0/805	1.67	13/1082 (1.2%)
11	K	0.78	0/900	1.23	7/1213 (0.6%)
12	L	0.57	0/986	1.06	4/1320 (0.3%)
13	M	0.76	0/947	1.16	2/1270 (0.2%)
14	N	0.59	0/501	1.01	0/664
15	O	0.65	0/745	1.26	1/992 (0.1%)
16	P	0.57	0/716	1.00	1/963 (0.1%)
17	Q	0.56	0/836	1.08	2/1117 (0.2%)
18	R	0.76	0/604	1.17	1/801 (0.1%)
19	S	0.91	0/661	1.35	3/890 (0.3%)
20	T	0.67	0/765	1.35	5/1007 (0.5%)
21	V	0.79	0/212	0.97	0/277
22	W	0.98	0/575	1.46	6/778 (0.8%)
23	X	1.01	1/1354 (0.1%)	1.28	11/1813 (0.6%)
24	Y	0.61	0/493	0.94	2/766 (0.3%)
25	Z	0.66	2/1719 (0.1%)	1.00	12/2674 (0.4%)
All	All	0.57	4/59976 (0.0%)	1.00	205/88871 (0.2%)

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
3	C	1	0
14	N	0	1
19	S	1	0
23	X	0	1
All	All	2	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	42	G	O3'-P	10.61	1.77	1.61
2	B	233	SER	C-N	5.67	1.38	1.33
25	Z	46	G7M	O3'-P	5.62	1.61	1.56
23	X	54	PRO	CA-C	5.58	1.57	1.52

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	15	ARG	N-CA-C	-23.22	71.68	109.76
19	S	70	LYS	CB-CA-C	23.20	156.58	110.42
9	I	7	THR	CB-CA-C	-22.34	74.42	111.51
10	J	60	ARG	CB-CA-C	-17.92	74.76	110.42
22	W	23	ARG	N-CA-C	-16.90	82.89	109.76
10	J	59	SER	N-CA-C	-16.31	81.34	109.06
10	J	71	LEU	N-CA-C	-16.18	83.03	109.40
3	C	65	ALA	N-CA-C	-16.08	83.19	109.40
5	E	16	THR	N-CA-CB	-15.59	86.64	111.43
10	J	72	VAL	N-CA-C	-14.28	79.64	109.34
10	J	72	VAL	CB-CA-C	-13.99	88.35	111.29
22	W	33	LEU	CB-CA-C	-13.88	87.94	110.14
4	D	34	GLU	N-CA-C	13.78	133.96	111.37
3	C	14	ILE	N-CA-C	13.67	137.78	109.34
22	W	33	LEU	N-CA-C	-12.67	87.56	108.34
10	J	73	ASP	N-CA-CB	-12.33	91.23	111.20
4	D	35	ARG	N-CA-CB	-11.37	93.81	110.53
1	A	1498	U	C2'-C3'-O3'	10.81	125.72	109.50
1	A	266	G	C2'-C3'-O3'	10.10	124.64	109.50
1	A	1301	U	C2'-C3'-O3'	10.09	124.64	109.50
19	S	70	LYS	N-CA-C	-9.88	89.77	110.80
1	A	748	C	C2'-C3'-O3'	9.70	124.05	109.50
1	A	1049	U	C4'-C3'-O3'	9.62	123.82	109.40
11	K	89	ALA	N-CA-C	9.41	122.71	111.33
1	A	1182	G	C2'-C3'-O3'	9.37	123.56	109.50
1	A	1145	C	C2'-C3'-O3'	9.35	123.52	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	60	ARG	N-CA-CB	9.33	126.26	110.49
1	A	965	A	C2'-C3'-O3'	9.05	123.08	109.50
1	A	1346	A	C2'-C3'-O3'	9.02	123.03	109.50
11	K	17	GLY	N-CA-C	8.96	122.60	110.69
1	A	1067	A	C2'-C3'-O3'	8.93	122.90	109.50
1	A	428	G	C2'-C3'-O3'	8.91	122.86	109.50
10	J	59	SER	CB-CA-C	-8.90	91.32	109.38
1	A	792	A	C2'-C3'-O3'	8.71	122.56	109.50
1	A	328	C	C2'-C3'-O3'	8.70	122.56	109.50
1	A	281	G	C2'-C3'-O3'	8.66	122.49	109.50
1	A	1065	U	C2'-C3'-O3'	8.64	122.45	109.50
1	A	960	U	C2'-C3'-O3'	8.55	122.33	109.50
1	A	559	A	C2'-C3'-O3'	8.53	122.30	109.50
1	A	1201	A	C2'-C3'-O3'	8.38	122.07	109.50
22	W	24	VAL	N-CA-CB	-8.25	99.48	111.52
10	J	61	GLU	N-CA-C	-8.22	96.57	109.72
1	A	575	G	C2'-C3'-O3'	8.19	121.78	109.50
10	J	71	LEU	CB-CA-C	-8.10	93.89	109.37
1	A	181	G	C2'-C3'-O3'	8.03	121.55	109.50
1	A	51	A	C4'-C3'-O3'	7.91	121.26	109.40
25	Z	36	U	C2'-C3'-O3'	7.82	125.44	113.70
1	A	1534	A	C2'-C3'-O3'	7.81	125.42	113.70
1	A	60	A	C2'-C3'-O3'	7.76	121.14	109.50
1	A	1397	C	C4'-C3'-O3'	7.70	120.95	109.40
25	Z	47	U	C2'-C3'-O3'	7.68	121.02	109.50
1	A	351	G	C2'-C3'-O3'	7.62	120.94	109.50
6	F	67	MET	N-CA-C	7.58	115.04	108.22
3	C	15	THR	N-CA-CB	-7.51	99.69	110.81
1	A	197	A	C2'-C3'-O3'	7.50	120.75	109.50
10	J	61	GLU	N-CA-CB	-7.50	98.26	111.08
1	A	509	A	C4'-C3'-O3'	7.45	124.17	113.00
11	K	125	PHE	N-CA-C	-7.32	105.26	114.56
2	B	90	MET	CA-C-N	7.22	127.22	119.78
2	B	90	MET	C-N-CA	7.22	127.22	119.78
1	A	993	G	C4'-C3'-O3'	7.22	120.23	109.40
3	C	65	ALA	CB-CA-C	-7.21	95.60	109.37
1	A	701	C	C2'-C3'-O3'	7.19	124.48	113.70
15	O	18	PHE	N-CA-C	7.13	116.53	108.25
3	C	28	GLN	N-CA-C	7.10	123.60	113.02
23	X	54	PRO	N-CA-C	7.09	119.35	110.70
3	C	66	VAL	N-CA-C	-7.03	97.31	107.78
7	G	113	GLU	N-CA-C	6.96	120.24	109.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1285	A	C4'-C3'-O3'	6.94	119.81	109.40
1	A	1190	G	C2'-C3'-O3'	6.92	124.09	113.70
19	S	71	LEU	N-CA-CB	-6.90	94.54	110.83
1	A	792	A	C4'-C3'-O3'	6.89	119.73	109.40
25	Z	17(A)	U	C2'-C3'-O3'	6.86	119.78	109.50
12	L	26	ALA	N-CA-C	-6.85	103.91	113.37
5	E	21	ALA	N-CA-C	6.83	118.73	111.28
20	T	74	LYS	CB-CA-C	-6.72	108.81	116.54
25	Z	47	U	C4'-C3'-O3'	6.70	119.46	109.40
1	A	243	A	C2'-C3'-O3'	6.70	119.54	109.50
17	Q	98	LEU	N-CA-C	6.69	120.90	112.87
20	T	97	ALA	CA-C-N	6.65	128.15	119.84
20	T	97	ALA	C-N-CA	6.65	128.15	119.84
1	A	129(A)	G	C2'-C3'-O3'	6.61	119.41	109.50
20	T	55	ILE	CB-CA-C	6.59	121.03	112.14
4	D	135	LEU	CA-C-N	6.56	126.25	119.56
4	D	135	LEU	C-N-CA	6.56	126.25	119.56
3	C	6	HIS	CA-C-N	6.53	126.11	119.19
3	C	6	HIS	C-N-CA	6.53	126.11	119.19
1	A	687	A	C2'-C3'-O3'	6.52	119.27	109.50
1	A	181	G	C4'-C3'-O3'	6.49	119.14	109.40
3	C	27	LYS	N-CA-C	6.46	118.40	111.36
5	E	78	HIS	N-CA-C	6.41	117.89	108.86
2	B	130	ARG	CA-C-N	6.39	127.83	119.84
2	B	130	ARG	C-N-CA	6.39	127.83	119.84
1	A	1101	A	C4'-C3'-O3'	6.37	118.96	109.40
4	D	171	GLY	CA-C-N	6.37	127.81	119.84
4	D	171	GLY	C-N-CA	6.37	127.81	119.84
1	A	326	G	C4'-C3'-O3'	-6.36	103.46	113.00
1	A	1285	A	C2'-C3'-O3'	6.35	119.03	109.50
10	J	60	ARG	N-CA-C	-6.34	97.30	110.80
1	A	279	A	C4'-C3'-O3'	6.33	118.89	109.40
22	W	23	ARG	CB-CA-C	-6.30	99.57	109.84
9	I	70	LYS	N-CA-C	6.27	118.67	111.02
1	A	975	A	C2'-C3'-O3'	6.25	118.88	109.50
4	D	24	GLU	N-CA-C	-6.21	102.30	110.43
5	E	41	VAL	N-CA-C	6.20	116.94	107.77
1	A	372	C	C2'-C3'-O3'	6.19	118.79	109.50
4	D	208	SER	N-CA-C	6.16	119.21	107.75
1	A	250	A	C4'-C3'-O3'	6.16	118.63	109.40
4	D	16	GLY	N-CA-C	6.12	123.17	115.21
1	A	743	U	C4'-C3'-O3'	-6.11	103.83	113.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	812	C	C2'-C3'-O3'	6.09	122.84	113.70
25	Z	42	G	O3'-P-O5'	6.08	113.12	104.00
23	X	94	ILE	N-CA-C	6.07	117.41	109.58
1	A	60	A	C4'-C3'-O3'	6.01	118.42	109.40
25	Z	59	A	N9-C1'-C2'	6.01	121.02	112.00
2	B	24	TRP	N-CA-C	6.00	123.59	110.80
3	C	170	GLN	N-CA-C	6.00	118.31	109.24
13	M	60	VAL	N-CA-C	5.98	116.04	110.42
6	F	95	GLU	CA-C-N	5.96	125.98	119.90
6	F	95	GLU	C-N-CA	5.96	125.98	119.90
1	A	1380	U	C4'-C3'-O3'	5.95	118.33	109.40
25	Z	17(A)	U	C4'-C3'-O3'	5.86	118.19	109.40
1	A	484	G	C4'-C3'-O3'	5.86	118.18	109.40
5	E	99	GLY	N-CA-C	5.85	119.28	110.97
8	H	63	LEU	N-CA-C	5.81	118.43	109.07
11	K	33	THR	N-CA-C	5.74	117.69	109.14
1	A	840	C	C2'-C3'-O3'	-5.71	105.14	113.70
1	A	653	A	C2'-C3'-O3'	5.69	118.03	109.50
12	L	84	LEU	N-CA-C	5.68	118.36	108.76
23	X	136	ILE	CB-CA-C	5.65	119.42	112.02
1	A	484	G	C2'-C3'-O3'	5.63	117.95	109.50
23	X	7	THR	N-CA-C	5.63	118.73	109.72
1	A	1065	U	C4'-C3'-O3'	5.62	117.83	109.40
1	A	1305	G	C4'-C3'-O3'	-5.62	104.57	113.00
1	A	351	G	C4'-C3'-O3'	5.61	117.82	109.40
1	A	1101	A	C2'-C3'-O3'	5.59	117.88	109.50
13	M	108	ARG	N-CA-C	5.57	117.16	111.14
23	X	54	PRO	CA-C-N	5.57	125.50	119.76
23	X	54	PRO	C-N-CA	5.57	125.50	119.76
17	Q	32	TYR	N-CA-C	5.57	119.70	113.02
25	Z	66	C	N1-C1'-C2'	5.56	120.34	112.00
1	A	288	A	C4'-C3'-O3'	-5.55	104.68	113.00
25	Z	67	C	C4'-C3'-O3'	-5.54	104.69	113.00
1	A	496	A	C4'-C3'-O3'	5.53	117.70	109.40
1	A	368	U	C4'-C3'-O3'	-5.52	104.71	113.00
20	T	33	ILE	N-CA-C	-5.51	104.95	110.30
1	A	1201	A	C4'-C3'-O3'	5.50	117.64	109.40
16	P	22	THR	N-CA-C	5.49	116.31	108.74
1	A	71	C	C2'-C3'-O3'	-5.48	105.48	113.70
8	H	75	ARG	CA-C-N	5.44	126.64	119.84
8	H	75	ARG	C-N-CA	5.44	126.64	119.84
25	Z	7	G	C2'-C3'-O3'	5.44	117.66	109.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	30	ALA	CA-C-N	5.42	125.06	119.05
12	L	30	ALA	C-N-CA	5.42	125.06	119.05
1	A	1504	G	C4'-C3'-O3'	5.41	117.52	109.40
1	A	568	G	C4'-C3'-O3'	-5.41	104.88	113.00
1	A	780	A	C4'-C3'-O3'	-5.41	104.89	113.00
1	A	1257	U	C4'-C3'-O3'	5.41	117.51	109.40
3	C	180	ALA	N-CA-C	5.40	116.85	111.07
1	A	1504	G	C2'-C3'-O3'	5.39	117.59	109.50
1	A	1001	A	O4'-C4'-C3'	-5.39	98.61	104.00
1	A	366	C	C2'-C3'-O3'	5.38	117.56	109.50
2	B	233	SER	N-CA-C	5.36	121.66	109.81
23	X	53	ASP	CA-C-N	5.34	125.88	120.38
23	X	53	ASP	C-N-CA	5.34	125.88	120.38
23	X	56	VAL	N-CA-C	5.34	116.05	107.73
1	A	1125	U	C2'-C3'-O3'	-5.31	105.74	113.70
1	A	202	U	C4'-C3'-O3'	5.31	117.36	109.40
25	Z	17	C	C2'-C3'-O3'	5.31	117.46	109.50
1	A	572	A	C4'-C3'-O3'	-5.29	105.06	113.00
7	G	103	TRP	CB-CA-C	5.28	119.83	110.85
2	B	210	SER	N-CA-C	5.27	117.83	111.40
1	A	10	A	C4'-C3'-O3'	-5.24	105.14	113.00
25	Z	51	C	C4'-C3'-O3'	5.24	120.86	113.00
1	A	687	A	C4'-C3'-O3'	5.23	117.24	109.40
3	C	70	VAL	N-CA-C	5.21	117.55	108.95
1	A	965	A	C4'-C3'-O3'	5.19	117.19	109.40
1	A	883	C	C4'-C3'-O3'	-5.18	105.24	113.00
1	A	991	U	C4'-C3'-O3'	-5.16	105.26	113.00
1	A	7	G	C4'-C3'-O3'	5.14	117.11	109.40
24	Y	38	G	C2'-C3'-O3'	5.13	117.20	109.50
1	A	429	U	C4'-C3'-O3'	5.13	117.09	109.40
1	A	1145	C	C4'-C3'-O3'	-5.12	101.71	109.40
7	G	8	GLU	N-CA-C	5.12	117.64	109.96
23	X	49	GLY	CA-C-N	5.11	124.61	119.19
23	X	49	GLY	C-N-CA	5.11	124.61	119.19
1	A	992	U	C2'-C3'-O3'	5.09	117.14	109.50
11	K	80	VAL	N-CA-C	5.09	115.18	107.75
1	A	115	G	C2'-C3'-O3'	5.08	117.12	109.50
4	D	43	HIS	N-CA-C	-5.08	106.67	112.92
24	Y	31	U	C4'-C3'-O3'	5.08	120.61	113.00
1	A	1526	G	C4'-C3'-O3'	-5.07	105.40	113.00
18	R	24	ALA	N-CA-C	5.06	116.88	111.36
6	F	55	ASP	CA-C-N	5.05	124.55	119.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	55	ASP	C-N-CA	5.05	124.55	119.19
22	W	46	ARG	N-CA-C	5.05	117.19	110.53
1	A	964	A	C4'-C3'-O3'	-5.05	105.43	113.00
10	J	38	ILE	N-CA-CB	5.05	114.77	110.08
3	C	144	SER	N-CA-C	5.04	118.92	112.87
5	E	95	ALA	CA-C-N	5.03	125.03	119.90
5	E	95	ALA	C-N-CA	5.03	125.03	119.90
11	K	90	GLY	CA-C-N	-5.01	113.17	120.29
11	K	90	GLY	C-N-CA	-5.01	113.17	120.29
1	A	25	C	C4'-C3'-O3'	-5.01	105.49	113.00
1	A	1403	C	C4'-C3'-O3'	-5.01	105.49	113.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	14	ILE	CA
19	S	70	LYS	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	13	THR	Peptide
23	X	53	ASP	Peptide

5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32522	0	16436	1209	0
2	B	1900	0	1951	45	0
3	C	1612	0	1677	68	0
4	D	1703	0	1766	59	0
5	E	1146	0	1207	37	0
6	F	843	0	857	25	0
7	G	1257	0	1296	30	0
8	H	1116	0	1177	45	0
9	I	1010	0	1037	35	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	792	0	835	34	0
11	K	885	0	904	18	0
12	L	970	0	1057	34	0
13	M	937	0	995	17	0
14	N	492	0	530	30	0
15	O	734	0	771	18	0
16	P	700	0	720	16	0
17	Q	823	0	891	21	0
18	R	598	0	670	28	0
19	S	647	0	673	28	0
20	T	763	0	861	32	0
21	V	208	0	221	1	0
22	W	565	0	588	10	0
23	X	1336	0	1389	56	0
24	Y	439	0	219	38	0
25	Z	1646	0	845	119	0
26	D	1	0	0	1	0
26	N	1	0	0	0	0
27	W	1	0	0	0	0
27	Z	1	0	0	0	0
All	All	55648	0	39573	1854	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1854) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:199:ASN:ND2	4:D:202:LEU:HG	1.25	1.43
3:C:29:TYR:CE1	3:C:33:LEU:HD12	1.67	1.30
1:A:1345:U:N3	1:A:1375:A:N6	1.80	1.28
1:A:72:C:C2'	1:A:73:G:H5'	1.65	1.23
23:X:5:TYR:OH	25:Z:20:U:C6	1.92	1.21
4:D:199:ASN:HD22	4:D:202:LEU:CG	1.54	1.19
3:C:28:GLN:HG2	3:C:31:HIS:CD2	1.77	1.18
1:A:72:C:H2'	1:A:73:G:C5'	1.75	1.17
4:D:199:ASN:ND2	4:D:202:LEU:CG	2.09	1.14
1:A:1022:G:H2'	1:A:1023:G:C8	1.84	1.11
19:S:40:ILE:CD1	19:S:70:LYS:O	1.97	1.11
20:T:41:ILE:HD13	20:T:87:LYS:HZ3	1.15	1.10
3:C:29:TYR:HE1	3:C:33:LEU:HD12	0.93	1.09

