



Full wwPDB EM Validation Report ⓘ

Aug 4, 2025 – 08:57 PM JST

PDB ID : 8Y5M / pdb_00008y5m
EMDB ID : EMD-38942
Title : E.coli transcription translation coupling complex in TTC-B state 2 containing mRNA with 27-mer spacer, NusG, NusA, fMet-tRNA(iMet), Phe-tRNA(Phe), and viomycin
Authors : Zhang, J.; Lu, G.; Wang, C.; Lin, J.
Deposited on : 2024-01-31
Resolution : 4.50 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.dev126
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

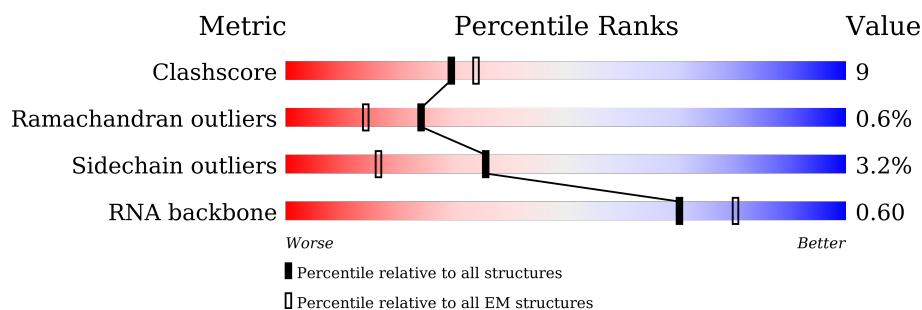
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.50 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A	70	 64% 29% 6%
2	B	57	 81% 18%
3	C	55	 75% 16% 9%
4	D	46	 67% 30%
5	E	65	 80% 18%
6	F	38	 71% 29%
7	G	241	 70% 18% 10%



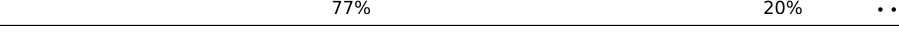
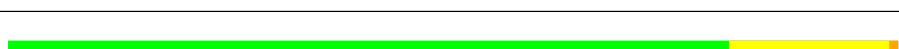



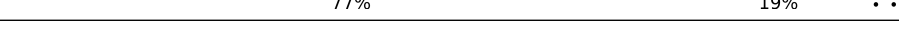



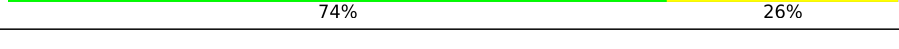

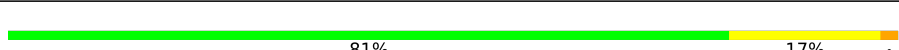


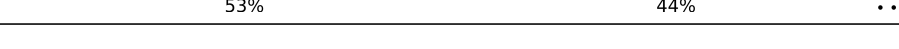
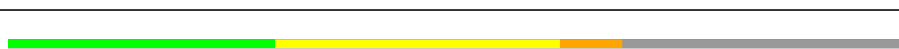
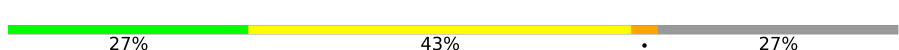





Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	H	233	
9	I	206	
10	J	167	
11	K	135	
12	L	179	
13	M	130	
14	N	130	
15	O	103	
16	P	129	
17	Q	124	
18	R	118	
19	S	101	
20	T	89	
21	U	82	
22	V	84	
23	W	75	
24	X	92	
25	Y	87	
26	Z	71	
27	b	273	
28	c	209	
29	d	201	
30	e	179	
31	f	177	
32	g	149	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	i	142	
34	j	142	
35	k	123	
36	l	144	
37	m	136	
38	n	127	
39	o	117	
40	p	115	
41	q	118	
42	r	103	
43	s	110	
44	t	100	
45	u	104	
46	v	94	
47	w	85	
48	x	78	
49	y	63	
50	z	59	
51	1	2904	
52	2	120	
53	3	1542	
54	4	44	
55	8	37	
56	9	37	
57	A1	329	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
57	A2	329	
58	B1	1407	
59	B2	1342	
60	W0	91	
61	NA	495	
62	NG	181	
63	5	76	
64	6	77	
65	a	234	
66	0	716	
67	h	6	

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 183546 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 protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 3 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 4 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 5 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 6 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	206	Total	C	N	O	S	0	0
			1620	1025	304	288	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	157	Total	C	N	O	S	0	0
			1152	717	218	211	6		

- Molecule 11 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

- Molecule 12 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 15 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 18 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

- Molecule 19 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 24 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 26 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 33 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 34 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 35 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 36 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 37 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 38 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 39 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	o	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 40 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 41 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 42 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 43 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 44 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 45 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	u	102	Total	C	N	O	0	0
			776	489	146	141		

- Molecule 46 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	v	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 47 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 48 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	x	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 49 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 50 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 51 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1929590828

- Molecule 52 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	U	conflict	GB NR_103249

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	4	30	Total	C	N	O	P	0	0
			627	280	92	225	30		

- Molecule 55 is a DNA chain called templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	27	Total	C	N	O	P	0	0
			539	257	88	167	27		

- Molecule 56 is a DNA chain called non-templete DNA strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	9	20	Total	C	N	O	P	0	0
			417	195	84	118	20		

- Molecule 57 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	A1	301	Total	C	N	O	S	0	0
			2088	1293	380	409	6		
57	A2	288	Total	C	N	O	S	0	0
			2029	1257	366	400	6		

- Molecule 58 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	B1	1335	Total	C	N	O	S	0	0
			10353	6509	1842	1955	47		

- Molecule 59 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	B2	1340	Total	C	N	O	S	0	0
			10546	6616	1839	2048	43		

- Molecule 60 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	W0	82	Total	C	N	O	S	0	0
			650	396	122	131	1		

- Molecule 61 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms				AltConf	Trace
61	NA	492	Total	C	N	O	0	0
			2432	1448	492	492		

- Molecule 62 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms				AltConf	Trace
62	NG	154	Total	C	N	O	0	0
			758	450	154	154		

- Molecule 63 is a RNA chain called tRNA(Phe).

Mol	Chain	Residues	Atoms					AltConf	Trace
63	5	76	Total	C	N	O	P	0	0
			1622	723	290	533	76		

- Molecule 64 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
64	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 65 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	a	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 66 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	0	697	Total	C	N	O	S	0	0
			5399	3403	929	1042	25		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	705	GLY	-	expression tag	UNP P0A6M8
0	706	SER	-	expression tag	UNP P0A6M8
0	707	SER	-	expression tag	UNP P0A6M8
0	708	GLY	-	expression tag	UNP P0A6M8
0	709	HIS	-	expression tag	UNP P0A6M8
0	710	HIS	-	expression tag	UNP P0A6M8
0	711	HIS	-	expression tag	UNP P0A6M8
0	712	HIS	-	expression tag	UNP P0A6M8
0	713	HIS	-	expression tag	UNP P0A6M8
0	714	HIS	-	expression tag	UNP P0A6M8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
0	715	HIS	-	expression tag	UNP P0A6M8
0	716	HIS	-	expression tag	UNP P0A6M8

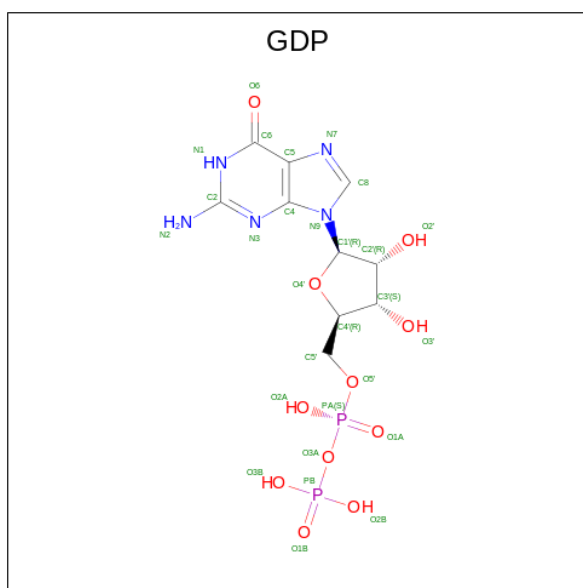
- Molecule 67 is a protein (with D amino acids) called Viomycin.

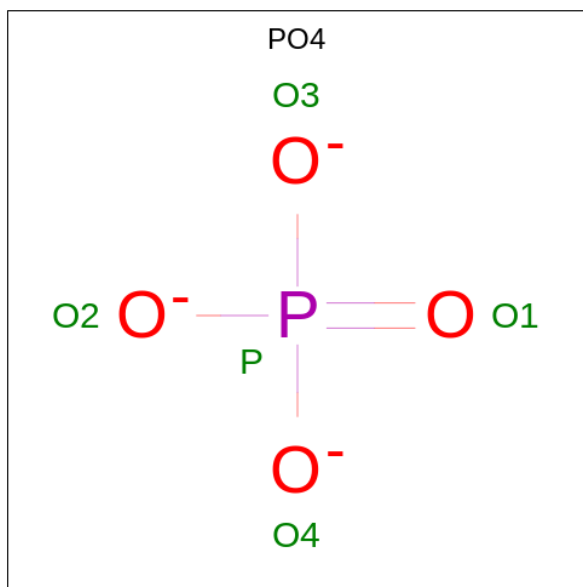
Mol	Chain	Residues	Atoms				AltConf	Trace
67	h	6	Total	C	N	O	0	0
			48	25	13	10		

- Molecule 68 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
68	B1	1	Total	Mg	0
			1	1	

- Molecule 69 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



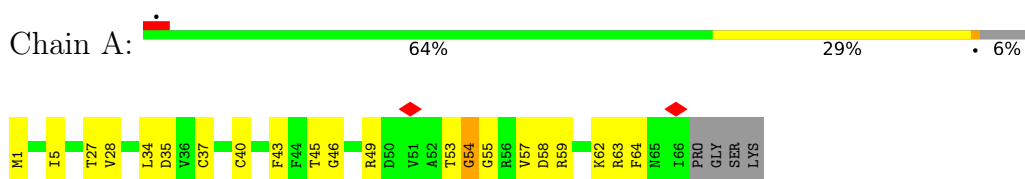


Mol	Chain	Residues	Atoms			AltConf
			Total	O	P	
70	0	1	5	4	1	0

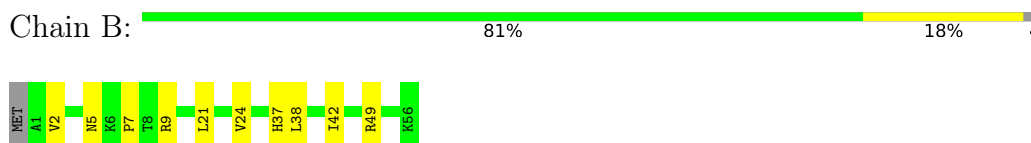
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

