



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 01:27 AM UTC

PDB ID : 6SGC / pdb_00006sgc
EMDB ID : EMD-10181
Title : Rabbit 80S ribosome stalled on a poly(A) tail
Authors : Chandrasekaran, V.; Juszkievicz, S.; Choi, J.; Puglisi, J.D.; Brown, A.; Shao, S.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2019-08-03
Resolution : 2.80 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:

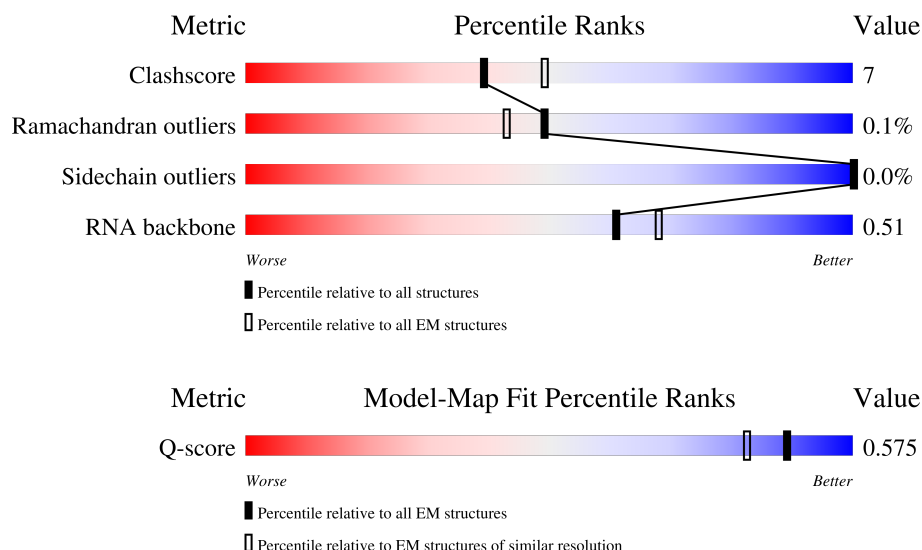
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 2.80 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.



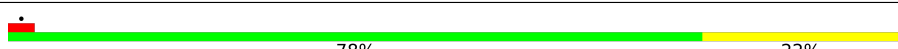
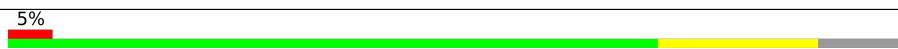
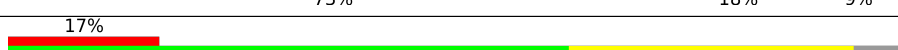
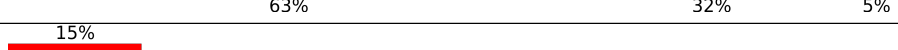
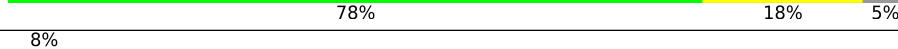
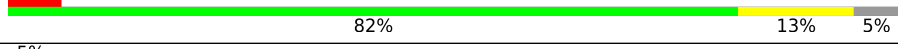
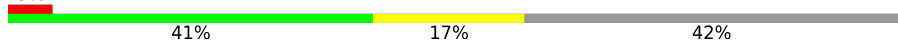
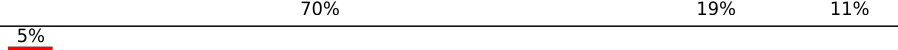
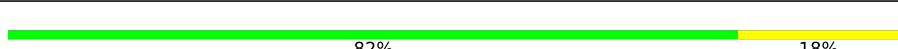
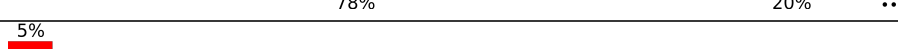
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

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	A1	1869	5% 59% 26% 6% 9%
2	B1	295	60% 14% 26%
3	C1	264	62% 19% 19%

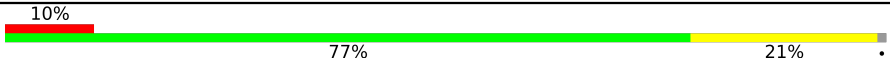
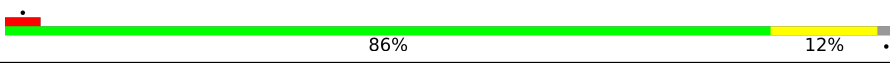
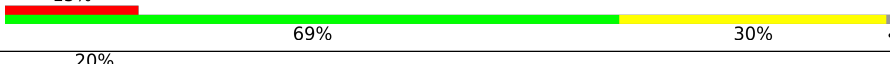
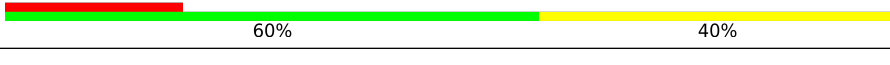
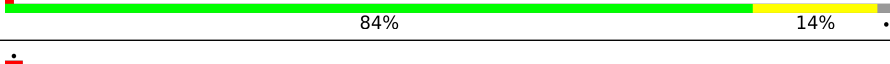
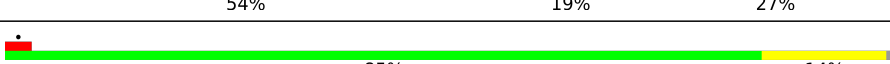
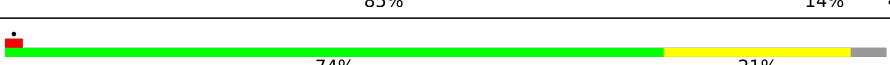
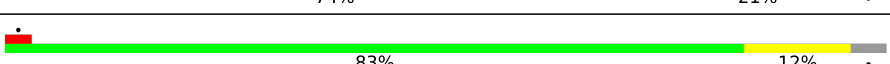
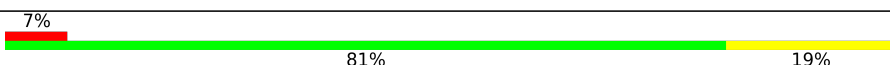
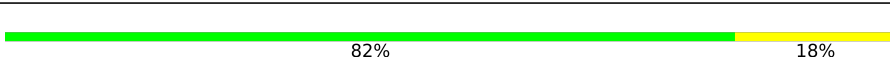
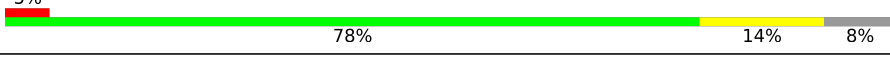
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D1	293	
5	E1	243	
6	F1	263	
7	G1	204	
8	H1	249	
9	I1	194	
10	J1	208	
11	K1	194	
12	L1	165	
13	M1	158	
14	N1	132	
15	O1	151	
16	P1	168	
17	Q1	145	
18	R1	146	
19	S1	135	
20	T1	152	
21	U1	145	
22	V1	119	
23	W1	83	
24	X1	130	
25	Y1	143	
26	Z1	130	
27	a1	125	
28	b1	115	

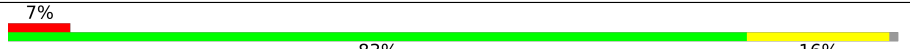
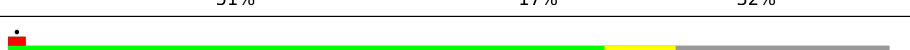
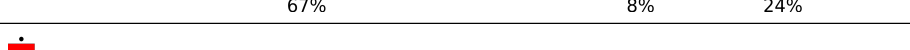
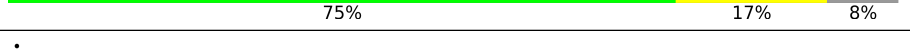
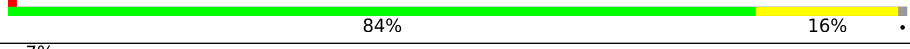
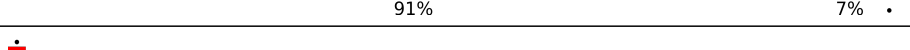
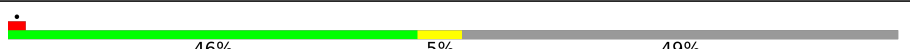
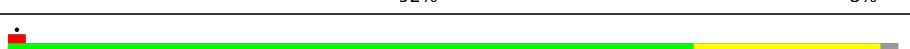
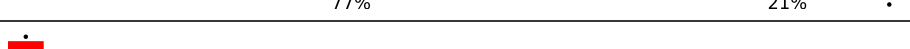
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	c1	84	
30	d1	69	
31	e1	56	
32	f1	133	
33	g1	156	
34	h1	317	
35	i1	10	
36	A2	257	
37	B2	403	
38	C2	425	
39	D2	297	
40	E2	291	
41	F2	247	
42	G2	319	
43	H2	192	
44	I2	214	
45	J2	178	
46	L2	211	
47	M2	218	
48	N2	204	
49	O2	203	
50	P2	184	
51	Q2	188	
52	R2	196	
53	S2	176	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	T2	160	
55	U2	128	
56	V2	140	
57	W2	157	
58	X2	156	
59	Y2	145	
60	Z2	136	
61	a2	148	
62	b2	245	
63	c2	115	
64	d2	125	
65	e2	135	
66	f2	110	
67	g2	116	
68	h2	123	
69	i2	105	
70	j2	97	
71	k2	70	
72	l2	51	
73	m2	102	
74	n2	25	
75	o2	106	
76	p2	92	
77	r2	137	
78	s2	318	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
79	t2	165	
80	54	3603	
81	74	120	
82	84	156	
83	XX	16	
84	B	217	
85	23	76	
85	33	76	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
85	70U	23	34	-	-	X	-
85	70U	33	34	-	-	X	-

2 Entry composition [i](#)

There are 88 unique types of molecules in this entry. The entry contains 218966 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 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A1	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 2 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 3 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C1	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 4 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D1	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 5 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 6 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F1	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F1	25	GLY	SER	conflict	UNP G1TK17
F1	51	ARG	LYS	conflict	UNP G1TK17
F1	78	THR	ALA	conflict	UNP G1TK17
F1	156	VAL	MET	conflict	UNP G1TK17

- Molecule 7 is a protein called Ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G1	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 8 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H1	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 9 is a protein called 40S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I1	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 10 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J1	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J1	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 11 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K1	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 12 is a protein called S10_ plectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L1	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 13 is a protein called Ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M1	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 14 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N1	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 15 is a protein called Ribosomal_S13_N domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O1	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 16 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P1	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

- Molecule 17 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q1	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 18 is a protein called Ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R1	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 19 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S1	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 20 is a protein called eS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T1	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 21 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U1	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
U1	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 22 is a protein called Ribosomal_S10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V1	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 23 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W1	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 24 is a protein called Ribosomal protein S15a.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X1	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 25 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y1	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 26 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z1	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 27 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a1	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 28 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b1	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 29 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c1	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 30 is a protein called Ribosomal protein S28.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d1	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 31 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e1	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 32 is a protein called 40S ribosomal protein S30.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f1	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 33 is a protein called Ribosomal protein S27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g1	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 34 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h1	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 35 is a RNA chain called polyA mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i1	10	Total	C	N	O	P	0	0
			220	100	50	60	10		

- Molecule 36 is a protein called Ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	A2	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 37 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	B2	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B2	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 38 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	C2	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

- Molecule 39 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	D2	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D2	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 40 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	E2	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 41 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	F2	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F2	61	ARG	GLY	conflict	UNP G1TUB1
F2	93	ARG	GLY	conflict	UNP G1TUB1
F2	131	MET	VAL	conflict	UNP G1TUB1
F2	153	ILE	VAL	conflict	UNP G1TUB1

- Molecule 42 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	G2	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

- Molecule 43 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	H2	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 44 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	I2	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 45 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	J2	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 46 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	L2	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 47 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	M2	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 48 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	N2	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 49 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	O2	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 50 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	P2	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 51 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Q2	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 52 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	R2	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 53 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S2	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 54 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	T2	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 55 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	U2	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 56 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	V2	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 57 is a protein called TRASH domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	W2	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 58 is a protein called Ribosomal_L23eN domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	X2	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 59 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	Y2	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 60 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	Z2	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 61 is a protein called Ribosomal_L18e/L15P domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	a2	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a2	1	MET	-	initiating methionine	UNP G1SNY0

- Molecule 62 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	b2	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

- Molecule 63 is a protein called Ribosomal_L7Ae domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	c2	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 64 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	d2	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 65 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	e2	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 66 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	f2	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 67 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	g2	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 68 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	h2	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 69 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	i2	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 70 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	j2	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 71 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	k2	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k2	24	LYS	ASN	conflict	UNP G1U001

- Molecule 72 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	l2	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 73 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	m2	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 74 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	n2	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 75 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	o2	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 76 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	p2	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 77 is a protein called Ribosomal_L28e domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	r2	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 78 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	s2	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 79 is a protein called Ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	t2	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 80 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	54	3603	Total	C	N	O	P	0	0
			77264	34409	14151	25101	3603		

- Molecule 81 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	74	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

- Molecule 82 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	84	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 83 is a protein called poly-lysine nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
83	XX	16	Total	C	N	O	0	0
			100	63	21	16		

- Molecule 84 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	B	206	Total	C	N	O	S	0	0
			1654	1058	297	291	8		

- Molecule 85 is a RNA chain called tRNA (Lys3).

Mol	Chain	Residues	Atoms						AltConf	Trace
85	23	76	Total	C	N	O	P	S	0	0
			1636	736	286	537	75	2		
85	33	76	Total	C	N	O	P	S	0	0
			1636	736	286	537	75	2		

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	A1	70	Total	Mg	0
			70	70	
86	A2	1	Total	Mg	0
			1	1	
86	B2	1	Total	Mg	0
			1	1	
86	I2	1	Total	Mg	0
			1	1	
86	P2	1	Total	Mg	0
			1	1	
86	V2	1	Total	Mg	0
			1	1	
86	a2	1	Total	Mg	0
			1	1	
86	g2	1	Total	Mg	0
			1	1	
86	j2	2	Total	Mg	0
			2	2	
86	54	185	Total	Mg	0
			185	185	
86	74	6	Total	Mg	0
			6	6	

Continued on next page...

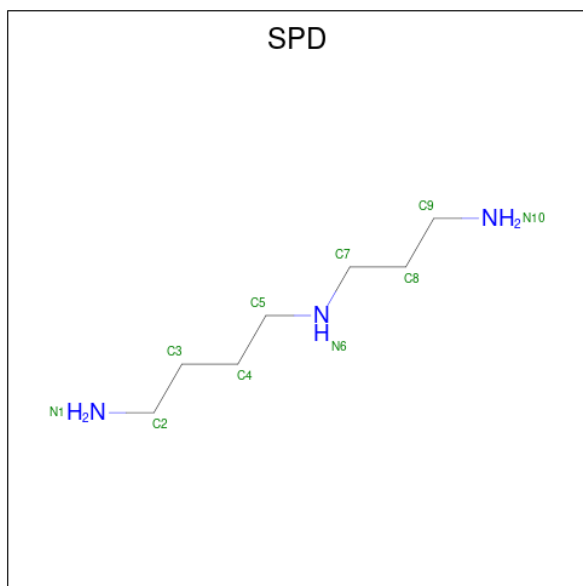
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
86	84	5	Total	Mg	0
			5	5	

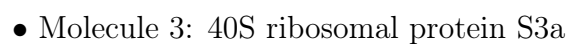
- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	b1	1	Total	Zn	0
			1	1	
87	e1	1	Total	Zn	0
			1	1	
87	g1	1	Total	Zn	0
			1	1	
87	g2	1	Total	Zn	0
			1	1	
87	j2	1	Total	Zn	0
			1	1	
87	m2	1	Total	Zn	0
			1	1	
87	o2	1	Total	Zn	0
			1	1	
87	p2	1	Total	Zn	0
			1	1	

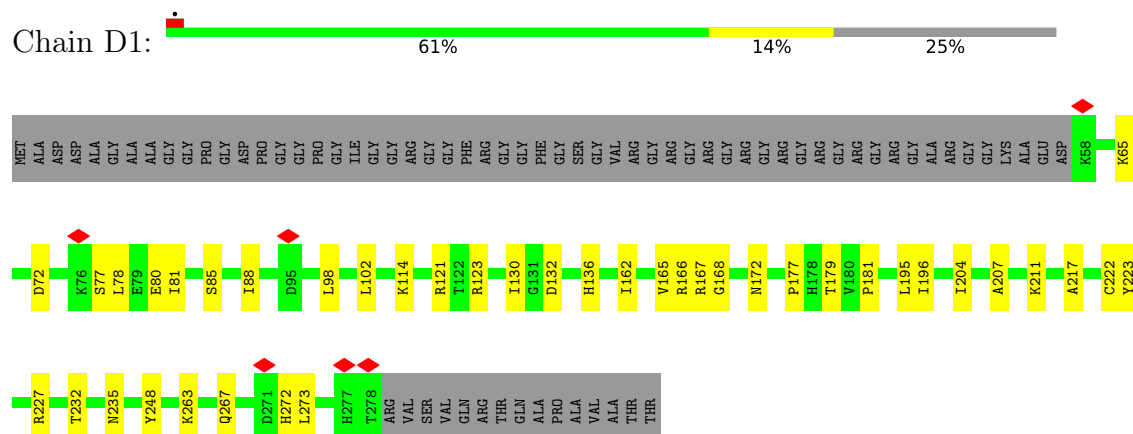
- Molecule 88 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



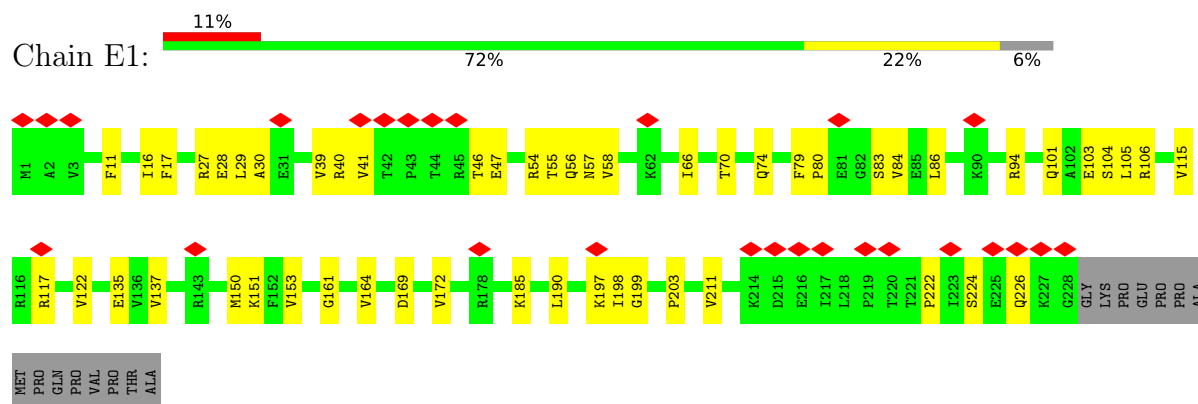
Mol	Chain	Residues	Atoms			AltConf
88	54	1	Total	C	N	0
			10	7	3	
88	54	1	Total	C	N	0
			10	7	3	



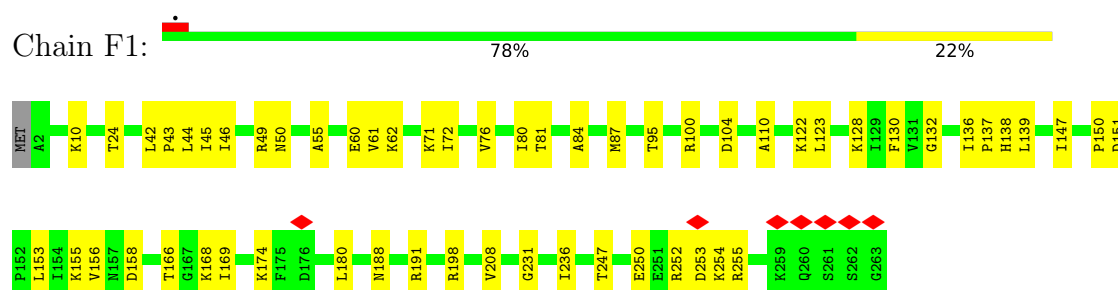
- Molecule 4: uS5



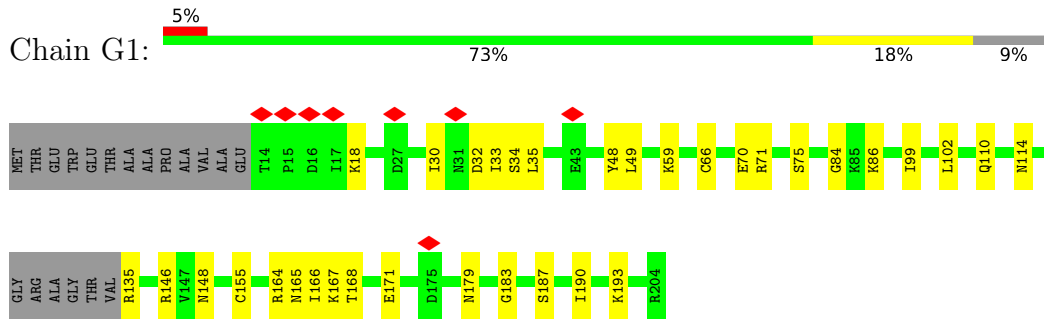
- Molecule 5: uS5



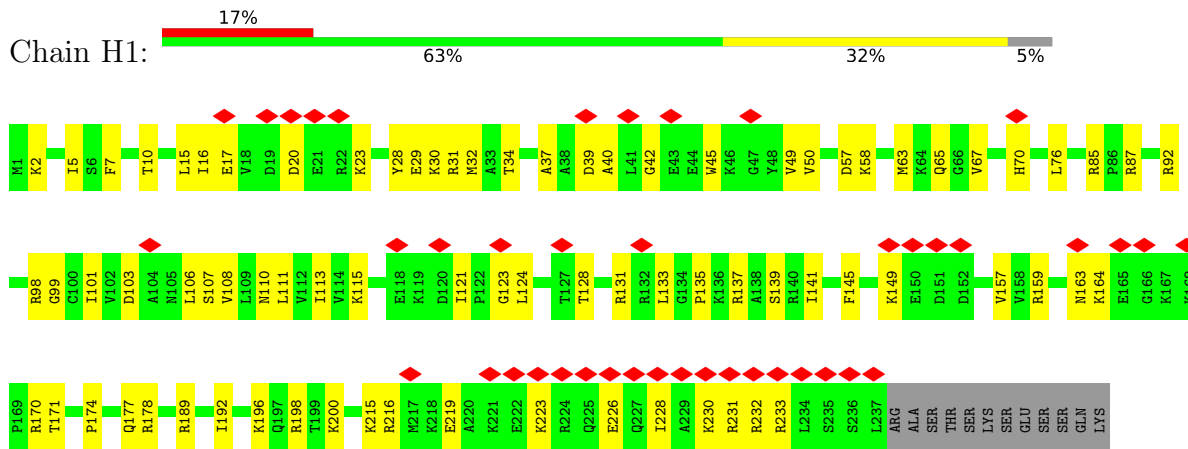
- Molecule 6: 40S ribosomal protein S4



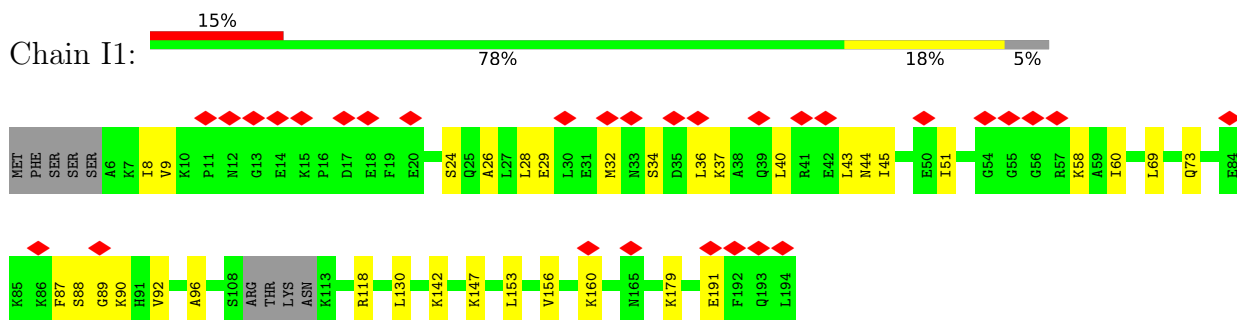
- Molecule 7: Ribosomal protein S5



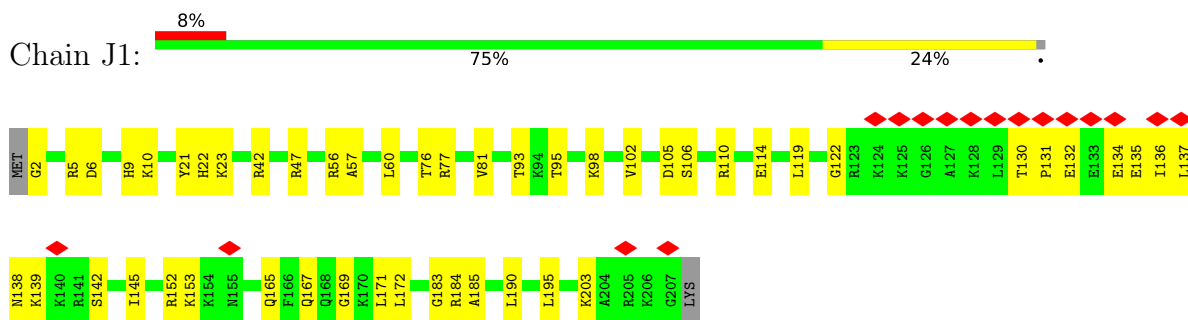
- Molecule 8: 40S ribosomal protein S6



- Molecule 9: 40S ribosomal protein S7



- Molecule 10: 40S ribosomal protein S8

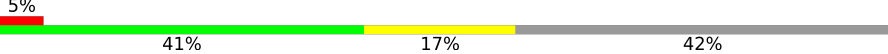


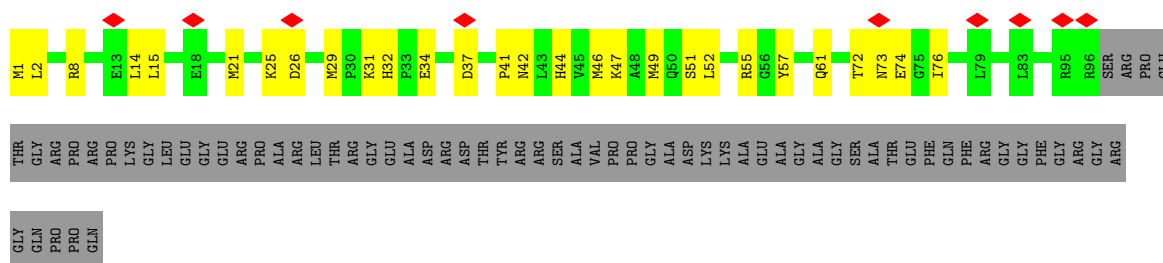
- Molecule 11: Ribosomal protein S9 (Predicted)

Chain K1: 



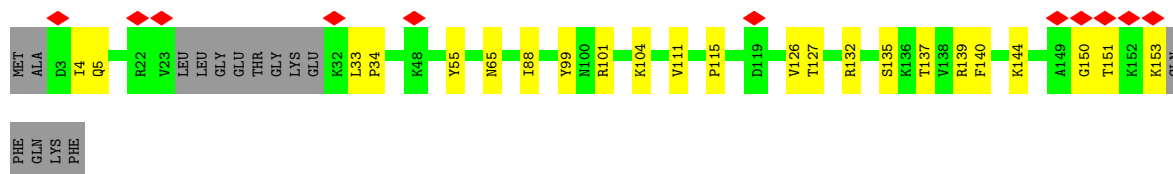
- Molecule 12: S10_pectin domain-containing protein

Chain L1: 



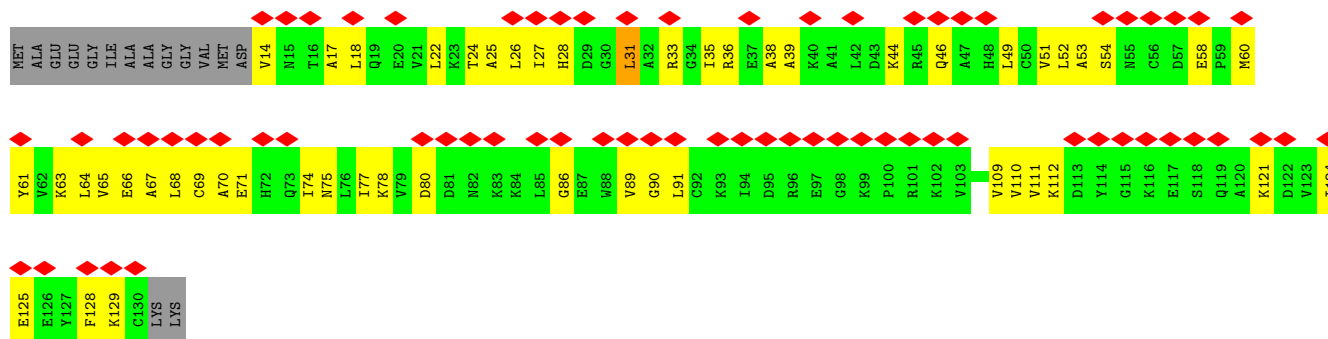
- Molecule 13: Ribosomal protein S11

Chain M1: 



- Molecule 14: 40S ribosomal protein S12

Chain N1: 



- Molecule 15: Ribosomal_S13_N domain-containing protein

Chain O1: 

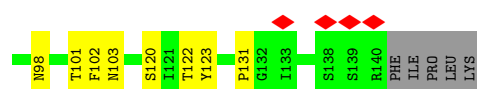
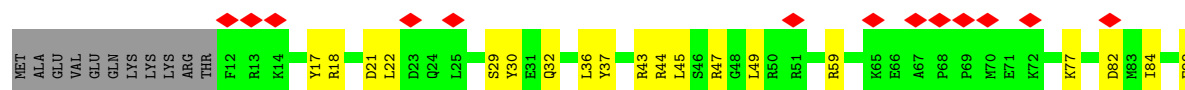
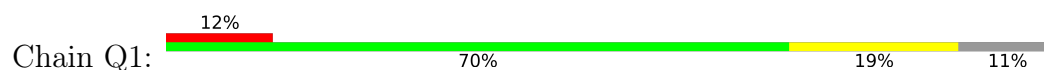




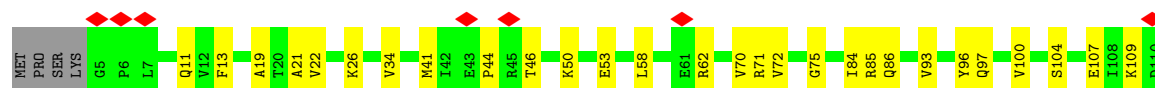
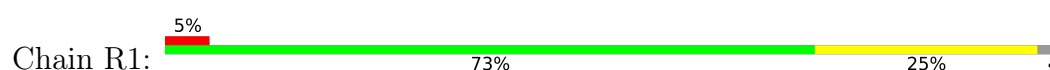
- Molecule 16: uS11



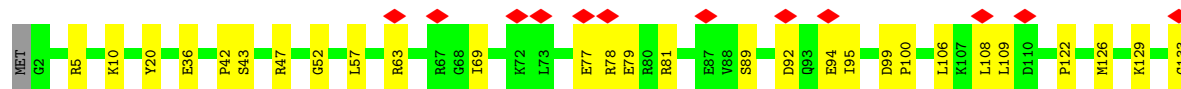
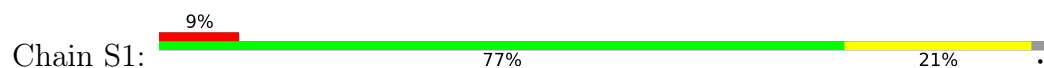
- Molecule 17: uS19



- Molecule 18: Ribosomal protein S16

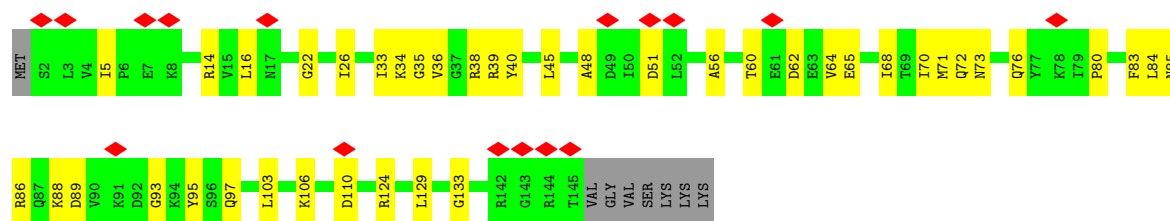


- Molecule 19: eS17

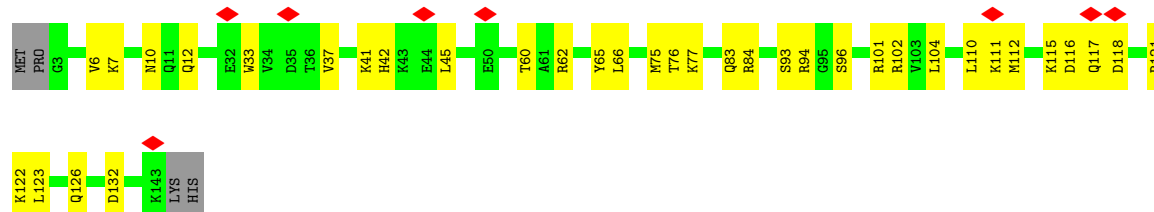
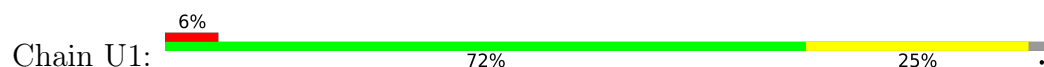


- Molecule 20: eS13

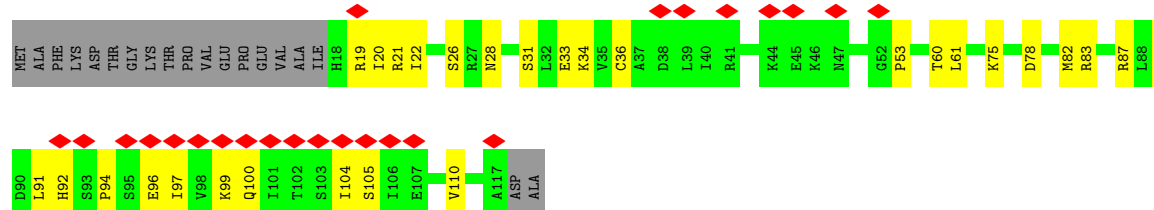




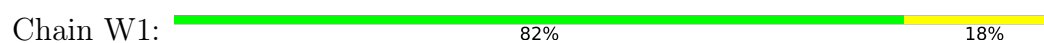
• Molecule 21: eS19



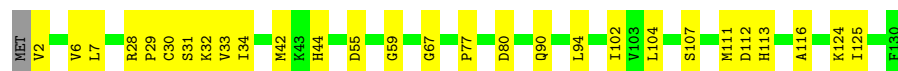
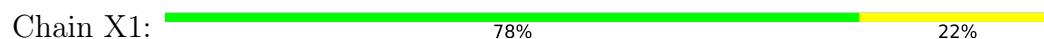
• Molecule 22: Ribosomal_S10 domain-containing protein



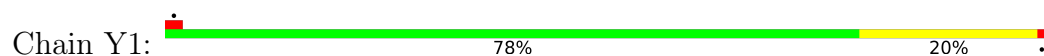
• Molecule 23: eS21



• Molecule 24: Ribosomal protein S15a

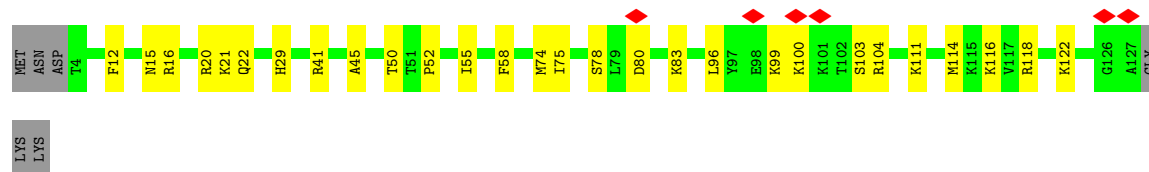


• Molecule 25: uS12

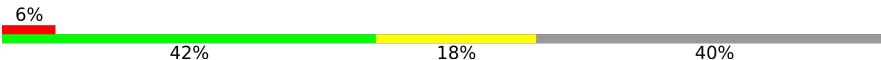


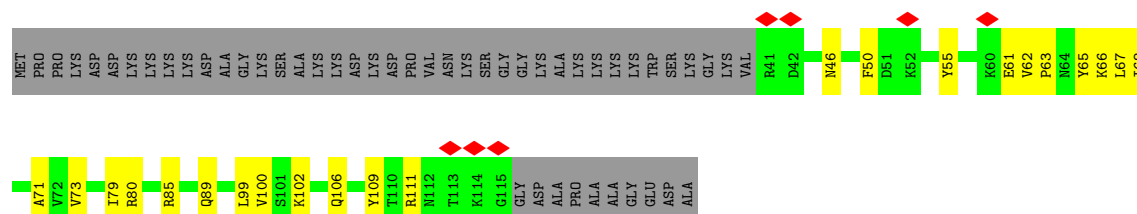
- Molecule 26: eS24

Chain Z1: 



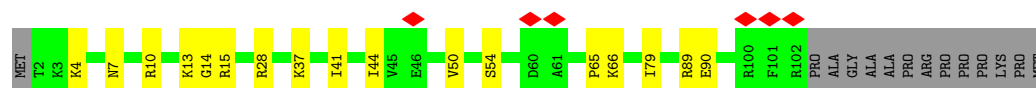
- Molecule 27: eS25

Chain a1: 



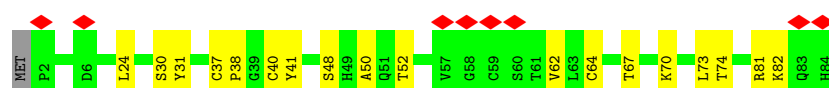
- Molecule 28: eS26

Chain b1: 



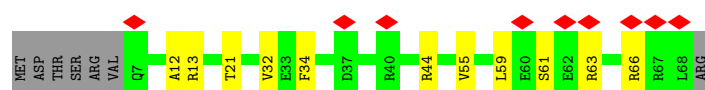
- Molecule 29: 40S ribosomal protein S27

Chain c1: 



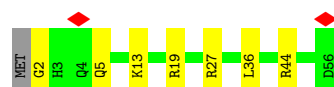
- Molecule 30: Ribosomal protein S28

Chain d1: 

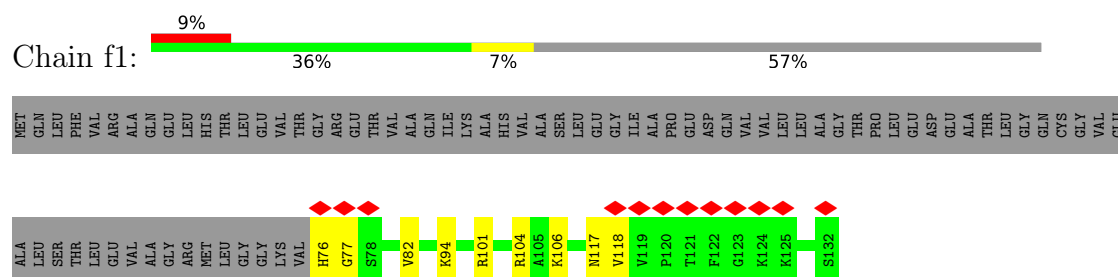


- Molecule 31: uS14

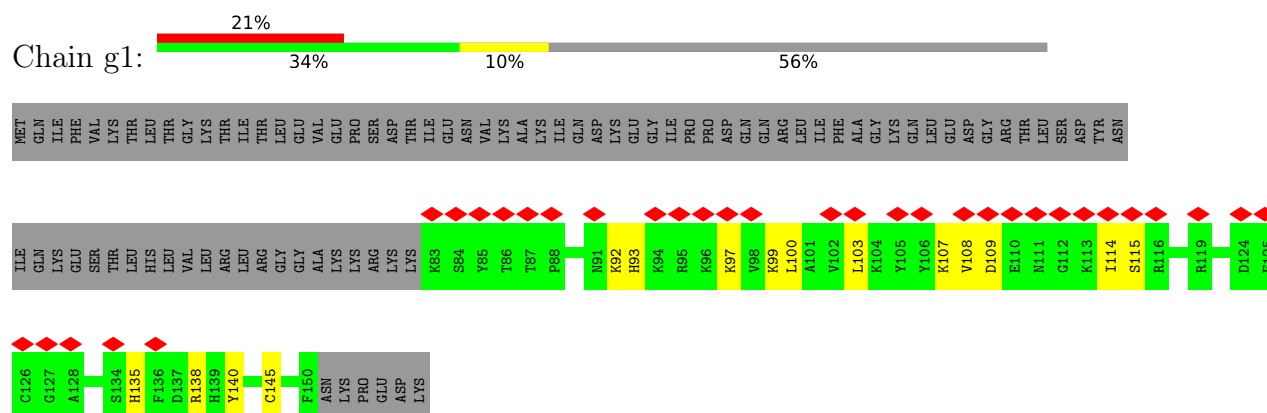
Chain e1: 



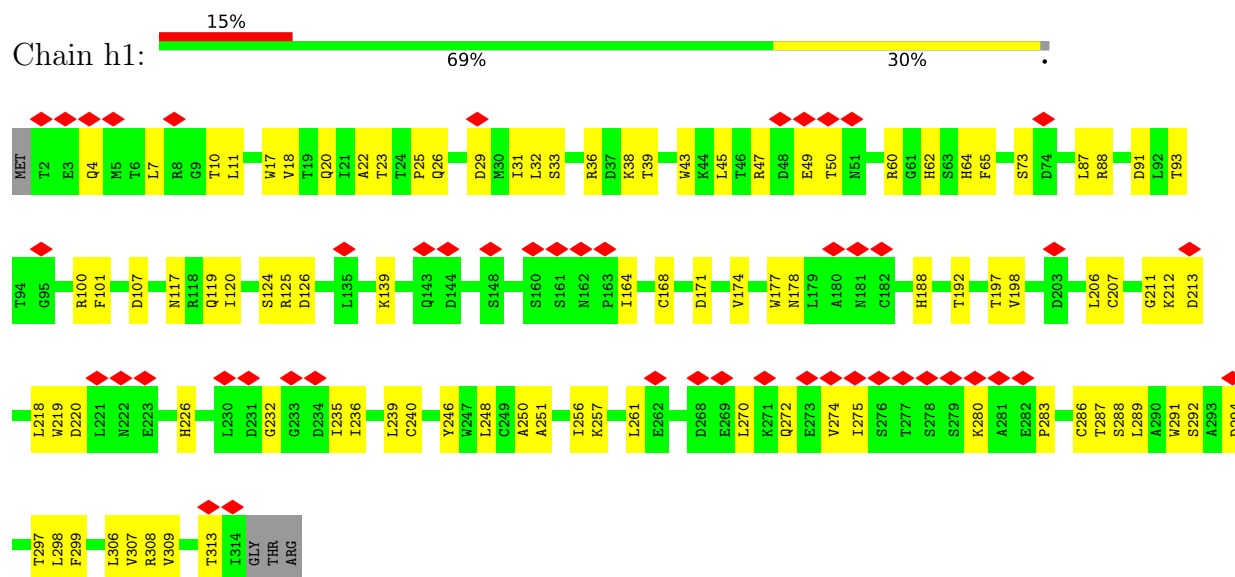
- Molecule 32: 40S ribosomal protein S30



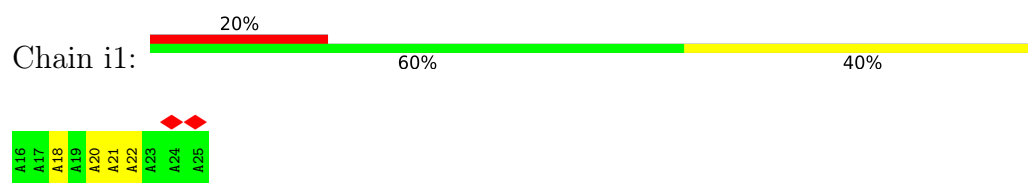
- Molecule 33: Ribosomal protein S27a



- Molecule 34: WD_REPEATS_REGION domain-containing protein



- Molecule 35: polyA mRNA



- Molecule 36: Ribosomal protein L8

	MET	G2	V15	A27	E36	I41	L48 L49	K60	F63	R72	E80	V101	V104	G105	T106	M107	P108	E117	R123	G124	R128	I137	S138	H139	E142	T143	K149	I158	N162	R163	A164	V165	A170	G173	L180	G182
	M194	C195	V196	P197	A198	V199	R200	V207	E208	N215	H216	Q217	K234	I238	R241	R242	T243	G244	T249	LYS	THR	VAL	GLN	GLU	LYS	GLU	ASN									

Chain B2: 84% 14%

[illegible]

Chain C2: 75% 11% 15%

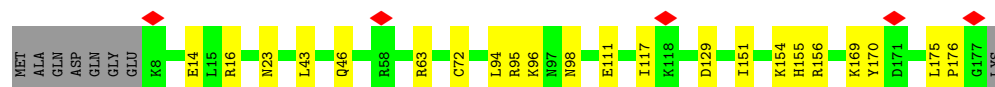
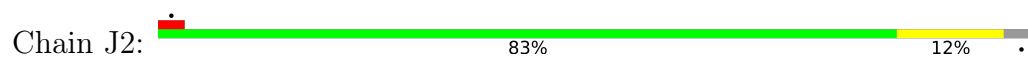
Protein	Position	Residue	Score	Label
Met	1	Met	1.00	Met
	2	Ala	0.99	A2
	3	Cys	0.98	C3
	20	Lys	0.97	K20
	29	Lys	0.96	K29
	39	Phe	0.95	F39
	43	Asn	0.94	N43
	69	Thr	0.93	T69
	78	Arg	0.92	R78
	81	Gln	0.91	Q81
	82	Gly	0.90	G82
	88	Gly	0.89	G88
	94	Asn	0.88	N94
	100	Arg	0.87	R100
	101	His	0.86	H101
	102	Asp	0.85	D102
	132	Ala	0.84	A132
	140	Lys	0.83	K140
	150	Lys	0.82	K150
	151	Pro	0.81	P151
	152	Lys	0.80	K152
	195	Lys	0.79	K195
	200	Arg	0.78	R200
	204	Lys	0.77	K204
	224	Lys	0.76	K224
227	Lys	0.75	K227	
235	Lys	0.74	K235	
240	Lys	0.73	K240	
241	His	0.72	H241	
242	Pro	0.71	P242	
245	Arg	0.70	R245	
251	Ala	0.69	A251	
262	Gly	0.68	G262	
Pro	1	Pro	1.00	Pro
	2	Lys	0.99	K2
	3	Thr	0.98	T3
	4	Ala	0.97	A4
	5	Ala	0.96	A5
	6	Ala	0.95	A6
	7	Ala	0.94	A7
	8	Ala	0.93	A8
	9	Ala	0.92	A9
	10	Ala	0.91	A10
	11	Ala	0.90	A11
	12	Ala	0.89	A12
	13	Ala	0.88	A13
	14	Ala	0.87	A14
	15	Ala	0.86	A15
	16	Ala	0.85	A16
	17	Ala	0.84	A17
	18	Ala	0.83	A18
	19	Ala	0.82	A19
	20	Ala	0.81	A20
	21	Ala	0.80	A21
	22	Ala	0.79	A22
	23	Ala	0.78	A23
	24	Ala	0.77	A24
	25	Ala	0.76	A25
Gln	1	Gln	1.00	G1
	2	Lys	0.99	K2
	3	Lys	0.98	K3
	4	Lys	0.97	K4
	5	Pro	0.96	P5
	6	Val	0.95	V6
	7	Val	0.94	V7
	8	Lys	0.93	K8
	9	Arg	0.92	R9
	10	Lys	0.91	K10
	11	Ala	0.90	A11
	12	Ala	0.89	A12
	13	Ala	0.88	A13
	14	Ala	0.87	A14
	15	Ala	0.86	A15
	16	Ala	0.85	A16
	17	Ala	0.84	A17
	18	Ala	0.83	A18
	19	Ala	0.82	A19
	20	Ala	0.81	A20
	21	Ala	0.80	A21
	22	Ala	0.79	A22
	23	Ala	0.78	A23
	24	Ala	0.77	A24
	25	Ala	0.76	A25

Chain D2: 79% 20%

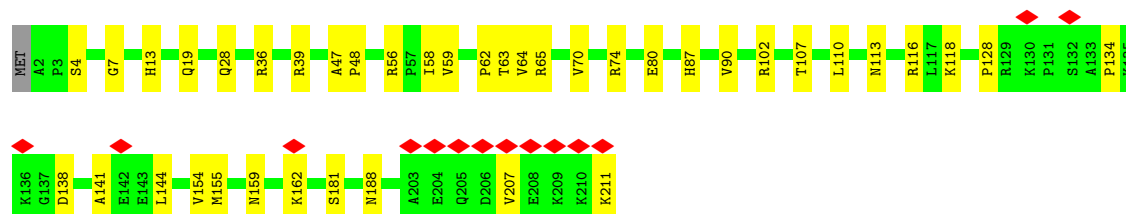
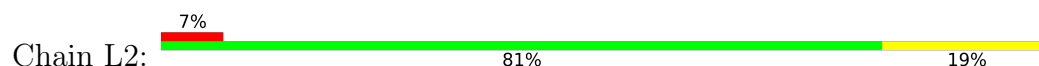
[illegible]

Chain E2:

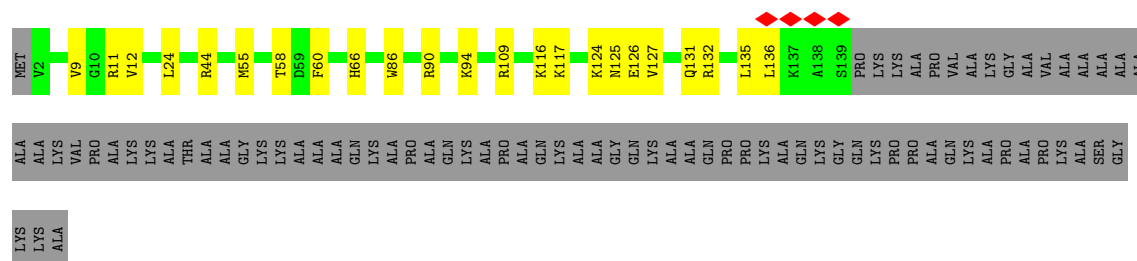
- Molecule 45: Ribosomal protein L11



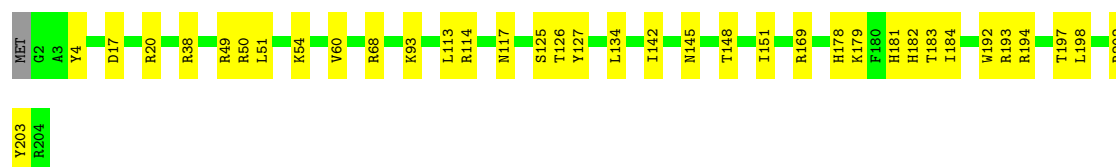
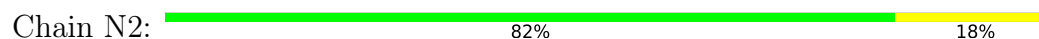
- Molecule 46: eL13



- Molecule 47: Ribosomal protein L14

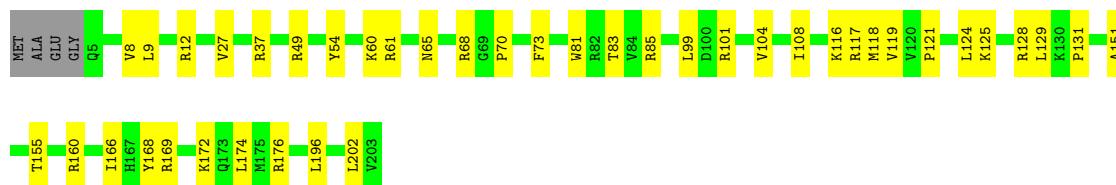


- Molecule 48: Ribosomal protein L15



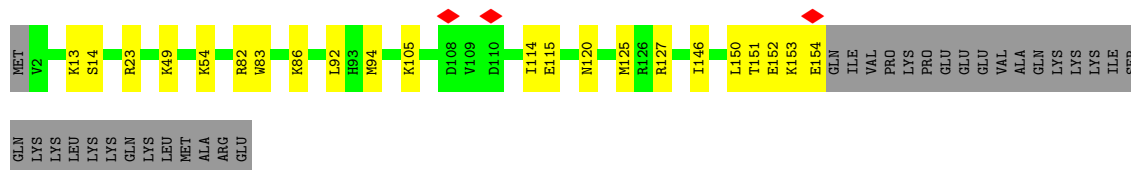
- Molecule 49: uL13

Chain O2:  78% 20% .