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:29:TYR:HE1	3:C:33:LEU:CD1	1.66	1.08
1:A:1022:G:H2'	1:A:1023:G:H8	0.98	1.08
1:A:1219:U:H2'	1:A:1220:G:C8	1.89	1.06
1:A:1014:A:H5''	19:S:14:HIS:HB3	1.17	1.06
1:A:92:C:H2'	1:A:93:G:H8	1.21	1.04
1:A:1459:C:OP1	20:T:28:ALA:HA	1.57	1.03
1:A:664:G:N2	1:A:741:G:H1	1.57	1.03
20:T:41:ILE:HD13	20:T:87:LYS:NZ	1.74	1.02
1:A:1219:U:H2'	1:A:1220:G:H8	1.18	1.01
1:A:1256:A:H62	1:A:1278:U:H1'	1.26	1.00
1:A:974:A:H8	1:A:974:A:OP1	1.44	1.00
3:C:28:GLN:OE1	3:C:32:LEU:HD11	1.60	1.00
1:A:600:C:H2'	1:A:601:C:H6	1.27	0.99
23:X:65:TRP:CD1	25:Z:17(A):U:H3	1.81	0.99
1:A:1345:U:H3	1:A:1375:A:N6	1.49	0.99
19:S:40:ILE:HD11	19:S:70:LYS:O	1.57	0.98
1:A:917:G:H2'	1:A:918:A:C8	1.97	0.98
1:A:711:G:H2'	1:A:712:A:H8	1.30	0.96
1:A:225:C:H2'	1:A:226:G:H8	1.27	0.95
1:A:92:C:H2'	1:A:93:G:C8	2.01	0.94
4:D:199:ASN:HD22	4:D:202:LEU:CD1	1.80	0.94
25:Z:21:A:N7	25:Z:48:C:C4	2.36	0.94
1:A:1539:C:H42	24:Y:26:G:H1	1.14	0.93
1:A:674:G:H2'	1:A:675:A:H8	1.32	0.93
1:A:21:G:H2'	1:A:22:G:C8	2.04	0.93
1:A:80:G:H3'	1:A:81:U:H5''	1.51	0.93
4:D:201:GLN:HE22	5:E:116:THR:HG23	1.34	0.92
19:S:40:ILE:CG1	19:S:70:LYS:O	2.17	0.92
25:Z:51:C:H42	25:Z:63:G:H1	1.17	0.92
1:A:1030:C:H42	1:A:1031:G:H1	1.15	0.91
23:X:17:ARG:CZ	25:Z:56:C:N4	2.34	0.91
1:A:1014:A:C5'	19:S:14:HIS:HB3	2.01	0.91
1:A:79:G:H2'	1:A:80:G:H8	1.34	0.90
3:C:28:GLN:HG2	3:C:31:HIS:HD2	1.35	0.90
19:S:40:ILE:HG13	19:S:70:LYS:O	1.72	0.90
1:A:34:C:H2'	1:A:35:G:C8	2.06	0.90
1:A:745:C:H2'	1:A:746:A:C8	2.06	0.89
1:A:170:U:H2'	1:A:171:A:H8	1.36	0.89
1:A:920:U:H2'	1:A:921:U:C6	2.07	0.89
1:A:125:U:H2'	1:A:126:G:C8	2.08	0.89
1:A:1500:A:OP1	1:A:1508:G:OP1	1.90	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:C:H2'	1:A:73:G:H5'	0.90	0.89
8:H:29:SER:HB3	8:H:32:LYS:HG3	1.56	0.88
23:X:72:ALA:HB1	25:Z:14:A:O3'	1.73	0.88
23:X:56:VAL:HG21	25:Z:19:G:C5	2.09	0.87
1:A:600:C:H2'	1:A:601:C:C6	2.10	0.87
1:A:999:C:O2	1:A:1043:C:O2	1.91	0.87
12:L:25:PRO:C	12:L:27:LEU:H	1.75	0.87
23:X:5:TYR:OH	25:Z:20:U:H6	1.41	0.87
1:A:72:C:C2'	1:A:73:G:C5'	2.43	0.87
1:A:1345:U:C2	1:A:1375:A:N6	2.42	0.86
1:A:1264:C:H2'	1:A:1265:G:H8	1.38	0.86
5:E:106:PRO:HA	5:E:109:ILE:HD12	1.55	0.86
1:A:173:U:OP1	1:A:198:G:H4'	1.74	0.86
1:A:736:C:H2'	1:A:737:A:H8	1.40	0.86
12:L:9:GLN:HA	12:L:12:ARG:HE	1.40	0.85
1:A:34:C:H2'	1:A:35:G:H8	1.37	0.85
4:D:26:CYS:HA	4:D:31:CYS:HB2	1.58	0.84
25:Z:23:C:H2'	25:Z:24:U:C6	2.12	0.84
1:A:1007:C:H42	1:A:1022:G:H1	1.23	0.84
23:X:56:VAL:CG2	25:Z:19:G:C6	2.61	0.84
3:C:92:ALA:O	3:C:95:THR:O	1.94	0.84
1:A:243:A:H4'	1:A:244:U:O5'	1.75	0.84
1:A:743:U:H2'	1:A:744:C:C6	2.11	0.84
1:A:559:A:H4'	1:A:560:U:H5''	1.57	0.84
1:A:1128:C:H4'	9:I:16:ARG:HH22	1.39	0.84
1:A:711:G:H2'	1:A:712:A:C8	2.13	0.83
1:A:1040:U:H2'	1:A:1041:A:C8	2.13	0.83
1:A:1386:G:H2'	1:A:1387:G:H8	1.42	0.83
25:Z:21:A:C8	25:Z:48:C:N4	2.47	0.83
4:D:97:LEU:O	4:D:100:ARG:HB2	1.79	0.83
25:Z:27:U:C2'	25:Z:28:C:H5'	2.08	0.83
1:A:864:A:H2'	1:A:865:A:C8	2.14	0.83
2:B:178:ARG:HE	8:H:74:PRO:HB3	1.44	0.82
3:C:28:GLN:OE1	3:C:32:LEU:CD1	2.26	0.82
6:F:99:ALA:HB2	18:R:31:LEU:HG	1.61	0.82
4:D:199:ASN:HD22	4:D:202:LEU:HG	0.99	0.82
3:C:29:TYR:OH	14:N:54:PRO:HG2	1.79	0.82
23:X:56:VAL:HG21	25:Z:19:G:C6	2.13	0.82
1:A:256:U:H2'	1:A:257:G:C8	2.15	0.81
1:A:736:C:H2'	1:A:737:A:C8	2.15	0.81
1:A:773:G:H1	1:A:806:C:H42	1.24	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:A:H2'	1:A:540:G:H8	1.43	0.81
25:Z:51:C:H2'	25:Z:52:G:O4'	1.81	0.81
1:A:1264:C:H2'	1:A:1265:G:C8	2.15	0.81
1:A:1539:C:N4	24:Y:26:G:H1	1.79	0.80
2:B:61:LEU:HD11	2:B:160:ASP:HB3	1.63	0.80
1:A:1356:G:H2'	1:A:1357:A:C8	2.17	0.80
1:A:155:C:H2'	1:A:156:G:C8	2.17	0.80
10:J:51:ARG:HB2	10:J:59:SER:HB3	1.61	0.80
25:Z:21:A:N7	25:Z:48:C:N4	2.30	0.80
22:W:50:GLY:HA3	23:X:128:ALA:HB3	1.64	0.80
23:X:65:TRP:NE1	25:Z:17(A):U:H3	1.79	0.80
25:Z:68:C:H2'	25:Z:69:C:C6	2.17	0.80
1:A:1457:G:N2	1:A:1458:G:H1'	1.96	0.79
25:Z:22:G:OP2	25:Z:46:G7M:N1	2.15	0.79
1:A:269:C:H2'	1:A:270:A:C8	2.17	0.78
1:A:979:C:H2'	1:A:980:C:O4'	1.81	0.78
1:A:1488:G:H2'	1:A:1489:G:H8	1.47	0.78
3:C:29:TYR:OH	14:N:54:PRO:CG	2.31	0.78
1:A:524:G:C6	1:A:525:C:N4	2.51	0.78
1:A:1020:U:H2'	1:A:1021:G:H8	1.47	0.78
18:R:53:ARG:HH21	18:R:60:ALA:HB2	1.48	0.78
1:A:155:C:H2'	1:A:156:G:H8	1.49	0.78
1:A:1407:C:H2'	1:A:1408:A:H8	1.49	0.78
1:A:170:U:H2'	1:A:171:A:C8	2.19	0.77
13:M:61:GLU:HA	13:M:66:LEU:HD11	1.66	0.77
1:A:834:C:H5''	18:R:60:ALA:CB	2.14	0.77
1:A:1059:C:H2'	1:A:1060:C:C6	2.20	0.77
1:A:1151:A:HO2'	1:A:1152:A:H8	1.32	0.77
1:A:1488:G:H2'	1:A:1489:G:C8	2.20	0.77
17:Q:27:PHE:HE1	17:Q:38:ARG:HB2	1.50	0.77
24:Y:36:A:N6	25:Z:37:A:C6	2.51	0.77
1:A:865:A:H2'	1:A:866:C:C6	2.20	0.77
1:A:1311:G:N7	19:S:2:PRO:HA	1.99	0.77
8:H:12:ARG:HA	8:H:15:ASN:HD22	1.50	0.77
1:A:501:C:H2'	1:A:502:G:H8	1.47	0.76
1:A:1127:G:N2	1:A:1144:G:N2	2.33	0.76
16:P:59:TRP:O	16:P:62:VAL:HG23	1.84	0.76
23:X:157:LEU:HB2	25:Z:27:U:OP1	1.86	0.76
1:A:1099:G:C6	1:A:1100:C:N3	2.53	0.76
1:A:967:C:H2'	1:A:968:A:C8	2.20	0.76
4:D:26:CYS:SG	26:D:300:ZN:ZN	1.73	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:26:G:C5	25:Z:27:U:C5	2.74	0.76
1:A:1039:C:H2'	1:A:1040:U:C6	2.21	0.76
1:A:1097:C:H2'	1:A:1098:C:C6	2.21	0.75
19:S:22:LEU:HD13	19:S:28:LYS:HB3	1.69	0.75
1:A:313:A:H2'	1:A:314:C:C6	2.22	0.75
1:A:544:G:H2'	1:A:545:C:O4'	1.86	0.75
1:A:944:G:O6	1:A:1337:G:H8	1.69	0.75
1:A:90:U:H2'	1:A:91:C:C6	2.21	0.75
1:A:539:A:H2'	1:A:540:G:C8	2.21	0.75
1:A:524:G:C2	1:A:525:C:N3	2.55	0.75
3:C:97:LYS:NZ	3:C:97:LYS:HB3	2.01	0.75
1:A:1396:A:O3'	1:A:1397:C:H5''	1.87	0.74
23:X:65:TRP:CD1	25:Z:17(A):U:N3	2.54	0.74
25:Z:20:U:H5''	25:Z:21:A:OP2	1.88	0.74
25:Z:27:U:H2'	25:Z:28:C:H5'	1.69	0.74
25:Z:27:U:O2'	25:Z:28:C:H5'	1.87	0.74
1:A:1102:A:H2'	1:A:1103:C:C6	2.22	0.74
1:A:674:G:H2'	1:A:675:A:C8	2.21	0.74
4:D:115:ARG:O	4:D:118:ARG:HG2	1.87	0.74
1:A:125:U:H2'	1:A:126:G:H8	1.52	0.74
20:T:70:SER:HA	20:T:73:HIS:CD2	2.23	0.73
1:A:974:A:OP1	1:A:974:A:C8	2.36	0.73
25:Z:21:A:C5	25:Z:48:C:N3	2.56	0.73
2:B:80:ILE:HG21	2:B:212:GLN:HA	1.70	0.73
23:X:17:ARG:CZ	25:Z:56:C:H41	2.02	0.73
1:A:1128:C:H4'	9:I:16:ARG:NH2	2.02	0.73
1:A:1262:C:H42	1:A:1273:G:H1	1.36	0.73
13:M:61:GLU:HA	13:M:66:LEU:CD1	2.17	0.73
1:A:40:C:H2'	1:A:41:G:H8	1.52	0.73
1:A:571:U:H3'	1:A:572:A:H5''	1.68	0.73
23:X:48:VAL:HG21	23:X:58:ARG:HE	1.52	0.73
23:X:17:ARG:NE	25:Z:56:C:N4	2.36	0.73
1:A:1445:C:C2	1:A:1458:G:C2	2.77	0.72
1:A:269:C:H2'	1:A:270:A:H8	1.53	0.72
1:A:1496:C:OP1	23:X:91:ARG:HB2	1.89	0.72
23:X:157:LEU:HD13	25:Z:27:U:C5'	2.20	0.72
1:A:80:G:H3'	1:A:81:U:C5'	2.19	0.72
25:Z:51:C:N4	25:Z:63:G:H1	1.87	0.72
3:C:59:ARG:HH12	3:C:97:LYS:HD3	1.54	0.72
12:L:45:PRO:HG2	12:L:51:ALA:H	1.55	0.72
20:T:83:ARG:HA	20:T:86:ARG:HH11	1.55	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:C:O2'	8:H:15:ASN:ND2	2.23	0.72
1:A:1314:C:H2'	1:A:1315:U:C6	2.25	0.72
1:A:438:G:N1	1:A:495:A:OP2	2.21	0.71
1:A:1030:C:N4	1:A:1031:G:H1	1.88	0.71
4:D:199:ASN:HD21	4:D:202:LEU:HG	1.52	0.71
1:A:1338:G:N2	25:Z:42:G:H1'	2.05	0.71
6:F:50:TYR:HB2	6:F:51:PRO:HD2	1.73	0.71
1:A:131:C:H2'	1:A:132:C:C6	2.25	0.71
15:O:15:PHE:CZ	15:O:84:LYS:HB3	2.26	0.71
24:Y:39:U:O4	25:Z:35:A:H1'	1.91	0.71
1:A:312:C:H2'	1:A:313:A:C8	2.26	0.71
1:A:1513:A:H2'	1:A:1514:C:C6	2.25	0.71
10:J:79:ARG:HH11	10:J:79:ARG:HA	1.56	0.71
1:A:72:C:C3'	1:A:73:G:H5'	2.20	0.71
23:X:17:ARG:NH2	23:X:19:VAL:HG22	2.05	0.70
1:A:1389:C:H2'	1:A:1390:U:O4'	1.90	0.70
1:A:1457:G:C4	1:A:1458:G:C8	2.79	0.70
25:Z:53:G:H1	25:Z:61:C:H42	1.36	0.70
1:A:1475:G:H2'	1:A:1476:G:H8	1.55	0.70
4:D:201:GLN:NE2	5:E:116:THR:HG23	2.05	0.70
1:A:533:A:O2'	1:A:535:A:OP2	2.10	0.70
25:Z:5:G:H1	25:Z:68:C:H42	1.37	0.70
4:D:201:GLN:HE22	5:E:116:THR:CG2	2.04	0.70
1:A:105:G:H2'	1:A:106:C:C6	2.26	0.70
1:A:868:C:H2'	1:A:869:G:O4'	1.91	0.70
2:B:72:GLY:HA3	2:B:81:VAL:HG21	1.74	0.70
7:G:53:LYS:HD2	7:G:125:MET:HE1	1.74	0.70
8:H:6:ILE:HB	8:H:85:ARG:HH12	1.57	0.69
10:J:27:ALA:HB2	10:J:85:LEU:HD21	1.74	0.69
11:K:23:ALA:HB1	11:K:88:GLY:H	1.55	0.69
16:P:59:TRP:O	16:P:62:VAL:CG2	2.40	0.69
1:A:255:G:H2'	1:A:256:U:C6	2.27	0.69
1:A:917:G:H2'	1:A:918:A:H8	1.58	0.69
8:H:48:TYR:HD2	8:H:59:LEU:HD21	1.57	0.69
15:O:38:ARG:HB3	15:O:38:ARG:HH11	1.57	0.69
23:X:5:TYR:OH	25:Z:20:U:C5	2.45	0.69
25:Z:21:A:C6	25:Z:48:C:C2	2.80	0.69
1:A:977:A:H1'	1:A:982:U:O4	1.93	0.69
1:A:70:G:C2	1:A:100:C:O2	2.46	0.69
1:A:728:A:H2'	1:A:729:A:C8	2.28	0.69
1:A:1124:G:O2'	1:A:1126:U:O4	2.11	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1463:C:H2'	1:A:1464:G:H8	1.57	0.69
20:T:50:GLU:HG3	20:T:100:ILE:HB	1.75	0.69
1:A:373:A:H2'	1:A:374:A:H8	1.56	0.69
1:A:407:G:H2'	1:A:408:A:H8	1.57	0.69
1:A:442:C:H2'	1:A:443:C:C6	2.28	0.69
1:A:521:G:N2	1:A:522:C:C2	2.60	0.69
1:A:1457:G:C2	1:A:1458:G:N9	2.60	0.69
1:A:79:G:H2'	1:A:80:G:C8	2.25	0.68
1:A:189(A):C:H2'	1:A:189(B):C:C6	2.28	0.68
1:A:614:A:H2'	1:A:615:C:C6	2.27	0.68
13:M:22:ILE:HG22	13:M:24:GLY:H	1.57	0.68
1:A:500:G:H2'	1:A:501:C:C6	2.28	0.68
1:A:1162:C:C2	1:A:1175:G:N2	2.61	0.68
1:A:1345:U:O4	1:A:1375:A:N1	2.26	0.68
2:B:112:VAL:HG13	2:B:153:ARG:HB3	1.74	0.68
20:T:10:LEU:HD12	20:T:11:SER:H	1.58	0.68
1:A:525:C:H2'	1:A:526:C:C6	2.28	0.68
1:A:745:C:H2'	1:A:746:A:H8	1.54	0.68
1:A:922:G:H2'	1:A:923:A:C8	2.29	0.68
3:C:29:TYR:CZ	3:C:33:LEU:HD12	2.25	0.68
2:B:68:ILE:HG12	2:B:161:ALA:HB3	1.75	0.68
1:A:70:G:C6	1:A:100:C:N3	2.62	0.68
1:A:778:G:H2'	1:A:779:C:O4'	1.93	0.68
25:Z:67:C:H2'	25:Z:68:C:C6	2.29	0.68
1:A:501:C:H2'	1:A:502:G:C8	2.28	0.68
1:A:571:U:C3'	1:A:572:A:H5''	2.24	0.68
1:A:834:C:H2'	1:A:835:U:C6	2.29	0.68
1:A:1124:G:H2'	1:A:1145:C:H5	1.56	0.68
25:Z:69:C:H2'	25:Z:70:G:C8	2.28	0.68
1:A:287:U:H2'	1:A:288:A:H8	1.59	0.67
1:A:424:G:H2'	1:A:425:G:H8	1.58	0.67
1:A:1407:C:H2'	1:A:1408:A:C8	2.29	0.67
24:Y:32:A:H3'	24:Y:33:A:H5''	1.76	0.67
1:A:240:C:H2'	1:A:241:C:H6	1.59	0.67
25:Z:1:C:H2'	25:Z:2:G:H8	1.59	0.67
1:A:183:G:H2'	1:A:184:G:O4'	1.94	0.67
1:A:613:C:H42	1:A:627:G:H1	1.43	0.67
1:A:1256:A:H62	1:A:1278:U:C1'	2.04	0.67
3:C:26:LYS:HD3	14:N:36:PHE:HE1	1.58	0.67
25:Z:21:A:C5	25:Z:48:C:C4	2.81	0.67
10:J:49:VAL:HB	14:N:41:ARG:HB2	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:C:O2'	1:A:1000:U:H5'	1.94	0.67
1:A:948:C:H2'	1:A:949:A:H8	1.60	0.67
1:A:1392:G:N2	1:A:1502:A:H8	1.92	0.67
1:A:1534:A:H2'	1:A:1535:C:C6	2.30	0.67
10:J:38:ILE:HG23	10:J:71:LEU:HB3	1.77	0.67
1:A:784:C:C2	1:A:799:G:N2	2.63	0.67
1:A:1410:G:H2'	1:A:1411:C:C6	2.30	0.67
1:A:1464:G:N2	1:A:1465:C:C2	2.63	0.67
19:S:40:ILE:HD13	19:S:62:ILE:HD11	1.76	0.67
25:Z:6:G:H2'	25:Z:7:G:C8	2.29	0.67
1:A:1059:C:H2'	1:A:1060:C:H6	1.60	0.66
19:S:11:VAL:HA	19:S:38:SER:HB2	1.77	0.66
1:A:671:G:N2	1:A:736:C:C2	2.63	0.66
1:A:683:G:N2	1:A:708:C:C2	2.63	0.66
1:A:1475:G:H2'	1:A:1476:G:C8	2.30	0.66
8:H:12:ARG:HB3	8:H:24:THR:HG21	1.75	0.66
10:J:62:HIS:HB2	14:N:59:ALA:HB3	1.76	0.66
25:Z:26:G:C6	25:Z:27:U:C5	2.83	0.66
1:A:728:A:H2'	1:A:729:A:H8	1.60	0.66
1:A:860:A:H3'	1:A:861:G:H8	1.61	0.66
1:A:1163:C:C2	1:A:1174:G:N2	2.64	0.66
23:X:5:TYR:CZ	25:Z:20:U:H6	2.13	0.66
1:A:313:A:H2'	1:A:314:C:H6	1.60	0.66
1:A:546:G:OP2	4:D:72:GLU:HB3	1.95	0.66
15:O:26:GLU:O	15:O:29:VAL:HG12	1.95	0.66
20:T:25:ARG:O	20:T:29:LYS:HG2	1.96	0.66
23:X:106:ILE:HG23	23:X:116:VAL:HG11	1.77	0.66
1:A:1063:C:H2'	1:A:1064:G:C8	2.31	0.66
1:A:1046:A:H3'	1:A:1047:G:H8	1.61	0.66
1:A:1525:G:H2'	1:A:1526:G:H8	1.61	0.66
20:T:41:ILE:CD1	20:T:87:LYS:NZ	2.56	0.66
1:A:773:G:H1	1:A:806:C:N4	1.92	0.65
10:J:53:PRO:HA	14:N:41:ARG:HH21	1.61	0.65
1:A:955:U:H2'	1:A:956:U:O4'	1.96	0.65
2:B:223:ILE:HG21	2:B:230:VAL:HB	1.78	0.65
23:X:56:VAL:HG22	25:Z:19:G:C6	2.31	0.65
1:A:737:A:H2'	1:A:738:C:C6	2.31	0.65
1:A:1030:C:C2	1:A:1032:G:N2	2.64	0.65
1:A:1395:C:H2'	1:A:1396:A:C8	2.32	0.65
1:A:1511:G:H2'	1:A:1512:U:C6	2.31	0.65
1:A:234:C:H2'	1:A:235:C:C6	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:C:H5''	18:R:60:ALA:HB2	1.77	0.65
1:A:834:C:H2'	1:A:835:U:H6	1.61	0.65
1:A:670:G:H1	1:A:736:C:H42	1.43	0.65
1:A:225:C:H2'	1:A:226:G:C8	2.20	0.65
25:Z:59:A:H2'	25:Z:60:U:O4'	1.95	0.65
1:A:849:C:H2'	1:A:850:U:O4'	1.95	0.65
8:H:64:LYS:HB3	8:H:79:VAL:HG11	1.79	0.65
16:P:81:ARG:HH11	16:P:81:ARG:HB2	1.62	0.65
1:A:256:U:H2'	1:A:257:G:H8	1.61	0.65
1:A:880:C:H2'	1:A:881:G:H8	1.61	0.65
1:A:1198:G:H2'	1:A:1199:U:O4'	1.96	0.65
12:L:24:VAL:HG12	12:L:26:ALA:H	1.63	0.65
1:A:1221:G:H5''	1:A:1321:C:O2	1.98	0.64
3:C:28:GLN:O	3:C:31:HIS:HD2	1.80	0.64
1:A:1137:C:H4'	1:A:1138:G:C2	2.32	0.64
6:F:27:GLN:HA	6:F:30:LEU:HD12	1.78	0.64
24:Y:30:G:H2'	24:Y:31:U:H5''	1.79	0.64
25:Z:23:C:H2'	25:Z:24:U:H6	1.60	0.64
1:A:1143:G:H2'	1:A:1144:G:C8	2.32	0.64
2:B:59:GLU:HG3	2:B:225:ALA:HB2	1.79	0.64
1:A:911:U:H2'	1:A:912:C:C6	2.33	0.64
1:A:1071:C:H2'	1:A:1072:G:H8	1.62	0.64
1:A:1415:G:N2	1:A:1486:G:H1'	2.12	0.64
3:C:64:VAL:HB	3:C:99:VAL:HG23	1.79	0.64
1:A:132:C:C2	1:A:231:G:N2	2.66	0.64
1:A:677:U:H3	1:A:713:G:H22	1.44	0.64
5:E:145:LYS:HA	8:H:107:LEU:HD21	1.80	0.64
1:A:324:G:N2	1:A:326:G:H3'	2.12	0.64
1:A:329:A:H4'	1:A:330:C:OP1	1.96	0.64
1:A:1157:A:H4'	1:A:1158:C:O5'	1.96	0.64
9:I:53:VAL:HG12	9:I:95:LYS:HB3	1.79	0.64
1:A:1166:G:N2	1:A:1170:A:OP2	2.31	0.64
1:A:1283:G:N2	1:A:1284:C:C2	2.65	0.64
7:G:65:ALA:O	7:G:69:VAL:HG23	1.98	0.64
1:A:1392:G:H21	1:A:1502:A:H8	1.43	0.64
4:D:30:LYS:C	4:D:32:ALA:H	2.04	0.64
1:A:481:G:O2'	1:A:483:C:N4	2.31	0.64
1:A:1201:A:H4'	1:A:1202:G:H5''	1.78	0.64
3:C:148:GLY:HA3	3:C:172:ARG:O	1.97	0.64
1:A:299:G:H2'	1:A:300:A:C8	2.33	0.63
1:A:1005:A:O4'	1:A:1036:G:N2	2.31	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1312:G:N2	1:A:1326:C:C2	2.66	0.63
1:A:1464:G:N1	1:A:1465:C:C4	2.66	0.63
1:A:1507:A:H2'	1:A:1508:G:H8	1.63	0.63
17:Q:92:ARG:O	17:Q:95:TYR:HB2	1.97	0.63
1:A:1274:G:H2'	1:A:1275:A:H8	1.62	0.63
5:E:31:LEU:HD23	5:E:45:PHE:HD1	1.63	0.63
1:A:1530:G:H2'	1:A:1531:A:H8	1.63	0.63
1:A:925:G:H1	1:A:1391:U:H3	1.46	0.63
1:A:971:G:H1'	1:A:1365:G:O2'	1.98	0.63
6:F:49:ALA:CB	18:R:80:PRO:HA	2.27	0.63
1:A:537:G:H5''	12:L:113:ARG:HH12	1.63	0.63
1:A:1252:A:H2'	1:A:1253:G:O4'	1.97	0.63
1:A:1151:A:O2'	1:A:1152:A:H8	1.81	0.63
1:A:1244:C:H2'	1:A:1245:A:H8	1.64	0.63
1:A:1464:G:C2	1:A:1465:C:C4	2.87	0.63
1:A:1007:C:C2	1:A:1023:G:N1	2.66	0.63
1:A:217:C:O2'	1:A:470:C:N4	2.32	0.63
1:A:715:A:H2'	1:A:716:A:C8	2.34	0.63
1:A:1067:A:H8	1:A:1067:A:O5'	1.82	0.63
25:Z:68:C:H2'	25:Z:69:C:H6	1.61	0.63
1:A:243:A:H2	1:A:245:C:H2'	1.62	0.62
1:A:370:C:C2	1:A:392:G:N2	2.67	0.62
1:A:407:G:H2'	1:A:408:A:C8	2.34	0.62
1:A:994:A:C2	14:N:5:ALA:HA	2.34	0.62
1:A:1509:C:H2'	1:A:1510:U:O4'	1.99	0.62
1:A:29:G:N2	1:A:555:C:C2	2.67	0.62
1:A:522:C:H41	12:L:53:ARG:HH22	1.47	0.62
1:A:738:C:H2'	1:A:739:C:C6	2.35	0.62
1:A:987:G:H1	1:A:1218:C:H42	1.47	0.62
1:A:1039:C:H2'	1:A:1040:U:H6	1.62	0.62
1:A:1457:G:H21	1:A:1458:G:H1'	1.62	0.62
4:D:31:CYS:C	4:D:33:MET:H	2.05	0.62
1:A:785:G:H8	1:A:785:G:H5''	1.64	0.62
1:A:1386:G:H2'	1:A:1387:G:C8	2.29	0.62
12:L:87:GLY:HA2	12:L:98:TYR:HA	1.81	0.62
17:Q:27:PHE:CE1	17:Q:38:ARG:HB2	2.33	0.62
1:A:42:G:H2'	1:A:43:C:O4'	1.99	0.62
1:A:189(K):U:H2'	1:A:189(L):G:C8	2.35	0.62
1:A:1382:C:H2'	1:A:1383:C:C6	2.35	0.62
17:Q:15:MET:HB3	17:Q:18:THR:HB	1.80	0.62
1:A:17:U:H2'	1:A:18:C:C6	2.34	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:U:H2'	1:A:297:G:C8	2.35	0.62
1:A:895:G:H1	1:A:904:C:H42	1.48	0.62
1:A:1217:C:N4	1:A:1218:C:N4	2.47	0.62
1:A:1432:G:O2'	1:A:1468:A:N6	2.33	0.62
1:A:1493:A:H4'	1:A:1494:G:H5'	1.81	0.62
4:D:18:LYS:HA	4:D:33:MET:HG3	1.81	0.62
1:A:639:G:H2'	1:A:640:A:H8	1.65	0.62
1:A:40:C:H2'	1:A:41:G:C8	2.33	0.62
1:A:834:C:H5''	18:R:60:ALA:HB3	1.82	0.62
1:A:1536:C:H42	24:Y:29:G:H1	1.46	0.62
1:A:778:G:C6	1:A:779:C:N3	2.68	0.61
1:A:1119:C:H2'	1:A:1120:G:H8	1.65	0.61
1:A:1240:U:OP1	7:G:116:ALA:HB2	2.00	0.61
1:A:131:C:H2'	1:A:132:C:H6	1.64	0.61
1:A:240:C:H2'	1:A:241:C:C6	2.35	0.61
1:A:401:C:H2'	1:A:402:G:H8	1.65	0.61
3:C:150:LYS:HB2	3:C:173:VAL:HG21	1.81	0.61
1:A:1127:G:N2	1:A:1144:G:H22	1.97	0.61
1:A:1311:G:N7	19:S:2:PRO:CA	2.63	0.61
1:A:1391:U:H2'	1:A:1392:G:C8	2.35	0.61
4:D:24:GLU:O	4:D:25:ARG:HB3	1.99	0.61
20:T:65:LYS:O	20:T:68:LYS:HB3	2.00	0.61
1:A:1000:U:C6	1:A:1000:U:H3'	2.36	0.61
14:N:41:ARG:HG3	14:N:42:ILE:N	2.14	0.61
1:A:372:C:H4'	1:A:373:A:O5'	2.01	0.61
1:A:927:G:H1	1:A:1390:U:H3	1.48	0.61
1:A:1367:C:H4'	10:J:48:THR:HG21	1.83	0.61
1:A:1536:C:N4	24:Y:29:G:H1	1.98	0.61
1:A:19:C:H2'	1:A:20:U:C6	2.36	0.61
1:A:69:G:H1	1:A:100:C:N4	1.99	0.61
1:A:391:G:H2'	1:A:392:G:O4'	2.01	0.61
1:A:770:C:H2'	1:A:771:G:H8	1.65	0.61
1:A:1457:G:C2	1:A:1458:G:C8	2.89	0.61
13:M:34:LEU:HD13	13:M:41:PRO:HG3	1.82	0.61
1:A:392:G:H2'	1:A:393:A:C8	2.36	0.61
1:A:398:C:H2'	1:A:399:G:H8	1.66	0.61
1:A:1020:U:H2'	1:A:1021:G:C8	2.33	0.61
1:A:1266:G:N2	1:A:1270:C:C2	2.69	0.61
9:I:4:TYR:HE2	9:I:21:PRO:HG3	1.66	0.61
20:T:83:ARG:HA	20:T:86:ARG:NH1	2.15	0.61
1:A:1323:G:H2'	1:A:1324:A:C8	2.36	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:G:H2'	1:A:1531:A:C8	2.36	0.61
20:T:73:HIS:HB3	20:T:74:LYS:HE3	1.82	0.61
23:X:47:LEU:HA	23:X:56:VAL:O	2.01	0.61
1:A:1244:C:H2'	1:A:1245:A:C8	2.37	0.60
1:A:1342:C:H2'	1:A:1343:G:H8	1.66	0.60
5:E:127:ASN:O	5:E:131:ILE:HG12	2.01	0.60
11:K:99:GLN:HA	11:K:105:VAL:HG21	1.83	0.60
14:N:37:PHE:HB3	14:N:39:LEU:HB2	1.83	0.60
1:A:417:C:N4	1:A:418:C:N4	2.49	0.60
1:A:521:G:N1	1:A:522:C:C4	2.69	0.60
1:A:824:C:H2'	1:A:825:G:H8	1.65	0.60
1:A:1369:C:H2'	1:A:1370:G:C8	2.36	0.60
3:C:29:TYR:CE1	3:C:33:LEU:CD1	2.54	0.60
10:J:50:ILE:HA	10:J:60:ARG:HA	1.84	0.60
1:A:785:G:H5''	1:A:785:G:C8	2.36	0.60
2:B:8:LYS:HD2	2:B:9:GLU:H	1.66	0.60
1:A:628:G:H2'	1:A:629:G:C8	2.37	0.60
1:A:720:C:H2'	1:A:721:G:C8	2.36	0.60
1:A:1447:A:H4'	1:A:1452:C:OP2	1.99	0.60
19:S:12:ASP:HB3	19:S:14:HIS:CD2	2.36	0.60
1:A:725:G:N2	1:A:726:C:C2	2.70	0.60
1:A:939:G:C6	1:A:940:C:N4	2.69	0.60
1:A:1084:G:H2'	1:A:1085:U:C6	2.37	0.60
1:A:1347:G:HO2'	1:A:1348:U:P	2.25	0.60
1:A:1525:G:H2'	1:A:1526:G:C8	2.36	0.60
11:K:100:ALA:O	11:K:102:GLY:N	2.33	0.60
25:Z:26:G:C5	25:Z:27:U:H5	2.20	0.60
1:A:664:G:H22	1:A:741:G:H1	0.74	0.60
1:A:926:G:H2'	1:A:1505:G:N3	2.16	0.60
1:A:1412:C:H2'	1:A:1413:A:C8	2.37	0.60
6:F:49:ALA:HB3	6:F:50:TYR:HD1	1.67	0.60
7:G:16:LEU:HB3	9:I:44:VAL:HG23	1.83	0.60
1:A:1105:A:H2'	1:A:1106:G:H8	1.67	0.60
12:L:45:PRO:HG3	12:L:53:ARG:HD3	1.83	0.60
15:O:34:LEU:O	15:O:38:ARG:HG2	2.02	0.60
1:A:455:C:C6	1:A:455:C:O5'	2.55	0.60
1:A:690:G:OP2	11:K:27:ASN:HB3	2.02	0.60
1:A:1537:U:O2	24:Y:28:A:N1	2.35	0.60
8:H:104:ARG:HB2	8:H:108:GLY:H	1.66	0.60
23:X:157:LEU:HD13	25:Z:27:U:H5'	1.84	0.60
1:A:1218:C:H2'	1:A:1219:U:C6	2.37	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:187:LEU:HD11	2:B:214:ILE:HD12	1.83	0.60
7:G:40:ALA:HB3	9:I:41:VAL:HG21	1.83	0.60
1:A:20:U:H2'	1:A:21:G:O4'	2.02	0.59
1:A:588:G:N2	1:A:589:C:C2	2.70	0.59
1:A:924:C:H2'	1:A:925:G:C8	2.38	0.59
1:A:1081:G:H5''	1:A:1081:G:H8	1.68	0.59
23:X:16:VAL:HG12	23:X:55:PRO:HB2	1.84	0.59
1:A:113:G:H1'	1:A:354:G:H5''	1.84	0.59
25:Z:41:C:H2'	25:Z:42:G:O4'	2.01	0.59
1:A:939:G:C2	1:A:940:C:N3	2.71	0.59
1:A:986:A:H2'	1:A:987:G:O4'	2.02	0.59
1:A:1342:C:H2'	1:A:1343:G:C8	2.38	0.59
1:A:246:A:O2'	17:Q:99:SER:HB2	2.02	0.59
1:A:334:C:H2'	1:A:335:C:C6	2.38	0.59
1:A:442:C:H2'	1:A:443:C:H6	1.68	0.59
1:A:1255:G:C6	1:A:1279:A:C8	2.90	0.59
1:A:1443:G:N2	1:A:1444:C:C2	2.71	0.59
22:W:40:MET:HE3	22:W:70:ARG:HA	1.83	0.59
1:A:32:A:H2'	1:A:33:A:C8	2.37	0.59
3:C:97:LYS:HB3	3:C:97:LYS:HZ3	1.66	0.59
9:I:19:LEU:HD22	9:I:59:PHE:HB3	1.85	0.59
11:K:87:THR:HG21	24:Y:28:A:O2'	2.03	0.59
1:A:24:U:H2'	1:A:25:C:C6	2.38	0.59
1:A:1106:G:N2	1:A:1107:C:C2	2.70	0.59
1:A:1126:U:OP1	1:A:1280:A:C8	2.56	0.59
3:C:187:ALA:HB3	3:C:198:VAL:HB	1.83	0.59
1:A:1040:U:H2'	1:A:1041:A:H8	1.63	0.59
1:A:1395:C:H2'	1:A:1396:A:H8	1.68	0.59
6:F:7:ASN:ND2	18:R:34:TYR:HE1	2.00	0.59
22:W:33:LEU:O	22:W:64:ARG:HA	2.03	0.59
1:A:529:G:H5'	1:A:530:G:OP2	2.02	0.59
1:A:838:G:N2	1:A:849:C:C2	2.71	0.59
1:A:953:G:H2'	1:A:954:G:O4'	2.02	0.59
2:B:201:ILE:HG21	2:B:214:ILE:HG21	1.85	0.59
8:H:91:ARG:HD3	12:L:7:ILE:HD12	1.84	0.59
25:Z:7:G:H1	25:Z:66:C:H42	1.51	0.59
1:A:601:C:H42	1:A:637:G:H1	1.51	0.58
1:A:616:G:H2'	1:A:617:G:H8	1.68	0.58
1:A:1124:G:H2'	1:A:1145:C:C5	2.38	0.58
1:A:1463:C:H2'	1:A:1464:G:C8	2.38	0.58
8:H:49:GLU:HG3	8:H:60:ARG:HB2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:G:N2	1:A:177:C:C2	2.72	0.58
1:A:312:C:H2'	1:A:313:A:H8	1.65	0.58
1:A:1249:C:H6	1:A:1249:C:H5''	1.68	0.58
1:A:1507:A:H2'	1:A:1508:G:C8	2.39	0.58
11:K:21:ILE:HG12	11:K:30:VAL:HG22	1.83	0.58
1:A:514:C:H2'	1:A:515:G:H8	1.68	0.58
1:A:551:U:H2'	1:A:552:U:C6	2.38	0.58
1:A:1443:G:C6	1:A:1444:C:N4	2.71	0.58
1:A:518:C:H4'	1:A:519:C:O5'	2.02	0.58
1:A:1016:A:H2'	1:A:1017:G:O4'	2.02	0.58
1:A:189(A):C:H2'	1:A:189(B):C:H6	1.69	0.58
3:C:59:ARG:NH1	3:C:97:LYS:HD3	2.18	0.58
1:A:504:C:C2	1:A:542:G:N2	2.71	0.58
1:A:1305:G:N2	1:A:1331:G:H1'	2.19	0.58
4:D:201:GLN:NE2	5:E:116:THR:CG2	2.65	0.58
20:T:56:MET:HE2	20:T:85:MET:HG2	1.84	0.58
23:X:9:GLU:HA	23:X:35:LEU:HD11	1.85	0.58
1:A:553:A:H2'	1:A:554:C:C6	2.38	0.58
1:A:584:G:H2'	1:A:585:G:H8	1.68	0.58
1:A:1112:C:N3	3:C:177:THR:HA	2.19	0.58
2:B:16:HIS:HE2	2:B:214:ILE:HD11	1.67	0.58
6:F:9:VAL:HB	6:F:87:ARG:HB2	1.84	0.58
25:Z:53:G:H1	25:Z:61:C:N4	2.02	0.58
1:A:643:C:H2'	1:A:644:G:H8	1.67	0.58
1:A:1201:A:H4'	1:A:1202:G:C5'	2.34	0.58
1:A:1293:G:H2'	1:A:1294:G:C8	2.38	0.58
1:A:1466:C:H2'	1:A:1467:G:O4'	2.04	0.58
1:A:334:C:H2'	1:A:335:C:H6	1.68	0.58
1:A:955:U:O5'	1:A:955:U:H6	1.87	0.58
1:A:500:G:C6	1:A:501:C:N4	2.72	0.58
1:A:969:A:H2'	1:A:970:C:O4'	2.01	0.58
1:A:124:G:H2'	1:A:125:U:O4'	2.03	0.57
1:A:750:G:N3	15:O:23:GLY:HA3	2.19	0.57
1:A:836:G:H2'	1:A:837:G:C8	2.38	0.57
9:I:11:LYS:HE2	9:I:109:VAL:HG23	1.85	0.57
1:A:397:A:H3'	1:A:397:A:N3	2.19	0.57
1:A:652:U:O4	1:A:752:G:O2'	2.17	0.57
1:A:417:C:N4	1:A:418:C:H41	2.02	0.57
1:A:767:A:H2'	1:A:768:A:O4'	2.05	0.57
1:A:1119:C:H2'	1:A:1120:G:C8	2.39	0.57
1:A:148:G:H2'	1:A:149:A:C8	2.39	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:C:H2'	1:A:166:G:H8	1.68	0.57
1:A:987:G:H2'	1:A:988:G:C8	2.38	0.57
1:A:1258:G:C6	1:A:1259:C:N4	2.73	0.57
1:A:1113:C:O4'	3:C:178:LEU:HG	2.04	0.57
23:X:17:ARG:NH2	25:Z:56:C:N4	2.52	0.57
1:A:1485:U:H2'	1:A:1486:G:H8	1.69	0.57
4:D:98:GLU:O	4:D:104:VAL:HG23	2.05	0.57
1:A:61:G:H2'	1:A:62:U:O4'	2.05	0.57
7:G:65:ALA:HA	7:G:127:ALA:HB1	1.87	0.57
23:X:168:VAL:HG12	23:X:169:LYS:HG3	1.87	0.57
1:A:69:G:H1	1:A:100:C:H42	1.51	0.57
1:A:426:G:H2'	1:A:427:U:O4'	2.04	0.57
1:A:649:G:H2'	1:A:650:G:O4'	2.05	0.57
1:A:1041:A:H2'	1:A:1042:G:H8	1.70	0.57
1:A:1345:U:N3	1:A:1375:A:C6	2.63	0.57
8:H:6:ILE:HB	8:H:85:ARG:NH1	2.20	0.57
11:K:123:LYS:HA	11:K:126:ARG:HB2	1.87	0.57
1:A:122:G:C6	1:A:123:C:C4	2.93	0.57
1:A:232:G:H2'	1:A:233:C:C6	2.40	0.57
1:A:504:C:N3	1:A:542:G:C2	2.73	0.57
10:J:53:PRO:HA	14:N:41:ARG:NH2	2.20	0.57
1:A:541:G:H2'	1:A:542:G:O4'	2.05	0.56
1:A:616:G:H2'	1:A:617:G:C8	2.40	0.56
1:A:663:A:H5''	18:R:61:LYS:HE3	1.86	0.56
1:A:1081:G:H5''	1:A:1081:G:C8	2.40	0.56
1:A:1512:U:H2'	1:A:1513:A:H8	1.69	0.56
2:B:44:LEU:HA	2:B:47:THR:HB	1.87	0.56
23:X:157:LEU:CD1	25:Z:27:U:OP1	2.53	0.56
1:A:1004:A:H5''	1:A:1025:U:C5	2.41	0.56
1:A:1163:C:N3	1:A:1174:G:C2	2.74	0.56
1:A:1241:G:N2	1:A:1242:C:C2	2.73	0.56
10:J:79:ARG:HH12	10:J:82:ILE:HB	1.70	0.56
15:O:19:PRO:C	15:O:21:ASP:H	2.13	0.56
1:A:129(A):G:H1	1:A:189(D):C:H2'	1.71	0.56
1:A:1081:G:H2'	1:A:1082:G:H8	1.71	0.56
1:A:1190:G:H5'	3:C:176:HIS:CE1	2.40	0.56
1:A:1521:G:H2'	1:A:1522:U:C6	2.40	0.56
7:G:71:PRO:HG3	7:G:103:TRP:HZ3	1.69	0.56
12:L:60:LEU:HD11	12:L:85:ILE:HD12	1.86	0.56
24:Y:36:A:N6	25:Z:37:A:N6	2.53	0.56
1:A:408:A:H2'	1:A:409:G:C8	2.40	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:22:G:P	25:Z:22:G:H8	2.28	0.56
1:A:165:C:H2'	1:A:166:G:C8	2.40	0.56
1:A:821:G:H2'	1:A:822:C:C6	2.41	0.56
4:D:101:LEU:HB2	4:D:138:TYR:HB3	1.88	0.56
1:A:10:A:H2'	1:A:11:G:C8	2.40	0.56
1:A:571:U:O5'	1:A:571:U:H6	1.89	0.56
1:A:671:G:C2	1:A:736:C:N3	2.74	0.56
1:A:755:G:N2	1:A:756:C:C2	2.74	0.56
1:A:781:A:N6	1:A:802:A:H1'	2.20	0.56
1:A:830:G:H2'	1:A:831:U:O4'	2.06	0.56
1:A:1076:C:C2	1:A:1082:G:N2	2.73	0.56
1:A:64:G:H4'	1:A:65:U:H5''	1.88	0.56
1:A:687:A:H2	1:A:700:G:N3	2.04	0.56
1:A:824:C:H2'	1:A:825:G:C8	2.41	0.56
1:A:874:G:N2	1:A:875:C:C2	2.73	0.56
1:A:837:G:H1	1:A:849:C:H42	1.52	0.56
1:A:877:C:H2'	1:A:878:G:H8	1.70	0.56
3:C:29:TYR:OH	14:N:54:PRO:HD2	2.05	0.56
6:F:11:ASN:HD21	6:F:13:ASN:HD22	1.51	0.56
1:A:275:G:H2'	1:A:276:G:H8	1.70	0.56
1:A:377:G:H1	1:A:386:C:H42	1.54	0.56
1:A:893:C:H2'	1:A:894:G:O4'	2.05	0.56
8:H:122:ARG:HB3	8:H:122:ARG:HH11	1.71	0.56
1:A:21:G:H2'	1:A:22:G:H8	1.64	0.56
1:A:613:C:H2'	1:A:614:A:H8	1.70	0.56
1:A:1103:C:H2'	1:A:1104:G:O4'	2.06	0.56
11:K:22:HIS:HB3	11:K:29:ILE:HG22	1.88	0.56
23:X:56:VAL:HG11	25:Z:19:G:N7	2.21	0.56
1:A:258:G:N2	1:A:269:C:C2	2.74	0.55
1:A:548:G:C6	1:A:549:C:N4	2.75	0.55
1:A:613:C:H2'	1:A:614:A:C8	2.40	0.55
1:A:835:U:OP1	18:R:61:LYS:HB2	2.06	0.55
1:A:926:G:N2	24:Y:35:A:H5'	2.22	0.55
1:A:939:G:H1	1:A:1344:C:H42	1.54	0.55
1:A:1401:G:H2'	1:A:1402:C:O4'	2.07	0.55
9:I:22:GLY:HA3	9:I:60:ASP:HB2	1.87	0.55
1:A:377:G:H1	1:A:386:C:N4	2.04	0.55
1:A:1412:C:H2'	1:A:1413:A:H8	1.69	0.55
1:A:69:G:H2'	1:A:70:G:H8	1.70	0.55
1:A:317:G:C2	1:A:337:C:C2	2.95	0.55
1:A:584:G:H2'	1:A:585:G:C8	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1001(A):G:N1	1:A:1002:G:C6	2.74	0.55
1:A:1380:U:C4	7:G:3:ARG:HG2	2.41	0.55
23:X:17:ARG:HH22	23:X:19:VAL:HG22	1.69	0.55
1:A:601:C:C2	1:A:638:G:N2	2.75	0.55
1:A:860:A:H3'	1:A:861:G:C8	2.41	0.55
1:A:987:G:H1	1:A:1218:C:N4	2.04	0.55
1:A:1257:U:H4'	1:A:1258:G:O5'	2.06	0.55
1:A:864:A:C2'	1:A:865:A:C8	2.87	0.55
1:A:948:C:H2'	1:A:949:A:C8	2.41	0.55
1:A:1409:C:H2'	1:A:1410:G:C8	2.42	0.55
23:X:5:TYR:HH	25:Z:20:U:H6	0.60	0.55
1:A:1126:U:H5'	1:A:1280:A:O2'	2.07	0.55
4:D:23:GLY:H	4:D:26:CYS:HB2	1.71	0.55
24:Y:38:G:O6	25:Z:34:C:N3	2.40	0.55
1:A:1102:A:H2'	1:A:1103:C:H6	1.72	0.55
1:A:1225:A:H2'	1:A:1225:A:N3	2.21	0.55
4:D:157:LEU:HA	4:D:160:GLN:HE21	1.72	0.55
1:A:296:U:H2'	1:A:297:G:H8	1.72	0.55
3:C:29:TYR:HH	14:N:54:PRO:HG2	1.72	0.55
1:A:174:C:H2'	1:A:175:C:C6	2.42	0.55
1:A:424:G:H2'	1:A:425:G:C8	2.40	0.55
4:D:187:ARG:HB2	4:D:187:ARG:NH1	2.22	0.55
12:L:25:PRO:C	12:L:27:LEU:N	2.48	0.55
19:S:81:ARG:HH11	19:S:81:ARG:HB2	1.70	0.55
25:Z:49:G:C2	25:Z:66:C:C2	2.95	0.55
1:A:1068:G:N2	1:A:1069:C:C2	2.75	0.54
1:A:1115:C:H2'	1:A:1116:C:C6	2.41	0.54
1:A:1256:A:N6	1:A:1278:U:C2	2.75	0.54
1:A:1262:C:N4	1:A:1273:G:H1	2.02	0.54
1:A:105:G:C6	1:A:106:C:N4	2.76	0.54
1:A:502:G:H2'	1:A:503:C:O4'	2.07	0.54
1:A:591:U:H2'	1:A:592:G:C8	2.42	0.54
1:A:1512:U:H2'	1:A:1513:A:C8	2.42	0.54
1:A:105:G:C5	1:A:106:C:C4	2.95	0.54
1:A:216:G:C2	1:A:217:C:N3	2.75	0.54
1:A:354:G:N2	1:A:355:C:C2	2.75	0.54
19:S:22:LEU:HD22	19:S:28:LYS:HD2	1.88	0.54
1:A:687:A:C2	1:A:700:G:N3	2.75	0.54
1:A:983:A:H2	1:A:1222:G:H22	1.53	0.54
1:A:532:A:H2'	1:A:532:A:N3	2.22	0.54
1:A:880:C:H2'	1:A:881:G:C8	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:C:H1'	1:A:1132:C:H5	1.72	0.54
1:A:1353:G:N2	1:A:1354:C:C2	2.76	0.54
25:Z:5:G:H1	25:Z:68:C:N4	2.05	0.54
1:A:998:G:N2	1:A:999:C:C2	2.75	0.54
1:A:1271:G:C6	1:A:1272:G:C5	2.96	0.54
1:A:45:U:H2'	1:A:46:G:C8	2.43	0.54
1:A:129(A):G:O2'	1:A:130:A:OP2	2.24	0.54
1:A:613:C:N4	1:A:627:G:H1	2.05	0.54
1:A:1111:A:N6	3:C:176:HIS:O	2.41	0.54
1:A:1504:G:H3'	1:A:1504:G:P	2.48	0.54
4:D:8:VAL:HG13	4:D:9:CYS:H	1.72	0.54
1:A:568:G:C6	1:A:569:C:N4	2.76	0.54
9:I:28:VAL:HA	9:I:63:ILE:O	2.08	0.54
24:Y:23:C:H2'	24:Y:24:A:O4'	2.07	0.54
1:A:988:G:C6	1:A:989:C:N3	2.76	0.54
1:A:1128:C:H1'	1:A:1146:A:H61	1.73	0.54
16:P:12:LYS:C	16:P:14:ASN:H	2.16	0.54
20:T:14:LYS:HE2	20:T:18:GLN:HE22	1.73	0.54
1:A:72:C:C3'	1:A:73:G:C5'	2.81	0.54
1:A:275:G:H2'	1:A:276:G:C8	2.42	0.54
1:A:742:G:H2'	1:A:743:U:O4'	2.08	0.54
1:A:926:G:H22	24:Y:35:A:H5'	1.73	0.54
1:A:976:G:H22	1:A:1363:C:H5''	1.73	0.54
1:A:1097:C:H2'	1:A:1098:C:H6	1.71	0.54
1:A:1115:C:H2'	1:A:1116:C:H6	1.72	0.54
1:A:1248:A:C6	1:A:1249:C:N4	2.76	0.54
23:X:89:LYS:HA	23:X:119:THR:O	2.07	0.54
24:Y:28:A:N6	24:Y:29:G:N1	2.56	0.54
25:Z:12:G:C6	25:Z:13:C:N3	2.76	0.54
1:A:243:A:C2	1:A:245:C:H2'	2.42	0.53
1:A:730:G:N2	1:A:765:G:H5''	2.23	0.53
1:A:1283:G:N1	1:A:1284:C:C4	2.76	0.53
25:Z:37:A:H3'	25:Z:38:A:H8	1.72	0.53
25:Z:38:A:H2'	25:Z:39:C:O4'	2.08	0.53
1:A:257:G:H1	1:A:269:C:H42	1.56	0.53
1:A:300:A:H2'	1:A:301:G:O4'	2.08	0.53
1:A:562:C:H41	1:A:884:U:H2'	1.73	0.53
1:A:731:G:N2	1:A:732:C:C2	2.77	0.53
1:A:1415:G:H22	1:A:1486:G:H1'	1.73	0.53
8:H:14:ARG:HG3	8:H:83:ILE:HG22	1.91	0.53
11:K:25:TYR:HB2	11:K:26:ASN:ND2	2.23	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:56:VAL:HG13	25:Z:19:G:O6	2.08	0.53
25:Z:54:5MU:H73	25:Z:55:PSU:C2	2.44	0.53
25:Z:69:C:H2'	25:Z:70:G:H8	1.71	0.53
1:A:661:G:C2	1:A:745:C:N3	2.77	0.53
1:A:971:G:H1'	1:A:1365:G:HO2'	1.73	0.53
1:A:1101:A:H4'	1:A:1102:A:O5'	2.07	0.53
1:A:1424:C:H42	1:A:1476:G:H1	1.56	0.53
10:J:39:PRO:O	10:J:40:LEU:HB2	2.07	0.53
1:A:822:C:H2'	1:A:823:G:H8	1.74	0.53
3:C:29:TYR:CD1	3:C:29:TYR:C	2.86	0.53
3:C:39:ILE:HD11	3:C:95:THR:HG21	1.90	0.53
1:A:18:C:H6	1:A:18:C:O5'	1.92	0.53
1:A:60:A:H4'	1:A:61:G:O5'	2.09	0.53
1:A:132:C:N3	1:A:231:G:C2	2.76	0.53
13:M:88:ARG:HA	13:M:98:VAL:HG11	1.91	0.53
1:A:333:G:N2	1:A:334:C:C2	2.76	0.53
1:A:1081:G:H2'	1:A:1082:G:C8	2.43	0.53
4:D:90:GLY:HA2	4:D:204:ILE:HD11	1.89	0.53
5:E:63:ARG:HA	5:E:66:MET:HE2	1.90	0.53
18:R:51:LEU:HD13	18:R:55:ARG:HD2	1.91	0.53
25:Z:22:G:OP2	25:Z:46:G7M:N2	2.42	0.53
4:D:132:ARG:HD3	4:D:151:LYS:NZ	2.24	0.53
1:A:335:C:H2'	1:A:336:C:C6	2.44	0.53
1:A:687:A:H4'	1:A:688:G:O5'	2.09	0.53
1:A:1258:G:C2	1:A:1259:C:N3	2.76	0.53
1:A:1443:G:C2	1:A:1444:C:C4	2.97	0.53
7:G:50:ILE:HA	7:G:125:MET:HE2	1.91	0.53
22:W:6:THR:HB	22:W:56:GLU:HG2	1.90	0.53
1:A:258:G:C2	1:A:269:C:N3	2.77	0.53
1:A:761:G:C2	1:A:762:C:C2	2.96	0.53
3:C:56:ASP:HB2	3:C:67:THR:HB	1.90	0.53
6:F:49:ALA:HB2	18:R:80:PRO:HA	1.89	0.53
23:X:21:PRO:HG2	23:X:41:MET:HE2	1.91	0.53
1:A:580:U:H2'	1:A:581:G:O4'	2.08	0.53
1:A:1141:C:H2'	1:A:1142:G:H8	1.73	0.53
3:C:29:TYR:OH	14:N:54:PRO:CD	2.55	0.53
6:F:48:LEU:HD13	6:F:52:ILE:HD12	1.91	0.53
23:X:137:LEU:HD13	23:X:163:MET:HG3	1.91	0.53
1:A:66:G:N2	1:A:67:C:C2	2.77	0.52
1:A:278:G:N7	17:Q:92:ARG:NH1	2.57	0.52
1:A:455:C:O5'	1:A:455:C:H6	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:G:H2'	1:A:558:G:C8	2.43	0.52
10:J:30:SER:HB2	10:J:80:LYS:O	2.08	0.52
1:A:559:A:O2'	1:A:560:U:OP2	2.23	0.52
1:A:1256:A:H8	3:C:27:LYS:NZ	2.08	0.52
1:A:1392:G:N2	1:A:1502:A:C8	2.75	0.52
17:Q:56:VAL:HG13	17:Q:77:VAL:HB	1.91	0.52
1:A:41:G:H1	1:A:401:C:H42	1.56	0.52
1:A:502:G:C2	1:A:503:C:C2	2.97	0.52
1:A:790:A:H2'	1:A:791:G:C8	2.45	0.52
1:A:855:G:N1	1:A:856:C:C2	2.78	0.52
1:A:216:G:C6	1:A:217:C:N4	2.77	0.52
1:A:298:A:H2'	1:A:299:G:C8	2.45	0.52
1:A:1008:C:N3	1:A:1022:G:N2	2.57	0.52
1:A:1194:U:H4'	5:E:22:GLY:HA3	1.92	0.52
1:A:1464:G:N2	1:A:1465:C:N3	2.58	0.52
12:L:6:THR:O	12:L:9:GLN:HB3	2.10	0.52
23:X:157:LEU:HD13	25:Z:27:U:OP1	2.10	0.52
1:A:566:G:O3'	1:A:567:G:H5'	2.08	0.52
1:A:1018:C:H2'	1:A:1019:C:C6	2.44	0.52
1:A:1048:G:H2'	1:A:1050:G:C8	2.44	0.52
1:A:1132:C:H2'	1:A:1133:G:C8	2.45	0.52
1:A:1241:G:C6	1:A:1242:C:N4	2.78	0.52
1:A:1355:G:H2'	1:A:1356:G:C8	2.44	0.52
6:F:8:ILE:HD11	6:F:79:LEU:HD13	1.91	0.52
9:I:3:GLN:HG3	9:I:20:ARG:HG3	1.91	0.52
1:A:199:G:N2	1:A:219:C:C2	2.78	0.52
1:A:729:A:H2'	1:A:730:G:H8	1.75	0.52
1:A:967:C:C4	1:A:968:A:C6	2.98	0.52
1:A:1305:G:O2'	1:A:1306:A:H8	1.92	0.52
3:C:174:PRO:HB2	3:C:177:THR:HG22	1.92	0.52
1:A:53:A:H2'	1:A:54:C:O4'	2.09	0.52
1:A:1198:G:C5	1:A:1199:U:C4	2.98	0.52
1:A:918:A:H2'	1:A:919:A:C8	2.44	0.52
8:H:6:ILE:HD13	8:H:6:ILE:N	2.24	0.52
23:X:157:LEU:HD13	25:Z:27:U:H5''	1.91	0.52
1:A:44:G:H2'	1:A:45:U:O4'	2.10	0.52
1:A:1518:A:H2'	1:A:1519:A:C8	2.45	0.52
6:F:37:VAL:HA	6:F:65:VAL:HG12	1.92	0.52
11:K:62:GLN:HG3	11:K:97:ALA:HB2	1.92	0.52
1:A:21:G:H21	1:A:914:A:H62	1.58	0.52
1:A:70:G:N1	1:A:100:C:C2	2.78	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:C:H2'	1:A:111:G:O4'	2.09	0.52
1:A:829:G:H5''	1:A:829:G:C8	2.45	0.52
1:A:1502:A:H2'	1:A:1504:G:C8	2.44	0.52
9:I:26:VAL:HG22	9:I:61:ALA:HB3	1.92	0.52
1:A:333:G:C6	1:A:334:C:N4	2.79	0.51
1:A:633:G:H2'	1:A:634:C:H6	1.75	0.51
1:A:663:A:H2'	1:A:664:G:O4'	2.09	0.51
1:A:774:G:N2	1:A:806:C:C2	2.77	0.51
1:A:1500:A:H5''	1:A:1508:G:H5''	1.92	0.51
6:F:30:LEU:HD22	6:F:65:VAL:HG11	1.92	0.51
10:J:6:ILE:HA	10:J:97:GLU:O	2.09	0.51
1:A:662:G:H2'	1:A:663:A:C8	2.46	0.51
1:A:983:A:H2	1:A:1222:G:N2	2.07	0.51
1:A:1347:G:C2'	1:A:1373:G:H1	2.23	0.51
1:A:1375:A:N3	1:A:1375:A:H2'	2.24	0.51
8:H:14:ARG:O	8:H:18:ARG:HD2	2.10	0.51
9:I:24:GLY:HA3	9:I:57:GLY:HA2	1.91	0.51
12:L:51:ALA:HB3	12:L:53:ARG:HE	1.75	0.51
1:A:143:A:H2	1:A:220:G:H1	1.58	0.51
1:A:590:C:C2	1:A:650:G:N2	2.78	0.51
1:A:1457:G:C2	1:A:1458:G:C1'	2.93	0.51
9:I:4:TYR:CE2	9:I:21:PRO:HG3	2.45	0.51
13:M:97:PRO:HA	13:M:110:ARG:NH1	2.25	0.51
18:R:51:LEU:HB3	18:R:55:ARG:HB3	1.92	0.51
1:A:416:G:H1	1:A:427:U:H3	1.58	0.51
1:A:499:A:C6	1:A:547:A:C8	2.98	0.51
1:A:520:A:H62	1:A:529:G:H21	1.58	0.51
1:A:548:G:N2	1:A:549:C:C2	2.78	0.51
1:A:554:C:H2'	1:A:555:C:C6	2.45	0.51
1:A:696:A:O5'	1:A:696:A:H8	1.92	0.51
1:A:725:G:N1	1:A:726:C:C4	2.79	0.51
1:A:784:C:N3	1:A:799:G:C2	2.79	0.51
1:A:983:A:C2	1:A:1222:G:N2	2.77	0.51
1:A:1001(A):G:N2	1:A:1040:U:C2	2.77	0.51
1:A:1536:C:H2'	1:A:1537:U:C6	2.46	0.51
1:A:24:U:H2'	1:A:25:C:H6	1.76	0.51
1:A:105:G:C5	1:A:106:C:N4	2.79	0.51
1:A:233:C:H2'	1:A:234:C:C6	2.46	0.51
1:A:564:C:P	12:L:15:ARG:HH21	2.32	0.51
1:A:985:C:H2'	1:A:986:A:C8	2.46	0.51
1:A:988:G:N1	1:A:989:C:C2	2.79	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:46:ARG:HH12	10:J:64:GLU:HB3	1.74	0.51
1:A:22:G:C2	1:A:23:C:C2	2.99	0.51
1:A:101:A:O2'	1:A:102:G:H5'	2.10	0.51
1:A:186:C:H5'	20:T:78:ALA:HB1	1.92	0.51
1:A:624:C:H2'	1:A:625:G:H8	1.75	0.51
4:D:3:ARG:HB2	4:D:5:ILE:HD12	1.92	0.51
20:T:41:ILE:HD13	20:T:87:LYS:HZ2	1.72	0.51
1:A:22:G:C6	1:A:23:C:C4	2.99	0.51
1:A:599:C:H4'	8:H:130:GLY:C	2.36	0.51
1:A:1120:G:H2'	1:A:1121:U:C6	2.46	0.51
1:A:1457:G:N3	1:A:1458:G:C8	2.79	0.51
4:D:61:LYS:HA	4:D:203:VAL:HG22	1.91	0.51
12:L:83:VAL:HG22	12:L:84:LEU:H	1.75	0.51
14:N:50:LYS:HD2	14:N:52:GLN:NE2	2.25	0.51
18:R:53:ARG:NH2	18:R:60:ALA:HB2	2.21	0.51
23:X:137:LEU:HB3	23:X:163:MET:SD	2.51	0.51
24:Y:36:A:H2'	24:Y:37:U:C6	2.45	0.51
1:A:238:G:H2'	1:A:239:U:O4'	2.11	0.51
1:A:590:C:N3	1:A:650:G:C2	2.79	0.51
1:A:604:G:H2'	1:A:605:U:O4'	2.10	0.51
1:A:1007:C:O2	1:A:1023:G:C2	2.64	0.51
1:A:1190:G:H5'	3:C:176:HIS:NE2	2.25	0.51
1:A:138:G:H2'	1:A:139:G:O4'	2.11	0.51
1:A:984:C:N3	1:A:1222:G:C2	2.79	0.51
1:A:1008:C:H2'	1:A:1009:G:O4'	2.11	0.51
2:B:88:ALA:HB2	2:B:219:VAL:HG13	1.93	0.51
2:B:130:ARG:NH2	3:C:207:VAL:HG21	2.26	0.51
6:F:7:ASN:ND2	18:R:34:TYR:CE1	2.79	0.51
8:H:79:VAL:HG13	8:H:80:ILE:HG13	1.93	0.51
9:I:89:ASN:C	9:I:91:ASP:H	2.19	0.51
17:Q:40:LYS:HB3	17:Q:42:TYR:HE1	1.76	0.51
1:A:500:G:C2	1:A:501:C:N3	2.79	0.51
1:A:772:U:H3	1:A:807:A:H61	1.59	0.51
3:C:23:TYR:HE2	10:J:9:ARG:HD3	1.76	0.51
15:O:62:GLN:HA	15:O:65:ARG:HD3	1.93	0.51
24:Y:22:G:C6	24:Y:23:C:N3	2.79	0.51
24:Y:36:A:C6	25:Z:37:A:C6	2.99	0.51
1:A:344:A:H4'	1:A:345:C:OP2	2.10	0.50
1:A:413:G:O2'	1:A:428:G:N2	2.44	0.50
1:A:748:C:H1'	1:A:749:C:C5	2.46	0.50
1:A:903:G:H2'	1:A:904:C:C6	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:975:A:N6	1:A:1366:C:O2'	2.39	0.50
1:A:1041:A:H2'	1:A:1042:G:C8	2.46	0.50
2:B:167:PRO:HG3	2:B:186:ALA:HB1	1.93	0.50
3:C:6:HIS:HB3	14:N:49:HIS:HB3	1.93	0.50
5:E:139:LEU:HA	5:E:142:LEU:HD12	1.92	0.50
7:G:93:PRO:O	7:G:96:GLN:HG2	2.10	0.50
1:A:122:G:C2	1:A:123:C:C2	2.99	0.50
1:A:457:C:H2'	1:A:458:C:H6	1.76	0.50
1:A:524:G:C2	1:A:525:C:C4	2.98	0.50
1:A:1328:C:H5''	13:M:28:ALA:HB3	1.93	0.50
1:A:1534:A:H2'	1:A:1535:C:H6	1.75	0.50
1:A:502:G:C6	1:A:503:C:C4	3.00	0.50
1:A:591:U:H2'	1:A:592:G:H8	1.76	0.50
1:A:976:G:N2	1:A:1363:C:H5''	2.27	0.50
1:A:1023:G:H2'	1:A:1023:G:N3	2.26	0.50
2:B:124:SER:HB2	2:B:125:PRO:HD2	1.93	0.50
1:A:471:G:O2'	1:A:472:A:H5'	2.11	0.50
1:A:886:G:C6	1:A:887:G:C5	2.98	0.50
1:A:910:C:H4'	1:A:1413:A:H4'	1.93	0.50
1:A:1243:C:H2'	1:A:1244:C:O4'	2.12	0.50
3:C:113:ALA:N	3:C:114:PRO:CD	2.74	0.50
24:Y:30:G:H3'	24:Y:31:U:H5''	1.94	0.50
25:Z:27:U:H2'	25:Z:28:C:C5'	2.41	0.50
1:A:141:A:H2'	1:A:142:G:O4'	2.11	0.50
1:A:369:C:H2'	1:A:370:C:C6	2.46	0.50
1:A:554:C:C2	1:A:555:C:C5	3.00	0.50
1:A:778:G:N1	1:A:779:C:C2	2.80	0.50
1:A:1004:A:N7	1:A:1037:C:N3	2.59	0.50
1:A:1148:U:H2'	1:A:1149:C:O4'	2.12	0.50
1:A:1240:U:P	7:G:116:ALA:H	2.34	0.50
1:A:303:A:H2'	1:A:304:U:C6	2.47	0.50
1:A:1374:A:C5	1:A:1375:A:C8	3.00	0.50
1:A:1457:G:H2'	1:A:1458:G:O4'	2.12	0.50
4:D:64:LEU:HA	4:D:67:ILE:HD12	1.94	0.50
4:D:185:PHE:HZ	4:D:189:PRO:HD3	1.77	0.50
9:I:42:ARG:O	9:I:74:ILE:HG21	2.12	0.50
18:R:40:LEU:HA	18:R:43:PHE:HD2	1.76	0.50
1:A:358:U:H2'	1:A:359:U:C6	2.46	0.50
1:A:441:A:H5''	1:A:441:A:H8	1.77	0.50
1:A:992:U:H1'	1:A:993:G:C2	2.46	0.50
1:A:1001:A:H2'	1:A:1001(A):G:C8	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1071:C:H2'	1:A:1072:G:C8	2.45	0.50
1:A:1338:G:H21	25:Z:42:G:H1'	1.76	0.50
6:F:3:ARG:HB3	6:F:93:SER:HB2	1.93	0.50
10:J:50:ILE:HG23	10:J:59:SER:HB2	1.94	0.50
20:T:43:LEU:HB3	20:T:52:ALA:HB2	1.94	0.50
1:A:855:G:C6	1:A:856:C:C4	2.99	0.50
1:A:1007:C:N3	1:A:1023:G:C6	2.80	0.50
1:A:370:C:N3	1:A:392:G:C2	2.80	0.50
1:A:798:G:H2'	1:A:799:G:O4'	2.12	0.50
4:D:7:PRO:HB2	4:D:10:ARG:HD2	1.94	0.50
8:H:82:HIS:NE2	8:H:84:ARG:HB2	2.27	0.50
1:A:100:C:H2'	1:A:101:A:C8	2.47	0.49
1:A:255:G:H2'	1:A:256:U:H6	1.75	0.49
1:A:721:G:H4'	1:A:722:A:O4'	2.12	0.49
1:A:858:G:H5''	1:A:869:G:O6	2.12	0.49
1:A:902:G:H2'	1:A:903:G:H8	1.77	0.49
1:A:1293:G:H2'	1:A:1294:G:H8	1.76	0.49
1:A:1346:A:C8	1:A:1348:U:C2	3.00	0.49
1:A:1346:A:H2'	7:G:10:ARG:HH22	1.76	0.49
7:G:30:ILE:HG22	7:G:39:ALA:HB1	1.94	0.49
8:H:14:ARG:NH2	8:H:83:ILE:O	2.45	0.49
12:L:84:LEU:HB2	12:L:105:TYR:HD2	1.77	0.49
25:Z:32:OMC:N3	25:Z:38:A:N6	2.60	0.49
25:Z:67:C:C2	25:Z:68:C:C5	3.00	0.49
1:A:200:G:C6	1:A:201:C:N3	2.80	0.49
1:A:399:G:C6	1:A:400:C:N4	2.80	0.49
1:A:608:A:C4	1:A:609:A:C8	3.00	0.49
1:A:761:G:C6	1:A:762:C:C4	3.01	0.49
7:G:113:GLU:HG2	7:G:119:ARG:HG2	1.93	0.49
1:A:33:A:H2'	1:A:34:C:C6	2.48	0.49
1:A:504:C:C2	1:A:542:G:C2	3.00	0.49
1:A:623:C:H2'	1:A:624:C:O4'	2.12	0.49
1:A:855:G:C2	1:A:856:C:C2	3.01	0.49
1:A:861:G:N2	1:A:862:C:C2	2.79	0.49
1:A:1025:U:H2'	1:A:1026:G:C8	2.47	0.49
1:A:1399:C:C2	1:A:1502:A:N6	2.81	0.49
15:O:82:ILE:HA	15:O:87:ILE:HD12	1.93	0.49
1:A:460:G:H1'	1:A:472:A:H61	1.78	0.49
1:A:550:G:H2'	1:A:551:U:C6	2.46	0.49
1:A:767:A:H2'	1:A:768:A:C8	2.48	0.49
1:A:823:G:N2	1:A:824:C:C2	2.80	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:825:G:H1	1:A:875:C:H42	1.61	0.49
1:A:1060:C:H2'	1:A:1061:G:H8	1.78	0.49
3:C:116:VAL:O	3:C:120:VAL:HG23	2.12	0.49
8:H:12:ARG:HA	8:H:15:ASN:ND2	2.22	0.49
9:I:55:ALA:HB1	9:I:59:PHE:HD2	1.77	0.49
17:Q:38:ARG:HA	17:Q:38:ARG:HE	1.77	0.49
1:A:621:A:C6	1:A:622:A:C6	3.01	0.49
1:A:738:C:H5''	6:F:69:GLU:HB3	1.95	0.49
1:A:939:G:H1'	1:A:1375:A:C2	2.48	0.49
1:A:1000:U:C6	1:A:1000:U:C3'	2.96	0.49
1:A:1114:C:C2	1:A:1187:G:C2	3.01	0.49
8:H:87:SER:HB2	8:H:133:LEU:O	2.13	0.49
9:I:63:ILE:HG21	9:I:77:ILE:HG12	1.95	0.49
1:A:1351:U:H2'	1:A:1352:C:H6	1.76	0.49
13:M:45:VAL:HA	13:M:48:LEU:HD12	1.94	0.49
1:A:303:A:H2'	1:A:304:U:H6	1.77	0.49
1:A:769:G:N2	1:A:770:C:C2	2.81	0.49
1:A:1189:C:H5'	14:N:58:LYS:NZ	2.28	0.49
1:A:1276:G:H2'	1:A:1277:C:O4'	2.12	0.49
1:A:1347:G:C4	1:A:1373:G:C6	3.01	0.49
25:Z:22:G:N2	25:Z:23:C:C2	2.80	0.49
1:A:636:U:H2'	1:A:637:G:C8	2.48	0.49
1:A:954:G:H21	1:A:1227:A:H62	1.60	0.49
1:A:1281:U:H3	10:J:5:ARG:HH12	1.59	0.49
1:A:1347:G:H8	9:I:107:ARG:O	1.96	0.49
1:A:1371:G:H2'	1:A:1372:U:H6	1.77	0.49
1:A:1464:G:N1	1:A:1465:C:N4	2.61	0.49
1:A:1484:C:H2'	1:A:1485:U:O4'	2.13	0.49
4:D:8:VAL:HG13	4:D:9:CYS:N	2.27	0.49
7:G:54:THR:O	7:G:56:GLN:N	2.44	0.49
11:K:79:SER:HA	11:K:104:GLN:HB3	1.95	0.49
1:A:232:G:H2'	1:A:233:C:H6	1.77	0.49
1:A:460:G:H1'	1:A:472:A:N6	2.28	0.49
1:A:514:C:H2'	1:A:515:G:C8	2.48	0.49
1:A:734:G:C2	1:A:735:C:C2	3.01	0.49
1:A:974:A:H4'	1:A:975:A:H3'	1.93	0.49
1:A:975:A:H62	1:A:1366:C:HO2'	1.59	0.49
1:A:1464:G:C2	1:A:1465:C:N3	2.81	0.49
22:W:10:GLU:HG2	22:W:54:VAL:HG22	1.95	0.49
1:A:67:C:H2'	1:A:68:G:C8	2.48	0.49
1:A:236:G:C2	1:A:237:C:C2	3.01	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:610:G:C4	1:A:611:A:C8	3.01	0.49
1:A:883:C:H2'	1:A:884:U:C6	2.48	0.49
1:A:1057:G:H2'	1:A:1058:G:H8	1.78	0.49
2:B:63:MET:HG3	2:B:64:ARG:HH11	1.78	0.49
20:T:89:ARG:O	20:T:93:GLU:HG2	2.13	0.49
1:A:187:C:N3	20:T:105:SER:HB2	2.28	0.48
1:A:355:C:H2'	1:A:356:A:O4'	2.13	0.48
1:A:427:U:O2'	1:A:541:G:OP1	2.30	0.48
1:A:443:C:C2	1:A:492:G:C2	3.00	0.48
1:A:682:G:H2'	1:A:683:G:O4'	2.13	0.48
1:A:942:G:C2	1:A:1342:C:O2	2.66	0.48
1:A:962:C:H2'	1:A:963:G:O4'	2.13	0.48
1:A:1001:A:C6	1:A:1001(A):G:C6	3.01	0.48
1:A:1233:G:C6	1:A:1234:C:N4	2.81	0.48
1:A:1347:G:C2'	1:A:1348:U:OP2	2.61	0.48
5:E:103:GLY:O	5:E:106:PRO:HD2	2.12	0.48
6:F:97:PHE:HB2	18:R:32:ARG:CZ	2.43	0.48
10:J:65:LEU:HD23	14:N:56:VAL:HG22	1.95	0.48
18:R:37:VAL:HG21	18:R:78:LEU:HD22	1.95	0.48
1:A:253:U:H2'	1:A:254:G:H8	1.78	0.48
1:A:373:A:H2'	1:A:374:A:C8	2.44	0.48
1:A:987:G:H2'	1:A:988:G:H8	1.76	0.48
1:A:1087:G:H2'	1:A:1088:G:H8	1.77	0.48
1:A:1222:G:OP2	1:A:1322:C:C5	2.66	0.48
22:W:8:ARG:HD3	22:W:56:GLU:HG3	1.96	0.48
1:A:146:G:H2'	1:A:147:G:H8	1.78	0.48
1:A:473:G:OP1	16:P:81:ARG:NH1	2.46	0.48
1:A:632:A:H2'	1:A:633:G:O4'	2.13	0.48
1:A:639:G:H2'	1:A:640:A:C8	2.48	0.48
1:A:778:G:C6	1:A:779:C:C4	3.02	0.48
1:A:1063:C:H2'	1:A:1064:G:N7	2.29	0.48
1:A:1074:G:C6	1:A:1075:C:C4	3.02	0.48
1:A:1502:A:H2'	1:A:1504:G:N7	2.27	0.48
16:P:81:ARG:HB2	16:P:81:ARG:NH1	2.27	0.48
1:A:309:G:H2'	1:A:310:G:H8	1.77	0.48
1:A:522:C:H41	12:L:53:ARG:NH2	2.10	0.48
1:A:874:G:N1	1:A:875:C:C4	2.81	0.48
1:A:942:G:C6	1:A:1342:C:N3	2.81	0.48
6:F:75:LEU:O	6:F:79:LEU:HG	2.13	0.48
24:Y:36:A:H61	25:Z:37:A:N6	2.10	0.48
1:A:392:G:H2'	1:A:393:A:H8	1.74	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:633:G:H2'	1:A:634:C:C6	2.49	0.48
1:A:792:A:C6	1:A:794:A:C6	3.02	0.48
1:A:881:G:P	12:L:12:ARG:HH22	2.36	0.48
1:A:1457:G:C2	1:A:1458:G:H1'	2.48	0.48
8:H:103:VAL:HG21	8:H:110:ALA:HB2	1.96	0.48
1:A:555:C:H2'	1:A:556:C:C6	2.48	0.48
1:A:1241:G:C2	1:A:1242:C:C4	3.01	0.48
1:A:1245:A:H2'	1:A:1246:C:C6	2.48	0.48
1:A:1366:C:H2'	1:A:1367:C:C6	2.49	0.48
12:L:102:ARG:HB2	12:L:120:TYR:O	2.13	0.48
23:X:9:GLU:HG2	23:X:35:LEU:CD2	2.43	0.48
1:A:512:U:H2'	1:A:513:C:C6	2.49	0.48
1:A:1164:G:N2	1:A:1165:C:C2	2.81	0.48
1:A:1369:C:H2'	1:A:1370:G:O4'	2.14	0.48
1:A:1464:G:C6	1:A:1465:C:N4	2.82	0.48
1:A:1487:G:H2'	1:A:1488:G:C8	2.48	0.48
2:B:29:ALA:HA	2:B:32:ILE:HD12	1.96	0.48
12:L:9:GLN:HG3	12:L:12:ARG:HH21	1.79	0.48
25:Z:22:G:H8	25:Z:22:G:O5'	1.96	0.48
1:A:7:G:H5'	1:A:298:A:O4'	2.13	0.48
1:A:199:G:C2	1:A:219:C:N3	2.81	0.48
1:A:653:A:C4	8:H:56:LYS:HG2	2.48	0.48
23:X:157:LEU:HD22	25:Z:27:U:H5''	1.94	0.48
1:A:47:C:C6	1:A:365:U:H2'	2.49	0.48
1:A:548:G:H2'	1:A:549:C:C6	2.49	0.48
4:D:83:SER:HA	4:D:89:THR:CG2	2.44	0.48
7:G:65:ALA:HB1	7:G:127:ALA:CB	2.43	0.48
17:Q:64:PRO:HA	17:Q:70:ARG:HG3	1.95	0.48
20:T:45:GLN:HA	20:T:91:LEU:HD22	1.95	0.48
24:Y:36:A:C6	25:Z:37:A:N1	2.82	0.48
1:A:289:G:N2	1:A:290:C:C2	2.82	0.48
1:A:575:G:H4'	1:A:576:G:O5'	2.13	0.48
1:A:1351:U:H2'	1:A:1352:C:C6	2.48	0.48
1:A:1481:U:H2'	1:A:1482:G:O4'	2.14	0.48
5:E:148:VAL:O	5:E:152:ARG:HG2	2.13	0.48
20:T:53:LEU:HD21	20:T:104:LEU:HD12	1.96	0.48
1:A:289:G:C6	1:A:290:C:N4	2.82	0.47
1:A:919:A:H2'	1:A:920:U:C6	2.49	0.47
1:A:1078:U:H2'	1:A:1079:G:O4'	2.13	0.47
1:A:1162:C:C2	1:A:1175:G:C2	3.02	0.47
9:I:33:PHE:HZ	9:I:46:ALA:HB3	1.79	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:94:ILE:HG22	23:X:136:ILE:HD13	1.96	0.47
1:A:230:G:O2'	16:P:25:ARG:NH2	2.47	0.47
1:A:1053:G:C2	1:A:1199:U:C4	3.02	0.47
1:A:1099:G:C2	1:A:1100:C:O2	2.67	0.47
7:G:22:LEU:HB3	7:G:62:PHE:HZ	1.78	0.47
1:A:384:G:H2'	1:A:385:C:C6	2.49	0.47
1:A:1286:A:H2'	1:A:1287:A:H4'	1.96	0.47
4:D:64:LEU:HD12	4:D:198:VAL:HG21	1.97	0.47
6:F:7:ASN:ND2	6:F:62:TRP:HD1	2.13	0.47
13:M:23:TYR:HE1	13:M:70:LEU:HB3	1.80	0.47
17:Q:32:TYR:C	17:Q:34:LYS:H	2.22	0.47
1:A:829:G:H5''	1:A:829:G:H8	1.78	0.47
1:A:1074:G:C2	1:A:1075:C:C2	3.02	0.47
1:A:1312:G:H2'	1:A:1313:U:C6	2.49	0.47
1:A:1355:G:H2'	1:A:1356:G:H8	1.79	0.47
7:G:65:ALA:CB	7:G:127:ALA:HB3	2.44	0.47
20:T:54:LYS:HA	20:T:57:ARG:HD3	1.96	0.47
23:X:71:MET:O	23:X:75:GLU:HG2	2.15	0.47
24:Y:21:G:H2'	24:Y:22:G:H8	1.78	0.47
1:A:8:A:H5'	5:E:101:ILE:HG22	1.97	0.47
1:A:513:C:H2'	1:A:514:C:C6	2.50	0.47
1:A:629:G:H2'	1:A:630:G:O4'	2.15	0.47
1:A:690:G:H2'	1:A:691:G:O4'	2.14	0.47
1:A:878:G:H2'	1:A:879:C:C6	2.49	0.47
1:A:1419:G:C2	1:A:1420:C:C2	3.02	0.47
4:D:29:PRO:HB3	4:D:35:ARG:CZ	2.44	0.47
4:D:80:GLU:HB3	4:D:84:LYS:NZ	2.30	0.47
8:H:88:LYS:HB2	8:H:91:ARG:HB3	1.97	0.47
9:I:46:ALA:HA	9:I:78:LYS:HB2	1.97	0.47
12:L:7:ILE:HA	12:L:10:LEU:HD12	1.96	0.47
20:T:41:ILE:CD1	20:T:87:LYS:HZ2	2.26	0.47
1:A:41:G:H2'	1:A:42:G:C8	2.49	0.47
1:A:750:G:H1'	15:O:23:GLY:H	1.80	0.47
1:A:1106:G:N1	1:A:1107:C:C4	2.82	0.47
4:D:200:GLU:HG2	4:D:201:GLN:N	2.29	0.47
13:M:84:ILE:HD12	19:S:74:PHE:HE1	1.80	0.47
1:A:562:C:N4	1:A:884:U:H2'	2.29	0.47
1:A:1046:A:H3'	1:A:1047:G:C8	2.45	0.47
1:A:1057:G:H2'	1:A:1058:G:C8	2.49	0.47
1:A:1370:G:C2	1:A:1371:G:N7	2.83	0.47
1:A:1470:G:H2'	1:A:1471:G:O4'	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:76:ILE:HG13	5:E:142:LEU:HD21	1.96	0.47
22:W:37:SER:HB3	22:W:40:MET:HG3	1.97	0.47
23:X:56:VAL:CG1	25:Z:19:G:O6	2.62	0.47
24:Y:21:G:H2'	24:Y:22:G:C8	2.49	0.47
1:A:448:A:OP2	1:A:485:G:N2	2.48	0.47
1:A:670:G:H1	1:A:736:C:N4	2.09	0.47
1:A:967:C:O2'	9:I:128:ARG:NH2	2.47	0.47
1:A:1387:G:C6	1:A:1388:C:N4	2.83	0.47
1:A:1457:G:C5	1:A:1458:G:C8	3.03	0.47
2:B:185:ILE:HG13	2:B:199:TYR:HB2	1.97	0.47
6:F:62:TRP:CH2	6:F:64:GLN:HB2	2.50	0.47
20:T:12:ALA:O	20:T:15:ARG:HB2	2.15	0.47
1:A:568:G:H2'	1:A:569:C:C6	2.49	0.47
1:A:673:G:H2'	1:A:674:G:C8	2.49	0.47
1:A:895:G:H1	1:A:904:C:N4	2.10	0.47
1:A:979:C:H41	1:A:1360:A:N6	2.13	0.47
15:O:74:ASP:HA	15:O:75:PRO:HD3	1.84	0.47
1:A:351:G:H4'	1:A:352:C:OP1	2.15	0.47
1:A:473:G:H5''	16:P:81:ARG:NH2	2.30	0.47
1:A:588:G:N1	1:A:589:C:C4	2.83	0.47
1:A:1328:C:H2'	1:A:1329:A:H8	1.79	0.47
1:A:1334:G:H8	1:A:1334:G:O5'	1.98	0.47
4:D:9:CYS:SG	4:D:22:LYS:HG2	2.55	0.47
5:E:115:VAL:HG11	5:E:118:ILE:HG12	1.97	0.47
13:M:91:ARG:HG3	13:M:98:VAL:HG13	1.96	0.47
13:M:107:ALA:HB3	13:M:111:LYS:HD2	1.97	0.47
25:Z:22:G:OP2	25:Z:46:G7M:C2	2.63	0.47
1:A:235:C:H2'	1:A:236:G:H8	1.81	0.46
1:A:316:G:H1	1:A:337:C:H42	1.61	0.46
1:A:739:C:O2'	15:O:42:HIS:ND1	2.43	0.46
1:A:743:U:H2'	1:A:744:C:H6	1.77	0.46
1:A:1347:G:O2'	1:A:1348:U:P	2.73	0.46
12:L:53:ARG:HG2	12:L:53:ARG:HH11	1.80	0.46
20:T:33:ILE:HG13	20:T:62:LEU:HD22	1.96	0.46
1:A:27:G:H2'	1:A:28:G:O4'	2.14	0.46
1:A:319:G:N2	1:A:320:C:C2	2.83	0.46
1:A:486:U:C2	1:A:487:A:C8	3.04	0.46
1:A:761:G:H2'	1:A:762:C:C6	2.50	0.46
1:A:778:G:C2	1:A:779:C:C2	3.03	0.46
1:A:864:A:C3'	1:A:865:A:C8	2.98	0.46
1:A:865:A:P	1:A:865:A:H8	2.38	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:G:H2'	1:A:948:C:C6	2.50	0.46
1:A:1067:A:H1'	1:A:1068:G:O4'	2.14	0.46
1:A:1075:C:H4'	1:A:1101:A:N6	2.30	0.46
1:A:1099:G:C6	1:A:1100:C:C2	3.03	0.46
1:A:1251:A:H2'	1:A:1252:A:C8	2.49	0.46
1:A:1309:G:C6	1:A:1329:A:C6	3.03	0.46
3:C:184:TYR:HE1	3:C:186:PHE:HB2	1.80	0.46
5:E:70:PRO:HG2	5:E:142:LEU:HD22	1.97	0.46
7:G:78:ARG:NH1	7:G:154:TYR:HB3	2.30	0.46
15:O:77:ARG:HG2	15:O:77:ARG:HH11	1.79	0.46
19:S:36:ARG:HB2	19:S:72:GLY:HA3	1.97	0.46
1:A:17:U:H2'	1:A:18:C:C5	2.50	0.46
1:A:500:G:C2	1:A:501:C:C2	3.04	0.46
1:A:509:A:H4'	1:A:510:A:OP1	2.15	0.46
1:A:1419:G:C6	1:A:1420:C:C4	3.03	0.46
2:B:209:ARG:HD3	2:B:239:VAL:HG11	1.97	0.46
7:G:65:ALA:CB	7:G:127:ALA:CB	2.94	0.46
1:A:112:G:H1	1:A:315:A:H61	1.63	0.46
1:A:116:A:H2'	1:A:117:G:H8	1.80	0.46
1:A:661:G:N2	1:A:745:C:C2	2.84	0.46
1:A:734:G:C6	1:A:735:C:C4	3.03	0.46
1:A:1178:G:OP2	9:I:97:LYS:HD2	2.15	0.46
1:A:1256:A:C8	3:C:27:LYS:NZ	2.78	0.46
1:A:1312:G:C2	1:A:1326:C:C2	3.03	0.46
2:B:84:GLU:HB3	2:B:219:VAL:HG21	1.97	0.46
3:C:26:LYS:HD3	14:N:36:PHE:CE1	2.46	0.46
8:H:46:LYS:HB3	8:H:62:TYR:HB3	1.97	0.46
9:I:50:LEU:HB3	9:I:56:LEU:H	1.79	0.46
1:A:146:G:H2'	1:A:147:G:C8	2.50	0.46
1:A:320:C:H2'	1:A:321:A:O4'	2.15	0.46
1:A:398:C:H2'	1:A:399:G:C8	2.48	0.46
1:A:416:G:C6	1:A:417:C:C4	3.03	0.46
1:A:834:C:C2	1:A:853:G:C2	3.04	0.46
4:D:31:CYS:C	4:D:33:MET:N	2.71	0.46
5:E:80:ILE:HG23	8:H:104:ARG:HH12	1.81	0.46
16:P:8:ARG:HE	16:P:15:PRO:HB3	1.80	0.46
25:Z:33:U:C6	25:Z:35:A:OP2	2.68	0.46
1:A:603:U:H2'	1:A:604:G:H8	1.80	0.46
1:A:914:A:H2'	1:A:915:A:H8	1.80	0.46
1:A:1288:A:N1	1:A:1371:G:H1'	2.31	0.46
1:A:1306:A:N6	1:A:1331:G:O4'	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:10:LEU:HA	8:H:13:ILE:HD12	1.97	0.46
16:P:19:ILE:O	16:P:36:ILE:HG13	2.16	0.46
25:Z:64:G:C6	25:Z:65:C:C4	3.03	0.46
1:A:90:U:H2'	1:A:91:C:C5	2.49	0.46
1:A:682:G:H1	1:A:708:C:H42	1.64	0.46
1:A:942:G:N1	1:A:1342:C:C2	2.82	0.46
1:A:1087:G:H2'	1:A:1088:G:C8	2.51	0.46
1:A:1298:C:OP1	1:A:1299:A:C8	2.69	0.46
24:Y:39:U:O4	25:Z:35:A:C1'	2.63	0.46
25:Z:64:G:C2	25:Z:65:C:C2	3.04	0.46
1:A:36:C:H4'	12:L:117:ARG:HH21	1.81	0.46
1:A:519:C:H2'	1:A:520:A:O4'	2.16	0.46
1:A:527:G:N2	1:A:528:C:C2	2.84	0.46
1:A:799:G:H3'	1:A:800:G:H8	1.80	0.46
1:A:800:G:H2'	1:A:801:U:C5	2.51	0.46
1:A:918:A:N6	1:A:919:A:N6	2.64	0.46
1:A:920:U:H2'	1:A:921:U:H6	1.71	0.46
1:A:1076:C:N3	1:A:1082:G:C2	2.84	0.46
1:A:1297:C:H1'	1:A:1298:C:H5	1.79	0.46
1:A:1537:U:N3	24:Y:28:A:N6	2.63	0.46
14:N:50:LYS:HD2	14:N:52:GLN:HE21	1.81	0.46
1:A:321:A:H2'	1:A:322:C:C6	2.51	0.46
1:A:402:G:N2	1:A:403:C:C2	2.83	0.46
1:A:1017:G:C2	1:A:1018:C:C2	3.03	0.46
1:A:1274:G:H2'	1:A:1275:A:C8	2.47	0.46
1:A:1493:A:H4'	1:A:1494:G:C5'	2.45	0.46
1:A:1517:G:H2'	1:A:1518:A:O4'	2.15	0.46
3:C:23:TYR:HD1	10:J:11:PHE:HZ	1.64	0.46
4:D:67:ILE:HG21	4:D:196:LEU:HD13	1.97	0.46
4:D:158:ILE:H	4:D:158:ILE:HD12	1.80	0.46
10:J:6:ILE:HD11	10:J:23:ILE:HG21	1.97	0.46
15:O:50:HIS:O	15:O:53:HIS:HB3	2.16	0.46
20:T:71:THR:HB	20:T:72:LEU:HG	1.97	0.46
24:Y:28:A:C6	24:Y:29:G:C6	3.04	0.46
1:A:105:G:C2	1:A:106:C:C2	3.04	0.46
1:A:257:G:H1	1:A:269:C:N4	2.13	0.46
1:A:522:C:OP2	12:L:69:TYR:OH	2.29	0.46
1:A:524:G:C5	1:A:525:C:N4	2.84	0.46
1:A:524:G:H2'	1:A:525:C:C6	2.51	0.46
1:A:544:G:C2	1:A:545:C:C2	3.04	0.46
1:A:999:C:N3	1:A:1043:C:N3	2.63	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1187:G:H2'	1:A:1188:A:C8	2.51	0.46
1:A:1430:C:C2	1:A:1471:G:N2	2.83	0.46
2:B:15:VAL:HG11	2:B:209:ARG:HB3	1.98	0.46
2:B:196:LEU:HG	8:H:74:PRO:HG3	1.97	0.46
8:H:82:HIS:CE1	8:H:84:ARG:HB2	2.51	0.46
1:A:456:C:C2	1:A:476:G:N2	2.84	0.45
1:A:939:G:H2'	1:A:940:C:C6	2.51	0.45
1:A:1539:C:N3	24:Y:26:G:N2	2.47	0.45
8:H:13:ILE:O	8:H:17:THR:HG23	2.16	0.45
25:Z:52:G:C2	25:Z:63:G:C2	3.04	0.45
1:A:447:G:H3'	1:A:485:G:H22	1.81	0.45
1:A:765:G:N1	1:A:812:C:H2'	2.31	0.45
1:A:1190:G:OP1	3:C:5:ILE:HG13	2.16	0.45
1:A:1303:C:H42	1:A:1334:G:H1	1.63	0.45
3:C:150:LYS:HB3	3:C:201:TYR:HB2	1.98	0.45
4:D:50:ARG:HH21	5:E:10:MET:HB3	1.82	0.45
5:E:50:GLU:HG2	5:E:52:PRO:HD2	1.98	0.45
6:F:22:GLU:HA	6:F:25:ILE:HD12	1.96	0.45
8:H:48:TYR:HA	8:H:60:ARG:O	2.15	0.45
1:A:200:G:C2	1:A:201:C:O2	2.70	0.45
1:A:250:A:H4'	1:A:251:G:O5'	2.16	0.45
1:A:558:G:H2'	1:A:559:A:C2	2.52	0.45
1:A:1241:G:N1	1:A:1242:C:C4	2.85	0.45
1:A:1387:G:H2'	1:A:1388:C:C6	2.50	0.45
5:E:51:VAL:HG12	5:E:52:PRO:HD3	1.97	0.45
9:I:9:ARG:HD2	9:I:104:ARG:HH21	1.81	0.45
11:K:84:VAL:HG11	11:K:95:ILE:HD11	1.98	0.45
24:Y:37:U:H2'	24:Y:38:G:C8	2.52	0.45
25:Z:21:A:N6	25:Z:46:G7M:O2'	2.50	0.45
1:A:41:G:H1	1:A:401:C:N4	2.14	0.45
1:A:51:A:H4'	1:A:52:G:O5'	2.16	0.45
1:A:70:G:C2	1:A:100:C:C2	3.04	0.45
1:A:76:C:N4	1:A:77:G:O6	2.49	0.45
1:A:276:G:H2'	1:A:277:C:C6	2.51	0.45
1:A:323:U:O5'	1:A:323:U:H6	2.00	0.45
1:A:363:A:OP2	12:L:34:ARG:HG3	2.16	0.45
1:A:447:G:H2'	1:A:485:G:N2	2.31	0.45
1:A:577:G:C2	1:A:578:C:C2	3.04	0.45
1:A:724:G:H8	1:A:724:G:O5'	2.00	0.45
1:A:1147:C:O2	9:I:16:ARG:NH1	2.50	0.45
1:A:1311:G:N7	19:S:2:PRO:N	2.64	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1324:A:H2'	1:A:1325:C:O4'	2.16	0.45
1:A:1517:G:H2'	1:A:1518:A:C8	2.52	0.45
4:D:76:ARG:HD2	4:D:207:TYR:CE1	2.51	0.45
5:E:37:ARG:HH12	5:E:111:GLU:HB3	1.80	0.45
23:X:34:ALA:HB1	23:X:45:LEU:HD11	1.99	0.45
25:Z:37:A:H3'	25:Z:38:A:C8	2.51	0.45
1:A:391:G:C6	1:A:392:G:C5	3.05	0.45
1:A:1168:A:H2'	1:A:1169:A:C8	2.52	0.45
1:A:43:C:H2'	1:A:44:G:H8	1.81	0.45
1:A:198:G:H2'	1:A:199:G:O4'	2.17	0.45
1:A:626:U:H2'	1:A:627:G:C8	2.51	0.45
1:A:941:G:H1	1:A:1342:C:H42	1.65	0.45
1:A:1002:G:O6	1:A:1039:C:N3	2.49	0.45
1:A:1162:C:N3	1:A:1175:G:C2	2.84	0.45
1:A:1371:G:O3'	9:I:69:GLY:HA3	2.17	0.45
1:A:1508:G:H2'	1:A:1509:C:C6	2.52	0.45
2:B:96:ARG:CG	2:B:98:LEU:HG	2.47	0.45
7:G:124:LEU:HD23	7:G:124:LEU:HA	1.90	0.45
25:Z:7:G:P	25:Z:16:C:H42	2.40	0.45
25:Z:21:A:N6	25:Z:48:C:C6	2.85	0.45
1:A:242:C:C2	1:A:285:G:N2	2.85	0.45
1:A:544:G:C6	1:A:545:C:C4	3.05	0.45
1:A:748:C:H1'	1:A:749:C:H5	1.81	0.45
1:A:909:A:H2'	1:A:910:C:O4'	2.16	0.45
1:A:1219:U:OP1	14:N:19:ARG:NH2	2.49	0.45
2:B:130:ARG:NH2	3:C:207:VAL:CG2	2.80	0.45
5:E:117:ASP:O	5:E:118:ILE:HG23	2.16	0.45
6:F:100:ASN:HD22	18:R:23:LYS:HG2	1.81	0.45
17:Q:67:LYS:O	17:Q:68:ARG:HG3	2.15	0.45
25:Z:47:U:H4'	25:Z:48:C:O5'	2.17	0.45
25:Z:67:C:H2'	25:Z:68:C:H6	1.81	0.45
1:A:72:C:C2'	1:A:73:G:H5''	2.43	0.45
1:A:450:G:N7	1:A:481:G:C6	2.85	0.45
1:A:874:G:C2	1:A:875:C:C2	3.05	0.45
1:A:1217:C:H2'	1:A:1218:C:O4'	2.15	0.45
5:E:148:VAL:HG11	8:H:107:LEU:CD2	2.47	0.45
17:Q:59:ILE:HG22	17:Q:71:PHE:HB3	1.98	0.45
18:R:59:SER:HB3	18:R:62:GLU:HB2	1.98	0.45
23:X:99:TYR:HE1	23:X:140:VAL:HG22	1.82	0.45
1:A:129(A):G:O2'	1:A:189(F):U:H5''	2.17	0.45
1:A:190:U:H2'	1:A:191:G:C8	2.52	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:G:C2	1:A:417:C:C2	3.04	0.45
1:A:998:G:N1	1:A:999:C:C4	2.85	0.45
1:A:1001(A):G:C6	1:A:1002:G:O6	2.70	0.45
1:A:1096:C:H2'	1:A:1097:C:C6	2.52	0.45
1:A:1266:G:C2	1:A:1270:C:N3	2.85	0.45
8:H:41:ARG:HG2	8:H:42:GLU:N	2.31	0.45
10:J:33:GLN:HB3	10:J:75:ILE:HD12	1.98	0.45
11:K:126:ARG:C	11:K:128:ALA:H	2.25	0.45
17:Q:92:ARG:HA	17:Q:95:TYR:CD2	2.51	0.45
1:A:519:C:H4'	22:W:66:ARG:CZ	2.47	0.45
1:A:838:G:C2	1:A:849:C:C2	3.04	0.45
1:A:1255:G:O2'	1:A:1258:G:H1'	2.17	0.45
1:A:1492:A:H3'	1:A:1493:A:H3'	1.99	0.45
1:A:1510:U:H2'	1:A:1511:G:C8	2.52	0.45
3:C:52:LEU:HA	3:C:70:VAL:HG12	1.99	0.45
10:J:79:ARG:NH1	10:J:82:ILE:HB	2.32	0.45
23:X:66:ARG:HD2	23:X:66:ARG:HA	1.93	0.45
1:A:166:G:N1	1:A:167:G:C6	2.84	0.44
1:A:417:C:H42	1:A:418:C:N4	2.15	0.44
1:A:1305:G:H22	1:A:1331:G:H1'	1.81	0.44
12:L:93:LEU:HA	12:L:94:PRO:HD3	1.79	0.44
1:A:157:G:N1	1:A:165:C:C2	2.85	0.44
1:A:189:G:C2	1:A:189(A):C:C2	3.05	0.44
1:A:262:A:H5''	20:T:76:ALA:HB2	2.00	0.44
1:A:394:G:N2	1:A:395:C:C2	2.85	0.44
1:A:557:G:C6	1:A:558:G:N1	2.85	0.44
1:A:947:G:C2	1:A:948:C:C2	3.05	0.44
1:A:1110:A:H2'	1:A:1111:A:O4'	2.17	0.44
1:A:1184:G:H8	1:A:1184:G:O5'	1.99	0.44
1:A:1508:G:C2	1:A:1509:C:C2	3.05	0.44
3:C:67:THR:HA	3:C:102:ASN:HB2	1.99	0.44
5:E:145:LYS:O	5:E:148:VAL:HG12	2.16	0.44
10:J:50:ILE:HG22	10:J:52:GLY:H	1.80	0.44
1:A:354:G:C6	1:A:355:C:N4	2.85	0.44
1:A:491:G:H2'	1:A:492:G:H8	1.82	0.44
1:A:545:C:O2'	1:A:549:C:H5''	2.16	0.44
1:A:778:G:C6	1:A:779:C:C2	3.06	0.44
1:A:973:G:H3'	1:A:974:A:H5''	2.00	0.44
1:A:1061:G:H1	1:A:1195:C:H42	1.66	0.44
1:A:1233:G:N2	1:A:1234:C:C2	2.86	0.44
2:B:15:VAL:HG21	2:B:209:ARG:HG2	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:10:MET:HA	5:E:32:VAL:HG23	1.98	0.44
15:O:70:LEU:O	15:O:74:ASP:N	2.50	0.44
19:S:19:VAL:HG21	19:S:44:MET:HG2	1.99	0.44
25:Z:62:C:H2'	25:Z:63:G:C8	2.53	0.44
1:A:35:G:C6	1:A:36:C:N4	2.85	0.44
1:A:146:G:C2	1:A:177:C:N3	2.85	0.44
1:A:157:G:C6	1:A:165:C:N3	2.85	0.44
1:A:568:G:N2	1:A:569:C:C2	2.85	0.44
1:A:618:C:H4'	16:P:42:ARG:HH22	1.82	0.44
1:A:785:G:C8	1:A:785:G:C5'	3.00	0.44
1:A:1263:C:N4	1:A:1264:C:N4	2.66	0.44
1:A:1339:A:H1'	25:Z:41:C:O2'	2.17	0.44
1:A:1468:A:H2'	1:A:1469:G:O4'	2.18	0.44
1:A:1536:C:N3	24:Y:29:G:N2	2.61	0.44
10:J:43:ARG:HD3	10:J:43:ARG:HA	1.78	0.44
12:L:35:GLY:HA3	12:L:60:LEU:HD13	1.99	0.44
22:W:17:LEU:HB2	22:W:21:THR:O	2.18	0.44
1:A:13:U:N3	1:A:915:A:N6	2.65	0.44
1:A:149:A:H2'	1:A:150:C:C6	2.52	0.44
1:A:537:G:H2'	1:A:538:G:O4'	2.16	0.44
1:A:573:A:H2'	1:A:574:A:O4'	2.17	0.44
1:A:774:G:C2	1:A:806:C:C2	3.05	0.44
1:A:977:A:H3'	1:A:977:A:N3	2.32	0.44
1:A:1305:G:O2'	1:A:1306:A:C8	2.70	0.44
2:B:127:ILE:H	2:B:127:ILE:HG13	1.66	0.44
12:L:77:LEU:HD13	12:L:107:ALA:HB2	1.99	0.44
20:T:49:ALA:O	20:T:53:LEU:HB2	2.18	0.44
24:Y:35:A:H4'	24:Y:36:A:OP2	2.16	0.44
25:Z:1:C:H2'	25:Z:2:G:C8	2.46	0.44
25:Z:20:U:O2	25:Z:20:U:H3'	2.16	0.44
1:A:119:A:H2'	1:A:240:C:H41	1.82	0.44
1:A:548:G:C2	1:A:549:C:C4	3.05	0.44
1:A:764:C:H2'	1:A:765:G:O4'	2.17	0.44
1:A:1048:G:H1	1:A:1209:C:N4	2.16	0.44
9:I:127:LYS:HG3	25:Z:32:OMC:OP2	2.18	0.44
13:M:87:TYR:HD1	19:S:76:PRO:HB3	1.83	0.44
19:S:51:VAL:HG11	19:S:72:GLY:HA2	1.99	0.44
1:A:189(B):C:H2'	1:A:189(C):C:C6	2.53	0.44
1:A:363:A:H2'	1:A:364:A:C8	2.53	0.44
1:A:554:C:H2'	1:A:555:C:H6	1.83	0.44
1:A:939:G:H1	1:A:1344:C:N4	2.13	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:G:N2	1:A:1217:C:C2	2.85	0.44
2:B:19:HIS:CD2	2:B:20:GLU:HG2	2.53	0.44
2:B:221:LEU:HD12	2:B:221:LEU:HA	1.76	0.44
4:D:30:LYS:C	4:D:32:ALA:N	2.73	0.44
14:N:42:ILE:H	14:N:42:ILE:HD12	1.83	0.44
25:Z:7:G:C6	25:Z:49:G:N7	2.86	0.44
1:A:41:G:H2'	1:A:42:G:H8	1.83	0.44
1:A:44:G:OP2	16:P:12:LYS:HD2	2.18	0.44
1:A:276:G:C2	1:A:277:C:C2	3.05	0.44
1:A:729:A:H2'	1:A:730:G:C8	2.53	0.44
1:A:999:C:C2	1:A:1043:C:O2	2.69	0.44
1:A:1029:C:H2'	1:A:1030:C:C6	2.53	0.44
1:A:1142:G:H2'	1:A:1143:G:O4'	2.17	0.44
1:A:1222:G:OP2	1:A:1322:C:H5	2.01	0.44
1:A:500:G:H2'	1:A:501:C:H6	1.82	0.44
1:A:683:G:C2	1:A:708:C:N3	2.86	0.44
1:A:769:G:C2	1:A:770:C:C2	3.05	0.44
1:A:881:G:C2	1:A:882:C:C2	3.06	0.44
1:A:994:A:N7	1:A:1216:G:H4'	2.33	0.44
2:B:90:MET:HA	2:B:91:PRO:HD2	1.78	0.44
2:B:112:VAL:HG23	2:B:149:LEU:HD23	1.99	0.44
5:E:12:LEU:HD13	5:E:13:ILE:H	1.83	0.44
5:E:43:LEU:HD22	5:E:136:MET:HG3	2.00	0.44
1:A:189(B):C:C2	1:A:189(J):G:N2	2.86	0.43
1:A:241:C:C2	1:A:286:G:N2	2.86	0.43
1:A:568:G:C2	1:A:569:C:N3	2.86	0.43
1:A:1000:U:H3'	1:A:1000:U:H6	1.79	0.43
1:A:1048:G:H2'	1:A:1050:G:H8	1.81	0.43
3:C:155:GLY:HA2	3:C:163:ALA:HB1	1.99	0.43
7:G:80:VAL:HG23	7:G:85:TYR:CD2	2.53	0.43
10:J:50:ILE:HG12	10:J:57:LYS:HA	2.00	0.43
10:J:51:ARG:HA	14:N:45:ARG:HD2	2.00	0.43
11:K:109:VAL:HG13	18:R:84:LYS:HB3	1.99	0.43
1:A:31:G:O2'	1:A:48:C:N4	2.52	0.43
1:A:903:G:C2	1:A:904:C:C2	3.05	0.43
1:A:947:G:H2'	1:A:948:C:O4'	2.18	0.43
1:A:1347:G:O2'	1:A:1348:U:OP2	2.32	0.43
1:A:1504:G:H4'	1:A:1505:G:O5'	2.18	0.43
4:D:108:LEU:HB3	4:D:110:PHE:CD1	2.54	0.43
1:A:189:G:C6	1:A:189(A):C:C4	3.07	0.43
1:A:585:G:C2	1:A:586:C:C2	3.06	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:G:N1	1:A:862:C:C4	2.86	0.43
1:A:872:A:C8	1:A:874:G:C8	3.07	0.43
1:A:1423:G:N2	1:A:1424:C:C2	2.86	0.43
1:A:1520:G:H2'	1:A:1521:G:C8	2.53	0.43
15:O:15:PHE:CE2	15:O:84:LYS:HB3	2.52	0.43
17:Q:46:ASP:HA	17:Q:47:PRO:HD2	1.90	0.43
18:R:53:ARG:HH21	18:R:60:ALA:CB	2.23	0.43
1:A:19:C:H5''	5:E:86:ALA:HB3	1.99	0.43
1:A:28:G:C2	1:A:556:C:N3	2.86	0.43
1:A:89:C:H2'	1:A:90:U:O4'	2.18	0.43
1:A:378:G:C6	1:A:379:C:N4	2.87	0.43
1:A:1263:C:C4	1:A:1264:C:N4	2.86	0.43
3:C:19:GLU:HB2	14:N:52:GLN:HA	2.00	0.43
5:E:76:ILE:HG22	5:E:93:PRO:HB3	2.00	0.43
5:E:79:GLU:HG3	5:E:93:PRO:HD2	1.99	0.43
12:L:118:SER:C	12:L:120:TYR:H	2.26	0.43
25:Z:28:C:C2	25:Z:43:A:C2	3.06	0.43
1:A:157:G:C2	1:A:165:C:O2	2.72	0.43
1:A:333:G:C2	1:A:334:C:C4	3.06	0.43
1:A:340:U:H2'	1:A:341:C:C6	2.53	0.43
1:A:548:G:C2	1:A:549:C:N3	2.86	0.43
1:A:893:C:H6	1:A:893:C:O5'	2.02	0.43
1:A:1009:G:C6	1:A:1021:G:C5	3.07	0.43
1:A:1311:G:OP2	19:S:3:ARG:HG3	2.19	0.43
3:C:50:ALA:HB2	3:C:75:VAL:HB	1.99	0.43
6:F:50:TYR:CE1	18:R:77:GLY:HA2	2.54	0.43
1:A:457:C:H2'	1:A:458:C:C6	2.53	0.43
1:A:564:C:C2	17:Q:31:LEU:HD11	2.53	0.43
1:A:601:C:C2	1:A:638:G:C2	3.07	0.43
1:A:823:G:C2	1:A:824:C:C2	3.07	0.43
3:C:56:ASP:O	3:C:66:VAL:HA	2.19	0.43
1:A:306:G:C2	1:A:307:C:C2	3.06	0.43
1:A:1095:U:C4	1:A:1096:C:C4	3.06	0.43
1:A:1445:C:N3	1:A:1458:G:C2	2.86	0.43
16:P:20:VAL:HG23	16:P:35:LYS:HA	2.00	0.43
1:A:21:G:C2	1:A:22:G:C5	3.07	0.43
1:A:127:G:C2	1:A:235:C:N3	2.86	0.43
1:A:279:A:OP2	17:Q:95:TYR:OH	2.35	0.43
1:A:410:G:OP2	4:D:25:ARG:NE	2.44	0.43
1:A:542:G:N2	1:A:543:C:C2	2.87	0.43
1:A:821:G:C2	1:A:822:C:C2	3.07	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:G:O3'	1:A:1025:U:H4'	2.16	0.43
1:A:1302:U:H3'	1:A:1303:C:H5''	2.01	0.43
1:A:1402:C:H2'	1:A:1403:C:O4'	2.19	0.43
2:B:17:PHE:HD1	2:B:18:GLY:H	1.67	0.43
2:B:79:ASP:HB3	2:B:238:LEU:HD23	2.01	0.43
12:L:23:LYS:O	12:L:97:ARG:NH1	2.51	0.43
15:O:53:HIS:HA	15:O:56:LEU:HD23	1.99	0.43
18:R:52:PRO:HD2	18:R:55:ARG:HB2	2.00	0.43
25:Z:22:G:N1	25:Z:23:C:C4	2.87	0.43
1:A:287:U:H2'	1:A:288:A:C8	2.47	0.43
1:A:306:G:C6	1:A:307:C:C4	3.07	0.43
1:A:320:C:H2'	1:A:321:A:C8	2.54	0.43
1:A:518:C:O2'	1:A:519:C:OP2	2.29	0.43
1:A:820:U:N3	1:A:873:A:N7	2.67	0.43
1:A:1198:G:H2'	1:A:1199:U:C6	2.54	0.43
1:A:1281:U:H4'	1:A:1282:C:OP2	2.19	0.43
1:A:1298:C:H4'	1:A:1299:A:C4	2.54	0.43
1:A:1305:G:C5'	21:V:4:GLY:HA3	2.49	0.43
1:A:1353:G:C6	1:A:1354:C:N4	2.87	0.43
1:A:1502:A:C2	1:A:1504:G:C4	3.06	0.43
10:J:24:VAL:HG21	10:J:37:PRO:HD3	2.00	0.43
20:T:74:LYS:HB2	20:T:75:ASN:H	1.49	0.43
22:W:13:VAL:HG22	22:W:24:VAL:HG22	2.01	0.43
23:X:167:PRO:HG2	23:X:170:VAL:HG22	2.01	0.43
1:A:22:G:H2'	1:A:23:C:C6	2.54	0.43
1:A:41:G:C6	1:A:402:G:C6	3.07	0.43
1:A:603:U:H2'	1:A:604:G:C8	2.54	0.43
1:A:620:C:N4	1:A:621:A:C6	2.87	0.43
1:A:628:G:H2'	1:A:629:G:H8	1.84	0.43
1:A:1171:G:C6	1:A:1172:C:N4	2.87	0.43
1:A:1343:G:OP1	9:I:125:TYR:HE2	2.02	0.43
1:A:1520:G:H2'	1:A:1521:G:H8	1.84	0.43
4:D:185:PHE:CZ	4:D:189:PRO:HD3	2.54	0.43
9:I:13:ALA:HB2	9:I:68:GLY:HA3	2.01	0.43
1:A:579:G:H2'	1:A:580:U:C6	2.54	0.42
1:A:679:C:N4	1:A:680:C:N4	2.67	0.42
1:A:1187:G:H3'	1:A:1188:A:C8	2.54	0.42
5:E:79:GLU:HA	5:E:91:LEU:O	2.18	0.42
19:S:40:ILE:CD1	19:S:62:ILE:HD11	2.45	0.42
1:A:262:A:H5'	20:T:74:LYS:HZ2	1.84	0.42
1:A:542:G:C2	1:A:543:C:C2	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:660:G:H1	1:A:745:C:N4	2.17	0.42
13:M:91:ARG:HD2	13:M:96:LEU:HD12	2.00	0.42
25:Z:51:C:N3	25:Z:63:G:N2	2.54	0.42
1:A:102:G:C2	1:A:103:C:C2	3.07	0.42
1:A:515:G:C6	1:A:516:U:N3	2.87	0.42
1:A:585:G:C6	1:A:586:C:C4	3.07	0.42
1:A:774:G:C2	1:A:806:C:N3	2.88	0.42
1:A:874:G:C6	1:A:875:C:C4	3.07	0.42
1:A:877:C:H2'	1:A:878:G:C8	2.52	0.42
1:A:1076:C:C2	1:A:1082:G:C2	3.08	0.42
1:A:1279:A:H1'	1:A:1282:C:N4	2.34	0.42
1:A:1290:G:H5'	7:G:35:LYS:NZ	2.34	0.42
1:A:1468:A:H3'	1:A:1469:G:H8	1.82	0.42
14:N:32:SER:HB3	14:N:41:ARG:HG2	2.02	0.42
1:A:96:U:H2'	1:A:97:G:H8	1.84	0.42
1:A:502:G:H2'	1:A:503:C:C6	2.55	0.42
1:A:545:C:N4	1:A:546:G:C6	2.87	0.42
1:A:866:C:C4	1:A:867:G:H1'	2.55	0.42
1:A:887:G:H2'	1:A:888:G:O4'	2.19	0.42
1:A:924:C:H2'	1:A:925:G:H8	1.80	0.42
1:A:1300:G:O2'	1:A:1303:C:N4	2.52	0.42
1:A:1526:G:C2	1:A:1527:C:C2	3.08	0.42
3:C:23:TYR:CD1	10:J:11:PHE:HZ	2.38	0.42
3:C:26:LYS:H	3:C:26:LYS:HG2	1.59	0.42
3:C:64:VAL:HG21	3:C:97:LYS:HD2	2.01	0.42
8:H:95:VAL:HB	8:H:99:GLU:HB3	2.01	0.42
25:Z:21:A:C5	25:Z:48:C:C2	3.06	0.42
1:A:858:G:H3'	1:A:869:G:H1	1.85	0.42
1:A:966:G:C4	25:Z:34:C:H5'	2.54	0.42
10:J:4:ILE:HD11	10:J:77:PRO:HB3	2.02	0.42
19:S:80:TYR:CZ	19:S:81:ARG:HD3	2.54	0.42
23:X:17:ARG:HG3	23:X:28:ILE:HG13	2.02	0.42
1:A:340:U:H2'	1:A:341:C:H6	1.84	0.42
1:A:370:C:H2'	1:A:371:G:C8	2.55	0.42
1:A:429:U:H1'	1:A:430:A:H5''	2.01	0.42
1:A:918:A:C6	1:A:919:A:C6	3.08	0.42
1:A:1110:A:N6	1:A:1111:A:N1	2.67	0.42
1:A:1370:G:C5'	9:I:12:GLU:HG3	2.50	0.42
1:A:1387:G:C2	1:A:1388:C:C2	3.08	0.42
1:A:1494:G:C6	1:A:1495:U:C4	3.07	0.42
2:B:16:HIS:NE2	2:B:214:ILE:HD11	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:139:GLN:HE22	3:C:170:GLN:HE22	1.67	0.42
7:G:65:ALA:CA	7:G:127:ALA:HB1	2.48	0.42
18:R:31:LEU:O	18:R:69:THR:HG21	2.20	0.42
23:X:16:VAL:HG22	23:X:31:THR:HA	2.00	0.42
24:Y:32:A:H3'	24:Y:33:A:C5'	2.47	0.42
1:A:9:G:H2'	1:A:10:A:O4'	2.20	0.42
1:A:104:G:H4'	1:A:174:C:H5'	2.00	0.42
1:A:120:A:C5	1:A:122:G:C6	3.07	0.42
1:A:236:G:C6	1:A:237:C:C4	3.08	0.42
1:A:319:G:C2	1:A:320:C:C2	3.08	0.42
1:A:402:G:C2	1:A:403:C:C2	3.08	0.42
1:A:451:A:C6	1:A:480:U:H2'	2.54	0.42
1:A:721:G:H1'	1:A:722:A:C2	2.53	0.42
1:A:761:G:C5	1:A:762:C:C4	3.07	0.42
16:P:7:ALA:O	16:P:17:TYR:HA	2.20	0.42
16:P:13:HIS:C	16:P:15:PRO:HD3	2.44	0.42
23:X:95:ASP:HB3	23:X:96:GLU:H	1.74	0.42
25:Z:41:C:C2'	25:Z:42:G:O4'	2.67	0.42
25:Z:64:G:C5	25:Z:65:C:C4	3.07	0.42
1:A:19:C:H2'	1:A:20:U:H6	1.82	0.42
1:A:42:G:C2	1:A:43:C:C2	3.08	0.42
1:A:132:C:C4	1:A:231:G:N1	2.87	0.42
1:A:577:G:C6	1:A:578:C:C4	3.07	0.42
1:A:755:G:N1	1:A:756:C:C4	2.87	0.42
1:A:975:A:N6	1:A:1367:C:O4'	2.52	0.42
1:A:1001:A:C2	1:A:1041:A:C6	3.08	0.42
4:D:3:ARG:HD2	4:D:118:ARG:CZ	2.50	0.42
5:E:78:HIS:NE2	5:E:142:LEU:HD23	2.35	0.42
8:H:75:ARG:HA	8:H:76:PRO:HD3	1.95	0.42
25:Z:13:C:H2'	25:Z:14:A:H8	1.85	0.42
1:A:116:A:H2'	1:A:117:G:C8	2.54	0.42
1:A:354:G:N1	1:A:355:C:C4	2.88	0.42
1:A:429:U:P	4:D:36:ARG:HH12	2.42	0.42
1:A:590:C:C2	1:A:650:G:C2	3.08	0.42
1:A:1103:C:C5'	2:B:98:LEU:HD13	2.50	0.42
1:A:1114:C:C2	1:A:1187:G:N2	2.88	0.42
1:A:1154:G:H2'	1:A:1155:G:C8	2.54	0.42
1:A:1291:G:O2'	9:I:38:GLN:O	2.32	0.42
3:C:28:GLN:OE1	3:C:32:LEU:CG	2.68	0.42
8:H:85:ARG:HH11	8:H:85:ARG:HG3	1.85	0.42
12:L:7:ILE:H	12:L:7:ILE:HG12	1.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:12:ASP:HB3	19:S:14:HIS:HD2	1.81	0.42
1:A:77:G:H1	1:A:92:C:N4	2.18	0.42
1:A:289:G:C2	1:A:290:C:C2	3.07	0.42
1:A:348:G:H2'	1:A:349:A:H8	1.85	0.42
1:A:433:C:H2'	1:A:434:U:C6	2.55	0.42
1:A:657:G:H4'	15:O:28:GLN:HG3	2.02	0.42
1:A:863:U:H2'	1:A:865:A:OP2	2.19	0.42
1:A:1251:A:H2'	1:A:1252:A:O4'	2.19	0.42
1:A:1278:U:H5''	1:A:1279:A:O4'	2.19	0.42
1:A:1292:U:H2'	1:A:1293:G:C8	2.54	0.42
1:A:1368:G:N2	1:A:1369:C:C2	2.88	0.42
1:A:1513:A:C6	1:A:1523:G:C6	3.08	0.42
3:C:29:TYR:CE1	3:C:33:LEU:HB2	2.54	0.42
3:C:29:TYR:HA	3:C:32:LEU:HD12	2.02	0.42
4:D:53:ASP:O	4:D:57:ARG:HD2	2.20	0.42
7:G:140:ASP:O	7:G:144:MET:HG2	2.20	0.42
11:K:62:GLN:CG	11:K:97:ALA:HB2	2.50	0.42
13:M:91:ARG:HE	13:M:96:LEU:HB2	1.83	0.42
17:Q:17:LYS:HA	17:Q:49:GLU:HG3	2.01	0.42
19:S:6:LYS:HB2	19:S:7:LYS:H	1.72	0.42
25:Z:54:5MU:C2	25:Z:58:A:N7	2.86	0.42
1:A:400:C:H2'	1:A:401:C:O4'	2.19	0.41
1:A:719:C:N3	18:R:74:ARG:NH1	2.62	0.41
1:A:951:G:C2	1:A:952:U:C2	3.08	0.41
1:A:1110:A:N6	1:A:1111:A:C6	2.88	0.41
1:A:1283:G:C2	1:A:1284:C:C4	3.07	0.41
1:A:1409:C:H2'	1:A:1410:G:H8	1.83	0.41
8:H:73:ASP:HA	8:H:74:PRO:HD2	1.87	0.41
9:I:26:VAL:HA	9:I:61:ALA:O	2.20	0.41
11:K:84:VAL:HG23	11:K:110:ASP:HA	2.02	0.41
25:Z:36:U:H2'	25:Z:37:A:O4'	2.20	0.41
1:A:13:U:H3	1:A:915:A:N6	2.17	0.41
1:A:181:G:H4'	1:A:182:U:H5'	2.02	0.41
1:A:333:G:N1	1:A:334:C:C4	2.88	0.41
1:A:681:C:C2	1:A:710:G:N2	2.87	0.41
1:A:926:G:C2	24:Y:35:A:C8	3.08	0.41
1:A:1017:G:C6	1:A:1018:C:C4	3.08	0.41
1:A:1141:C:H2'	1:A:1142:G:C8	2.55	0.41
1:A:1425:U:H2'	1:A:1426:C:C6	2.55	0.41
1:A:1443:G:N1	1:A:1444:C:C4	2.88	0.41
3:C:6:HIS:CB	14:N:49:HIS:HB3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:132:ARG:HG3	4:D:132:ARG:O	2.20	0.41
8:H:16:ALA:O	8:H:20:TYR:N	2.51	0.41
23:X:9:GLU:HG2	23:X:35:LEU:HD22	2.01	0.41
23:X:11:ILE:HG21	23:X:16:VAL:HG11	2.01	0.41
25:Z:7:G:N1	25:Z:49:G:C5	2.88	0.41
25:Z:31:G:C2	25:Z:40:C:C2	3.08	0.41
1:A:43:C:H2'	1:A:44:G:C8	2.55	0.41
1:A:189(J):G:C6	1:A:189(K):U:C4	3.09	0.41
1:A:251:G:N1	1:A:266:G:C6	2.89	0.41
1:A:276:G:C6	1:A:277:C:C4	3.09	0.41
1:A:406:G:H1	1:A:436:C:H42	1.67	0.41
1:A:1015:A:H2'	1:A:1016:A:C8	2.55	0.41
1:A:1255:G:H2'	1:A:1279:A:N6	2.35	0.41
1:A:1374:A:C6	1:A:1375:A:C8	3.08	0.41
9:I:18:PHE:HD2	9:I:62:TYR:CD2	2.37	0.41
17:Q:59:ILE:CG2	17:Q:71:PHE:HB3	2.50	0.41
25:Z:65:C:H2'	25:Z:66:C:O4'	2.20	0.41
1:A:91:C:N4	1:A:92:C:N4	2.68	0.41
1:A:761:G:C6	1:A:762:C:N3	2.88	0.41
1:A:891:U:H2'	1:A:892:A:H8	1.84	0.41
1:A:903:G:C6	1:A:904:C:C4	3.08	0.41
1:A:925:G:C2	1:A:927:G:C8	3.08	0.41
1:A:1116:C:H2'	1:A:1117:G:O4'	2.21	0.41
1:A:1177:G:H3'	1:A:1178:G:H8	1.86	0.41
1:A:1206:G:C6	1:A:1207:G:C5	3.08	0.41
2:B:53:ARG:NH1	2:B:53:ARG:HG2	2.36	0.41
14:N:9:LYS:HE3	14:N:20:ALA:HA	2.02	0.41
24:Y:31:U:H3'	24:Y:32:A:C5'	2.50	0.41
1:A:29:G:C2	1:A:555:C:N3	2.88	0.41
1:A:52:G:C6	1:A:53:A:C5	3.09	0.41
1:A:112:G:H21	1:A:354:G:H5'	1.85	0.41
1:A:583:A:H2'	1:A:584:G:O4'	2.20	0.41
1:A:731:G:O5'	1:A:731:G:H8	2.03	0.41
1:A:825:G:C2	1:A:826:C:C2	3.08	0.41
1:A:886:G:O6	1:A:887:G:C6	2.73	0.41
1:A:938:A:H5'	7:G:76:ARG:HH21	1.86	0.41
1:A:947:G:C5	1:A:948:C:C4	3.08	0.41
1:A:1019:C:H2'	1:A:1020:U:O4'	2.20	0.41
1:A:1058:G:C6	1:A:1059:C:C4	3.09	0.41
1:A:1105:A:N3	1:A:1106:G:C8	2.88	0.41
1:A:1291:G:H4'	9:I:39:GLY:HA3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1353:G:N1	1:A:1354:C:C4	2.88	0.41
8:H:97:VAL:HA	8:H:100:ILE:HD11	2.01	0.41
11:K:58:PRO:HB2	11:K:93:GLN:HG3	2.01	0.41
15:O:75:PRO:O	15:O:78:TYR:HB3	2.21	0.41
25:Z:14:A:N3	25:Z:14:A:H2'	2.34	0.41
25:Z:41:C:H2'	25:Z:42:G:C8	2.55	0.41
1:A:241:C:C2	1:A:286:G:C2	3.09	0.41
1:A:399:G:H2'	1:A:400:C:C6	2.55	0.41
1:A:456:C:C2	1:A:476:G:C2	3.09	0.41
1:A:505:G:OP2	1:A:535:A:H5'	2.19	0.41
1:A:864:A:H2'	1:A:865:A:N9	2.34	0.41
1:A:988:G:C6	1:A:989:C:C4	3.08	0.41
1:A:1001(A):G:C6	1:A:1002:G:C6	3.09	0.41
1:A:1127:G:H21	1:A:1147:C:N4	2.17	0.41
1:A:1233:G:C2	1:A:1234:C:C2	3.09	0.41
1:A:1366:C:O2'	10:J:60:ARG:NH2	2.53	0.41
2:B:158:LEU:HA	2:B:159:PRO:HD2	1.98	0.41
5:E:82:VAL:HG21	5:E:138:ALA:HA	2.03	0.41
1:A:66:G:N1	1:A:67:C:C4	2.88	0.41
1:A:127:G:N2	1:A:235:C:C2	2.89	0.41
1:A:563:A:C2	1:A:567:G:C5	3.08	0.41
1:A:636:U:H2'	1:A:637:G:H8	1.86	0.41
1:A:683:G:C2	1:A:708:C:C2	3.09	0.41
1:A:748:C:H4'	1:A:749:C:H5'	2.02	0.41
1:A:865:A:H8	1:A:865:A:O5'	2.04	0.41
1:A:942:G:N3	1:A:942:G:H2'	2.35	0.41
1:A:1205:U:H4'	3:C:195:VAL:CG2	2.51	0.41
1:A:1235:U:O2'	1:A:1305:G:O5'	2.39	0.41
1:A:1443:G:C2	1:A:1444:C:N3	2.88	0.41
2:B:55:PHE:HB3	2:B:221:LEU:HD23	2.03	0.41
3:C:34:LEU:HD12	14:N:25:VAL:HG21	2.03	0.41
5:E:125:SER:O	5:E:126:ARG:HD3	2.20	0.41
12:L:40:VAL:HG23	12:L:56:ALA:HB2	2.03	0.41
23:X:123:ARG:HD2	24:Y:39:U:O2	2.21	0.41
25:Z:17:C:O2	25:Z:17:C:C2'	2.68	0.41
1:A:83:U:H2'	1:A:84:U:O4'	2.21	0.41
1:A:333:G:C2	1:A:334:C:C2	3.08	0.41
1:A:384:G:C6	1:A:385:C:N4	2.89	0.41
1:A:471:G:C2'	1:A:472:A:H5'	2.50	0.41
1:A:980:C:H1'	14:N:19:ARG:HG2	2.02	0.41
1:A:1060:C:H5''	10:J:51:ARG:HH11	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1205:U:H4'	3:C:195:VAL:HG21	2.02	0.41
1:A:1207:G:C6	1:A:1208:C:C4	3.08	0.41
1:A:1243:C:C2	1:A:1295:G:C2	3.09	0.41
1:A:1309:G:N7	13:M:99:ARG:NH2	2.68	0.41
1:A:1387:G:N2	1:A:1388:C:C2	2.88	0.41
1:A:1445:C:O2	1:A:1458:G:C2	2.73	0.41
2:B:96:ARG:HG2	2:B:98:LEU:HG	2.03	0.41
3:C:34:LEU:HD23	3:C:35:GLU:HG3	2.03	0.41
4:D:201:GLN:HA	4:D:204:ILE:HD12	2.03	0.41
6:F:43:LEU:HD21	18:R:35:ARG:HB3	2.01	0.41
8:H:6:ILE:HD12	8:H:31:PHE:HD2	1.85	0.41
23:X:162:ASN:CG	25:Z:26:G:H5''	2.46	0.41
1:A:399:G:N2	1:A:400:C:C2	2.88	0.41
1:A:402:G:C6	1:A:403:C:C4	3.09	0.41
1:A:443:C:C2	1:A:492:G:N2	2.89	0.41
1:A:455:C:N4	1:A:456:C:H41	2.19	0.41
1:A:555:C:N3	1:A:556:C:C4	2.88	0.41
1:A:576:G:H3'	1:A:577:G:C5'	2.51	0.41
1:A:769:G:N1	1:A:770:C:C4	2.89	0.41
1:A:944:G:O6	1:A:1337:G:C8	2.60	0.41
1:A:1050:G:C2	1:A:1209:C:O2	2.74	0.41
1:A:1067:A:O5'	1:A:1067:A:C8	2.67	0.41
1:A:1164:G:N1	1:A:1165:C:C4	2.89	0.41
1:A:1177:G:H3'	1:A:1178:G:C8	2.55	0.41
1:A:1271:G:H8	1:A:1271:G:O5'	2.03	0.41
1:A:1414:U:O4	1:A:1487:G:N2	2.53	0.41
1:A:1423:G:C2	1:A:1424:C:C2	3.09	0.41
1:A:1472:U:H2'	1:A:1473:A:C8	2.56	0.41
2:B:9:GLU:HB2	2:B:217:ARG:HH21	1.86	0.41
2:B:156:LYS:HD3	2:B:157:ARG:HG2	2.03	0.41
3:C:95:THR:HB	3:C:97:LYS:HE3	2.03	0.41
4:D:10:ARG:HG3	4:D:11:LEU:N	2.36	0.41
7:G:99:LEU:HA	7:G:102:ARG:NH1	2.35	0.41
8:H:4:ASP:HA	8:H:5:PRO:HD3	1.91	0.41
13:M:84:ILE:HD12	19:S:74:PHE:CE1	2.56	0.41
18:R:38:GLU:HA	18:R:41:LYS:HB2	2.03	0.41
18:R:51:LEU:HA	18:R:52:PRO:HD3	1.94	0.41
20:T:60:GLU:HG3	20:T:81:LYS:HE3	2.02	0.41
24:Y:30:G:C3'	24:Y:31:U:H5''	2.49	0.41
1:A:802:A:C8	1:A:803:G:C8	3.09	0.41
1:A:890:G:O2'	1:A:906:G:O6	2.31	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1134:G:N2	1:A:1141:C:C2	2.89	0.41
1:A:1236:A:H2'	1:A:1237:C:C6	2.56	0.41
1:A:1241:G:C2	1:A:1242:C:C2	3.09	0.41
1:A:1316:G:H4'	14:N:18:VAL:HG11	2.02	0.41
1:A:1347:G:H22	1:A:1374:A:P	2.44	0.41
2:B:68:ILE:H	2:B:90:MET:HG2	1.85	0.41
4:D:128:VAL:HG12	4:D:129:ASN:HD22	1.85	0.41
8:H:9:MET:HE3	8:H:10:LEU:HD23	2.03	0.41
17:Q:56:VAL:HG12	17:Q:78:GLU:HB3	2.03	0.41
23:X:58:ARG:HD2	23:X:60:MET:HE2	2.02	0.41
24:Y:30:G:C2'	24:Y:31:U:H5''	2.48	0.41
1:A:19:C:O2	1:A:917:G:C2	2.74	0.40
1:A:384:G:C2	1:A:385:C:C2	3.09	0.40
1:A:557:G:N1	1:A:558:G:C2	2.89	0.40
1:A:731:G:N1	1:A:732:C:C4	2.89	0.40
1:A:807:A:H2'	1:A:808:C:C6	2.57	0.40
1:A:1110:A:C5	1:A:1111:A:C5	3.09	0.40
1:A:1207:G:C2	1:A:1208:C:C2	3.09	0.40
1:A:1263:C:H2'	1:A:1264:C:C6	2.56	0.40
3:C:177:THR:HG23	3:C:180:ALA:HB2	2.02	0.40
7:G:74:GLU:HG2	7:G:91:VAL:HG22	2.01	0.40
20:T:79:ARG:NH2	20:T:80:ARG:HG2	2.36	0.40
25:Z:63:G:C2	25:Z:64:G:C5	3.09	0.40
1:A:145:G:N2	1:A:178:C:C2	2.90	0.40
1:A:289:G:H2'	1:A:290:C:C6	2.55	0.40
1:A:499:A:O3'	1:A:500:G:H8	2.05	0.40
1:A:590:C:H42	1:A:649:G:H1	1.69	0.40
1:A:832:C:O2	1:A:855:G:C2	2.74	0.40
1:A:838:G:C2	1:A:849:C:N3	2.89	0.40
1:A:1491:G:H5''	12:L:47:LYS:HB2	2.03	0.40
1:A:1508:G:C6	1:A:1509:C:C4	3.09	0.40
5:E:87:SER:HA	5:E:125:SER:HB3	2.03	0.40
7:G:85:TYR:HB3	7:G:151:TYR:CD2	2.56	0.40
10:J:10:GLY:O	10:J:67:THR:HA	2.21	0.40
19:S:80:TYR:CE2	19:S:81:ARG:NH1	2.89	0.40
25:Z:2:G:N2	25:Z:3:C:C2	2.89	0.40
1:A:189:G:C6	1:A:189(L):G:C6	3.09	0.40
1:A:311:C:H2'	1:A:312:C:C6	2.56	0.40
1:A:491:G:O2'	1:A:492:G:H5'	2.21	0.40
1:A:543:C:OP2	4:D:10:ARG:NH2	2.53	0.40
1:A:577:G:C8	1:A:816:A:C6	3.09	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:947:G:C6	1:A:948:C:C4	3.09	0.40
1:A:1081:G:H2'	1:A:1082:G:O4'	2.22	0.40
1:A:1387:G:N1	1:A:1388:C:C4	2.90	0.40
1:A:1429:C:H2'	1:A:1430:C:C6	2.57	0.40
2:B:208:ILE:H	2:B:208:ILE:HG13	1.44	0.40
6:F:14:LEU:HD11	6:F:84:ASN:HB3	2.04	0.40
8:H:37:ARG:HG2	8:H:41:ARG:HH12	1.87	0.40
19:S:32:LYS:H	19:S:32:LYS:HG2	1.69	0.40
25:Z:68:C:H2'	25:Z:69:C:O4'	2.22	0.40
1:A:98:G:C2	1:A:99:U:C2	3.09	0.40
1:A:254:G:OP1	17:Q:69:LYS:HB2	2.22	0.40
1:A:309:G:H2'	1:A:310:G:C8	2.55	0.40
1:A:658:G:H2'	1:A:659:U:C6	2.56	0.40
1:A:694:A:H5'	11:K:53:SER:HB2	2.03	0.40
1:A:725:G:C2	1:A:726:C:C2	3.09	0.40
1:A:823:G:C6	1:A:824:C:N4	2.90	0.40
1:A:988:G:C2	1:A:989:C:C2	3.09	0.40
2:B:25:ASN:HA	2:B:26:PRO:HD3	1.87	0.40
4:D:83:SER:HA	4:D:89:THR:HG23	2.03	0.40
4:D:101:LEU:O	4:D:105:VAL:HG23	2.20	0.40
4:D:173:TRP:CD1	4:D:174:LEU:HG	2.56	0.40
16:P:39:TYR:CD1	16:P:73:LEU:HD21	2.56	0.40
24:Y:22:G:C2	24:Y:23:C:O2	2.75	0.40
1:A:143:A:H8	1:A:143:A:O5'	2.04	0.40
1:A:168:G:C6	1:A:169:C:N4	2.90	0.40
1:A:568:G:C2	1:A:569:C:C4	3.10	0.40
1:A:912:C:H2'	1:A:913:A:C8	2.57	0.40
1:A:946:A:H2'	1:A:947:G:C8	2.56	0.40
1:A:1084:G:H2'	1:A:1085:U:C5	2.57	0.40
1:A:1283:G:C6	1:A:1284:C:N4	2.90	0.40
1:A:1343:G:C6	1:A:1344:C:N4	2.90	0.40
1:A:1491:G:H4'	12:L:47:LYS:HB2	2.04	0.40
3:C:156:ARG:HB3	3:C:159:GLY:HA2	2.03	0.40
5:E:42:GLY:HA2	5:E:65:ASN:O	2.22	0.40
7:G:29:LYS:HB3	7:G:105:VAL:HG21	2.04	0.40
10:J:39:PRO:HB2	10:J:40:LEU:H	1.78	0.40
14:N:13:THR:HG22	14:N:15:LYS:HB2	2.03	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 PDB entries followed by that with respect to all EM entries.