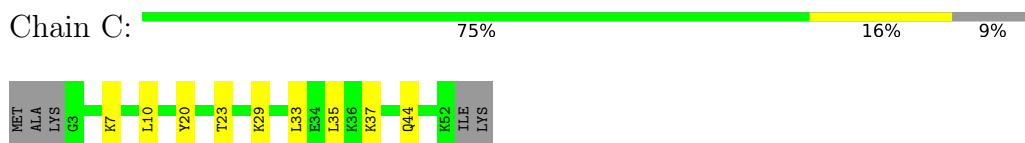
- Molecule 1: 50S ribosomal protein L31



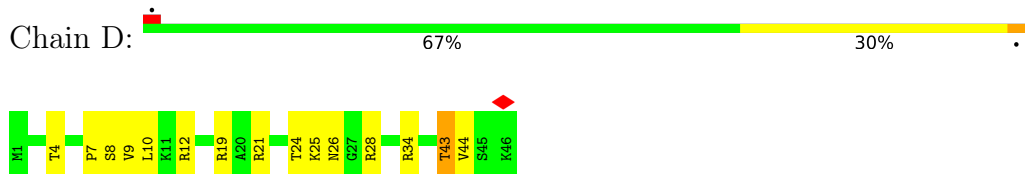
- Molecule 2: 50S ribosomal protein L32



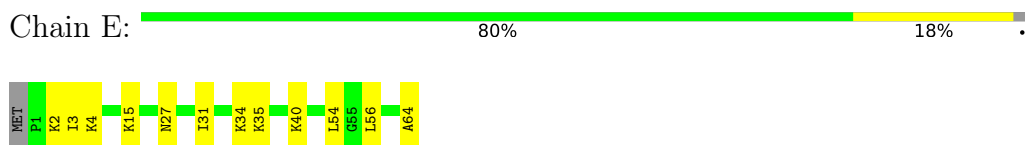
- Molecule 3: 50S ribosomal protein L33



- Molecule 4: 50S ribosomal protein L34



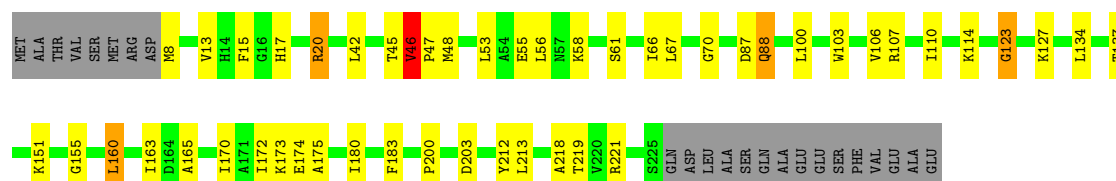
- Molecule 5: 50S ribosomal protein L35



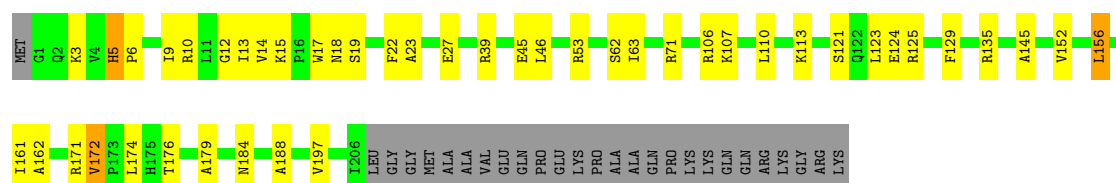
- Molecule 6: 50S ribosomal protein L36

M1 K2 V3 R4 C11 C14 K18 I23 A29 K32 Q35 G38

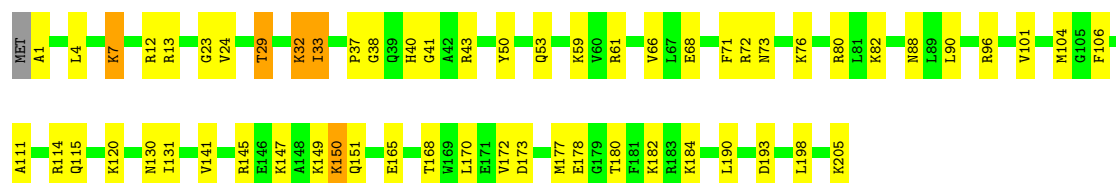
- Chain G:  70% 18% 2% 10%



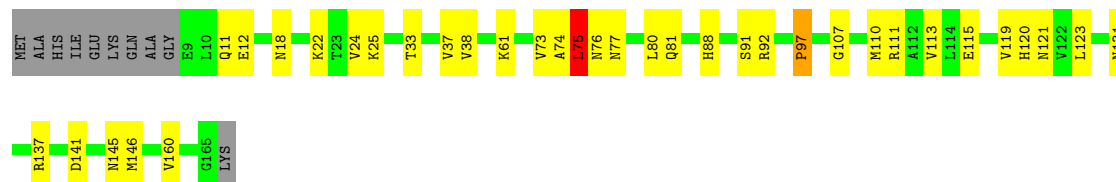
- Chain H: 69% 18% 12%



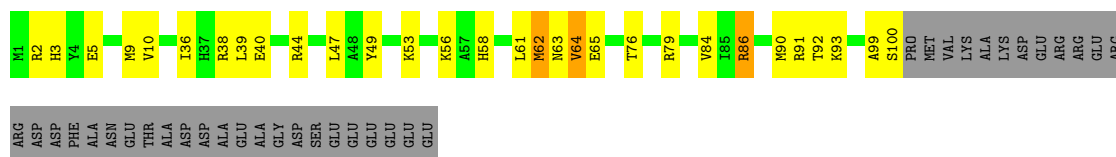
- Chain I: 71% 26%



- Chain J:  72% 20% .. 6%

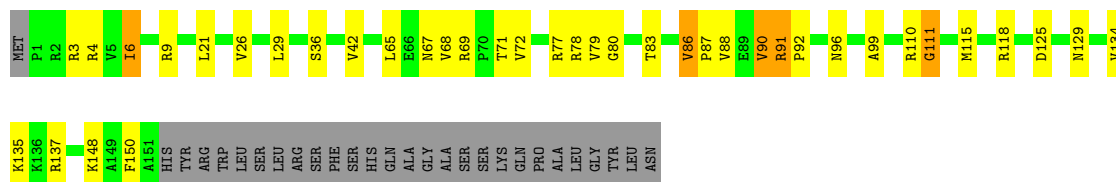


- Chain K:  52% 20% 2% 26%



- Molecule 12: 30S ribosomal protein S7

Chain L: 63% 19% 16%



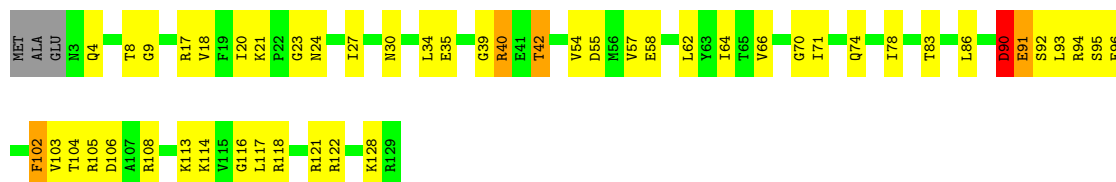
- Molecule 13: 30S ribosomal protein S8

Chain M: 84% 15%



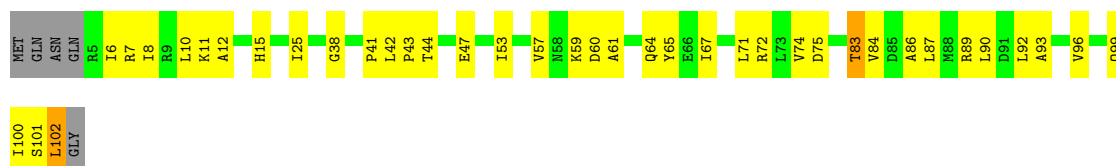
- Molecule 14: 30S ribosomal protein S9

Chain N: 59% 35%



- Molecule 15: 30S ribosomal protein S10

Chain O: 57% 36% 5%



- Molecule 16: 30S ribosomal protein S11

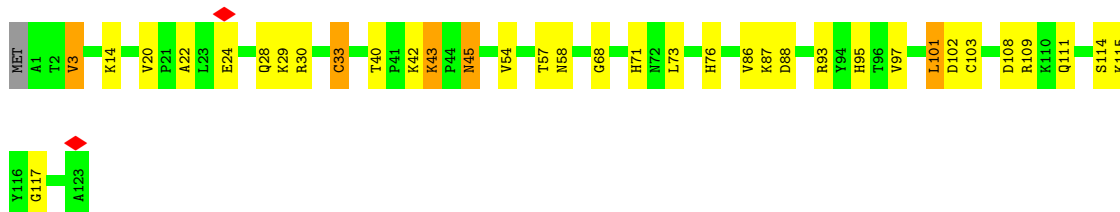
Chain P: 65% 23% 10%





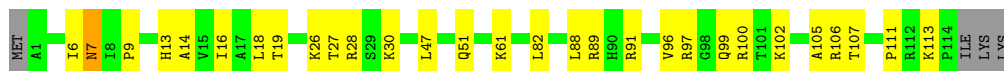
- Molecule 17: 30S ribosomal protein S12

Chain Q: 71% 24% . .



- Molecule 18: 30S ribosomal protein S13

Chain R: 72% 24% . .



- Molecule 19: 30S ribosomal protein S14

Chain S: 72% 27% .



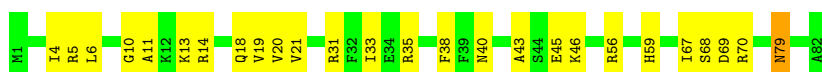
- Molecule 20: 30S ribosomal protein S15

Chain T: 78% 19% . .



- Molecule 21: 30S ribosomal protein S16

Chain U: 68% 30% .



- Molecule 22: 30S ribosomal protein S17

Chain V: 63% 32% 5%



- Molecule 23: 30S ribosomal protein S18

Chain W:  64% 19% 13%



- Molecule 24: 30S ribosomal protein S19

Chain X:  60% 25% 14%



- Molecule 25: 30S ribosomal protein S20

Chain Y:  72% 25% 3%



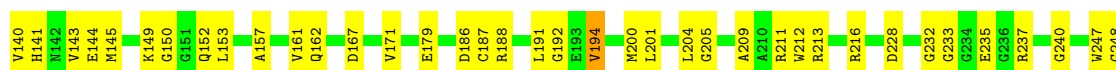
- Molecule 26: 30S ribosomal protein S21

Chain Z:  70% 18% 8%




- Molecule 27: 50S ribosomal protein L2

Chain b:  72% 26% 2%



- Molecule 28: 50S ribosomal protein L3

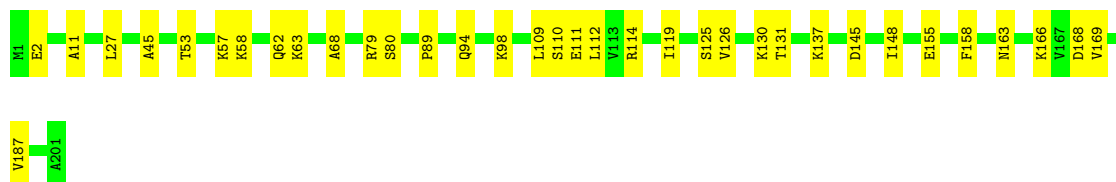
Chain c:  78% 21% 1%





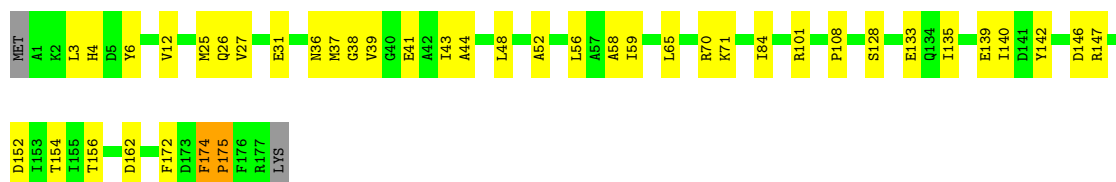
- Molecule 29: 50S ribosomal protein L4

Chain d: 83% 17%



- Molecule 30: 50S ribosomal protein L5

Chain e: 76% 22% ..



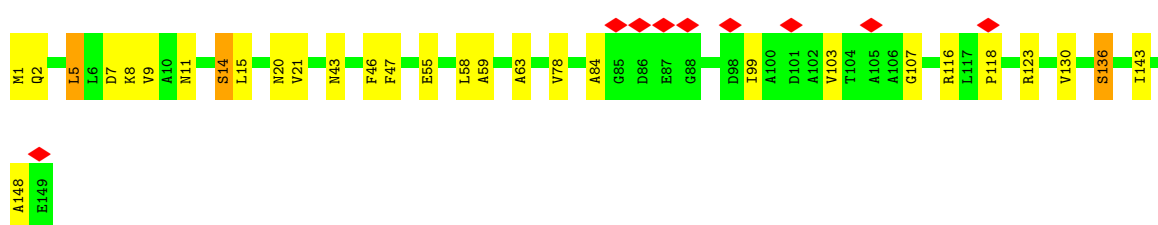
- Molecule 31: 50S ribosomal protein L6

Chain f: 85% 14% ...



- Molecule 32: 50S ribosomal protein L9

Chain g: 6% 80% 18% .



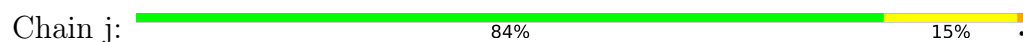
- Molecule 33: 50S ribosomal protein L11

Chain i: 54% 38% 6% ..

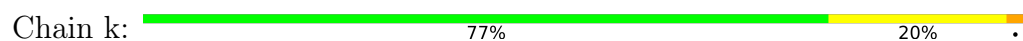




- Molecule 34: 50S ribosomal protein L13



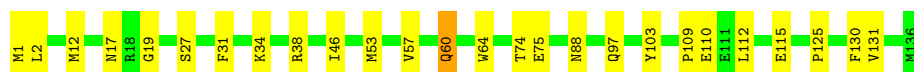
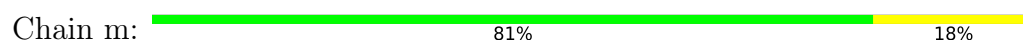
- Molecule 35: 50S ribosomal protein L14



- Molecule 36: 50S ribosomal protein L15



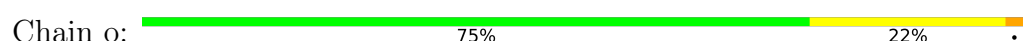
- Molecule 37: 50S ribosomal protein L16




- Molecule 38: 50S ribosomal protein L17

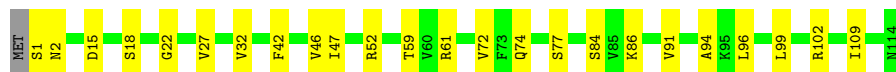


- Molecule 39: 50S ribosomal protein L18




- Molecule 40: 50S ribosomal protein L19

Chain p:  78% 21%



- Molecule 41: 50S ribosomal protein L20

Chain q:  77% 19%




- Molecule 42: 50S ribosomal protein L21

Chain r:  75% 23%



- Molecule 43: 50S ribosomal protein L22

Chain s:  79% 21%




- Molecule 44: 50S ribosomal protein L23

Chain t:  73% 20% 7%



- Molecule 45: 50S ribosomal protein L24

Chain u:  84% 13%



- Molecule 46: 50S ribosomal protein L25

Chain v:  74% 26%




- Molecule 47: 50S ribosomal protein L27

Chain w:  69% 18% 12%


MET ALA HIS LYS LYS ALA GLY GLY SER THR R7 S12 E15 A14 G18 V19 K20 T33 V34 R35 G38 V47 K58 K62 P70 T76 S77 I78 E81

- Molecule 48: 50S ribosomal protein L28

Chain x:  79% 17% ..


MET S1 Q5 V6 L21 T7 G8 K9 M16 R17 S18 N22 K25 P30 N31 L32 R36 T47 V57 K60 R73 Y77

- Molecule 49: 50S ribosomal protein L29

Chain y:  81% 17% .

M1 L19 N20 L21 L22 R23 E24 Q25 R29 M30 Q31 A32 Q36 L37 H41 A63

- Molecule 50: 50S ribosomal protein L30

Chain z:  78% 19% ..