• Molecule 50: uL22

Chain P2:  71% 12% 17%



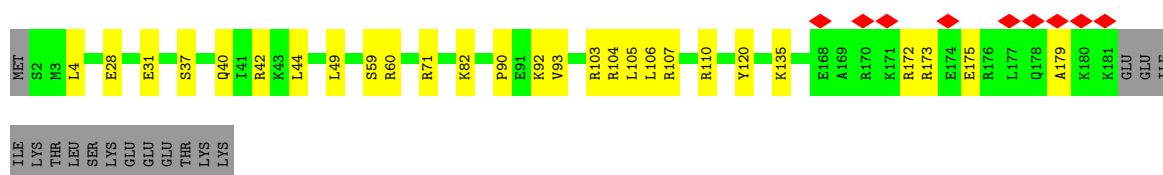
• Molecule 51: eL18

Chain Q2:  84% 16% .



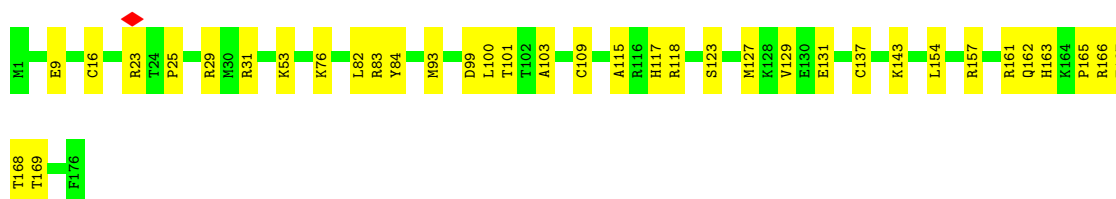
• Molecule 52: eL19

Chain R2:  5% 78% 14% 8%



• Molecule 53: eL20

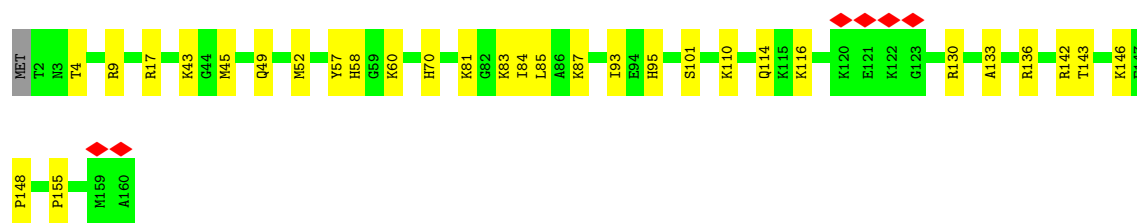
Chain S2:  80% 20%



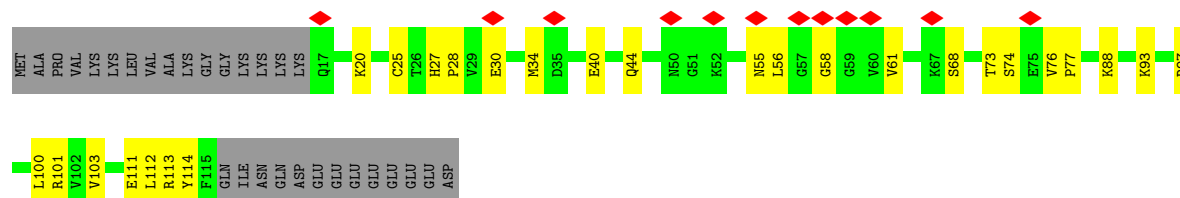
• Molecule 54: eL21

Chain T2:  81% 19%

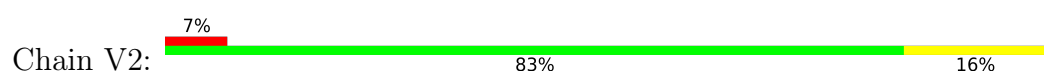




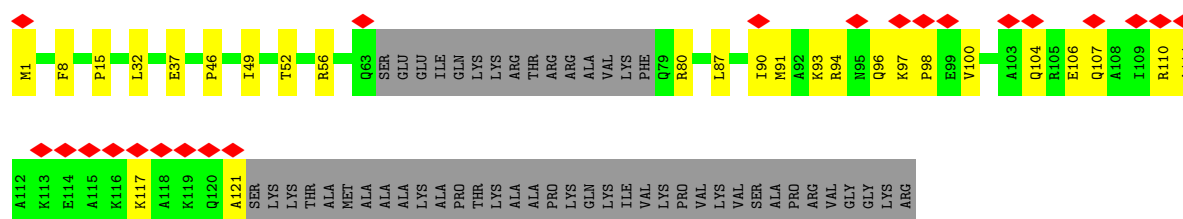
- Molecule 55: eL22



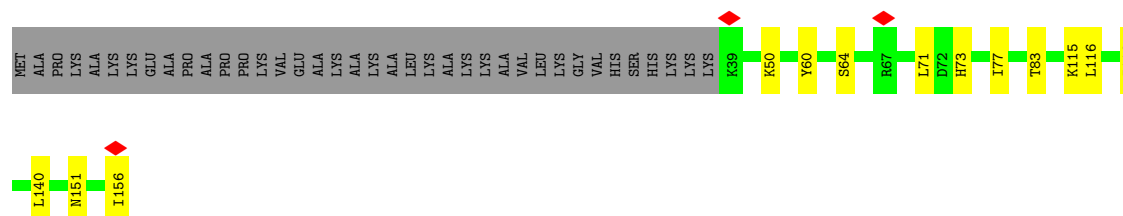
- Molecule 56: Ribosomal protein L23



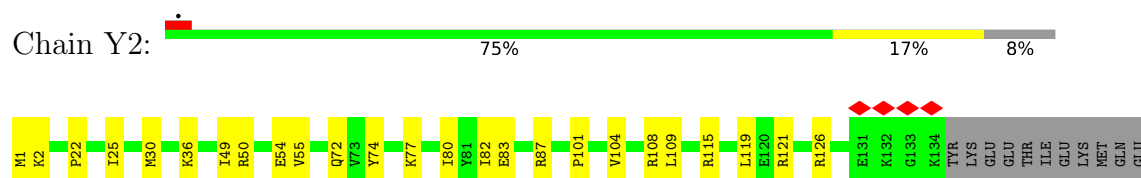
- Molecule 57: TRASH domain-containing protein



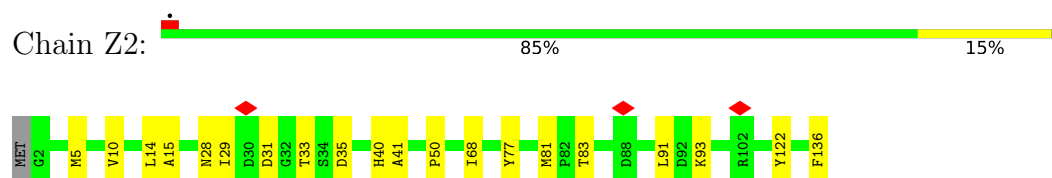
- Molecule 58: Ribosomal_L23eN domain-containing protein



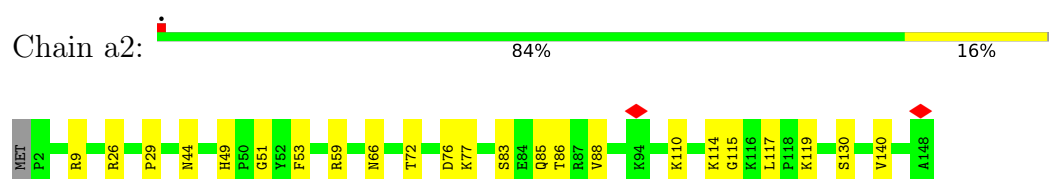
- Molecule 59: Ribosomal protein L26



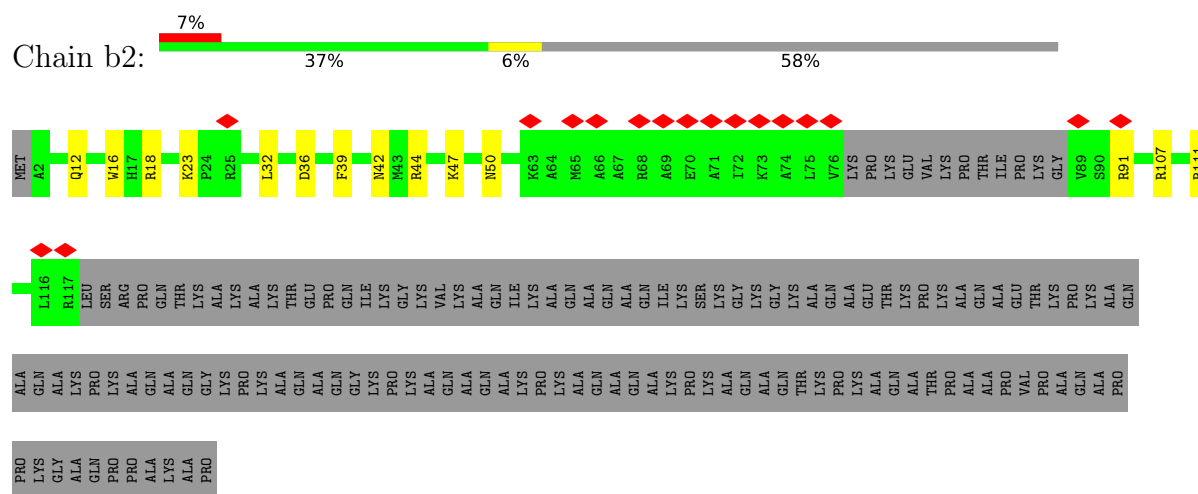
- Molecule 60: 60S ribosomal protein L27



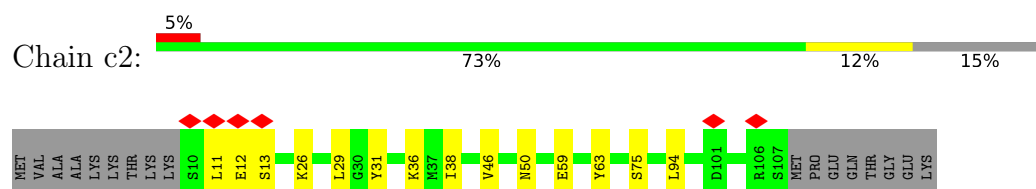
- Molecule 61: Ribosomal_L18e/L15P domain-containing protein



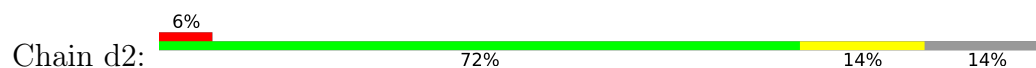
- Molecule 62: eL29



- Molecule 63: Ribosomal_L7Ae domain-containing protein

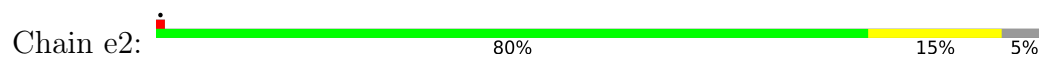


- Molecule 64: eL31

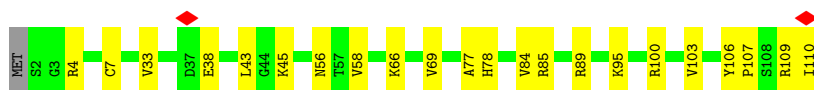
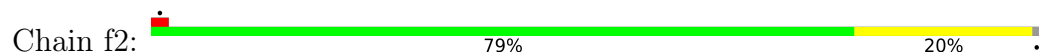




- Molecule 65: eL32



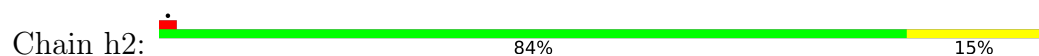
- Molecule 66: eL33



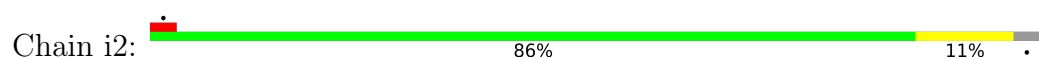
- Molecule 67: eL34



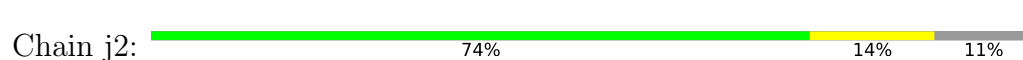
- Molecule 68: uL29



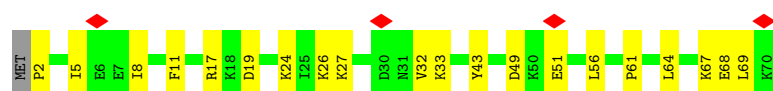
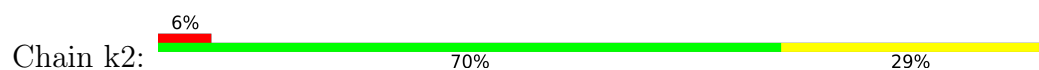
- Molecule 69: 60S ribosomal protein L36



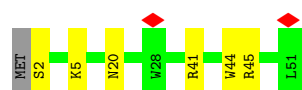
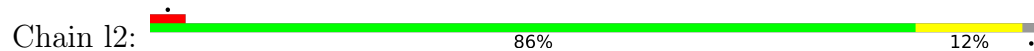
- Molecule 70: Ribosomal protein L37



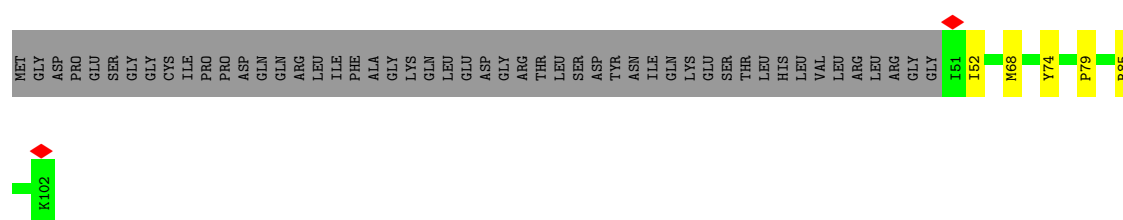
- Molecule 71: eL38



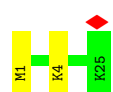
- Molecule 72: eL39



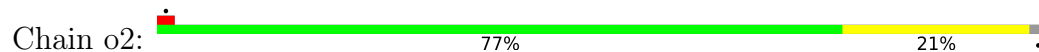
- Molecule 73: eL40



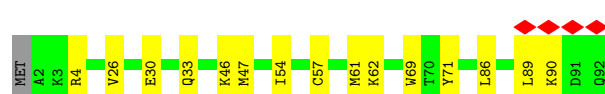
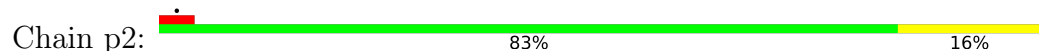
- Molecule 74: 60s ribosomal protein l41



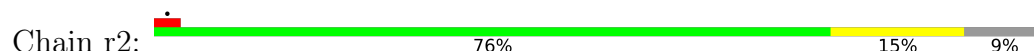
- Molecule 75: eL42

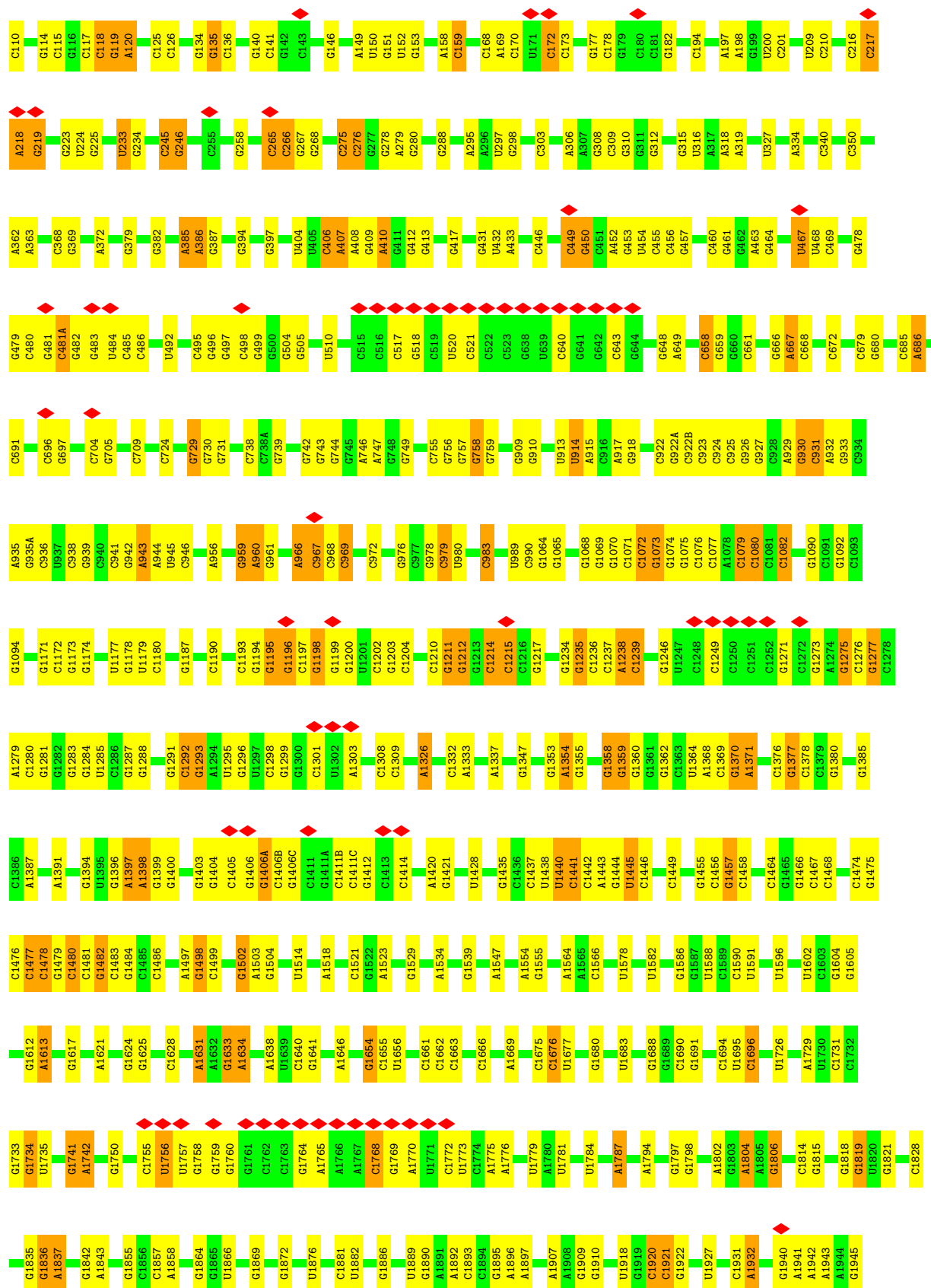


- Molecule 76: eL43

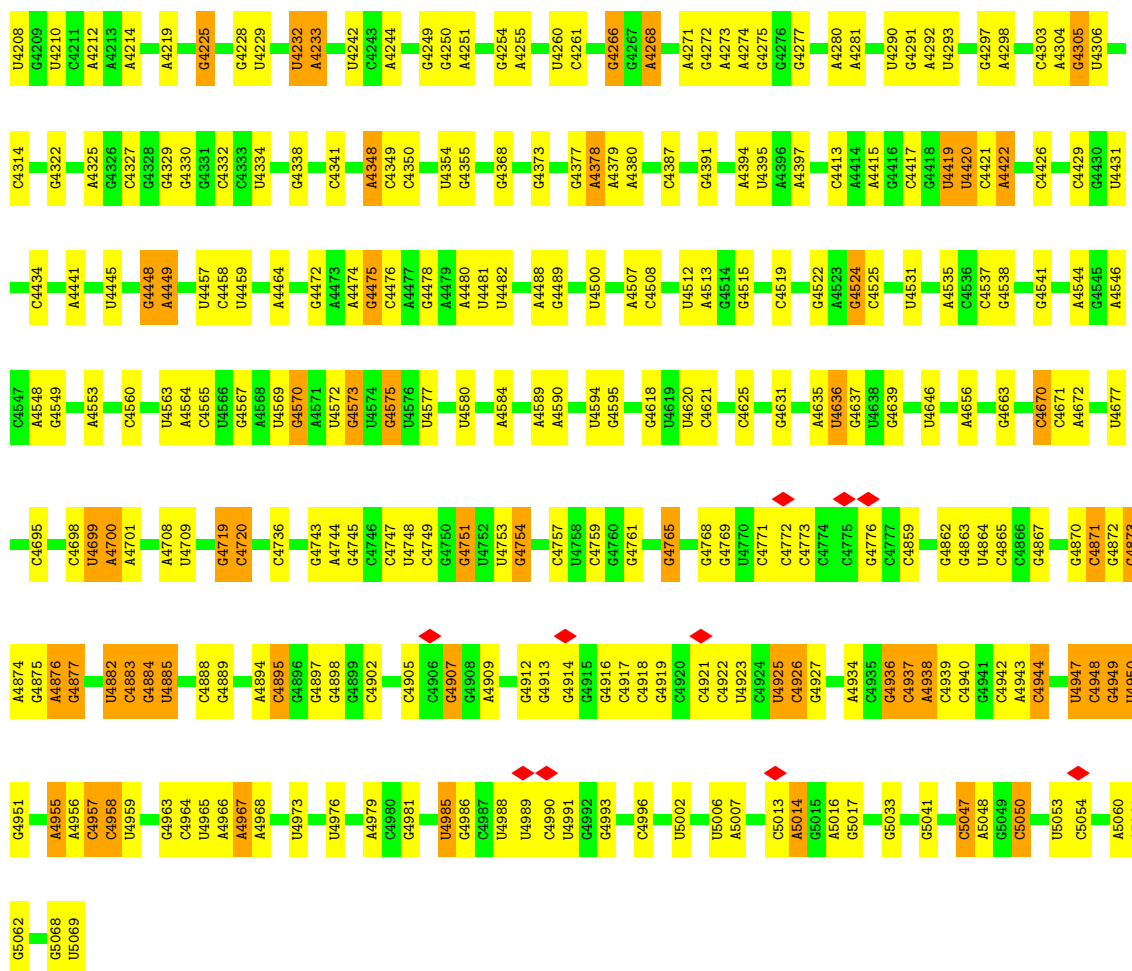


- Molecule 77: Ribosomal_L28e domain-containing protein









- Molecule 81: 5S ribosomal RNA

Chain 74: 81% 17% ..



- Molecule 82: 5.8S ribosomal RNA

Chain 84: 63% 28% 5% .

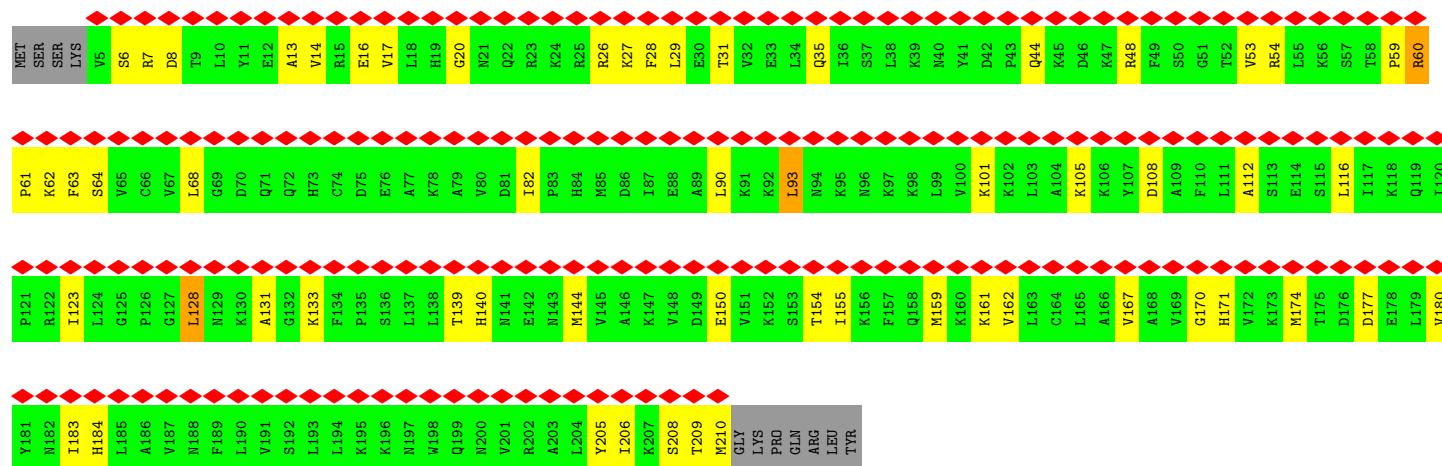


- Molecule 83: poly-lysine nascent chain

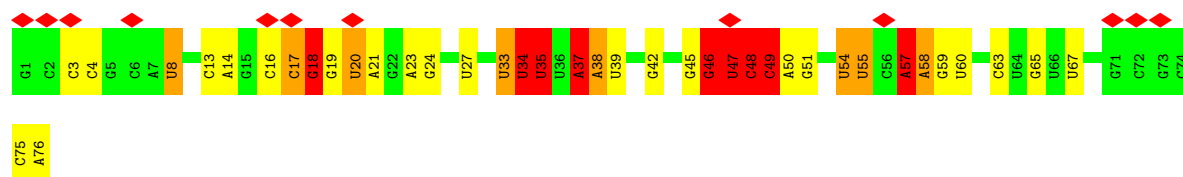
Chain XX: 94% 50% 38% 12%



• Molecule 84: Ribosomal protein



• Molecule 85: tRNA (Lys3)



• Molecule 85: tRNA (Lys3)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	148615	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	41.8, 41.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k), FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.573	Depositor
Minimum map value	-0.276	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	555.52, 555.52, 555.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.085, 1.085, 1.085	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 12A, MG, PSU, 7MG, 70U, 2MU, H2U, 1MA, ZN, SPD, 5MC

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	A1	0.12	0/40502	0.23	0/63100
2	B1	0.13	0/1747	0.31	0/2374
3	C1	0.13	0/1756	0.34	0/2350
4	D1	0.13	0/1753	0.32	0/2369
5	E1	0.13	0/1796	0.36	0/2417
6	F1	0.13	0/2118	0.33	0/2849
7	G1	0.12	0/1492	0.36	0/2005
8	H1	0.14	0/1946	0.39	0/2590
9	I1	0.13	0/1510	0.35	0/2022
10	J1	0.14	0/1715	0.38	0/2287
11	K1	0.12	0/1550	0.35	0/2069
12	L1	0.12	0/834	0.33	0/1125
13	M1	0.14	0/1195	0.33	0/1597
14	N1	0.18	0/918	0.47	0/1233
15	O1	0.13	0/1226	0.31	0/1649
16	P1	0.14	0/1029	0.35	0/1380
17	Q1	0.14	0/1079	0.40	0/1441
18	R1	0.13	0/1146	0.37	0/1534
19	S1	0.12	0/1082	0.35	0/1452
20	T1	0.14	0/1208	0.39	0/1618
21	U1	0.13	0/1115	0.35	0/1493
22	V1	0.15	0/805	0.38	0/1081
23	W1	0.12	0/643	0.30	0/860
24	X1	0.14	0/1051	0.32	0/1406
25	Y1	0.14	0/1116	0.35	0/1490
26	Z1	0.11	0/1028	0.32	0/1366
27	a1	0.13	0/604	0.36	0/810
28	b1	0.16	0/828	0.39	0/1109
29	c1	0.12	0/665	0.29	0/891
30	d1	0.12	0/490	0.35	0/656
31	e1	0.13	0/470	0.33	0/623
32	f1	0.13	0/462	0.37	0/607

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g1	0.12	0/567	0.40	0/753
34	h1	0.20	1/2493 (0.0%)	0.38	1/3394 (0.0%)
35	i1	0.11	0/249	0.23	0/386
36	A2	0.16	0/1936	0.40	1/2596 (0.0%)
37	B2	0.15	0/3240	0.36	0/4339
38	C2	0.15	0/2937	0.37	0/3946
39	D2	0.13	0/2437	0.31	0/3264
40	E2	0.14	0/1762	0.35	0/2362
41	F2	0.14	0/1911	0.33	0/2549
42	G2	0.14	0/1910	0.35	0/2569
43	H2	0.13	0/1535	0.34	0/2063
44	I2	0.14	0/1702	0.31	0/2272
45	J2	0.12	0/1385	0.32	0/1852
46	L2	0.15	0/1733	0.38	0/2316
47	M2	0.13	0/1158	0.33	0/1547
48	N2	0.16	0/1746	0.34	0/2338
49	O2	0.14	0/1662	0.33	0/2222
50	P2	0.15	0/1268	0.34	0/1700
51	Q2	0.15	0/1539	0.37	0/2054
52	R2	0.14	0/1524	0.35	0/2013
53	S2	0.15	0/1501	0.34	0/2012
54	T2	0.16	0/1326	0.38	0/1770
55	U2	0.13	0/823	0.40	0/1104
56	V2	0.14	0/1048	0.32	0/1402
57	W2	0.16	0/873	0.38	0/1158
58	X2	0.14	0/984	0.29	0/1323
59	Y2	0.15	0/1132	0.33	0/1504
60	Z2	0.13	0/1130	0.30	0/1507
61	a2	0.16	0/1191	0.36	0/1590
62	b2	0.14	0/861	0.36	0/1138
63	c2	0.12	0/771	0.26	0/1034
64	d2	0.15	0/903	0.33	0/1216
65	e2	0.14	0/1071	0.33	0/1429
66	f2	0.16	0/895	0.39	0/1198
67	g2	0.14	0/916	0.35	0/1220
68	h2	0.12	0/1021	0.32	0/1348
69	i2	0.12	0/841	0.32	0/1112
70	j2	0.15	0/720	0.36	0/952
71	k2	0.13	0/575	0.32	0/761
72	l2	0.14	0/459	0.37	0/608
73	m2	0.13	0/435	0.35	0/575
74	n2	0.17	0/240	0.41	0/305
75	o2	0.13	0/864	0.29	0/1140

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	p2	0.13	0/718	0.34	0/953
77	r2	0.15	0/1010	0.34	0/1354
78	s2	0.18	0/1530	0.41	0/2064
79	t2	0.17	0/1174	0.51	0/1582
80	54	0.14	0/86419	0.24	0/134760
81	74	0.13	0/2836	0.17	0/4421
82	84	0.13	0/3581	0.19	0/5577
83	XX	0.43	0/99	1.14	0/129
84	B	0.32	0/1680	0.86	1/2255 (0.0%)
85	23	0.74	5/1525 (0.3%)	1.10	13/2372 (0.5%)
85	33	0.74	5/1525 (0.3%)	1.10	13/2372 (0.5%)
All	All	0.16	11/234250 (0.0%)	0.32	29/343633 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
19	S1	0	1
25	Y1	0	1
37	B2	0	1
66	f2	0	1
84	B	0	3
All	All	0	7

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	33	35	U	O5'-C5'	18.54	1.70	1.42
85	23	35	U	O5'-C5'	18.48	1.70	1.42
85	23	35	U	C5'-C4'	10.65	1.67	1.51
85	33	35	U	C5'-C4'	10.61	1.67	1.51
85	33	35	U	C3'-O3'	8.94	1.55	1.42
85	23	35	U	C3'-O3'	8.92	1.55	1.42
85	23	35	U	P-O5'	7.53	1.71	1.59
85	33	35	U	P-O5'	7.52	1.71	1.59
34	h1	283	PRO	CA-C	-6.98	1.48	1.51
85	23	35	U	C4'-C3'	6.60	1.62	1.52
85	33	35	U	C4'-C3'	6.57	1.62	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	33	35	U	C2'-C3'-O3'	-22.90	79.35	113.70
85	23	35	U	C2'-C3'-O3'	-22.90	79.36	113.70
85	23	35	U	C4'-C3'-O3'	21.34	145.02	113.00
85	33	35	U	C4'-C3'-O3'	21.33	145.00	113.00
85	23	35	U	O5'-P-OP1	-20.35	46.94	108.00
85	33	35	U	O5'-P-OP1	-20.35	46.95	108.00
85	23	35	U	P-O5'-C5'	11.34	137.91	120.90
85	33	35	U	P-O5'-C5'	11.33	137.89	120.90
85	33	35	U	O5'-C5'-C4'	10.95	127.93	111.50
85	23	35	U	O5'-C5'-C4'	10.94	127.91	111.50
85	33	35	U	C5'-C4'-C3'	10.88	132.32	116.00
85	23	35	U	C5'-C4'-C3'	10.87	132.30	116.00
85	33	35	U	O5'-P-OP2	10.14	138.41	108.00
85	23	35	U	O5'-P-OP2	10.13	138.38	108.00
85	33	35	U	C3'-C2'-O2'	9.71	125.27	110.70
85	23	35	U	C3'-C2'-O2'	9.69	125.23	110.70
85	23	35	U	OP1-P-OP2	-8.01	95.57	119.60
85	33	35	U	OP1-P-OP2	-8.00	95.60	119.60
36	A2	15	VAL	N-CA-C	-7.64	106.45	113.71
84	B	123	ILE	N-CA-C	-7.32	106.76	113.71
85	23	38	A	C1'-C2'-O2'	-6.73	98.31	108.40
85	33	38	A	C1'-C2'-O2'	-6.70	98.35	108.40
85	33	18	G	C4'-C3'-O3'	-6.33	99.91	109.40
85	23	18	G	C4'-C3'-O3'	-6.29	99.96	109.40
85	33	18	G	O4'-C4'-C3'	-6.22	99.88	106.10
85	23	18	G	O4'-C4'-C3'	-6.21	99.89	106.10
85	33	57	A	C4'-C3'-O3'	-5.99	104.01	113.00
85	23	57	A	C4'-C3'-O3'	-5.98	104.03	113.00
34	h1	283	PRO	O-C-N	-5.30	118.87	121.31

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
84	B	128	LEU	Peptide
84	B	20	GLY	Peptide
84	B	60	ARG	Peptide
37	B2	258	HIS	Peptide
19	S1	108	LEU	Peptide
25	Y1	61	GLN	Peptide
66	f2	106	TYR	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	A1	36229	0	18306	321	0
2	B1	1710	0	1708	29	0
3	C1	1729	0	1803	32	0
4	D1	1716	0	1806	27	0
5	E1	1768	0	1866	37	0
6	F1	2076	0	2177	38	0
7	G1	1471	0	1522	26	0
8	H1	1923	0	2089	67	0
9	I1	1488	0	1582	21	0
10	J1	1686	0	1772	37	0
11	K1	1525	0	1640	20	0
12	L1	810	0	836	19	0
13	M1	1175	0	1249	14	0
14	N1	908	0	939	48	0
15	O1	1202	0	1289	13	0
16	P1	1016	0	1039	22	0
17	Q1	1058	0	1104	27	0
18	R1	1128	0	1195	24	0
19	S1	1068	0	1121	22	0
20	T1	1190	0	1249	32	0
21	U1	1097	0	1132	30	0
22	V1	795	0	862	21	0
23	W1	636	0	637	12	0
24	X1	1034	0	1080	24	0
25	Y1	1098	0	1167	22	0
26	Z1	1011	0	1083	23	0
27	a1	598	0	654	46	0
28	b1	814	0	864	18	0
29	c1	651	0	672	11	0
30	d1	488	0	514	7	0
31	e1	459	0	448	5	0
32	f1	457	0	502	8	0
33	g1	555	0	565	16	0
34	h1	2436	0	2393	65	0
35	i1	220	0	111	6	0
36	A2	1898	0	1993	36	0
37	B2	3172	0	3310	39	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	C2	2883	0	3053	37	0
39	D2	2391	0	2424	43	0
40	E2	1729	0	1887	40	0
41	F2	1875	0	1995	26	0
42	G2	1879	0	2027	44	0
43	H2	1516	0	1597	23	0
44	I2	1664	0	1712	32	0
45	J2	1362	0	1399	15	0
46	L2	1702	0	1820	31	0
47	M2	1137	0	1211	20	0
48	N2	1701	0	1749	31	0
49	O2	1630	0	1778	32	0
50	P2	1242	0	1274	14	0
51	Q2	1515	0	1634	33	0
52	R2	1508	0	1664	21	0
53	S2	1462	0	1508	28	0
54	T2	1298	0	1366	27	0
55	U2	809	0	833	19	0
56	V2	1034	0	1097	18	0
57	W2	860	0	903	19	0
58	X2	967	0	1040	10	0
59	Y2	1115	0	1205	18	0
60	Z2	1107	0	1182	14	0
61	a2	1162	0	1209	20	0
62	b2	848	0	920	12	0
63	c2	761	0	794	10	0
64	d2	888	0	930	10	0
65	e2	1053	0	1147	15	0
66	f2	876	0	912	16	0
67	g2	906	0	999	8	0
68	h2	1013	0	1147	16	0
69	i2	830	0	916	9	0
70	j2	705	0	737	12	0
71	k2	569	0	637	15	0
72	l2	447	0	480	5	0
73	m2	429	0	465	4	0
74	n2	239	0	289	2	0
75	o2	851	0	920	15	0
76	p2	708	0	756	14	0
77	r2	994	0	1051	14	0
78	s2	1507	0	1564	54	0
79	t2	1160	0	1218	56	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
80	54	77264	0	39043	746	0
81	74	2538	0	1286	18	0
82	84	3208	0	1629	33	0
83	XX	100	0	86	8	0
84	B	1654	0	1760	50	0
85	23	1636	0	848	54	0
85	33	1636	0	847	86	0
86	54	185	0	0	0	0
86	74	6	0	0	0	0
86	84	5	0	0	0	0
86	A1	70	0	0	0	0
86	A2	1	0	0	0	0
86	B2	1	0	0	0	0
86	I2	1	0	0	0	0
86	P2	1	0	0	0	0
86	V2	1	0	0	0	0
86	a2	1	0	0	0	0
86	g2	1	0	0	0	0
86	j2	2	0	0	0	0
87	b1	1	0	0	0	0
87	e1	1	0	0	0	0
87	g1	1	0	0	0	0
87	g2	1	0	0	0	0
87	j2	1	0	0	0	0
87	m2	1	0	0	0	0
87	o2	1	0	0	0	0
87	p2	1	0	0	0	0
88	54	20	0	38	2	0
All	All	218966	0	163265	2540	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 7.

All (2540) 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)
27:a1:67:LEU:H	85:33:34:70U:C9	1.06	1.60
27:a1:67:LEU:N	85:33:34:70U:H91	1.16	1.41
85:33:35:U:C5'	85:33:35:U:O5'	1.70	1.40
85:23:35:U:O5'	85:23:35:U:C5'	1.70	1.38
80:54:4041:C:OP1	84:B:105:LYS:CE	1.73	1.34