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	232/256 (91%)	178 (77%)	41 (18%)	13 (6%)	1	14
3	C	204/239 (85%)	173 (85%)	25 (12%)	6 (3%)	3	23
4	D	206/209 (99%)	174 (84%)	25 (12%)	7 (3%)	3	20
5	E	148/162 (91%)	130 (88%)	16 (11%)	2 (1%)	9	38
6	F	99/101 (98%)	91 (92%)	6 (6%)	2 (2%)	6	30
7	G	153/156 (98%)	133 (87%)	17 (11%)	3 (2%)	6	30
8	H	136/138 (99%)	117 (86%)	17 (12%)	2 (2%)	8	38
9	I	125/128 (98%)	101 (81%)	18 (14%)	6 (5%)	2	16
10	J	96/105 (91%)	77 (80%)	11 (12%)	8 (8%)	0	9
11	K	117/129 (91%)	97 (83%)	16 (14%)	4 (3%)	3	20
12	L	122/132 (92%)	95 (78%)	24 (20%)	3 (2%)	4	25
13	M	116/126 (92%)	94 (81%)	19 (16%)	3 (3%)	4	25
14	N	58/61 (95%)	44 (76%)	14 (24%)	0	100	100
15	O	86/89 (97%)	79 (92%)	6 (7%)	1 (1%)	10	42
16	P	81/88 (92%)	76 (94%)	5 (6%)	0	100	100
17	Q	97/105 (92%)	85 (88%)	11 (11%)	1 (1%)	12	47
18	R	71/88 (81%)	59 (83%)	9 (13%)	3 (4%)	2	17
19	S	78/93 (84%)	62 (80%)	15 (19%)	1 (1%)	9	40
20	T	97/106 (92%)	81 (84%)	10 (10%)	6 (6%)	1	13
21	V	22/27 (82%)	19 (86%)	3 (14%)	0	100	100
22	W	69/72 (96%)	58 (84%)	9 (13%)	2 (3%)	3	23
23	X	160/171 (94%)	135 (84%)	21 (13%)	4 (2%)	4	25
All	All	2573/2781 (92%)	2158 (84%)	338 (13%)	77 (3%)	5	22