MET A1 R10 S11 A12 I13 G14 R15 L16 P17 K20 G27 R37 T40 P41 A42 I43 M53 E58

- Molecule 51: 23S rRNA

Chain 1:  56% 38% 7%

G1 U4 A5 A6 G7 A10 C11 U12 G17 U18 A19 C20 A21 G26 C32 C33 U34 G35 C41 A42 A43 G44 G45 G46 G47 G48 G51 A63 C69 G70 A71 A74 G75 G76 G77 G85 A91 A94 A95 C96 C97 C98 U99 U100 A101 U102 A103

A118 A119 A120 A121 G122 G123 G124 U133 G134 U135 G136 U139 C140 G141 A142 A149 U150 C151 A152 U153 U154 A155 A156 C157 U158 A161 U162 C163 U174 G175 G178 G179 G180 A181 A182 G186 G187 G188 G189 A195 A196 A197 A198 A199 U200 A207 C208 C209 G214

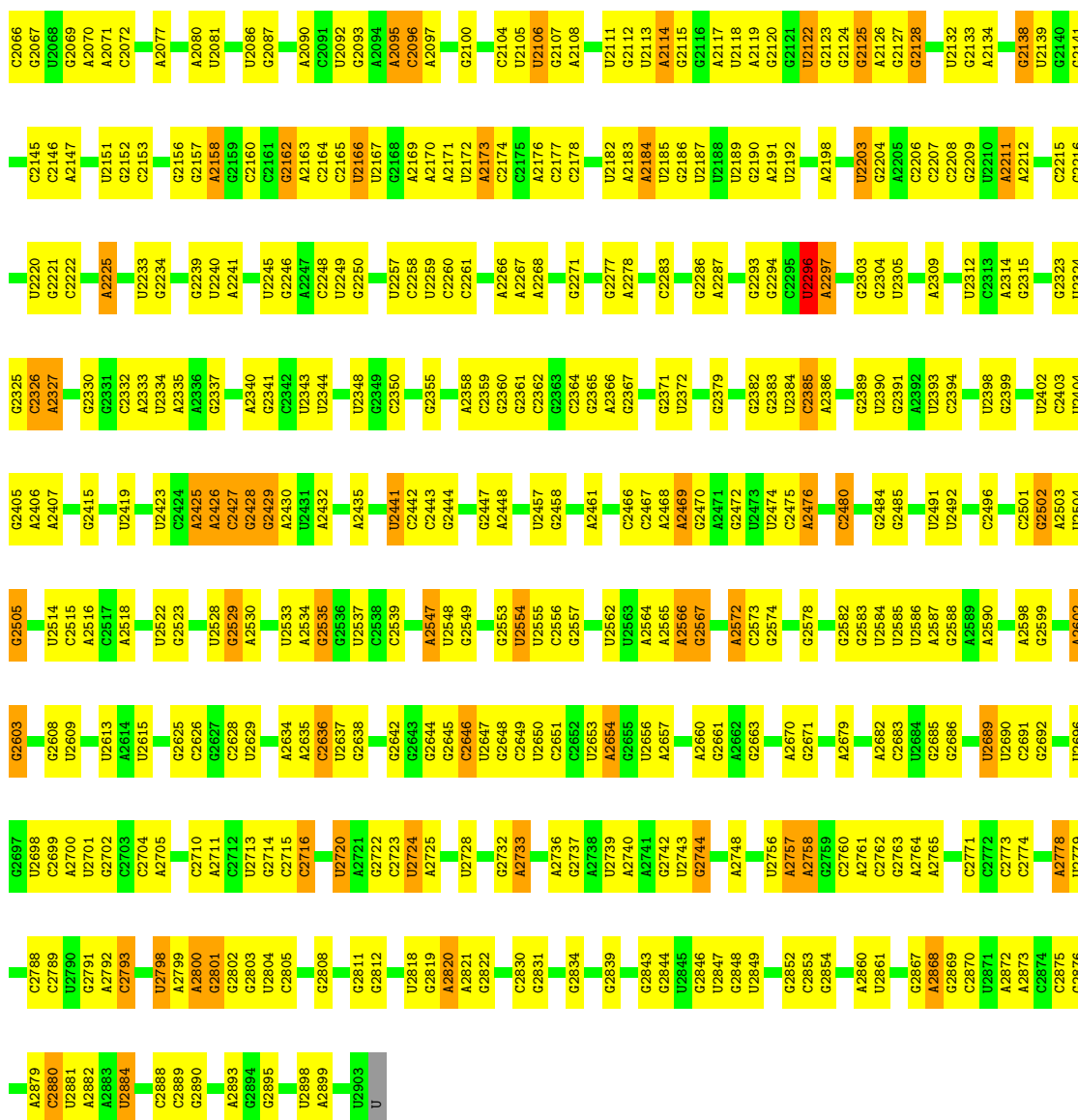
G215 A216 A217 A218 A219 G220 A221 A222 C225 A226 A227 C228 C229 G232 A233 U234 U235 C239 C240 A241 G242 G248 C249 G250 A251 A255 A256 C257 G266 A272 G273 C274 C275 U276 G277 A278 C281 A282 C283 U284 G285 U286 G287 C289 U294 A295 U296 G297 A300

A310 A311 G312 A320 U321 A322 C323 A324 G327 U328 C329 A330 C334 C335 C336 C337 C338 U339 A340 A341 C341 A342 A346 A353 A354 C355 U355 G356 A361 A362 G367 A368 A369 G370 A371 G372 U373 A374 G380 G386 U387 U395 U396 U399 A404 U405 G411 A412

C413 C414 A415 U416 U419 C420 G424 C435 C436 U437 A449 G450 U451 G452 C455 A456 A466 A467 G468 A472 G473 G474 A479 A480 G481 C490 G491 G494 A503 A504 A505 A508 A515 U518 U519 G520 G524 U525 A526 A527 A528 A529 G530 A532

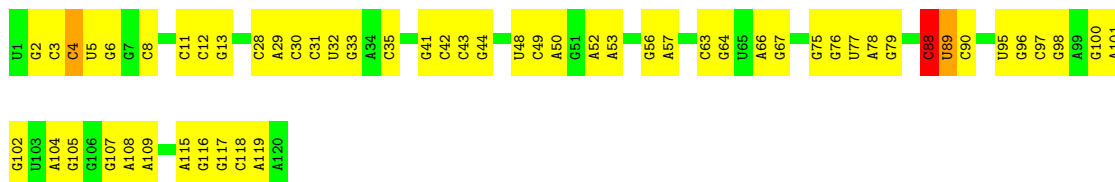
G533 U534 G535 G536 G539 G543 C544 U545 U552 G553 U554 G555 U562 A563 C564 A565 U566 U567 A572 U573 A574 A575 A576 U580 C581 G584 G585 A586 C587 U588 A592 A596 G597 U598 A599 G600 A603 U606 U607 A608 A609 C610 C611 A614 U615

C1967	G1873	U1775	A1669	G1555	U1488	C1357	G1252	G1122	G1056	A975	A878	A792	U694	A616
A1970	A1877	G1776	A1656	C1556	G1459	G1358	A1253	C1123	A1057	A979	G879	A793	G695	G617
G1971	G1878	A1780	C1557	U1558	U1460	G1358	A1254	G1124	U1058		C885	G797	G700	A621
G1972	U1781	A1782	G1673	C1558	C1461	C1363	U1255	G1125	G1059		C886	G798	G701	G622
C1974	U1882	U1783	G1674	G1560	U1468	G1364	G1256	U1130	U1061	C982	C885	G799	U702	A826
	U1883	A1784	G1675	G1564	U1469	A1365	C1287	G1131	G1062	A983	U887	A800	U703	A627
U1991	C1893	A1785	A1676	C1564	A1470	U1375	U1258	G1132	C985	A984	A892	G801	G704	A826
G1992	C1894	A1786	U1680	C1565	G1471	C1376	G1259	A1133	U1063	C986	C893	A802	A716	G628
U1993			G1681	G1568	G1472	G1376	U1263	A1134	U1065	C987	U894	U803	G629	G630
	A1899	C1790	G1682	A1569	U1474	G1378	U1263	G1135	U1066	A988	U895	A804	C717	G630
C1996	A1900	A1791	U1687	U1578	G1475	U1379	G1271	G1136	A1067	C989	A896	G805	A718	A631
C1997	A1901	C1792	A1698	U1579	G1476	U1379	A1272	G1137	G1068	A990	C897	C806	C719	
A1998		A1794	A1698	U1584	G1478	G1380	U1272	G1138	A1069			U807	G726	G634
C1999	G1906	C1795	U1796	U1584		A1383	U1273	G1139	A1070	C994	C903	G808	G726	G635
G2004	G1907	U1796	G1701	U1587	G1482		A1274	G1140	G1071	C995	G904	G809	A637	G636
A2005	C1908	U1797	G1702	G1587		C1386	A1275	U1141	C1072	A996		U810	G729	G637
	C1909	U1798			A1490	A1387	A1276	A1142	A1073		G907	U811	A730	G638
	G1910			C1595	G1491	U1394	G1277	A1143	G1074	U999	C908	C812	C731	U639
G2010	U1911	A1800	U1709	A1596	G1492	U1394	C1278		C1075	A1000	A909	U813	C732	C840
U2011	A1912	A1801	G1710	A1597	C1493	U1394	G1279	G1162	A1076	A1001	A910	C814	G733	
G2012	C1913	C1805	G1715	A1598	A1494	U1397	A1278	G1157	U1078	C1006	G914	C816	C740	A644
	A1914	A1805	U1716	G1601	A1495	C1398	G1286	C1158	C1079		C915	C817	C645	C646
A2020	U1915	C1806	A1717	U1602	A1504	U1409	C1289	U1159	A1080	G1011	G916	G818	A743	C650
C2021	A1916	G1807	G1718	A1603	A1505	C1409	G1292	G1160	U1081	U1012	A917	U827	U744	
U2022	U1917	A1808	U1725	U1603	U1506	G1410	C1292	C1161	U1082	C1013	A918	U828	A654	A655
C2023	A1918	A1809	C1726	C1507	C1507	G1416	C1293	G1162	A1083	U1014	A920	U829	G748	
G2024		A1810	U1726	A1608	U1508	C1417	G1296	C1172	A1085	G1016	U929	A829	A749	U658
C2025		G1811	C1727	C1611	A1509	G1418	C1297	U1173	A1086	U1017	U930	G830	A750	G659
U2026	U1923		G1728	A1616	G1510	A1419	A1300	U1174	G1087	U1018	U931	U831	A752	C660
G2027	C1924	C1816	U1729	U1616		A1420	A1301	U1175	A1088		U932	U832	A752	G661
U2028	U1925	A1819	G1730	C1617	A1515		G1301	U1176	A1020	A933	U933	A833		A661
A2030	C1926	U1820	C1732	A1618		G1424	G1309	C1178	G1091	A1021	U934	U839	G757	G662
G2031	A1821	C1822	G1733	C1625	A1522	G1425	U1309	G1179	C1092	C935		U839	G760	G663
C2032	C1823	G1734	C1735	U1626	U1523	G1426	U1318	G1179	A1095	A936		U839	G760	
U2033	U1930	A1735	A1626	A1626	G1524	A1427	C1319	U1180	C937	G1024	C937	U845	A761	A668
U2034	C1931	U1736	G1627	C1627		G1428	U1181	U1181	A1096	G1025	U938	U846	U762	G669
G2035	A1932	G1737	G1628	G1628	A1528	G1429	C1320	U1182	U1097	G1026	G939	G763	G763	G669
C2036	C1933	G1828	G1738	U1636	G1529	A1430	A1321	U1183	A1098	A1027	G940	G855	A764	A670
	C1934	A1829		U1636		G1430	A1322	U1183	G1099	A1028	A941	G856	A764	C671
U2039		U1747	A1637	C1637	C1533	A1433	A1322	G1186			A942	G857	G770	C672
G2040	A1937	C1837	C1748	C1638	U1534	A1434	U1326	G1187	C1102	C1030	G942	U857		
U2041	C1938	C1838	A1749	C1638	A1535	G1435	A1327	U1188	A1103	G1031	A943	G858	U773	A676
A2042	G1839			G1645	C1536	G1436	A1327	A1189	C1104	A1032	C946	U860	G774	A677
C2043	U1944			G1646	G1537	U1437	C1330	G1190	U105	U1033	C947	A861	G775	
	G1945			U1647	C1538	U1438	C1330	G1190	G1106	G1034	C948	G862	G776	G681
G2048	C1843	G1843	U1753	U1648	U1539	A1439	C1335	U1201		U1035	G949	G863	G777	G682
G2049	A1952	C1844	A1755	G1649	G1540	U1440	A1336	G1202	C1109	G1036		G864	G778	U683
C2050	G1845	G1756	A1650	C1541	G1541	G1441	U1336	G1202	C1109	G1036		G865	G779	G684
A2051	U1955	G1846	G1651	U1542	U1542	U1442	U1336	G1211	C1109	G1036	C961		G780	A685
	U1847	A1847	U1758	G1543	G1543	U1443	U1336	G1212	A1111	U1113	U967	G869	A781	U686
	A1759		A1759	A1544	A1544	G1444	U1341	C1212	G1112	C1045	U967	U870	A782	C687
C2055	A1960	C1857	C1760	A1654	A1545	G1444	A1342	G1221	U1113	C1045	C968	U871	A782	C687
G2056	C1961		U1655	A1655	G1546	C1447	A1342	C1221	U1046	G1047	C969	U872	A783	U688
A2060	U1963	G1869	C1764	C1658	U1546	G1448	A1343	G1225	C1117	G1047	U970	U872	G784	A689
G2061	C1963	A1870	A1773	C1658	C1550	G1449	U1344	G1225	U1119	C1053	A972	C873	G785	C690
C1965	A1871		A1773	A1665	A1551	G1450	U1345	G1248	U1119	C1053	A972	C873	G785	C691
A2062	U1966	A1872	C1773	A1666	A1551	G1450	U1345	U1249	G1120	A1054	G974	C876	A788	C692
							U1350	U1249	C1120	C1055		A877		A693