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a1:66:LYS:HE2	85:33:34:70U:OP1	1.34	1.25
27:a1:66:LYS:HG3	85:33:34:70U:OP1	1.36	1.23
80:54:4041:C:OP1	84:B:105:LYS:HE2	1.27	1.18
80:54:3958:G:C8	85:33:20:H2U:OP1	2.03	1.11
27:a1:66:LYS:CG	85:33:34:70U:OP1	1.98	1.10
27:a1:66:LYS:CE	85:33:34:70U:OP1	2.00	1.10
27:a1:67:LEU:CA	85:33:34:70U:H91	1.84	1.06
84:B:44:GLN:OE1	85:33:62:C:C4'	2.08	1.02
84:B:161:LYS:HG3	85:33:54:2MU:H6'1	1.42	1.01
18:R1:146:ARG:NH2	85:23:33:U:OP2	1.94	1.01
27:a1:67:LEU:H	85:33:34:70U:H92	1.24	0.99
1:A1:1473:G:H2'	1:A1:1475:G:H22	1.28	0.98
1:A1:1091:C:HO2'	24:X1:2:VAL:N	1.60	0.98
27:a1:66:LYS:CD	85:33:34:70U:OP1	2.13	0.96
80:54:3974:G:H5'	84:B:28:PHE:CZ	2.01	0.96
84:B:44:GLN:OE1	85:33:62:C:H5'	1.66	0.95
85:33:33:U:O3'	85:33:35:U:P	2.24	0.95
85:23:33:U:C3'	85:23:35:U:P	2.54	0.95
85:23:33:U:O3'	85:23:35:U:P	2.24	0.95
85:33:33:U:C3'	85:33:35:U:P	2.54	0.95
78:s2:57:LYS:HB3	80:54:2020:U:H5'	1.47	0.94
84:B:53:VAL:O	84:B:154:THR:HA	1.66	0.94
35:i1:20:A:N6	85:23:35:U:O4	2.00	0.93
85:33:35:U:C5'	85:33:35:U:OP1	2.17	0.93
85:23:35:U:C5'	85:23:35:U:OP1	2.16	0.92
27:a1:67:LEU:N	85:33:34:70U:C9	1.90	0.92
27:a1:65:TYR:HA	85:33:34:70U:H6	1.53	0.91
80:54:2638:G:N2	80:54:2697:A:N1	2.20	0.90
27:a1:65:TYR:HA	85:33:34:70U:C6	1.92	0.89
84:B:44:GLN:OE1	85:33:62:C:C5'	2.20	0.89
80:54:4093:G:H1	80:54:4115:G:H22	1.23	0.86
14:N1:66:GLU:HA	14:N1:69:CYS:HB3	1.56	0.85
35:i1:21:A:N6	85:23:34:70U:O4	2.09	0.85
1:A1:1858:G:OP2	16:P1:146:ARG:NH2	2.10	0.85
85:23:33:U:H3'	85:23:35:U:P	2.16	0.85
85:33:33:U:H3'	85:33:35:U:P	2.16	0.85
85:23:34:70U:P	85:23:35:U:P	2.75	0.85
66:f2:58:VAL:O	80:54:4944:C:N4	2.10	0.84
85:33:34:70U:P	85:33:35:U:P	2.75	0.84
1:A1:1701:C:H5	85:23:34:70U:H93	1.42	0.84
46:L2:58:ILE:H	46:L2:113:ASN:HD21	1.24	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:T2:45:MET:H	54:T2:95:HIS:HD2	1.25	0.83
84:B:44:GLN:CD	85:33:62:C:H4'	2.03	0.83
80:54:4041:C:OP1	84:B:105:LYS:HE3	1.77	0.82
1:A1:1701:C:C5	85:23:34:70U:H93	2.15	0.82
80:54:4949:G:H4'	80:54:4950:U:H5'	1.60	0.81
27:a1:65:TYR:C	85:33:34:70U:H5''	2.04	0.81
2:B1:6:ASP:HA	2:B1:9:GLN:HG2	1.63	0.81
80:54:3751:G:H21	80:54:3775:A:H8	1.27	0.80
51:Q2:67:ILE:HD12	51:Q2:96:PRO:HD2	1.62	0.80
1:A1:1292:C:N3	33:g1:138:ARG:NH1	2.30	0.80
80:54:989:U:H3	80:54:1065:G:H1	1.29	0.80
77:r2:98:ARG:NH2	80:54:2262:G:OP2	2.15	0.80
84:B:161:LYS:CG	85:33:54:2MU:H6'1	2.13	0.79
27:a1:111:ARG:HE	85:33:34:70U:C5'	1.95	0.79
85:33:33:U:H2'	85:33:35:U:O5'	1.83	0.78
34:h1:107:ASP:HB2	34:h1:125:ARG:HG3	1.66	0.78
1:A1:1488:C:O2'	1:A1:1490:G:OP2	2.01	0.78
35:i1:21:A:H61	85:23:34:70U:C4	1.96	0.78
40:E2:185:ASN:ND2	40:E2:274:LEU:O	2.17	0.78
42:G2:314:LEU:HA	42:G2:317:LYS:HD3	1.66	0.78
85:23:33:U:H2'	85:23:35:U:O5'	1.83	0.77
46:L2:56:ARG:O	46:L2:116:ARG:NH2	2.17	0.77
46:L2:116:ARG:NH1	46:L2:155:MET:O	2.17	0.77
80:54:3641:U:OP2	80:54:3646:A:N6	2.15	0.77
8:H1:7:PHE:HB2	8:H1:124:LEU:HD23	1.65	0.77
85:23:54:2MU:O5'	85:23:54:2MU:H6	1.85	0.77
80:54:1967:A:N6	80:54:2020:U:O4	2.18	0.77
85:33:54:2MU:O5'	85:33:54:2MU:H6	1.85	0.77
80:54:1199:G:H2'	80:54:1200:G:H8	1.49	0.76
4:D1:196:ILE:HB	4:D1:223:TYR:HB2	1.65	0.76
50:P2:23:ARG:NH1	50:P2:125:MET:SD	2.58	0.76
61:a2:76:ASP:HB3	61:a2:115:GLY:HA3	1.67	0.76
27:a1:67:LEU:H	85:33:34:70U:H91	0.61	0.76
38:C2:78:ARG:HB3	38:C2:88:GLY:HA2	1.67	0.75
1:A1:1396:A:O2'	1:A1:1398:G:N7	2.18	0.75
1:A1:984:C:O2'	16:P1:138:ASP:OD2	2.04	0.75
6:F1:130:PHE:HB2	6:F1:138:HIS:HB2	1.69	0.74
27:a1:66:LYS:N	85:33:34:70U:H92	2.02	0.74
77:r2:107:ARG:NH1	80:54:2263:A:OP1	2.20	0.74
16:P1:94:HIS:HD2	16:P1:128:ARG:H	1.35	0.74
34:h1:256:ILE:HB	34:h1:270:LEU:HB2	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:925:G:H1	1:A1:1017:U:H3	1.33	0.74
62:b2:32:LEU:HD12	80:54:1464:C:H5'	1.69	0.74
1:A1:928:G:H1	1:A1:1013:U:H3	1.35	0.74
28:b1:44:ILE:HD12	28:b1:65:PRO:HG2	1.69	0.74
59:Y2:74:TYR:OH	82:84:75:G:OP2	2.06	0.74
80:54:3692:A:H62	80:54:3823:G:H21	1.35	0.74
3:C1:150:ILE:HD13	19:S1:129:LYS:HB2	1.69	0.74
36:A2:234:LYS:HG2	36:A2:238:ILE:HD12	1.68	0.74
46:L2:39:ARG:NH2	80:54:1362:G:OP1	2.21	0.74
78:s2:59:THR:HA	78:s2:62:ARG:HD2	1.70	0.73
9:I1:160:LYS:HE2	9:I1:191:GLU:HA	1.68	0.73
84:B:44:GLN:OE1	85:33:62:C:O4'	2.05	0.73
1:A1:1475:G:OP2	1:A1:1475:G:N2	2.21	0.73
38:C2:323:ARG:HH11	80:54:976:G:H22	1.35	0.73
80:54:4925:U:H4'	80:54:4926:C:H5'	1.70	0.73
80:54:115:C:O2'	80:54:276:C:OP1	2.06	0.73
80:54:1073:G:H22	80:54:1238:A:H2	1.36	0.73
1:A1:952:G:H21	16:P1:52:THR:HG21	1.54	0.73
80:54:4055:U:O2'	84:B:162:VAL:CG2	2.38	0.72
38:C2:100:ARG:NH2	80:54:1521:C:OP1	2.23	0.72
80:54:4635:A:H2	80:54:4663:G:H21	1.35	0.72
80:54:2638:G:H1	80:54:2697:A:H61	1.37	0.72
24:X1:102:ILE:H	24:X1:113:HIS:HD2	1.37	0.72
80:54:2758:G:O2'	80:54:2765:A:N3	2.23	0.72
5:E1:135:GLU:HG3	5:E1:153:VAL:HG22	1.70	0.72
1:A1:561:A:H5'	11:K1:171:GLY:HA3	1.69	0.72
55:U2:111:GLU:OE2	55:U2:113:ARG:NH1	2.22	0.71
6:F1:104:ASP:HB3	6:F1:110:ALA:HB2	1.71	0.71
18:R1:19:ALA:HB2	18:R1:75:GLY:HA3	1.71	0.71
80:54:1435:G:O2'	80:54:2105:A:N1	2.23	0.71
83:XX:1010:LYS:HG2	83:XX:1011:LYS:H	1.55	0.71
1:A1:581:U:OP1	11:K1:133:ARG:NH2	2.23	0.71
44:I2:14:ASN:O	44:I2:128:ARG:NH2	2.19	0.71
80:54:980:U:H3	80:54:1275:G:H1	1.37	0.71
80:54:4872:G:H4'	80:54:4873:G:H5'	1.73	0.71
43:H2:27:VAL:HG11	43:H2:80:MET:HB3	1.71	0.71
51:Q2:104:ARG:NH2	80:54:1353:G:N7	2.38	0.71
76:p2:4:ARG:NH1	80:54:1554:A:OP2	2.24	0.71
12:L1:21:MET:HG2	12:L1:49:MET:HE3	1.72	0.71
14:N1:121:LYS:HA	14:N1:124:ILE:HD12	1.72	0.71
78:s2:37:SER:HB2	80:54:1999:A:H61	1.53	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:3974:G:H5'	84:B:28:PHE:HZ	1.51	0.71
79:t2:32:ILE:HD11	79:t2:42:VAL:HG21	1.71	0.70
80:54:4041:C:OP1	84:B:105:LYS:NZ	2.23	0.70
6:F1:153:LEU:O	6:F1:174:LYS:NZ	2.21	0.70
14:N1:54:SER:H	14:N1:80:ASP:HA	1.56	0.70
80:54:5047:C:O2'	80:54:5050:C:OP2	2.10	0.70
21:U1:116:ASP:HB2	21:U1:122:LYS:HB2	1.73	0.70
49:O2:60:LYS:HE3	80:54:2046:G:H5'	1.72	0.70
79:t2:109:ILE:HD11	79:t2:143:VAL:HG21	1.73	0.70
77:r2:119:ARG:HH22	80:54:456:C:H5''	1.56	0.70
55:U2:28:PRO:HB3	55:U2:100:LEU:HD21	1.73	0.70
20:T1:36:VAL:HG21	20:T1:71:MET:HE3	1.74	0.70
9:I1:34:SER:O	9:I1:37:LYS:NZ	2.25	0.70
34:h1:124:SER:OG	34:h1:126:ASP:OD1	2.08	0.69
55:U2:101:ARG:NH2	80:54:2702:C:OP1	2.24	0.69
36:A2:215:ASN:ND2	80:54:4546:A:N7	2.39	0.69
2:B1:80:ARG:NH2	2:B1:165:ASN:O	2.25	0.69
42:G2:90:LYS:NZ	80:54:4126:C:OP1	2.25	0.69
13:M1:104:LYS:O	25:Y1:11:ARG:NH2	2.25	0.69
19:S1:100:PRO:HG2	19:S1:122:PRO:HD3	1.74	0.69
39:D2:120:GLU:O	39:D2:248:ARG:NH2	2.25	0.69
63:c2:36:LYS:NZ	80:54:2657:G:OP2	2.26	0.69
78:s2:106:LYS:HB3	78:s2:184:SER:HB2	1.74	0.69
75:o2:99:ARG:HE	75:o2:102:GLN:HG3	1.58	0.69
39:D2:224:SER:HB3	81:74:49:A:H5''	1.75	0.69
80:54:2553:A:H2	80:54:2765:A:H62	1.39	0.69
1:A1:540:U:O2'	1:A1:543:C:N4	2.26	0.69
1:A1:1617:G:N1	1:A1:1620:A:OP2	2.25	0.69
27:a1:66:LYS:HG3	85:33:34:70U:P	2.33	0.69
40:E2:159:ARG:NH1	80:54:4940:C:OP1	2.26	0.69
80:54:4055:U:O2'	84:B:162:VAL:HG23	1.92	0.69
72:l2:2:SER:O	72:l2:5:LYS:NZ	2.25	0.68
80:54:1171:G:H1	80:54:1190:C:H42	1.41	0.68
14:N1:46:GLN:HE22	14:N1:112:LYS:HD3	1.58	0.68
34:h1:64:HIS:CD2	34:h1:65:PHE:H	2.11	0.68
80:54:483:G:H3'	80:54:484:U:H2'	1.75	0.68
84:B:44:GLN:CD	85:33:62:C:C4'	2.63	0.68
45:J2:129:ASP:OD1	80:54:4250:G:O2'	2.10	0.68
55:U2:55:ASN:OD1	55:U2:58:GLY:N	2.27	0.68
64:d2:38:PHE:HB3	64:d2:78:ARG:HG2	1.75	0.68
34:h1:17:TRP:H	34:h1:36:ARG:HB2	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h1:107:ASP:OD2	34:h1:125:ARG:NH1	2.27	0.68
49:O2:85:ARG:HG3	49:O2:99:LEU:HD11	1.75	0.68
11:K1:121:LYS:H	11:K1:125:HIS:HD2	1.42	0.68
80:54:481(A):C:H4'	80:54:483:G:H4'	1.76	0.68
72:l2:41:ARG:NH1	80:54:2431:A:OP1	2.27	0.68
1:A1:67:C:H41	8:H1:163:ASN:HA	1.59	0.67
1:A1:1455:A:OP1	19:S1:5:ARG:NH1	2.27	0.67
59:Y2:1:MET:HE2	80:54:1368:A:H1'	1.76	0.67
5:E1:105:LEU:HB2	5:E1:122:VAL:HG21	1.75	0.67
78:s2:13:TYR:OH	78:s2:55:MET:O	2.12	0.67
80:54:2579:G:N2	80:54:2582:A:OP2	2.24	0.67
53:S2:9:GLU:OE1	53:S2:31:ARG:NH2	2.27	0.67
59:Y2:54:GLU:HB2	59:Y2:108:ARG:HB3	1.77	0.67
80:54:1405:C:H2'	80:54:1406:G:C8	2.29	0.67
80:54:4348:A:O2'	80:54:4350:C:OP2	2.13	0.67
1:A1:64:A:H2	1:A1:83:A:H62	1.41	0.67
18:R1:34:VAL:HG21	18:R1:84:ILE:HD12	1.77	0.67
34:h1:206:LEU:HA	34:h1:220:ASP:HA	1.77	0.67
42:G2:96:GLN:O	80:54:4124:G:N2	2.28	0.67
80:54:969:C:H42	80:54:2095:A:H61	1.41	0.67
1:A1:532:C:H2'	1:A1:533:A:C8	2.29	0.67
7:G1:35:LEU:HD21	7:G1:146:ARG:HD3	1.75	0.67
22:V1:78:ASP:OD2	31:e1:44:ARG:NH1	2.27	0.67
1:A1:1616:U:OP2	17:Q1:43:ARG:NH2	2.27	0.67
6:F1:45:ILE:HG13	6:F1:61:VAL:HG21	1.76	0.67
51:Q2:178:ARG:H	61:a2:51:GLY:HA2	1.58	0.67
39:D2:217:ASP:HA	39:D2:220:LYS:HB2	1.76	0.67
54:T2:130:ARG:NH1	80:54:1802:A:N3	2.43	0.67
80:54:1976:G:H22	80:54:1991:A:H1'	1.59	0.67
79:t2:32:ILE:HA	79:t2:35:LEU:HD23	1.76	0.67
37:B2:337:VAL:HG21	37:B2:345:LEU:HD21	1.76	0.67
80:54:2786:C:H5''	80:54:2787:A:H5'	1.75	0.67
77:r2:53:PRO:HD3	77:r2:117:ILE:HD12	1.76	0.66
80:54:3960:A:H2'	80:54:4048:A:H61	1.60	0.66
8:H1:70:HIS:HA	8:H1:98:ARG:HH12	1.59	0.66
1:A1:398:A:H5''	1:A1:399:C:H3'	1.77	0.66
1:A1:1138:C:OP1	2:B1:155:ARG:NH2	2.29	0.66
13:M1:153:LYS:HB2	15:O1:133:ARG:HH22	1.60	0.66
58:X2:50:LYS:NZ	80:54:2474:G:O2'	2.27	0.66
80:54:4272:G:OP2	80:54:4272:G:N2	2.22	0.66
12:L1:72:THR:HG22	12:L1:74:GLU:H	1.59	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:D2:33:ARG:NH2	81:74:7:G:OP1	2.28	0.66
1:A1:583:A:OP1	11:K1:162:ARG:NH2	2.28	0.66
1:A1:1161:U:O4	25:Y1:3:LYS:NZ	2.22	0.66
38:C2:323:ARG:NH1	80:54:1279:A:N3	2.44	0.66
1:A1:453:C:O2'	8:H1:92:ARG:O	2.13	0.66
65:e2:128:ARG:NH2	80:54:2306:G:OP1	2.29	0.66
80:54:3904:G:O2'	80:54:3905:A:OP1	2.13	0.66
1:A1:1553:C:O2'	1:A1:1554:C:O4'	2.13	0.65
17:Q1:29:SER:H	17:Q1:32:GLN:HE21	1.44	0.65
43:H2:23:ARG:HE	43:H2:39:ASN:HA	1.61	0.65
21:U1:60:THR:HG23	21:U1:75:MET:HE2	1.78	0.65
7:G1:102:LEU:HD11	27:a1:100:VAL:HG21	1.78	0.65
57:W2:96:GLN:HE21	57:W2:100:VAL:HG12	1.60	0.65
78:s2:27:CYS:HB2	78:s2:193:PHE:HB3	1.78	0.65
14:N1:69:CYS:SG	14:N1:70:ALA:N	2.69	0.65
34:h1:39:THR:HG22	34:h1:60:ARG:HG2	1.78	0.65
59:Y2:50:ARG:NH2	82:84:85:U:O4	2.30	0.65
73:m2:74:TYR:O	80:54:4472:G:O2'	2.15	0.65
80:54:976:G:H1	80:54:1279:A:H2	1.45	0.65
80:54:1076:C:O2	80:54:1235:G:N2	2.30	0.65
53:S2:163:HIS:HD2	53:S2:166:ARG:HE	1.45	0.65
37:B2:35:ASP:OD2	37:B2:193:LYS:NZ	2.27	0.65
56:V2:15:ARG:NH2	80:54:4670:C:O2'	2.30	0.65
80:54:245:C:O2'	80:54:246:G:OP2	2.15	0.65
23:W1:60:ARG:HA	23:W1:65:SER:HB2	1.77	0.65
1:A1:165:G:N2	1:A1:165:G:OP2	2.26	0.65
1:A1:1394:G:H21	1:A1:1475:G:H1'	1.62	0.64
20:T1:33:ILE:HD12	20:T1:71:MET:HE1	1.78	0.64
2:B1:3:GLY:HA3	23:W1:80:SER:HB3	1.79	0.64
7:G1:71:ARG:NH1	7:G1:148:ASN:OD1	2.29	0.64
26:Z1:20:ARG:NH1	26:Z1:22:GLN:OE1	2.28	0.64
52:R2:105:LEU:HD12	52:R2:135:LYS:HE2	1.79	0.64
68:h2:12:LYS:NZ	68:h2:20:GLN:OE1	2.29	0.64
80:54:3968:U:O2'	80:54:3969:G:OP1	2.13	0.64
80:54:3958:G:N2	80:54:4046:A:OP1	2.30	0.64
1:A1:190:G:O2'	1:A1:209:A:N6	2.30	0.64
20:T1:35:GLY:O	20:T1:97:GLN:NE2	2.30	0.64
66:f2:7:CYS:HB2	66:f2:103:VAL:HB	1.80	0.64
1:A1:507:G:OP2	26:Z1:104:ARG:NH2	2.30	0.64
56:V2:15:ARG:HB2	80:54:4618:G:H5''	1.79	0.64
80:54:2647:A:H62	80:54:2686:G:H8	1.44	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:943:U:O2'	16:P1:135:ILE:O	2.15	0.64
66:f2:43:LEU:O	66:f2:109:ARG:NH1	2.30	0.64
80:54:1886:G:HO2'	80:54:1909:G:HO2'	1.46	0.64
80:54:2465:C:H1'	80:54:3672:G:H22	1.62	0.64
85:23:34:70U:P	85:23:35:U:OP2	2.56	0.64
14:N1:54:SER:OG	14:N1:78:LYS:NZ	2.31	0.64
45:J2:154:LYS:NZ	81:74:55:A:OP1	2.25	0.64
80:54:308:G:OP2	80:54:308:G:N2	2.27	0.64
1:A1:1285:G:OP2	14:N1:35:ILE:N	2.31	0.64
9:I1:69:LEU:HD22	9:I1:96:ALA:HB2	1.79	0.64
17:Q1:18:ARG:HD2	20:T1:88:LYS:HG2	1.80	0.64
42:G2:198:THR:O	42:G2:202:ASN:ND2	2.31	0.64
46:L2:87:HIS:HB3	46:L2:90:VAL:HG22	1.78	0.63
69:i2:30:ARG:NH1	80:54:327:U:O2'	2.31	0.63
43:H2:107:GLU:OE1	43:H2:127:ARG:NH2	2.31	0.63
71:k2:33:LYS:NZ	80:54:2695:A:OP2	2.27	0.63
80:54:3961:G:O2'	80:54:4043:G:N2	2.31	0.63
48:N2:68:ARG:NH2	80:54:303:C:OP2	2.32	0.63
78:s2:62:ARG:NH2	78:s2:82:ILE:O	2.30	0.63
1:A1:994:C:N4	28:b1:14:GLY:O	2.31	0.63
25:Y1:52:LEU:HD11	25:Y1:73:GLN:HB2	1.78	0.63
85:23:34:70U:C3'	85:23:34:70U:C6	2.76	0.63
85:33:34:70U:P	85:33:35:U:OP2	2.56	0.63
49:O2:128:ARG:NH2	53:S2:162:GLN:OE1	2.31	0.63
55:U2:28:PRO:HB2	55:U2:34:MET:HG2	1.79	0.63
65:e2:103:VAL:O	65:e2:108:ARG:NH2	2.30	0.63
39:D2:267:ASN:HD21	81:74:2:U:H5'	1.63	0.63
1:A1:1568:C:OP1	21:U1:96:SER:OG	2.17	0.63
27:a1:68:ILE:HB	27:a1:109:TYR:HB2	1.79	0.63
55:U2:28:PRO:HG3	55:U2:112:LEU:HD12	1.79	0.63
80:54:449:C:H4'	80:54:450:G:OP2	1.98	0.63
80:54:1481:C:O2'	80:54:1482:G:N3	2.25	0.63
37:B2:108:GLU:OE2	37:B2:138:GLN:NE2	2.31	0.63
80:54:2545:U:H3'	80:54:2546:G:H4'	1.81	0.63
44:I2:59:GLN:HB3	44:I2:126:VAL:HG11	1.80	0.62
45:J2:46:GLN:NE2	45:J2:72:CYS:SG	2.71	0.62
46:L2:59:VAL:HB	80:54:74:G:H5'	1.81	0.62
66:f2:69:VAL:HG21	80:54:4944:C:H1'	1.81	0.62
80:54:2482:C:O2	80:54:2496:G:N2	2.28	0.62
1:A1:1137:U:O2'	1:A1:1138:C:OP1	2.14	0.62
20:T1:48:ALA:HB2	20:T1:70:ILE:HD12	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:k2:67:LYS:NZ	71:k2:68:GLU:O	2.32	0.62
8:H1:5:ILE:HD12	8:H1:16:ILE:HD13	1.81	0.62
41:F2:104:VAL:HG13	41:F2:135:VAL:HG12	1.82	0.62
80:54:1279:A:O2'	80:54:1281:G:N7	2.30	0.62
25:Y1:93:PHE:O	25:Y1:140:ARG:NH1	2.33	0.62
63:c2:38:ILE:HG21	63:c2:63:TYR:HB3	1.81	0.62
46:L2:80:GLU:HG3	46:L2:110:LEU:HD12	1.81	0.62
80:54:178:C:O2	80:54:258:G:N2	2.30	0.62
5:E1:74:GLN:HB3	5:E1:84:VAL:HG11	1.82	0.62
29:c1:62:VAL:O	29:c1:74:THR:OG1	2.16	0.62
36:A2:101:VAL:HG22	36:A2:165:VAL:HG22	1.81	0.62
84:B:68:LEU:O	84:B:112:ALA:HA	2.00	0.62
72:l2:2:SER:N	80:54:2406:G:N7	2.48	0.62
39:D2:52:ILE:HD13	81:74:6:C:H4'	1.81	0.62
80:54:658:C:N4	80:54:659:G:O6	2.33	0.62
1:A1:1566:G:N7	21:U1:101:ARG:NH2	2.48	0.62
4:D1:121:ARG:HH12	4:D1:123:ARG:HH21	1.47	0.62
14:N1:25:ALA:HB3	14:N1:31:LEU:HD23	1.81	0.62
75:o2:39:ARG:NH1	80:54:295:A:OP2	2.32	0.62
79:t2:146:ARG:HB3	79:t2:148:PRO:HD2	1.81	0.62
1:A1:126:G:OP2	8:H1:198:ARG:NH2	2.31	0.62
18:R1:116:ASP:OD1	18:R1:118:THR:OG1	2.17	0.62
20:T1:38:ARG:HD2	21:U1:45:LEU:HD11	1.81	0.62
21:U1:104:LEU:HD13	21:U1:121:ARG:HD3	1.82	0.62
22:V1:104:ILE:HG13	22:V1:105:SER:H	1.65	0.62
78:s2:15:LEU:HD23	78:s2:18:ILE:HD13	1.80	0.62
80:54:2378:G:N2	80:54:2381:A:OP2	2.33	0.62
80:54:3949:A:C4	80:54:4065:G:H1'	2.34	0.62
1:A1:1605:G:OP1	21:U1:84:ARG:NH1	2.33	0.61
42:G2:215:ASP:HB2	80:54:150:U:H3	1.65	0.61
58:X2:64:SER:HB3	68:h2:69:LEU:HD13	1.82	0.61
65:e2:107:ASN:ND2	80:54:2303:C:OP1	2.33	0.61
1:A1:919:A:OP2	15:O1:64:ARG:NH2	2.32	0.61
1:A1:1248:U:C2	85:23:34:70U:H4'	2.35	0.61
15:O1:99:ARG:NH2	15:O1:119:GLU:OE2	2.30	0.61
43:H2:42:ASN:HD21	49:O2:131:PRO:HB2	1.65	0.61
64:d2:19:GLU:OE2	64:d2:92:ARG:NH2	2.33	0.61
65:e2:91:CYS:HB3	65:e2:95:TYR:HD2	1.65	0.61
27:a1:67:LEU:CB	85:33:34:70U:H91	2.28	0.61
79:t2:15:LEU:HD13	79:t2:46:ILE:HG12	1.81	0.61
85:33:34:70U:C6	85:33:34:70U:C3'	2.76	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:L2:36:ARG:NH2	80:54:1364:U:OP2	2.28	0.61
46:L2:47:ALA:HB3	46:L2:48:PRO:HD3	1.83	0.61
49:O2:27:VAL:O	49:O2:101:ARG:NH1	2.34	0.61
1:A1:454:U:H4'	8:H1:76:LEU:HD21	1.82	0.61
1:A1:560:A:OP2	11:K1:177:ASN:ND2	2.33	0.61
1:A1:1299:A:OP2	17:Q1:59:ARG:NH2	2.34	0.61
2:B1:77:ILE:HG12	2:B1:99:ILE:HB	1.81	0.61
16:P1:113:GLN:NE2	28:b1:44:ILE:O	2.32	0.61
24:X1:6:VAL:HG12	24:X1:34:ILE:HD11	1.83	0.61
34:h1:87:LEU:HB2	34:h1:101:PHE:HB2	1.82	0.61
39:D2:256:LYS:HD2	81:74:117:G:H5'	1.81	0.61
80:54:2547:G:N2	80:54:2772:C:O2	2.17	0.61
80:54:3811:G:O2'	80:54:3814:U:OP2	2.18	0.61
80:54:2495:U:H2'	80:54:2496:G:H8	1.66	0.61
80:54:4138:C:N3	80:54:4146:G:N1	2.49	0.61
6:F1:166:THR:HG22	6:F1:168:LYS:HG2	1.83	0.61
20:T1:5:ILE:N	27:a1:50:PHE:O	2.23	0.61
44:I2:162:ARG:NH1	80:54:2033:A:OP1	2.32	0.61
69:i2:74:LYS:HE2	69:i2:80:HIS:HB2	1.83	0.61
80:54:3961:G:N2	80:54:3965:A:OP2	2.34	0.61
1:A1:146:G:O2'	1:A1:147:A:O5'	2.18	0.61
1:A1:1298:G:O2'	1:A1:1299:A:O5'	2.18	0.61
1:A1:1314:U:O2'	12:L1:8:ARG:NH2	2.34	0.61
1:A1:1623:A:H5''	20:T1:133:GLY:HA3	1.83	0.61
44:I2:103:LEU:HD23	44:I2:112:GLN:HE21	1.66	0.61
68:h2:86:LYS:NZ	82:84:38:U:O2'	2.34	0.61
82:84:126:C:O2'	82:84:127:U:O5'	2.18	0.61
14:N1:51:VAL:HG22	14:N1:77:ILE:HD13	1.82	0.61
36:A2:200:ARG:NH2	36:A2:217:GLN:OE1	2.33	0.61
46:L2:188:ASN:ND2	80:54:1482:G:O6	2.34	0.61
49:O2:9:LEU:HD23	49:O2:118:MET:HB2	1.83	0.61
78:s2:41:GLN:NE2	80:54:1996:C:O2	2.34	0.61
80:54:3967:G:O6	80:54:4054:C:N4	2.34	0.61
1:A1:1441:U:O2	1:A1:1443:C:N4	2.33	0.60
10:J1:76:THR:HG22	10:J1:77:ARG:H	1.65	0.60
39:D2:50:ARG:NH1	39:D2:72:ASP:OD2	2.29	0.60
59:Y2:1:MET:HE3	59:Y2:2:LYS:H	1.67	0.60
1:A1:788:G:H2'	1:A1:789:G:H8	1.65	0.60
40:E2:144:ARG:NH1	40:E2:194:GLN:O	2.26	0.60
1:A1:1331:C:O2	1:A1:1489:A:O2'	2.16	0.60
36:A2:200:ARG:NH1	80:54:3651:A:OP2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S2:23:ARG:NH1	80:54:1199:G:O3'	2.34	0.60
61:a2:72:THR:HG22	61:a2:110:LYS:HB3	1.83	0.60
2:B1:76:VAL:HG12	2:B1:123:VAL:HB	1.83	0.60
47:M2:11:ARG:NH2	47:M2:58:THR:O	2.35	0.60
69:i2:63:VAL:HG23	69:i2:65:LYS:HG3	1.83	0.60
1:A1:1259:A:N6	1:A1:1519:U:OP1	2.21	0.60
1:A1:1701:C:H5	85:23:34:70U:C9	2.13	0.60
3:C1:106:THR:OG1	3:C1:108:ASP:OD1	2.11	0.60
38:C2:326:LEU:O	41:F2:46:ARG:NH2	2.35	0.60
49:O2:166:ILE:HG12	49:O2:169:ARG:HH12	1.66	0.60
1:A1:940:U:H3	1:A1:1002:U:H3	1.50	0.60
41:F2:49:ILE:HD12	41:F2:185:CYS:HB3	1.82	0.60
41:F2:150:ASN:ND2	80:54:943:A:N7	2.49	0.60
45:J2:95:ARG:NH2	45:J2:176:PRO:O	2.34	0.60
46:L2:118:LYS:NZ	80:54:520:U:OP1	2.34	0.60
2:B1:37:TYR:OH	2:B1:57:LYS:NZ	2.34	0.60
34:h1:246:TYR:CE2	34:h1:261:LEU:HB2	2.36	0.60
39:D2:208:MET:HB2	39:D2:233:PRO:HG3	1.84	0.60
79:t2:90:ARG:HD3	79:t2:90:ARG:H	1.66	0.60
4:D1:81:ILE:HG21	4:D1:88:ILE:HD11	1.83	0.60
80:54:3958:G:H8	85:33:19:G:HO2'	1.48	0.60
6:F1:137:PRO:HB2	6:F1:150:PRO:HD2	1.84	0.60
17:Q1:18:ARG:NH1	20:T1:88:LYS:O	2.35	0.60
39:D2:107:ARG:NH1	39:D2:169:GLY:O	2.32	0.60
80:54:4522:G:O2'	80:54:4525:C:OP2	2.13	0.60
1:A1:1091:C:O2'	24:X1:2:VAL:N	2.33	0.60
1:A1:1637:A:H4'	1:A1:1638:G:O5'	2.02	0.60
4:D1:168:GLY:N	4:D1:179:THR:O	2.32	0.60
18:R1:11:GLN:HE21	18:R1:71:ARG:HH12	1.49	0.60
80:54:956:A:H1'	80:54:2076:G:H5''	1.84	0.60
80:54:1197:C:H2'	80:54:1198:G:C8	2.36	0.60
48:N2:125:SER:HB3	80:54:3937:C:H1'	1.84	0.59
51:Q2:99:LYS:HE2	51:Q2:121:LEU:HD11	1.83	0.59
80:54:4572:U:O2'	80:54:4573:G:O4'	2.20	0.59
85:23:54:2MU:H6'2	85:23:55:PSU:H5''	1.84	0.59
1:A1:472:C:O2'	1:A1:474:G:OP1	2.18	0.59
4:D1:167:ARG:HB3	4:D1:177:PRO:HB2	1.85	0.59
24:X1:30:CYS:N	24:X1:59:GLY:O	2.35	0.59
80:54:3908:A:H2	83:XX:1021:LYS:HA	1.67	0.59
80:54:4541:G:N2	80:54:4544:A:OP2	2.29	0.59
34:h1:18:VAL:O	34:h1:287:THR:OG1	2.17	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:E2:64:MET:HE3	40:E2:68:LYS:HD2	1.84	0.59
40:E2:193:HIS:HD2	40:E2:195:LYS:H	1.49	0.59
47:M2:117:LYS:NZ	80:54:4882:U:OP1	2.32	0.59
48:N2:182:HIS:HD2	48:N2:183:THR:HG23	1.67	0.59
70:j2:49:TRP:O	80:54:1646:A:O2'	2.19	0.59
1:A1:754:G:H22	1:A1:791:C:H1'	1.67	0.59
1:A1:872:A:O2'	1:A1:874:G:OP2	2.21	0.59
1:A1:874:G:H2'	1:A1:875:A:H8	1.66	0.59
34:h1:174:VAL:HB	34:h1:188:HIS:HB2	1.83	0.59
39:D2:115:MET:SD	80:54:1819:G:O2'	2.61	0.59
80:54:408:A:H4'	80:54:409:G:H3'	1.85	0.59
80:54:4751:G:H1	80:54:4948:C:H5	1.50	0.59
1:A1:4:C:O2'	11:K1:18:ARG:NH1	2.36	0.59
53:S2:101:THR:HG22	53:S2:103:ALA:H	1.68	0.59
54:T2:83:LYS:HE2	54:T2:85:LEU:HD21	1.84	0.59
79:t2:11:LYS:HB3	79:t2:64:ILE:HB	1.83	0.59
1:A1:1693:G:H21	1:A1:1834:A:H8	1.51	0.59
5:E1:137:VAL:HG22	5:E1:151:LYS:HG3	1.84	0.59
10:J1:6:ASP:OD1	10:J1:9:HIS:ND1	2.34	0.59
19:S1:78:ARG:NH1	19:S1:79:GLU:OE2	2.35	0.59
29:c1:67:THR:OG1	29:c1:70:LYS:O	2.20	0.59
80:54:369:G:N2	80:54:372:A:OP2	2.32	0.59
42:G2:126:ARG:NE	80:54:4076:G:OP1	2.27	0.59
44:I2:24:ARG:NH2	80:54:4225:G:OP1	2.33	0.59
85:33:54:2MU:H6'2	85:33:55:PSU:H5''	1.84	0.59
20:T1:65:GLU:HA	20:T1:68:ILE:HG12	1.84	0.59
42:G2:105:THR:O	82:84:150:C:N4	2.36	0.59
75:o2:81:ARG:NH2	80:54:4293:U:O2'	2.36	0.59
2:B1:128:ARG:NH2	2:B1:151:ASP:O	2.36	0.58
37:B2:385:LYS:NZ	80:54:5002:U:OP2	2.36	0.58
47:M2:132:ARG:NH2	80:54:4895:C:N3	2.50	0.58
49:O2:168:TYR:OH	80:54:4768:G:OP1	2.21	0.58
78:s2:58:ASN:O	78:s2:62:ARG:N	2.31	0.58
80:54:67:C:OP2	80:54:312:G:N2	2.36	0.58
80:54:3809:G:OP2	80:54:3809:G:N2	2.34	0.58
85:33:33:U:H3'	85:33:35:U:OP1	2.02	0.58
2:B1:38:ILE:HD11	2:B1:150:THR:HG22	1.85	0.58
36:A2:108:PRO:HD3	76:p2:90:LYS:HD2	1.85	0.58
38:C2:262:ASP:HB3	38:C2:273:LEU:HD13	1.84	0.58
40:E2:290:VAL:O	47:M2:109:ARG:NH1	2.36	0.58
49:O2:81:TRP:HB2	49:O2:104:VAL:HG21	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t2:154:ASP:HA	79:t2:158:GLY:HA3	1.85	0.58
85:23:33:U:HO2'	85:23:35:U:H5	1.50	0.58
1:A1:874:G:H2'	1:A1:875:A:C8	2.38	0.58
35:i1:21:A:H61	85:23:34:70U:HN3	1.51	0.58
36:A2:27:ALA:O	36:A2:128:ARG:NH1	2.30	0.58
57:W2:1:MET:HE3	57:W2:15:PRO:HB3	1.85	0.58
63:c2:11:LEU:HD13	63:c2:75:SER:HB2	1.85	0.58
51:Q2:12:LYS:HB2	51:Q2:14:ARG:HH11	1.68	0.58
80:54:990:C:N4	80:54:1064:G:O6	2.32	0.58
80:54:4039:G:H3'	80:54:4041:C:H41	1.67	0.58
1:A1:1354:G:N2	1:A1:1357:A:OP2	2.30	0.58
6:F1:60:GLU:OE2	26:Z1:20:ARG:NH2	2.37	0.58
27:a1:65:TYR:C	85:33:34:70U:C5'	2.72	0.58
40:E2:154:ILE:HB	40:E2:198:ILE:HB	1.85	0.58
80:54:233:U:O2'	80:54:2304:U:O4	2.19	0.58
80:54:1397:A:O2'	80:54:1467:C:O2'	2.20	0.58
1:A1:144:U:OP2	8:H1:139:SER:OG	2.22	0.58
1:A1:433:A:H5''	10:J1:22:HIS:HB3	1.85	0.58
18:R1:53:GLU:OE2	18:R1:85:ARG:NH1	2.34	0.58
39:D2:278:ASP:OD2	39:D2:282:GLN:NE2	2.36	0.58
61:a2:26:ARG:NH1	80:54:1655:C:OP2	2.36	0.58
79:t2:64:ILE:HA	79:t2:69:ALA:HA	1.85	0.58
85:23:33:U:H3'	85:23:35:U:OP1	2.03	0.58
36:A2:106:THR:O	76:p2:90:LYS:NZ	2.33	0.58
84:B:48:ARG:NH2	84:B:159:MET:O	2.30	0.58
1:A1:520:A:O2'	1:A1:825:A:N3	2.36	0.58
3:C1:63:LYS:HE2	3:C1:90:ASP:HA	1.85	0.58
8:H1:42:GLY:HA3	8:H1:45:TRP:HE3	1.69	0.58
48:N2:184:ILE:O	48:N2:194:ARG:NH1	2.37	0.58
61:a2:44:ASN:ND2	80:54:1683:U:OP1	2.34	0.58
72:l2:20:ASN:O	72:l2:41:ARG:NH2	2.37	0.58
80:54:1092:G:N2	80:54:1204:C:O2	2.19	0.58
39:D2:28:THR:O	80:54:4280:A:N6	2.35	0.58
40:E2:108:ARG:NH2	80:54:469:C:N3	2.51	0.58
1:A1:1083:A:N7	1:A1:1841:C:O2'	2.36	0.57
22:V1:22:ILE:N	22:V1:89:ILE:O	2.36	0.57
24:X1:111:MET:HE3	24:X1:116:ALA:HA	1.86	0.57
36:A2:137:ILE:HD11	36:A2:149:LYS:HB2	1.85	0.57
40:E2:144:ARG:NH2	66:f2:110:ILE:OXT	2.34	0.57
42:G2:142:ARG:NH2	82:84:155:C:OP2	2.37	0.57
44:I2:141:LYS:HD3	44:I2:143:GLN:HE22	1.68	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:s2:34:ASN:HB3	80:54:1968:G:H4'	1.86	0.57
80:54:4036:G:O2'	80:54:4037:C:OP1	2.22	0.57
82:84:93:C:HO2'	82:84:94:G:H8	1.51	0.57
1:A1:183:G:O2'	1:A1:184:G:O5'	2.22	0.57
1:A1:635:G:OP1	32:f1:94:LYS:NZ	2.37	0.57
38:C2:323:ARG:HE	80:54:976:G:H21	1.51	0.57
80:54:3765:G:O2'	80:54:3767:C:N4	2.37	0.57
8:H1:5:ILE:HG12	8:H1:111:LEU:HB2	1.85	0.57
45:J2:151:ILE:HD11	45:J2:156:ARG:HG2	1.87	0.57
75:o2:11:PHE:O	75:o2:81:ARG:NH1	2.32	0.57
78:s2:28:PHE:HZ	78:s2:95:LEU:HA	1.69	0.57
79:t2:117:ARG:HB2	79:t2:125:LEU:HD12	1.84	0.57
80:54:1283:G:N1	80:54:2076:G:OP1	2.31	0.57
22:V1:36:CYS:SG	22:V1:53:PRO:HB3	2.44	0.57
38:C2:29:LYS:NZ	80:54:667:A:O2'	2.34	0.57
80:54:1676:C:O2'	80:54:3914:U:N3	2.37	0.57
2:B1:52:LYS:HB2	19:S1:109:LEU:HD21	1.85	0.57
5:E1:103:GLU:HA	5:E1:106:ARG:HB3	1.86	0.57
11:K1:136:ARG:NH1	11:K1:159:PHE:O	2.37	0.57
14:N1:67:ALA:HB1	33:g1:114:ILE:HB	1.85	0.57
26:Z1:55:ILE:HG12	26:Z1:75:ILE:HG22	1.86	0.57
78:s2:43:ILE:HG12	78:s2:105:ASN:HD21	1.69	0.57
9:I1:60:ILE:HB	9:I1:92:VAL:HG12	1.87	0.57
24:X1:80:ASP:OD1	24:X1:124:LYS:NZ	2.31	0.57
60:Z2:33:THR:OG1	60:Z2:35:ASP:OD1	2.21	0.57
78:s2:29:ILE:HD13	78:s2:82:ILE:HD11	1.86	0.57
80:54:1326:A:OP2	80:54:4445:U:O2'	2.22	0.57
80:54:4322:G:N2	80:54:4325:A:OP2	2.36	0.57
6:F1:71:LYS:HG2	6:F1:76:VAL:HG22	1.87	0.57
38:C2:317:ASN:HD22	38:C2:320:LYS:HE2	1.70	0.57
48:N2:49:ARG:HH12	80:54:152:U:P	2.28	0.57
51:Q2:75:ARG:NH2	80:54:1457:G:O2'	2.37	0.57
80:54:1755:C:O2'	80:54:1768:C:N4	2.37	0.57
1:A1:64:A:OP1	8:H1:177:GLN:NE2	2.38	0.57
3:C1:152:LYS:HD3	19:S1:133:GLY:HA3	1.87	0.57
17:Q1:44:ARG:NH1	17:Q1:82:ASP:O	2.30	0.57
27:a1:99:LEU:HD21	27:a1:102:LYS:HG3	1.86	0.57
36:A2:244:GLY:HA3	80:54:3746:A:H5''	1.86	0.57
48:N2:38:ARG:NH2	82:84:142:U:OP1	2.34	0.57
50:P2:115:GLU:HG2	50:P2:151:THR:HG23	1.87	0.57
79:t2:99:LYS:HD3	79:t2:140:GLY:HA3	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:1377:G:H21	80:54:1380:G:H5'	1.68	0.57
80:54:2738:C:O2'	80:54:2740:U:O2	2.22	0.57
17:Q1:29:SER:HB3	17:Q1:32:GLN:HG2	1.85	0.57
34:h1:197:THR:HG21	34:h1:239:LEU:H	1.69	0.57
41:F2:244:ARG:NH1	80:54:942:G:OP1	2.38	0.57
78:s2:50:LYS:HD2	78:s2:93:GLU:HG3	1.87	0.57
79:t2:117:ARG:O	79:t2:120:SER:OG	2.18	0.57
11:K1:82:VAL:HG21	11:K1:92:MET:HE2	1.85	0.56
26:Z1:41:ARG:NH2	26:Z1:52:PRO:O	2.38	0.56
48:N2:192:TRP:NE1	80:54:48:G:OP1	2.36	0.56
80:54:667:A:OP1	80:54:668:C:N4	2.33	0.56
39:D2:267:ASN:ND2	81:74:2:U:H5'	2.19	0.56
48:N2:50:ARG:NH2	80:54:279:A:OP1	2.38	0.56
51:Q2:181:ARG:HH12	80:54:1391:A:H5'	1.70	0.56
47:M2:125:ASN:OD1	47:M2:126:GLU:N	2.37	0.56
50:P2:49:LYS:HE2	50:P2:92:LEU:HD21	1.86	0.56
53:S2:83:ARG:HB2	53:S2:127:MET:HE3	1.88	0.56
56:V2:111:GLU:HG2	56:V2:131:ARG:HG3	1.86	0.56
80:54:1503:A:H4'	80:54:1504:G:H5'	1.87	0.56
84:B:131:ALA:HB3	84:B:133:LYS:HB2	1.87	0.56
1:A1:1749:G:H1	1:A1:1785:C:H42	1.53	0.56
10:J1:190:LEU:HB3	10:J1:195:LEU:HB2	1.87	0.56
27:a1:66:LYS:HE2	85:33:34:70U:P	2.43	0.56
33:g1:100:LEU:HB3	33:g1:103:LEU:HD23	1.88	0.56
46:L2:102:ARG:HG3	80:54:75:G:N7	2.21	0.56
1:A1:629:A:O2'	1:A1:631:U:OP1	2.24	0.56
8:H1:159:ARG:HH11	8:H1:171:THR:HG23	1.70	0.56
14:N1:52:LEU:CD1	14:N1:65:VAL:HG11	2.35	0.56
34:h1:207:CYS:N	34:h1:219:TRP:O	2.25	0.56
38:C2:82:GLY:HA2	80:54:368:C:H1'	1.88	0.56
38:C2:305:PRO:HD3	51:Q2:38:ARG:HH21	1.70	0.56
42:G2:156:ARG:NH2	42:G2:245:ARG:O	2.35	0.56
1:A1:49:C:N4	1:A1:473:A:OP2	2.34	0.56
25:Y1:61:GLN:O	25:Y1:63:ASN:N	2.39	0.56
39:D2:226:TYR:OH	81:74:48:G:OP1	2.21	0.56
49:O2:54:TYR:OH	49:O2:73:PHE:O	2.23	0.56
80:54:1397:A:N1	80:54:1498:G:O2'	2.34	0.56
80:54:1590:C:H4'	80:54:2857:A:H5'	1.87	0.56
1:A1:1171:G:O2'	1:A1:1187:G:O6	2.23	0.56
3:C1:129:THR:OG1	3:C1:131:ASP:O	2.22	0.56
22:V1:28:ASN:HD22	22:V1:31:SER:HB3	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:I2:87:ILE:HG12	44:I2:138:ILE:HG12	1.86	0.56
19:S1:57:LEU:HD13	19:S1:69:ILE:HD11	1.88	0.56
48:N2:4:TYR:OH	80:54:151:G:OP2	2.20	0.56
85:23:49:5MC:HN41	85:23:65:G:H1	1.54	0.56
8:H1:223:LYS:HA	8:H1:226:GLU:HB2	1.87	0.56
62:b2:91:ARG:NH2	80:54:1214:C:OP2	2.39	0.56
11:K1:113:GLN:OE1	11:K1:154:GLN:NE2	2.39	0.56
38:C2:275:SER:N	80:54:1376:C:OP1	2.39	0.56
80:54:3692:A:H62	80:54:3823:G:N2	2.02	0.56
7:G1:75:SER:OG	7:G1:155:CYS:SG	2.64	0.55
40:E2:164:ARG:NH2	40:E2:276:SER:OG	2.40	0.55
53:S2:127:MET:HE1	54:T2:155:PRO:HA	1.87	0.55
5:E1:169:ASP:HB2	5:E1:190:LEU:HD11	1.87	0.55
6:F1:87:MET:HE3	6:F1:123:LEU:HB2	1.86	0.55
16:P1:59:GLY:HA2	16:P1:68:GLU:HG2	1.87	0.55
48:N2:93:LYS:NZ	80:54:4177:C:OP1	2.32	0.55
49:O2:116:LYS:HE3	53:S2:169:THR:HB	1.88	0.55
61:a2:114:LYS:HG3	80:54:1397:A:H8	1.70	0.55
79:t2:58:ILE:HD11	79:t2:76:SER:H	1.70	0.55
80:54:1656:U:O2'	80:54:3906:A:N1	2.37	0.55
1:A1:161:U:H5'	26:Z1:116:LYS:HB3	1.87	0.55
80:54:1804:A:H5'	80:54:1806:G:O4'	2.06	0.55
4:D1:204:ILE:O	4:D1:211:LYS:NZ	2.33	0.55
5:E1:39:VAL:HG12	5:E1:41:VAL:HG13	1.87	0.55
48:N2:114:ARG:NH1	48:N2:151:ILE:O	2.40	0.55
84:B:54:ARG:NH2	84:B:150:GLU:OE2	2.40	0.55
1:A1:54:A:OP1	26:Z1:111:LYS:NZ	2.38	0.55
36:A2:173:GLY:O	76:p2:69:TRP:NE1	2.39	0.55
41:F2:126:LYS:HB2	54:T2:133:ALA:HB3	1.88	0.55
44:I2:74:LYS:HD3	80:54:4415:A:H4'	1.88	0.55
46:L2:63:THR:O	46:L2:65:ARG:N	2.39	0.55
48:N2:178:HIS:ND1	80:54:68:U:OP1	2.36	0.55
50:P2:94:MET:HE1	50:P2:146:ILE:HB	1.88	0.55
79:t2:56:LEU:HD11	80:54:1977:C:H5'	1.89	0.55
80:54:1999:A:O2'	80:54:2018:C:O2'	2.21	0.55
1:A1:1834:A:H2	1:A1:1837:G:H1	1.55	0.55
10:J1:134:GLU:HA	10:J1:137:LEU:HD12	1.88	0.55
14:N1:35:ILE:O	14:N1:39:ALA:N	2.22	0.55
40:E2:189:LEU:H	40:E2:253:GLN:HE22	1.54	0.55
60:Z2:15:ALA:HB2	67:g2:88:ARG:HH21	1.70	0.55
80:54:4378:A:O2'	80:54:4379:A:H2'	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:71:G:O6	8:H1:170:ARG:NH1	2.40	0.55
1:A1:183:G:O2'	1:A1:184:G:O4'	2.23	0.55
7:G1:110:GLN:HE21	7:G1:114:ASN:HD21	1.54	0.55
10:J1:119:LEU:HD21	10:J1:153:LYS:HD3	1.88	0.55
17:Q1:44:ARG:HD3	17:Q1:84:ILE:HD11	1.87	0.55
37:B2:228:TYR:O	80:54:2835:A:O2'	2.25	0.55
78:s2:171:GLU:HA	78:s2:174:LEU:HD13	1.88	0.55
1:A1:1060:A:O2'	1:A1:1062:A:N7	2.28	0.55
22:V1:33:GLU:OE1	22:V1:87:ARG:NE	2.40	0.55
28:b1:14:GLY:H	28:b1:15:ARG:HH11	1.55	0.55
51:Q2:88:ASP:OD2	51:Q2:108:ARG:NE	2.38	0.55
54:T2:146:LYS:H	54:T2:146:LYS:HD2	1.72	0.55
63:c2:31:TYR:OH	63:c2:59:GLU:OE2	2.23	0.55
76:p2:4:ARG:NH2	80:54:1555:G:O6	2.40	0.55
78:s2:18:ILE:HA	78:s2:21:LEU:HB3	1.89	0.55
78:s2:146:LYS:O	78:s2:153:GLU:HB3	2.07	0.55
80:54:1794:A:H5''	80:54:4214:A:H61	1.72	0.55
80:54:4635:A:H8	80:54:5048:A:H61	1.54	0.55
10:J1:57:ALA:HB2	10:J1:183:GLY:HA2	1.88	0.55
22:V1:61:LEU:HB2	22:V1:82:MET:HB3	1.88	0.55
46:L2:4:SER:O	61:a2:44:ASN:ND2	2.37	0.55
50:P2:13:LYS:HB3	50:P2:152:GLU:HG2	1.89	0.55
79:t2:129:ILE:HG13	79:t2:130:LYS:HD3	1.89	0.55
80:54:1481:C:O2'	80:54:1482:G:O4'	2.24	0.55
1:A1:1498:A:OP2	5:E1:27:ARG:NH2	2.39	0.55
5:E1:70:THR:HG22	5:E1:86:LEU:HD13	1.89	0.55
18:R1:44:PRO:HB2	18:R1:46:THR:HG22	1.89	0.55
39:D2:253:TYR:OH	81:74:117:G:OP1	2.24	0.55
65:e2:69:MET:HB2	65:e2:75:ARG:HE	1.72	0.55
80:54:1193:C:H2'	80:54:1194:G:C8	2.41	0.55
40:E2:94:THR:OG1	80:54:2258:C:O2	2.24	0.54
44:I2:38:ARG:NH2	44:I2:45:GLU:OE2	2.39	0.54
59:Y2:121:ARG:NH2	80:54:194:C:O2	2.40	0.54
80:54:1666:C:O2'	80:54:1688:G:OP1	2.22	0.54
1:A1:1016:U:OP1	29:c1:30:SER:OG	2.24	0.54
6:F1:253:ASP:OD1	6:F1:254:LYS:N	2.40	0.54
20:T1:60:THR:OG1	20:T1:62:ASP:OD1	2.20	0.54
26:Z1:20:ARG:NH2	26:Z1:74:MET:SD	2.80	0.54
31:e1:19:ARG:O	31:e1:27:ARG:NH1	2.40	0.54
37:B2:117:ARG:HG2	37:B2:180:LEU:HD13	1.88	0.54
41:F2:134:ILE:HD11	80:54:1726:U:H5'	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:R2:28:GLU:HG3	52:R2:49:LEU:HD22	1.89	0.54
80:54:3654:G:O2'	80:54:3693:U:OP1	2.22	0.54
1:A1:1863:A:H1'	28:b1:79:ILE:HD13	1.89	0.54
10:J1:22:HIS:ND1	10:J1:23:LYS:O	2.38	0.54
36:A2:183:GLY:HA2	80:54:1613:A:H5''	1.89	0.54
55:U2:113:ARG:NH2	80:54:2702:C:O3'	2.40	0.54
80:54:1211:G:H2'	80:54:1212:G:H8	1.71	0.54
80:54:2749:C:H2'	80:54:2750:G:H8	1.72	0.54
85:33:49:5MC:HN41	85:33:65:G:H1	1.54	0.54
11:K1:63:LEU:O	11:K1:70:ARG:NH1	2.37	0.54
78:s2:175:LEU:HD23	78:s2:180:ILE:HB	1.89	0.54
80:54:1077:C:OP1	80:54:1215:C:O2'	2.23	0.54
14:N1:60:MET:O	14:N1:64:LEU:N	2.37	0.54
34:h1:256:ILE:HD12	34:h1:289:LEU:HD13	1.90	0.54
34:h1:292:SER:OG	34:h1:297:THR:OG1	2.26	0.54
44:I2:38:ARG:HG3	44:I2:83:ASP:HB3	1.90	0.54
76:p2:47:MET:SD	76:p2:57:CYS:HB2	2.47	0.54
80:54:983:C:H42	80:54:1071:C:H42	1.54	0.54
80:54:1633:G:H5'	80:54:1634:A:OP1	2.08	0.54
80:54:2845:A:H61	80:54:3843:C:H42	1.53	0.54
1:A1:681:U:H4'	25:Y1:9:THR:HG22	1.89	0.54
1:A1:1497:G:N7	12:L1:25:LYS:NZ	2.52	0.54
5:E1:16:ILE:HD11	31:e1:36:LEU:HD23	1.88	0.54
7:G1:70:GLU:OE2	7:G1:86:LYS:NZ	2.26	0.54
20:T1:73:ASN:ND2	20:T1:76:GLN:OE1	2.40	0.54
36:A2:196:TRP:HB3	36:A2:197:PRO:HD3	1.88	0.54
41:F2:161:ILE:HB	41:F2:166:ILE:HD12	1.88	0.54
51:Q2:178:ARG:N	61:a2:51:GLY:HA2	2.23	0.54
57:W2:93:LYS:HA	57:W2:96:GLN:HB2	1.90	0.54
66:f2:4:ARG:NH1	80:54:4754:G:OP1	2.41	0.54
80:54:1985:G:H1'	80:54:2003:G:H2'	1.89	0.54
1:A1:1693:G:N2	1:A1:1834:A:H8	2.04	0.54
80:54:85:G:O2'	80:54:97:G:O6	2.22	0.54
36:A2:15:VAL:HG12	36:A2:194:ASN:HD22	1.73	0.54
60:Z2:10:VAL:O	60:Z2:83:THR:OG1	2.24	0.54
62:b2:18:ARG:NH2	80:54:1669:A:OP1	2.31	0.54
80:54:394:G:N2	80:54:397:G:OP2	2.33	0.54
80:54:2093:G:H22	80:54:2262:G:H1	1.55	0.54
80:54:4045:G:H22	80:54:4047:A:H3'	1.73	0.54
19:S1:94:GLU:HG2	19:S1:95:ILE:HG12	1.90	0.54
42:G2:139:VAL:HG12	42:G2:236:ILE:HG22	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:k2:26:LYS:HE2	80:54:2696:A:H5'	1.89	0.54
79:t2:14:TYR:HA	79:t2:61:LYS:HG3	1.90	0.54
80:54:4044:U:O2'	80:54:4048:A:N6	2.41	0.54
80:54:4948:C:H3'	80:54:4949:G:C5'	2.38	0.54
8:H1:219:GLU:HG2	8:H1:223:LYS:NZ	2.23	0.54
12:L1:15:LEU:HD22	12:L1:49:MET:HE1	1.91	0.54
28:b1:89:ARG:NH2	28:b1:90:GLU:OE2	2.41	0.54
51:Q2:13:VAL:O	80:54:1691:G:H5''	2.08	0.54
80:54:2382:A:N1	80:54:2829:U:O2'	2.31	0.54
80:54:4947:U:O2'	80:54:4948:C:OP1	2.24	0.54
1:A1:377:G:H5'	10:J1:98:LYS:HB3	1.90	0.53
27:a1:111:ARG:HE	85:33:34:70U:H5''	1.71	0.53
43:H2:23:ARG:HG3	80:54:4765:G:OP1	2.08	0.53
80:54:1211:G:H2'	80:54:1212:G:C8	2.43	0.53
1:A1:446:G:OP2	10:J1:47:ARG:NH1	2.40	0.53
1:A1:1475:G:H21	1:A1:1475:G:P	2.31	0.53
5:E1:80:PRO:O	5:E1:83:SER:OG	2.25	0.53
34:h1:292:SER:OG	34:h1:294:ASP:OD1	2.26	0.53
4:D1:121:ARG:NH1	4:D1:123:ARG:HD3	2.24	0.53
20:T1:26:ILE:HG13	20:T1:45:LEU:HD21	1.91	0.53
38:C2:224:ILE:HB	38:C2:227:ILE:HD12	1.90	0.53
42:G2:139:VAL:HG11	42:G2:238:LYS:HG3	1.90	0.53
51:Q2:108:ARG:NH2	80:54:1354:A:H5'	2.24	0.53
70:j2:31:LYS:HB3	70:j2:33:THR:HG22	1.89	0.53
80:54:2368:A:N6	80:54:2827:G:O2'	2.41	0.53
80:54:3888:G:O2'	80:54:3889:G:OP1	2.25	0.53
1:A1:86:C:O2'	1:A1:171:A:N1	2.38	0.53
5:E1:29:LEU:HD22	5:E1:58:VAL:HG23	1.89	0.53
13:M1:127:THR:HB	13:M1:144:LYS:HG2	1.89	0.53
1:A1:167:G:H4'	57:W2:80:ARG:HH22	1.74	0.53
36:A2:123:ARG:NH1	80:54:4083:U:OP1	2.42	0.53
59:Y2:87:ARG:NH1	80:54:404:U:O2'	2.41	0.53
80:54:407:A:O2'	80:54:410:A:OP1	2.20	0.53
23:W1:32:ILE:HG12	23:W1:60:ARG:HD2	1.91	0.53
50:P2:120:ASN:ND2	82:84:12:G:H21	2.07	0.53
57:W2:8:PHE:HZ	57:W2:49:ILE:HD12	1.74	0.53
65:e2:108:ARG:NH1	80:54:2326:G:OP1	2.42	0.53
67:g2:37:LYS:NZ	80:54:2515:G:OP1	2.27	0.53
85:23:57:A:O5'	85:23:57:A:H8	1.92	0.53
1:A1:1692:U:H2'	1:A1:1693:G:C8	2.43	0.53
1:A1:1741:U:OP1	10:J1:42:ARG:NH1	2.41	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F1:252:ARG:HG2	6:F1:255:ARG:HH21	1.73	0.53
79:t2:114:ARG:HA	79:t2:125:LEU:HD11	1.90	0.53
1:A1:167:G:O2'	57:W2:80:ARG:NH1	2.33	0.53
36:A2:117:GLU:HB2	36:A2:162:ASN:HB2	1.90	0.53
68:h2:95:LEU:O	80:54:135:G:N2	2.36	0.53
79:t2:80:LEU:HG	79:t2:112:ILE:HD12	1.90	0.53
80:54:1675:C:C4	80:54:1677:U:H1'	2.43	0.53
80:54:1197:C:H2'	80:54:1198:G:H8	1.73	0.53
80:54:1755:C:H1'	80:54:1756:U:H3'	1.91	0.53
80:54:2478:C:N4	80:54:2479:G:O6	2.41	0.53
80:54:4303:C:H2'	80:54:4305:G:C8	2.44	0.53
1:A1:1738:C:OP1	8:H1:92:ARG:NH1	2.33	0.53
4:D1:77:SER:OG	4:D1:80:GLU:OE1	2.19	0.53
14:N1:52:LEU:HD13	14:N1:65:VAL:HG11	1.91	0.53
24:X1:102:ILE:H	24:X1:113:HIS:CD2	2.22	0.53
42:G2:88:ARG:NH1	80:54:4128:A:O2'	2.41	0.53
80:54:1369:C:OP2	80:54:1370:G:O2'	2.19	0.53
80:54:1406(B):C:H2'	80:54:1406(C):G:C8	2.44	0.53
80:54:4232:U:H4'	80:54:4233:A:O5'	2.08	0.53
84:B:29:LEU:HD13	84:B:62:LYS:HD2	1.91	0.53
1:A1:190:G:H5''	10:J1:145:ILE:HD13	1.90	0.52
1:A1:1550:G:H3'	1:A1:1579:A:H61	1.73	0.52
1:A1:1757:G:O6	1:A1:1774:C:N4	2.35	0.52
23:W1:62:MET:HG2	23:W1:64:GLU:HG2	1.91	0.52
26:Z1:83:LYS:HE3	26:Z1:96:LEU:HD12	1.92	0.52
36:A2:15:VAL:HG21	80:54:1628:C:H5''	1.90	0.52
37:B2:128:LYS:O	37:B2:131:THR:OG1	2.26	0.52
40:E2:193:HIS:HB3	40:E2:196:PHE:HD2	1.75	0.52
58:X2:77:ILE:HD12	58:X2:116:LEU:HD12	1.92	0.52
68:h2:55:ALA:O	68:h2:59:THR:OG1	2.25	0.52
75:o2:47:GLY:HA2	80:54:288:G:H5''	1.90	0.52
77:r2:38:PHE:O	77:r2:45:HIS:HE1	1.92	0.52
80:54:1927:U:OP1	80:54:1949:U:O2'	2.27	0.52
80:54:2483:G:H2'	80:54:2484:A:H8	1.74	0.52
80:54:2564:G:H2'	80:54:2565:A:C8	2.44	0.52
80:54:2811:G:N1	80:54:2814:C:OP2	2.39	0.52
1:A1:901:G:H2'	1:A1:902:G:H8	1.74	0.52
3:C1:226:GLY:HA3	42:G2:316:THR:HG22	1.90	0.52
36:A2:243:THR:HB	80:54:3748:A:H5''	1.90	0.52
40:E2:184:LEU:O	80:54:4883:C:N4	2.42	0.52
42:G2:276:ARG:HG3	42:G2:280:ASN:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:Q2:14:ARG:NH2	80:54:2083:C:OP2	2.39	0.52
1:A1:1005:G:OP2	3:C1:162:ARG:NH1	2.36	0.52
5:E1:203:PRO:HG2	19:S1:42:PRO:HB3	1.92	0.52
23:W1:20:SER:HB3	23:W1:59:ILE:HD11	1.90	0.52
36:A2:72:ARG:NH2	80:54:4084:G:O6	2.30	0.52
53:S2:31:ARG:HH11	53:S2:129:VAL:HB	1.75	0.52
1:A1:145:G:O6	8:H1:178:ARG:NH1	2.38	0.52
2:B1:126:ASP:OD1	2:B1:165:ASN:ND2	2.42	0.52
3:C1:60:ASP:OD1	3:C1:60:ASP:N	2.42	0.52
14:N1:65:VAL:O	14:N1:69:CYS:N	2.42	0.52
16:P1:46:ASP:OD2	16:P1:48:SER:OG	2.26	0.52
80:54:2724:G:O2'	80:54:2726:G:OP2	2.26	0.52
80:54:2844:A:O2'	80:54:4631:G:H4'	2.10	0.52
80:54:3690:U:O2'	80:54:3817:A:N3	2.40	0.52
80:54:3717:A:OP2	80:54:3735:G:N2	2.42	0.52
1:A1:110:U:O2'	1:A1:111:A:OP1	2.28	0.52
1:A1:1075:C:OP1	15:O1:107:LYS:NZ	2.42	0.52
25:Y1:24:ASP:HB3	25:Y1:27:TYR:HB3	1.91	0.52
36:A2:207:VAL:HG13	36:A2:208:GLU:HG3	1.89	0.52
46:L2:181:SER:HB3	69:i2:7:MET:HE1	1.92	0.52
80:54:4045:G:H1	80:54:4048:A:H5''	1.74	0.52
85:33:57:A:H8	85:33:57:A:O5'	1.92	0.52
1:A1:1286:G:H3'	33:g1:97:LYS:HE3	1.91	0.52
1:A1:1560:U:O2'	1:A1:1583:C:O2'	2.26	0.52
14:N1:36:ARG:NH1	14:N1:36:ARG:O	2.43	0.52
28:b1:41:ILE:HG22	28:b1:66:LYS:HD3	1.90	0.52
36:A2:241:ARG:NH1	80:54:3659:G:OP1	2.43	0.52
51:Q2:160:HIS:NE2	80:54:4298:A:OP1	2.41	0.52
1:A1:1115:U:H1'	1:A1:1116:C:H2'	1.92	0.52
3:C1:57:ILE:HG22	3:C1:59:SER:H	1.74	0.52
6:F1:55:ALA:HB1	6:F1:60:GLU:HB3	1.92	0.52
14:N1:18:LEU:HD11	14:N1:51:VAL:HG21	1.92	0.52
45:J2:98:ASN:HD22	80:54:4250:G:H5''	1.74	0.52
53:S2:99:ASP:OD1	53:S2:100:LEU:N	2.40	0.52
57:W2:104:GLN:O	57:W2:107:GLN:HG3	2.10	0.52
64:d2:64:ILE:HG23	64:d2:68:LEU:HD23	1.91	0.52
84:B:60:ARG:HG2	84:B:63:PHE:HD1	1.74	0.52
1:A1:63:U:O2'	1:A1:170:A:N3	2.41	0.52
14:N1:31:LEU:HD12	14:N1:33:ARG:HH11	1.74	0.52
18:R1:21:ALA:HB2	18:R1:72:VAL:HG23	1.92	0.52
18:R1:146:ARG:HH22	85:23:33:U:H3'	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:a1:66:LYS:N	85:33:34:70U:H5''	2.23	0.52
64:d2:114:PHE:HA	64:d2:117:LEU:HD12	1.91	0.52
80:54:4040:C:OP1	80:54:4048:A:O2'	2.28	0.52
38:C2:323:ARG:HH12	80:54:1279:A:H1'	1.74	0.52
54:T2:81:LYS:O	62:b2:16:TRP:CD2	2.63	0.52
80:54:3784:A:O2'	80:54:3785:A:H3'	2.10	0.52
80:54:4948:C:H3'	80:54:4949:G:H5''	1.92	0.52
84:B:31:THR:HA	84:B:171:HIS:HA	1.92	0.52
1:A1:623:G:O6	25:Y1:63:ASN:ND2	2.43	0.52
3:C1:46:LYS:HE2	16:P1:19:PRO:HG2	1.91	0.52
5:E1:94:ARG:O	5:E1:101:GLN:NE2	2.43	0.52
20:T1:89:ASP:OD2	20:T1:106:LYS:NZ	2.43	0.52
38:C2:94:ASN:HD22	38:C2:102:PHE:HB2	1.75	0.52
56:V2:82:ILE:HB	56:V2:121:VAL:HG13	1.91	0.52
61:a2:85:GLN:HA	61:a2:88:VAL:HG22	1.91	0.52
67:g2:76:ARG:NH1	80:54:2583:C:OP2	2.41	0.52
71:k2:49:ASP:OD1	71:k2:51:GLU:N	2.43	0.52
14:N1:63:LYS:HZ2	33:g1:109:ASP:H	1.58	0.51
16:P1:20:GLN:HE22	16:P1:25:GLU:HB2	1.74	0.51
39:D2:56:THR:HG21	81:74:26:C:H5''	1.92	0.51
40:E2:142:LYS:O	40:E2:194:GLN:NE2	2.32	0.51
42:G2:126:ARG:HH12	80:54:4162:C:H5	1.57	0.51
77:r2:65:LYS:O	77:r2:102:TYR:OH	2.24	0.51
80:54:1449:C:HO2'	80:54:2105:A:HO2'	1.51	0.51
80:54:1733:G:N3	80:54:4214:A:H2'	2.25	0.51
80:54:1734:G:N2	80:54:1735:U:O4	2.29	0.51
80:54:4537:C:H2'	80:54:4538:G:C8	2.44	0.51
82:84:121:G:H3'	82:84:122:G:H8	1.74	0.51
3:C1:52:THR:HG23	3:C1:57:ILE:HA	1.92	0.51
13:M1:135:SER:O	13:M1:139:ARG:NH1	2.42	0.51
24:X1:44:HIS:NE2	24:X1:112:ASP:OD2	2.43	0.51
29:c1:40:CYS:SG	29:c1:41:TYR:N	2.82	0.51
40:E2:146:SER:OG	66:f2:110:ILE:O	2.26	0.51
42:G2:263:GLU:OE1	42:G2:263:GLU:N	2.41	0.51
44:I2:16:PRO:HA	44:I2:95:HIS:HD2	1.75	0.51
44:I2:55:ASP:OD2	44:I2:164:LYS:NZ	2.33	0.51
48:N2:60:VAL:HG11	82:84:141:C:H5''	1.92	0.51
59:Y2:109:LEU:HD13	59:Y2:119:LEU:HD21	1.92	0.51
80:54:1990:A:H2'	80:54:1991:A:H5''	1.90	0.51
80:54:2483:G:H2'	80:54:2484:A:C8	2.46	0.51
80:54:2490:U:O2'	80:54:2491:C:O4'	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:4745:G:H1	80:54:4955:A:H61	1.57	0.51
85:33:48:5MC:OP2	85:33:48:5MC:H6	1.94	0.51
1:A1:380:G:OP2	10:J1:56:ARG:NH2	2.38	0.51
10:J1:60:LEU:HD21	10:J1:185:ALA:HB2	1.91	0.51
34:h1:291:TRP:CE2	34:h1:298:LEU:HD13	2.46	0.51
44:I2:184:MET:HE3	44:I2:190:LEU:HD11	1.92	0.51
80:54:217:C:H4'	80:54:218:A:O5'	2.10	0.51
80:54:1478:C:H2'	80:54:1479:G:H8	1.76	0.51
80:54:2520:C:O2	80:54:2640:G:N2	2.42	0.51
15:O1:46:THR:H	15:O1:49:GLN:HE21	1.57	0.51
39:D2:62:CYS:HB3	39:D2:105:LEU:HD22	1.91	0.51
44:I2:68:ALA:HB1	44:I2:155:ALA:HB1	1.92	0.51
51:Q2:12:LYS:HB2	51:Q2:14:ARG:NH1	2.25	0.51
52:R2:31:GLU:OE1	52:R2:31:GLU:N	2.44	0.51
61:a2:77:LYS:HE3	80:54:1502:G:H22	1.76	0.51
71:k2:8:ILE:HG23	71:k2:56:LEU:HD21	1.93	0.51
78:s2:45:MET:SD	78:s2:48:ARG:NH2	2.76	0.51
80:54:4888:C:H2'	80:54:4889:G:H8	1.75	0.51
1:A1:866:U:H2'	1:A1:867:G:C8	2.46	0.51
41:F2:155:LYS:NZ	41:F2:247:ASN:OXT	2.34	0.51
80:54:3959:U:O2'	80:54:3960:A:O5'	2.27	0.51
5:E1:172:VAL:HG22	5:E1:185:LYS:HG2	1.93	0.51
20:T1:14:ARG:NH2	45:J2:111:GLU:OE1	2.40	0.51
30:d1:44:ARG:NH2	30:d1:63:ARG:O	2.40	0.51
44:I2:93:PRO:HB2	44:I2:125:THR:HG22	1.92	0.51
44:I2:114:GLY:HA2	80:54:4441:A:H5''	1.93	0.51
51:Q2:68:ARG:NH2	80:54:1421:G:OP1	2.44	0.51
52:R2:60:ARG:NH1	80:54:2808:G:O3'	2.44	0.51
62:b2:111:ARG:NH1	80:54:1246:G:O6	2.37	0.51
68:h2:66:LYS:HD2	82:84:96:C:H5''	1.92	0.51
18:R1:34:VAL:HG22	18:R1:70:VAL:HB	1.91	0.51
35:i1:18:A:O2'	85:23:37:12A:OG1	2.29	0.51
38:C2:39:PHE:O	38:C2:43:ASN:ND2	2.39	0.51
41:F2:222:LYS:HE3	80:54:1907:A:H4'	1.91	0.51
42:G2:139:VAL:HG21	42:G2:238:LYS:HG3	1.91	0.51
53:S2:93:MET:HE1	53:S2:117:HIS:CE1	2.46	0.51
80:54:1406:G:O6	80:54:1411(B):C:N4	2.42	0.51
80:54:4776:G:N2	80:54:4859:C:N3	2.53	0.51
85:23:58:1MA:O2'	85:23:60:U:OP2	2.29	0.51
1:A1:1232:U:H2'	1:A1:1233:G:C8	2.46	0.51
2:B1:38:ILE:HD12	2:B1:47:TYR:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R1:93:VAL:HG11	18:R1:109:LYS:HD3	1.93	0.51
34:h1:232:GLY:HA2	34:h1:257:LYS:HD2	1.93	0.51
48:N2:51:LEU:O	48:N2:117:ASN:ND2	2.36	0.51
54:T2:45:MET:H	54:T2:95:HIS:CD2	2.16	0.51
60:Z2:91:LEU:O	60:Z2:93:LYS:NZ	2.35	0.51
68:h2:112:ARG:NH2	80:54:172:C:O2	2.43	0.51
79:t2:104:ILE:HB	79:t2:143:VAL:HG22	1.93	0.51
80:54:318:A:H2'	80:54:319:A:C8	2.46	0.51
80:54:478:G:H2'	80:54:479:G:C8	2.46	0.51
80:54:1802:A:O2'	80:54:1837:A:OP1	2.26	0.51
84:B:6:SER:OG	84:B:8:ASP:OD1	2.26	0.51
16:P1:34:PHE:HB3	16:P1:41:PHE:HB2	1.92	0.51
55:U2:100:LEU:HD23	55:U2:112:LEU:HB3	1.92	0.51
80:54:924:C:N4	80:54:927:G:H5''	2.26	0.51
80:54:1983:A:H5'	80:54:1984:A:OP1	2.11	0.51
80:54:2477:A:H2'	80:54:2478:C:C6	2.46	0.51
80:54:2558:C:H2'	80:54:2559:G:H8	1.76	0.51
80:54:4936:G:H1'	80:54:4937:C:OP1	2.10	0.51
85:23:48:5MC:OP2	85:23:48:5MC:H6	1.94	0.51
1:A1:441:C:OP2	10:J1:2:GLY:N	2.44	0.51
8:H1:215:LYS:O	8:H1:219:GLU:HB2	2.11	0.51
25:Y1:84:PHE:CE2	25:Y1:86:PRO:HA	2.46	0.51
42:G2:243:LEU:HD11	42:G2:255:VAL:HG22	1.92	0.51
80:54:520:U:H2'	80:54:521:C:C6	2.46	0.51
84:B:155:ILE:HG21	84:B:167:VAL:HG13	1.93	0.51
1:A1:1013:U:OP1	1:A1:1129:G:O2'	2.28	0.50
1:A1:1228:A:H2'	1:A1:1229:G:C8	2.46	0.50
6:F1:247:THR:HG23	6:F1:250:GLU:H	1.76	0.50
8:H1:230:LYS:HD2	8:H1:233:ARG:HB3	1.93	0.50
46:L2:107:THR:HG23	69:i2:20:ASN:HB3	1.92	0.50
47:M2:116:LYS:HG3	49:O2:196:LEU:HD21	1.93	0.50
80:54:2485:U:H2'	80:54:2486:G:C8	2.47	0.50
1:A1:1673:U:O2'	7:G1:84:GLY:O	2.21	0.50
14:N1:125:GLU:O	14:N1:129:LYS:N	2.44	0.50
32:f1:117:ASN:OD1	32:f1:118:VAL:N	2.45	0.50
40:E2:286:PRO:HG2	66:f2:7:CYS:SG	2.52	0.50
46:L2:128:PRO:HA	46:L2:138:ASP:OD2	2.11	0.50
59:Y2:30:MET:HB3	59:Y2:101:PRO:HG2	1.93	0.50
79:t2:79:ALA:HA	79:t2:82:ILE:HB	1.93	0.50
80:54:2491:C:H2'	80:54:2492:C:O4'	2.11	0.50
80:54:3909:C:H1'	83:XX:1023:LYS:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1423:C:H2'	1:A1:1424:G:O4'	2.11	0.50
5:E1:211:VAL:O	19:S1:20:TYR:OH	2.24	0.50
38:C2:323:ARG:HE	80:54:976:G:N2	2.09	0.50
47:M2:9:VAL:HG11	47:M2:66:HIS:HA	1.93	0.50
53:S2:118:ARG:NH2	80:54:2034:G:O2'	2.44	0.50
61:a2:130:SER:OG	80:54:1397:A:OP1	2.24	0.50
70:j2:20:ARG:NH2	70:j2:39:TYR:OH	2.44	0.50
78:s2:24:TYR:HD2	78:s2:90:PHE:HB3	1.74	0.50
79:t2:41:LYS:O	79:t2:45:ASP:HB2	2.12	0.50
1:A1:1834:A:H2	1:A1:1837:G:N1	2.08	0.50
8:H1:58:LYS:NZ	8:H1:106:LEU:O	2.42	0.50
19:S1:77:GLU:O	19:S1:81:ARG:NH2	2.45	0.50
21:U1:115:LYS:HG2	21:U1:121:ARG:NH2	2.26	0.50
44:I2:118:ALA:O	80:54:1864:G:O2'	2.23	0.50
78:s2:175:LEU:O	78:s2:179:ASN:N	2.45	0.50
80:54:966:A:H1'	80:54:968:C:N4	2.26	0.50
80:54:2553:A:O2'	80:54:2554:U:OP2	2.28	0.50
80:54:3648:A:H1'	80:54:3785:A:N6	2.27	0.50
80:54:4098:A:H2'	80:54:4099:G:C8	2.47	0.50
1:A1:219:U:O4'	10:J1:184:ARG:NH1	2.44	0.50
1:A1:935:G:O2'	15:O1:108:ASP:OD1	2.24	0.50
80:54:1787:A:N3	80:54:4210:U:O2'	2.45	0.50
80:54:4907:G:N2	80:54:4913:G:H2'	2.27	0.50
1:A1:1252:C:OP1	22:V1:75:LYS:NZ	2.38	0.50
1:A1:1597:C:H4'	1:A1:1603:G:O6	2.11	0.50
2:B1:205:ARG:NH2	2:B1:213:GLU:OE2	2.44	0.50
13:M1:55:TYR:CD2	13:M1:115:PRO:HG2	2.46	0.50
39:D2:261:VAL:HG11	81:74:119:U:C2	2.46	0.50
62:b2:107:ARG:NH1	80:54:1271:G:OP1	2.37	0.50
66:f2:89:ARG:NH1	80:54:709:C:OP1	2.45	0.50
80:54:2007:G:H1'	80:54:2013:A:C6	2.46	0.50
1:A1:371:A:OP2	10:J1:10:LYS:HB2	2.12	0.50
13:M1:4:ILE:HG13	13:M1:5:GLN:OE1	2.12	0.50
21:U1:10:ASN:ND2	21:U1:12:GLN:HB2	2.27	0.50
21:U1:117:GLN:O	21:U1:118:ASP:HB2	2.11	0.50
34:h1:10:THR:HG22	34:h1:308:ARG:HG2	1.93	0.50
37:B2:107:ALA:HB1	37:B2:202:GLU:HG3	1.93	0.50
79:t2:133:LEU:HD11	79:t2:150:ASP:HB3	1.93	0.50
80:54:1477:C:O2'	80:54:1478:C:OP1	2.28	0.50
1:A1:819:G:OP2	11:K1:80:ARG:NH2	2.45	0.50
1:A1:1076:G:H5''	15:O1:106:ARG:HH22	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1786:U:H2'	1:A1:1787:G:C8	2.47	0.50
2:B1:118:GLU:OE1	4:D1:65:LYS:N	2.43	0.50
7:G1:110:GLN:HE21	7:G1:114:ASN:ND2	2.09	0.50
8:H1:135:PRO:HB2	8:H1:141:ILE:HG12	1.93	0.50
39:D2:275:GLN:HE21	80:54:1187:G:H1'	1.76	0.50
80:54:460:C:H2'	80:54:461:G:C8	2.47	0.50
80:54:1478:C:H2'	80:54:1479:G:C8	2.47	0.50
1:A1:910:G:OP2	52:R2:173:ARG:NH2	2.44	0.50
1:A1:1308:U:H1'	33:g1:135:HIS:NE2	2.27	0.50
1:A1:1337:C:H2'	1:A1:1338:G:C8	2.47	0.50
30:d1:21:THR:OG1	30:d1:66:ARG:NH1	2.42	0.50
34:h1:168:CYS:SG	34:h1:198:VAL:HB	2.52	0.50
51:Q2:75:ARG:HA	51:Q2:78:LYS:HD2	1.94	0.50
55:U2:101:ARG:HG2	55:U2:103:VAL:HG13	1.93	0.50
62:b2:36:ASP:HB3	62:b2:39:PHE:HB3	1.93	0.50
80:54:406:C:O2'	80:54:407:A:OP1	2.26	0.50
1:A1:24:C:O2'	1:A1:25:A:OP1	2.27	0.49
1:A1:830:A:OP2	1:A1:846:G:N2	2.45	0.49
1:A1:912:C:H3'	1:A1:913:A:H5''	1.93	0.49
1:A1:1543:U:OP2	21:U1:62:ARG:NH1	2.39	0.49
3:C1:29:ASP:OD1	3:C1:94:LYS:NZ	2.45	0.49
17:Q1:123:TYR:OH	20:T1:124:ARG:NH1	2.45	0.49
29:c1:31:TYR:O	29:c1:48:SER:OG	2.29	0.49
37:B2:224:LYS:HG3	80:54:4625:C:OP1	2.12	0.49
44:I2:177:ASN:HB2	44:I2:180:GLU:HG2	1.94	0.49
78:s2:121:VAL:O	78:s2:160:LEU:N	2.45	0.49
80:54:1411(C):C:N4	80:54:1412:G:O6	2.45	0.49
80:54:1996:C:H42	80:54:2000:G:H22	1.60	0.49
80:54:2529:A:O2'	80:54:2531:C:OP2	2.30	0.49
1:A1:429:C:O2'	1:A1:811:A:N1	2.42	0.49
1:A1:695:C:H2'	1:A1:696:G:C8	2.47	0.49
7:G1:32:ASP:OD1	7:G1:33:ILE:N	2.45	0.49
19:S1:36:GLU:HG2	19:S1:47:ARG:HD2	1.94	0.49
43:H2:103:VAL:HG11	43:H2:144:LEU:HD21	1.94	0.49
46:L2:19:GLN:HE22	80:54:1518:A:H61	1.60	0.49
49:O2:121:PRO:HD3	53:S2:168:THR:HG22	1.94	0.49
79:t2:134:GLY:HA2	79:t2:147:HIS:HE1	1.77	0.49
80:54:149:A:H5''	80:54:151:G:O4'	2.12	0.49
1:A1:1579:A:O2'	1:A1:1581:C:OP2	2.21	0.49
14:N1:63:LYS:HD2	33:g1:108:VAL:HG23	1.93	0.49
27:a1:111:ARG:NE	85:33:34:70U:C5'	2.72	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:h1:17:TRP:HB2	34:h1:36:ARG:HG3	1.93	0.49
39:D2:272:SER:HB3	39:D2:275:GLN:HG3	1.94	0.49
41:F2:147:LYS:O	41:F2:151:GLU:HG2	2.11	0.49
42:G2:161:GLN:O	42:G2:164:LYS:HG3	2.12	0.49
43:H2:23:ARG:NH1	43:H2:39:ASN:HD22	2.10	0.49
43:H2:42:ASN:ND2	49:O2:131:PRO:HB2	2.27	0.49
45:J2:63:ARG:HE	75:o2:103:VAL:HG21	1.78	0.49
52:R2:82:LYS:O	80:54:2863:G:O2'	2.29	0.49
79:t2:28:LEU:O	79:t2:32:ILE:HG12	2.12	0.49
80:54:969:C:N4	80:54:2095:A:H61	2.09	0.49
80:54:1195:G:H2'	80:54:1196:G:C8	2.46	0.49
80:54:3692:A:N6	80:54:3823:G:H21	2.08	0.49
80:54:3962:A:N7	80:54:4038:C:O2'	2.45	0.49
1:A1:1533:A:OP2	7:G1:164:ARG:NH2	2.45	0.49
1:A1:1863:A:H8	28:b1:79:ILE:HG21	1.78	0.49
8:H1:49:VAL:HG12	8:H1:115:LYS:HB2	1.93	0.49
39:D2:70:GLU:OE1	39:D2:70:GLU:N	2.44	0.49
45:J2:43:LEU:HD13	45:J2:117:ILE:HD11	1.94	0.49
80:54:959:G:H4'	80:54:960:A:O5'	2.13	0.49
80:54:4589:A:N1	80:54:4621:C:O2'	2.41	0.49
80:54:4888:C:H2'	80:54:4889:G:C8	2.47	0.49
82:84:67:U:H2'	82:84:68:G:C8	2.47	0.49
1:A1:1130:G:N2	1:A1:1130:G:OP2	2.42	0.49
1:A1:1808:U:H2'	1:A1:1809:A:C8	2.47	0.49
17:Q1:18:ARG:O	20:T1:93:GLY:N	2.45	0.49
44:I2:3:ARG:NH2	80:54:4431:U:OP2	2.45	0.49
51:Q2:63:LEU:O	51:Q2:67:ILE:HG12	2.12	0.49
80:54:2008:U:H1'	80:54:2011:C:H5	1.77	0.49
80:54:4055:U:O2'	84:B:162:VAL:HG21	2.10	0.49
1:A1:1658:G:OP2	1:A1:1660:C:N4	2.46	0.49
3:C1:179:ASN:HB3	3:C1:183:GLU:HB3	1.94	0.49
4:D1:130:ILE:HG23	4:D1:162:ILE:HD11	1.93	0.49
6:F1:49:ARG:NH2	6:F1:50:ASN:OD1	2.45	0.49
38:C2:204:ARG:HH21	80:54:2298:U:H5''	1.77	0.49
80:54:2503:G:H5'	80:54:2504:C:OP2	2.12	0.49
1:A1:67:C:N4	8:H1:163:ASN:HA	2.27	0.49
1:A1:809:A:H2'	1:A1:810:A:O4'	2.13	0.49
2:B1:42:LYS:NZ	19:S1:99:ASP:OD2	2.32	0.49
8:H1:39:ASP:OD1	8:H1:40:ALA:N	2.45	0.49
21:U1:41:LYS:HE3	21:U1:93:SER:HB2	1.94	0.49
34:h1:10:THR:HB	34:h1:306:LEU:HD12	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:C2:307:LYS:NZ	80:54:2090:U:OP2	2.34	0.49
39:D2:57:ASN:OD1	81:74:27:G:H5'	2.13	0.49
42:G2:103:ASP:OD1	42:G2:105:THR:HG23	2.12	0.49
44:I2:17:TYR:H	44:I2:95:HIS:CD2	2.29	0.49
54:T2:84:ILE:HD12	62:b2:23:LYS:HG2	1.94	0.49
80:54:1481:C:O2'	80:54:1482:G:O5'	2.30	0.49
80:54:2266:C:H4'	80:54:2267:U:O5'	2.13	0.49
80:54:2749:C:H2'	80:54:2750:G:C8	2.47	0.49
80:54:4413:C:H5	80:54:4429:C:H42	1.60	0.49
82:84:122:G:H21	82:84:128:C:H5	1.61	0.49
1:A1:17:C:O2'	1:A1:1194:A:N1	2.43	0.49
4:D1:78:LEU:HD12	4:D1:81:ILE:HD12	1.94	0.49
14:N1:63:LYS:NZ	33:g1:109:ASP:H	2.10	0.49
30:d1:12:ALA:HB1	30:d1:32:VAL:HB	1.94	0.49
34:h1:240:CYS:HG	34:h1:291:TRP:CD1	2.31	0.49
38:C2:338:ASN:C	38:C2:340:ILE:H	2.21	0.49
51:Q2:64:SER:OG	51:Q2:89:ASP:OD2	2.24	0.49
54:T2:87:LYS:NZ	80:54:4305:G:H22	2.09	0.49
59:Y2:55:VAL:HB	59:Y2:104:VAL:HG13	1.95	0.49
63:c2:38:ILE:HD11	63:c2:46:VAL:HG21	1.95	0.49
80:54:4474:A:H2'	80:54:4476:C:O5'	2.13	0.49
1:A1:77:A:O2'	8:H1:174:PRO:O	2.31	0.49
1:A1:1283:C:H4'	1:A1:1287:A:H5'	1.93	0.49
1:A1:1401:A:N6	1:A1:1441:U:O2'	2.45	0.49
12:L1:73:ASN:HA	12:L1:76:ILE:HG12	1.93	0.49
34:h1:20:GLN:OE1	34:h1:288:SER:OG	2.31	0.49
51:Q2:69:LYS:HD2	80:54:1458:C:H5'	1.95	0.49
71:k2:5:ILE:HD12	71:k2:11:PHE:HD1	1.78	0.49
80:54:1617:G:H1'	80:54:2513:A:N6	2.28	0.49
80:54:2258:C:H3'	80:54:2259:G:C8	2.48	0.49
1:A1:1520:G:H5'	1:A1:1521:C:OP2	2.11	0.49
4:D1:165:VAL:HG11	4:D1:217:ALA:HB1	1.94	0.49
11:K1:149:VAL:HG11	11:K1:157:ILE:HD11	1.93	0.49
42:G2:229:LYS:HE3	69:i2:39:PHE:HE1	1.78	0.49
57:W2:117:LYS:HE2	57:W2:121:ALA:HA	1.95	0.49
80:54:197:A:N1	80:54:225:G:O2'	2.41	0.49
80:54:3955:G:N2	80:54:4058:U:O2	2.46	0.49
85:33:8:U:H1'	85:33:48:5MC:H1'	1.94	0.49
1:A1:191:A:N6	1:A1:208:G:O2'	2.46	0.48
1:A1:550:C:O2'	1:A1:551:U:O4'	2.29	0.48
1:A1:1010:G:H2'	1:A1:1011:A:C8	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1842:C:OP2	74:n2:4:LYS:HB2	2.13	0.48
23:W1:42:VAL:HG23	23:W1:43:THR:HG23	1.95	0.48
50:P2:153:LYS:HG3	50:P2:154:GLU:H	1.78	0.48
62:b2:12:GLN:HB3	62:b2:16:TRP:CZ2	2.48	0.48
78:s2:44:ARG:O	78:s2:48:ARG:HB2	2.13	0.48
1:A1:1598:G:OP1	27:a1:80:ARG:NH2	2.45	0.48
7:G1:168:THR:OG1	27:a1:106:GLN:OE1	2.29	0.48
45:J2:14:GLU:OE2	45:J2:16:ARG:NH2	2.36	0.48
50:P2:54:LYS:HA	50:P2:83:TRP:CD1	2.48	0.48
54:T2:4:THR:O	54:T2:9:ARG:NE	2.46	0.48
79:t2:134:GLY:HA2	79:t2:147:HIS:CE1	2.48	0.48
80:54:467:U:O2	80:54:686:A:N6	2.46	0.48
80:54:2740:U:O2'	80:54:2742:G:N2	2.47	0.48
84:B:14:VAL:HA	84:B:17:VAL:HG22	1.95	0.48
84:B:90:LEU:HA	84:B:93:LEU:HB2	1.94	0.48
85:23:34:70U:C3'	85:23:34:70U:H6	2.43	0.48
1:A1:163:U:OP2	8:H1:87:ARG:NH1	2.46	0.48
1:A1:1786:U:H2'	1:A1:1787:G:H8	1.78	0.48
7:G1:66:CYS:SG	7:G1:70:GLU:HG2	2.53	0.48
20:T1:22:GLY:HA2	20:T1:56:ALA:HB3	1.93	0.48
39:D2:128:ASP:OD1	39:D2:129:GLU:N	2.45	0.48
42:G2:152:ALA:HB1	42:G2:189:LEU:HD11	1.95	0.48
50:P2:14:SER:O	50:P2:105:LYS:NZ	2.28	0.48
79:t2:61:LYS:NZ	80:54:1975:G:N7	2.61	0.48
80:54:1199:G:H2'	80:54:1200:G:C8	2.39	0.48
1:A1:531:A:H3'	1:A1:532:C:H5''	1.96	0.48
1:A1:1585:U:O2'	1:A1:1587:G:OP2	2.26	0.48
6:F1:147:ILE:HG21	6:F1:169:ILE:HD11	1.95	0.48
24:X1:104:LEU:HD23	24:X1:125:ILE:HA	1.95	0.48
26:Z1:29:HIS:ND1	26:Z1:29:HIS:O	2.47	0.48
27:a1:46:ASN:ND2	27:a1:79:ILE:O	2.46	0.48
51:Q2:150:ARG:NH2	80:54:1499:C:OP1	2.45	0.48
55:U2:25:CYS:O	55:U2:68:SER:OG	2.31	0.48
65:e2:127:ALA:HB1	80:54:2326:G:H5''	1.95	0.48
71:k2:61:PRO:HG2	71:k2:64:LEU:HD22	1.96	0.48
80:54:3773:U:H2'	80:54:3775:A:H2	1.77	0.48
85:23:8:U:H1'	85:23:48:5MC:H1'	1.94	0.48
5:E1:28:GLU:HG2	12:L1:61:GLN:HG2	1.96	0.48
27:a1:67:LEU:HB3	85:33:34:70U:H91	1.94	0.48
39:D2:244:HIS:O	39:D2:248:ARG:HG3	2.14	0.48
42:G2:234:TYR:CZ	42:G2:279:TYR:HB3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:Z2:136:PHE:OXT	80:54:4122:G:O2'	2.30	0.48
65:e2:26:ASP:OD1	65:e2:26:ASP:N	2.43	0.48
68:h2:63:GLN:NE2	82:84:95:A:N3	2.61	0.48
79:t2:146:ARG:HG2	79:t2:147:HIS:H	1.78	0.48
80:54:959:G:H8	80:54:959:G:OP2	1.95	0.48
82:84:47:C:H1'	82:84:61:A:H2'	1.96	0.48
1:A1:196:C:O2	1:A1:203:G:N2	2.38	0.48
1:A1:220:U:H2'	1:A1:221:A:C8	2.47	0.48
1:A1:909:G:OP2	52:R2:172:ARG:NE	2.29	0.48
1:A1:1706:G:H5'	74:n2:1:MET:HG3	1.96	0.48
6:F1:132:GLY:N	6:F1:136:ILE:O	2.29	0.48
17:Q1:21:ASP:OD1	17:Q1:22:LEU:N	2.46	0.48
20:T1:86:ARG:NH2	20:T1:110:ASP:OD2	2.29	0.48
26:Z1:103:SER:OG	26:Z1:104:ARG:N	2.47	0.48
34:h1:192:THR:OG1	34:h1:213:ASP:OD2	2.31	0.48
36:A2:199:VAL:HG21	80:54:1631:A:N7	2.28	0.48
80:54:4489:G:N3	80:54:4708:A:H2'	2.28	0.48
80:54:4884:G:H2'	80:54:4885:U:O4'	2.13	0.48
82:84:121:G:H3'	82:84:122:G:C8	2.49	0.48
1:A1:189:U:OP1	10:J1:152:ARG:NH2	2.42	0.48
1:A1:332:G:O6	8:H1:189:ARG:NH2	2.44	0.48
1:A1:882:U:H3	1:A1:904:A:H61	1.61	0.48
1:A1:1646:C:H5''	18:R1:138:ARG:HH11	1.78	0.48
6:F1:158:ASP:OD2	6:F1:174:LYS:NZ	2.37	0.48
7:G1:123:GLU:HG3	30:d1:59:LEU:HG	1.95	0.48
9:I1:9:VAL:HB	9:I1:44:ASN:HD21	1.78	0.48
9:I1:69:LEU:O	9:I1:73:GLN:HG2	2.14	0.48
39:D2:211:LEU:HB3	39:D2:219:TYR:HB2	1.95	0.48
42:G2:269:ALA:O	42:G2:273:GLU:HG3	2.14	0.48
46:L2:28:GLN:HE21	48:N2:202:ARG:HD3	1.79	0.48
62:b2:44:ARG:NH2	80:54:1466:G:OP2	2.46	0.48
78:s2:41:GLN:HE22	80:54:1996:C:H1'	1.79	0.48
79:t2:110:VAL:HA	79:t2:113:ALA:HB3	1.96	0.48
80:54:158:A:N1	80:54:276:C:O2'	2.46	0.48
80:54:1872:G:O2'	80:54:4219:A:N3	2.40	0.48
5:E1:115:VAL:HG13	5:E1:150:MET:HE1	1.94	0.48
36:A2:117:GLU:HG2	36:A2:124:GLY:H	1.78	0.48
71:k2:5:ILE:HD11	71:k2:43:TYR:HB3	1.93	0.48
72:l2:44:TRP:CZ3	72:l2:45:ARG:HD3	2.49	0.48
80:54:265:C:H4'	80:54:266:C:OP2	2.07	0.48
80:54:4244:A:O2'	80:54:4268:A:OP1	2.23	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:E2:182:LEU:HD12	40:E2:186:ARG:HA	1.96	0.48
48:N2:145:ASN:HB3	48:N2:148:THR:HG22	1.94	0.48
51:Q2:42:THR:OG1	80:54:1428:U:H5'	2.14	0.48
78:s2:44:ARG:HG3	80:54:1996:C:O2'	2.14	0.48
80:54:1794:A:H5''	80:54:4214:A:N6	2.28	0.48
80:54:1972:G:H1	80:54:1994:C:H42	1.60	0.48
80:54:1982:G:N2	80:54:2009:A:O3'	2.46	0.48
80:54:2479:G:H2'	80:54:2480:G:H8	1.77	0.48
84:B:44:GLN:CG	85:33:62:C:H4'	2.43	0.48
84:B:68:LEU:HB3	84:B:116:LEU:HD23	1.96	0.48
85:33:34:70U:H6	85:33:34:70U:C3'	2.43	0.48
1:A1:10:G:H21	4:D1:114:LYS:HA	1.79	0.48
1:A1:1126:G:OP2	19:S1:129:LYS:NZ	2.36	0.48
2:B1:142:LEU:O	23:W1:60:ARG:NH2	2.47	0.48
3:C1:110:MET:HE1	3:C1:140:VAL:HG21	1.96	0.48
9:I1:40:LEU:HD23	9:I1:43:LEU:HD12	1.95	0.48
12:L1:52:LEU:HD22	12:L1:57:TYR:HD2	1.79	0.48
35:i1:21:A:N6	85:23:34:70U:HN3	2.12	0.48
42:G2:136:PHE:HA	42:G2:236:ILE:HD13	1.96	0.48
43:H2:91:LYS:HG2	43:H2:145:VAL:HG22	1.96	0.48
51:Q2:133:GLY:O	51:Q2:136:THR:OG1	2.27	0.48
80:54:709:C:H1'	80:54:4942:C:H5	1.78	0.48
80:54:4635:A:OP1	80:54:4636:U:O2'	2.31	0.48
80:54:4897:G:H1	80:54:4923:U:H3	1.61	0.48
1:A1:57:U:OP1	1:A1:504:G:O2'	2.31	0.47
1:A1:1016:U:H5''	15:O1:14:SER:HB3	1.95	0.47
1:A1:1606:G:N2	1:A1:1632:G:H1'	2.28	0.47
6:F1:151:ASP:OD2	8:H1:216:ARG:NE	2.47	0.47
14:N1:38:ALA:HB1	14:N1:110:VAL:HG23	1.96	0.47
37:B2:161:ARG:HG2	37:B2:184:GLN:HA	1.94	0.47
43:H2:23:ARG:NE	43:H2:39:ASN:HA	2.27	0.47
50:P2:83:TRP:O	80:54:3856:A:H5''	2.13	0.47
64:d2:75:LYS:HB2	64:d2:79:ASN:O	2.13	0.47
70:j2:28:HIS:CD2	70:j2:31:LYS:H	2.33	0.47
80:54:3607:U:H2'	80:54:3608:A:C8	2.49	0.47
80:54:3958:G:N7	85:33:20:H2U:OP1	2.42	0.47
80:54:4397:A:H2	83:XX:1023:LYS:HD3	1.79	0.47
80:54:5016:A:N6	80:54:5033:G:O2'	2.47	0.47
8:H1:98:ARG:NH2	8:H1:103:ASP:OD1	2.47	0.47
15:O1:100:LYS:O	15:O1:103:GLU:HG2	2.13	0.47
37:B2:94:GLU:H	37:B2:158:GLN:NE2	2.12	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B2:94:GLU:H	37:B2:158:GLN:HE21	1.62	0.47
51:Q2:88:ASP:OD1	51:Q2:89:ASP:N	2.47	0.47
65:e2:35:TRP:CZ2	65:e2:56:PRO:HD2	2.49	0.47
78:s2:121:VAL:HB	78:s2:160:LEU:HB3	1.96	0.47
79:t2:110:VAL:O	79:t2:114:ARG:HD3	2.13	0.47
80:54:478:G:H2'	80:54:479:G:H8	1.77	0.47
80:54:978:G:N2	80:54:1277:G:H1	2.12	0.47
80:54:3732:A:H2'	80:54:3733:A:C8	2.49	0.47
1:A1:791:C:H2'	1:A1:792:C:C6	2.49	0.47
42:G2:308:LYS:HA	42:G2:311:ALA:HB3	1.95	0.47
52:R2:104:ARG:NH1	80:54:2898:G:OP1	2.44	0.47
54:T2:130:ARG:NH2	80:54:1837:A:OP1	2.47	0.47
80:54:5068:G:N2	80:54:5069:U:O4	2.39	0.47
1:A1:343:A:H4'	6:F1:130:PHE:HZ	1.78	0.47
1:A1:587:A:H5'	1:A1:592:C:H41	1.78	0.47
1:A1:1179:G:N2	1:A1:1182:A:OP2	2.42	0.47
1:A1:1587:G:H5''	21:U1:77:LYS:HD3	1.95	0.47
1:A1:1617:G:N7	17:Q1:47:ARG:NH1	2.59	0.47
2:B1:198:MET:HG2	2:B1:200:ASP:H	1.79	0.47
4:D1:114:LYS:HD2	4:D1:121:ARG:NH2	2.28	0.47
4:D1:195:LEU:HB3	4:D1:222:CYS:SG	2.54	0.47
7:G1:18:LYS:HG3	7:G1:48:TYR:CZ	2.49	0.47
10:J1:135:GLU:HG3	10:J1:139:LYS:NZ	2.29	0.47
14:N1:26:LEU:HD11	14:N1:90:GLY:HA3	1.96	0.47
17:Q1:98:ASN:HB3	17:Q1:101:THR:H	1.78	0.47
34:h1:17:TRP:N	34:h1:36:ARG:HB2	2.26	0.47
40:E2:155:ILE:HD12	40:E2:192:THR:HG21	1.96	0.47
43:H2:59:LYS:HE3	43:H2:66:GLU:HB3	1.95	0.47
80:54:2503:G:H2'	80:54:2504:C:C2	2.50	0.47
80:54:4927:G:OP2	80:54:4927:G:N2	2.42	0.47
84:B:44:GLN:CD	85:33:62:C:C5'	2.86	0.47
1:A1:170:A:OP1	8:H1:137:ARG:N	2.40	0.47
1:A1:551:U:H2'	1:A1:552:G:H8	1.78	0.47
1:A1:1759:G:N2	1:A1:1773:C:O2	2.47	0.47
2:B1:85:ARG:HD3	2:B1:203:PHE:O	2.14	0.47
37:B2:378:ARG:HE	57:W2:32:LEU:HD21	1.79	0.47
52:R2:106:LEU:HG	52:R2:120:TYR:CD1	2.49	0.47
76:p2:86:LEU:HD23	76:p2:89:LEU:HD21	1.95	0.47
78:s2:53:VAL:HG22	78:s2:89:VAL:HG22	1.95	0.47
80:54:2487:G:O2'	82:84:126:C:OP1	2.32	0.47
80:54:4060:U:H2'	80:54:4061:G:C8	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N1:54:SER:H	14:N1:80:ASP:CA	2.26	0.47
34:h1:91:ASP:OD2	34:h1:93:THR:OG1	2.25	0.47
42:G2:106:ARG:HG3	42:G2:106:ARG:HH11	1.79	0.47
80:54:4417:C:N4	80:54:4422:A:O2'	2.47	0.47
80:54:5006:U:H4'	80:54:5007:A:H5'	1.96	0.47
85:23:34:70U:O5'	85:23:35:U:P	2.73	0.47
1:A1:444:G:N2	1:A1:447:A:OP2	2.47	0.47
1:A1:1232:U:H2'	1:A1:1233:G:H8	1.79	0.47
5:E1:66:ILE:O	5:E1:70:THR:HG23	2.15	0.47
13:M1:33:LEU:HD12	13:M1:34:PRO:HD2	1.95	0.47
20:T1:51:ASP:OD1	20:T1:51:ASP:N	2.46	0.47
22:V1:96:GLU:HA	22:V1:99:LYS:HB2	1.96	0.47
25:Y1:68:LYS:HE2	32:f1:82:VAL:HG12	1.97	0.47
34:h1:23:THR:HG22	34:h1:31:ILE:HG22	1.97	0.47
37:B2:260:ALA:C	37:B2:261:ARG:HD3	2.40	0.47
38:C2:140:LYS:NZ	38:C2:242:PRO:O	2.44	0.47
49:O2:65:ASN:ND2	80:54:4565:C:OP1	2.40	0.47
59:Y2:82:ILE:HG22	59:Y2:83:GLU:H	1.80	0.47
60:Z2:5:MET:O	60:Z2:28:ASN:ND2	2.48	0.47
79:t2:10:ILE:HG23	79:t2:63:THR:HG23	1.95	0.47
79:t2:53:TRP:O	79:t2:55:GLY:N	2.48	0.47
80:54:978:G:N2	80:54:1277:G:H22	2.13	0.47
80:54:1068:G:H2'	80:54:1069:G:H8	1.79	0.47
80:54:1082:C:H42	80:54:1217:G:H1	1.61	0.47
80:54:1991:A:H2'	80:54:1992:U:O4'	2.14	0.47
80:54:2558:C:H2'	80:54:2559:G:C8	2.50	0.47
80:54:4507:A:H2'	80:54:4508:C:C6	2.50	0.47
1:A1:68:A:OP2	8:H1:164:LYS:NZ	2.44	0.47
3:C1:131:ASP:O	3:C1:133:TYR:N	2.44	0.47
6:F1:100:ARG:HH12	6:F1:122:LYS:HA	1.80	0.47
10:J1:122:GLY:HA2	10:J1:167:GLN:HG2	1.97	0.47
34:h1:4:GLN:O	34:h1:313:THR:OG1	2.31	0.47
37:B2:122:TRP:CE2	37:B2:127:LYS:HE3	2.50	0.47
37:B2:354:GLN:HB3	37:B2:359:ALA:HB1	1.96	0.47
39:D2:106:ALA:HB2	39:D2:166:ALA:HA	1.96	0.47
42:G2:303:ILE:O	42:G2:307:GLU:HG3	2.15	0.47
49:O2:125:LYS:HG2	49:O2:129:LEU:HD12	1.96	0.47
77:r2:28:GLU:CG	77:r2:31:ASN:HB2	2.44	0.47
79:t2:56:LEU:HD22	79:t2:82:ILE:HG21	1.97	0.47
80:54:456:C:H2'	80:54:457:G:C8	2.50	0.47
80:54:2848:G:O2'	80:54:3838:U:O4	2.30	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:220:U:H2'	1:A1:221:A:H8	1.80	0.47
3:C1:25:PHE:HZ	16:P1:53:ILE:HA	1.79	0.47
7:G1:49:LEU:HD12	18:R1:50:LYS:HG2	1.97	0.47
14:N1:27:ILE:HG13	14:N1:28:HIS:HD2	1.80	0.47
19:S1:89:SER:HB3	19:S1:92:ASP:CG	2.40	0.47
21:U1:33:TRP:CE3	21:U1:37:VAL:HG11	2.50	0.47
34:h1:29:ASP:OD2	34:h1:47:ARG:NH2	2.46	0.47
43:H2:111:LEU:HD12	43:H2:127:ARG:HH21	1.80	0.47
52:R2:59:SER:N	80:54:4646:U:OP1	2.40	0.47
52:R2:90:PRO:HG2	52:R2:93:VAL:HG22	1.97	0.47
53:S2:115:ALA:HB2	80:54:2060:G:N2	2.30	0.47
54:T2:17:ARG:HG2	80:54:4277:G:H5''	1.96	0.47
63:c2:50:ASN:ND2	63:c2:75:SER:O	2.48	0.47
80:54:1444:G:H2'	80:54:1445:U:C6	2.50	0.47
80:54:4093:G:H22	80:54:4115:G:N2	2.12	0.47
85:33:58:1MA:O2'	85:33:60:U:OP2	2.29	0.47
6:F1:45:ILE:HA	6:F1:61:VAL:HG11	1.97	0.47
8:H1:57:ASP:OD1	8:H1:58:LYS:N	2.42	0.47
11:K1:78:LEU:HB3	11:K1:92:MET:HG3	1.96	0.47
22:V1:31:SER:HA	22:V1:34:LYS:HG2	1.97	0.47
26:Z1:114:MET:O	26:Z1:122:LYS:NZ	2.42	0.47
51:Q2:16:LYS:O	51:Q2:33:ARG:NH2	2.48	0.47
54:T2:70:HIS:NE2	80:54:4327:C:OP1	2.47	0.47
78:s2:37:SER:OG	80:54:1970:A:OP1	2.32	0.47
80:54:1769:G:H2'	80:54:1770:A:C8	2.50	0.47
80:54:3648:A:H1'	80:54:3785:A:H61	1.79	0.47
80:54:4419:U:OP1	80:54:4421:C:N4	2.48	0.47
88:54:5286:SPD:H92	88:54:5286:SPD:H41	1.97	0.47
85:23:47:H2U:H5''	85:23:47:H2U:H62	1.97	0.47
1:A1:379:C:O2	10:J1:5:ARG:NE	2.48	0.46
14:N1:49:LEU:HD11	14:N1:77:ILE:HD11	1.97	0.46
25:Y1:101:LEU:HB3	25:Y1:124:LYS:HB2	1.96	0.46
27:a1:111:ARG:NE	85:33:34:70U:H5'	2.29	0.46
37:B2:160:ILE:HD11	37:B2:190:VAL:HG13	1.96	0.46
52:R2:175:GLU:O	52:R2:179:ALA:N	2.48	0.46
79:t2:80:LEU:HG	79:t2:112:ILE:HB	1.97	0.46
80:54:62:A:N3	80:54:77:U:O2'	2.42	0.46
80:54:4862:G:H2'	80:54:4863:G:C8	2.50	0.46
80:54:5047:C:H5''	80:54:5050:C:H5	1.80	0.46
85:23:37:12A:H8	85:23:37:12A:H5''	1.98	0.46
85:33:37:12A:H5''	85:33:37:12A:H8	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:15:U:H2'	1:A1:16:G:O4'	2.16	0.46
1:A1:1166:G:N7	25:Y1:25:LYS:HE2	2.29	0.46
1:A1:1521:C:OP1	20:T1:129:LEU:HD13	2.16	0.46
22:V1:60:THR:HG22	22:V1:83:ARG:HG2	1.97	0.46
40:E2:49:ASN:ND2	80:54:979:C:OP1	2.48	0.46
80:54:1238:A:HO2'	80:54:1239:C:P	2.38	0.46
80:54:4083:U:O2'	80:54:4086:G:OP1	2.24	0.46
80:54:4208:U:OP1	80:54:4334:U:O2'	2.33	0.46
14:N1:44:LYS:HG3	14:N1:46:GLN:HG3	1.97	0.46
14:N1:68:LEU:HA	14:N1:71:GLU:HB3	1.98	0.46
16:P1:101:GLY:HA3	16:P1:134:PRO:HG2	1.96	0.46
43:H2:50:LYS:HD2	43:H2:51:LYS:HG3	1.96	0.46
58:X2:73:HIS:CG	58:X2:115:LYS:HD2	2.50	0.46
80:54:1758:G:H2'	80:54:1759:G:C8	2.51	0.46
85:23:33:U:C3'	85:23:35:U:OP1	2.62	0.46
85:23:33:U:C2'	85:23:35:U:P	3.04	0.46
85:33:33:U:O2'	85:33:35:U:H5	1.98	0.46
14:N1:60:MET:SD	14:N1:60:MET:N	2.81	0.46
17:Q1:37:TYR:OH	17:Q1:45:LEU:HD12	2.15	0.46
21:U1:42:HIS:HB2	21:U1:83:GLN:HA	1.98	0.46
33:g1:107:LYS:HG3	33:g1:115:SER:HB3	1.97	0.46
37:B2:90:VAL:HG22	37:B2:104:THR:HG23	1.97	0.46
41:F2:79:ASN:HA	54:T2:143:THR:HG22	1.96	0.46
50:P2:127:ARG:NH2	80:54:2422:C:OP1	2.39	0.46
60:Z2:83:THR:HG22	67:g2:95:PHE:CZ	2.50	0.46
78:s2:39:GLN:O	78:s2:43:ILE:HG13	2.16	0.46
79:t2:77:ALA:HA	79:t2:80:LEU:HB2	1.96	0.46
1:A1:492:C:H5	26:Z1:104:ARG:HH21	1.64	0.46
2:B1:57:LYS:HA	2:B1:57:LYS:HD2	1.80	0.46
3:C1:103:MET:HG3	3:C1:215:VAL:HB	1.98	0.46
5:E1:190:LEU:HD23	5:E1:199:GLY:HA2	1.96	0.46
9:I1:130:LEU:HD21	9:I1:156:VAL:HG21	1.98	0.46
13:M1:150:GLY:O	13:M1:151:THR:HG22	2.16	0.46
14:N1:58:GLU:HG2	14:N1:61:TYR:CB	2.45	0.46
21:U1:33:TRP:HZ2	21:U1:102:ARG:HD2	1.81	0.46
3:C1:25:PHE:HA	3:C1:28:LYS:HG2	1.97	0.46
21:U1:77:LYS:HB2	21:U1:94:ARG:HH12	1.79	0.46
37:B2:174:ARG:NH1	80:54:4985:U:O2	2.41	0.46
41:F2:85:GLU:OE1	54:T2:136:ARG:NH1	2.48	0.46
48:N2:49:ARG:HH21	80:54:114:G:P	2.38	0.46
57:W2:91:MET:HA	57:W2:94:ARG:HB3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:s2:59:THR:HG21	80:54:1961:G:H5''	1.97	0.46
1:A1:51:U:H2'	1:A1:52:G:C8	2.51	0.46
1:A1:549:C:H5'	1:A1:550:C:OP2	2.15	0.46
1:A1:1410:C:H2'	1:A1:1411:G:C8	2.51	0.46
1:A1:1473:G:N1	1:A1:1476:A:OP2	2.49	0.46
6:F1:80:ILE:HG13	6:F1:81:THR:HG23	1.97	0.46
10:J1:165:GLN:HE22	10:J1:172:LEU:H	1.63	0.46
17:Q1:30:TYR:OH	17:Q1:88:GLU:OE2	2.26	0.46
21:U1:7:LYS:HE2	21:U1:66:LEU:HD22	1.97	0.46
33:g1:109:ASP:N	33:g1:109:ASP:OD1	2.48	0.46
37:B2:80:GLU:OE1	37:B2:323:TYR:OH	2.23	0.46
38:C2:110:ARG:O	38:C2:113:ARG:NH1	2.49	0.46
43:H2:41:ILE:HG22	43:H2:43:VAL:HG13	1.96	0.46
48:N2:184:ILE:HD12	80:54:99:A:H5''	1.98	0.46
75:o2:51:GLN:HG2	75:o2:55:ILE:HD11	1.97	0.46
80:54:1755:C:O2'	80:54:1757:U:OP2	2.26	0.46
80:54:1857:C:H2'	80:54:1858:A:C8	2.51	0.46
80:54:1979:A:O2'	80:54:1980:U:OP1	2.31	0.46
80:54:4448:G:H5''	80:54:4449:A:H5'	1.96	0.46
80:54:4874:A:C5	80:54:4877:G:H4'	2.51	0.46
82:84:102:G:OP2	82:84:104:A:O2'	2.31	0.46
83:XX:1021:LYS:O	83:XX:1022:LYS:HB2	2.14	0.46
1:A1:1446:A:O2'	1:A1:1447:G:H5''	2.15	0.46
36:A2:128:ARG:NH2	80:54:3681:G:OP2	2.47	0.46
36:A2:158:ILE:HB	36:A2:162:ASN:HD21	1.81	0.46
42:G2:318:LEU:HD23	42:G2:318:LEU:H	1.81	0.46
49:O2:68:ARG:NH2	80:54:4565:C:OP2	2.48	0.46
51:Q2:2:GLY:N	80:54:2072:C:OP1	2.49	0.46
80:54:1202:C:H2'	80:54:1203:G:H8	1.81	0.46
80:54:2745:A:H2'	80:54:2746:A:C8	2.51	0.46
80:54:3599:A:H2'	80:54:3600:G:C8	2.51	0.46
80:54:4260:U:H2'	80:54:4261:C:C6	2.50	0.46
80:54:4905:C:H42	80:54:4916:G:H1	1.64	0.46
1:A1:150:A:N6	1:A1:169:U:O2	2.49	0.46
1:A1:860:G:N2	24:X1:107:SER:HG	2.14	0.46
5:E1:17:PHE:HE2	5:E1:39:VAL:HG11	1.81	0.46
31:e1:2:GLY:N	31:e1:5:GLN:OE1	2.48	0.46
39:D2:64:ILE:HG12	39:D2:105:LEU:HD11	1.98	0.46
48:N2:113:LEU:HB2	48:N2:134:LEU:HD23	1.98	0.46
54:T2:130:ARG:HG2	80:54:1837:A:OP2	2.16	0.46
66:f2:56:ASN:OD1	66:f2:66:LYS:NZ	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
79:t2:35:LEU:HB3	79:t2:37:LEU:HD23	1.98	0.46
80:54:3777:G:O2'	80:54:3815:G:O6	2.31	0.46
85:33:34:70U:O5'	85:33:35:U:P	2.73	0.46
1:A1:373:G:OP1	13:M1:137:THR:OG1	2.32	0.46
1:A1:1114:U:H3	1:A1:1119:A:H61	1.64	0.46
2:B1:5:LEU:HD21	23:W1:41:LYS:HA	1.97	0.46
2:B1:102:ARG:HA	2:B1:102:ARG:HD2	1.80	0.46
8:H1:219:GLU:HG2	8:H1:223:LYS:HZ3	1.80	0.46
14:N1:24:THR:O	14:N1:27:ILE:HG12	2.15	0.46
37:B2:57:VAL:HB	37:B2:367:PHE:HB3	1.98	0.46
38:C2:356:ALA:O	38:C2:360:ALA:N	2.42	0.46
49:O2:168:TYR:CE2	49:O2:172:LYS:HD3	2.51	0.46
55:U2:76:VAL:HG22	55:U2:77:PRO:HD2	1.98	0.46
79:t2:132:ILE:HA	79:t2:135:THR:HB	1.97	0.46
80:54:1484:G:O2'	80:54:1486:C:OP2	2.34	0.46
80:54:1604:G:H2'	80:54:1605:G:C8	2.52	0.46
80:54:1980:U:O2'	80:54:1982:G:O6	2.26	0.46
80:54:2566:G:H2'	80:54:2567:G:H8	1.81	0.46
1:A1:4:C:H4'	4:D1:207:ALA:HB2	1.98	0.45
1:A1:1864:U:OP2	28:b1:4:LYS:NZ	2.45	0.45
7:G1:59:LYS:HD3	7:G1:59:LYS:HA	1.72	0.45
14:N1:22:LEU:HD13	14:N1:89:VAL:HA	1.98	0.45
14:N1:86:GLY:HA2	14:N1:89:VAL:HG12	1.99	0.45
21:U1:122:LYS:HG2	21:U1:123:LEU:H	1.80	0.45
46:L2:13:HIS:NE2	80:54:97:G:N7	2.58	0.45
80:54:1941:A:C2	80:54:4434:C:H5'	2.52	0.45
80:54:4135:G:H2'	80:54:4136:G:H8	1.81	0.45
14:N1:22:LEU:HD22	14:N1:89:VAL:HG23	1.98	0.45
18:R1:58:LEU:O	18:R1:62:ARG:HD3	2.16	0.45
34:h1:64:HIS:HD2	34:h1:65:PHE:H	1.58	0.45
42:G2:111:PRO:HD2	42:G2:114:ILE:HD12	1.98	0.45
46:L2:70:VAL:HG22	46:L2:159:ASN:HB3	1.98	0.45
49:O2:61:ARG:HA	49:O2:70:PRO:HD2	1.98	0.45
51:Q2:108:ARG:NH1	80:54:1355:G:OP1	2.33	0.45
57:W2:107:GLN:O	57:W2:111:ALA:N	2.43	0.45
60:Z2:50:PRO:HD3	60:Z2:68:ILE:HG12	1.97	0.45
61:a2:9:ARG:NH1	80:54:2345:G:N7	2.64	0.45
78:s2:31:GLY:HA3	78:s2:190:GLN:HE21	1.81	0.45
80:54:4045:G:C2	80:54:4047:A:H5''	2.51	0.45
85:33:33:U:C2'	85:33:35:U:P	3.04	0.45
1:A1:1007:C:H2'	1:A1:1008:A:C8	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1101:U:OP1	3:C1:151:ARG:HG3	2.17	0.45
1:A1:1780:G:H2'	1:A1:1781:A:O4'	2.17	0.45
3:C1:83:LYS:HD2	3:C1:106:THR:HG22	1.99	0.45
7:G1:165:ASN:OD1	7:G1:166:ILE:N	2.49	0.45
11:K1:124:HIS:HD2	32:f1:104:ARG:HH21	1.63	0.45
20:T1:16:LEU:HD21	20:T1:72:GLN:HE21	1.81	0.45
36:A2:194:ASN:HB2	80:54:1539:G:H4'	1.98	0.45
37:B2:182:GLU:OE2	80:54:4580:U:O2'	2.21	0.45
40:E2:201:SER:N	40:E2:291:PHE:O	2.49	0.45
41:F2:143:TYR:N	41:F2:236:GLU:O	2.44	0.45
58:X2:83:THR:HG21	80:54:2434:G:H5'	1.99	0.45
60:Z2:41:ALA:HB2	60:Z2:77:TYR:HE1	1.82	0.45
66:f2:100:ARG:NH1	80:54:4753:U:OP1	2.49	0.45
76:p2:30:GLU:HA	76:p2:33:GLN:HG2	1.98	0.45
78:s2:69:LEU:HG	78:s2:70:GLU:CD	2.42	0.45
80:54:168:C:H2'	80:54:169:A:C8	2.52	0.45
80:54:922:C:H2'	80:54:922(A):G:C8	2.51	0.45
80:54:1442:C:H2'	80:54:1443:A:O4'	2.17	0.45
80:54:2318:G:N2	80:54:2321:G:OP2	2.29	0.45
80:54:2411:C:H2'	80:54:2412:A:C8	2.51	0.45
80:54:3875:G:H2'	80:54:3876:A:H3'	1.99	0.45
82:84:67:U:H2'	82:84:68:G:H8	1.80	0.45
1:A1:110:U:H3	1:A1:351:G:H1	1.63	0.45
1:A1:207:G:H2'	1:A1:208:G:O4'	2.16	0.45
1:A1:1399:C:H4'	34:h1:100:ARG:NH1	2.30	0.45
16:P1:53:ILE:HG23	16:P1:88:LEU:HD12	1.98	0.45
26:Z1:15:ASN:ND2	26:Z1:22:GLN:OE1	2.41	0.45
27:a1:66:LYS:N	85:33:34:70U:C5'	2.78	0.45
68:h2:70:ARG:HB3	68:h2:83:LEU:HD22	1.99	0.45
77:r2:113:ARG:O	77:r2:117:ILE:HG12	2.16	0.45
80:54:648:G:H2'	80:54:649:A:H8	1.82	0.45
80:54:968:C:H42	80:54:2096:G:H1	1.63	0.45
80:54:1484:G:N3	80:54:1484:G:H2'	2.32	0.45
80:54:1942:A:H61	80:54:2039:G:H2'	1.80	0.45
80:54:3974:G:H2'	80:54:3975:C:O4'	2.17	0.45
80:54:4266:G:H2'	80:54:4266:G:N3	2.32	0.45
84:B:48:ARG:HH12	85:33:54:2MU:H5''	1.81	0.45
1:A1:1137:U:O2'	1:A1:1138:C:H3'	2.17	0.45
3:C1:136:ARG:HB3	3:C1:216:LYS:HB2	1.97	0.45
4:D1:248:TYR:OH	23:W1:11:LEU:HB2	2.17	0.45
5:E1:55:THR:HA	5:E1:58:VAL:HG12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H1:50:VAL:HG12	8:H1:113:ILE:HA	1.98	0.45
18:R1:146:ARG:CZ	85:23:33:U:OP2	2.63	0.45
25:Y1:100:VAL:HG12	25:Y1:125:VAL:HG23	1.98	0.45
34:h1:248:LEU:HB3	34:h1:261:LEU:HD21	1.97	0.45
39:D2:41:LYS:HG3	54:T2:93:ILE:HG13	1.97	0.45
40:E2:156:LEU:HD11	40:E2:198:ILE:HG13	1.97	0.45
40:E2:275:ARG:NH2	80:54:4884:G:O6	2.50	0.45
40:E2:289:LEU:HD12	47:M2:109:ARG:CZ	2.47	0.45
41:F2:143:TYR:CE2	41:F2:236:GLU:HB3	2.52	0.45
44:I2:77:VAL:HG13	44:I2:82:LYS:HA	1.98	0.45
47:M2:12:VAL:HB	47:M2:60:PHE:HB2	1.98	0.45
54:T2:116:LYS:NZ	80:54:1836:G:O6	2.50	0.45
80:54:3707:U:H2'	80:54:3708:C:C6	2.52	0.45
80:54:4743:G:H2'	80:54:4744:A:O4'	2.16	0.45
1:A1:1335:G:OP1	5:E1:185:LYS:NZ	2.49	0.45
10:J1:130:THR:HG22	10:J1:131:PRO:HD3	1.98	0.45
18:R1:104:SER:O	18:R1:107:GLU:HG2	2.17	0.45
24:X1:7:LEU:HD21	24:X1:33:VAL:HG12	1.98	0.45
24:X1:28:ARG:HB2	24:X1:29:PRO:HD3	1.99	0.45
34:h1:164:ILE:HA	34:h1:178:ASN:HA	1.98	0.45
34:h1:171:ASP:OD1	34:h1:171:ASP:N	2.47	0.45
36:A2:41:ILE:HG12	36:A2:63:PHE:HD2	1.82	0.45
49:O2:12:ARG:HD3	49:O2:37:ARG:NH1	2.32	0.45
79:t2:113:ALA:HA	79:t2:116:MET:HG2	1.99	0.45
80:54:679:C:H2'	80:54:680:G:C8	2.52	0.45
80:54:2089:G:H1'	80:54:2090:U:OP2	2.17	0.45
80:54:2557:G:H1	80:54:2570:U:H3	1.65	0.45
80:54:4719:G:O2'	80:54:4720:C:O5'	2.26	0.45
82:84:93:C:O2'	82:84:94:G:H8	1.99	0.45
1:A1:969:U:OP1	1:A1:970:G:O2'	2.20	0.45
1:A1:1404:U:P	22:V1:21:ARG:HH12	2.40	0.45
8:H1:49:VAL:HG12	8:H1:115:LYS:CB	2.46	0.45
8:H1:121:ILE:HG22	8:H1:123:GLY:H	1.81	0.45
11:K1:129:LEU:HB3	11:K1:135:ILE:HD11	1.99	0.45
15:O1:83:ASP:OD1	15:O1:83:ASP:N	2.50	0.45
27:a1:66:LYS:H	85:33:34:70U:H6	1.81	0.45
45:J2:155:HIS:HB2	81:74:55:A:H4'	1.99	0.45
46:L2:141:ALA:HA	46:L2:144:LEU:HD12	1.99	0.45
52:R2:42:ARG:NH1	80:54:2525:U:OP2	2.49	0.45
52:R2:92:LYS:NZ	80:54:2667:C:O2	2.45	0.45
53:S2:161:ARG:HH12	80:54:4876:A:N6	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
71:k2:17:ARG:HD2	71:k2:19:ASP:OD1	2.16	0.45
78:s2:69:LEU:HG	78:s2:70:GLU:OE1	2.17	0.45
80:54:417:G:H1'	82:84:16:G:N2	2.31	0.45
80:54:922:C:H2'	80:54:922(A):G:H8	1.82	0.45
80:54:1443:A:H3'	80:54:1444:G:C8	2.52	0.45
80:54:4135:G:H2'	80:54:4136:G:C8	2.51	0.45
80:54:4476:C:O2'	80:54:4478:G:OP2	2.32	0.45
81:74:38:U:N3	81:74:41:G:OP2	2.38	0.45
85:33:17:C:H3'	85:33:17:C:OP2	2.16	0.45
1:A1:191:A:OP1	10:J1:142:SER:OG	2.26	0.45
1:A1:1265:A:H5''	1:A1:1266:C:OP2	2.16	0.45
16:P1:36:SER:OG	16:P1:37:PHE:N	2.49	0.45
22:V1:19:ARG:HG2	22:V1:92:HIS:CD2	2.52	0.45
27:a1:111:ARG:HE	85:33:34:70U:H5'	1.76	0.45
41:F2:23:ASN:O	80:54:966:A:H5''	2.17	0.45
44:I2:51:HIS:ND1	44:I2:137:SER:OG	2.42	0.45
46:L2:63:THR:HG21	61:a2:66:ASN:HD22	1.82	0.45
52:R2:103:ARG:O	52:R2:107:ARG:HB2	2.16	0.45
70:j2:63:ARG:NH1	82:84:58:G:O6	2.47	0.45
80:54:1443:A:H3'	80:54:1444:G:H8	1.82	0.45
80:54:1769:G:H2'	80:54:1770:A:H8	1.81	0.45
80:54:2045:G:O6	80:54:3870:C:O2'	2.35	0.45
80:54:2258:C:H3'	80:54:2259:G:H8	1.80	0.45
82:84:32:C:H2'	82:84:33:G:O4'	2.16	0.45
1:A1:143:U:OP1	8:H1:149:LYS:NZ	2.40	0.45
6:F1:43:PRO:HD2	6:F1:46:ILE:HD12	1.98	0.45
8:H1:228:ILE:HA	8:H1:231:ARG:HB2	1.99	0.45
24:X1:90:GLN:HB2	24:X1:94:LEU:HD12	1.98	0.45
25:Y1:87:ASN:HB2	25:Y1:90:CYS:SG	2.56	0.45
43:H2:45:LEU:HD22	43:H2:57:VAL:HG22	1.99	0.45
75:o2:4:VAL:O	75:o2:94:GLY:N	2.49	0.45
80:54:2710:C:H2'	80:54:2712:G:H5'	1.99	0.45
80:54:4065:G:H3'	80:54:4066:U:C6	2.51	0.45
80:54:4397:A:C5	88:54:5287:SPD:H31	2.52	0.45
85:33:47:H2U:H62	85:33:47:H2U:H5''	1.97	0.45
1:A1:756:C:N4	1:A1:788:G:O6	2.50	0.45
5:E1:56:GLN:H	5:E1:56:GLN:CD	2.25	0.45
14:N1:89:VAL:HG21	14:N1:109:VAL:HG21	1.99	0.45
20:T1:34:LYS:HG2	20:T1:103:LEU:HD23	1.99	0.45
34:h1:212:LYS:HA	34:h1:235:ILE:HG13	1.98	0.45
37:B2:160:ILE:HD13	37:B2:194:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:S2:82:LEU:HD21	53:S2:109:CYS:SG	2.57	0.45
66:f2:78:HIS:HB2	66:f2:85:ARG:HG3	1.97	0.45
70:j2:2:THR:O	70:j2:7:SER:OG	2.29	0.45
80:54:119:G:H3'	80:54:120:A:H5''	1.99	0.45
85:23:37:12A:N1	85:23:37:12A:HA	2.32	0.45
1:A1:656:G:H5'	1:A1:662:G:N2	2.32	0.44
1:A1:1617:G:N7	17:Q1:43:ARG:NH1	2.64	0.44
3:C1:36:PRO:HG2	3:C1:39:PHE:HE1	1.82	0.44
9:I1:44:ASN:OD1	9:I1:45:ILE:N	2.50	0.44
9:I1:130:LEU:HD23	9:I1:142:LYS:HE2	1.99	0.44
34:h1:73:SER:HB3	34:h1:117:ASN:HD21	1.82	0.44
37:B2:252:ALA:HB3	80:54:4457:U:H1'	1.99	0.44
38:C2:323:ARG:NH2	80:54:1279:A:O3'	2.49	0.44
39:D2:64:ILE:HG13	39:D2:109:LEU:HD13	1.99	0.44
80:54:1332:C:H2'	80:54:1333:A:C8	2.52	0.44
80:54:1354:A:N1	80:54:1385:G:O2'	2.44	0.44
80:54:2402:G:H5''	80:54:2786:C:N4	2.32	0.44
80:54:3641:U:H5	80:54:3646:A:N7	2.15	0.44
80:54:4098:A:H2'	80:54:4099:G:H8	1.81	0.44
80:54:4274:A:H2'	80:54:4275:G:C8	2.52	0.44
80:54:4575:G:O2'	80:54:5069:U:OP1	2.35	0.44
80:54:4699:U:H1'	80:54:4700:A:H5''	1.98	0.44
82:84:60:G:O6	82:84:96:C:O2'	2.29	0.44
85:33:37:12A:HA	85:33:37:12A:N1	2.32	0.44
1:A1:1117:C:O2'	1:A1:1118:C:O2	2.31	0.44
1:A1:1314:U:H2'	12:L1:2:LEU:HA	1.99	0.44
5:E1:54:ARG:HB3	5:E1:57:ASN:ND2	2.32	0.44
13:M1:101:ARG:HB2	25:Y1:10:ALA:HB2	1.99	0.44
26:Z1:21:LYS:HD2	26:Z1:75:ILE:HD11	1.98	0.44
42:G2:213:ASP:N	42:G2:213:ASP:OD1	2.51	0.44
48:N2:50:ARG:HD3	80:54:278:G:O4'	2.18	0.44
52:R2:44:LEU:HD22	52:R2:49:LEU:HD12	1.99	0.44
54:T2:57:TYR:OH	54:T2:87:LYS:HE3	2.17	0.44
79:t2:45:ASP:O	79:t2:48:LYS:HG3	2.16	0.44
80:54:4864:U:H2'	80:54:4865:C:O4'	2.18	0.44
80:54:4897:G:H2'	80:54:4898:G:C8	2.52	0.44
85:33:33:U:C3'	85:33:35:U:OP1	2.62	0.44
1:A1:465:A:H4'	1:A1:466:G:O5'	2.18	0.44
1:A1:1109:C:N3	19:S1:126:MET:HG3	2.33	0.44
1:A1:1432:U:O2'	1:A1:1438:A:OP1	2.30	0.44
1:A1:1622:U:H3'	1:A1:1623:A:H4'	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H1:32:MET:HB3	8:H1:65:GLN:NE2	2.31	0.44
29:c1:64:CYS:HB3	29:c1:73:LEU:HD23	1.98	0.44
40:E2:132:GLY:C	40:E2:133:LYS:HD2	2.42	0.44
53:S2:76:LYS:HD2	53:S2:131:GLU:OE1	2.17	0.44
55:U2:56:LEU:HD22	55:U2:61:VAL:O	2.18	0.44
63:c2:26:LYS:HE3	63:c2:26:LYS:HB3	1.71	0.44
68:h2:97:LYS:HB2	68:h2:97:LYS:HE3	1.78	0.44
80:54:2544:G:H2'	80:54:2545:U:O4'	2.18	0.44
80:54:3970:G:H5'	84:B:60:ARG:NH2	2.33	0.44
80:54:3972:A:H4'	80:54:3973:G:O4'	2.18	0.44
80:54:4188:U:H2'	80:54:4189:U:C6	2.52	0.44
80:54:4594:U:H2'	80:54:4595:G:H8	1.81	0.44
84:B:7:ARG:HH12	84:B:184:HIS:HB2	1.82	0.44
84:B:59:PRO:HB2	84:B:170:GLY:H	1.82	0.44
2:B1:108:PHE:HB2	2:B1:136:GLU:HG2	1.98	0.44
4:D1:166:ARG:O	4:D1:181:PRO:HD3	2.17	0.44
5:E1:11:PHE:HB3	22:V1:82:MET:HE2	1.99	0.44
6:F1:45:ILE:HD12	6:F1:80:ILE:HD12	2.00	0.44
8:H1:5:ILE:HG22	8:H1:124:LEU:HD21	1.98	0.44
12:L1:31:LYS:HA	12:L1:41:PRO:HA	1.99	0.44
27:a1:66:LYS:HB2	85:33:34:70U:H72	1.99	0.44
42:G2:185:ARG:HB3	80:54:119:G:C6	2.52	0.44
44:I2:193:ASP:N	44:I2:193:ASP:OD1	2.51	0.44
52:R2:110:ARG:NH1	80:54:2664:G:OP1	2.46	0.44
67:g2:62:LYS:NZ	80:54:2516:G:O2'	2.51	0.44
68:h2:8:ASP:OD1	68:h2:8:ASP:N	2.44	0.44
78:s2:138:PHE:HD1	78:s2:174:LEU:HD23	1.83	0.44
80:54:517:C:H2'	80:54:518:G:C8	2.52	0.44
80:54:914:U:H1'	80:54:915:A:C5	2.53	0.44
80:54:2561:C:N4	80:54:2562:G:O6	2.50	0.44
80:54:2588:C:H5''	80:54:2589:C:H5''	2.00	0.44
80:54:4092:G:H3'	80:54:4093:G:H8	1.81	0.44
84:B:171:HIS:CE1	84:B:174:MET:HE2	2.52	0.44
1:A1:1284:A:H61	1:A1:1313:A:H2'	1.82	0.44
10:J1:106:SER:HB3	10:J1:171:LEU:HG	1.99	0.44
16:P1:96:LYS:HD3	16:P1:132:VAL:HG11	1.98	0.44
16:P1:129:ILE:O	28:b1:65:PRO:HG3	2.18	0.44
24:X1:42:MET:HE2	24:X1:42:MET:HB3	1.87	0.44
26:Z1:58:PHE:CE1	26:Z1:74:MET:HE2	2.52	0.44
34:h1:11:LEU:HB2	34:h1:307:VAL:HG13	1.99	0.44
34:h1:256:ILE:HD11	34:h1:286:CYS:SG	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:B2:21:ARG:NH2	80:54:4981:G:O6	2.50	0.44
37:B2:80:GLU:OE2	37:B2:328:ASN:ND2	2.50	0.44
45:J2:94:LEU:O	45:J2:175:LEU:N	2.39	0.44
46:L2:48:PRO:HB2	68:h2:120:ALA:HB2	2.00	0.44
47:M2:135:LEU:HD12	47:M2:136:LEU:HD23	1.99	0.44
56:V2:42:VAL:HB	56:V2:45:ILE:HD12	2.00	0.44
59:Y2:72:GLN:HE21	59:Y2:74:TYR:HD1	1.64	0.44
67:g2:36:LYS:NZ	80:54:2519:U:OP2	2.39	0.44
70:j2:34:CYS:HB3	70:j2:39:TYR:H	1.83	0.44
78:s2:16:LYS:HE2	78:s2:16:LYS:HB3	1.84	0.44
78:s2:28:PHE:CZ	78:s2:95:LEU:HA	2.52	0.44
80:54:1440:U:O2'	80:54:1441:C:OP1	2.33	0.44
80:54:1973:G:OP2	80:54:1974:U:H3'	2.17	0.44
80:54:3890:A:N6	80:54:4570:G:O2'	2.48	0.44
80:54:4115:G:H4'	80:54:4116:C:H5'	1.98	0.44
82:84:92:U:H2'	82:84:93:C:O4'	2.17	0.44
85:23:33:U:O2'	85:23:35:U:H5	1.98	0.44
4:D1:263:LYS:HE2	4:D1:267:GLN:HG2	2.00	0.44
6:F1:155:LYS:HD3	6:F1:155:LYS:HA	1.71	0.44
7:G1:34:SER:HA	30:d1:55:VAL:HB	1.98	0.44
14:N1:31:LEU:HA	14:N1:111:VAL:HA	1.99	0.44
40:E2:66:SER:HB2	80:54:1072:C:H41	1.82	0.44
41:F2:225:HIS:NE2	41:F2:233:GLY:HA3	2.32	0.44
44:I2:4:ARG:NH2	80:54:1866:U:OP1	2.39	0.44
67:g2:50:PRO:HG3	76:p2:61:MET:HE3	1.99	0.44
80:54:1292:C:H5'	80:54:1293:G:OP2	2.17	0.44
80:54:4169:G:H4'	80:54:4171:C:C2	2.52	0.44
3:C1:146:ARG:HH11	3:C1:206:PRO:HG3	1.82	0.44
8:H1:32:MET:HE2	8:H1:63:MET:HE2	1.99	0.44
14:N1:77:ILE:HG22	14:N1:78:LYS:H	1.83	0.44
37:B2:49:TYR:OH	37:B2:179:HIS:ND1	2.44	0.44
37:B2:95:THR:HG22	37:B2:97:ARG:H	1.83	0.44
40:E2:135:PRO:HB2	80:54:1288:G:OP1	2.17	0.44
46:L2:162:LYS:NZ	80:54:643:C:OP1	2.43	0.44
47:M2:24:LEU:HD11	47:M2:86:TRP:CG	2.52	0.44
52:R2:4:LEU:HB2	80:54:2386:U:H5'	1.99	0.44
53:S2:29:ARG:HB2	54:T2:148:PRO:HB2	2.00	0.44
56:V2:87:SER:HA	56:V2:97:TYR:HB3	1.99	0.44
56:V2:106:VAL:HG12	56:V2:112:MET:HA	2.00	0.44
56:V2:109:LYS:HB3	56:V2:109:LYS:HE2	1.80	0.44
64:d2:70:LYS:HG3	80:54:2389:A:H4'	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:679:C:H2'	80:54:680:G:H8	1.82	0.44
80:54:1358:G:O2'	80:54:1360:G:O6	2.32	0.44
80:54:1396:G:HO2'	80:54:1468:C:HO2'	1.62	0.44
80:54:1480:C:O2'	80:54:1482:G:OP2	2.36	0.44
80:54:1741:G:H3'	80:54:1742:A:C5'	2.48	0.44
80:54:2003:G:H22	80:54:2016:C:H42	1.66	0.44
80:54:4413:C:H5	80:54:4429:C:N4	2.15	0.44
83:XX:1015:LYS:O	83:XX:1016:LYS:CB	2.65	0.44
85:23:17:C:H3'	85:23:17:C:OP2	2.16	0.44
1:A1:65:C:N4	8:H1:133:LEU:HD13	2.33	0.44
1:A1:380:G:N1	1:A1:383:G:OP2	2.41	0.44
1:A1:417:C:O2'	1:A1:418:A:OP1	2.35	0.44
1:A1:921:G:C6	24:X1:28:ARG:HD2	2.53	0.44
1:A1:1298:G:O2'	1:A1:1299:A:C8	2.70	0.44
1:A1:1836:G:OP1	1:A1:1839:U:H4'	2.17	0.44
3:C1:149:GLN:OE1	3:C1:154:SER:HB2	2.17	0.44
4:D1:232:THR:HG22	4:D1:235:ASN:H	1.83	0.44
9:I1:51:ILE:HG21	9:I1:179:LYS:HG2	1.99	0.44
17:Q1:36:LEU:O	20:T1:88:LYS:HD3	2.17	0.44
34:h1:25:PRO:HG2	34:h1:26:GLN:NE2	2.33	0.44
48:N2:169:ARG:NH1	80:54:63:G:OP1	2.50	0.44
54:T2:101:SER:HB2	80:54:1729:A:H2	1.82	0.44
70:j2:45:ARG:NH1	80:54:372:A:O3'	2.51	0.44
80:54:3625:G:O2'	80:54:3626:G:OP1	2.31	0.44
80:54:3932:U:H2'	80:54:3933:G:C8	2.53	0.44
1:A1:686:U:OP1	24:X1:32:LYS:N	2.47	0.44
1:A1:1236:G:O2'	17:Q1:131:PRO:O	2.23	0.44
7:G1:167:LYS:HA	27:a1:71:ALA:HB1	1.99	0.44
8:H1:2:LYS:HB2	8:H1:108:VAL:HG23	2.00	0.44
24:X1:30:CYS:SG	24:X1:31:SER:N	2.91	0.44
26:Z1:99:LYS:HD3	26:Z1:100:LYS:N	2.32	0.44
42:G2:134:ASN:O	42:G2:137:THR:OG1	2.34	0.44
43:H2:53:LYS:NZ	80:54:758:G:OP1	2.39	0.44
54:T2:43:LYS:HG3	54:T2:58:HIS:CE1	2.53	0.44
56:V2:82:ILE:HD12	56:V2:121:VAL:HG22	2.00	0.44
58:X2:156:ILE:HD12	58:X2:156:ILE:HA	1.86	0.44
66:f2:45:LYS:HD3	66:f2:107:PRO:HD2	2.00	0.44
70:j2:48:ASN:ND2	80:54:52:G:OP2	2.51	0.44
78:s2:175:LEU:HA	78:s2:178:LEU:HB2	2.00	0.44
80:54:106:A:H2'	80:54:107:G:O4'	2.18	0.44
80:54:2639:U:H2'	80:54:2694:G:H1	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:3879:G:O2'	80:54:3881:G:OP2	2.35	0.44
80:54:3961:G:N2	80:54:3963:A:N7	2.66	0.44
1:A1:67:C:H5	8:H1:164:LYS:H	1.64	0.43
1:A1:860:G:N2	24:X1:107:SER:OG	2.51	0.43
1:A1:1307:U:H2'	33:g1:135:HIS:CE1	2.53	0.43
1:A1:1511:U:H2'	1:A1:1512:C:C6	2.53	0.43
8:H1:10:THR:HB	8:H1:128:THR:HG22	1.99	0.43
9:I1:88:SER:OG	9:I1:89:GLY:N	2.51	0.43
24:X1:55:ASP:OD1	24:X1:59:GLY:HA2	2.18	0.43
42:G2:170:ARG:O	42:G2:174:LYS:HG2	2.18	0.43
44:I2:90:ARG:NH2	80:54:1784:U:OP1	2.50	0.43
48:N2:178:HIS:HA	48:N2:181:HIS:NE2	2.33	0.43
51:Q2:146:ARG:HH22	80:54:1347:G:P	2.41	0.43
53:S2:53:LYS:NZ	81:74:74:A:N3	2.64	0.43
62:b2:42:ASN:OD1	80:54:1814:C:O2'	2.30	0.43
78:s2:24:TYR:CD2	78:s2:90:PHE:HB3	2.53	0.43
80:54:114:G:N2	80:54:158:A:H61	2.16	0.43
80:54:1079:C:H2'	80:54:1080:C:C6	2.53	0.43
80:54:2276:A:H2'	80:54:2277:C:O4'	2.17	0.43
1:A1:922:A:OP1	24:X1:28:ARG:NH2	2.50	0.43
1:A1:1447:G:OP1	22:V1:87:ARG:NH1	2.51	0.43
1:A1:1839:U:O4	28:b1:28:ARG:NH2	2.51	0.43
9:I1:8:ILE:HB	9:I1:24:SER:HB3	1.99	0.43
10:J1:10:LYS:HB2	10:J1:10:LYS:HE3	1.76	0.43
12:L1:41:PRO:HD2	12:L1:44:HIS:ND1	2.34	0.43
14:N1:77:ILE:HG22	14:N1:78:LYS:N	2.33	0.43
34:h1:22:ALA:HB3	34:h1:32:LEU:HB3	2.00	0.43
36:A2:183:GLY:CA	80:54:1613:A:H5''	2.48	0.43
47:M2:90:ARG:O	47:M2:94:LYS:HG2	2.18	0.43
47:M2:132:ARG:NE	80:54:4895:C:O2	2.51	0.43
48:N2:126:THR:HG23	48:N2:127:TYR:CD2	2.54	0.43
55:U2:40:GLU:O	55:U2:44:GLN:HG3	2.18	0.43
58:X2:60:TYR:CD1	68:h2:78:TYR:HB3	2.53	0.43
71:k2:2:PRO:HD2	80:54:2642:A:C2	2.53	0.43
79:t2:153:ASP:O	79:t2:157:SER:OG	2.28	0.43
80:54:1238:A:O2'	80:54:1239:C:OP1	2.30	0.43
80:54:1741:G:H3'	80:54:1742:A:H5''	2.00	0.43
80:54:2001:G:N2	80:54:2017:A:H1'	2.32	0.43
80:54:2862:G:N3	80:54:3624:A:H2'	2.32	0.43
80:54:3700:C:O2'	80:54:3774:A:N3	2.44	0.43
80:54:3784:A:H61	80:54:3814:U:H1'	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:B:13:ALA:HA	84:B:16:GLU:HG2	2.00	0.43
85:23:46:7MG:OP2	85:23:46:7MG:H82	2.18	0.43
1:A1:65:C:C4	8:H1:133:LEU:HD13	2.54	0.43
1:A1:1531:A:H4'	1:A1:1605:G:H4'	2.00	0.43
5:E1:54:ARG:HB3	5:E1:57:ASN:HD22	1.83	0.43
5:E1:161:GLY:O	5:E1:164:VAL:HG22	2.18	0.43
6:F1:87:MET:HE1	6:F1:236:ILE:HD13	2.00	0.43
8:H1:58:LYS:HA	8:H1:107:SER:HB3	1.99	0.43
9:I1:147:LYS:HE3	9:I1:153:LEU:HD13	2.00	0.43
22:V1:100:GLN:O	22:V1:104:ILE:HG22	2.18	0.43
25:Y1:107:ARG:HD3	25:Y1:112:VAL:HG22	1.98	0.43
36:A2:180:LEU:HD11	76:p2:26:VAL:HG11	1.99	0.43
38:C2:20:LYS:HA	38:C2:20:LYS:HD3	1.87	0.43
52:R2:42:ARG:HH12	80:54:2525:U:P	2.40	0.43
60:Z2:14:LEU:HD13	67:g2:92:LYS:HE3	2.00	0.43
69:i2:50:PHE:HZ	69:i2:93:VAL:HG21	1.83	0.43
80:54:1072:C:O2'	80:54:1073:G:O5'	2.31	0.43
80:54:1094:G:H1	80:54:1202:C:H42	1.66	0.43
80:54:3848:U:H2'	80:54:3849:A:C8	2.53	0.43
80:54:4107:G:H2'	80:54:4108:G:H8	1.83	0.43
85:33:46:7MG:H82	85:33:46:7MG:OP2	2.18	0.43
1:A1:1255:G:OP1	1:A1:1256:G:O2'	2.24	0.43
1:A1:1636:G:H2'	1:A1:1636:G:N3	2.34	0.43
1:A1:1798:C:O2'	10:J1:2:GLY:HA2	2.19	0.43
3:C1:30:TRP:CD2	16:P1:19:PRO:HG3	2.54	0.43
5:E1:74:GLN:HA	5:E1:79:PHE:HB2	2.00	0.43
6:F1:198:ARG:HG3	6:F1:208:VAL:HG22	2.01	0.43
8:H1:31:ARG:HB3	8:H1:101:ILE:HD13	2.00	0.43
9:I1:36:LEU:H	9:I1:36:LEU:HD23	1.83	0.43
18:R1:26:LYS:HB3	18:R1:26:LYS:HE2	1.81	0.43
21:U1:110:LEU:HD23	21:U1:110:LEU:H	1.82	0.43
21:U1:110:LEU:HG	21:U1:112:MET:HG2	1.99	0.43
36:A2:49:ILE:HD13	36:A2:60:LYS:HE3	2.00	0.43
37:B2:252:ALA:HB1	80:54:4524:G:N3	2.33	0.43
41:F2:45:ARG:O	41:F2:49:ILE:HG12	2.18	0.43
43:H2:40:HIS:ND1	80:54:4701:A:O2'	2.35	0.43
49:O2:172:LYS:HG2	80:54:4873:G:H21	1.84	0.43
53:S2:154:LEU:HD13	53:S2:157:ARG:NH1	2.33	0.43
56:V2:97:TYR:OH	57:W2:37:GLU:OE2	2.21	0.43
57:W2:106:GLU:OE1	57:W2:106:GLU:N	2.52	0.43
78:s2:54:LEU:O	78:s2:55:MET:HE2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:1677:U:H4'	80:54:1680:G:N1	2.34	0.43
80:54:2438:A:O2'	80:54:2440:U:OP2	2.35	0.43
80:54:2730:U:H2'	80:54:2731:C:C6	2.52	0.43
1:A1:77:A:H4'	8:H1:157:VAL:HG11	1.99	0.43
1:A1:495:U:H4'	6:F1:24:THR:HG22	2.01	0.43
1:A1:917:U:O4'	9:I1:118:ARG:HG3	2.19	0.43
10:J1:119:LEU:HD11	10:J1:153:LYS:HG3	2.00	0.43
13:M1:99:TYR:O	13:M1:101:ARG:N	2.44	0.43
16:P1:45:THR:HG22	16:P1:52:THR:HG22	2.00	0.43
26:Z1:12:PHE:HZ	26:Z1:21:LYS:HD3	1.83	0.43
37:B2:17:LEU:HD12	37:B2:17:LEU:HA	1.79	0.43
40:E2:271:GLN:O	40:E2:275:ARG:HG3	2.18	0.43
44:I2:113:THR:HB	44:I2:116:ARG:HB3	2.00	0.43
77:r2:84:LYS:HE2	77:r2:88:ALA:HB1	2.00	0.43
78:s2:158:VAL:HG23	78:s2:158:VAL:O	2.19	0.43
1:A1:901:G:H2'	1:A1:902:G:C8	2.54	0.43
1:A1:1284:A:P	1:A1:1286:G:H5'	2.59	0.43
1:A1:1811:C:OP1	25:Y1:37:LYS:HE3	2.18	0.43
2:B1:5:LEU:HB3	2:B1:7:VAL:HG12	2.00	0.43
7:G1:179:ASN:HB2	7:G1:187:SER:HB3	2.01	0.43
12:L1:26:ASP:H	12:L1:46:MET:HE1	1.83	0.43
14:N1:49:LEU:HB3	14:N1:111:VAL:HB	2.01	0.43
15:O1:25:TRP:CE2	29:c1:82:LYS:HD2	2.54	0.43
17:Q1:103:ASN:OD1	17:Q1:120:SER:OG	2.25	0.43
18:R1:97:GLN:NE2	34:h1:60:ARG:HE	2.16	0.43
39:D2:158:LYS:HG3	81:74:46:C:OP1	2.18	0.43
56:V2:91:LYS:HD3	56:V2:91:LYS:HA	1.71	0.43
60:Z2:29:ILE:HD13	60:Z2:40:HIS:CD2	2.53	0.43
63:c2:29:LEU:HD23	63:c2:94:LEU:HD13	2.01	0.43
65:e2:48:ARG:NH2	80:54:2280:G:OP1	2.51	0.43
69:i2:90:LEU:HA	69:i2:93:VAL:HG12	1.99	0.43
75:o2:69:ARG:HH11	75:o2:80:LYS:HD3	1.84	0.43
79:t2:15:LEU:HD22	79:t2:28:LEU:HD11	2.01	0.43
80:54:433:A:C2	80:54:3867:A:H4'	2.54	0.43
80:54:1195:G:C6	80:54:1196:G:C6	3.07	0.43
80:54:1956:A:O2'	80:54:1957:U:OP2	2.32	0.43
80:54:2259:G:H5'	80:54:2260:C:OP2	2.19	0.43
85:23:17:C:C2	85:23:17:C:H5'	2.54	0.43
1:A1:31:U:O2'	1:A1:643:A:N1	2.50	0.43
1:A1:501:C:O2	1:A1:501:C:H2'	2.18	0.43
6:F1:42:LEU:N	6:F1:84:ALA:O	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N1:69:CYS:O	14:N1:74:ILE:HB	2.19	0.43
18:R1:86:GLN:HE22	18:R1:122:ALA:HA	1.84	0.43
23:W1:1:MET:HE3	23:W1:1:MET:HB2	1.79	0.43
41:F2:216:ARG:O	41:F2:245:ARG:HD2	2.19	0.43
42:G2:220:VAL:HG12	42:G2:223:LEU:HD12	1.99	0.43
46:L2:154:VAL:HG12	46:L2:155:MET:HG3	2.00	0.43
51:Q2:13:VAL:HG11	80:54:1690:C:C5	2.53	0.43
53:S2:84:TYR:HA	53:S2:123:SER:O	2.18	0.43
75:o2:3:ASN:O	80:54:4232:U:H2'	2.19	0.43
78:s2:77:LYS:HD3	78:s2:198:ILE:HG12	2.01	0.43
80:54:3598:C:H2'	80:54:3599:A:C8	2.52	0.43
80:54:3786:U:O2	80:54:3814:U:H4'	2.19	0.43
80:54:4917:C:H2'	80:54:4918:C:C6	2.54	0.43
84:B:44:GLN:HG2	85:33:62:C:H4'	2.00	0.43
5:E1:30:ALA:HB1	5:E1:106:ARG:HH12	1.83	0.43
10:J1:21:TYR:CZ	10:J1:22:HIS:HD2	2.37	0.43
14:N1:44:LYS:HG2	14:N1:46:GLN:HE21	1.84	0.43
28:b1:15:ARG:HD2	28:b1:15:ARG:N	2.32	0.43
39:D2:60:ILE:HB	39:D2:80:ALA:HB2	2.01	0.43
39:D2:160:PHE:HA	39:D2:163:LEU:HB3	2.01	0.43
46:L2:58:ILE:N	46:L2:113:ASN:HD21	2.04	0.43
52:R2:37:SER:OG	52:R2:40:GLN:HG3	2.19	0.43
53:S2:76:LYS:NZ	53:S2:100:LEU:O	2.50	0.43
57:W2:87:LEU:HA	57:W2:90:ILE:HG12	2.01	0.43
66:f2:77:ALA:HA	66:f2:84:VAL:HG23	2.01	0.43
80:54:52:G:H4'	80:54:1529:G:H4'	2.01	0.43
80:54:1187:G:OP2	80:54:1187:G:N2	2.35	0.43
80:54:1403:G:H2'	80:54:1404:G:C8	2.54	0.43
80:54:4034:G:H2'	80:54:4035:G:O4'	2.18	0.43
1:A1:168:C:OP1	8:H1:131:ARG:NE	2.52	0.43
1:A1:566:U:H2'	1:A1:567:C:O4'	2.17	0.43
6:F1:44:LEU:HD21	6:F1:72:ILE:HD11	2.01	0.43
12:L1:14:LEU:HD23	12:L1:21:MET:HE1	2.00	0.43
14:N1:14:VAL:HB	14:N1:17:ALA:HB3	1.99	0.43
17:Q1:44:ARG:HD3	17:Q1:84:ILE:CD1	2.49	0.43
34:h1:211:GLY:H	34:h1:236:ILE:HB	1.84	0.43
44:I2:116:ARG:HG3	80:54:4195:G:OP1	2.18	0.43
48:N2:17:ASP:OD1	48:N2:20:ARG:NH2	2.51	0.43
55:U2:27:HIS:HB3	55:U2:114:TYR:HE1	1.83	0.43
68:h2:80:PRO:HD2	68:h2:83:LEU:HD12	2.00	0.43
79:t2:111:ASN:OD1	79:t2:112:ILE:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:406:C:HO2'	80:54:407:A:P	2.40	0.43
80:54:2001:G:H22	80:54:2017:A:H1'	1.83	0.43
80:54:2664:G:H4'	80:54:2677:G:H4'	2.01	0.43
80:54:3770:U:H2'	80:54:3771:C:C6	2.54	0.43
80:54:4973:U:H1'	80:54:4986:G:C2	2.54	0.43
1:A1:1098:C:H2'	1:A1:1099:G:C8	2.54	0.43
6:F1:174:LYS:HB2	6:F1:174:LYS:HE2	1.92	0.43
6:F1:180:LEU:HB2	6:F1:231:GLY:O	2.19	0.43
17:Q1:36:LEU:HA	17:Q1:36:LEU:HD23	1.80	0.43
36:A2:80:GLU:HB2	36:A2:170:ALA:HA	2.01	0.43
36:A2:104:VAL:O	36:A2:139:HIS:HE1	2.02	0.43
44:I2:103:LEU:HD23	44:I2:112:GLN:NE2	2.32	0.43
52:R2:71:ARG:HH22	80:54:3604:A:H5''	1.83	0.43
59:Y2:22:PRO:HD2	59:Y2:25:ILE:HD12	2.01	0.43
59:Y2:36:LYS:HA	59:Y2:36:LYS:HD2	1.84	0.43
80:54:755:C:H2'	80:54:756:G:C8	2.54	0.43
80:54:1982:G:N2	80:54:2009:A:O2'	2.51	0.43
80:54:2765:A:H2'	80:54:2766:A:C8	2.54	0.43
80:54:3765:G:H21	80:54:3766:A:N6	2.16	0.43
84:B:161:LYS:HG3	85:33:54:2MU:C6'	2.31	0.43
85:33:17:C:C2	85:33:17:C:H5'	2.54	0.43
85:33:23:A:H2'	85:33:24:G:C8	2.54	0.43
1:A1:165:G:O4'	8:H1:110:ASN:ND2	2.52	0.42
1:A1:1061:U:H4'	1:A1:1062:A:OP2	2.18	0.42
1:A1:1329:U:O2'	1:A1:1332:A:OP2	2.29	0.42
8:H1:85:ARG:HH21	26:Z1:118:ARG:HD2	1.84	0.42
18:R1:13:PHE:HA	18:R1:22:VAL:HA	2.01	0.42
28:b1:7:ASN:ND2	28:b1:10:ARG:O	2.51	0.42
33:g1:92:LYS:HD2	33:g1:92:LYS:HA	1.92	0.42
38:C2:150:LEU:HB3	38:C2:151:PRO:HD3	2.01	0.42
42:G2:155:TYR:OH	42:G2:264:ASP:OD2	2.31	0.42
45:J2:23:ASN:OD1	45:J2:129:ASP:HB3	2.19	0.42
54:T2:49:GLN:HA	54:T2:52:MET:HE3	2.02	0.42
56:V2:21:PRO:HA	56:V2:54:ALA:HA	1.99	0.42
65:e2:57:ASN:O	80:54:2319:C:H1'	2.19	0.42
79:t2:11:LYS:HG2	79:t2:35:LEU:HD11	2.01	0.42
79:t2:16:ARG:HD2	80:54:1975:G:N2	2.33	0.42
80:54:2394:G:O2'	80:54:2819:U:O4	2.31	0.42
80:54:3905:A:C2	83:XX:1018:LYS:HD2	2.54	0.42
85:33:50:A:H2'	85:33:51:G:H8	1.84	0.42
1:A1:1650:A:H5''	18:R1:139:ALA:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J1:105:ASP:HA	10:J1:169:GLY:O	2.19	0.42
16:P1:20:GLN:HG2	16:P1:21:VAL:H	1.84	0.42
26:Z1:78:SER:OG	26:Z1:80:ASP:OD1	2.21	0.42
33:g1:99:LYS:HG2	33:g1:100:LEU:HD23	2.01	0.42
34:h1:29:ASP:HA	34:h1:45:LEU:HD12	2.01	0.42
47:M2:55:MET:O	53:S2:157:ARG:NH2	2.52	0.42
47:M2:94:LYS:HE3	80:54:4872:G:OP2	2.19	0.42
48:N2:203:TYR:HB2	80:54:1359:G:H4'	2.00	0.42
53:S2:165:PRO:C	53:S2:167:PHE:H	2.27	0.42
59:Y2:49:ILE:HD13	59:Y2:80:ILE:HD13	2.01	0.42
61:a2:83:SER:OG	61:a2:86:THR:OG1	2.34	0.42
75:o2:63:THR:O	75:o2:87:ARG:NH1	2.52	0.42
78:s2:139:GLN:HE22	78:s2:145:THR:HB	1.85	0.42
79:t2:78:SER:OG	80:54:1976:G:O2'	2.32	0.42
80:54:223:G:H4'	80:54:225:G:N7	2.35	0.42
80:54:1202:C:H2'	80:54:1203:G:C8	2.54	0.42
80:54:4967:A:H2'	80:54:4968:A:C8	2.54	0.42
84:B:139:THR:OG1	84:B:140:HIS:N	2.51	0.42
85:23:47:H2U:H62	85:23:47:H2U:C5'	2.49	0.42
1:A1:732:U:H2'	1:A1:733:C:C6	2.53	0.42
1:A1:1620:A:H4'	1:A1:1621:U:C5	2.54	0.42
4:D1:72:ASP:OD2	4:D1:272:HIS:HE1	2.02	0.42
8:H1:28:TYR:HB3	8:H1:29:GLU:OE1	2.19	0.42
8:H1:67:VAL:CG2	8:H1:99:GLY:HA2	2.49	0.42
9:I1:26:ALA:HA	9:I1:29:GLU:HB2	2.01	0.42
10:J1:138:ASN:C	10:J1:139:LYS:HD3	2.44	0.42
22:V1:20:ILE:O	22:V1:91:LEU:N	2.38	0.42
22:V1:96:GLU:HA	22:V1:99:LYS:CB	2.49	0.42
39:D2:158:LYS:HE2	81:74:47:G:OP2	2.19	0.42
46:L2:7:GLY:O	61:a2:49:HIS:NE2	2.45	0.42
46:L2:207:VAL:HG12	46:L2:211:LYS:HB2	2.01	0.42
54:T2:57:TYR:HA	54:T2:60:LYS:HG3	2.01	0.42
56:V2:50:ASN:ND2	80:54:4457:U:OP1	2.47	0.42
58:X2:151:ASN:HD21	58:X2:156:ILE:HG12	1.84	0.42
60:Z2:31:ASP:OD1	60:Z2:31:ASP:N	2.51	0.42
70:j2:30:GLN:NE2	80:54:1621:A:OP2	2.51	0.42
78:s2:139:GLN:HG3	78:s2:143:ILE:O	2.19	0.42
80:54:1662:C:H2'	80:54:1663:C:C6	2.54	0.42
80:54:2495:U:H2'	80:54:2496:G:C8	2.51	0.42
1:A1:581:U:H2'	1:A1:582:U:O4'	2.19	0.42
1:A1:1029:G:O2'	80:54:1564:A:N1	2.48	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1088:U:H4'	1:A1:1089:G:OP2	2.19	0.42
4:D1:85:SER:OG	23:W1:25:GLY:O	2.32	0.42
8:H1:2:LYS:HG2	8:H1:17:GLU:OE1	2.19	0.42
16:P1:78:ALA:HB3	16:P1:118:ALA:HB3	2.00	0.42
20:T1:64:VAL:O	20:T1:68:ILE:HG23	2.20	0.42
29:c1:31:TYR:CD2	29:c1:81:ARG:HG3	2.54	0.42
34:h1:220:ASP:OD1	34:h1:220:ASP:N	2.50	0.42
36:A2:142:GLU:O	36:A2:143:THR:OG1	2.23	0.42
37:B2:86:VAL:HG12	37:B2:201:LEU:HD12	2.01	0.42
41:F2:102:PRO:HD3	80:54:1876:U:O3'	2.19	0.42
49:O2:8:VAL:HG12	49:O2:117:ARG:HG3	2.00	0.42
65:e2:102:ASN:O	80:54:2302:C:O2'	2.37	0.42
70:j2:76:HIS:CE1	82:84:93:C:H5''	2.55	0.42
79:t2:137:GLN:NE2	79:t2:142:ASN:HA	2.34	0.42
80:54:924:C:H41	80:54:927:G:H5''	1.84	0.42
81:74:27:G:H21	81:74:55:A:N6	2.17	0.42
85:23:23:A:H2'	85:23:24:G:C8	2.54	0.42
85:33:18:G:C5'	85:33:18:G:C8	3.02	0.42
1:A1:993:G:O6	28:b1:15:ARG:HG3	2.20	0.42
1:A1:1299:A:O2'	1:A1:1301:A:OP1	2.31	0.42
1:A1:1610:G:N2	20:T1:85:ASN:O	2.52	0.42
6:F1:139:LEU:HB2	6:F1:147:ILE:HB	2.02	0.42
9:I1:58:LYS:HB2	9:I1:90:LYS:HG2	2.01	0.42
10:J1:81:VAL:HG22	10:J1:102:VAL:HG12	2.02	0.42
11:K1:127:ARG:HD3	32:f1:104:ARG:HD3	2.02	0.42
28:b1:50:VAL:O	28:b1:54:SER:OG	2.23	0.42
34:h1:272:GLN:HE22	34:h1:275:ILE:HD11	1.84	0.42
37:B2:350:SER:OG	37:B2:354:GLN:NE2	2.52	0.42
38:C2:235:LEU:HD22	38:C2:240:LEU:HD11	2.01	0.42
40:E2:152:ILE:HD13	40:E2:274:LEU:HD21	2.02	0.42
49:O2:176:ARG:HD3	80:54:4769:G:H5'	2.01	0.42
61:a2:117:LEU:HD23	61:a2:140:VAL:HG11	2.01	0.42
68:h2:82:ASP:OD1	68:h2:82:ASP:N	2.48	0.42
77:r2:28:GLU:HG3	77:r2:31:ASN:HB2	2.00	0.42
80:54:1370:G:H4'	80:54:1371:A:O5'	2.19	0.42
80:54:3603:G:H2'	80:54:3604:A:C8	2.55	0.42
80:54:3645:U:O2'	80:54:4553:A:O2'	2.31	0.42
80:54:4947:U:HO2'	80:54:4948:C:P	2.42	0.42
82:84:140:C:H2'	82:84:141:C:C6	2.55	0.42
84:B:35:GLN:N	84:B:205:TYR:O	2.49	0.42
85:33:47:H2U:H62	85:33:47:H2U:C5'	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:522:A:OP2	11:K1:45:ARG:NH2	2.52	0.42
1:A1:551:U:H2'	1:A1:552:G:C8	2.53	0.42
1:A1:1556:A:C8	31:e1:13:LYS:HE3	2.53	0.42
3:C1:47:THR:OG1	3:C1:65:ARG:NH1	2.52	0.42
7:G1:118:ASN:O	7:G1:193:LYS:HE2	2.19	0.42
8:H1:145:PHE:HA	57:W2:94:ARG:HG3	2.01	0.42
12:L1:37:ASP:N	12:L1:37:ASP:OD1	2.52	0.42
18:R1:113:ILE:HG12	18:R1:120:LEU:HD12	2.01	0.42
21:U1:76:THR:HB	21:U1:94:ARG:HB3	2.02	0.42
34:h1:236:ILE:HD12	34:h1:250:ALA:HB1	2.02	0.42
38:C2:69:THR:HG21	80:54:3906:A:H2'	2.01	0.42
39:D2:10:LYS:O	39:D2:14:LYS:HG3	2.19	0.42
41:F2:219:MET:HB3	41:F2:231:ASP:OD2	2.20	0.42
51:Q2:178:ARG:HB2	61:a2:53:PHE:O	2.20	0.42
77:r2:45:HIS:HB2	77:r2:48:THR:HG22	2.01	0.42
77:r2:54:ALA:HA	77:r2:61:VAL:HG23	2.00	0.42
80:54:1405:C:H2'	80:54:1406:G:H8	1.80	0.42
80:54:4115:G:H5''	80:54:4116:C:OP1	2.19	0.42
80:54:4480:A:H2'	80:54:4481:U:O4'	2.20	0.42
84:B:64:SER:HB3	84:B:108:ASP:H	1.84	0.42
1:A1:156:G:OP1	8:H1:2:LYS:NZ	2.31	0.42
1:A1:1101:U:H2'	1:A1:1102:G:C8	2.54	0.42
2:B1:10:MET:SD	2:B1:15:VAL:HG22	2.60	0.42
8:H1:37:ALA:HA	8:H1:49:VAL:HA	2.01	0.42
8:H1:192:ILE:HG22	8:H1:196:LYS:HE3	2.01	0.42
10:J1:110:ARG:O	10:J1:114:GLU:HG3	2.19	0.42
12:L1:47:LYS:HA	12:L1:47:LYS:HD3	1.77	0.42
38:C2:140:LYS:HG3	38:C2:140:LYS:O	2.19	0.42
40:E2:69:ALA:HA	40:E2:71:TYR:CE1	2.55	0.42
40:E2:167:PHE:HA	40:E2:178:VAL:HG23	2.00	0.42
41:F2:30:LYS:HE2	41:F2:30:LYS:HB3	1.73	0.42
53:S2:154:LEU:HB3	53:S2:157:ARG:HD3	2.01	0.42
55:U2:93:LYS:NZ	80:54:2628:U:OP1	2.52	0.42
56:V2:82:ILE:HG13	56:V2:83:ARG:HG3	2.01	0.42
59:Y2:126:ARG:NH2	80:54:198:A:OP2	2.52	0.42
66:f2:95:LYS:HE3	66:f2:95:LYS:HB2	1.83	0.42
78:s2:55:MET:N	80:54:1998:A:OP1	2.52	0.42
79:t2:82:ILE:HG23	79:t2:100:HIS:NE2	2.34	0.42
80:54:4045:G:N2	80:54:4047:A:H3'	2.34	0.42
80:54:4563:U:H2'	80:54:4564:A:C8	2.54	0.42
82:84:122:G:C6	82:84:123:U:H1'	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
84:B:82:ILE:HG13	84:B:144:MET:HE1	2.02	0.42
85:33:37:12A:H3'	85:33:38:A:H8	1.85	0.42
1:A1:407:G:N3	1:A1:407:G:H2'	2.34	0.42
1:A1:1567:G:H2'	1:A1:1568:C:O4'	2.20	0.42
2:B1:132:GLN:HB3	2:B1:133:PRO:HD3	2.02	0.42
5:E1:197:LYS:HG3	5:E1:198:ILE:HG23	2.01	0.42
6:F1:95:THR:HG22	26:Z1:16:ARG:HB2	2.00	0.42
13:M1:65:ASN:O	13:M1:132:ARG:NH1	2.39	0.42
13:M1:88:ILE:HG21	13:M1:126:VAL:HG11	2.02	0.42
17:Q1:17:TYR:CD2	17:Q1:18:ARG:HG2	2.55	0.42
18:R1:41:MET:HE2	21:U1:10:ASN:HB2	2.01	0.42
21:U1:10:ASN:HD21	21:U1:12:GLN:HB2	1.84	0.42
25:Y1:59:ALA:HB1	25:Y1:114:ASP:HB3	2.01	0.42
27:a1:62:VAL:HG22	27:a1:63:PRO:HD3	2.01	0.42
32:f1:101:ARG:O	32:f1:106:LYS:HB2	2.19	0.42
37:B2:92:TYR:OH	37:B2:182:GLU:OE1	2.31	0.42
38:C2:132:ALA:C	38:C2:150:LEU:HD23	2.44	0.42
38:C2:195:LYS:HB3	38:C2:200:ARG:NE	2.35	0.42
38:C2:283:LYS:HE2	38:C2:283:LYS:HB2	1.85	0.42
41:F2:56:TYR:OH	41:F2:188:ASP:OD1	2.36	0.42
54:T2:142:ARG:NH1	80:54:1090:G:OP1	2.49	0.42
57:W2:107:GLN:O	57:W2:110:ARG:HG2	2.20	0.42
60:Z2:81:MET:HE1	63:c2:59:GLU:HG3	2.01	0.42
64:d2:32:ARG:NH1	80:54:4996:C:OP1	2.52	0.42
76:p2:47:MET:HE2	76:p2:71:TYR:CE1	2.55	0.42
78:s2:147:ILE:HG12	78:s2:152:ILE:HA	2.02	0.42
79:t2:81:ILE:CD1	79:t2:136:ALA:HA	2.49	0.42
80:54:1177:U:H2'	80:54:1178:G:C8	2.55	0.42
80:54:1406(A):G:H2'	80:54:1406(B):C:O4'	2.19	0.42
80:54:4620:U:OP2	80:54:4670:C:N4	2.50	0.42
80:54:4964:C:N4	80:54:4965:U:O4	2.52	0.42
85:23:18:G:C5'	85:23:18:G:C8	3.02	0.42
1:A1:1021:U:OP1	15:O1:132:LYS:NZ	2.50	0.42
22:V1:26:SER:HB2	22:V1:110:VAL:HA	2.02	0.42
23:W1:21:ASN:HB3	24:X1:67:GLY:HA3	2.02	0.42
34:h1:119:GLN:HE22	34:h1:139:LYS:NZ	2.18	0.42
40:E2:64:MET:HE2	80:54:979:C:OP1	2.20	0.42
42:G2:250:LYS:HB3	80:54:6:C:H5''	2.01	0.42
56:V2:89:ARG:HB2	56:V2:95:PHE:CE2	2.55	0.42
57:W2:97:LYS:HE2	57:W2:98:PRO:HD2	2.01	0.42
78:s2:47:LEU:HD22	78:s2:50:LYS:HE2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
78:s2:136:SER:O	78:s2:140:ALA:N	2.53	0.42
80:54:140:G:H2'	80:54:141:C:O4'	2.19	0.42
80:54:2539:C:H2'	80:54:2540:C:C6	2.55	0.42
80:54:2565:A:C5	80:54:2566:G:H1'	2.54	0.42
80:54:2588:C:OP1	80:54:2768:C:O2'	2.32	0.42
1:A1:429:C:OP1	6:F1:10:LYS:NZ	2.43	0.42
2:B1:19:LEU:HD11	19:S1:106:LEU:HD11	2.01	0.42
4:D1:65:LYS:HD2	4:D1:273:LEU:HD13	2.02	0.42
10:J1:77:ARG:HB3	10:J1:105:ASP:OD2	2.20	0.42
14:N1:53:ALA:HB1	14:N1:80:ASP:O	2.20	0.42
27:a1:65:TYR:CA	85:33:34:70U:C6	2.82	0.42
30:d1:34:PHE:CZ	30:d1:61:SER:HB2	2.55	0.42
34:h1:49:GLU:HG3	34:h1:50:THR:HG23	2.01	0.42
39:D2:51:MET:HE1	39:D2:163:LEU:HA	2.02	0.42
39:D2:193:GLU:O	39:D2:197:LYS:HG2	2.20	0.42
40:E2:189:LEU:N	40:E2:253:GLN:HE22	2.17	0.42
41:F2:181:TYR:CZ	41:F2:202:GLU:HG2	2.54	0.42
49:O2:151:ALA:O	49:O2:155:THR:HG23	2.20	0.42
50:P2:114:ILE:HG12	50:P2:150:LEU:HD22	2.02	0.42
78:s2:146:LYS:HG3	78:s2:155:LEU:HB2	2.02	0.42
79:t2:58:ILE:HG23	79:t2:60:VAL:HG23	2.01	0.42
80:54:1172:C:H2'	80:54:1173:G:C8	2.55	0.42
80:54:1398:A:C2	80:54:1399:G:H1'	2.55	0.42
80:54:2408:U:H4'	80:54:2409:U:O5'	2.20	0.42
80:54:2457:G:H21	80:54:3672:G:N2	2.18	0.42
85:23:17:C:H6	85:23:17:C:H2'	1.71	0.42
1:A1:78:C:OP1	8:H1:159:ARG:NH2	2.53	0.41
1:A1:553:U:O2'	1:A1:554:A:H8	2.01	0.41
1:A1:1389:C:OP1	19:S1:43:SER:OG	2.28	0.41
1:A1:1597:C:H4'	1:A1:1603:G:C6	2.55	0.41
22:V1:94:PRO:HG2	22:V1:97:ILE:HD12	2.02	0.41
24:X1:7:LEU:HD23	24:X1:34:ILE:HG12	2.01	0.41
34:h1:211:GLY:N	34:h1:236:ILE:HB	2.34	0.41
37:B2:306:ASP:OD1	37:B2:306:ASP:N	2.51	0.41
38:C2:150:LEU:O	38:C2:152:LEU:N	2.52	0.41
42:G2:113:TYR:OH	82:84:148:A:N3	2.40	0.41
54:T2:110:LYS:O	54:T2:114:GLN:HG2	2.20	0.41
62:b2:47:LYS:HA	62:b2:50:ASN:ND2	2.34	0.41
80:54:757:G:H1'	80:54:758:G:H5'	2.02	0.41
80:54:909:G:H2'	80:54:910:G:C8	2.55	0.41
80:54:1198:G:H2'	80:54:1199:G:C8	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:1308:C:H2'	80:54:1309:C:C6	2.55	0.41
80:54:4069:U:H2'	80:54:4070:U:C6	2.55	0.41
84:B:177:ASP:HA	84:B:180:VAL:HG22	2.02	0.41
84:B:208:SER:OG	84:B:210:MET:O	2.35	0.41
85:23:50:A:H2'	85:23:51:G:H8	1.84	0.41
85:33:34:70U:OP2	85:33:35:U:OP2	2.39	0.41
3:C1:133:TYR:HB3	3:C1:217:MET:HE1	2.02	0.41
5:E1:40:ARG:HB2	5:E1:47:GLU:HG2	2.02	0.41
7:G1:127:ARG:HD3	7:G1:135:ARG:O	2.20	0.41
8:H1:20:ASP:HB2	8:H1:23:LYS:HB3	2.01	0.41
8:H1:63:MET:HG2	8:H1:99:GLY:O	2.19	0.41
8:H1:85:ARG:NH2	26:Z1:118:ARG:HD2	2.35	0.41
34:h1:299:PHE:CD1	34:h1:309:VAL:HG12	2.55	0.41
36:A2:48:ILE:HG22	76:p2:54:ILE:HG12	2.02	0.41
37:B2:206:PRO:HG2	37:B2:209:GLN:HG2	2.02	0.41
39:D2:6:VAL:HG12	80:54:1779:U:OP1	2.19	0.41
39:D2:83:LEU:HB3	39:D2:88:VAL:HB	2.01	0.41
39:D2:152:ARG:HG3	39:D2:154:THR:HG23	2.02	0.41
49:O2:119:VAL:N	53:S2:168:THR:O	2.49	0.41
55:U2:27:HIS:O	55:U2:30:GLU:HG3	2.19	0.41
71:k2:24:LYS:HD3	71:k2:69:LEU:HD11	2.02	0.41
78:s2:78:LEU:HD12	78:s2:78:LEU:HA	1.88	0.41
78:s2:133:GLU:CD	78:s2:134:LYS:H	2.27	0.41
80:54:1441:C:H2'	80:54:1442:C:C6	2.54	0.41
80:54:1983:A:H4'	80:54:1984:A:O5'	2.20	0.41
80:54:2538:U:H2'	80:54:2539:C:C6	2.55	0.41
80:54:3961:G:O2'	80:54:4049:U:O4	2.24	0.41
80:54:4420:U:H3'	80:54:4421:C:C6	2.55	0.41
83:XX:1010:LYS:HG2	83:XX:1011:LYS:N	2.30	0.41
84:B:27:LYS:H	84:B:27:LYS:HG2	1.70	0.41
84:B:101:LYS:HB3	84:B:128:LEU:HD21	2.01	0.41
1:A1:107:A:H2'	1:A1:108:G:C8	2.55	0.41
1:A1:1201:U:H2'	1:A1:1202:U:C6	2.56	0.41
1:A1:1284:A:C8	14:N1:91:LEU:HD11	2.55	0.41
3:C1:34:LYS:O	3:C1:98:THR:OG1	2.30	0.41
3:C1:153:THR:HB	3:C1:155:TYR:CD2	2.56	0.41
7:G1:30:ILE:HD12	7:G1:30:ILE:H	1.85	0.41
9:I1:28:LEU:O	9:I1:32:MET:HG2	2.20	0.41
34:h1:36:ARG:HD3	34:h1:65:PHE:CE2	2.55	0.41
34:h1:164:ILE:HB	34:h1:177:TRP:O	2.20	0.41
40:E2:160:HIS:HB3	40:E2:163:LYS:HD2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:E2:168:LEU:HD11	40:E2:179:THR:HG22	2.02	0.41
55:U2:88:LYS:HD2	55:U2:97:ARG:NH2	2.35	0.41
58:X2:119:ILE:HD12	58:X2:140:LEU:HD22	2.01	0.41
64:d2:32:ARG:HG2	64:d2:48:GLU:HB3	2.02	0.41
73:m2:68:MET:HG2	73:m2:79:PRO:HA	2.02	0.41
79:t2:81:ILE:HD11	79:t2:139:VAL:HG21	2.02	0.41
80:54:275:C:H2'	80:54:276:C:C6	2.55	0.41
80:54:956:A:N6	80:54:1283:G:H1'	2.36	0.41
80:54:2461:G:H2'	80:54:2462:C:C6	2.55	0.41
80:54:2768:C:H5'	80:54:2769:U:OP1	2.20	0.41
80:54:4748:U:H2'	80:54:4749:C:C6	2.55	0.41
80:54:4776:G:H1	80:54:4859:C:H42	1.68	0.41
85:33:59:G:C2'	85:33:60:U:H5'	2.51	0.41
1:A1:191:A:N6	1:A1:192:C:O2	2.53	0.41
1:A1:671:A:H4'	1:A1:672:A:H5''	2.02	0.41
1:A1:1612:G:OP1	17:Q1:18:ARG:NH1	2.47	0.41
1:A1:1629:C:H5''	20:T1:39:ARG:HG2	2.02	0.41
2:B1:149:ASN:HB2	2:B1:165:ASN:OD1	2.20	0.41
7:G1:49:LEU:HD23	7:G1:49:LEU:HA	1.92	0.41
8:H1:30:LYS:HB3	8:H1:34:THR:HG21	2.02	0.41
21:U1:111:LYS:O	21:U1:126:GLN:NE2	2.53	0.41
26:Z1:45:ALA:HB1	26:Z1:50:THR:O	2.20	0.41
27:a1:50:PHE:HB3	27:a1:55:TYR:HB2	2.01	0.41
27:a1:65:TYR:CG	85:33:34:70U:C2	2.86	0.41
27:a1:73:VAL:HG12	27:a1:79:ILE:HD11	2.03	0.41
27:a1:85:ARG:O	27:a1:89:GLN:HG3	2.20	0.41
43:H2:71:ARG:HH22	80:54:4695:C:P	2.44	0.41
49:O2:172:LYS:HG2	80:54:4873:G:N2	2.34	0.41
71:k2:19:ASP:OD2	80:54:2773:G:H5''	2.21	0.41
79:t2:62:LEU:HA	79:t2:72:GLU:HB2	2.03	0.41
80:54:521:C:N4	80:54:640:C:H42	2.18	0.41
80:54:966:A:H4'	80:54:967:C:H5''	2.02	0.41
80:54:2390:G:H22	80:54:2825:A:H2	1.66	0.41
80:54:2439:G:H5'	80:54:2778:G:OP2	2.20	0.41
80:54:3717:A:H2'	80:54:3718:A:C8	2.54	0.41
80:54:3938:G:H4'	80:54:3939:G:O5'	2.20	0.41
1:A1:92:A:C6	1:A1:446:G:C6	3.08	0.41
1:A1:792:C:H2'	1:A1:793:G:H8	1.85	0.41
1:A1:1154:U:O4	4:D1:227:ARG:HD2	2.20	0.41
1:A1:1298:G:O2'	1:A1:1299:A:H8	2.03	0.41
3:C1:171:ILE:O	3:C1:175:GLU:HG2	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E1:101:GLN:HA	5:E1:104:SER:HB3	2.02	0.41
8:H1:2:LYS:HD3	8:H1:15:LEU:HD21	2.02	0.41
13:M1:111:VAL:HG12	13:M1:140:PHE:HB2	2.02	0.41
20:T1:5:ILE:HG22	27:a1:50:PHE:O	2.20	0.41
24:X1:77:PRO:HD3	25:Y1:5:ARG:O	2.20	0.41
32:f1:76:HIS:CG	32:f1:77:GLY:H	2.39	0.41
34:h1:251:ALA:HA	34:h1:256:ILE:HD13	2.01	0.41
58:X2:71:LEU:HD12	58:X2:71:LEU:HA	1.94	0.41
65:e2:98:GLU:HG3	65:e2:123:THR:HB	2.03	0.41
80:54:92:C:OP2	80:54:4341:C:O2'	2.34	0.41
80:54:158:A:H5''	80:54:159:C:H2'	2.02	0.41
80:54:1068:G:H2'	80:54:1069:G:C8	2.56	0.41
80:54:1920:C:H3'	80:54:1921:C:H5''	2.02	0.41
80:54:2601:A:N6	80:54:2743:A:H3'	2.35	0.41
80:54:2697:A:O3'	80:54:2711:G:N2	2.53	0.41
82:84:123:U:H3'	82:84:124:U:C6	2.55	0.41
85:23:37:12A:H3'	85:23:38:A:H8	1.85	0.41
1:A1:616:A:OP1	25:Y1:68:LYS:NZ	2.53	0.41
1:A1:640:A:H2'	1:A1:641:A:C8	2.56	0.41
1:A1:1415:C:O2'	21:U1:132:ASP:OD2	2.26	0.41
1:A1:1445:U:O4	1:A1:1446:A:N6	2.54	0.41
1:A1:1490:G:OP2	1:A1:1490:G:H8	2.04	0.41
7:G1:183:GLY:HA2	7:G1:190:ILE:HG13	2.03	0.41
11:K1:121:LYS:H	11:K1:125:HIS:CD2	2.31	0.41
17:Q1:49:LEU:HD12	17:Q1:49:LEU:HA	1.96	0.41
19:S1:5:ARG:HB2	19:S1:10:LYS:HE2	2.02	0.41
37:B2:193:LYS:HE3	37:B2:193:LYS:HB2	1.90	0.41
40:E2:186:ARG:HH21	80:54:4938:A:P	2.44	0.41
42:G2:84:LEU:HD21	60:Z2:122:TYR:O	2.21	0.41
43:H2:50:LYS:HG3	80:54:759:G:H5'	2.02	0.41
49:O2:121:PRO:HA	49:O2:124:LEU:HD12	2.02	0.41
59:Y2:50:ARG:HD2	59:Y2:115:ARG:HH11	1.86	0.41
61:a2:29:PRO:HG3	80:54:1654:G:H5''	2.02	0.41
65:e2:104:SER:OG	65:e2:107:ASN:ND2	2.53	0.41
66:f2:33:VAL:HG13	66:f2:38:GLU:HB2	2.03	0.41
68:h2:12:LYS:HE2	68:h2:16:GLU:HG3	2.02	0.41
80:54:909:G:H2'	80:54:910:G:H8	1.84	0.41
80:54:1881:C:H5'	80:54:2281:U:H1'	2.02	0.41
80:54:2845:A:H61	80:54:3843:C:N4	2.18	0.41
80:54:3956:G:N2	80:54:4057:C:O2	2.53	0.41
1:A1:992:A:H3'	28:b1:15:ARG:HH22	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1759:G:H2'	1:A1:1760:G:H8	1.84	0.41
6:F1:188:ASN:HB3	6:F1:191:ARG:HG3	2.01	0.41
10:J1:203:LYS:HB3	10:J1:203:LYS:HE3	1.87	0.41
12:L1:32:HIS:CE1	12:L1:34:GLU:HB2	2.56	0.41
21:U1:42:HIS:ND1	21:U1:93:SER:OG	2.52	0.41
25:Y1:90:CYS:HA	25:Y1:93:PHE:CD2	2.55	0.41
27:a1:61:GLU:O	85:33:34:70U:O2'	2.37	0.41
33:g1:135:HIS:CD2	33:g1:138:ARG:NH2	2.89	0.41
38:C2:140:LYS:HZ3	38:C2:245:HIS:HB2	1.85	0.41
42:G2:253:THR:OG1	80:54:150:U:OP2	2.37	0.41
43:H2:137:SER:HB3	43:H2:145:VAL:CG2	2.51	0.41
44:I2:17:TYR:H	44:I2:95:HIS:HD2	1.68	0.41
45:J2:96:LYS:HE3	45:J2:96:LYS:HB2	1.88	0.41
51:Q2:13:VAL:O	51:Q2:13:VAL:HG12	2.21	0.41
53:S2:137:CYS:O	53:S2:143:LYS:NZ	2.48	0.41
57:W2:52:THR:O	57:W2:56:ARG:HG3	2.21	0.41
78:s2:57:LYS:O	78:s2:61:MET:HG3	2.20	0.41
78:s2:101:MET:O	78:s2:105:ASN:HB2	2.21	0.41
79:t2:121:LEU:HD13	80:54:1972:G:H4'	2.03	0.41
80:54:32:G:H21	80:54:50:C:H5	1.69	0.41
80:54:385:A:H4'	80:54:386:A:OP1	2.20	0.41
80:54:1980:U:H2'	80:54:1982:G:N7	2.36	0.41
80:54:3607:U:H2'	80:54:3608:A:H8	1.85	0.41
80:54:3927:U:H2'	80:54:3928:A:C8	2.55	0.41
85:23:59:G:H2'	85:23:60:U:H5'	2.02	0.41
1:A1:28:U:H2'	1:A1:29:G:H8	1.85	0.41
1:A1:1189:A:H2'	1:A1:1190:A:C8	2.56	0.41
7:G1:99:ILE:HD13	7:G1:171:GLU:HG2	2.02	0.41
11:K1:139:LYS:HE2	11:K1:139:LYS:HB2	1.91	0.41
28:b1:37:LYS:HB2	28:b1:37:LYS:HE2	1.85	0.41
36:A2:117:GLU:OE2	36:A2:163:ARG:NH2	2.41	0.41
37:B2:8:ALA:HB1	56:V2:48:ARG:HH22	1.86	0.41
43:H2:25:VAL:HB	43:H2:80:MET:HE1	2.03	0.41
46:L2:74:ARG:NH2	80:54:109:G:OP2	2.45	0.41
47:M2:44:ARG:HE	47:M2:44:ARG:HB2	1.63	0.41
56:V2:83:ARG:NH1	56:V2:120:PRO:O	2.41	0.41
78:s2:18:ILE:HA	78:s2:21:LEU:CB	2.51	0.41
79:t2:60:VAL:C	79:t2:61:LYS:HD3	2.46	0.41
80:54:1474:C:H2'	80:54:1475:G:O4'	2.21	0.41
80:54:1695:U:H2'	80:54:1696:C:O4'	2.21	0.41
80:54:1895:G:H2'	80:54:1896:A:O4'	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:2424:G:H8	80:54:2424:G:O5'	2.04	0.41
80:54:2547:G:H2'	80:54:2548:C:C6	2.56	0.41
82:84:31:G:H2'	82:84:32:C:O4'	2.21	0.41
84:B:26:ARG:HH22	84:B:209:THR:H	1.68	0.41
1:A1:183:G:HO2'	1:A1:184:G:C4'	2.32	0.41
1:A1:223:C:H2'	1:A1:224:A:C8	2.56	0.41
1:A1:338:G:H2'	1:A1:339:A:H8	1.86	0.41
1:A1:659:G:H21	25:Y1:17:ARG:NH1	2.19	0.41
1:A1:1144:A:H2'	1:A1:1145:A:C8	2.56	0.41
1:A1:1298:G:H5''	17:Q1:77:LYS:HB2	2.01	0.41
1:A1:1486:A:H2'	1:A1:1487:A:O4'	2.21	0.41
1:A1:1613:G:OP1	20:T1:88:LYS:NZ	2.34	0.41
2:B1:34:MET:HE3	2:B1:34:MET:HB3	1.96	0.41
3:C1:48:LEU:O	16:P1:51:GLU:HG3	2.21	0.41
3:C1:87:ILE:HG22	3:C1:101:HIS:HB2	2.02	0.41
5:E1:117:ARG:HD2	5:E1:117:ARG:HA	1.86	0.41
6:F1:128:LYS:HA	6:F1:156:VAL:HG23	2.03	0.41
9:I1:179:LYS:HB2	9:I1:179:LYS:HE2	1.84	0.41
14:N1:75:ASN:HB3	14:N1:128:PHE:CZ	2.56	0.41
18:R1:96:TYR:HA	18:R1:100:VAL:HG22	2.03	0.41
21:U1:6:VAL:HB	21:U1:65:TYR:CE2	2.56	0.41
21:U1:33:TRP:CZ2	21:U1:102:ARG:HD2	2.56	0.41
27:a1:99:LEU:HD12	27:a1:109:TYR:HE1	1.86	0.41
29:c1:24:LEU:HD12	29:c1:24:LEU:HA	1.91	0.41
38:C2:289:LEU:HB3	77:r2:4:HIS:CD2	2.56	0.41
39:D2:289:ARG:NH1	80:54:1180:C:OP2	2.53	0.41
40:E2:219:TYR:OH	40:E2:249:ARG:HD3	2.20	0.41
43:H2:111:LEU:HD12	43:H2:127:ARG:HD2	2.03	0.41
47:M2:124:LYS:HA	47:M2:127:VAL:HG12	2.02	0.41
49:O2:83:THR:HG23	80:54:2052:G:H5'	2.03	0.41
51:Q2:63:LEU:HD23	51:Q2:63:LEU:HA	1.88	0.41
71:k2:8:ILE:HG12	71:k2:56:LEU:HD11	2.02	0.41
75:o2:23:VAL:HG13	75:o2:68:LEU:HB3	2.03	0.41
75:o2:53:LYS:HE2	80:54:91:G:H4'	2.03	0.41
76:p2:46:LYS:HE3	76:p2:46:LYS:HB3	1.74	0.41
77:r2:66:ARG:NE	77:r2:75:THR:O	2.51	0.41
79:t2:151:ILE:O	79:t2:155:ILE:HG12	2.20	0.41
80:54:86:U:H2'	80:54:87:A:C8	2.56	0.41
80:54:495:C:H2'	80:54:496:G:H8	1.85	0.41
80:54:1074:G:H2'	80:54:1075:G:C8	2.55	0.41
80:54:1196:G:H2'	80:54:1197:C:O4'	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:2335:C:H2'	80:54:2336:G:H8	1.85	0.41
80:54:2553:A:H1'	80:54:2554:U:O4'	2.21	0.41
80:54:3960:A:H5''	80:54:3961:G:OP2	2.20	0.41
80:54:4957:C:H3'	80:54:4958:C:H5''	2.02	0.41
80:54:5013:C:H4'	80:54:5014:A:H5''	2.01	0.41
1:A1:996:A:P	15:O1:114:ARG:HH12	2.42	0.41
1:A1:1293:A:H3'	1:A1:1294:G:H8	1.86	0.41
8:H1:200:LYS:HE3	8:H1:200:LYS:HB3	1.91	0.41
12:L1:51:SER:O	12:L1:55:ARG:HG3	2.20	0.41
17:Q1:98:ASN:OD1	17:Q1:122:THR:HA	2.22	0.41
19:S1:94:GLU:N	19:S1:94:GLU:OE1	2.53	0.41
20:T1:36:VAL:HG22	20:T1:40:TYR:CD2	2.56	0.41
29:c1:37:CYS:SG	29:c1:38:PRO:HD2	2.61	0.41
33:g1:140:TYR:HE1	33:g1:145:CYS:HA	1.85	0.41
34:h1:62:HIS:CE1	34:h1:88:ARG:HG3	2.56	0.41
34:h1:101:PHE:CE2	34:h1:120:ILE:HD11	2.56	0.41
34:h1:206:LEU:HD13	34:h1:218:LEU:HD12	2.03	0.41
34:h1:272:GLN:OE1	34:h1:274:VAL:HG12	2.20	0.41
38:C2:152:LEU:HD23	38:C2:251:ILE:HG12	2.02	0.41
48:N2:38:ARG:HD2	82:84:141:C:OP1	2.21	0.41
48:N2:54:LYS:NZ	80:54:153:G:OP2	2.54	0.41
48:N2:142:ILE:HG21	48:N2:151:ILE:HD11	2.03	0.41
65:e2:84:GLU:O	65:e2:87:VAL:HG22	2.21	0.41
75:o2:9:ARG:HA	75:o2:20:PRO:HA	2.03	0.41
80:54:930:G:H2'	80:54:931:C:O4'	2.21	0.41
80:54:2000:G:H4'	80:54:2017:A:H2	1.86	0.41
80:54:4458:C:H2'	80:54:4459:U:C6	2.56	0.41
85:23:59:G:C2'	85:23:60:U:H5'	2.51	0.41
4:D1:98:LEU:O	4:D1:102:LEU:HB2	2.21	0.40
17:Q1:101:THR:HG22	17:Q1:102:PHE:N	2.36	0.40
20:T1:80:PRO:HD2	20:T1:83:PHE:CD2	2.56	0.40
20:T1:84:LEU:HD12	20:T1:95:TYR:HB3	2.03	0.40
42:G2:212:HIS:ND1	42:G2:238:LYS:HA	2.36	0.40
42:G2:214:VAL:HG21	42:G2:220:VAL:HG22	2.03	0.40
44:I2:48:LEU:O	44:I2:139:ARG:HA	2.21	0.40
44:I2:160:PRO:HB3	80:54:4431:U:O3'	2.21	0.40
46:L2:128:PRO:HB3	46:L2:134:PRO:HA	2.03	0.40
47:M2:131:GLN:NE2	49:O2:174:LEU:HD21	2.35	0.40
48:N2:198:LEU:HD23	48:N2:198:LEU:HA	1.93	0.40
50:P2:82:ARG:NH2	80:54:2362:U:OP1	2.46	0.40
57:W2:8:PHE:CD1	57:W2:46:PRO:HG3	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
80:54:481(A):C:C4'	80:54:483:G:H4'	2.48	0.40
80:54:1298:C:H2'	80:54:1299:G:C8	2.56	0.40
80:54:1443:A:H61	80:54:2111:U:H3	1.69	0.40
80:54:2480:G:H2'	80:54:2481:G:C8	2.55	0.40
80:54:2744:A:H8	80:54:2744:A:OP2	2.04	0.40
80:54:3672:G:O2'	80:54:3673:C:OP1	2.32	0.40
80:54:4670:C:O3'	80:54:4671:C:H3'	2.21	0.40
80:54:4948:C:H2'	80:54:4949:G:N2	2.36	0.40
85:23:3:C:H2'	85:23:4:C:C6	2.56	0.40
85:33:59:G:H2'	85:33:60:U:H5'	2.02	0.40
1:A1:1304:U:H5''	33:g1:93:HIS:HB2	2.04	0.40
1:A1:1842:C:H2'	1:A1:1843:G:C8	2.56	0.40
2:B1:103:PHE:CG	2:B1:133:PRO:HG3	2.56	0.40
5:E1:222:PRO:HG2	34:h1:226:HIS:CG	2.56	0.40
5:E1:224:SER:HB3	5:E1:226:GLN:OE1	2.21	0.40
12:L1:29:MET:SD	12:L1:42:ASN:ND2	2.84	0.40
14:N1:26:LEU:HD23	14:N1:26:LEU:HA	1.87	0.40
14:N1:33:ARG:H	14:N1:33:ARG:HD3	1.87	0.40
34:h1:7:LEU:HA	34:h1:309:VAL:O	2.21	0.40
34:h1:38:LYS:HB3	34:h1:62:HIS:O	2.22	0.40
36:A2:36:GLU:OE2	36:A2:163:ARG:NH1	2.54	0.40
37:B2:194:LEU:HD12	37:B2:194:LEU:HA	1.91	0.40
38:C2:343:GLN:HG2	80:54:724:C:H1'	2.03	0.40
40:E2:180:GLY:O	40:E2:181:PRO:C	2.64	0.40
42:G2:196:VAL:O	42:G2:200:VAL:HG23	2.21	0.40
50:P2:86:LYS:HB2	80:54:3857:G:H5''	2.03	0.40
55:U2:74:SER:OG	55:U2:76:VAL:HG12	2.20	0.40
64:d2:37:GLY:O	64:d2:41:ARG:HG3	2.21	0.40
71:k2:26:LYS:HB2	71:k2:69:LEU:HD12	2.03	0.40
71:k2:27:LYS:HB2	71:k2:32:VAL:HG22	2.04	0.40
76:p2:62:LYS:HE2	76:p2:62:LYS:HB2	1.89	0.40
79:t2:121:LEU:HD22	80:54:1972:G:O2'	2.21	0.40
80:54:464:G:H1	80:54:691:C:H42	1.68	0.40
80:54:743:G:H2'	80:54:744:G:O4'	2.21	0.40
80:54:1968:G:C2	80:54:1969:G:C4	3.10	0.40
80:54:2323:C:H2'	80:54:2324:C:C6	2.56	0.40
80:54:4036:G:HO2'	80:54:4037:C:P	2.42	0.40
80:54:4420:U:O4	80:54:4475:G:N2	2.54	0.40
80:54:4862:G:H2'	80:54:4863:G:H8	1.86	0.40
80:54:4897:G:H2'	80:54:4898:G:H8	1.86	0.40
85:33:33:U:H2'	85:33:35:U:OP1	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:1453:C:O2'	19:S1:52:GLY:HA3	2.22	0.40
1:A1:1782:G:H2'	1:A1:1783:C:H4'	2.03	0.40
1:A1:1798:C:H2'	1:A1:1799:G:O4'	2.21	0.40
1:A1:1839:U:H2'	1:A1:1840:U:C6	2.57	0.40
4:D1:132:ASP:OD1	4:D1:136:HIS:HB2	2.21	0.40
4:D1:172:ASN:HD22	4:D1:172:ASN:HA	1.71	0.40
5:E1:46:THR:O	5:E1:46:THR:OG1	2.36	0.40
8:H1:231:ARG:NH2	8:H1:232:ARG:HH21	2.19	0.40
9:I1:87:PHE:HB3	9:I1:90:LYS:HD3	2.03	0.40
10:J1:93:THR:O	10:J1:95:THR:N	2.53	0.40
11:K1:124:HIS:CD2	32:f1:104:ARG:HH21	2.38	0.40
22:V1:34:LYS:HE3	22:V1:34:LYS:HB2	1.95	0.40
29:c1:50:ALA:C	29:c1:52:THR:H	2.29	0.40
30:d1:13:ARG:HG2	30:d1:55:VAL:HG22	2.03	0.40
39:D2:89:LYS:HE2	39:D2:89:LYS:HB3	1.90	0.40
40:E2:111:LYS:HE2	40:E2:111:LYS:HB3	1.78	0.40
41:F2:75:ARG:HD2	80:54:729:G:H5''	2.04	0.40
41:F2:114:ARG:NH1	51:Q2:4:ASP:O	2.49	0.40
42:G2:87:LYS:O	42:G2:89:PRO:HD3	2.21	0.40
49:O2:108:ILE:HD12	49:O2:160:ARG:CZ	2.51	0.40
53:S2:16:CYS:O	53:S2:25:PRO:HG2	2.22	0.40
56:V2:72:LEU:O	56:V2:77:HIS:HE1	2.04	0.40
59:Y2:74:TYR:HD2	59:Y2:77:LYS:HB2	1.87	0.40
61:a2:59:ARG:NH2	75:o2:36:GLN:OE1	2.44	0.40
61:a2:119:LYS:HA	61:a2:140:VAL:HG23	2.01	0.40
70:j2:28:HIS:HD2	70:j2:30:GLN:H	1.69	0.40
80:54:93:G:H2'	80:54:94:A:C8	2.57	0.40
80:54:118:C:H5'	80:54:119:G:OP2	2.22	0.40
80:54:1440:U:HO2'	80:54:1441:C:P	2.44	0.40
80:54:4042:G:H3'	80:54:4043:G:C8	2.56	0.40
80:54:4060:U:H2'	80:54:4061:G:H8	1.86	0.40
85:23:46:7MG:H81	85:23:46:7MG:H2'	1.70	0.40
1:A1:53:C:O2'	1:A1:507:G:N7	2.42	0.40
1:A1:869:A:C4	1:A1:915:G:H1'	2.57	0.40
1:A1:1784:G:H8	1:A1:1784:G:OP1	2.05	0.40
10:J1:132:GLU:O	10:J1:136:ILE:HG13	2.21	0.40
19:S1:63:ARG:NH1	34:h1:280:LYS:HG3	2.36	0.40
34:h1:11:LEU:HB3	34:h1:43:TRP:CZ3	2.56	0.40
39:D2:196:ARG:O	39:D2:200:MET:HG2	2.21	0.40
48:N2:193:ARG:O	48:N2:197:THR:OG1	2.39	0.40
55:U2:20:LYS:HG2	55:U2:73:THR:HB	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:c2:12:GLU:HG2	63:c2:13:SER:N	2.36	0.40
64:d2:25:TYR:CD2	64:d2:88:LEU:HD13	2.56	0.40
69:i2:71:LYS:HB3	69:i2:71:LYS:HE3	1.91	0.40
73:m2:85:ARG:NH2	80:54:4698:C:H3'	2.36	0.40
79:t2:137:GLN:HB2	79:t2:147:HIS:NE2	2.35	0.40
80:54:218:A:O2'	80:54:219:G:H5'	2.22	0.40
80:54:382:G:N1	80:54:385:A:OP2	2.50	0.40
84:B:26:ARG:NH1	84:B:31:THR:H	2.19	0.40
85:23:34:70U:H6	85:23:34:70U:C4'	2.52	0.40
85:33:34:70U:C5'	85:33:35:U:P	3.09	0.40
1:A1:503:C:OP1	6:F1:62:LYS:HE2	2.21	0.40
1:A1:886:A:N6	1:A1:900:C:O2	2.47	0.40
1:A1:1337:C:H2'	1:A1:1338:G:H8	1.85	0.40
12:L1:1:MET:HE3	12:L1:44:HIS:HD2	1.87	0.40
21:U1:33:TRP:HE3	21:U1:37:VAL:HG11	1.87	0.40
28:b1:13:LYS:HD3	28:b1:13:LYS:HA	1.71	0.40
34:h1:33:SER:HB2	34:h1:43:TRP:HE1	1.86	0.40
37:B2:89:ILE:HD12	37:B2:197:ALA:HB1	2.03	0.40
40:E2:289:LEU:HD12	47:M2:109:ARG:NH2	2.37	0.40
43:H2:95:VAL:HG13	73:m2:52:ILE:HD11	2.04	0.40
44:I2:30:LYS:HG3	44:I2:66:GLU:OE1	2.22	0.40
45:J2:169:LYS:HD2	45:J2:170:TYR:CE1	2.57	0.40
47:M2:94:LYS:HE2	80:54:4871:C:OP1	2.21	0.40
48:N2:179:LYS:HD3	80:54:298:G:OP1	2.22	0.40
49:O2:49:ARG:NH1	80:54:1932:A:OP2	2.55	0.40
49:O2:202:LEU:HD23	49:O2:202:LEU:HA	1.90	0.40
79:t2:42:VAL:HA	79:t2:45:ASP:HB2	2.04	0.40
80:54:755:C:H2'	80:54:756:G:H8	1.87	0.40
80:54:969:C:H2'	80:54:2259:G:O6	2.22	0.40
80:54:1942:A:H2'	80:54:1943:A:C8	2.56	0.40
80:54:1989:G:C2	80:54:1990:A:C4	3.09	0.40
80:54:3823:G:H8	80:54:3823:G:O5'	2.04	0.40
80:54:4944:C:OP1	80:54:4944:C:H4'	2.20	0.40
85:23:55:PSU:H6	85:23:55:PSU:H3'	1.86	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	B1	215/295 (73%)	211 (98%)	4 (2%)	0	100	100
3	C1	211/264 (80%)	201 (95%)	10 (5%)	0	100	100
4	D1	219/293 (75%)	215 (98%)	4 (2%)	0	100	100
5	E1	226/243 (93%)	215 (95%)	11 (5%)	0	100	100
6	F1	260/263 (99%)	252 (97%)	8 (3%)	0	100	100
7	G1	181/204 (89%)	168 (93%)	13 (7%)	0	100	100
8	H1	235/249 (94%)	229 (97%)	6 (3%)	0	100	100
9	I1	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
10	J1	204/208 (98%)	194 (95%)	10 (5%)	0	100	100
11	K1	183/194 (94%)	181 (99%)	2 (1%)	0	100	100
12	L1	94/165 (57%)	90 (96%)	4 (4%)	0	100	100
13	M1	139/158 (88%)	131 (94%)	8 (6%)	0	100	100
14	N1	115/132 (87%)	100 (87%)	15 (13%)	0	100	100
15	O1	147/151 (97%)	145 (99%)	2 (1%)	0	100	100
16	P1	134/168 (80%)	130 (97%)	4 (3%)	0	100	100
17	Q1	127/145 (88%)	122 (96%)	5 (4%)	0	100	100
18	R1	140/146 (96%)	136 (97%)	4 (3%)	0	100	100
19	S1	130/135 (96%)	123 (95%)	7 (5%)	0	100	100
20	T1	142/152 (93%)	136 (96%)	6 (4%)	0	100	100
21	U1	139/145 (96%)	132 (95%)	7 (5%)	0	100	100
22	V1	98/119 (82%)	93 (95%)	5 (5%)	0	100	100
23	W1	81/83 (98%)	80 (99%)	1 (1%)	0	100	100
24	X1	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
25	Y1	139/143 (97%)	133 (96%)	4 (3%)	2 (1%)	9	30
26	Z1	122/130 (94%)	119 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	a1	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
28	b1	99/115 (86%)	95 (96%)	4 (4%)	0	100	100
29	c1	81/84 (96%)	79 (98%)	2 (2%)	0	100	100
30	d1	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
31	e1	53/56 (95%)	53 (100%)	0	0	100	100
32	f1	55/133 (41%)	54 (98%)	1 (2%)	0	100	100
33	g1	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
34	h1	311/317 (98%)	288 (93%)	23 (7%)	0	100	100
36	A2	246/257 (96%)	235 (96%)	11 (4%)	0	100	100
37	B2	392/403 (97%)	382 (97%)	10 (3%)	0	100	100
38	C2	360/425 (85%)	349 (97%)	10 (3%)	1 (0%)	36	66
39	D2	291/297 (98%)	286 (98%)	5 (2%)	0	100	100
40	E2	208/291 (72%)	203 (98%)	5 (2%)	0	100	100
41	F2	223/247 (90%)	216 (97%)	7 (3%)	0	100	100
42	G2	229/319 (72%)	228 (100%)	1 (0%)	0	100	100
43	H2	188/192 (98%)	180 (96%)	8 (4%)	0	100	100
44	I2	201/214 (94%)	197 (98%)	4 (2%)	0	100	100
45	J2	168/178 (94%)	166 (99%)	2 (1%)	0	100	100
46	L2	208/211 (99%)	197 (95%)	9 (4%)	2 (1%)	12	38
47	M2	136/218 (62%)	131 (96%)	5 (4%)	0	100	100
48	N2	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
49	O2	197/203 (97%)	195 (99%)	2 (1%)	0	100	100
50	P2	151/184 (82%)	146 (97%)	5 (3%)	0	100	100
51	Q2	185/188 (98%)	176 (95%)	9 (5%)	0	100	100
52	R2	178/196 (91%)	175 (98%)	3 (2%)	0	100	100
53	S2	174/176 (99%)	167 (96%)	7 (4%)	0	100	100
54	T2	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
55	U2	97/128 (76%)	91 (94%)	6 (6%)	0	100	100
56	V2	137/140 (98%)	135 (98%)	2 (2%)	0	100	100
57	W2	102/157 (65%)	99 (97%)	3 (3%)	0	100	100
58	X2	116/156 (74%)	115 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
59	Y2	132/145 (91%)	130 (98%)	2 (2%)	0	100	100
60	Z2	133/136 (98%)	127 (96%)	6 (4%)	0	100	100
61	a2	145/148 (98%)	135 (93%)	10 (7%)	0	100	100
62	b2	100/245 (41%)	96 (96%)	4 (4%)	0	100	100
63	c2	96/115 (84%)	95 (99%)	1 (1%)	0	100	100
64	d2	105/125 (84%)	100 (95%)	5 (5%)	0	100	100
65	e2	126/135 (93%)	122 (97%)	4 (3%)	0	100	100
66	f2	107/110 (97%)	105 (98%)	2 (2%)	0	100	100
67	g2	112/116 (97%)	112 (100%)	0	0	100	100
68	h2	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
69	i2	100/105 (95%)	98 (98%)	2 (2%)	0	100	100
70	j2	84/97 (87%)	84 (100%)	0	0	100	100
71	k2	67/70 (96%)	64 (96%)	3 (4%)	0	100	100
72	l2	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
73	m2	50/102 (49%)	49 (98%)	1 (2%)	0	100	100
74	n2	23/25 (92%)	23 (100%)	0	0	100	100
75	o2	102/106 (96%)	100 (98%)	2 (2%)	0	100	100
76	p2	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
77	r2	122/137 (89%)	120 (98%)	2 (2%)	0	100	100
78	s2	194/318 (61%)	179 (92%)	15 (8%)	0	100	100
79	t2	151/165 (92%)	126 (83%)	24 (16%)	1 (1%)	18	47
83	XX	14/16 (88%)	5 (36%)	7 (50%)	2 (14%)	0	0
84	B	204/217 (94%)	171 (84%)	32 (16%)	1 (0%)	24	55
All	All	11756/13607 (86%)	11295 (96%)	452 (4%)	9 (0%)	49	77