All (77) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	21	ARG
2	B	24	TRP
8	H	105	ARG
10	J	39	PRO
10	J	40	LEU
10	J	60	ARG
11	K	101	SER
18	R	87	ARG
23	X	54	PRO
2	B	16	HIS
2	B	17	PHE
2	B	132	LYS
2	B	207	ALA
4	D	5	ILE
4	D	32	ALA
7	G	7	ALA
7	G	55	GLY
9	I	56	LEU
13	M	99	ARG
17	Q	99	SER
20	T	70	SER
22	W	2	LYS
3	C	12	LEU
3	C	168	ALA
5	E	142	LEU
9	I	33	PHE
10	J	55	LYS
10	J	72	VAL
12	L	27	LEU
20	T	49	ALA
23	X	8	ASN
2	B	183	PRO
2	B	228	GLY
3	C	108	ASN
4	D	129	ASN
9	I	44	VAL
10	J	34	VAL
11	K	14	VAL
11	K	37	GLY
11	K	117	ASN
13	M	14	ARG
18	R	17	SER
20	T	95	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	T	97	ALA
23	X	154	PRO
2	B	9	GLU
2	B	130	ARG
2	B	194	PRO
2	B	229	VAL
3	C	127	ARG
3	C	181	ASN
4	D	18	LYS
4	D	30	LYS
6	F	51	PRO
6	F	70	ASP
8	H	54	ASP
9	I	54	ASP
9	I	121	ARG
10	J	54	PHE
12	L	25	PRO
12	L	26	ALA
13	M	5	ALA
18	R	45	SER
23	X	125	ARG
2	B	131	PRO
5	E	124	GLY
19	S	8	GLY
9	I	90	PRO
10	J	31	GLY
4	D	167	GLY
20	T	96	GLY
3	C	14	ILE
22	W	49	PRO
7	G	112	PRO
15	O	75	PRO
20	T	69	GLY
4	D	172	PRO