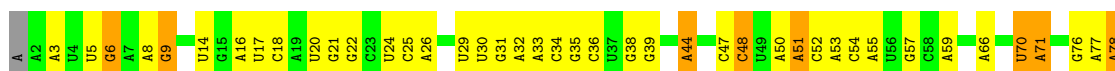
• Molecule 52: 5S rRNA

Chain 2: 53% 44% 3%



• Molecule 53: 16S rRNA

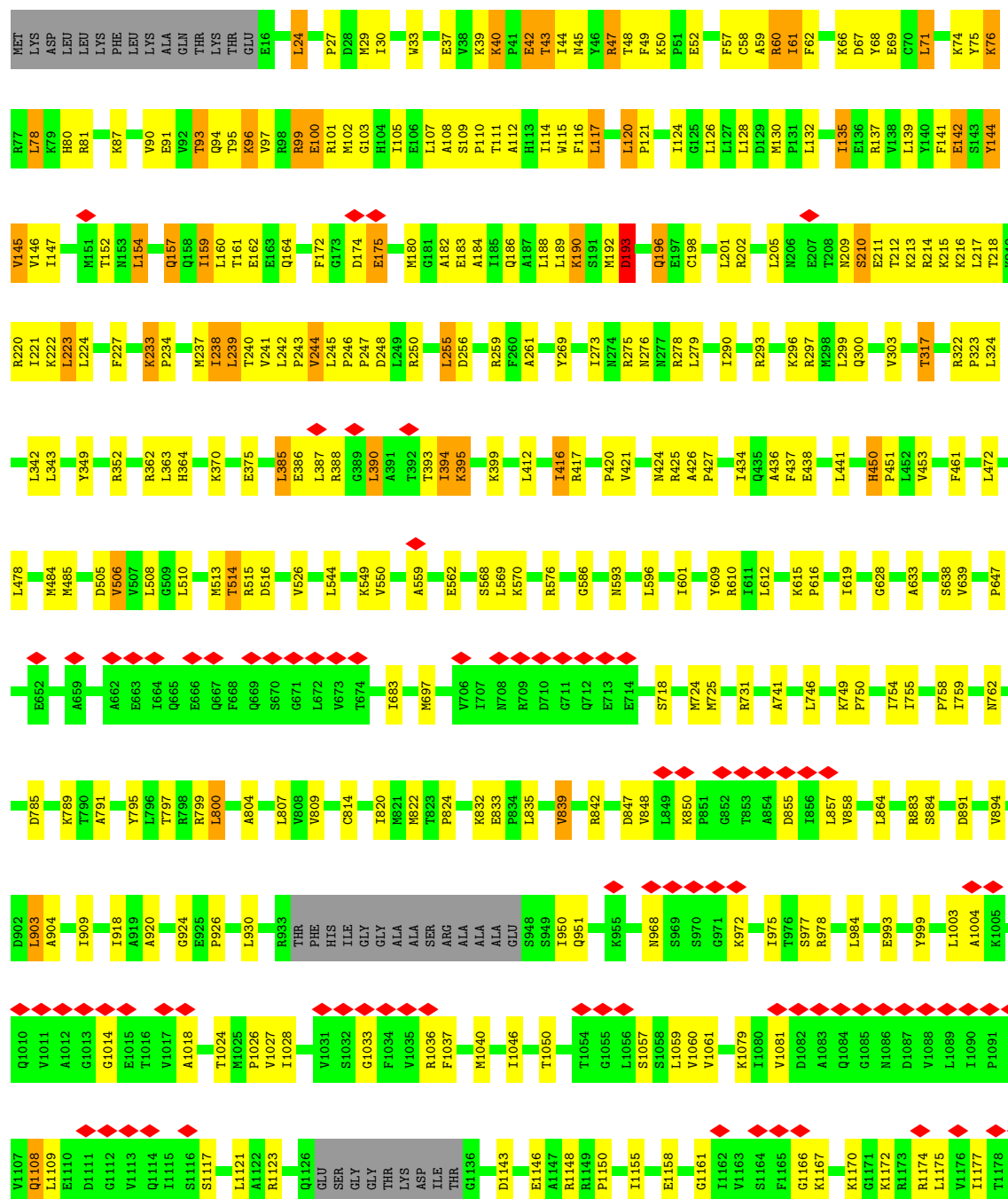
Chain 3: 55% 39% 6%



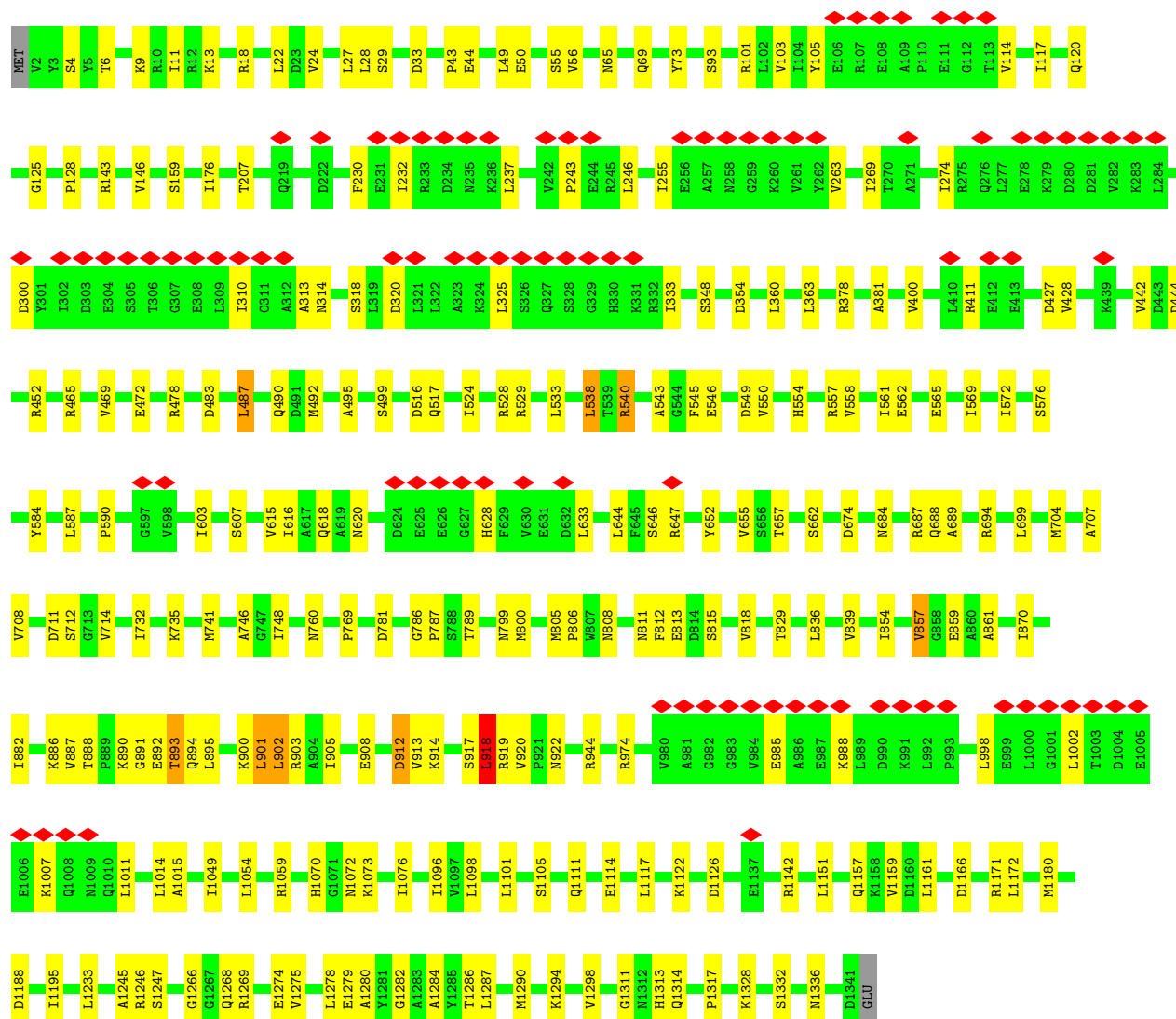
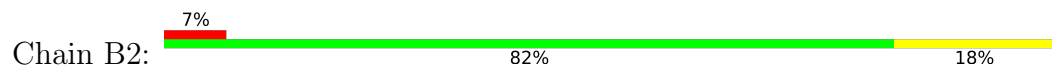




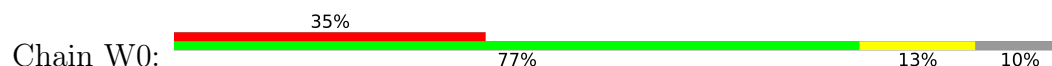
• Molecule 58: DNA-directed RNA polymerase subunit beta'

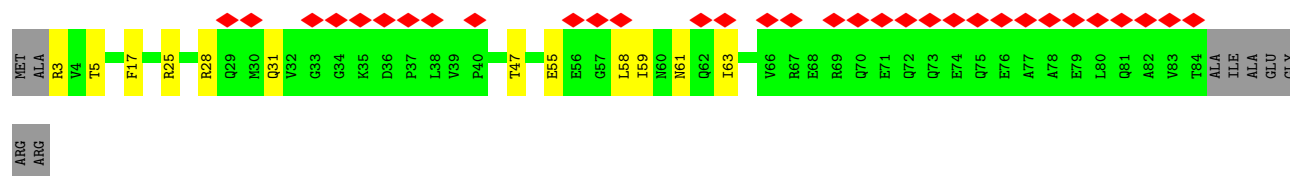


- Molecule 59: DNA-directed RNA polymerase subunit beta

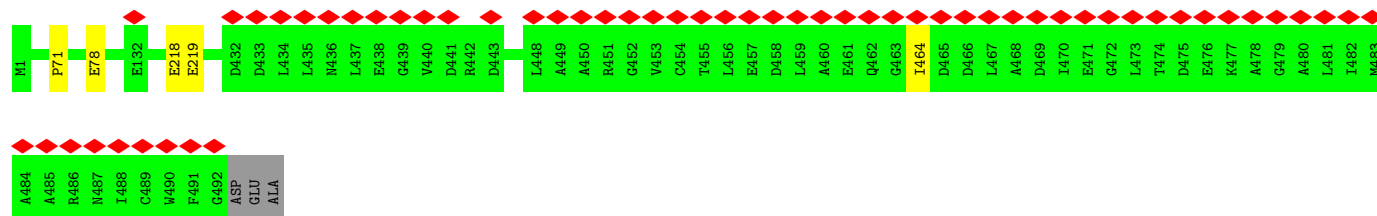


- Molecule 60: DNA-directed RNA polymerase subunit omega

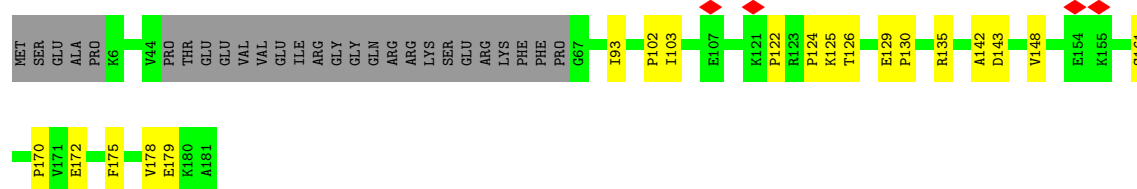
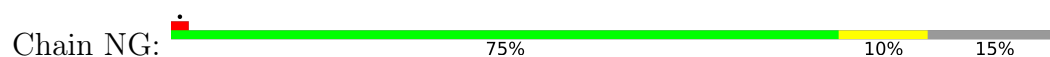




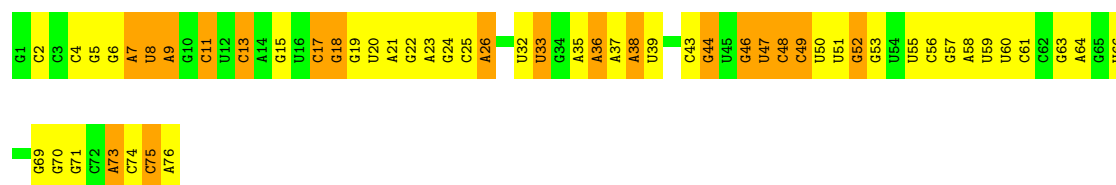
- Molecule 61: Transcription termination/antitermination protein NusA



- Molecule 62: Transcription termination/antitermination protein NusG



- Molecule 63: tRNA(Phe)

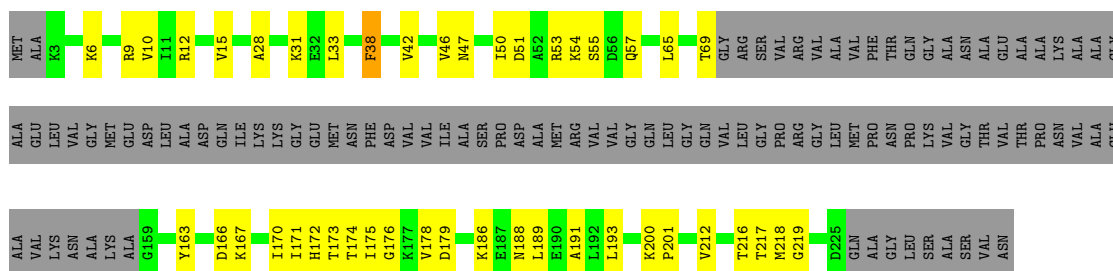


- Molecule 64: tRNA(fMet)