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
83	XX	1016	LYS
46	L2	64	VAL
83	XX	1022	LYS
25	Y1	62	PRO
25	Y1	61	GLN
84	B	61	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
79	t2	54	LYS
38	C2	81	GLY
46	L2	62	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	B1	180/245 (74%)	180 (100%)	0	100	100
3	C1	194/231 (84%)	194 (100%)	0	100	100
4	D1	187/225 (83%)	187 (100%)	0	100	100
5	E1	190/202 (94%)	190 (100%)	0	100	100
6	F1	224/225 (100%)	224 (100%)	0	100	100
7	G1	158/170 (93%)	158 (100%)	0	100	100
8	H1	207/218 (95%)	207 (100%)	0	100	100
9	I1	165/174 (95%)	165 (100%)	0	100	100
10	J1	178/180 (99%)	178 (100%)	0	100	100
11	K1	161/168 (96%)	161 (100%)	0	100	100
12	L1	87/136 (64%)	87 (100%)	0	100	100
13	M1	130/142 (92%)	130 (100%)	0	100	100
14	N1	99/108 (92%)	98 (99%)	1 (1%)	68	88
15	O1	130/131 (99%)	130 (100%)	0	100	100
16	P1	106/130 (82%)	106 (100%)	0	100	100
17	Q1	115/130 (88%)	115 (100%)	0	100	100
18	R1	117/121 (97%)	117 (100%)	0	100	100
19	S1	119/121 (98%)	119 (100%)	0	100	100
20	T1	125/132 (95%)	125 (100%)	0	100	100
21	U1	111/115 (96%)	111 (100%)	0	100	100
22	V1	92/107 (86%)	92 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	W1	67/67 (100%)	67 (100%)	0	100	100
24	X1	112/113 (99%)	112 (100%)	0	100	100
25	Y1	113/115 (98%)	113 (100%)	0	100	100
26	Z1	107/112 (96%)	107 (100%)	0	100	100
27	a1	66/103 (64%)	66 (100%)	0	100	100
28	b1	88/98 (90%)	88 (100%)	0	100	100
29	c1	75/76 (99%)	75 (100%)	0	100	100
30	d1	55/62 (89%)	55 (100%)	0	100	100
31	e1	48/49 (98%)	48 (100%)	0	100	100
32	f1	47/106 (44%)	47 (100%)	0	100	100
33	g1	61/140 (44%)	61 (100%)	0	100	100
34	h1	272/275 (99%)	272 (100%)	0	100	100
36	A2	190/199 (96%)	190 (100%)	0	100	100
37	B2	342/348 (98%)	342 (100%)	0	100	100
38	C2	302/347 (87%)	302 (100%)	0	100	100
39	D2	247/250 (99%)	247 (100%)	0	100	100
40	E2	190/251 (76%)	190 (100%)	0	100	100
41	F2	196/215 (91%)	196 (100%)	0	100	100
42	G2	200/272 (74%)	200 (100%)	0	100	100
43	H2	169/171 (99%)	169 (100%)	0	100	100
44	I2	175/181 (97%)	175 (100%)	0	100	100
45	J2	143/149 (96%)	143 (100%)	0	100	100
46	L2	175/176 (99%)	175 (100%)	0	100	100
47	M2	117/161 (73%)	117 (100%)	0	100	100
48	N2	171/172 (99%)	171 (100%)	0	100	100
49	O2	171/173 (99%)	171 (100%)	0	100	100
50	P2	134/163 (82%)	134 (100%)	0	100	100
51	Q2	164/165 (99%)	164 (100%)	0	100	100
52	R2	159/175 (91%)	159 (100%)	0	100	100
53	S2	157/157 (100%)	157 (100%)	0	100	100
54	T2	139/140 (99%)	139 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	U2	89/114 (78%)	89 (100%)	0	100	100
56	V2	106/107 (99%)	106 (100%)	0	100	100
57	W2	86/126 (68%)	86 (100%)	0	100	100
58	X2	106/134 (79%)	106 (100%)	0	100	100
59	Y2	124/135 (92%)	124 (100%)	0	100	100
60	Z2	117/118 (99%)	117 (100%)	0	100	100
61	a2	119/120 (99%)	119 (100%)	0	100	100
62	b2	84/184 (46%)	84 (100%)	0	100	100
63	c2	84/98 (86%)	84 (100%)	0	100	100
64	d2	98/110 (89%)	98 (100%)	0	100	100
65	e2	114/121 (94%)	114 (100%)	0	100	100
66	f2	88/89 (99%)	88 (100%)	0	100	100
67	g2	98/99 (99%)	98 (100%)	0	100	100
68	h2	109/110 (99%)	109 (100%)	0	100	100
69	i2	86/89 (97%)	86 (100%)	0	100	100
70	j2	73/80 (91%)	73 (100%)	0	100	100
71	k2	64/65 (98%)	64 (100%)	0	100	100
72	l2	47/48 (98%)	47 (100%)	0	100	100
73	m2	48/90 (53%)	48 (100%)	0	100	100
74	n2	24/24 (100%)	24 (100%)	0	100	100
75	o2	92/94 (98%)	92 (100%)	0	100	100
76	p2	74/75 (99%)	74 (100%)	0	100	100
77	r2	108/121 (89%)	108 (100%)	0	100	100
78	s2	164/258 (64%)	164 (100%)	0	100	100
79	t2	126/137 (92%)	126 (100%)	0	100	100
83	XX	5/16 (31%)	5 (100%)	0	100	100
84	B	186/196 (95%)	183 (98%)	3 (2%)	55	83
All	All	10246/11550 (89%)	10242 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	N1	31	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
84	B	93	LEU
84	B	183	ILE
84	B	206	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (190) such sidechains are listed below:

Mol	Chain	Res	Type
2	B1	113	GLN
2	B1	132	GLN
2	B1	141	ASN
3	C1	75	GLN
3	C1	163	GLN
4	D1	172	ASN
4	D1	178	HIS
4	D1	272	HIS
4	D1	277	HIS
5	E1	22	ASN
5	E1	57	ASN
5	E1	101	GLN
5	E1	207	HIS
6	F1	112	HIS
6	F1	161	GLN
7	G1	65	GLN
7	G1	114	ASN
8	H1	65	GLN
8	H1	197	GLN
9	I1	68	GLN
10	J1	52	ASN
10	J1	84	ASN
10	J1	88	ASN
10	J1	111	GLN
10	J1	165	GLN
11	K1	124	HIS
12	L1	66	HIS
13	M1	18	GLN
13	M1	19	ASN
13	M1	65	ASN
13	M1	112	HIS
13	M1	121	GLN
14	N1	28	HIS
14	N1	46	GLN
14	N1	75	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
15	O1	49	GLN
15	O1	58	HIS
15	O1	62	GLN
16	P1	32	HIS
16	P1	94	HIS
17	Q1	32	GLN
18	R1	8	GLN
18	R1	11	GLN
18	R1	24	HIS
18	R1	80	GLN
18	R1	97	GLN
19	S1	116	ASN
20	T1	11	HIS
20	T1	72	GLN
20	T1	105	ASN
21	U1	83	GLN
21	U1	85	ASN
22	V1	28	ASN
23	W1	21	ASN
24	X1	64	ASN
24	X1	90	GLN
24	X1	113	HIS
25	Y1	31	HIS
25	Y1	46	HIS
25	Y1	77	ASN
26	Z1	94	HIS
26	Z1	112	ASN
27	a1	89	GLN
27	a1	112	ASN
28	b1	17	HIS
29	c1	65	GLN
30	d1	7	GLN
30	d1	26	GLN
31	e1	4	GLN
31	e1	16	GLN
32	f1	76	HIS
32	f1	95	GLN
33	g1	135	HIS
34	h1	15	ASN
34	h1	26	GLN
34	h1	64	HIS
34	h1	117	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	h1	119	GLN
34	h1	272	GLN
34	h1	305	ASN
36	A2	22	HIS
36	A2	95	GLN
36	A2	205	ASN
36	A2	216	HIS
37	B2	3	HIS
37	B2	158	GLN
37	B2	184	GLN
37	B2	236	HIS
37	B2	258	HIS
37	B2	354	GLN
38	C2	38	ASN
38	C2	187	GLN
38	C2	212	ASN
38	C2	317	ASN
38	C2	329	ASN
39	D2	175	HIS
39	D2	198	HIS
39	D2	225	GLN
39	D2	267	ASN
39	D2	282	GLN
39	D2	291	GLN
40	E2	193	HIS
40	E2	214	HIS
40	E2	253	GLN
40	E2	287	HIS
41	F2	79	ASN
41	F2	115	GLN
41	F2	118	ASN
41	F2	191	HIS
41	F2	238	GLN
41	F2	247	ASN
42	G2	99	GLN
42	G2	134	ASN
42	G2	206	GLN
42	G2	261	ASN
42	G2	278	ASN
43	H2	39	ASN
43	H2	42	ASN
43	H2	156	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
44	I2	73	ASN
44	I2	95	HIS
44	I2	112	GLN
44	I2	163	GLN
44	I2	213	HIS
45	J2	10	ASN
45	J2	46	GLN
45	J2	104	ASN
46	L2	19	GLN
46	L2	28	GLN
46	L2	67	HIS
46	L2	113	ASN
46	L2	188	ASN
48	N2	15	GLN
48	N2	87	HIS
48	N2	182	HIS
48	N2	196	ASN
48	N2	201	HIS
49	O2	50	ASN
49	O2	63	ASN
49	O2	180	GLN
50	P2	21	ASN
50	P2	25	HIS
50	P2	28	ASN
50	P2	56	GLN
50	P2	80	GLN
50	P2	116	HIS
50	P2	133	HIS
51	Q2	93	GLN
51	Q2	125	GLN
51	Q2	188	ASN
52	R2	27	ASN
52	R2	75	HIS
52	R2	141	HIS
52	R2	143	HIS
53	S2	91	HIS
53	S2	156	HIS
53	S2	163	HIS
54	T2	95	HIS
55	U2	41	GLN
56	V2	27	ASN
56	V2	77	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
56	V2	135	ASN
57	W2	17	HIS
57	W2	95	ASN
57	W2	96	GLN
58	X2	107	HIS
58	X2	111	GLN
58	X2	151	ASN
59	Y2	14	ASN
61	a2	28	HIS
62	b2	27	GLN
62	b2	60	ASN
63	c2	72	HIS
64	d2	30	HIS
64	d2	100	ASN
65	e2	107	ASN
68	h2	98	HIS
68	h2	108	GLN
69	i2	15	HIS
69	i2	26	HIS
70	j2	28	HIS
70	j2	66	HIS
70	j2	76	HIS
72	l2	4	HIS
75	o2	76	ASN
77	r2	4	HIS
77	r2	45	HIS
78	s2	105	ASN
78	s2	190	GLN
79	t2	65	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A1	1680/1869 (89%)	302 (17%)	17 (1%)
35	i1	9/10 (90%)	1 (11%)	0
80	54	3577/3603 (99%)	685 (19%)	59 (1%)
81	74	118/120 (98%)	9 (7%)	0
82	84	149/156 (95%)	25 (16%)	1 (0%)
85	23	75/76 (98%)	24 (32%)	7 (9%)
85	33	75/76 (98%)	24 (32%)	7 (9%)
All	All	5683/5910 (96%)	1070 (18%)	91 (1%)