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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%)	148 (73%)	54 (27%)	0	3
3	C	160/188 (85%)	130 (81%)	30 (19%)	1	9
4	D	180/181 (99%)	141 (78%)	39 (22%)	1	6
5	E	115/123 (94%)	89 (77%)	26 (23%)	1	6
6	F	90/90 (100%)	71 (79%)	19 (21%)	1	7
7	G	126/127 (99%)	110 (87%)	16 (13%)	4	17
8	H	119/119 (100%)	89 (75%)	30 (25%)	0	4
9	I	98/99 (99%)	83 (85%)	15 (15%)	3	13
10	J	87/92 (95%)	73 (84%)	14 (16%)	2	12
11	K	90/99 (91%)	75 (83%)	15 (17%)	2	11
12	L	104/109 (95%)	82 (79%)	22 (21%)	1	7
13	M	94/101 (93%)	84 (89%)	10 (11%)	6	22
14	N	49/50 (98%)	39 (80%)	10 (20%)	1	8
15	O	79/80 (99%)	57 (72%)	22 (28%)	0	3
16	P	72/74 (97%)	56 (78%)	16 (22%)	1	6
17	Q	94/97 (97%)	78 (83%)	16 (17%)	2	11
18	R	64/77 (83%)	48 (75%)	16 (25%)	0	4
19	S	71/80 (89%)	55 (78%)	16 (22%)	1	6
20	T	76/82 (93%)	60 (79%)	16 (21%)	1	7
21	V	19/22 (86%)	16 (84%)	3 (16%)	2	12
22	W	61/63 (97%)	53 (87%)	8 (13%)	4	16
23	X	145/150 (97%)	115 (79%)	30 (21%)	1	7
All	All	2195/2323 (94%)	1752 (80%)	443 (20%)	3	8