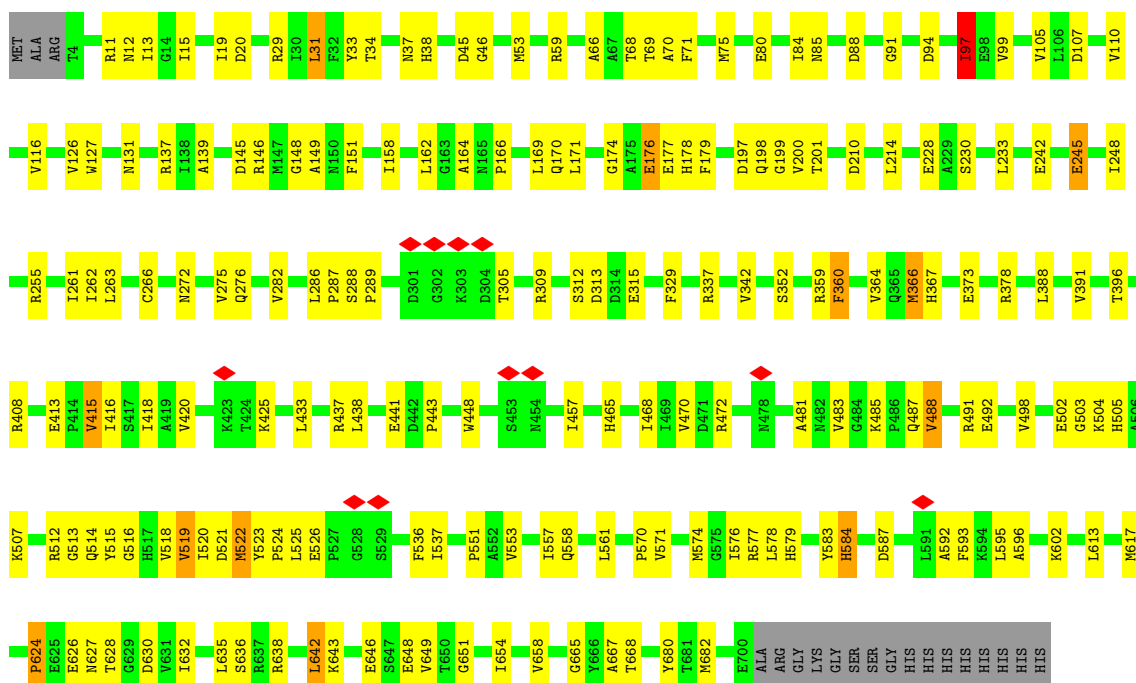


- Molecule 65: Large ribosomal subunit protein uL1

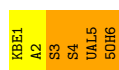




• Molecule 66: Elongation factor G



• Molecule 67: Viomycin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	31000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.091	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0075	Depositor
Map size (\AA)	753.60004, 753.60004, 753.60004	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.57, 1.57, 1.57	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: KBE, PO4, UAL, GDP, MG, 5OH, DPP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.47	0/531	0.99	4/709 (0.6%)
2	B	0.50	0/450	0.84	0/599
3	C	0.35	0/416	0.73	0/554
4	D	0.41	0/380	0.89	1/498 (0.2%)
5	E	0.40	0/513	0.86	0/676
6	F	0.35	0/303	0.77	0/397
7	G	0.48	0/1735	0.95	7/2338 (0.3%)
8	H	0.45	0/1647	0.88	3/2221 (0.1%)
9	I	0.45	0/1665	0.98	8/2227 (0.4%)
10	J	0.45	0/1165	0.95	7/1568 (0.4%)
11	K	0.58	0/835	1.02	5/1128 (0.4%)
12	L	0.44	0/1195	1.02	8/1602 (0.5%)
13	M	0.38	0/989	0.80	0/1326
14	N	0.48	0/1034	1.06	6/1375 (0.4%)
15	O	0.54	0/796	1.01	3/1077 (0.3%)
16	P	0.41	0/885	0.98	5/1195 (0.4%)
17	Q	0.51	1/969 (0.1%)	1.06	5/1300 (0.4%)
18	R	0.39	0/892	0.87	1/1193 (0.1%)
19	S	0.39	0/817	0.90	2/1088 (0.2%)
20	T	0.34	0/722	0.85	1/964 (0.1%)
21	U	0.40	0/659	0.91	2/884 (0.2%)
22	V	0.41	0/657	0.85	2/881 (0.2%)
23	W	0.47	0/544	0.95	2/731 (0.3%)
24	X	0.40	0/652	0.95	1/877 (0.1%)
25	Y	0.38	0/671	0.90	2/888 (0.2%)
26	Z	0.59	0/550	1.12	2/728 (0.3%)
27	b	0.45	0/2121	0.93	6/2852 (0.2%)
28	c	0.39	0/1586	0.84	3/2134 (0.1%)
29	d	0.43	0/1571	0.78	0/2113
30	e	0.44	1/1434 (0.1%)	0.91	5/1926 (0.3%)
31	f	0.41	0/1343	0.82	2/1816 (0.1%)
32	g	0.47	0/1122	0.93	3/1515 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.70	1/1046 (0.1%)	1.16	6/1410 (0.4%)
34	j	0.39	0/1152	0.86	4/1551 (0.3%)
35	k	0.49	0/947	0.95	2/1268 (0.2%)
36	l	0.40	0/1054	0.95	5/1403 (0.4%)
37	m	0.39	0/1093	0.85	3/1460 (0.2%)
38	n	0.39	0/973	0.92	3/1301 (0.2%)
39	o	0.39	0/902	0.92	3/1209 (0.2%)
40	p	0.40	0/929	0.85	1/1242 (0.1%)
41	q	0.46	0/960	0.90	3/1278 (0.2%)
42	r	0.45	0/829	0.96	4/1107 (0.4%)
43	s	0.38	0/864	0.84	2/1156 (0.2%)
44	t	0.39	0/744	0.78	0/994
45	u	0.41	0/784	0.92	3/1047 (0.3%)
46	v	0.39	0/766	0.78	0/1025
47	w	0.33	0/582	0.72	0/769
48	x	0.36	0/635	0.85	2/848 (0.2%)
49	y	0.34	0/510	0.87	1/677 (0.1%)
50	z	0.50	0/453	0.75	0/605
51	1	0.44	0/69796	0.54	8/108888 (0.0%)
52	2	0.45	0/2872	0.53	1/4479 (0.0%)
53	3	0.45	0/36963	0.53	3/57662 (0.0%)
54	4	0.56	0/695	0.72	0/1076
55	8	0.56	0/599	0.70	1/919 (0.1%)
56	9	0.48	0/468	0.53	0/719
57	A1	0.55	0/2106	0.82	0/2868
57	A2	0.48	0/2048	0.75	0/2786
58	B1	0.55	5/10510 (0.0%)	0.74	8/14196 (0.1%)
59	B2	0.45	0/10714	0.67	1/14459 (0.0%)
60	W0	0.29	0/652	0.61	0/879
61	NA	0.71	0/2431	1.20	0/3385
62	NG	1.12	0/756	1.03	2/1048 (0.2%)
63	5	0.56	0/1812	0.88	2/2823 (0.1%)
64	6	0.43	0/1832	0.56	0/2855
65	a	0.46	0/1033	0.98	5/1387 (0.4%)
66	0	0.51	0/5501	0.96	19/7446 (0.3%)
67	h	3.18	2/11 (18.2%)	0.75	0/13
All	All	0.46	10/196871 (0.0%)	0.69	188/289618 (0.1%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	3	SER	CA-C	-6.72	1.38	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	4	SER	CA-C	-6.20	1.40	1.52
30	e	174	PHE	N-CA	5.74	1.54	1.46
58	B1	1350	ASN	CG-ND2	-5.27	1.22	1.33
58	B1	424	ASN	CG-ND2	-5.16	1.22	1.33
33	i	2	LYS	N-CA	5.13	1.49	1.46
58	B1	777	HIS	ND1-CE1	5.13	1.37	1.32
58	B1	1108	GLN	CD-OE1	5.11	1.33	1.23
17	Q	43	LYS	N-CA	5.07	1.50	1.46
58	B1	1268	ASN	CG-OD1	5.01	1.33	1.23