All (1070) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A1	2	A
1	A1	3	C
1	A1	17	C
1	A1	23	G
1	A1	25	A
1	A1	33	G
1	A1	41	G
1	A1	44	U
1	A1	46	A
1	A1	56	G
1	A1	58	C
1	A1	67	C
1	A1	68	A
1	A1	72	C
1	A1	73	C
1	A1	74	G
1	A1	75	G
1	A1	77	A
1	A1	79	A
1	A1	100	U
1	A1	103	A
1	A1	111	A
1	A1	113	G
1	A1	114	G
1	A1	115	U
1	A1	116	U
1	A1	124	U
1	A1	126	G
1	A1	130	G
1	A1	143	U
1	A1	147	A
1	A1	155	G
1	A1	162	C
1	A1	163	U
1	A1	173	A
1	A1	180	G
1	A1	183	G
1	A1	184	G
1	A1	185	G
1	A1	186	C
1	A1	188	C
1	A1	192	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	206	G
1	A1	302	A
1	A1	307	G
1	A1	308	G
1	A1	309	G
1	A1	312	G
1	A1	319	C
1	A1	347	G
1	A1	362	C
1	A1	364	A
1	A1	368	U
1	A1	369	C
1	A1	370	G
1	A1	385	G
1	A1	386	C
1	A1	398	A
1	A1	400	C
1	A1	407	G
1	A1	408	A
1	A1	409	C
1	A1	418	A
1	A1	441	C
1	A1	447	A
1	A1	448	A
1	A1	450	C
1	A1	464	A
1	A1	465	A
1	A1	466	G
1	A1	471	G
1	A1	472	C
1	A1	473	A
1	A1	474	G
1	A1	482	G
1	A1	483	C
1	A1	487	U
1	A1	492	C
1	A1	516	A
1	A1	517	C
1	A1	531	A
1	A1	532	C
1	A1	533	A
1	A1	535	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	542	U
1	A1	547	G
1	A1	548	C
1	A1	549	C
1	A1	550	C
1	A1	551	U
1	A1	554	A
1	A1	556	U
1	A1	559	G
1	A1	561	A
1	A1	562	U
1	A1	568	C
1	A1	576	A
1	A1	583	A
1	A1	587	A
1	A1	588	G
1	A1	590	A
1	A1	591	U
1	A1	603	C
1	A1	606	G
1	A1	607	U
1	A1	608	C
1	A1	614	C
1	A1	621	C
1	A1	627	U
1	A1	628	A
1	A1	631	U
1	A1	632	C
1	A1	643	A
1	A1	644	G
1	A1	655	A
1	A1	660	C
1	A1	664	A
1	A1	668	A
1	A1	669	A
1	A1	670	A
1	A1	671	A
1	A1	672	A
1	A1	673	G
1	A1	684	G
1	A1	689	U
1	A1	752	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	753	C
1	A1	754	G
1	A1	808	A
1	A1	811	A
1	A1	821	G
1	A1	822	U
1	A1	830	A
1	A1	844	U
1	A1	847	A
1	A1	859	G
1	A1	868	G
1	A1	870	A
1	A1	871	U
1	A1	872	A
1	A1	874	G
1	A1	875	A
1	A1	878	G
1	A1	879	C
1	A1	887	U
1	A1	888	U
1	A1	889	U
1	A1	893	U
1	A1	898	U
1	A1	901	G
1	A1	908	A
1	A1	909	G
1	A1	913	A
1	A1	914	U
1	A1	920	A
1	A1	922	A
1	A1	933	G
1	A1	963	A
1	A1	971	G
1	A1	978	G
1	A1	990	A
1	A1	992	A
1	A1	999	G
1	A1	1017	U
1	A1	1023	A
1	A1	1060	A
1	A1	1062	A
1	A1	1078	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1080	A
1	A1	1083	A
1	A1	1085	C
1	A1	1107	G
1	A1	1115	U
1	A1	1116	C
1	A1	1117	C
1	A1	1118	C
1	A1	1121	G
1	A1	1126	G
1	A1	1138	C
1	A1	1148	A
1	A1	1153	C
1	A1	1154	U
1	A1	1195	A
1	A1	1203	G
1	A1	1207	G
1	A1	1208	A
1	A1	1215	C
1	A1	1221	G
1	A1	1224	G
1	A1	1242	U
1	A1	1248	U
1	A1	1251	A
1	A1	1253	A
1	A1	1256	G
1	A1	1257	G
1	A1	1259	A
1	A1	1265	A
1	A1	1274	G
1	A1	1275	G
1	A1	1282	A
1	A1	1284	A
1	A1	1285	G
1	A1	1286	G
1	A1	1292	C
1	A1	1299	A
1	A1	1301	A
1	A1	1302	G
1	A1	1303	C
1	A1	1308	U
1	A1	1309	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1310	U
1	A1	1313	A
1	A1	1318	G
1	A1	1341	C
1	A1	1342	U
1	A1	1348	G
1	A1	1371	U
1	A1	1372	U
1	A1	1378	A
1	A1	1395	C
1	A1	1396	A
1	A1	1397	U
1	A1	1401	A
1	A1	1402	A
1	A1	1404	U
1	A1	1406	G
1	A1	1428	G
1	A1	1429	G
1	A1	1447	G
1	A1	1452	A
1	A1	1454	A
1	A1	1462	U
1	A1	1463	U
1	A1	1466	G
1	A1	1476	A
1	A1	1480	A
1	A1	1487	A
1	A1	1489	A
1	A1	1490	G
1	A1	1495	G
1	A1	1497	G
1	A1	1498	A
1	A1	1519	U
1	A1	1521	C
1	A1	1533	A
1	A1	1544	C
1	A1	1548	G
1	A1	1552	G
1	A1	1553	C
1	A1	1554	C
1	A1	1555	U
1	A1	1556	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1560	U
1	A1	1570	G
1	A1	1574	C
1	A1	1580	A
1	A1	1585	U
1	A1	1586	U
1	A1	1587	G
1	A1	1588	A
1	A1	1601	A
1	A1	1603	G
1	A1	1621	U
1	A1	1623	A
1	A1	1637	A
1	A1	1638	G
1	A1	1639	G
1	A1	1648	G
1	A1	1654	G
1	A1	1664	A
1	A1	1665	G
1	A1	1671	G
1	A1	1680	G
1	A1	1697	A
1	A1	1699	A
1	A1	1721	U
1	A1	1722	G
1	A1	1726	G
1	A1	1744	G
1	A1	1748	G
1	A1	1750	C
1	A1	1753	C
1	A1	1774	C
1	A1	1783	C
1	A1	1784	G
1	A1	1785	C
1	A1	1805	G
1	A1	1823	A
1	A1	1825	A
1	A1	1829	G
1	A1	1831	A
1	A1	1835	A
1	A1	1836	G
1	A1	1838	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A1	1849	G
1	A1	1851	A
1	A1	1860	A
1	A1	1861	G
1	A1	1862	G
1	A1	1863	A
1	A1	1865	C
1	A1	1869	A
35	i1	22	A
80	54	17	A
80	54	25	A
80	54	35	U
80	54	39	A
80	54	42	A
80	54	56	A
80	54	58	G
80	54	59	A
80	54	64	A
80	54	65	A
80	54	66	A
80	54	73	A
80	54	74	G
80	54	91	G
80	54	98	A
80	54	104	G
80	54	108	A
80	54	109	G
80	54	110	C
80	54	117	C
80	54	118	C
80	54	119	G
80	54	120	A
80	54	126	C
80	54	134	G
80	54	135	G
80	54	136	C
80	54	146	G
80	54	159	C
80	54	170	C
80	54	172	C
80	54	173	C
80	54	177	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	182	G
80	54	200	U
80	54	201	C
80	54	209	U
80	54	210	C
80	54	216	C
80	54	218	A
80	54	219	G
80	54	224	U
80	54	233	U
80	54	234	G
80	54	246	G
80	54	265	C
80	54	266	C
80	54	267	G
80	54	268	G
80	54	276	C
80	54	280	G
80	54	297	U
80	54	306	A
80	54	309	C
80	54	310	G
80	54	315	G
80	54	316	U
80	54	334	A
80	54	340	C
80	54	350	C
80	54	362	A
80	54	363	A
80	54	379	G
80	54	386	A
80	54	387	G
80	54	407	A
80	54	410	A
80	54	412	G
80	54	413	G
80	54	431	G
80	54	432	U
80	54	446	C
80	54	449	C
80	54	450	G
80	54	452	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	453	G
80	54	454	U
80	54	455	C
80	54	463	A
80	54	467	U
80	54	468	U
80	54	481	G
80	54	481(A)	C
80	54	482	G
80	54	485	C
80	54	486	C
80	54	492	U
80	54	497	G
80	54	498	C
80	54	499	G
80	54	505	G
80	54	510	U
80	54	658	C
80	54	661	C
80	54	666	G
80	54	667	A
80	54	672	C
80	54	685	C
80	54	686	A
80	54	696	C
80	54	697	G
80	54	704	C
80	54	705	G
80	54	729	G
80	54	730	G
80	54	731	G
80	54	738	C
80	54	739	G
80	54	742	G
80	54	746	A
80	54	747	A
80	54	749	G
80	54	758	G
80	54	913	U
80	54	914	U
80	54	917	A
80	54	918	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	923	C
80	54	925	C
80	54	926	G
80	54	929	A
80	54	931	C
80	54	932	A
80	54	933	G
80	54	935	A
80	54	935(A)	G
80	54	936	C
80	54	938	C
80	54	939	G
80	54	941	C
80	54	943	A
80	54	944	A
80	54	945	U
80	54	946	C
80	54	959	G
80	54	960	A
80	54	961	G
80	54	966	A
80	54	967	C
80	54	969	C
80	54	972	C
80	54	979	C
80	54	983	C
80	54	1070	G
80	54	1072	C
80	54	1073	G
80	54	1079	C
80	54	1080	C
80	54	1082	C
80	54	1174	G
80	54	1179	U
80	54	1195	G
80	54	1196	G
80	54	1198	G
80	54	1210	C
80	54	1211	G
80	54	1212	G
80	54	1214	C
80	54	1215	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	1234	G
80	54	1235	G
80	54	1236	C
80	54	1237	C
80	54	1239	C
80	54	1249	C
80	54	1273	G
80	54	1275	G
80	54	1276	C
80	54	1277	G
80	54	1280	C
80	54	1284	G
80	54	1285	U
80	54	1287	G
80	54	1292	C
80	54	1293	G
80	54	1295	U
80	54	1296	G
80	54	1301	C
80	54	1303	A
80	54	1326	A
80	54	1337	A
80	54	1354	A
80	54	1358	G
80	54	1359	G
80	54	1371	A
80	54	1377	G
80	54	1378	C
80	54	1387	A
80	54	1394	G
80	54	1397	A
80	54	1398	A
80	54	1400	G
80	54	1406(A)	G
80	54	1414	C
80	54	1420	A
80	54	1437	C
80	54	1438	U
80	54	1440	U
80	54	1441	C
80	54	1445	U
80	54	1446	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	1456	C
80	54	1457	G
80	54	1476	C
80	54	1477	C
80	54	1478	C
80	54	1480	C
80	54	1482	G
80	54	1483	C
80	54	1497	A
80	54	1498	G
80	54	1502	G
80	54	1514	U
80	54	1523	A
80	54	1534	A
80	54	1547	A
80	54	1566	C
80	54	1578	U
80	54	1582	U
80	54	1586	G
80	54	1588	U
80	54	1591	U
80	54	1596	U
80	54	1602	U
80	54	1612	G
80	54	1613	A
80	54	1624	G
80	54	1625	G
80	54	1631	A
80	54	1633	G
80	54	1634	A
80	54	1638	A
80	54	1640	C
80	54	1641	G
80	54	1654	G
80	54	1661	C
80	54	1676	C
80	54	1694	C
80	54	1696	C
80	54	1731	C
80	54	1734	G
80	54	1741	G
80	54	1742	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	1750	G
80	54	1756	U
80	54	1760	G
80	54	1764	G
80	54	1765	A
80	54	1768	C
80	54	1772	C
80	54	1773	U
80	54	1775	A
80	54	1776	A
80	54	1781	U
80	54	1787	A
80	54	1797	G
80	54	1798	G
80	54	1804	A
80	54	1806	G
80	54	1815	G
80	54	1819	G
80	54	1821	G
80	54	1828	C
80	54	1835	G
80	54	1836	G
80	54	1837	A
80	54	1842	G
80	54	1843	A
80	54	1855	G
80	54	1869	G
80	54	1882	U
80	54	1889	U
80	54	1890	G
80	54	1892	A
80	54	1893	C
80	54	1897	A
80	54	1910	G
80	54	1918	U
80	54	1920	C
80	54	1921	C
80	54	1922	G
80	54	1931	C
80	54	1932	A
80	54	1940	G
80	54	1945	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	1948	G
80	54	1951	G
80	54	1958	A
80	54	1961	G
80	54	1962	A
80	54	1964	A
80	54	1965	G
80	54	1967	A
80	54	1969	G
80	54	1972	G
80	54	1976	G
80	54	1977	C
80	54	1978	C
80	54	1979	A
80	54	1980	U
80	54	1983	A
80	54	1984	A
80	54	1985	G
80	54	1986	U
80	54	1987	C
80	54	1991	A
80	54	1997	U
80	54	2001	G
80	54	2002	A
80	54	2004	U
80	54	2007	G
80	54	2021	G
80	54	2025	A
80	54	2026	A
80	54	2044	U
80	54	2046	G
80	54	2047	A
80	54	2048	U
80	54	2052	G
80	54	2055	G
80	54	2056	G
80	54	2069	A
80	54	2071	A
80	54	2084	U
80	54	2090	U
80	54	2092	G
80	54	2093	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	2094	C
80	54	2097	A
80	54	2098	G
80	54	2100	G
80	54	2102	G
80	54	2104	A
80	54	2105	A
80	54	2106	G
80	54	2107	A
80	54	2108	G
80	54	2259	G
80	54	2260	C
80	54	2267	U
80	54	2268	A
80	54	2289	C
80	54	2300	A
80	54	2301	G
80	54	2313	A
80	54	2316	G
80	54	2332	A
80	54	2333	G
80	54	2345	G
80	54	2348	G
80	54	2351	C
80	54	2360	A
80	54	2364	G
80	54	2395	A
80	54	2396	A
80	54	2402	G
80	54	2409	U
80	54	2417	A
80	54	2422	C
80	54	2425	U
80	54	2433	G
80	54	2441	C
80	54	2447	U
80	54	2450	G
80	54	2453	A
80	54	2471	G
80	54	2475	G
80	54	2488	C
80	54	2489	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	2490	U
80	54	2491	C
80	54	2493	G
80	54	2503	G
80	54	2504	C
80	54	2505	C
80	54	2506	G
80	54	2513	A
80	54	2514	G
80	54	2529	A
80	54	2530	U
80	54	2537	A
80	54	2544	G
80	54	2546	G
80	54	2547	G
80	54	2554	U
80	54	2564	G
80	54	2566	G
80	54	2583	C
80	54	2586	G
80	54	2587	A
80	54	2601	A
80	54	2618	G
80	54	2627	C
80	54	2638	G
80	54	2640	G
80	54	2653	C
80	54	2662	G
80	54	2669	C
80	54	2681	G
80	54	2687	U
80	54	2694	G
80	54	2695	A
80	54	2696	A
80	54	2705	G
80	54	2707	U
80	54	2708	U
80	54	2709	C
80	54	2710	C
80	54	2711	G
80	54	2716	C
80	54	2723	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	2726	G
80	54	2735	G
80	54	2740	U
80	54	2743	A
80	54	2744	A
80	54	2754	G
80	54	2763	U
80	54	2764	A
80	54	2769	U
80	54	2787	A
80	54	2788	U
80	54	2790	U
80	54	2798	A
80	54	2803	U
80	54	2806	A
80	54	2807	A
80	54	2808	G
80	54	2814	C
80	54	2815	A
80	54	2826	U
80	54	2827	G
80	54	2828	U
80	54	2842	G
80	54	2855	G
80	54	2867	C
80	54	2869	U
80	54	3598	C
80	54	3602	C
80	54	3603	G
80	54	3604	A
80	54	3605	C
80	54	3606	U
80	54	3615	G
80	54	3616	U
80	54	3617	G
80	54	3618	C
80	54	3625	G
80	54	3626	G
80	54	3635	A
80	54	3644	U
80	54	3648	A
80	54	3657	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	3662	A
80	54	3670	C
80	54	3673	C
80	54	3696	C
80	54	3712	A
80	54	3713	U
80	54	3714	G
80	54	3743	G
80	54	3748	A
80	54	3753	G
80	54	3756	A
80	54	3760	A
80	54	3773	U
80	54	3774	A
80	54	3776	G
80	54	3777	G
80	54	3784	A
80	54	3786	U
80	54	3788	C
80	54	3810	C
80	54	3811	G
80	54	3812	C
80	54	3814	U
80	54	3817	A
80	54	3819	G
80	54	3838	U
80	54	3839	G
80	54	3840	U
80	54	3876	A
80	54	3877	A
80	54	3878	C
80	54	3879	G
80	54	3889	G
80	54	3897	G
80	54	3901	A
80	54	3905	A
80	54	3906	A
80	54	3907	G
80	54	3908	A
80	54	3915	U
80	54	3916	G
80	54	3938	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	3939	G
80	54	3951	G
80	54	3960	A
80	54	3962	A
80	54	3963	A
80	54	3964	U
80	54	3966	A
80	54	3967	G
80	54	3969	G
80	54	3972	A
80	54	3973	G
80	54	4037	C
80	54	4038	C
80	54	4039	G
80	54	4041	C
80	54	4043	G
80	54	4048	A
80	54	4056	A
80	54	4066	U
80	54	4073	A
80	54	4076	G
80	54	4086	G
80	54	4088	C
80	54	4097	G
80	54	4110	C
80	54	4116	C
80	54	4118	U
80	54	4119	C
80	54	4120	U
80	54	4122	G
80	54	4127	A
80	54	4138	C
80	54	4158	C
80	54	4162	C
80	54	4163	U
80	54	4170	A
80	54	4171	C
80	54	4183	G
80	54	4184	G
80	54	4191	G
80	54	4203	A
80	54	4212	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	4225	G
80	54	4228	G
80	54	4229	U
80	54	4232	U
80	54	4233	A
80	54	4242	U
80	54	4249	G
80	54	4251	A
80	54	4254	G
80	54	4255	A
80	54	4266	G
80	54	4268	A
80	54	4271	A
80	54	4273	A
80	54	4281	A
80	54	4290	U
80	54	4291	G
80	54	4292	A
80	54	4297	G
80	54	4304	A
80	54	4305	G
80	54	4306	U
80	54	4314	C
80	54	4329	G
80	54	4330	G
80	54	4332	C
80	54	4338	G
80	54	4348	A
80	54	4349	C
80	54	4354	U
80	54	4355	G
80	54	4368	G
80	54	4373	G
80	54	4377	G
80	54	4378	A
80	54	4380	A
80	54	4387	C
80	54	4391	G
80	54	4394	A
80	54	4395	U
80	54	4419	U
80	54	4420	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	4422	A
80	54	4426	C
80	54	4448	G
80	54	4449	A
80	54	4464	A
80	54	4475	G
80	54	4482	U
80	54	4488	A
80	54	4500	U
80	54	4512	U
80	54	4513	A
80	54	4515	G
80	54	4519	C
80	54	4524	G
80	54	4531	U
80	54	4535	A
80	54	4548	A
80	54	4549	G
80	54	4560	C
80	54	4567	G
80	54	4569	U
80	54	4570	G
80	54	4573	G
80	54	4575	G
80	54	4577	U
80	54	4584	A
80	54	4590	A
80	54	4636	U
80	54	4637	G
80	54	4639	G
80	54	4656	A
80	54	4670	C
80	54	4672	A
80	54	4677	U
80	54	4700	A
80	54	4709	U
80	54	4719	G
80	54	4720	C
80	54	4736	C
80	54	4747	C
80	54	4751	G
80	54	4754	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	4757	C
80	54	4759	C
80	54	4761	G
80	54	4765	G
80	54	4771	C
80	54	4772	C
80	54	4773	C
80	54	4867	G
80	54	4870	G
80	54	4871	C
80	54	4873	G
80	54	4875	G
80	54	4876	A
80	54	4877	G
80	54	4882	U
80	54	4883	C
80	54	4885	U
80	54	4894	A
80	54	4895	C
80	54	4902	C
80	54	4907	G
80	54	4909	A
80	54	4912	G
80	54	4914	G
80	54	4919	G
80	54	4921	C
80	54	4922	C
80	54	4926	C
80	54	4934	A
80	54	4937	C
80	54	4938	A
80	54	4939	C
80	54	4943	A
80	54	4944	C
80	54	4948	C
80	54	4949	G
80	54	4950	U
80	54	4951	G
80	54	4955	A
80	54	4956	A
80	54	4957	C
80	54	4958	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	4959	U
80	54	4963	G
80	54	4966	A
80	54	4967	A
80	54	4976	U
80	54	4979	A
80	54	4985	U
80	54	4988	U
80	54	4989	U
80	54	4990	C
80	54	4991	U
80	54	4993	G
80	54	5014	A
80	54	5017	G
80	54	5041	G
80	54	5047	C
80	54	5050	C
80	54	5053	U
80	54	5054	C
80	54	5060	A
80	54	5061	A
80	54	5062	G
81	74	2	U
81	74	7	G
81	74	25	G
81	74	53	U
81	74	54	A
81	74	64	G
81	74	100	A
81	74	110	G
81	74	111	C
82	84	2	G
82	84	3	A
82	84	23	C
82	84	34	U
82	84	35	C
82	84	52	A
82	84	59	A
82	84	60	G
82	84	62	A
82	84	63	U
82	84	74	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
82	84	75	G
82	84	87	G
82	84	103	A
82	84	105	C
82	84	110	U
82	84	111	U
82	84	114	G
82	84	121	G
82	84	123	U
82	84	125	C
82	84	126	C
82	84	127	U
82	84	128	C
82	84	147	G
85	23	8	U
85	23	13	C
85	23	14	A
85	23	16	C
85	23	17	C
85	23	18	G
85	23	19	G
85	23	20	H2U
85	23	21	A
85	23	33	U
85	23	34	70U
85	23	35	U
85	23	37	12A
85	23	42	G
85	23	45	G
85	23	46	7MG
85	23	47	H2U
85	23	48	5MC
85	23	49	5MC
85	23	57	A
85	23	63	C
85	23	67	U
85	23	75	C
85	23	76	A
85	33	8	U
85	33	13	C
85	33	14	A
85	33	16	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
85	33	17	C
85	33	18	G
85	33	19	G
85	33	20	H2U
85	33	21	A
85	33	33	U
85	33	34	70U
85	33	35	U
85	33	37	12A
85	33	42	G
85	33	45	G
85	33	46	7MG
85	33	47	H2U
85	33	48	5MC
85	33	49	5MC
85	33	57	A
85	33	63	C
85	33	67	U
85	33	75	C
85	33	76	A