All (443) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	15	VAL
2	B	16	HIS
2	B	21	ARG
2	B	23	ARG
2	B	24	TRP
2	B	25	ASN
2	B	28	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	44	LEU
2	B	53	ARG
2	B	61	LEU
2	B	64	ARG
2	B	67	THR
2	B	75	LYS
2	B	76	GLN
2	B	78	GLN
2	B	87	ARG
2	B	90	MET
2	B	93	VAL
2	B	96	ARG
2	B	97	TRP
2	B	102	LEU
2	B	108	ILE
2	B	112	VAL
2	B	114	ARG
2	B	126	GLU
2	B	127	ILE
2	B	140	HIS
2	B	141	GLU
2	B	142	LEU
2	B	149	LEU
2	B	153	ARG
2	B	155	LEU
2	B	160	ASP
2	B	165	VAL
2	B	174	VAL
2	B	178	ARG
2	B	179	LYS
2	B	180	LEU
2	B	182	ILE
2	B	185	ILE
2	B	187	LEU
2	B	190	THR
2	B	191	ASP
2	B	193	ASP
2	B	196	LEU
2	B	200	ILE
2	B	205	ASP
2	B	208	ILE
2	B	211	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	213	LEU
2	B	215	LEU
2	B	220	ASP
2	B	226	ARG
3	C	3	ASN
3	C	11	ARG
3	C	15	THR
3	C	31	HIS
3	C	33	LEU
3	C	34	LEU
3	C	43	LEU
3	C	52	LEU
3	C	55	VAL
3	C	64	VAL
3	C	68	VAL
3	C	87	LEU
3	C	90	GLU
3	C	91	LEU
3	C	94	LEU
3	C	97	LYS
3	C	98	ASN
3	C	108	ASN
3	C	111	LEU
3	C	126	ARG
3	C	144	SER
3	C	157	ILE
3	C	166	GLU
3	C	167	TRP
3	C	173	VAL
3	C	188	LEU
3	C	190	ARG
3	C	191	THR
3	C	196	LEU
3	C	207	VAL
4	D	13	ARG
4	D	14	ARG
4	D	15	GLU
4	D	19	LEU
4	D	28	SER
4	D	33	MET
4	D	35	ARG
4	D	36	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	43	HIS
4	D	45	GLN
4	D	47	ARG
4	D	59	ARG
4	D	64	LEU
4	D	66	ARG
4	D	70	ILE
4	D	73	ARG
4	D	78	LEU
4	D	83	SER
4	D	84	LYS
4	D	92	VAL
4	D	98	GLU
4	D	114	ARG
4	D	115	ARG
4	D	122	ARG
4	D	131	ARG
4	D	134	ASP
4	D	141	ARG
4	D	144	ASP
4	D	146	ILE
4	D	151	LYS
4	D	152	SER
4	D	153	ARG
4	D	162	LEU
4	D	165	MET
4	D	174	LEU
4	D	179	GLU
4	D	181	MET
4	D	190	ASP
4	D	200	GLU
5	E	5	ASP
5	E	12	LEU
5	E	13	ILE
5	E	15	ARG
5	E	19	MET
5	E	24	ARG
5	E	25	ARG
5	E	27	ARG
5	E	32	VAL
5	E	36	ASP
5	E	47	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	76	ILE
5	E	80	ILE
5	E	87	SER
5	E	100	VAL
5	E	107	ARG
5	E	118	ILE
5	E	120	THR
5	E	123	LEU
5	E	126	ARG
5	E	129	ILE
5	E	130	ASN
5	E	137	GLU
5	E	142	LEU
5	E	148	VAL
5	E	149	GLU
6	F	3	ARG
6	F	7	ASN
6	F	8	ILE
6	F	10	LEU
6	F	19	LEU
6	F	28	ARG
6	F	31	GLU
6	F	36	ARG
6	F	40	VAL
6	F	54	LYS
6	F	55	ASP
6	F	61	LEU
6	F	70	ASP
6	F	74	ASP
6	F	75	LEU
6	F	77	ARG
6	F	82	ARG
6	F	91	VAL
6	F	98	LEU
7	G	12	LEU
7	G	41	ARG
7	G	45	ASP
7	G	61	VAL
7	G	62	PHE
7	G	74	GLU
7	G	76	ARG
7	G	79	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	80	VAL
7	G	91	VAL
7	G	92	SER
7	G	96	GLN
7	G	104	LEU
7	G	129	GLU
7	G	136	LYS
7	G	149	ARG
8	H	2	LEU
8	H	6	ILE
8	H	10	LEU
8	H	11	THR
8	H	14	ARG
8	H	18	ARG
8	H	21	LYS
8	H	22	GLU
8	H	36	LEU
8	H	38	ILE
8	H	39	LEU
8	H	41	ARG
8	H	53	VAL
8	H	59	LEU
8	H	60	ARG
8	H	63	LEU
8	H	68	ARG
8	H	83	ILE
8	H	84	ARG
8	H	92	ARG
8	H	93	VAL
8	H	100	ILE
8	H	109	ILE
8	H	112	LEU
8	H	119	LEU
8	H	122	ARG
8	H	127	LEU
8	H	129	VAL
8	H	133	LEU
8	H	134	ILE
9	I	32	ASP
9	I	38	GLN
9	I	44	VAL
9	I	56	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	I	64	THR
9	I	65	VAL
9	I	78	LYS
9	I	85	LEU
9	I	87	GLN
9	I	91	ASP
9	I	95	LYS
9	I	97	LYS
9	I	102	LEU
9	I	110	GLU
9	I	127	LYS
10	J	4	ILE
10	J	8	LEU
10	J	16	LEU
10	J	38	ILE
10	J	42	THR
10	J	48	THR
10	J	57	LYS
10	J	61	GLU
10	J	71	LEU
10	J	74	ILE
10	J	79	ARG
10	J	83	GLU
10	J	96	ILE
10	J	99	LYS
11	K	18	ARG
11	K	29	ILE
11	K	34	ASP
11	K	40	ILE
11	K	41	THR
11	K	48	ILE
11	K	57	THR
11	K	63	LEU
11	K	84	VAL
11	K	91	ARG
11	K	96	ARG
11	K	105	VAL
11	K	112	THR
11	K	117	ASN
11	K	126	ARG
12	L	6	THR
12	L	7	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	L	17	LYS
12	L	33	ARG
12	L	39	VAL
12	L	41	ARG
12	L	42	THR
12	L	46	LYS
12	L	58	VAL
12	L	59	ARG
12	L	66	VAL
12	L	79	GLU
12	L	80	HIS
12	L	89	ARG
12	L	90	VAL
12	L	91	LYS
12	L	92	ASP
12	L	97	ARG
12	L	104	VAL
12	L	110	VAL
12	L	113	ARG
12	L	117	ARG
13	M	15	VAL
13	M	47	ASP
13	M	56	LEU
13	M	66	LEU
13	M	90	LEU
13	M	98	VAL
13	M	102	ARG
13	M	109	THR
13	M	115	LYS
13	M	116	THR
14	N	9	LYS
14	N	13	THR
14	N	18	VAL
14	N	26	ARG
14	N	32	SER
14	N	33	VAL
14	N	35	ARG
14	N	42	ILE
14	N	46	GLU
14	N	58	LYS
15	O	14	GLU
15	O	17	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O	21	ASP
15	O	22	THR
15	O	27	VAL
15	O	31	LEU
15	O	32	LEU
15	O	38	ARG
15	O	39	LEU
15	O	41	GLU
15	O	43	LEU
15	O	48	LYS
15	O	54	ARG
15	O	56	LEU
15	O	58	MET
15	O	65	ARG
15	O	70	LEU
15	O	71	GLN
15	O	77	ARG
15	O	83	GLU
15	O	87	ILE
15	O	88	ARG
16	P	9	PHE
16	P	12	LYS
16	P	20	VAL
16	P	23	ASP
16	P	28	ARG
16	P	29	ASP
16	P	33	ILE
16	P	35	LYS
16	P	36	ILE
16	P	44	THR
16	P	57	ARG
16	P	62	VAL
16	P	67	THR
16	P	69	THR
16	P	72	ARG
16	P	73	LEU
17	Q	15	MET
17	Q	16	GLN
17	Q	21	VAL
17	Q	38	ARG
17	Q	41	LYS
17	Q	53	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	59	ILE
17	Q	63	ARG
17	Q	68	ARG
17	Q	70	ARG
17	Q	74	LEU
17	Q	82	MET
17	Q	89	LEU
17	Q	93	GLN
17	Q	98	LEU
17	Q	100	LYS
18	R	18	ARG
18	R	19	LYS
18	R	22	VAL
18	R	28	GLU
18	R	36	ASN
18	R	37	VAL
18	R	39	VAL
18	R	47	THR
18	R	53	ARG
18	R	54	ARG
18	R	59	SER
18	R	62	GLU
18	R	63	GLN
18	R	66	LEU
18	R	75	ILE
18	R	83	GLU
19	S	5	LEU
19	S	6	LYS
19	S	7	LYS
19	S	11	VAL
19	S	15	LEU
19	S	18	LYS
19	S	19	VAL
19	S	27	GLU
19	S	29	ARG
19	S	39	THR
19	S	41	VAL
19	S	43	GLU
19	S	62	ILE
19	S	63	THR
19	S	77	THR
19	S	81	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	T	10	LEU
20	T	18	GLN
20	T	20	LEU
20	T	23	ARG
20	T	25	ARG
20	T	42	GLN
20	T	45	GLN
20	T	56	MET
20	T	62	LEU
20	T	68	LYS
20	T	71	THR
20	T	72	LEU
20	T	73	HIS
20	T	74	LYS
20	T	75	ASN
20	T	84	LEU
21	V	12	LYS
21	V	13	ILE
21	V	21	TYR
22	W	4	LYS
22	W	8	ARG
22	W	12	VAL
22	W	19	ASN
22	W	23	ARG
22	W	27	ASP
22	W	32	ILE
22	W	68	VAL
23	X	3	LYS
23	X	4	GLU
23	X	19	VAL
23	X	22	ASP
23	X	26	LEU
23	X	31	THR
23	X	33	GLU
23	X	35	LEU
23	X	37	LEU
23	X	43	LEU
23	X	61	ASP
23	X	71	MET
23	X	73	GLU
23	X	74	LYS
23	X	87	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	X	91	ARG
23	X	103	LEU
23	X	117	LYS
23	X	118	VAL
23	X	119	THR
23	X	123	ARG
23	X	125	ARG
23	X	126	GLU
23	X	131	GLU
23	X	135	ARG
23	X	143	ASP
23	X	150	VAL
23	X	156	MET
23	X	164	LEU
23	X	170	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	19	HIS
2	B	45	GLN
2	B	76	GLN
2	B	95	GLN
2	B	204	ASN
3	C	3	ASN
3	C	31	HIS
3	C	104	GLN
3	C	123	GLN
3	C	139	GLN
3	C	170	GLN
4	D	42	GLN
4	D	43	HIS
4	D	77	ASN
4	D	103	ASN
4	D	116	GLN
4	D	129	ASN
4	D	160	GLN
4	D	199	ASN
4	D	201	GLN
5	E	130	ASN
6	F	7	ASN
6	F	13	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	64	GLN
6	F	100	ASN
7	G	68	ASN
7	G	96	GLN
7	G	110	GLN
7	G	122	HIS
8	H	15	ASN
8	H	82	HIS
9	I	89	ASN
9	I	124	GLN
10	J	68	HIS
10	J	84	GLN
11	K	13	GLN
11	K	26	ASN
11	K	62	GLN
11	K	78	GLN
11	K	116	HIS
13	M	77	ASN
13	M	101	GLN
15	O	50	HIS
15	O	71	GLN
16	P	65	GLN
17	Q	16	GLN
17	Q	26	GLN
17	Q	45	HIS
17	Q	94	ASN
18	R	36	ASN
18	R	63	GLN
19	S	53	ASN
20	T	18	GLN
20	T	73	HIS
20	T	75	ASN
23	X	114	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1508/1522 (99%)	447 (29%)	113 (7%)
24	Y	19/42 (45%)	15 (78%)	3 (15%)
25	Z	75/77 (97%)	32 (42%)	9 (12%)
All	All	1602/1641 (97%)	494 (30%)	125 (7%)