All (188) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	0	174	GLY	N-CA-C	10.08	123.45	111.35
11	K	99	ALA	N-CA-C	9.93	123.44	111.02
65	a	179	ASP	N-CA-C	-9.71	99.88	114.64
16	P	73	VAL	N-CA-C	-9.11	104.46	113.20
66	0	45	ASP	N-CA-C	-8.82	103.64	114.75
8	H	9	ILE	N-CA-C	8.69	115.51	106.21
12	L	111	GLY	N-CA-C	8.59	121.41	111.36
15	O	60	ASP	N-CA-C	-8.56	104.86	114.62
9	I	7	LYS	N-CA-C	8.47	121.73	111.40
39	o	22	GLY	N-CA-C	-8.43	101.23	111.35
43	s	24	ILE	N-CA-C	8.39	115.19	106.21
37	m	60	GLN	N-CA-C	8.24	122.37	110.10
1	A	45	THR	N-CA-C	-8.22	102.70	112.89
51	1	876	C	C2'-C3'-O3'	-8.11	101.54	113.70
66	0	38	HIS	N-CA-C	-7.89	97.55	109.94
66	0	413	GLU	N-CA-C	7.71	119.49	109.93
33	i	90	GLY	N-CA-C	-7.67	105.35	114.48
7	G	88	GLN	N-CA-C	7.66	121.74	110.17
31	f	46	ASP	N-CA-C	-7.53	103.01	111.14
51	1	1020	A	C2'-C3'-O3'	7.34	120.52	109.50
17	Q	22	ALA	N-CA-C	-7.30	102.93	111.03
9	I	168	THR	N-CA-C	7.29	122.24	111.96
34	j	105	VAL	N-CA-C	-7.11	106.14	111.90
4	D	7	PRO	N-CA-C	7.07	122.45	111.21
65	a	10	VAL	N-CA-C	-7.06	103.59	110.72
27	b	87	SER	N-CA-C	-6.97	105.30	113.88
19	S	39	ASP	N-CA-C	-6.92	103.84	112.90
16	P	126	ARG	N-CA-C	6.89	118.97	110.91
26	Z	66	ARG	N-CA-C	6.87	119.61	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	91	ARG	CA-C-N	6.85	126.09	118.97
12	L	91	ARG	C-N-CA	6.85	126.09	118.97
33	i	119	ALA	N-CA-C	6.83	120.39	110.42
66	0	366	MET	N-CA-C	6.82	118.89	110.91
39	o	10	ARG	N-CA-C	-6.80	105.13	113.50
1	A	54	GLY	N-CA-C	6.76	123.26	112.58
65	a	178	VAL	N-CA-C	6.75	113.43	106.21
21	U	46	LYS	N-CA-C	-6.63	99.02	109.50
34	j	81	ILE	N-CA-C	6.63	117.32	110.36
48	x	17	ARG	N-CA-C	6.54	119.20	111.02
27	b	30	ALA	N-CA-C	6.52	121.62	112.75
58	B1	450	HIS	CB-CG-CD2	-6.51	122.74	131.20
41	q	6	GLY	N-CA-C	6.48	116.11	110.21
27	b	121	ALA	N-CA-C	6.48	118.66	110.24
27	b	248	GLY	N-CA-C	6.47	122.93	113.48
21	U	79	ASN	N-CA-C	6.45	118.65	110.33
28	c	59	ARG	N-CA-C	-6.42	107.30	114.62
24	X	48	ILE	N-CA-C	6.41	118.03	109.37
58	B1	61	ILE	CA-C-N	-6.36	114.01	121.64
58	B1	61	ILE	C-N-CA	-6.36	114.01	121.64
30	e	147	ARG	N-CA-C	6.35	118.06	110.19
58	B1	777	HIS	CB-CG-CD2	-6.33	122.97	131.20
30	e	43	ILE	N-CA-C	-6.32	103.19	111.09
15	O	83	THR	CB-CA-C	-6.28	101.30	110.96
38	n	104	ALA	N-CA-C	6.26	118.91	111.71
25	Y	6	ALA	N-CA-C	-6.24	103.33	113.19
16	P	90	PRO	N-CA-C	-6.23	105.52	114.18
33	i	21	PRO	N-CA-C	6.23	118.30	110.70
36	l	95	LEU	N-CA-C	-6.20	105.55	113.23
12	L	86	VAL	N-CA-C	6.19	114.78	109.02
16	P	125	LYS	N-CA-C	6.13	123.86	110.80
10	J	11	GLN	N-CA-C	6.13	119.70	111.24
45	u	6	ARG	N-CA-C	6.11	123.82	110.80
23	W	68	PRO	N-CA-C	6.11	120.57	111.41
18	R	14	ALA	N-CA-C	6.07	118.69	111.71
38	n	14	SER	N-CA-C	6.07	117.56	111.07
10	J	110	MET	N-CA-C	-6.05	105.81	113.43
12	L	135	LYS	N-CA-C	-6.04	105.95	113.38
7	G	212	TYR	N-CA-C	6.04	117.73	111.03
66	0	408	ARG	N-CA-C	6.03	118.56	108.73
10	J	77	ASN	N-CA-C	6.02	119.54	111.24
34	j	31	GLU	N-CA-C	-6.01	104.84	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	177	MET	N-CA-C	6.00	117.93	110.91
37	m	110	GLU	N-CA-C	6.00	117.49	111.07
11	K	86	ARG	N-CA-C	5.99	117.92	110.91
10	J	74	ALA	N-CA-C	5.95	123.47	110.80
27	b	145	MET	N-CA-C	-5.93	106.69	114.04
42	r	54	VAL	N-CA-C	5.93	121.67	109.34
1	A	43	PHE	N-CA-C	-5.92	106.18	113.41
25	Y	43	LYS	N-CA-C	5.92	117.53	111.14
14	N	42	THR	N-CA-C	5.91	119.79	111.52
48	x	60	LYS	N-CA-C	-5.90	104.48	111.03
14	N	90	ASP	N-CA-C	5.89	123.35	110.80
30	e	4	HIS	N-CA-C	-5.86	104.49	111.69
36	l	115	GLU	N-CA-C	5.85	117.75	110.91
7	G	13	VAL	N-CA-C	5.84	121.48	109.34
8	H	10	ARG	N-CA-C	-5.80	105.57	114.16
52	2	88	C	C2'-C3'-O3'	-5.80	105.00	113.70
51	1	1085	A	C2'-C3'-O3'	-5.80	105.00	113.70
12	L	90	VAL	N-CA-C	5.79	117.66	108.87
45	u	89	GLY	N-CA-C	-5.78	107.17	114.16
28	c	86	GLU	N-CA-C	5.77	119.21	111.24
8	H	5	HIS	N-CA-C	5.77	116.67	109.57
17	Q	33	CYS	N-CA-C	5.74	117.62	110.91
7	G	123	GLY	N-CA-C	5.72	117.34	111.56
34	j	119	PHE	N-CA-C	-5.71	106.44	113.41
20	T	43	ALA	N-CA-C	-5.69	105.00	111.14
14	N	58	GLU	N-CA-C	-5.66	103.88	112.99
35	k	94	PRO	N-CA-C	5.66	124.13	112.47
16	P	89	GLY	N-CA-C	5.65	123.86	112.34
51	1	2296	U	C2'-C3'-O3'	-5.64	105.24	113.70
14	N	71	ILE	N-CA-C	5.63	116.08	110.23
30	e	172	PHE	N-CA-C	-5.62	106.42	113.28
33	i	53	PRO	N-CA-C	5.62	119.91	111.14
58	B1	450	HIS	CB-CG-ND1	5.62	131.13	122.70
41	q	75	TYR	N-CA-C	5.62	117.08	111.07
66	0	359	ARG	N-CA-C	5.62	117.16	110.19
22	V	58	VAL	N-CA-C	5.61	116.66	107.24
39	o	21	LEU	N-CA-C	-5.60	105.04	113.89
43	s	62	ASP	N-CA-C	5.60	118.46	111.24
66	0	635	LEU	N-CA-C	-5.59	104.88	110.97
33	i	124	MET	N-CA-C	-5.59	104.81	111.69
35	k	108	ARG	N-CA-C	5.55	118.69	108.58
7	G	151	LYS	N-CA-C	5.53	117.75	111.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	Q	115	LYS	N-CA-C	-5.53	101.53	110.32
17	Q	117	GLY	N-CA-C	5.52	122.44	114.10
30	e	175	PRO	N-CA-C	5.52	123.84	112.47
11	K	62	MET	N-CA-C	5.51	119.68	112.13
66	0	242	GLU	N-CA-C	-5.50	100.15	108.67
45	u	31	GLY	N-CA-C	-5.50	107.20	114.95
66	0	37	ASN	N-CA-C	5.49	118.35	109.40
66	0	31	LEU	N-CA-C	-5.49	105.71	112.90
11	K	39	LEU	N-CA-C	-5.48	104.46	113.50
63	5	73	A	C3'-C2'-O2'	5.48	118.92	110.70
41	q	6	GLY	O-C-N	5.47	124.91	121.85
26	Z	34	ARG	N-CA-C	5.46	122.43	110.80
66	0	287	PRO	N-CA-C	5.43	119.71	111.19
17	Q	3	VAL	N-CA-C	5.42	120.62	109.34
51	1	278	A	N9-C1'-C2'	5.42	120.13	112.00
58	B1	777	HIS	CB-CG-ND1	5.42	130.84	122.70
55	8	7	DC	C2'-C3'-O3'	-5.42	103.37	111.50
9	I	13	ARG	N-CA-C	-5.41	106.69	113.28
11	K	64	VAL	N-CA-C	5.40	115.72	108.17
23	W	51	GLN	N-CA-C	-5.39	106.38	113.12
22	V	79	GLU	N-CA-C	5.39	117.22	110.91
63	5	75	C	C4'-C3'-O3'	5.39	117.48	109.40
9	I	29	THR	N-CA-C	5.38	122.27	110.80
66	0	245	GLU	N-CA-C	5.38	118.64	111.75
49	y	24	GLU	N-CA-C	5.38	122.25	110.80
62	NG	103	ILE	CA-C-N	-5.36	114.02	122.76
62	NG	103	ILE	C-N-CA	-5.36	114.02	122.76
51	1	1104	C	C4'-C3'-O3'	5.36	121.03	113.00
42	r	50	GLY	N-CA-C	-5.36	105.92	112.77
28	c	174	SER	N-CA-C	5.35	117.17	110.91
12	L	6	ILE	N-CA-C	5.33	120.43	109.34
7	G	46	VAL	N-CA-CB	5.33	113.86	110.50
53	3	754	C	N1-C1'-C2'	5.32	119.98	112.00
42	r	53	PHE	CB-CA-C	5.32	121.00	110.42
33	i	72	THR	N-CA-C	-5.30	98.09	109.81
59	B2	891	GLY	O-C-N	5.30	124.82	121.85
9	I	150	LYS	N-CA-C	5.29	117.10	110.91
31	f	174	LYS	N-CA-C	5.27	122.02	110.80
66	0	46	GLY	N-CA-C	-5.26	108.06	115.32
58	B1	27	PRO	N-CA-C	-5.23	106.23	113.81
66	0	80	GLU	N-CA-C	-5.22	102.88	110.08
66	0	97	ILE	N-CA-C	-5.22	105.45	110.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	160	VAL	N-CA-C	5.21	115.93	110.62
66	0	441	GLU	N-CA-C	5.20	117.95	111.24
9	I	182	LYS	N-CA-C	5.20	119.26	112.13
12	L	129	ASN	N-CA-C	5.19	118.36	111.30
14	N	40	ARG	N-CA-C	-5.18	106.06	114.09
32	g	136	SER	N-CA-C	5.18	121.83	110.80
38	n	50	PRO	N-CA-C	-5.16	107.41	113.86
32	g	63	ALA	N-CA-C	-5.16	106.94	113.18
66	0	13	ILE	N-CA-C	5.15	116.72	108.89
66	0	624	PRO	N-CA-C	5.15	120.30	113.40
19	S	13	VAL	N-CA-C	-5.14	105.40	111.00
10	J	92	ARG	N-CA-CB	-5.13	104.46	111.65
51	1	100	U	N1-C1'-C2'	5.13	119.70	112.00
15	O	38	GLY	N-CA-C	5.12	122.80	112.34
65	a	38	PHE	N-CA-C	-5.12	100.83	109.07
58	B1	61	ILE	CA-C-O	-5.10	115.65	120.95
65	a	191	ALA	N-CA-C	-5.10	106.91	113.02
40	p	18	SER	N-CA-C	5.09	117.93	110.30
36	l	29	LYS	CA-C-N	5.08	131.24	121.54
36	l	29	LYS	C-N-CA	5.08	131.24	121.54
9	I	165	GLU	N-CA-C	5.08	121.61	110.80
51	1	1111	A	N9-C1'-C2'	5.07	119.61	112.00
7	G	56	LEU	N-CA-C	-5.07	105.84	111.36
14	N	103	VAL	N-CA-C	-5.06	107.87	112.12
1	A	5	ILE	N-CA-C	-5.06	107.87	112.12
27	b	157	ALA	N-CA-C	5.06	117.68	110.24
36	l	96	LYS	N-CA-C	-5.04	106.64	112.89
10	J	75	LEU	N-CA-C	5.04	121.54	110.80
37	m	27	SER	N-CA-C	5.04	119.43	113.28
32	g	14	SER	N-CA-C	5.03	117.26	110.06
53	3	368	U	N1-C1'-C2'	5.03	119.55	112.00
42	r	47	VAL	CA-C-O	-5.02	118.26	122.63
53	3	1301	U	C4'-C3'-O3'	5.01	116.92	109.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	522	0	524	18	0
2	B	444	0	461	8	0
3	C	409	0	440	7	0
4	D	377	0	418	14	0
5	E	504	0	574	9	0
6	F	302	0	341	10	0
7	G	1704	0	1732	27	0
8	H	1620	0	1688	28	0
9	I	1643	0	1710	43	0
10	J	1152	0	1195	19	0
11	K	817	0	808	15	0
12	L	1181	0	1240	26	0
13	M	979	0	1034	13	0
14	N	1022	0	1070	38	0
15	O	786	0	828	26	0
16	P	869	0	878	21	0
17	Q	955	0	1019	20	0
18	R	883	0	944	22	0
19	S	805	0	847	21	0
20	T	714	0	737	13	0
21	U	649	0	666	21	0
22	V	648	0	691	19	0
23	W	535	0	552	14	0
24	X	637	0	665	23	0
25	Y	665	0	714	20	0
26	Z	544	0	579	10	0
27	b	2082	0	2157	51	0
28	c	1565	0	1616	37	0
29	d	1552	0	1619	26	0
30	e	1410	0	1447	26	0
31	f	1323	0	1374	19	0
32	g	1111	0	1148	19	0
33	i	1032	0	1088	61	0
34	j	1129	0	1162	19	0
35	k	938	0	1012	17	0
36	l	1045	0	1117	29	0
37	m	1074	0	1157	17	0
38	n	960	0	1000	21	0
39	o	892	0	923	21	0
40	p	917	0	965	21	0
41	q	947	0	1022	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	r	816	0	839	16	0
43	s	857	0	922	16	0
44	t	738	0	807	12	0
45	u	776	0	825	7	0
46	v	753	0	780	17	0
47	w	575	0	592	16	0
48	x	625	0	655	15	0
49	y	509	0	543	8	0
50	z	449	0	491	9	0
51	1	62317	0	31346	968	0
52	2	2568	0	1303	58	0
53	3	33012	0	16618	568	0
54	4	627	0	313	8	0
55	8	539	0	305	29	0
56	9	417	0	224	1	0
57	A1	2088	0	1895	26	0
57	A2	2029	0	1864	14	0
58	B1	10353	0	10548	314	0
59	B2	10546	0	10550	161	0
60	W0	650	0	658	10	0
61	NA	2432	0	1171	8	0
62	NG	758	0	334	16	0
63	5	1622	0	821	23	0
64	6	1640	0	837	19	0
65	a	1026	0	1092	32	0
66	0	5399	0	5363	108	0
67	h	48	0	40	7	0
68	B1	1	0	0	0	0
69	0	28	0	12	2	0
70	0	5	0	0	1	0
All	All	183546	0	132910	2831	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 9.