All (91) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A1	24	C
1	A1	110	U
1	A1	417	C
1	A1	465	A
1	A1	532	C
1	A1	553	U
1	A1	561	A
1	A1	627	U
1	A1	688	U
1	A1	752	G
1	A1	870	A
1	A1	874	G
1	A1	1061	U
1	A1	1137	U
1	A1	1308	U
1	A1	1395	C
1	A1	1637	A
80	54	125	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	134	G
80	54	217	C
80	54	245	C
80	54	265	C
80	54	267	G
80	54	275	C
80	54	385	A
80	54	406	C
80	54	449	C
80	54	480	C
80	54	485	C
80	54	504	G
80	54	685	C
80	54	922(B)	C
80	54	930	G
80	54	959	G
80	54	1072	C
80	54	1211	G
80	54	1236	C
80	54	1238	A
80	54	1291	G
80	54	1370	G
80	54	1440	U
80	54	1445	U
80	54	1455	G
80	54	1477	C
80	54	1633	G
80	54	1818	G
80	54	1979	A
80	54	1983	A
80	54	2046	G
80	54	2068	C
80	54	2089	G
80	54	2258	C
80	54	2266	C
80	54	2502	A
80	54	2639	U
80	54	2695	A
80	54	3603	G
80	54	3625	G
80	54	3672	G
80	54	3876	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
80	54	3888	G
80	54	3904	G
80	54	3959	U
80	54	3968	U
80	54	4036	G
80	54	4042	G
80	54	4119	C
80	54	4232	U
80	54	4354	U
80	54	4448	G
80	54	4699	U
80	54	4719	G
80	54	4884	G
80	54	4925	U
80	54	4936	G
80	54	4947	U
82	84	124	U
85	23	16	C
85	23	17	C
85	23	18	G
85	23	19	G
85	23	35	U
85	23	47	H2U
85	23	48	5MC
85	33	16	C
85	33	17	C
85	33	18	G
85	33	19	G
85	33	35	U
85	33	47	H2U
85	33	48	5MC

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

24 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
85	5MC	23	48	85	19,22,23	1.53	2 (10%)	26,32,35	1.78	8 (30%)
85	1MA	33	58	85	21,25,26	1.37	4 (19%)	30,37,40	1.85	7 (23%)
85	PSU	33	27	85	18,21,22	2.03	4 (22%)	21,30,33	2.14	4 (19%)
85	70U	33	34	85	22,26,27	3.31	9 (40%)	27,37,40	3.70	12 (44%)
85	H2U	23	47	85	18,21,22	1.01	2 (11%)	19,30,33	1.23	3 (15%)
85	PSU	23	39	85	18,21,22	2.06	4 (22%)	21,30,33	2.10	4 (19%)
85	2MU	33	54	85	20,23,24	1.48	3 (15%)	27,33,36	2.56	7 (25%)
85	2MU	23	54	85	20,23,24	1.48	3 (15%)	27,33,36	2.54	7 (25%)
85	7MG	23	46	85	23,26,27	1.74	4 (17%)	27,39,42	2.84	9 (33%)
85	H2U	33	20	85	18,21,22	4.39	5 (27%)	19,30,33	4.06	6 (31%)
85	H2U	23	20	85	18,21,22	4.39	5 (27%)	19,30,33	4.06	6 (31%)
85	PSU	23	27	85	18,21,22	2.03	4 (22%)	21,30,33	2.12	4 (19%)
85	5MC	33	48	85	19,22,23	1.52	2 (10%)	26,32,35	1.78	8 (30%)
85	H2U	33	47	85	18,21,22	1.01	2 (11%)	19,30,33	1.23	3 (15%)
85	5MC	23	49	85	19,22,23	1.21	2 (10%)	26,32,35	1.63	7 (26%)
85	PSU	23	55	85	18,21,22	1.50	4 (22%)	21,30,33	2.38	6 (28%)
85	70U	23	34	35,85	22,26,27	3.31	9 (40%)	27,37,40	3.70	12 (44%)
85	12A	23	37	85	33,36,37	1.87	5 (15%)	46,52,55	2.13	13 (28%)
85	1MA	23	58	85	21,25,26	1.37	4 (19%)	30,37,40	1.85	7 (23%)
85	PSU	33	55	85	18,21,22	1.49	4 (22%)	21,30,33	2.38	6 (28%)
85	PSU	33	39	85	18,21,22	2.06	4 (22%)	21,30,33	2.09	4 (19%)
85	12A	33	37	85	33,36,37	1.87	5 (15%)	46,52,55	2.13	13 (28%)
85	5MC	33	49	85	19,22,23	1.21	2 (10%)	26,32,35	1.63	7 (26%)
85	7MG	33	46	85	23,26,27	1.74	4 (17%)	27,39,42	2.83	9 (33%)

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
85	5MC	23	48	85	-	2/7/25/26	0/2/2/2
85	1MA	33	58	85	-	0/7/25/26	0/3/3/3
85	PSU	33	27	85	-	0/7/25/26	0/2/2/2
85	70U	33	34	85	-	5/13/31/32	0/2/2/2
85	H2U	23	47	85	-	2/7/38/39	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
85	PSU	23	39	85	-	0/7/25/26	0/2/2/2
85	2MU	33	54	85	-	1/9/27/28	0/2/2/2
85	2MU	23	54	85	-	1/9/27/28	0/2/2/2
85	7MG	23	46	85	-	1/7/37/38	0/3/3/3
85	H2U	33	20	85	-	5/7/38/39	0/2/2/2
85	H2U	23	20	85	-	5/7/38/39	0/2/2/2
85	PSU	23	27	85	-	0/7/25/26	0/2/2/2
85	5MC	33	48	85	-	2/7/25/26	0/2/2/2
85	H2U	33	47	85	-	2/7/38/39	0/2/2/2
85	5MC	23	49	85	-	1/7/25/26	0/2/2/2
85	PSU	23	55	85	-	0/7/25/26	0/2/2/2
85	70U	23	34	35,85	-	5/13/31/32	0/2/2/2
85	12A	23	37	85	-	9/25/43/44	0/3/3/3
85	1MA	23	58	85	-	0/7/25/26	0/3/3/3
85	PSU	33	55	85	-	0/7/25/26	0/2/2/2
85	PSU	33	39	85	-	0/7/25/26	0/2/2/2
85	12A	33	37	85	-	9/25/43/44	0/3/3/3
85	5MC	33	49	85	-	1/7/25/26	0/2/2/2
85	7MG	33	46	85	-	1/7/37/38	0/3/3/3

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	33	20	H2U	O4-C4	10.40	1.43	1.23
85	23	20	H2U	O4-C4	10.38	1.43	1.23
85	33	20	H2U	C2-N1	9.28	1.48	1.35
85	23	20	H2U	C2-N1	9.27	1.48	1.35
85	23	34	70U	C2-S2	-8.87	1.53	1.67
85	33	34	70U	C2-S2	-8.83	1.53	1.67
85	33	20	H2U	O2-C2	8.68	1.38	1.23
85	23	20	H2U	O2-C2	8.67	1.38	1.23
85	23	37	12A	C2-S2	-6.97	1.70	1.75
85	33	37	12A	C2-S2	-6.94	1.70	1.75
85	23	20	H2U	C2-N3	6.74	1.49	1.38
85	33	20	H2U	C2-N3	6.72	1.49	1.38
85	33	34	70U	O3'-C3'	-6.08	1.27	1.43
85	23	34	70U	O3'-C3'	-6.06	1.27	1.43
85	23	34	70U	C4-N3	-5.69	1.28	1.38
85	33	34	70U	C4-N3	-5.68	1.28	1.38
85	23	20	H2U	C4-N3	5.45	1.46	1.37
85	33	20	H2U	C4-N3	5.44	1.46	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	23	46	7MG	C4-N9	-5.30	1.31	1.37
85	33	46	7MG	C4-N9	-5.30	1.31	1.37
85	33	39	PSU	C6-C5	4.71	1.40	1.35
85	33	27	PSU	C6-C5	4.67	1.40	1.35
85	23	39	PSU	C6-C5	4.66	1.40	1.35
85	23	27	PSU	C6-C5	4.63	1.40	1.35
85	33	37	12A	C5-C4	4.59	1.47	1.39
85	23	37	12A	C5-C4	4.57	1.47	1.39
85	33	34	70U	C6-N1	-4.50	1.30	1.38
85	23	34	70U	C6-N1	-4.49	1.30	1.38
85	23	39	PSU	C2-N1	-4.30	1.31	1.36
85	33	39	PSU	C2-N1	-4.28	1.31	1.36
85	33	27	PSU	C2-N1	-4.21	1.31	1.36
85	23	27	PSU	C2-N1	-4.21	1.31	1.36
85	33	34	70U	O9-C8	4.04	1.45	1.33
85	23	34	70U	O9-C8	4.02	1.45	1.33
85	23	39	PSU	O4-C4	-3.94	1.16	1.23
85	33	39	PSU	O4-C4	-3.92	1.16	1.23
85	23	27	PSU	O4-C4	-3.92	1.16	1.23
85	23	34	70U	C2-N3	-3.91	1.28	1.38
85	33	34	70U	C2-N3	-3.91	1.28	1.38
85	33	27	PSU	O4-C4	-3.88	1.16	1.23
85	23	46	7MG	C5-N7	-3.85	1.30	1.35
85	33	46	7MG	C5-N7	-3.82	1.30	1.35
85	23	48	5MC	C6-N1	-3.73	1.31	1.38
85	33	48	5MC	C6-N1	-3.70	1.31	1.38
85	23	48	5MC	C5-C4	3.63	1.46	1.44
85	23	54	2MU	C4-N3	-3.60	1.32	1.38
85	33	48	5MC	C5-C4	3.59	1.46	1.44
85	33	54	2MU	C4-N3	-3.59	1.32	1.38
85	33	34	70U	C3'-C4'	-3.49	1.44	1.53
85	23	34	70U	C3'-C4'	-3.49	1.44	1.53
85	23	46	7MG	C6-N1	-3.38	1.32	1.38
85	33	46	7MG	C6-N1	-3.37	1.32	1.38
85	23	49	5MC	C6-N1	-3.31	1.32	1.38
85	33	49	5MC	C6-N1	-3.29	1.32	1.38
85	33	55	PSU	C4-N3	-3.11	1.33	1.38
85	23	55	PSU	C4-N3	-3.10	1.33	1.38
85	33	54	2MU	C2-N3	-3.01	1.32	1.38
85	23	54	2MU	C2-N3	-2.99	1.32	1.38
85	23	39	PSU	C4-N3	-2.94	1.33	1.38
85	33	39	PSU	C4-N3	-2.91	1.33	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	23	27	PSU	C4-N3	-2.87	1.33	1.38
85	33	27	PSU	C4-N3	-2.87	1.33	1.38
85	23	49	5MC	C5-C4	2.79	1.46	1.44
85	33	49	5MC	C5-C4	2.79	1.46	1.44
85	23	47	H2U	C4-N3	-2.74	1.33	1.37
85	23	34	70U	C3'-C2'	-2.72	1.46	1.53
85	33	34	70U	C3'-C2'	-2.71	1.46	1.53
85	33	47	H2U	C4-N3	-2.71	1.33	1.37
85	33	58	1MA	C6-N6	2.69	1.34	1.28
85	23	58	1MA	C6-N6	2.68	1.34	1.28
85	33	55	PSU	C2-N1	-2.68	1.33	1.36
85	23	55	PSU	C2-N1	-2.68	1.33	1.36
85	23	37	12A	C5-C6	2.66	1.48	1.41
85	33	37	12A	C5-C6	2.65	1.48	1.41
85	23	54	2MU	C6-N1	-2.62	1.33	1.38
85	33	54	2MU	C6-N1	-2.61	1.33	1.38
85	23	58	1MA	C5-C4	2.52	1.45	1.38
85	33	58	1MA	C5-C4	2.52	1.45	1.38
85	23	55	PSU	C6-N1	-2.44	1.32	1.36
85	33	55	PSU	C6-N1	-2.41	1.32	1.36
85	33	58	1MA	C4-N9	-2.41	1.31	1.38
85	23	58	1MA	C4-N9	-2.39	1.32	1.38
85	33	37	12A	C5-N7	-2.37	1.34	1.39
85	23	37	12A	C5-N7	-2.35	1.34	1.39
85	33	37	12A	C8-N7	2.31	1.36	1.31
85	23	47	H2U	C2-N3	-2.29	1.34	1.38
85	33	34	70U	C5'-C4'	2.29	1.58	1.51
85	33	47	H2U	C2-N3	-2.28	1.34	1.38
85	23	37	12A	C8-N7	2.28	1.36	1.31
85	23	34	70U	C5'-C4'	2.28	1.58	1.51
85	23	46	7MG	C5-C4	2.27	1.44	1.37
85	33	46	7MG	C5-C4	2.26	1.44	1.37
85	23	58	1MA	C5-N7	-2.22	1.34	1.39
85	23	55	PSU	C2-N3	-2.20	1.33	1.37
85	33	55	PSU	C2-N3	-2.19	1.33	1.37
85	33	58	1MA	C5-N7	-2.19	1.34	1.39

All (172) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	33	20	H2U	O2-C2-N1	-11.47	109.31	123.10
85	23	20	H2U	O2-C2-N1	-11.46	109.32	123.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	23	46	7MG	N9-C4-N3	9.45	139.31	125.46
85	33	46	7MG	N9-C4-N3	9.39	139.22	125.46
85	33	34	70U	C3'-C2'-C1'	-8.82	84.78	101.46
85	23	34	70U	C3'-C2'-C1'	-8.82	84.78	101.46
85	23	34	70U	O4'-C4'-C3'	-7.99	89.29	105.15
85	33	34	70U	O4'-C4'-C3'	-7.98	89.32	105.15
85	23	34	70U	C2'-C3'-C4'	7.94	117.95	102.61
85	33	34	70U	C2'-C3'-C4'	7.92	117.91	102.61
85	23	37	12A	C5-C4-N3	-7.66	119.11	127.18
85	33	37	12A	C5-C4-N3	-7.64	119.13	127.18
85	23	20	H2U	O4-C4-N3	-7.51	108.72	120.30
85	33	20	H2U	O4-C4-N3	-7.51	108.72	120.30
85	23	20	H2U	O2-C2-N3	-7.04	108.50	121.49
85	33	20	H2U	O2-C2-N3	-7.04	108.50	121.49
85	23	55	PSU	N1-C2-N3	6.65	122.18	115.17
85	33	55	PSU	N1-C2-N3	6.63	122.16	115.17
85	33	46	7MG	N9-C8-N7	-6.50	94.16	103.37
85	23	46	7MG	N9-C8-N7	-6.50	94.17	103.37
85	33	27	PSU	N1-C2-N3	6.48	122.01	115.17
85	23	20	H2U	O4-C4-C5	-6.47	108.95	122.20
85	33	54	2MU	C5-C4-N3	6.47	120.94	115.32
85	33	20	H2U	O4-C4-C5	-6.46	108.98	122.20
85	23	54	2MU	C5-C4-N3	6.43	120.91	115.32
85	23	27	PSU	N1-C2-N3	6.42	121.94	115.17
85	23	39	PSU	N1-C2-N3	6.38	121.90	115.17
85	33	39	PSU	N1-C2-N3	6.34	121.86	115.17
85	33	37	12A	N3-C4-N9	6.13	134.77	126.99
85	23	37	12A	N3-C4-N9	6.13	134.77	126.99
85	33	54	2MU	C4-N3-C2	-6.12	119.32	127.34
85	23	54	2MU	C4-N3-C2	-6.08	119.36	127.34
85	23	46	7MG	C5-C4-N3	-5.51	117.79	128.13
85	33	46	7MG	C5-C4-N3	-5.49	117.82	128.13
85	33	54	2MU	N3-C2-N1	5.19	121.64	114.89
85	23	54	2MU	N3-C2-N1	5.13	121.57	114.89
85	33	54	2MU	O4-C4-C5	-4.92	119.29	124.92
85	23	54	2MU	O4-C4-C5	-4.91	119.30	124.92
85	23	48	5MC	C5-C6-N1	-4.75	118.16	123.31
85	33	48	5MC	C5-C6-N1	-4.74	118.16	123.31
85	23	34	70U	O9-C8-C5M	4.67	120.71	111.28
85	33	34	70U	O9-C8-C5M	4.66	120.69	111.28
85	23	34	70U	O3'-C3'-C4'	-4.66	97.69	111.08
85	33	34	70U	O3'-C3'-C4'	-4.66	97.70	111.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	33	20	H2U	N3-C2-N1	-4.60	112.02	116.65
85	23	55	PSU	O2-C2-N1	-4.59	118.06	122.79
85	33	55	PSU	O2-C2-N1	-4.57	118.08	122.79
85	33	55	PSU	C4-N3-C2	-4.57	120.08	126.37
85	23	55	PSU	C4-N3-C2	-4.56	120.08	126.37
85	23	20	H2U	N3-C2-N1	-4.56	112.06	116.65
85	23	34	70U	C5M-C5-C4	4.55	124.16	118.00
85	33	34	70U	O4'-C4'-C5'	4.54	123.89	109.33
85	33	34	70U	C5M-C5-C4	4.54	124.15	118.00
85	23	34	70U	O4'-C4'-C5'	4.54	123.86	109.33
85	33	58	1MA	C5-C4-N3	-4.53	120.61	127.27
85	23	58	1MA	C5-C4-N3	-4.52	120.61	127.27
85	33	27	PSU	C4-N3-C2	-4.31	120.43	126.37
85	23	34	70U	C5-C6-N1	-4.28	117.18	122.94
85	23	27	PSU	C4-N3-C2	-4.28	120.48	126.37
85	23	34	70U	C5-C4-N3	4.28	121.74	115.21
85	33	34	70U	C5-C4-N3	4.26	121.71	115.21
85	33	34	70U	C5-C6-N1	-4.26	117.21	122.94
85	23	58	1MA	C2-N3-C4	4.24	120.85	112.53
85	33	58	1MA	C2-N3-C4	4.23	120.82	112.53
85	23	39	PSU	C4-N3-C2	-4.16	120.64	126.37
85	33	39	PSU	C4-N3-C2	-4.16	120.65	126.37
85	23	54	2MU	C5-C6-N1	-3.98	118.99	123.31
85	33	54	2MU	C5-C6-N1	-3.96	119.01	123.31
85	23	46	7MG	C2-N3-C4	3.73	118.72	112.30
85	33	46	7MG	C2-N3-C4	3.70	118.67	112.30
85	23	39	PSU	O2-C2-N1	-3.60	119.07	122.79
85	33	27	PSU	O2-C2-N1	-3.60	119.07	122.79
85	33	39	PSU	O2-C2-N1	-3.58	119.09	122.79
85	23	27	PSU	O2-C2-N1	-3.55	119.13	122.79
85	23	37	12A	C4-C5-N7	-3.43	106.66	110.58
85	33	37	12A	C4-C5-N7	-3.42	106.67	110.58
85	33	58	1MA	C6-C5-N7	3.40	138.18	132.16
85	23	58	1MA	C6-C5-N7	3.40	138.18	132.16
85	23	37	12A	C2-N3-C4	3.34	121.03	112.29
85	33	37	12A	C2-N3-C4	3.34	121.03	112.29
85	33	37	12A	C6-C5-N7	3.33	136.06	132.43
85	33	49	5MC	O2-C2-N3	-3.33	117.08	122.33
85	23	37	12A	C6-C5-N7	3.33	136.05	132.43
85	23	49	5MC	O2-C2-N3	-3.31	117.11	122.33
85	33	58	1MA	C4-C5-N7	-3.22	105.57	110.67
85	23	58	1MA	C4-C5-N7	-3.20	105.59	110.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	23	20	H2U	C5-C4-N3	-3.19	113.29	116.69
85	23	34	70U	O4'-C1'-N1	-3.18	101.16	108.36
85	33	20	H2U	C5-C4-N3	-3.18	113.31	116.69
85	33	34	70U	O4'-C1'-N1	-3.16	101.20	108.36
85	33	37	12A	N6-CC-N	3.07	117.99	113.77
85	23	37	12A	N6-CC-N	3.06	117.98	113.77
85	33	37	12A	C2'-C1'-N9	-3.04	105.74	113.30
85	23	37	12A	C2'-C1'-N9	-3.04	105.74	113.30
85	33	37	12A	C4-N9-C8	3.01	108.90	105.74
85	23	37	12A	C4-N9-C8	2.98	108.87	105.74
85	33	37	12A	C2M-S2-C2	-2.95	100.03	102.25
85	23	49	5MC	O3'-C3'-C2'	2.93	121.19	111.82
85	23	37	12A	C2M-S2-C2	-2.92	100.06	102.25
85	33	49	5MC	O3'-C3'-C2'	2.91	121.16	111.82
85	23	48	5MC	C2'-C3'-C4'	2.89	108.19	102.61
85	33	48	5MC	C2'-C3'-C4'	2.89	108.19	102.61
85	33	48	5MC	O3'-C3'-C4'	2.88	119.34	111.08
85	33	48	5MC	O3'-C3'-C2'	2.87	121.00	111.82
85	23	48	5MC	O3'-C3'-C2'	2.86	121.00	111.82
85	23	48	5MC	O3'-C3'-C4'	2.86	119.31	111.08
85	33	46	7MG	O6-C6-C5	-2.86	120.60	127.62
85	23	46	7MG	O6-C6-C5	-2.86	120.61	127.62
85	33	34	70U	O4-C4-N3	-2.85	114.75	120.11
85	23	34	70U	O4-C4-N3	-2.85	114.76	120.11
85	23	54	2MU	C2'-C1'-N1	-2.84	108.86	114.24
85	23	55	PSU	O2'-C2'-C1'	-2.83	104.50	111.21
85	33	54	2MU	C2'-C1'-N1	-2.83	108.88	114.24
85	33	55	PSU	O2'-C2'-C1'	-2.82	104.53	111.21
85	23	49	5MC	C2'-C3'-C4'	2.79	107.99	102.61
85	33	49	5MC	C2'-C3'-C4'	2.78	107.98	102.61
85	23	49	5MC	C5-C6-N1	-2.73	120.35	123.31
85	33	49	5MC	C5-C6-N1	-2.69	120.39	123.31
85	23	48	5MC	CM5-C5-C6	-2.69	119.21	122.85
85	33	48	5MC	CM5-C5-C6	-2.68	119.22	122.85
85	23	46	7MG	C5-C4-N9	-2.68	102.90	106.33
85	33	46	7MG	C5-C4-N9	-2.64	102.95	106.33
85	33	49	5MC	O3'-C3'-C4'	2.63	118.63	111.08
85	23	49	5MC	O3'-C3'-C4'	2.61	118.58	111.08
85	23	37	12A	C5-N7-C8	2.59	107.53	103.45
85	23	46	7MG	C5-C6-N1	2.59	115.49	110.94
85	33	34	70U	O3'-C3'-C2'	2.58	120.09	111.82
85	33	37	12A	C5-N7-C8	2.58	107.50	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	23	34	70U	O3'-C3'-C2'	2.57	120.05	111.82
85	33	46	7MG	C5-C6-N1	2.57	115.46	110.94
85	23	48	5MC	O2-C2-N3	-2.48	118.42	122.33
85	33	48	5MC	O2-C2-N3	-2.46	118.45	122.33
85	33	27	PSU	C5-C6-N1	-2.44	118.76	122.14
85	33	55	PSU	C5-C6-N1	-2.43	118.77	122.14
85	33	37	12A	N3-C2-N1	-2.43	122.57	127.00
85	23	27	PSU	C5-C6-N1	-2.43	118.77	122.14
85	23	37	12A	C2-N1-C6	2.43	122.15	117.54
85	33	37	12A	C2-N1-C6	2.43	122.15	117.54
85	23	37	12A	N3-C2-N1	-2.42	122.58	127.00
85	23	55	PSU	C5-C6-N1	-2.41	118.80	122.14
85	23	58	1MA	C1'-N9-C4	-2.38	119.45	126.49
85	33	55	PSU	C5'-C4'-C3'	-2.38	106.63	115.21
85	23	55	PSU	C5'-C4'-C3'	-2.38	106.64	115.21
85	33	58	1MA	C1'-N9-C4	-2.36	119.50	126.49
85	33	49	5MC	C5-C4-N3	-2.35	119.34	121.75
85	23	49	5MC	C5-C4-N3	-2.34	119.36	121.75
85	33	39	PSU	C5-C6-N1	-2.30	118.94	122.14
85	23	39	PSU	C5-C6-N1	-2.27	118.99	122.14
85	33	54	2MU	O2-C2-N3	-2.23	117.38	121.49
85	23	54	2MU	O2-C2-N3	-2.23	117.38	121.49
85	23	37	12A	N9-C8-N7	-2.20	110.82	113.94
85	33	37	12A	N9-C8-N7	-2.19	110.84	113.94
85	33	47	H2U	C3'-C2'-C1'	2.18	105.59	101.46
85	23	48	5MC	C5'-C4'-C3'	-2.17	107.40	115.21
85	33	48	5MC	C5'-C4'-C3'	-2.16	107.42	115.21
85	23	47	H2U	C3'-C2'-C1'	2.16	105.55	101.46
85	23	47	H2U	C2'-C3'-C4'	2.16	106.77	102.61
85	23	46	7MG	C2-N1-C6	-2.15	121.21	125.11
85	33	46	7MG	C2-N1-C6	-2.14	121.24	125.11
85	33	47	H2U	C2'-C3'-C4'	2.13	106.73	102.61
85	23	58	1MA	N9-C4-N3	2.11	131.71	126.90
85	33	58	1MA	N9-C4-N3	2.10	131.68	126.90
85	23	58	1MA	C8-N7-C5	2.09	107.98	104.26
85	33	58	1MA	C8-N7-C5	2.08	107.97	104.26
85	33	46	7MG	O6-C6-N1	2.04	123.95	120.11
85	23	48	5MC	C5-C4-N3	-2.04	119.67	121.75
85	23	49	5MC	C1'-N1-C6	-2.03	117.81	121.15
85	23	47	H2U	O4-C4-N3	2.03	123.43	120.30
85	33	48	5MC	C5-C4-N3	-2.03	119.68	121.75
85	33	47	H2U	O4-C4-N3	2.03	123.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	33	49	5MC	C1'-N1-C6	-2.02	117.83	121.15
85	23	46	7MG	O6-C6-N1	2.01	123.90	120.11

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	23	20	H2U	O4'-C4'-C5'-O5'
85	23	20	H2U	O4'-C1'-N1-C2
85	23	20	H2U	O4'-C1'-N1-C6
85	33	20	H2U	O4'-C4'-C5'-O5'
85	33	20	H2U	O4'-C1'-N1-C2
85	33	20	H2U	O4'-C1'-N1-C6
85	23	34	70U	C5M-C8-O9-C9
85	33	34	70U	C5M-C8-O9-C9
85	23	37	12A	C5-C6-N6-CC
85	23	37	12A	OO-CC-N6-C6
85	23	37	12A	N-CC-N6-C6
85	23	37	12A	N6-CC-N-CA
85	33	37	12A	C5-C6-N6-CC
85	33	37	12A	OO-CC-N6-C6
85	33	37	12A	N-CC-N6-C6
85	33	37	12A	N6-CC-N-CA
85	23	34	70U	O8-C8-O9-C9
85	33	34	70U	O8-C8-O9-C9
85	23	37	12A	OO-CC-N-CA
85	33	37	12A	OO-CC-N-CA
85	23	48	5MC	O4'-C4'-C5'-O5'
85	23	48	5MC	C3'-C4'-C5'-O5'
85	33	48	5MC	O4'-C4'-C5'-O5'
85	33	48	5MC	C3'-C4'-C5'-O5'
85	23	37	12A	C3'-C4'-C5'-O5'
85	33	37	12A	C3'-C4'-C5'-O5'
85	23	20	H2U	C3'-C4'-C5'-O5'
85	33	20	H2U	C3'-C4'-C5'-O5'
85	23	37	12A	O4'-C4'-C5'-O5'
85	33	37	12A	O4'-C4'-C5'-O5'
85	23	20	H2U	C4'-C5'-O5'-P
85	33	20	H2U	C4'-C5'-O5'-P
85	23	47	H2U	C3'-C4'-C5'-O5'
85	33	47	H2U	C3'-C4'-C5'-O5'
85	23	34	70U	C4'-C5'-O5'-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
85	33	34	70U	C4'-C5'-O5'-P
85	23	54	2MU	C3'-C2'-O2'-C6'
85	33	54	2MU	C3'-C2'-O2'-C6'
85	33	49	5MC	O4'-C4'-C5'-O5'
85	23	49	5MC	O4'-C4'-C5'-O5'
85	23	34	70U	C3'-C4'-C5'-O5'
85	33	34	70U	C3'-C4'-C5'-O5'
85	23	47	H2U	O4'-C4'-C5'-O5'
85	33	47	H2U	O4'-C4'-C5'-O5'
85	23	37	12A	CB-CA-N-CC
85	33	37	12A	CB-CA-N-CC
85	23	37	12A	C-CA-N-CC
85	33	37	12A	C-CA-N-CC
85	23	46	7MG	C4'-C5'-O5'-P
85	33	46	7MG	C4'-C5'-O5'-P
85	23	34	70U	C5-C5M-C8-O9
85	33	34	70U	C5-C5M-C8-O9

There are no ring outliers.