All (494) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	6	G
1	A	7	G
1	A	8	A
1	A	9	G
1	A	13	U
1	A	16	A
1	A	18	C
1	A	22	G
1	A	31	G
1	A	32	A
1	A	39	G
1	A	40	C
1	A	47	C
1	A	48	C
1	A	49	U
1	A	50	A
1	A	51	A
1	A	52	G
1	A	54	C
1	A	55	A
1	A	58	C
1	A	60	A
1	A	61	G
1	A	72	C
1	A	73	G
1	A	81	U
1	A	90	U
1	A	91	C
1	A	97	G
1	A	100	C
1	A	116	A
1	A	120	A
1	A	121	C
1	A	122	G
1	A	127	G
1	A	129(A)	G
1	A	130	A
1	A	131	C
1	A	142	G
1	A	151	A
1	A	157	G
1	A	163	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	173	U
1	A	174	C
1	A	178	C
1	A	181	G
1	A	182	U
1	A	183	G
1	A	189(E)	U
1	A	189(F)	U
1	A	189(G)	G
1	A	189(H)	G
1	A	195	A
1	A	196	A
1	A	197	A
1	A	198	G
1	A	201	C
1	A	202	U
1	A	203	U
1	A	204	U
1	A	216	G
1	A	220	G
1	A	222	U
1	A	240	C
1	A	244	U
1	A	247	G
1	A	250	A
1	A	251	G
1	A	252	U
1	A	253	U
1	A	266	G
1	A	267	C
1	A	279	A
1	A	280	C
1	A	281	G
1	A	282	A
1	A	283	C
1	A	289	G
1	A	298	A
1	A	301	G
1	A	315	A
1	A	316	G
1	A	321	A
1	A	324	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	340	U
1	A	345	C
1	A	347	G
1	A	350	G
1	A	351	G
1	A	352	C
1	A	353	A
1	A	357	G
1	A	362	G
1	A	366	C
1	A	367	U
1	A	368	U
1	A	372	C
1	A	373	A
1	A	382	A
1	A	384	G
1	A	388	G
1	A	392	G
1	A	393	A
1	A	396	G
1	A	397	A
1	A	398	C
1	A	406	G
1	A	409	G
1	A	412	A
1	A	413	G
1	A	421	U
1	A	422	C
1	A	423	G
1	A	424	G
1	A	428	G
1	A	429	U
1	A	430	A
1	A	439	A
1	A	441	A
1	A	448	A
1	A	450	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	452	A
1	A	470	C
1	A	481	G
1	A	482	A
1	A	484	G
1	A	485	G
1	A	486	U
1	A	495	A
1	A	496	A
1	A	498	U
1	A	509	A
1	A	510	A
1	A	511	C
1	A	514	C
1	A	517	G
1	A	518	C
1	A	519	C
1	A	521	G
1	A	524	G
1	A	527	G
1	A	529	G
1	A	530	G
1	A	531	U
1	A	532	A
1	A	533	A
1	A	534	U
1	A	545	C
1	A	547	A
1	A	548	G
1	A	550	G
1	A	559	A
1	A	560	U
1	A	561	U
1	A	562	C
1	A	566	G
1	A	568	G
1	A	571	U
1	A	572	A
1	A	573	A
1	A	574	A
1	A	575	G
1	A	576	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	577	G
1	A	578	C
1	A	582	U
1	A	588	G
1	A	589	C
1	A	595	G
1	A	596	C
1	A	607	A
1	A	619	U
1	A	632	A
1	A	639	G
1	A	641	U
1	A	642	A
1	A	653	A
1	A	654	G
1	A	657	G
1	A	665	A
1	A	671	G
1	A	672	U
1	A	687	A
1	A	688	G
1	A	692	U
1	A	701	C
1	A	702	A
1	A	703	G
1	A	713	G
1	A	717	C
1	A	721	G
1	A	722	A
1	A	723	U
1	A	727	G
1	A	731	G
1	A	733	A
1	A	748	C
1	A	749	C
1	A	753	A
1	A	754	C
1	A	755	G
1	A	760	G
1	A	777	A
1	A	785	G
1	A	787	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	792	A
1	A	793	U
1	A	794	A
1	A	798	G
1	A	799	G
1	A	800	G
1	A	810	C
1	A	813	U
1	A	815	A
1	A	817	C
1	A	820	U
1	A	821	G
1	A	828	A
1	A	839	U
1	A	841	U
1	A	853	G
1	A	855	G
1	A	859	A
1	A	865	A
1	A	870	U
1	A	872	A
1	A	873	A
1	A	876	G
1	A	884	U
1	A	885	G
1	A	889	A
1	A	900	A
1	A	901	A
1	A	902	G
1	A	911	U
1	A	913	A
1	A	922	G
1	A	926	G
1	A	927	G
1	A	932	C
1	A	934	C
1	A	935	A
1	A	942	G
1	A	943	U
1	A	950	U
1	A	960	U
1	A	961	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	965	A
1	A	966	G
1	A	968	A
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	982	U
1	A	983	A
1	A	991	U
1	A	992	U
1	A	993	G
1	A	994	A
1	A	1000	U
1	A	1001	A
1	A	1002	G
1	A	1003	G
1	A	1004	A
1	A	1005	A
1	A	1016	A
1	A	1022	G
1	A	1023	G
1	A	1024	G
1	A	1025	U
1	A	1030	C
1	A	1030(C)	G
1	A	1031	G
1	A	1043	C
1	A	1045	C
1	A	1049	U
1	A	1050	G
1	A	1051	C
1	A	1053	G
1	A	1054	C
1	A	1064	G
1	A	1065	U
1	A	1066	C
1	A	1067	A
1	A	1068	G
1	A	1074	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1085	U
1	A	1089	G
1	A	1094	G
1	A	1095	U
1	A	1101	A
1	A	1102	A
1	A	1104	G
1	A	1117	G
1	A	1118	C
1	A	1124	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	1135	U
1	A	1136	U
1	A	1137	C
1	A	1138	G
1	A	1139	G
1	A	1140	C
1	A	1145	C
1	A	1146	A
1	A	1150	U
1	A	1152	A
1	A	1157	A
1	A	1159	U
1	A	1160	G
1	A	1169	A
1	A	1171	G
1	A	1176	A
1	A	1183	A
1	A	1184	G
1	A	1187	G
1	A	1191	A
1	A	1193	G
1	A	1196	U
1	A	1197	G
1	A	1200	C
1	A	1201	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1202	G
1	A	1212	U
1	A	1213	A
1	A	1214	C
1	A	1215	G
1	A	1224	G
1	A	1225	A
1	A	1226	C
1	A	1227	A
1	A	1228	C
1	A	1236	A
1	A	1237	C
1	A	1238	A
1	A	1249	C
1	A	1250	A
1	A	1253	G
1	A	1256	A
1	A	1257	U
1	A	1258	G
1	A	1260	C
1	A	1261	A
1	A	1268	A
1	A	1270	C
1	A	1275	A
1	A	1277	C
1	A	1279	A
1	A	1280	A
1	A	1281	U
1	A	1282	C
1	A	1285	A
1	A	1286	A
1	A	1287	A
1	A	1290	G
1	A	1296	C
1	A	1297	C
1	A	1298	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1302	U
1	A	1303	C
1	A	1304	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1305	G
1	A	1312	G
1	A	1318	A
1	A	1319	A
1	A	1320	C
1	A	1321	C
1	A	1323	G
1	A	1332	A
1	A	1335	C
1	A	1336	C
1	A	1337	G
1	A	1340	A
1	A	1341	U
1	A	1342	C
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1348	U
1	A	1351	U
1	A	1353	G
1	A	1357	A
1	A	1361	G
1	A	1362	C
1	A	1363	C
1	A	1363(A)	A
1	A	1364	U
1	A	1370	G
1	A	1376	U
1	A	1378	C
1	A	1379	G
1	A	1381	U
1	A	1394	A
1	A	1396	A
1	A	1398	A
1	A	1401	G
1	A	1412	C
1	A	1415	G
1	A	1440	C
1	A	1442	G
1	A	1443	G
1	A	1445	C
1	A	1446	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1447	A
1	A	1452	C
1	A	1456	G
1	A	1457	G
1	A	1459	C
1	A	1484	C
1	A	1488	G
1	A	1492	A
1	A	1493	A
1	A	1494	G
1	A	1497	G
1	A	1499	A
1	A	1502	A
1	A	1503	A
1	A	1504	G
1	A	1505	G
1	A	1506	U
1	A	1507	A
1	A	1508	G
1	A	1517	G
1	A	1520	G
1	A	1524	C
1	A	1529	G
1	A	1530	G
1	A	1531	A
1	A	1535	C
1	A	1538	C
24	Y	21	G
24	Y	23	C
24	Y	24	A
24	Y	26	G
24	Y	28	A
24	Y	29	G
24	Y	31	U
24	Y	32	A
24	Y	33	A
24	Y	34	A
24	Y	35	A
24	Y	36	A
24	Y	37	U
24	Y	38	G
24	Y	39	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	Z	3	C
25	Z	4	G
25	Z	6	G
25	Z	7	G
25	Z	9	G
25	Z	13	C
25	Z	14	A
25	Z	16	C
25	Z	17	C
25	Z	17(A)	U
25	Z	18	G
25	Z	19	G
25	Z	20	U
25	Z	21	A
25	Z	26	G
25	Z	34	C
25	Z	37	A
25	Z	40	C
25	Z	42	G
25	Z	46	G7M
25	Z	47	U
25	Z	48	C
25	Z	55	PSU
25	Z	57	A
25	Z	59	A
25	Z	60	U
25	Z	61	C
25	Z	67	C
25	Z	68	C
25	Z	74	C
25	Z	75	C
25	Z	76	A

All (125) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	30	U
1	A	48	C
1	A	49	U
1	A	51	A
1	A	60	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	115	G
1	A	119	A
1	A	125	U
1	A	129(A)	G
1	A	181	G
1	A	197	A
1	A	202	U
1	A	243	A
1	A	250	A
1	A	251	G
1	A	266	G
1	A	279	A
1	A	281	G
1	A	289	G
1	A	328	C
1	A	329	A
1	A	344	A
1	A	351	G
1	A	356	A
1	A	366	C
1	A	367	U
1	A	372	C
1	A	421	U
1	A	428	G
1	A	429	U
1	A	481	G
1	A	484	G
1	A	496	A
1	A	509	A
1	A	518	C
1	A	531	U
1	A	547	A
1	A	559	A
1	A	560	U
1	A	561	U
1	A	575	G
1	A	577	G
1	A	595	G
1	A	624	C
1	A	641	U
1	A	653	A
1	A	671	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	687	A
1	A	701	C
1	A	702	A
1	A	721	G
1	A	748	C
1	A	753	A
1	A	770	C
1	A	792	A
1	A	809	G
1	A	812	C
1	A	865	A
1	A	872	A
1	A	884	U
1	A	934	C
1	A	954	G
1	A	960	U
1	A	965	A
1	A	968	A
1	A	975	A
1	A	976	G
1	A	982	U
1	A	992	U
1	A	993	G
1	A	1001	A
1	A	1049	U
1	A	1065	U
1	A	1067	A
1	A	1101	A
1	A	1145	C
1	A	1151	A
1	A	1182	G
1	A	1190	G
1	A	1196	U
1	A	1200	C
1	A	1201	A
1	A	1213	A
1	A	1214	C
1	A	1224	G
1	A	1249	C
1	A	1256	A
1	A	1257	U
1	A	1285	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1297	C
1	A	1299	A
1	A	1300	G
1	A	1301	U
1	A	1303	C
1	A	1319	A
1	A	1335	C
1	A	1336	C
1	A	1345	U
1	A	1346	A
1	A	1347	G
1	A	1380	U
1	A	1397	C
1	A	1400	C
1	A	1442(B)	A
1	A	1447	A
1	A	1452	C
1	A	1488	G
1	A	1493	A
1	A	1498	U
1	A	1503	A
1	A	1504	G
1	A	1534	A
24	Y	31	U
24	Y	35	A
24	Y	38	G
25	Z	16	C
25	Z	17	C
25	Z	17(A)	U
25	Z	33	U
25	Z	36	U
25	Z	47	U
25	Z	51	C
25	Z	60	U
25	Z	62	C

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	5MU	Z	54	25	19,22,23	1.54	3 (15%)	27,32,35	1.90	6 (22%)
25	OMC	Z	32	25	19,22,23	1.03	2 (10%)	25,31,34	1.48	4 (16%)
25	G7M	Z	46	25	23,26,27	2.58	5 (21%)	34,39,42	2.86	13 (38%)
25	4SU	Z	8	25	18,21,22	1.90	5 (27%)	25,30,33	2.54	9 (36%)
25	PSU	Z	55	25	18,21,22	1.47	3 (16%)	21,30,33	2.22	6 (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
25	5MU	Z	54	25	-	0/7/25/26	0/2/2/2
25	OMC	Z	32	25	-	1/9/27/28	0/2/2/2
25	G7M	Z	46	25	-	2/7/25/26	0/3/3/3
25	4SU	Z	8	25	-	1/7/25/26	0/2/2/2
25	PSU	Z	55	25	-	4/7/25/26	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	46	G7M	C8-N7	8.57	1.47	1.33
25	Z	8	4SU	C4-S4	-4.89	1.60	1.68
25	Z	55	PSU	C6-C5	4.69	1.40	1.35
25	Z	46	G7M	C8-N9	4.63	1.48	1.35
25	Z	46	G7M	C5-C4	4.43	1.49	1.38
25	Z	46	G7M	C5-N7	-4.14	1.34	1.39
25	Z	54	5MU	C6-C5	4.02	1.41	1.34
25	Z	8	4SU	C2-N1	4.02	1.44	1.38
25	Z	54	5MU	C4-C5	2.76	1.49	1.44
25	Z	54	5MU	C4-N3	-2.57	1.34	1.38
25	Z	8	4SU	C5-C4	-2.46	1.39	1.42
25	Z	46	G7M	C5-C6	2.40	1.49	1.43
25	Z	55	PSU	C4-C5	2.38	1.50	1.44
25	Z	32	OMC	C6-C5	2.33	1.40	1.35
25	Z	55	PSU	C4-N3	-2.17	1.34	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Z	8	4SU	C4-N3	-2.16	1.35	1.37
25	Z	32	OMC	C2-N1	2.13	1.44	1.40
25	Z	8	4SU	C6-C5	2.04	1.39	1.35

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	46	G7M	CN7-N7-C8	-7.56	113.34	124.79
25	Z	46	G7M	N9-C8-N7	-6.26	97.28	112.48
25	Z	46	G7M	C8-N7-C5	6.21	115.55	107.78
25	Z	55	PSU	N1-C2-N3	5.76	121.25	115.17
25	Z	8	4SU	C4-N3-C2	-5.55	122.00	127.31
25	Z	8	4SU	C5-C4-N3	5.52	119.89	114.75
25	Z	54	5MU	N3-C2-N1	5.48	122.02	114.89
25	Z	46	G7M	N9-C4-N3	5.17	136.29	125.95
25	Z	46	G7M	C5-C4-N3	-5.17	118.38	128.15
25	Z	8	4SU	C5-C4-S4	-4.76	118.87	124.31
25	Z	8	4SU	C1'-N1-C2	4.58	125.82	117.59
25	Z	46	G7M	C2-N3-C4	4.51	120.06	112.30
25	Z	55	PSU	C4-N3-C2	-4.04	120.81	126.37
25	Z	8	4SU	N3-C2-N1	3.81	119.85	114.89
25	Z	54	5MU	C6-N1-C2	-3.70	117.62	121.30
25	Z	54	5MU	O2-C2-N1	-3.53	118.20	122.80
25	Z	32	OMC	O2-C2-N3	-3.52	116.78	122.33
25	Z	46	G7M	C8-N9-C4	3.51	115.79	107.09
25	Z	46	G7M	CN7-N7-C5	3.46	131.12	126.80
25	Z	55	PSU	C6-C5-C4	-3.39	115.88	118.17
25	Z	55	PSU	C3'-C2'-C1'	3.34	105.64	101.69
25	Z	8	4SU	C6-N1-C2	-3.17	117.14	121.00
25	Z	55	PSU	O4'-C4'-C5'	3.11	119.31	109.33
25	Z	55	PSU	O2-C2-N1	-3.03	119.67	122.79
25	Z	54	5MU	C4-N3-C2	-2.87	123.58	127.34
25	Z	46	G7M	O4'-C1'-N9	2.60	114.26	108.36
25	Z	32	OMC	C2'-C1'-N1	-2.41	109.67	114.24
25	Z	32	OMC	C1'-N1-C2	2.38	123.70	118.44
25	Z	46	G7M	C1'-N9-C8	-2.38	118.71	126.74
25	Z	8	4SU	O4'-C4'-C5'	2.37	116.92	109.33
25	Z	8	4SU	O2-C2-N3	-2.36	117.14	121.49
25	Z	8	4SU	O3'-C3'-C2'	2.31	119.23	111.82
25	Z	46	G7M	C3'-C2'-C1'	2.27	105.76	101.46
25	Z	32	OMC	O2-C2-N1	2.18	123.17	118.90
25	Z	54	5MU	C1'-N1-C6	2.17	124.72	121.15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Z	54	5MU	O4'-C1'-N1	2.12	113.16	108.36
25	Z	46	G7M	O6-C6-C5	-2.11	123.30	128.01
25	Z	46	G7M	C6-C5-N7	2.02	134.70	132.17

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	Z	55	PSU	O4'-C4'-C5'-O5'
25	Z	55	PSU	C3'-C4'-C5'-O5'
25	Z	46	G7M	C3'-C4'-C5'-O5'
25	Z	46	G7M	O4'-C4'-C5'-O5'
25	Z	55	PSU	O4'-C1'-C5-C4
25	Z	55	PSU	O4'-C1'-C5-C6
25	Z	32	OMC	C2'-C1'-N1-C2
25	Z	8	4SU	C2'-C1'-N1-C2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
25	Z	54	5MU	2	0
25	Z	32	OMC	2	0
25	Z	46	G7M	4	0
25	Z	55	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	6
25	Z	3
24	Y	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	55:PSU	O3'	56:C	P	5.82
1	A	841:U	O3'	848:C	P	5.50
1	A	93:G	O3'	96:U	P	4.90
1	A	84:U	O3'	88:A	P	4.32
1	A	1442(A):G	O3'	1442(B):A	P	3.51
1	Y	32:A	O3'	33:A	P	3.38
1	A	927:G	O3'	928:G	P	3.26
1	A	204:U	O3'	216:G	P	3.23
1	Z	14:A	O3'	15:G	P	3.20
1	Z	42:G	O3'	43:A	P	1.77

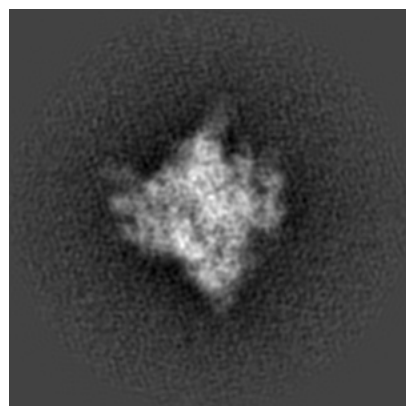
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4078. These allow visual inspection of the internal detail of the map and identification of artifacts.

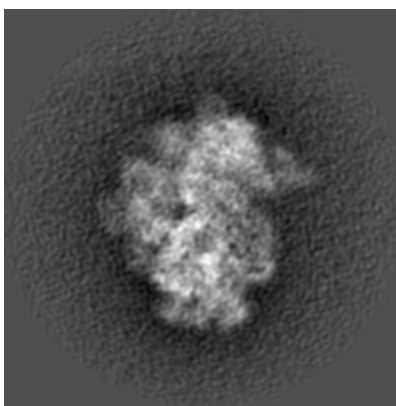
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

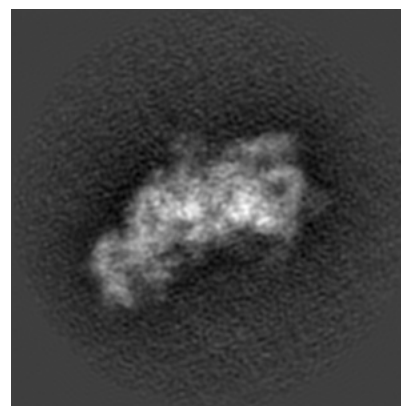
6.1.1 Primary map



X

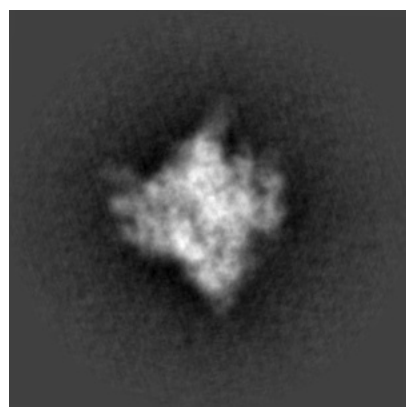


Y

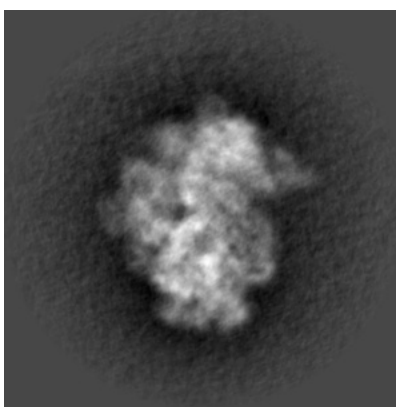


Z

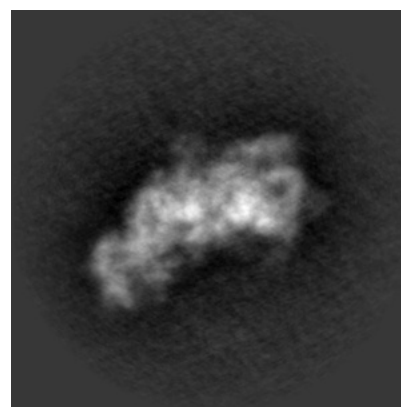
6.1.2 Raw map



X



Y

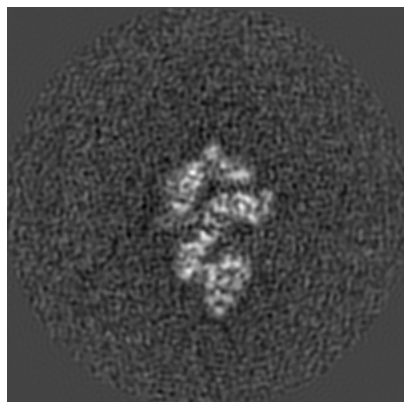


Z

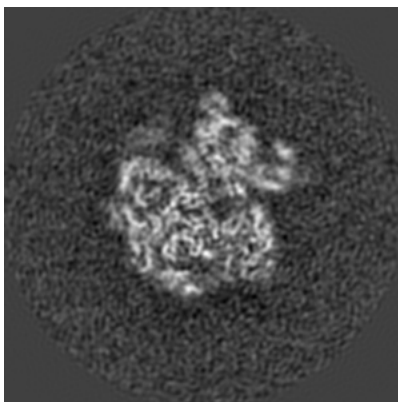
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

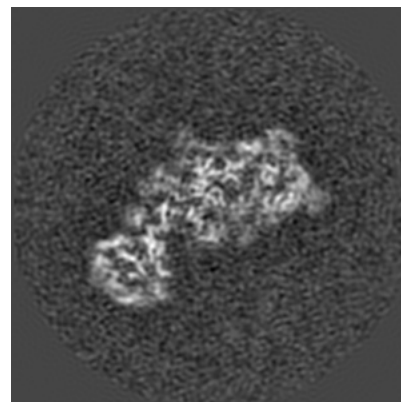
6.2.1 Primary map



X Index: 130

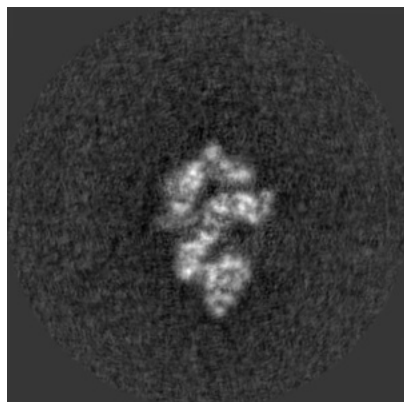


Y Index: 130

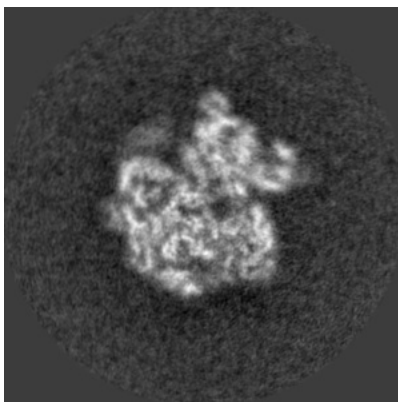


Z Index: 130

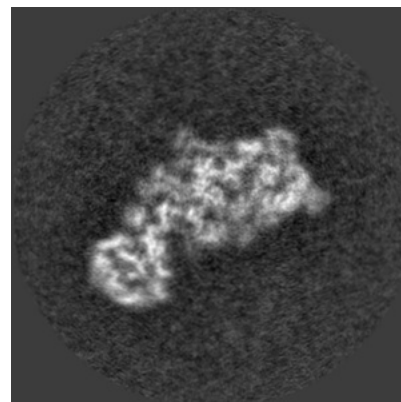
6.2.2 Raw map



X Index: 130



Y Index: 130

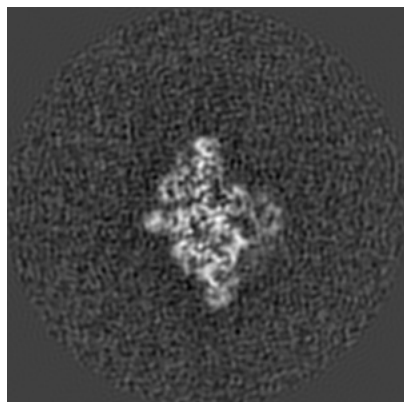


Z Index: 130

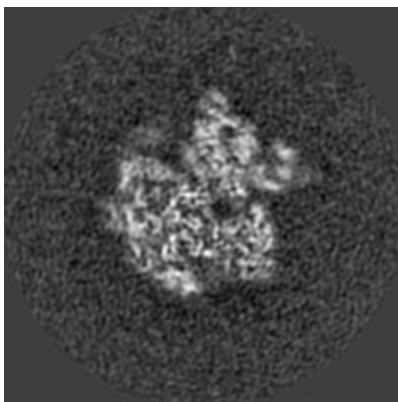
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

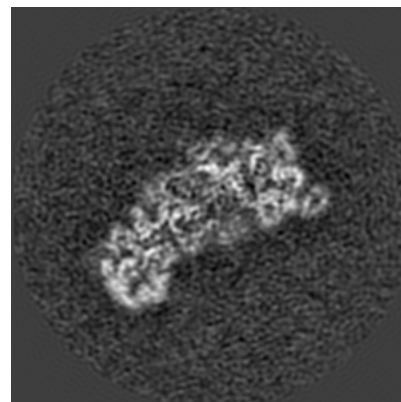
6.3.1 Primary map



X Index: 118

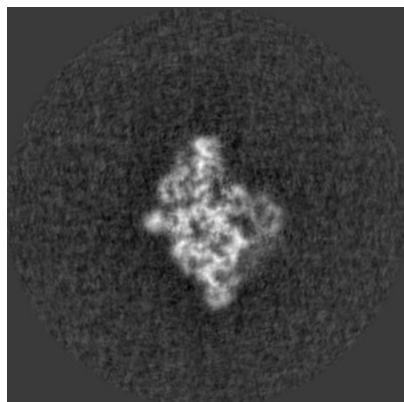


Y Index: 131

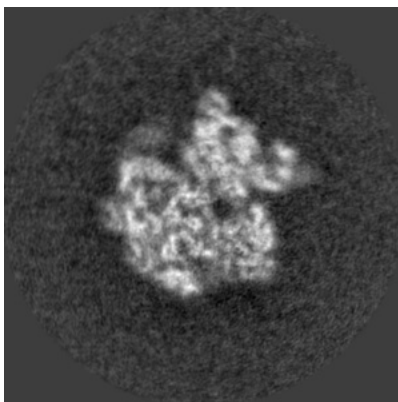


Z Index: 135

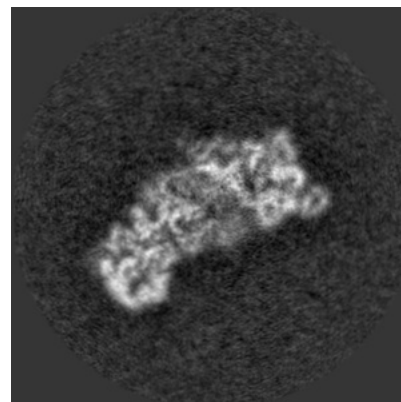
6.3.2 Raw map



X Index: 118



Y Index: 131

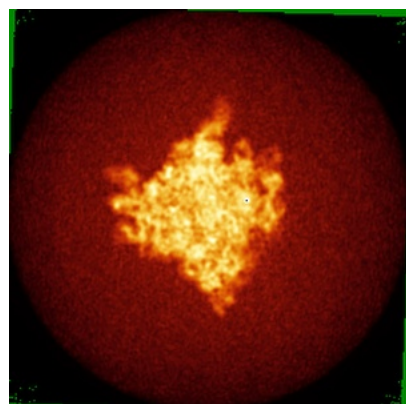


Z Index: 135

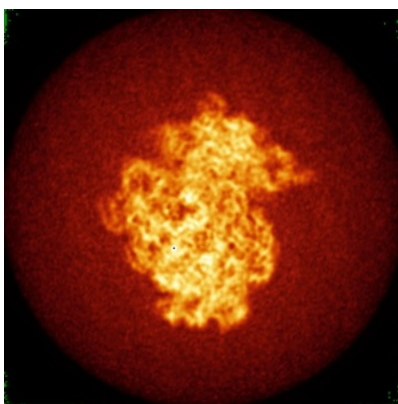
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