All (2831) 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)
23:W:42:ARG:NH2	53:3:721:G:H5''	1.59	1.18
35:k:48:PRO:HB3	53:3:1423:G:H5''	1.23	1.14
51:1:2682:A:H61	51:1:2728:U:H1'	1.18	1.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:42:ARG:HH21	53:3:721:G:H5''	0.97	1.08
33:i:93:ASN:HB2	51:1:1077:A:H5'	1.12	1.08
51:1:1064:C:H3'	51:1:1065:U:H5''	1.37	1.07
51:1:1019:U:OP1	51:1:1036:G:H5'	1.54	1.04
64:6:26:G:H2'	64:6:27:U:H5''	1.39	1.04
22:V:5:ARG:HH22	53:3:128:G:H5'	1.20	1.04
51:1:814:C:H1'	51:1:1225:G:H21	1.20	1.04
57:A1:287:VAL:CB	61:NA:78:GLU:CB	2.38	1.02
33:i:7:TYR:HE2	33:i:57:VAL:HB	1.24	1.02
51:1:1645:G:H5''	51:1:1646:C:H5'	1.42	1.01
58:B1:750:PRO:HB3	59:B2:549:ASP:OD2	1.60	1.01
33:i:123:ALA:HB1	51:1:1081:U:H4'	1.44	1.00
51:1:1557:C:H3'	51:1:1558:C:H5''	1.42	1.00
58:B1:111:THR:HG23	58:B1:300:GLN:CD	1.86	1.00
33:i:92:PRO:HB2	51:1:1077:A:O4'	1.62	0.99
53:3:1421:G:H3'	53:3:1422:G:H4'	1.44	0.99
15:O:41:PRO:HB3	53:3:1151:A:H1'	1.40	0.99
1:A:64:PHE:HD1	53:3:1011:C:H4'	1.26	0.98
33:i:93:ASN:HB2	51:1:1077:A:C5'	1.93	0.98
51:1:2382:G:H5''	51:1:2383:G:H5'	1.44	0.97
58:B1:352:ARG:HD2	59:B2:1268:GLN:NE2	1.79	0.97
34:j:27:ARG:HH22	51:1:1142:A:H4'	1.29	0.96
6:F:3:VAL:HG21	51:1:2539:C:H5'	1.47	0.96
22:V:5:ARG:NH2	53:3:128:G:H5'	1.83	0.94
58:B1:68:TYR:O	58:B1:75:TYR:CE2	2.20	0.94
51:1:562:U:H2'	51:1:572:A:H1'	1.50	0.94
51:1:1394:U:H4'	51:1:1603:A:H4'	1.49	0.94
66:0:524:PRO:HA	66:0:574:MET:HA	1.47	0.94
51:1:1098:A:H2'	51:1:1099:G:H5'	1.48	0.93
51:1:663:G:H2'	51:1:664:G:H5''	1.51	0.90
33:i:93:ASN:CB	51:1:1077:A:H5'	2.02	0.90
58:B1:68:TYR:C	58:B1:75:TYR:HE2	1.80	0.90
59:B2:854:ILE:HG21	59:B2:917:SER:HB3	1.54	0.90
21:U:31:ARG:HB2	53:3:310:G:H5''	1.53	0.89
58:B1:317:THR:HA	58:B1:323:PRO:HA	1.55	0.89
51:1:1697:G:H3'	51:1:1698:A:H5''	1.52	0.89
58:B1:202:ARG:HG2	58:B1:202:ARG:HH11	1.35	0.89
51:1:1045:C:H5'	51:1:1046:A:C8	2.09	0.88
51:1:45:G:H5''	51:1:46:G:H5'	1.51	0.88
54:4:44:G:H21	58:B1:427:PRO:HD3	1.38	0.88
63:5:9:A:H2'	63:5:11:C:H41	1.38	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
64:6:69:C:H2'	64:6:70:G:H5''	1.56	0.88
53:3:1421:G:N7	53:3:1422:G:H1'	1.88	0.87
53:3:813:U:H2'	53:3:814:A:H5''	1.58	0.85
51:1:2653:U:H3'	51:1:2654:A:H5''	1.58	0.85
51:1:1075:C:H3'	51:1:1076:C:H5''	1.58	0.85
51:1:876:C:H3'	51:1:877:A:C4'	2.06	0.84
17:Q:57:THR:HG21	53:3:362:G:H5''	1.57	0.84
46:v:49:ASN:HD21	51:1:1040:A:H4'	1.40	0.84
58:B1:68:TYR:HB3	58:B1:75:TYR:OH	1.76	0.84
51:1:2656:U:H5''	66:0:146:ARG:HE	1.40	0.83
15:O:43:PRO:HA	53:3:1151:A:H5'	1.59	0.83
58:B1:633:ALA:HB2	59:B2:808:ASN:H	1.41	0.83
2:B:5:ASN:HD22	51:1:2020:A:H62	1.23	0.83
21:U:5:ARG:HB2	53:3:376:G:H5''	1.59	0.83
21:U:14:ARG:HH12	53:3:618:C:H1'	1.43	0.83
51:1:740:C:H6	51:1:740:C:H5'	1.44	0.83
27:b:38:LYS:HB2	51:1:692:C:H5''	1.59	0.82
51:1:814:C:H1'	51:1:1225:G:N2	1.93	0.82
53:3:335:C:H2'	53:3:336:A:H8	1.44	0.82
52:2:3:C:H2'	52:2:4:C:H5''	1.62	0.82
58:B1:68:TYR:O	58:B1:75:TYR:HE2	1.58	0.82
58:B1:770:LEU:HD13	59:B2:618:GLN:HG3	1.61	0.82
51:1:161:A:H3'	51:1:162:U:H5''	1.62	0.82
55:8:1:DC:H5''	58:B1:210:SER:OG	1.80	0.82
53:3:405:U:H3'	53:3:406:G:H5'	1.61	0.81
51:1:2107:G:H2'	51:1:2108:A:H8	1.44	0.81
58:B1:144:TYR:HE1	58:B1:162:GLU:OE2	1.64	0.81
51:1:2553:G:H3'	51:1:2554:U:H5''	1.63	0.81
53:3:1422:G:H2'	53:3:1423:G:C8	2.15	0.81
58:B1:141:PHE:CE2	58:B1:296:LYS:HB2	2.15	0.80
51:1:2156:G:H2'	51:1:2157:G:H5'	1.63	0.80
58:B1:141:PHE:HE2	58:B1:296:LYS:HB2	1.44	0.80
58:B1:37:GLU:O	58:B1:61:ILE:HD11	1.81	0.80
58:B1:111:THR:HG23	58:B1:300:GLN:OE1	1.81	0.80
21:U:10:GLY:HA2	53:3:624:C:H4'	1.64	0.79
51:1:740:C:H42	51:1:757:G:H1	1.27	0.79
53:3:1088:G:H21	53:3:1167:A:H61	1.30	0.79
64:6:47:U:H2'	64:6:50:U:OP1	1.82	0.79
36:l:17:LYS:HD2	51:1:663:G:H5''	1.62	0.79
15:O:7:ARG:HB2	15:O:101:SER:HB2	1.62	0.79
62:NG:126:THR:CB	62:NG:175:PHE:O	2.31	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:186:GLN:HG3	58:B1:238:ILE:HG13	1.65	0.78
52:2:88:C:H5''	52:2:89:U:OP1	1.82	0.78
12:L:68:VAL:HG13	12:L:99:ALA:HB1	1.65	0.78
52:2:30:C:H2'	52:2:31:C:H5'	1.66	0.78
51:1:1064:C:H3'	51:1:1065:U:C5'	2.14	0.78
53:3:112:G:H21	53:3:354:G:H5'	1.47	0.77
33:i:7:TYR:CE2	33:i:57:VAL:HB	2.16	0.77
38:n:4:ARG:HB2	51:1:2722:G:H4'	1.64	0.77
51:1:2128:G:H1	51:1:2160:C:N4	1.82	0.77
51:1:2799:A:H2'	51:1:2800:A:H5'	1.65	0.77
58:B1:202:ARG:HG2	58:B1:202:ARG:NH1	1.99	0.77
66:0:632:ILE:HD11	66:0:654:ILE:HG12	1.66	0.77
2:B:49:ARG:HG3	51:1:2884:U:H6	1.48	0.76
51:1:1020:A:H1'	51:1:1021:A:OP2	1.86	0.76
53:3:1012:A:H5'	53:3:1012:A:H8	1.48	0.76
51:1:974:G:H1'	51:1:975:A:C8	2.20	0.76
51:1:2656:U:H5''	66:0:146:ARG:NE	2.01	0.76
39:o:33:ARG:HB2	52:2:52:A:N6	2.00	0.76
64:6:26:G:C2'	64:6:27:U:H5''	2.16	0.76
58:B1:110:PRO:HG2	58:B1:183:GLU:HG3	1.68	0.75
53:3:769:G:H4'	53:3:1513:A:H4'	1.67	0.75
55:8:13:DT:H72	58:B1:791:ALA:HB2	1.67	0.75
39:o:15:ARG:NH2	52:2:8:C:H5''	2.02	0.75
15:O:41:PRO:HB3	53:3:1151:A:C1'	2.16	0.75
43:s:6:LYS:HG3	51:1:494:G:H4'	1.68	0.75
51:1:855:G:H2'	51:1:856:G:H5''	1.67	0.75
55:8:15:DC:H1'	58:B1:426:ALA:HB1	1.67	0.75
14:N:30:ASN:HD21	14:N:66:VAL:H	1.35	0.75
51:1:1326:U:H2'	51:1:1327:A:H8	1.51	0.75
25:Y:55:PRO:HD3	53:3:193:C:H4'	1.69	0.75
55:8:3:DC:H2'	55:8:4:DT:H72	1.69	0.74
51:1:694:U:OP1	51:1:1569:A:H1'	1.86	0.74
51:1:572:A:H61	51:1:2029:G:H21	1.35	0.74
51:1:760:G:H5'	51:1:760:G:H8	1.50	0.74
9:I:38:GLY:HA3	53:3:542:G:H5'	1.69	0.74
51:1:940:G:H2'	51:1:941:A:H5''	1.68	0.74
31:f:174:LYS:HD2	51:1:2529:G:H5'	1.68	0.74
18:R:105:ALA:HA	53:3:948:C:OP1	1.88	0.74
53:3:1028:C:H3'	53:3:1029:U:H5''	1.68	0.74
66:0:448:TRP:HB2	66:0:457:ILE:HB	1.70	0.74
53:3:1421:G:H3'	53:3:1422:G:C4'	2.18	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:107:LEU:HD11	58:B1:242:LEU:HB2	1.70	0.73
58:B1:211:GLU:HG2	58:B1:215:LYS:HE3	1.70	0.73
51:1:1062:G:OP1	51:1:1063:G:OP2	2.06	0.73
58:B1:210:SER:HB3	58:B1:213:LYS:HB2	1.71	0.73
12:L:72:VAL:HG23	12:L:88:VAL:O	1.89	0.73
51:1:2163:A:H2'	51:1:2164:C:H5'	1.71	0.73
1:A:64:PHE:CD1	53:3:1011:C:H4'	2.17	0.73
58:B1:105:ILE:HD12	58:B1:242:LEU:HD22	1.71	0.73
58:B1:142:GLU:HG3	58:B1:142:GLU:O	1.89	0.73
58:B1:68:TYR:C	58:B1:75:TYR:CE2	2.65	0.73
64:6:44:A:H2'	64:6:45:G:C8	2.24	0.72
9:I:12:ARG:HG2	9:I:33:ILE:HA	1.71	0.72
51:1:2502:G:H5'	51:1:2503:A:H5''	1.70	0.72
53:3:352:C:H4'	53:3:354:G:OP1	1.89	0.72
55:8:3:DC:C2'	55:8:4:DT:H72	2.19	0.72
53:3:1088:G:N2	53:3:1167:A:H61	1.86	0.72
33:i:10:LEU:CD1	51:1:1061:U:H1'	2.20	0.72
58:B1:157:GLN:OE1	58:B1:157:GLN:HA	1.88	0.72
46:v:49:ASN:ND2	51:1:1040:A:H4'	2.05	0.72
51:1:1252:G:O2'	51:1:1253:A:H5''	1.90	0.72
58:B1:1143:ASP:OD1	58:B1:1148:ARG:NH1	2.21	0.72
47:w:38:GLY:HA2	51:1:2330:G:H21	1.53	0.72
8:H:71:ARG:HH12	54:4:17:U:H4'	1.54	0.72
31:f:70:LEU:HD11	51:1:2758:A:C2	2.25	0.72
33:i:79:LEU:HD21	33:i:132:ALA:HB2	1.71	0.71
51:1:663:G:C2'	51:1:664:G:H5''	2.20	0.71
33:i:130:GLY:HA3	51:1:1079:C:H1'	1.71	0.71
27:b:201:LEU:HD22	53:3:773:G:H5''	1.72	0.71
37:m:12:MET:HA	51:1:910:A:H62	1.55	0.71
51:1:414:C:H2'	51:1:415:A:H8	1.54	0.71
51:1:2743:U:H2'	51:1:2744:G:H5''	1.72	0.71
62:NG:125:LYS:O	62:NG:179:GLU:HA	1.89	0.71
14:N:70:GLY:HA3	53:3:1371:G:O3'	1.90	0.71
19:S:52:ARG:HH11	53:3:1317:C:H42	1.38	0.71
39:o:55:GLU:HG2	52:2:116:G:H5'	1.72	0.71
58:B1:93:THR:HB	58:B1:97:VAL:HG21	1.73	0.71
51:1:703:U:H2'	51:1:704:G:H5'	1.72	0.71
51:1:718:A:H2'	51:1:719:C:O4'	1.91	0.71
53:3:560:A:H5'	53:3:566:G:N2	2.05	0.71
35:k:87:LEU:HD12	35:k:92:GLU:HB3	1.72	0.71
36:l:19:LEU:HD23	51:1:587:C:C2	2.25	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2792:A:H2'	51:1:2793:C:H5''	1.72	0.70
53:3:1316:G:H2'	53:3:1317:C:H5''	1.73	0.70
4:D:34:ARG:HD3	51:1:467:G:OP2	1.91	0.70
33:i:92:PRO:CB	51:1:1077:A:H1'	2.22	0.70
52:2:115:A:H2'	52:2:116:G:C8	2.26	0.70
10:J:61:LYS:NZ	53:3:1073:U:OP2	2.24	0.70
15:O:44:THR:HG23	53:3:1151:A:H5''	1.71	0.70
51:1:2691:C:H2'	51:1:2692:G:C8	2.26	0.70
58:B1:128:LEU:HD11	58:B1:189:LEU:HG	1.73	0.70
53:3:1218:C:H2'	53:3:1219:A:C8	2.27	0.70