19 monomers are involved in 86 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
85	23	48	5MC	2	0
85	33	58	1MA	1	0
85	33	34	70U	39	0
85	23	47	H2U	2	0
85	33	54	2MU	6	0
85	23	54	2MU	2	0
85	23	46	7MG	2	0
85	33	20	H2U	2	0
85	33	48	5MC	2	0
85	33	47	H2U	2	0
85	23	49	5MC	1	0
85	23	55	PSU	2	0
85	23	34	70U	14	0
85	23	37	12A	4	0
85	23	58	1MA	1	0
85	33	55	PSU	1	0
85	33	37	12A	3	0
85	33	49	5MC	1	0
85	33	46	7MG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 285 ligands modelled in this entry, 283 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
88	SPD	54	5287	-	9,9,9	0.32	0	8,8,8	0.52	0
88	SPD	54	5286	-	9,9,9	0.32	0	8,8,8	0.40	0

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
88	SPD	54	5287	-	-	6/7/7/7	-
88	SPD	54	5286	-	-	6/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
88	54	5287	SPD	C8-C7-N6-C5
88	54	5286	SPD	C3-C4-C5-N6
88	54	5286	SPD	C8-C7-N6-C5
88	54	5287	SPD	C3-C4-C5-N6
88	54	5286	SPD	C7-C8-C9-N10
88	54	5286	SPD	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
88	54	5287	SPD	C2-C3-C4-C5
88	54	5287	SPD	C4-C5-N6-C7
88	54	5287	SPD	N6-C7-C8-C9
88	54	5286	SPD	N1-C2-C3-C4
88	54	5287	SPD	C7-C8-C9-N10
88	54	5286	SPD	C4-C5-N6-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
88	54	5287	SPD	1	0
88	54	5286	SPD	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
80	54	32
1	A1	7

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	54	2113:G	O3'	2258:C	P	42.26
1	54	1252:C	O3'	1271:G	P	35.14
1	54	1219:G	O3'	1233:G	P	20.13
1	54	523:C	O3'	638:G	P	18.09
1	54	1406(C):G	O3'	1411:C	P	17.23
1	54	4138:C	O3'	4146:G	P	17.14
1	54	3977:C	O3'	4034:G	P	17.10
1	54	990:C	O3'	1064:G	P	17.04
1	54	4777:C	O3'	4859:C	P	15.69
1	54	1696:C	O3'	1720:C	P	15.53
1	54	760:G	O3'	904:C	P	15.38

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	54	182:G	O3'	189:G	P	14.79
1	54	5022:U	O3'	5028:G	P	14.76
1	54	4101:C	O3'	4107:G	P	13.82
1	54	1364:U	O3'	1368:A	P	13.78
1	54	2901:G	O3'	3597:G	P	12.28
1	54	1180:C	O3'	1183:C	P	10.19
1	54	512:U	O3'	515:C	P	10.11
1	54	4729:A	O3'	4735:G	P	8.47
1	54	500:G	O3'	504:G	P	6.70
1	A1	689:U	O3'	690:G	P	6.53
1	54	4064:C	O3'	4065:G	P	6.26
1	A1	322:C	O3'	323:C	P	6.07
1	54	4740:G	O3'	4743:G	P	5.77
1	54	1956:A	O3'	1957:U	P	5.11
1	A1	798:G	O3'	799:U	P	4.57
1	54	3948:C	O3'	3949:A	P	4.51
1	54	1100:U	O3'	1168:G	P	4.36
1	A1	902:G	O3'	903:A	P	4.19
1	A1	304:C	O3'	305:U	P	4.03
1	54	1239:C	O3'	1244:G	P	3.87
1	54	5020:G	O3'	5021:C	P	3.59
1	54	1957:U	O3'	1958:A	P	3.48
1	54	170:C	O3'	171:U	P	3.39
1	54	1438:U	O3'	1440:U	P	3.39
1	A1	903:A	O3'	904:A	P	3.29
1	A1	886:A	O3'	887:U	P	3.27
1	54	751:G	O3'	752:G	P	3.27
1	54	4899:G	O3'	4902:C	P	3.13

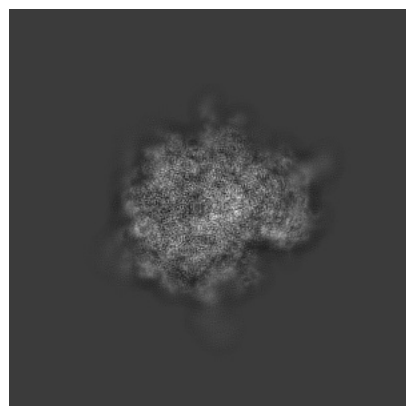
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10181. These allow visual inspection of the internal detail of the map and identification of artifacts.

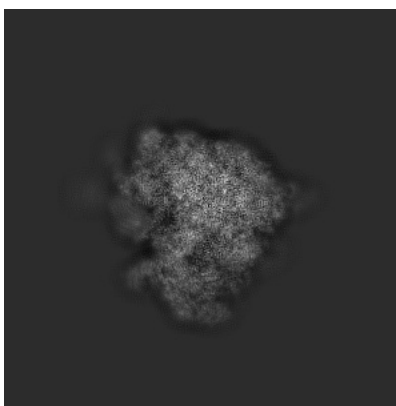
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

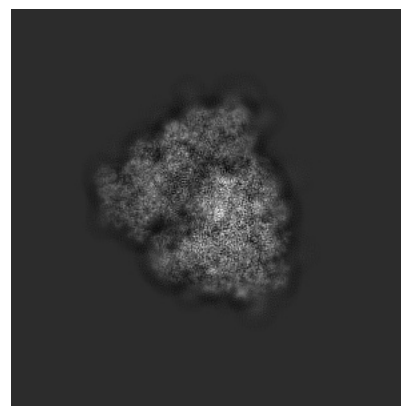
6.1.1 Primary map



X

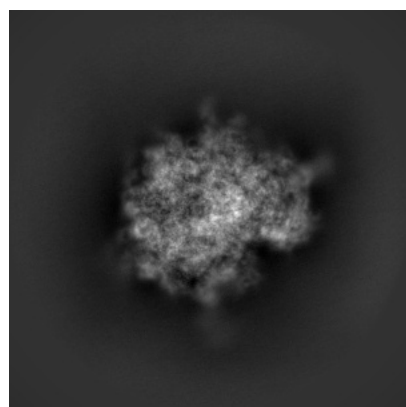


Y

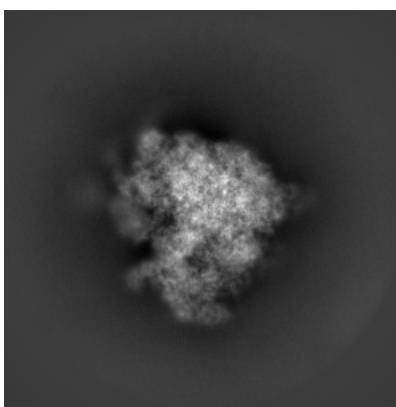


Z

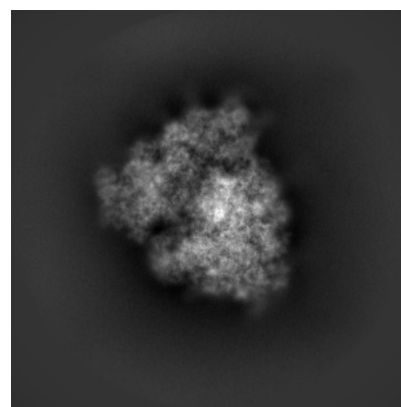
6.1.2 Raw map



X



Y

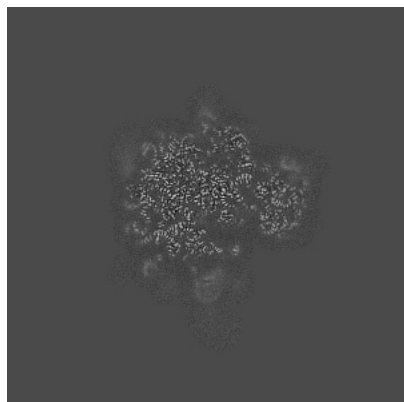


Z

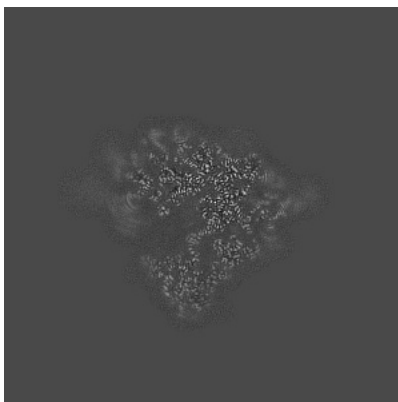
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

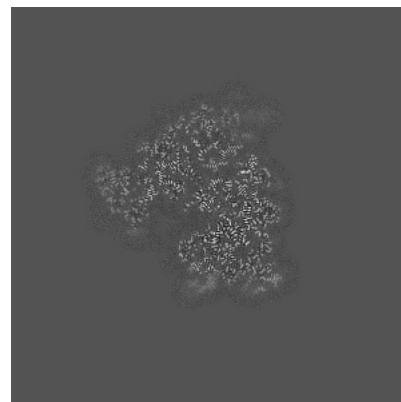
6.2.1 Primary map



X Index: 256

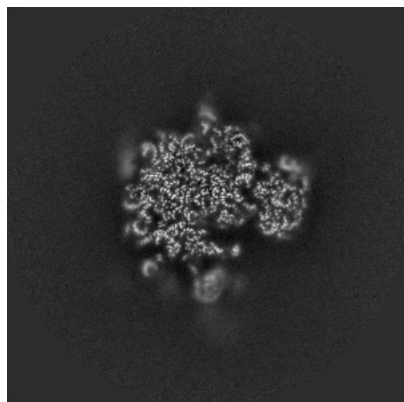


Y Index: 256

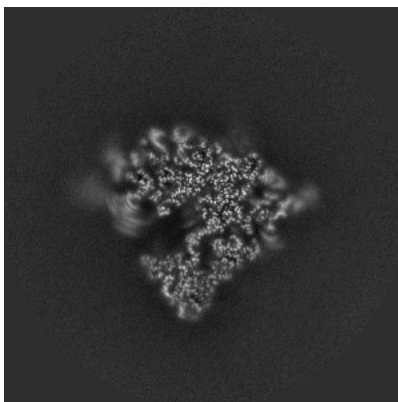


Z Index: 256

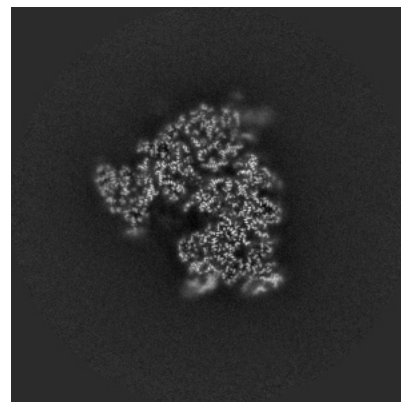
6.2.2 Raw map



X Index: 256



Y Index: 256

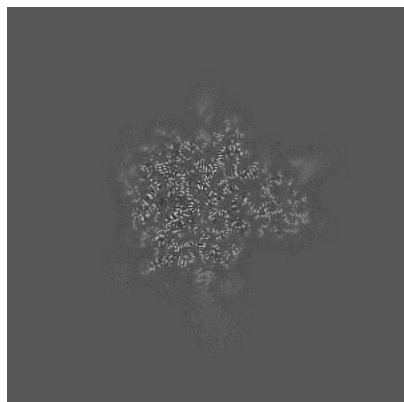


Z Index: 256

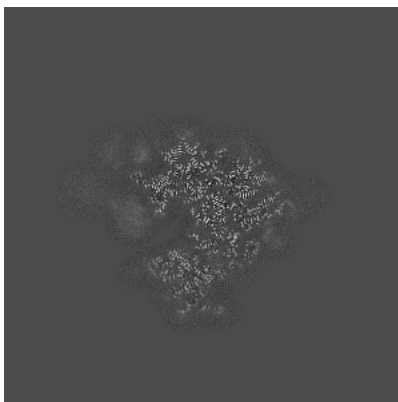
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

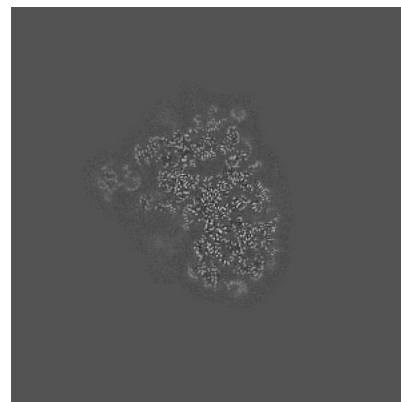
6.3.1 Primary map



X Index: 269

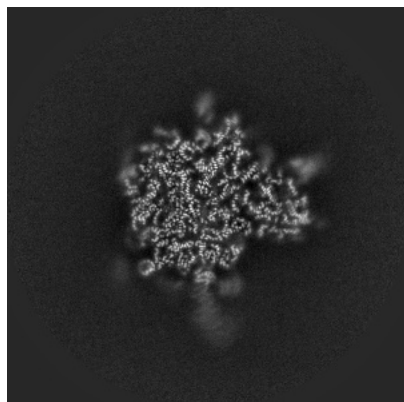


Y Index: 267

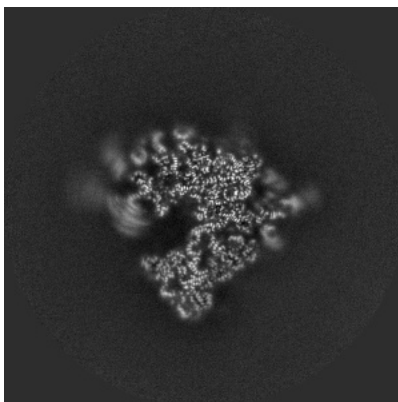


Z Index: 278

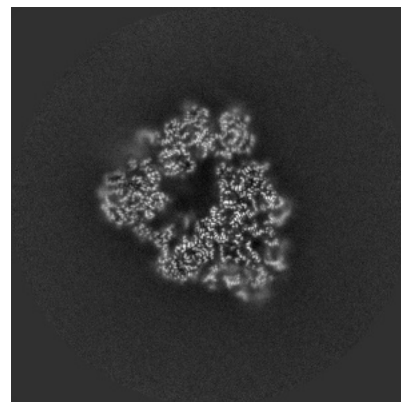
6.3.2 Raw map



X Index: 270



Y Index: 260

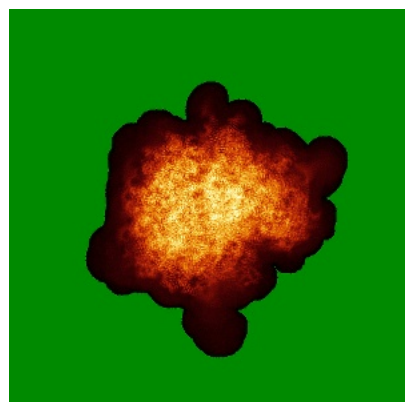


Z Index: 225

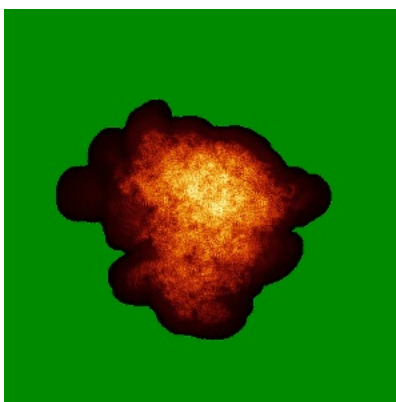
The images above show the largest variance slices of the map in three orthogonal directions.

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

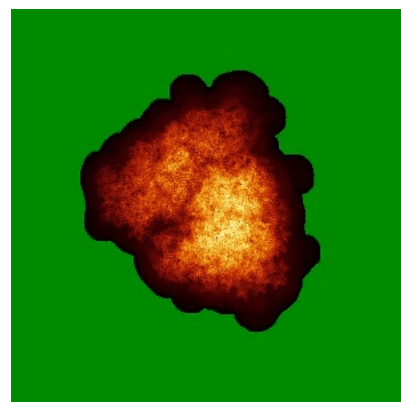
6.4.1 Primary map



X

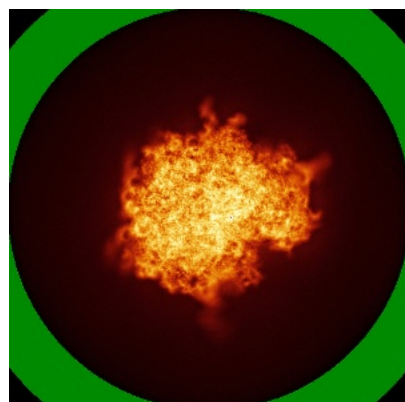


Y

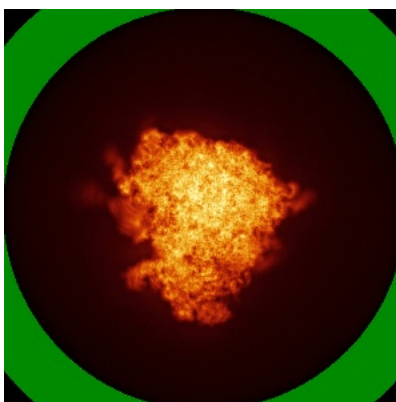


Z

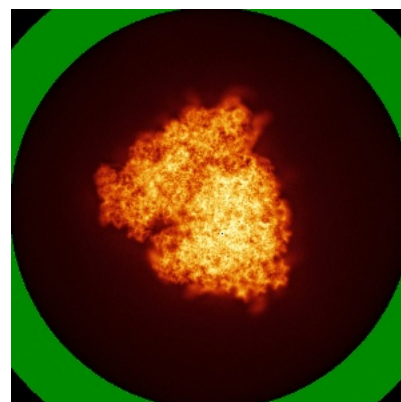
6.4.2 Raw map



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



X



Y



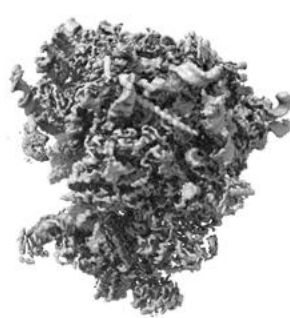
Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. 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



X



Y



Z

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.

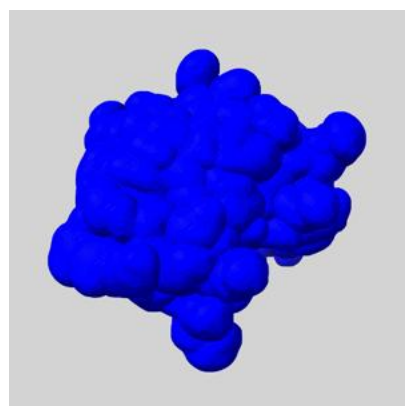
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

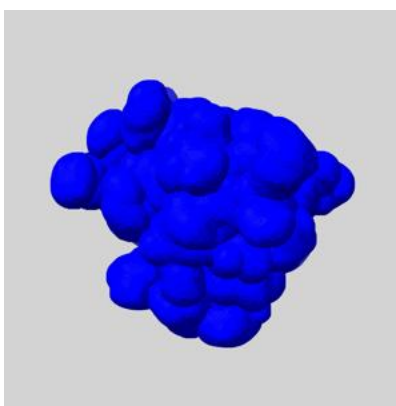
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

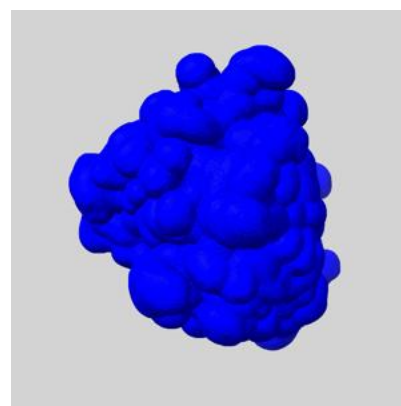
6.6.1 emd_10181_msk_1.map [i](#)



X



Y

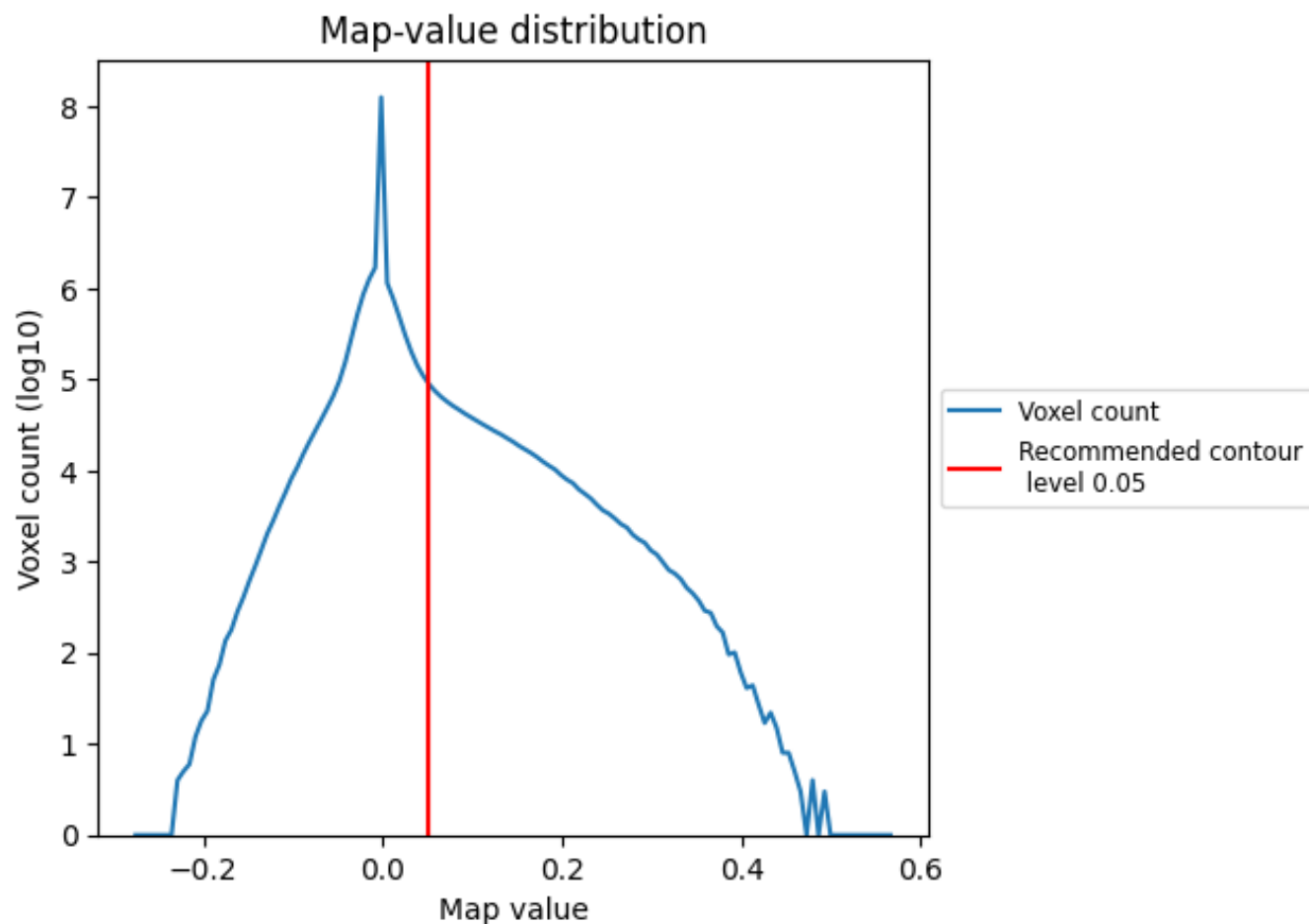


Z

7 Map analysis [i](#)

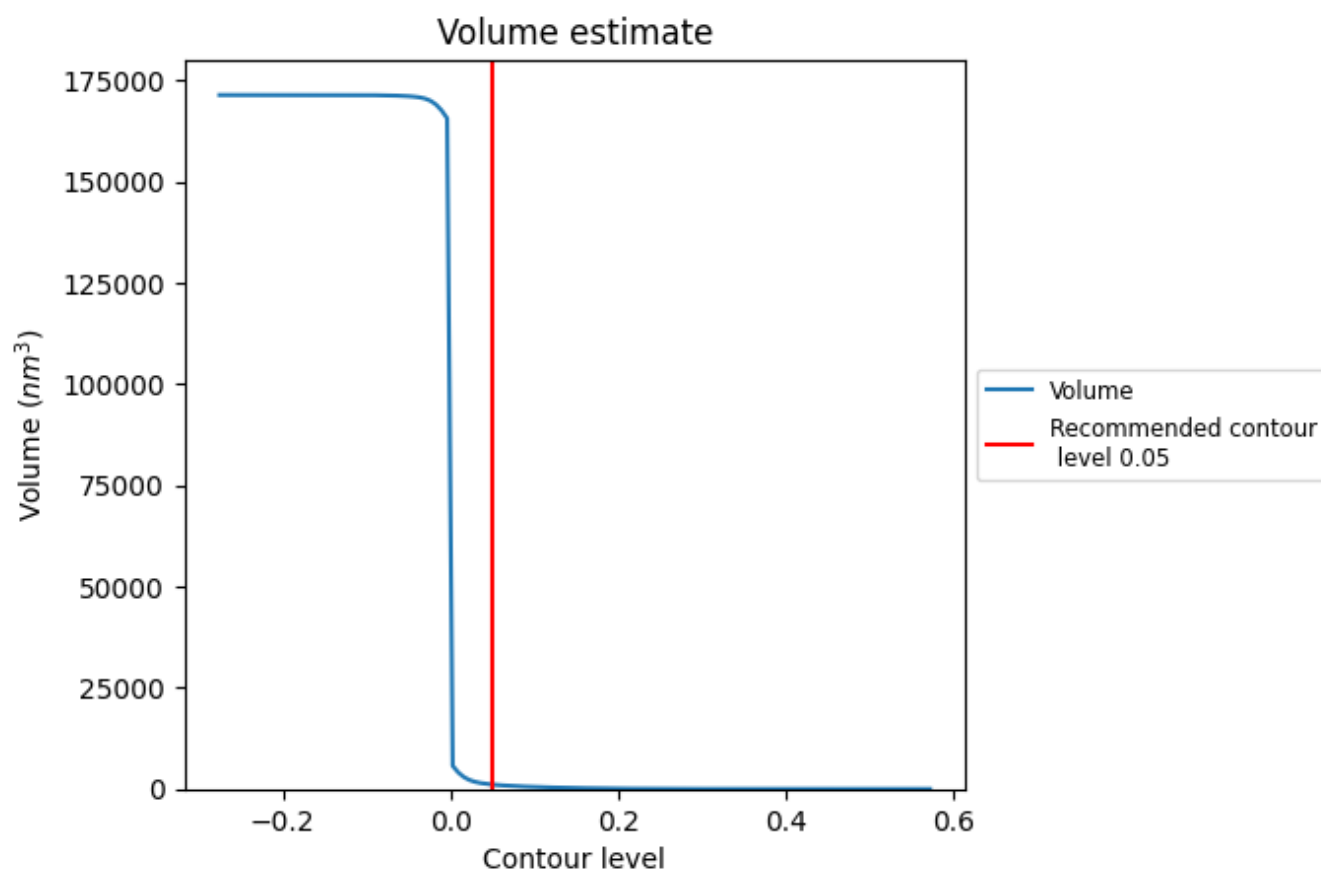
This section contains the results of statistical analysis of the map.

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.

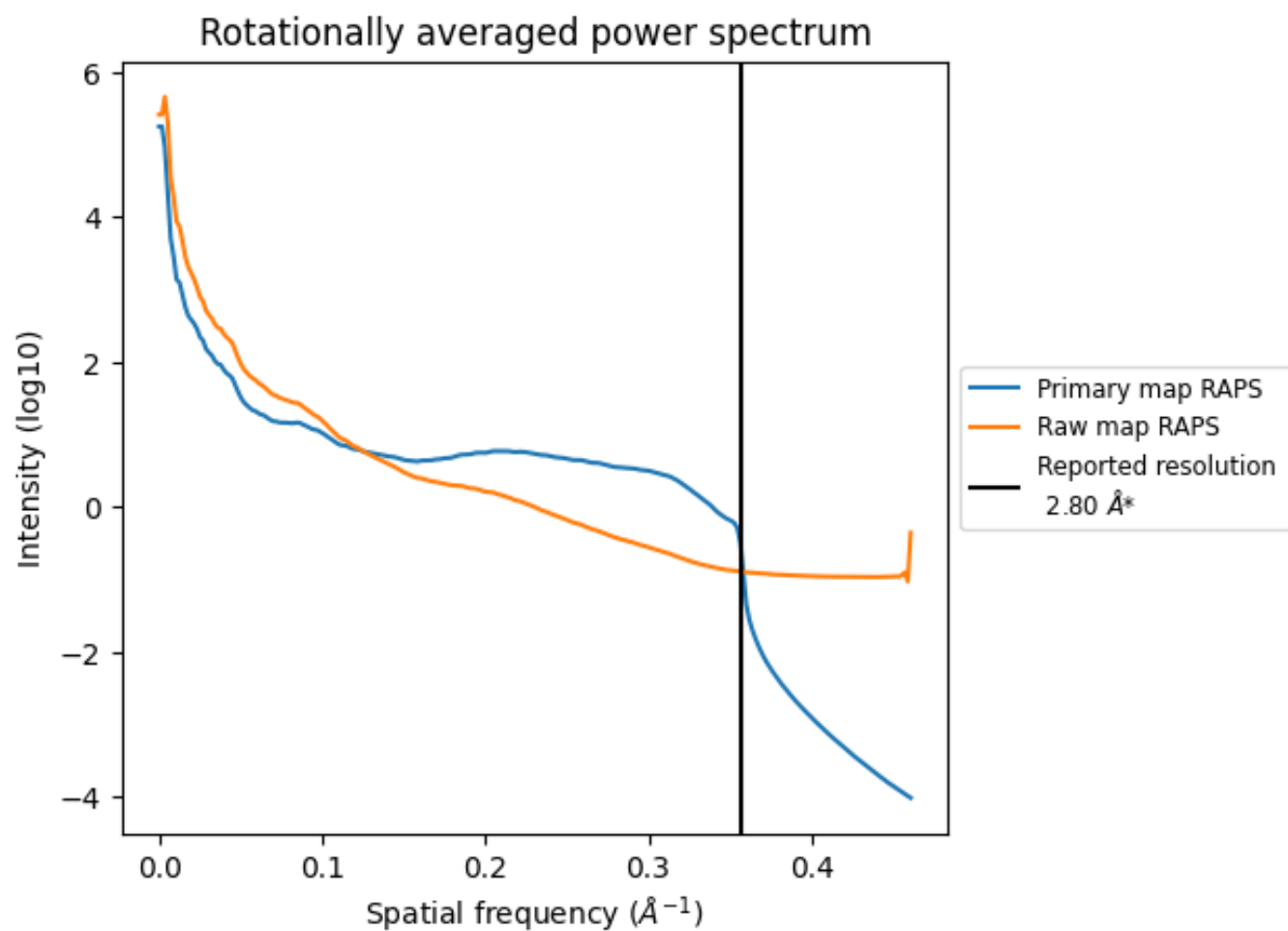
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1093 nm^3 ; this corresponds to an approximate mass of 988 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 ⓘ

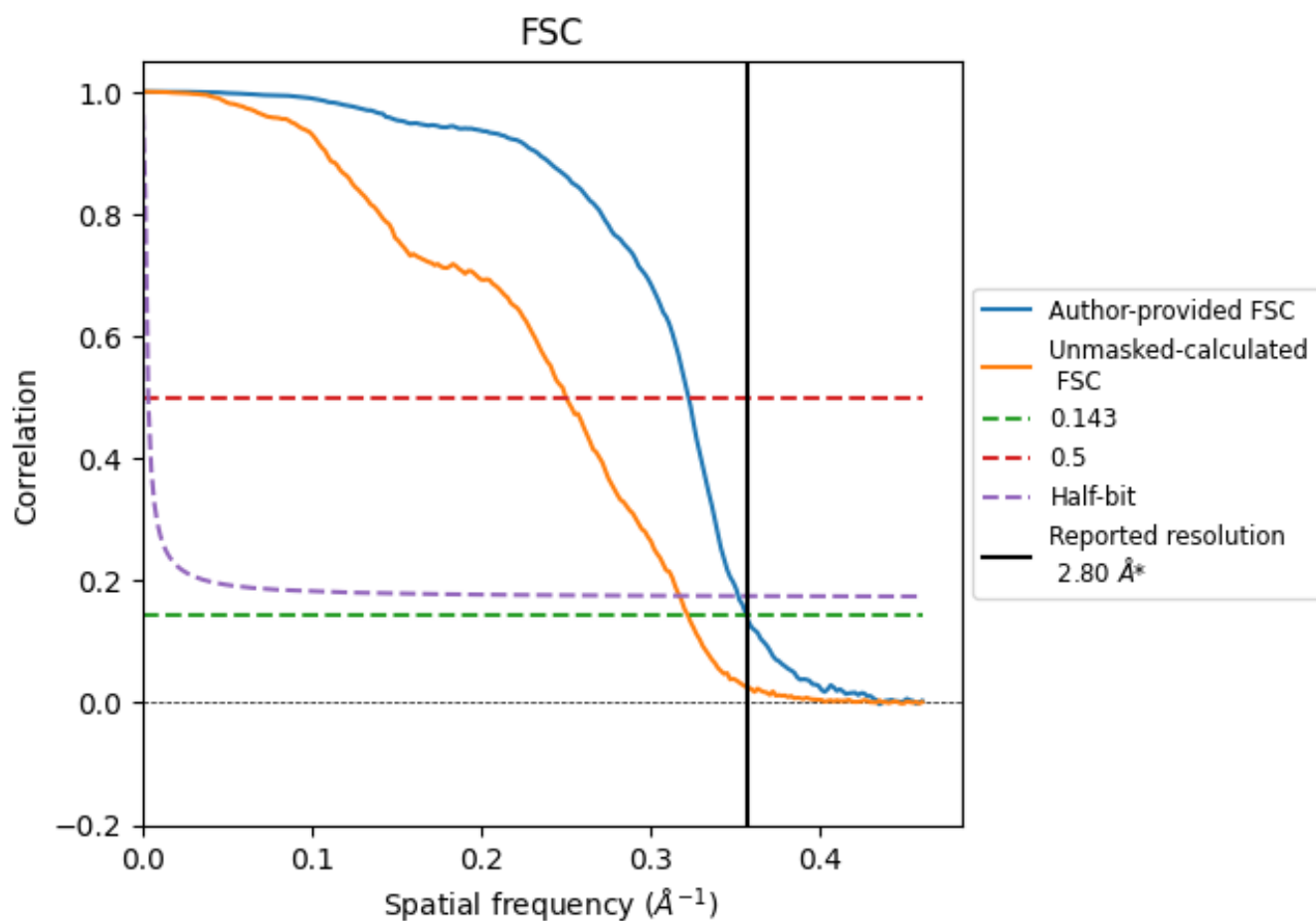


*Reported resolution corresponds to spatial frequency of $0.357 \text{ \AA}^{-1}$

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 $0.357 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

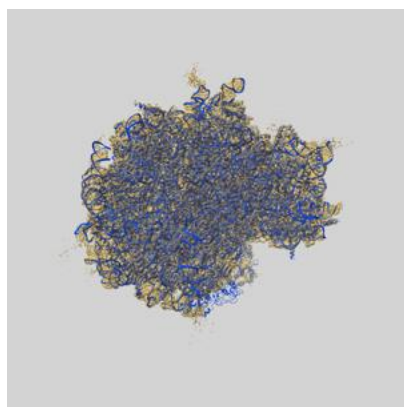
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	2.80	3.10	2.84
Unmasked-calculated*	3.10	4.00	3.15

*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 3.10 differs from the reported value 2.8 by more than 10 %

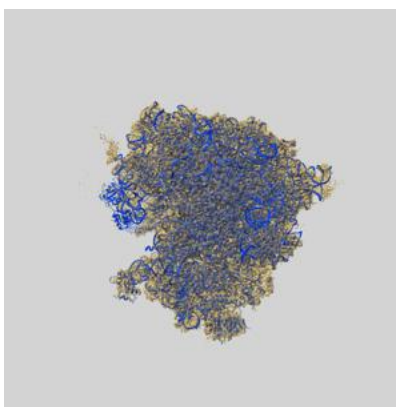
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10181 and PDB model 6SGC. Per-residue inclusion information can be found in section 3 on page 23.

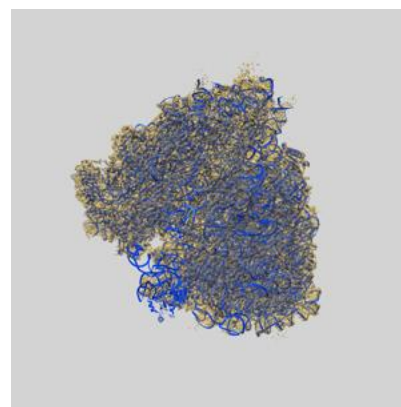
9.1 Map-model overlay [i](#)



X



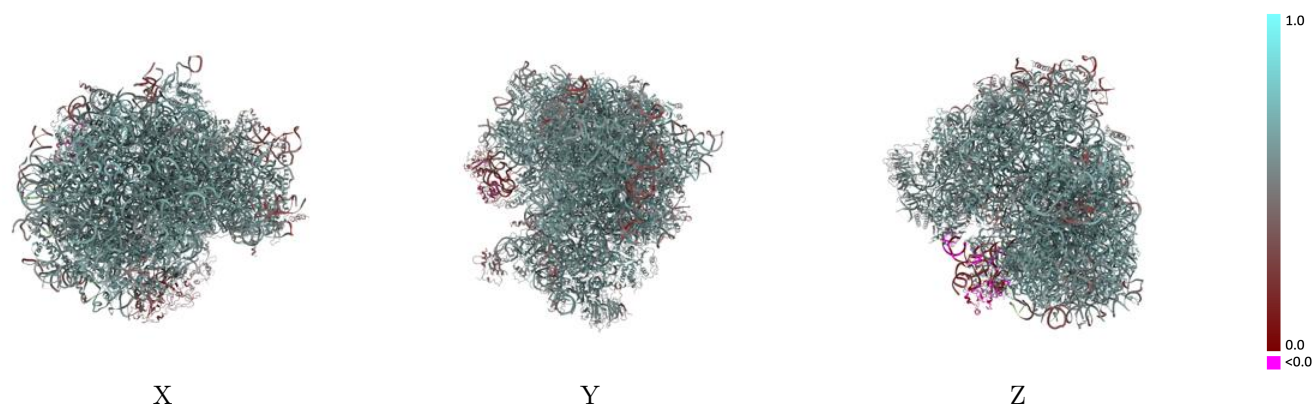
Y



Z

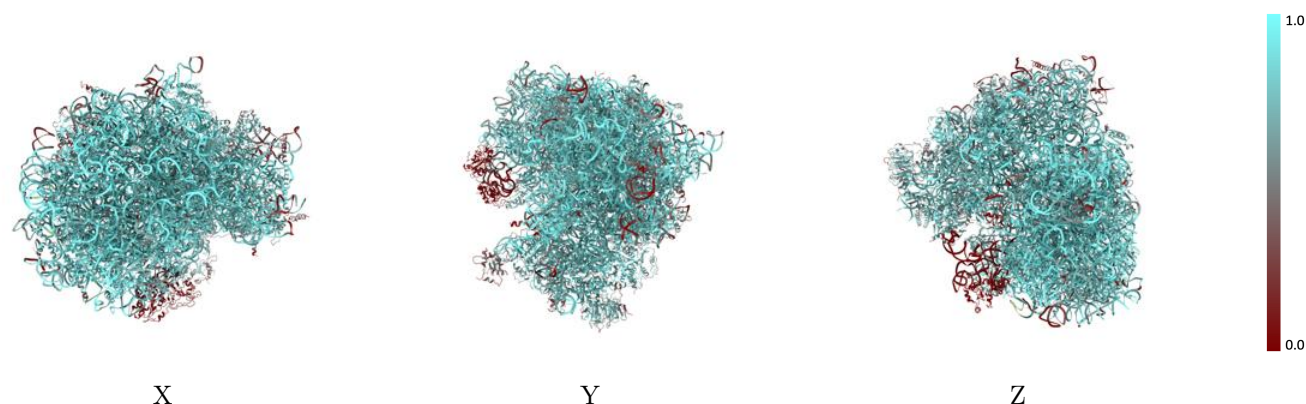
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



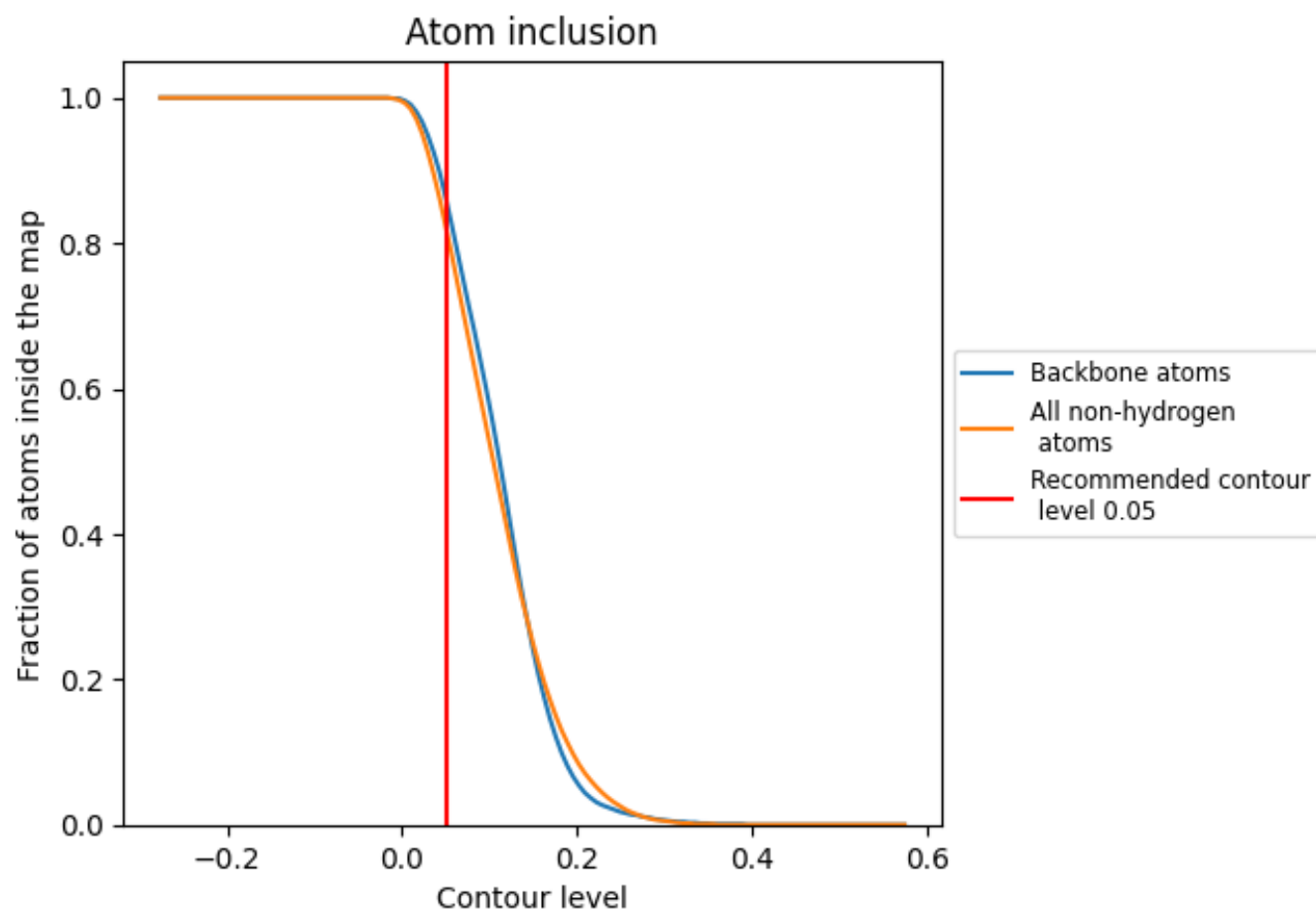
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 82% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8210	 0.5750
23	 0.6680	 0.5310
33	 0.0040	 0.0540
54	 0.8840	 0.5860
74	 0.9800	 0.6290
84	 0.9260	 0.6100
A1	 0.8890	 0.5850
A2	 0.9080	 0.6340
B	 0.0030	 0.0680
B1	 0.7990	 0.5880
B2	 0.8670	 0.6150
C1	 0.7700	 0.5790
C2	 0.8680	 0.6140
D1	 0.8090	 0.6010
D2	 0.8440	 0.5990
E1	 0.6430	 0.5400
E2	 0.8270	 0.5910
F1	 0.7710	 0.5860
F2	 0.8860	 0.6220
G1	 0.7190	 0.5660
G2	 0.7630	 0.5740
H1	 0.6570	 0.5250
H2	 0.8060	 0.5970
I1	 0.6640	 0.5370
I2	 0.8340	 0.6090
J1	 0.7740	 0.5770
J2	 0.7660	 0.5810
K1	 0.7750	 0.5810
L1	 0.6830	 0.5460
L2	 0.8160	 0.5950
M1	 0.8180	 0.6050
M2	 0.8440	 0.6020
N1	 0.3270	 0.3890
N2	 0.9170	 0.6330
O1	 0.8250	 0.6000



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
O2	 0.8860	 0.6190
P1	 0.7990	 0.5900
P2	 0.8830	 0.6190
Q1	 0.6680	 0.5450
Q2	 0.8700	 0.6220
R1	 0.7420	 0.5720
R2	 0.8130	 0.5980
S1	 0.6930	 0.5520
S2	 0.8810	 0.6210
T1	 0.7000	 0.5620
T2	 0.8160	 0.5950
U1	 0.7470	 0.5640
U2	 0.6900	 0.5250
V1	 0.6210	 0.5280
V2	 0.8130	 0.6100
W1	 0.7700	 0.5800
W2	 0.6930	 0.5400
X1	 0.8500	 0.6110
X2	 0.8160	 0.6050
XX	 0.0900	 0.3060
Y1	 0.8050	 0.6030
Y2	 0.8420	 0.6030
Z1	 0.7330	 0.5660
Z2	 0.8380	 0.5990
a1	 0.6740	 0.5460
a2	 0.9030	 0.6300
b1	 0.7900	 0.5910
b2	 0.7030	 0.5750
c1	 0.7170	 0.5730
c2	 0.8350	 0.6050
d1	 0.6550	 0.5620
d2	 0.8090	 0.6010
e1	 0.8330	 0.6020
e2	 0.8740	 0.6250
f1	 0.6090	 0.5280
f2	 0.9000	 0.6340
g1	 0.4010	 0.4320
g2	 0.8340	 0.6070
h1	 0.6130	 0.5120
h2	 0.8160	 0.6050
i1	 0.7320	 0.5530
i2	 0.7910	 0.5960

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
j2	 0.8960	 0.6280
k2	 0.7270	 0.5730
l2	 0.8410	 0.6110
m2	 0.8510	 0.6100
n2	 0.8170	 0.6170
o2	 0.8350	 0.6150
p2	 0.8160	 0.6130
r2	 0.8750	 0.6150
s2	 0.0460	 0.2920
t2	 0.0130	 0.2330