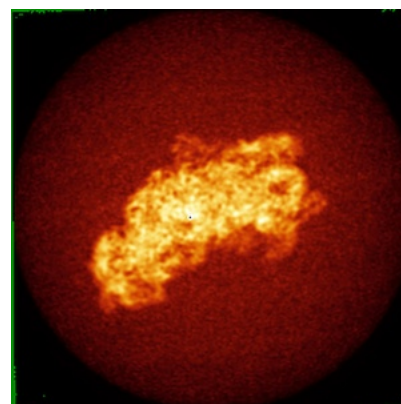
6.4.1 Primary map



X

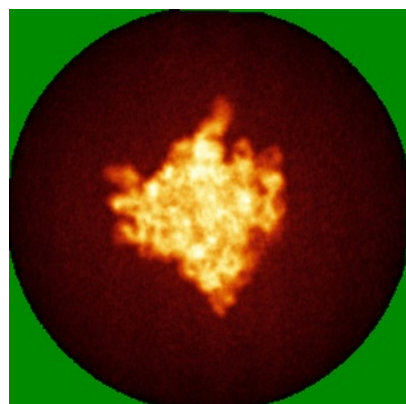


Y

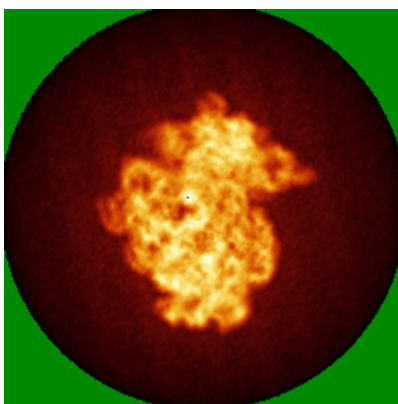


Z

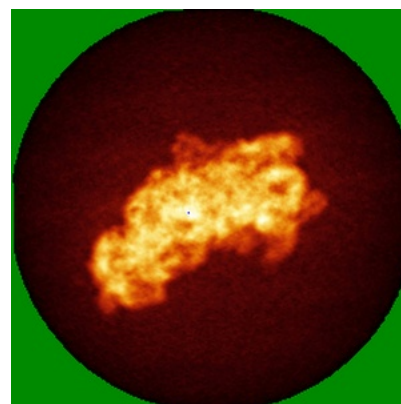
6.4.2 Raw map



X



Y

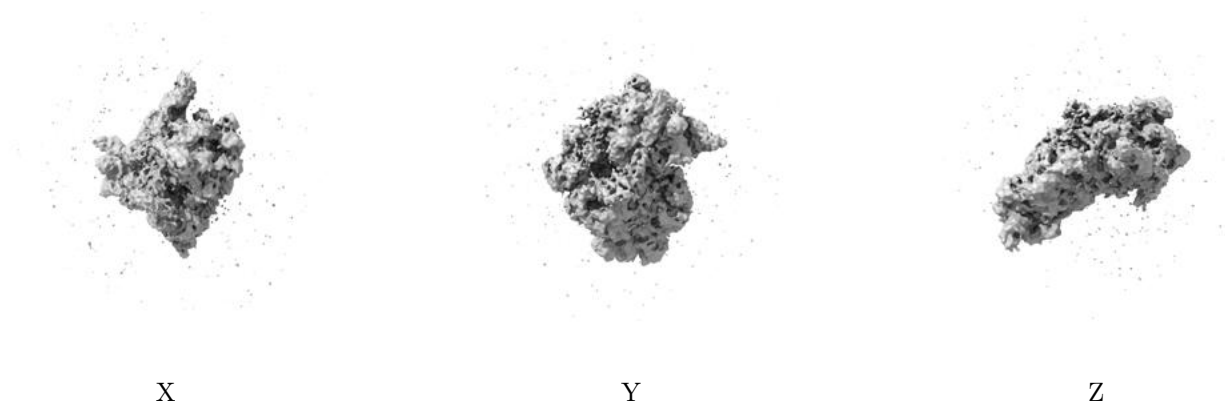


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

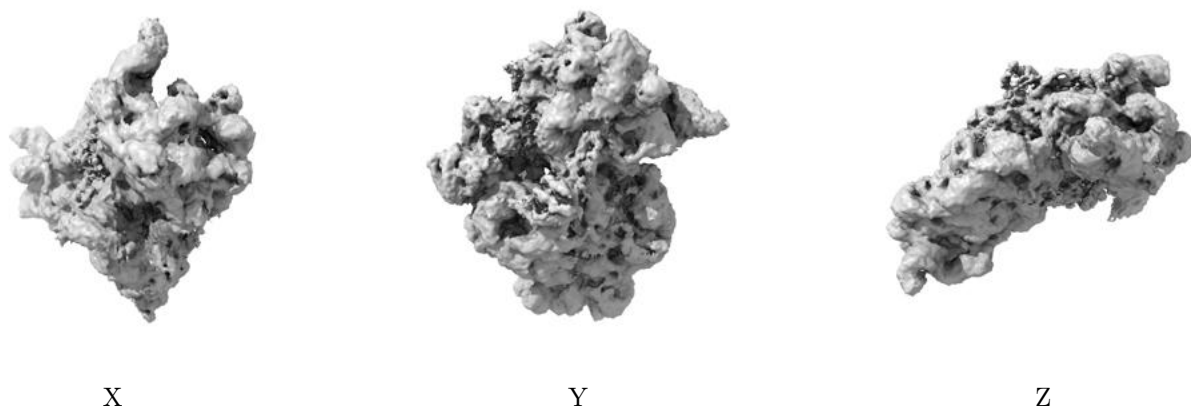
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

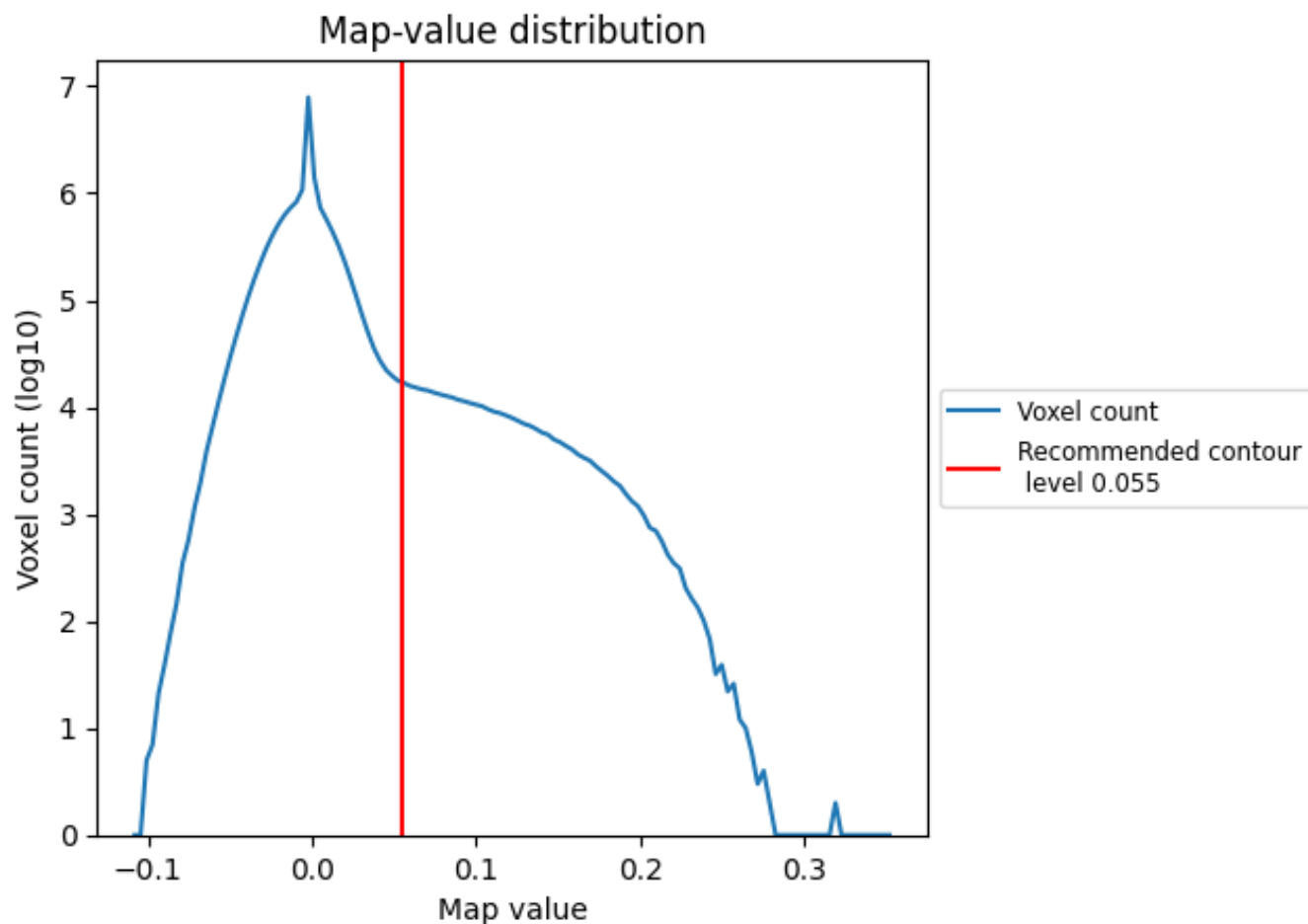
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

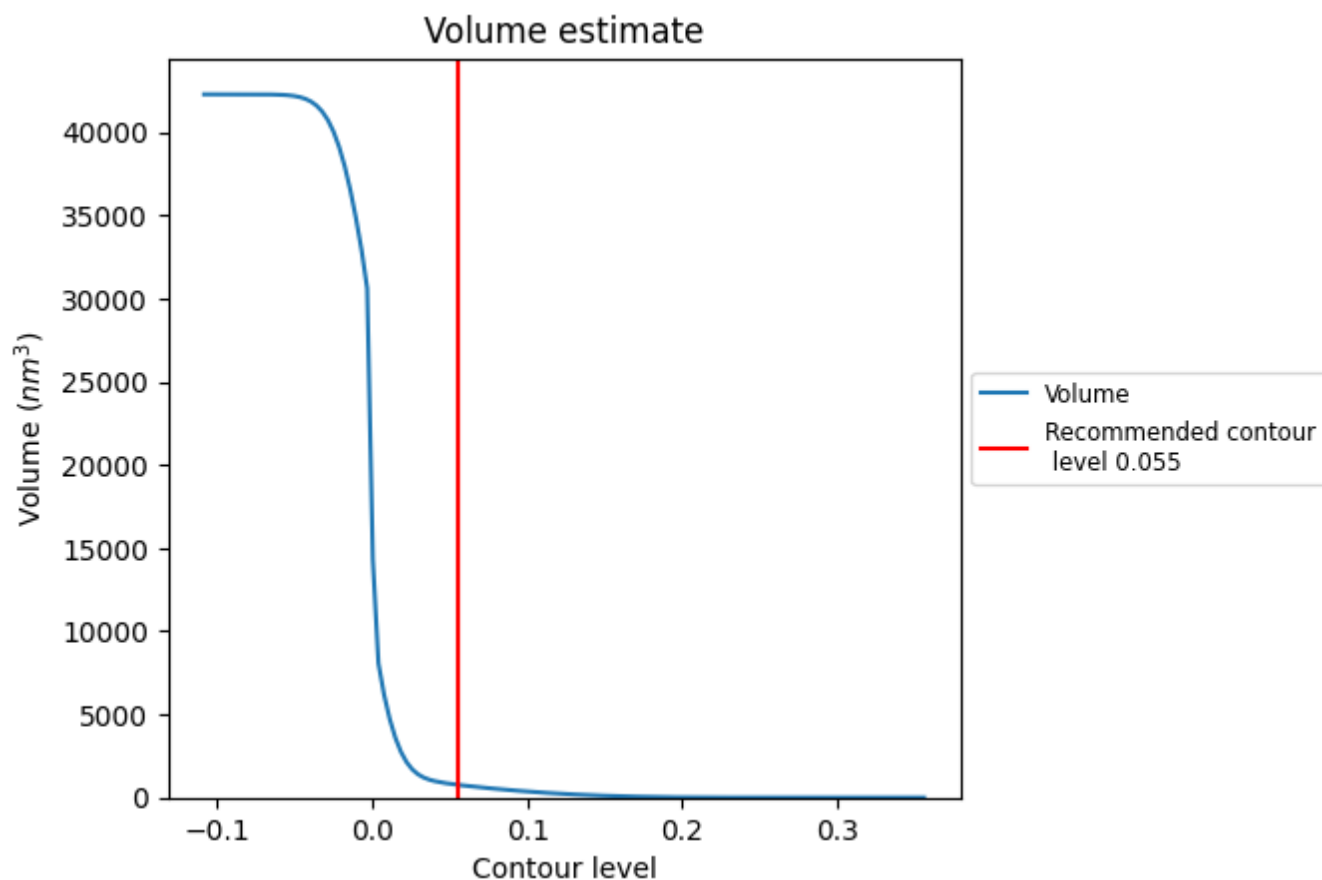
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

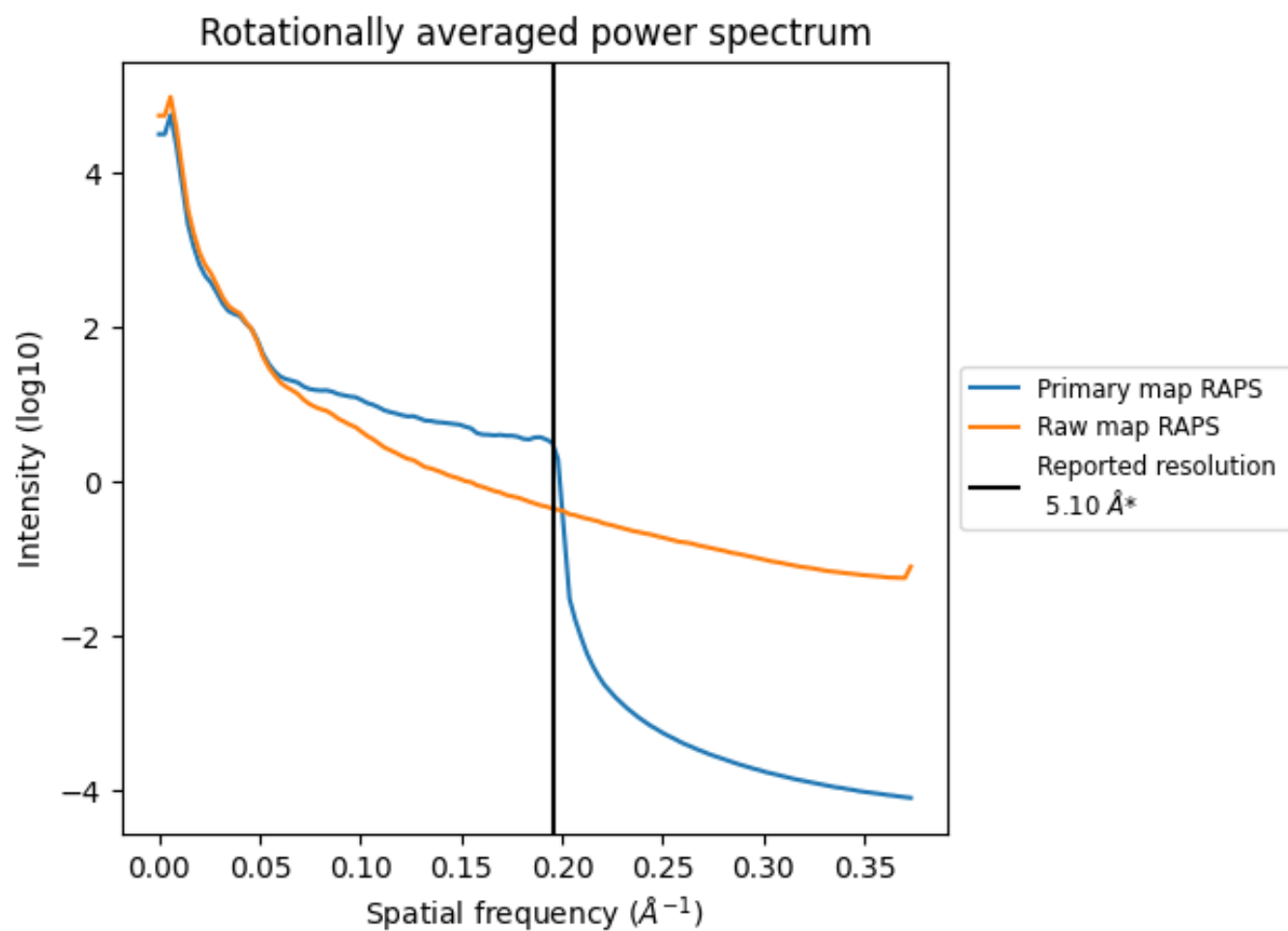
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 769 nm³; this corresponds to an approximate mass of 694 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

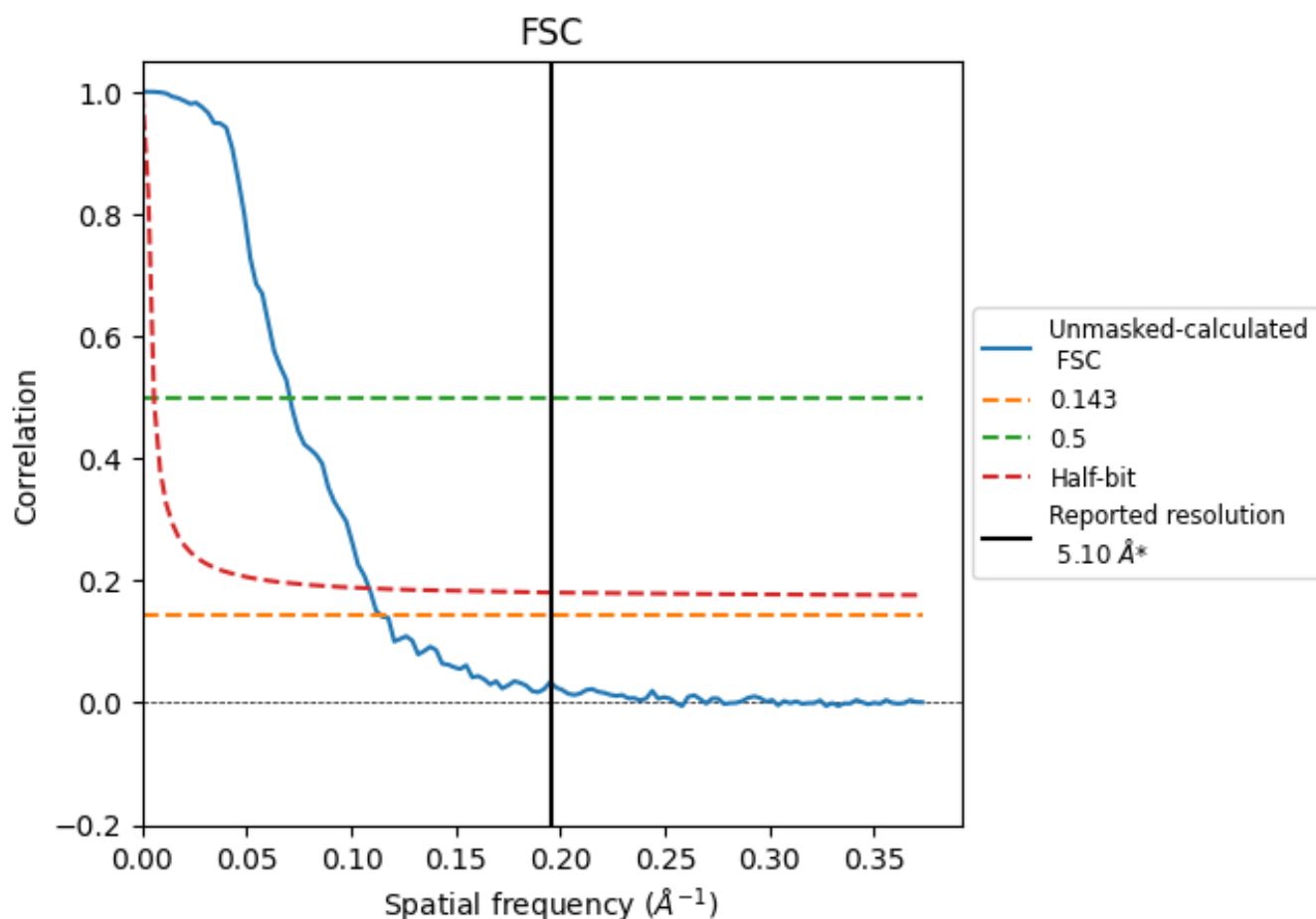


*Reported resolution corresponds to spatial frequency of 0.196 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.196 \text{ \AA}^{-1}$

8.2 Resolution estimates

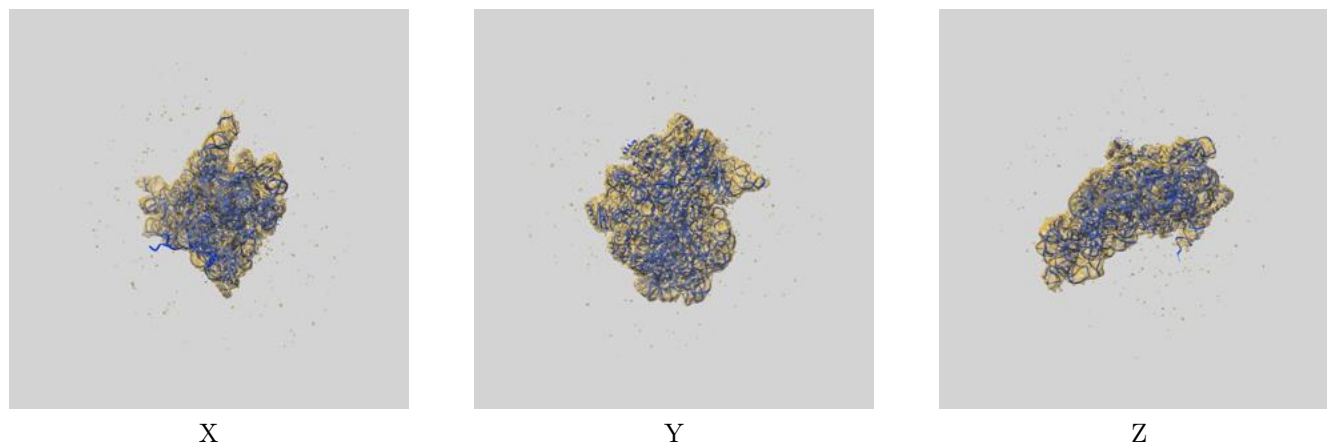
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.76	14.16	9.21

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.76 differs from the reported value 5.1 by more than 10 %

9 Map-model fit [i](#)

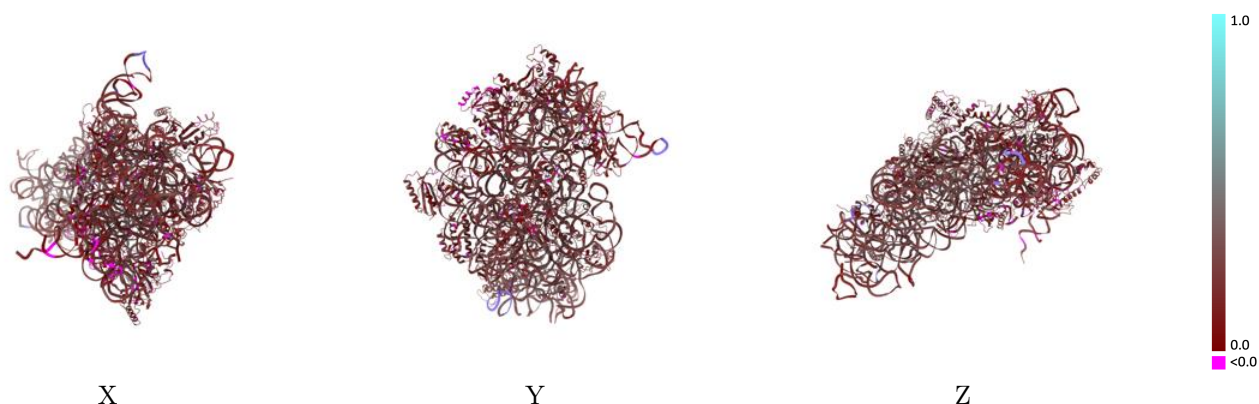
This section contains information regarding the fit between EMDB map EMD-4078 and PDB model 5LMS. Per-residue inclusion information can be found in section 3 on page 8.

9.1 Map-model overlay [i](#)



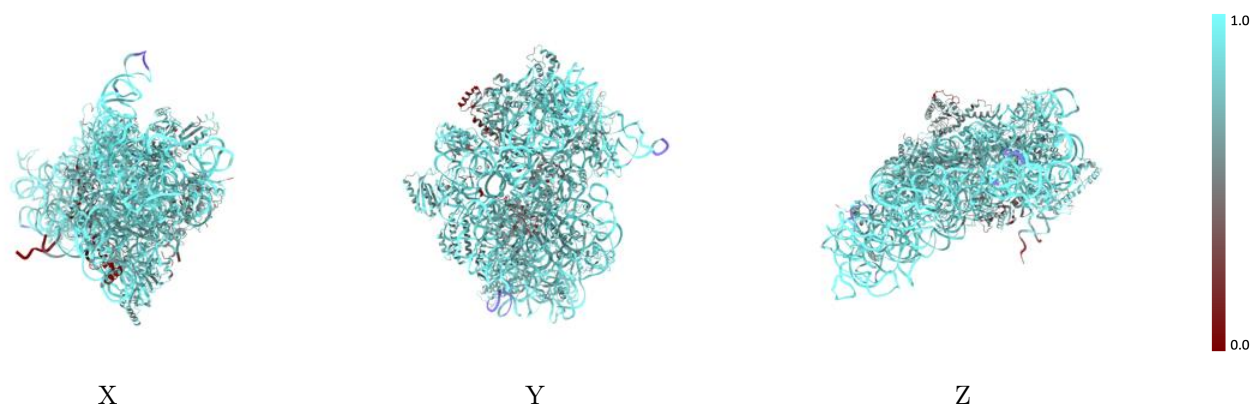
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



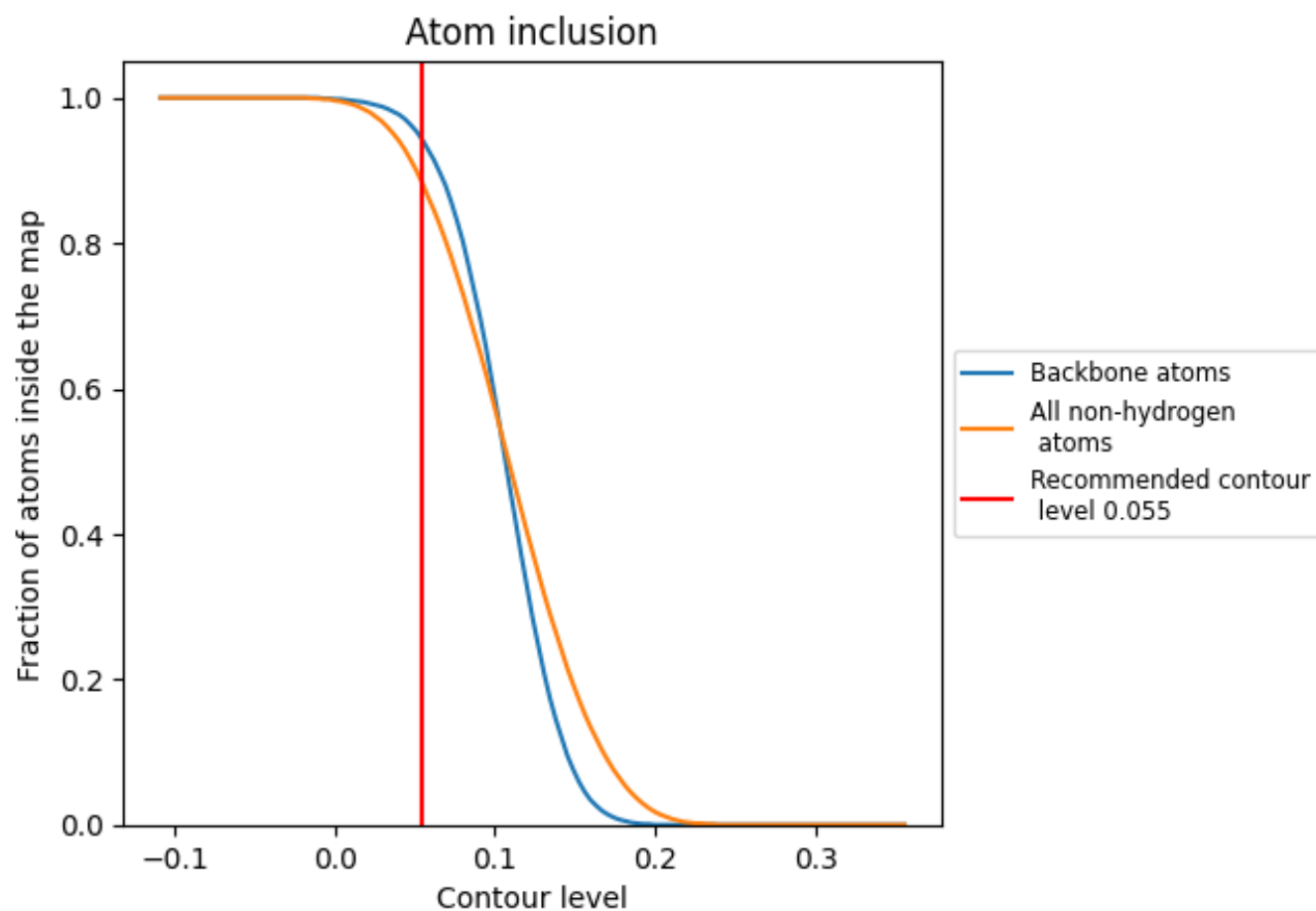
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.055).

9.4 Atom inclusion ⓘ



At the recommended contour level, 94% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.055) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8820	 0.2310
A	 0.9740	 0.2580
B	 0.5590	 0.1810
C	 0.7890	 0.2180
D	 0.8120	 0.2200
E	 0.7910	 0.2270
F	 0.7830	 0.2050
G	 0.7730	 0.2040
H	 0.8150	 0.2210
I	 0.7690	 0.1810
J	 0.7500	 0.2040
K	 0.8120	 0.1960
L	 0.7600	 0.2420
M	 0.8230	 0.1690
N	 0.8120	 0.2260
O	 0.7920	 0.2040
P	 0.7950	 0.2220
Q	 0.7980	 0.2210
R	 0.7580	 0.1790
S	 0.8260	 0.1670
T	 0.8130	 0.2010
V	 0.8220	 0.1600
W	 0.6300	 0.1670
X	 0.4700	 0.1210
Y	 0.8060	 0.1940
Z	 0.7500	 0.1210