58:B1:220:ARG:HG2	58:B1:220:ARG:HH11	1.55	0.70
38:n:20:MET:HE2	51:1:1277:G:H5'	1.74	0.70
51:1:807:U:H2'	51:1:808:G:H8	1.55	0.70
53:3:335:C:H2'	53:3:336:A:C8	2.26	0.70
53:3:1422:G:H2'	53:3:1423:G:H8	1.55	0.70
48:x:17:ARG:HG3	51:1:380:G:H5'	1.73	0.70
51:1:876:C:H3'	51:1:877:A:H4'	1.73	0.70
53:3:78:A:H2'	53:3:79:G:O4'	1.91	0.70
53:3:1421:G:C8	53:3:1422:G:H1'	2.26	0.69
51:1:2634:A:H2'	51:1:2635:A:O4'	1.91	0.69
67:h:6:5OH:N	67:h:6:5OH:HS	2.07	0.69
33:i:79:LEU:HD13	33:i:128:ILE:HG22	1.73	0.69
51:1:2123:G:N7	51:1:2170:A:H4'	2.07	0.69
33:i:92:PRO:CB	51:1:1077:A:C1'	2.70	0.69
51:1:760:G:H2'	51:1:761:A:H5'	1.73	0.69
51:1:2566:A:H4'	51:1:2567:G:H5''	1.74	0.69
53:3:483:C:H2'	53:3:484:G:C8	2.27	0.69
58:B1:352:ARG:HD2	59:B2:1268:GLN:HE22	1.55	0.69
53:3:358:U:H2'	53:3:359:G:C8	2.28	0.69
53:3:1293:C:H2'	53:3:1294:G:H8	1.58	0.69
40:p:1:SER:H1	51:1:2875:C:H4'	1.57	0.69
40:p:59:THR:HG22	40:p:72:VAL:HG12	1.75	0.69
59:B2:65:ASN:HB3	59:B2:105:TYR:HB2	1.73	0.69
53:3:837:U:H2'	53:3:838:G:H8	1.57	0.69
53:3:1513:A:H2'	53:3:1514:G:H8	1.58	0.69
58:B1:243:PRO:HG2	59:B2:1332:SER:O	1.93	0.69
58:B1:832:LYS:C	58:B1:1242:ARG:HH12	2.01	0.69
51:1:2296:U:H5''	51:1:2297:A:OP1	1.92	0.69
14:N:35:GLU:HA	14:N:39:GLY:HA3	1.75	0.68
51:1:1063:G:H5''	51:1:1064:C:C6	2.28	0.68
57:A2:294:ASN:HA	61:NA:464:ILE:H	1.57	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:39:LYS:O	58:B1:273:ILE:CG2	2.41	0.68
7:G:46:VAL:HG23	7:G:47:PRO:HD3	1.75	0.68
51:1:2691:C:H2'	51:1:2692:G:H8	1.58	0.68
52:2:3:C:C2'	52:2:4:C:H5''	2.23	0.68
28:c:13:ARG:HH11	51:1:2683:C:H4'	1.58	0.68
63:5:47:U:H4'	63:5:48:C:H5'	1.75	0.68
51:1:2638:G:H1'	51:1:2778:A:H61	1.58	0.68
9:I:111:ALA:HB1	53:3:407:U:H5''	1.75	0.68
53:3:207:C:H2'	53:3:208:U:H5''	1.74	0.68
39:o:12:THR:HB	51:1:2334:U:H5'	1.76	0.68
51:1:807:U:H2'	51:1:808:G:C8	2.28	0.68
67:h:4:SER:O	67:h:5:UAL:N1	2.26	0.68
32:g:8:LYS:HB2	32:g:15:LEU:HG	1.76	0.68
51:1:1869:G:H3'	51:1:1870:C:C5'	2.24	0.68
58:B1:141:PHE:CD2	58:B1:293:ARG:O	2.47	0.68
10:J:22:LYS:HG3	53:3:1081:A:H5'	1.75	0.68
58:B1:117:LEU:HD12	58:B1:117:LEU:O	1.94	0.68
66:0:515:TYR:HB3	66:0:584:HIS:CG	2.28	0.68
27:b:48:ILE:HG22	51:1:779:U:OP1	1.94	0.68
34:j:30:THR:HG21	51:1:1012:U:O4	1.94	0.67
51:1:1098:A:C2'	51:1:1099:G:H5'	2.22	0.67
35:k:48:PRO:HB3	53:3:1423:G:C5'	2.14	0.67
51:1:784:G:H5'	51:1:785:G:OP1	1.94	0.67
51:1:1550:C:H2'	51:1:1551:A:H8	1.60	0.67
53:3:603:U:H2'	53:3:604:G:H8	1.58	0.67
64:6:69:C:C2'	64:6:70:G:H5''	2.24	0.67
11:K:76:THR:HA	11:K:79:ARG:HG2	1.76	0.67
58:B1:1355:ARG:NH1	58:B1:1369:ARG:HH12	1.93	0.67
55:8:3:DC:C6	55:8:4:DT:H72	2.29	0.67
51:1:255:A:H2'	51:1:256:A:O4'	1.95	0.67
14:N:83:THR:HG21	14:N:102:PHE:HB3	1.77	0.67
51:1:1059:G:H3'	51:1:1060:U:H2'	1.77	0.67
53:3:76:G:H2'	53:3:77:A:H5'	1.76	0.67
58:B1:161:THR:HG22	58:B1:164:GLN:HB2	1.75	0.67
13:M:28:SER:HB2	13:M:56:PRO:HB2	1.78	0.66
51:1:729:G:H4'	51:1:763:G:H5'	1.78	0.66
55:8:23:DC:H2''	55:8:24:DC:C5	2.30	0.66
58:B1:1037:PHE:HB3	58:B1:1040:MET:HB2	1.78	0.66
66:0:66:ALA:HB3	66:0:88:ASP:HB3	1.76	0.66
51:1:635:C:H2'	51:1:636:G:C8	2.30	0.66
51:1:635:C:H2'	51:1:636:G:H8	1.58	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8:13:DT:OP2	58:B1:791:ALA:HB1	1.95	0.66
14:N:4:GLN:HE22	53:3:1131:G:H5'	1.61	0.66
58:B1:108:ALA:HB3	58:B1:279:LEU:HD22	1.77	0.66
53:3:948:C:H5'	53:3:1306:A:O2'	1.95	0.66
53:3:1333:A:H2'	53:3:1334:G:O4'	1.95	0.66
58:B1:193:ASP:HB3	58:B1:196:GLN:HB2	1.78	0.66
58:B1:108:ALA:CB	58:B1:279:LEU:HD22	2.25	0.66
51:1:1378:A:H1'	51:1:1379:U:C5	2.30	0.66
4:D:26:ASN:CG	51:1:682:G:H5'	2.20	0.65
51:1:1297:C:OP1	51:1:2710:C:H4'	1.97	0.65
51:1:2383:G:O2'	51:1:2384:U:H5'	1.97	0.65
51:1:855:G:C2'	51:1:856:G:H5''	2.26	0.65
53:3:29:U:O2'	53:3:30:U:H5'	1.96	0.65
53:3:813:U:C2'	53:3:814:A:H5''	2.26	0.65
58:B1:141:PHE:HD2	58:B1:293:ARG:O	1.80	0.65
51:1:1752:C:H2'	51:1:1753:G:C8	2.31	0.65
17:Q:76:HIS:HB2	66:0:425:LYS:HD2	1.77	0.65
52:2:3:C:H42	52:2:117:G:H1	1.44	0.65
53:3:884:U:H4'	53:3:885:G:H5''	1.77	0.65
66:0:558:GLN:HA	66:0:561:LEU:HD12	1.78	0.65
53:3:663:A:H5'	53:3:836:G:OP1	1.96	0.65
58:B1:984:LEU:HB3	58:B1:993:GLU:HB2	1.77	0.65
51:1:310:A:C2'	51:1:311:A:H5''	2.27	0.65
51:1:2177:C:O2'	65:a:170:ILE:HG21	1.97	0.65
58:B1:975:ILE:HG22	58:B1:977:SER:H	1.62	0.65
58:B1:162:GLU:HA	58:B1:162:GLU:OE1	1.97	0.65
9:I:101:VAL:HG13	9:I:106:PHE:HB2	1.79	0.65
51:1:414:C:H2'	51:1:415:A:C8	2.32	0.65
51:1:2715:C:H3'	51:1:2716:C:H5''	1.79	0.65
36:l:20:GLY:HA2	36:l:28:GLY:HA2	1.79	0.65
58:B1:68:TYR:HB3	58:B1:75:TYR:CE2	2.32	0.65
51:1:1139:G:O2'	51:1:1140:C:H5'	1.97	0.65
52:2:95:U:H2'	52:2:96:G:H8	1.63	0.65
58:B1:395:LYS:HZ2	58:B1:399:LYS:CD	2.10	0.64
51:1:1906:G:C3'	51:1:1907:G:H5''	2.27	0.64
53:3:1260:G:H4'	53:3:1284:C:H5'	1.80	0.64
55:8:3:DC:C2'	55:8:4:DT:C7	2.75	0.64
51:1:855:G:C3'	51:1:856:G:H5''	2.28	0.64
53:3:664:G:H22	53:3:741:G:H1	1.45	0.64
43:s:42:LYS:HB2	51:1:2010:G:H5''	1.80	0.64
51:1:2808:G:H2'	51:1:2890:G:C6	2.32	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:461:PHE:HD2	59:B2:813:GLU:HB2	1.61	0.64
51:1:1752:C:H2'	51:1:1753:G:H8	1.62	0.64
51:1:1827:U:H2'	51:1:1828:G:H5'	1.80	0.64
53:3:1012:A:H5'	53:3:1012:A:C8	2.31	0.64
53:3:1293:C:H2'	53:3:1294:G:C8	2.33	0.64
2:B:49:ARG:HG3	51:1:2884:U:C6	2.32	0.64
51:1:151:C:H2'	51:1:152:A:H8	1.62	0.64
51:1:310:A:H2'	51:1:311:A:H5''	1.79	0.64
23:W:42:ARG:NH2	53:3:721:G:C5'	2.51	0.64
51:1:1186:G:H2'	51:1:1187:G:O4'	1.97	0.64
51:1:2682:A:N6	51:1:2728:U:H1'	2.02	0.64
52:2:3:C:C3'	52:2:4:C:H5''	2.28	0.64
53:3:971:G:H1'	53:3:1365:G:O2'	1.98	0.64
53:3:1274:A:O2'	53:3:1275:A:H5''	1.98	0.64
7:G:155:GLY:CA	61:NA:219:GLU:CB	2.76	0.63
7:G:155:GLY:HA2	61:NA:219:GLU:CB	2.28	0.63
14:N:118:ARG:NH2	53:3:1233:G:H5'	2.13	0.63
30:e:84:ILE:HG21	51:1:2312:U:H4'	1.80	0.63
58:B1:918:ILE:HG22	59:B2:1280:ALA:HB1	1.79	0.63
58:B1:978:ARG:HG2	58:B1:1197:ASN:HD21	1.60	0.63
7:G:8:MET:HE3	7:G:46:VAL:HG11	1.79	0.63
53:3:662:U:H2'	53:3:663:A:C8	2.33	0.63
59:B2:314:ASN:HD21	59:B2:348:SER:HA	1.62	0.63
33:i:27:LEU:HD21	33:i:34:ILE:HB	1.79	0.63
53:3:1513:A:H2'	53:3:1514:G:C8	2.33	0.63
33:i:92:PRO:HB2	51:1:1077:A:C1'	2.27	0.63
51:1:876:C:H3'	51:1:877:A:O4'	1.99	0.63
51:1:1960:A:H2'	51:1:1961:C:H5''	1.81	0.63
14:N:118:ARG:HH22	53:3:1233:G:H5'	1.62	0.63
15:O:12:ALA:HB2	15:O:96:VAL:HG13	1.81	0.63
33:i:123:ALA:HA	33:i:126:ARG:HD2	1.80	0.63
35:k:5:GLN:HA	35:k:20:MET:HE3	1.80	0.63
58:B1:245:LEU:HG	58:B1:246:PRO:HD2	1.80	0.63
66:O:632:ILE:HG23	66:O:642:LEU:HB3	1.80	0.63
27:b:144:GLU:HB2	27:b:187:CYS:HB3	1.81	0.63
39:o:100:HIS:NE2	52:2:48:U:H4'	2.14	0.63
43:s:11:ARG:HG3	51:1:1322:A:OP1	1.99	0.63
53:3:1349:A:H2'	53:3:1350:A:O4'	1.98	0.63
58:B1:1355:ARG:NH1	58:B1:1369:ARG:NH1	2.47	0.63
28:c:35:THR:HG22	28:c:73:VAL:HG21	1.79	0.63
51:1:2831:G:OP1	51:1:2834:G:H4'	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:0:228:GLU:HB2	66:0:255:ARG:HH12	1.63	0.63
59:B2:1282:GLY:HA3	60:W0:17:PHE:HE1	1.63	0.63
14:N:105:ARG:HG3	53:3:1118:U:H5'	1.79	0.62
33:i:10:LEU:HG	51:1:1061:U:H1'	1.81	0.62
58:B1:111:THR:CG2	58:B1:300:GLN:CD	2.66	0.62
59:B2:120:GLN:NE2	59:B2:490:GLN:OE1	2.32	0.62
28:c:170:VAL:HG21	51:1:2679:A:H5'	1.81	0.62
35:k:76:VAL:H	40:p:72:VAL:HG22	1.63	0.62
53:3:583:A:H2'	53:3:584:G:O4'	1.99	0.62
53:3:1304:G:H2'	53:3:1305:G:H1'	1.80	0.62
53:3:1421:G:C3'	53:3:1422:G:H4'	2.27	0.62
35:k:66:LYS:NZ	35:k:80:ASP:O	2.32	0.62
40:p:2:ASN:HD21	51:1:2876:G:H4'	1.63	0.62
51:1:1078:U:H5''	51:1:1079:C:H5'	1.81	0.62
53:3:79:G:O2'	53:3:80:A:H5'	1.98	0.62
53:3:1073:U:H2'	53:3:1074:G:H8	1.64	0.62
58:B1:128:LEU:HA	58:B1:192:MET:HE1	1.81	0.62
19:S:48:GLN:HE22	24:X:11:ASP:HA	1.64	0.62
10:J:107:GLY:HA3	53:3:9:G:H5'	1.80	0.62
31:f:70:LEU:HD11	51:1:2758:A:H2	1.64	0.62
39:o:33:ARG:HB2	52:2:52:A:H62	1.62	0.62
46:v:21:ARG:HH22	52:2:77:U:P	2.23	0.62
53:3:1421:G:H3'	53:3:1422:G:C5'	2.30	0.62
58:B1:144:TYR:CE1	58:B1:162:GLU:OE2	2.51	0.62
27:b:200:MET:HG3	51:1:1820:U:O2	2.00	0.62
33:i:9:LYS:NZ	51:1:1061:U:OP1	2.30	0.62
51:1:1701:A:H2'	51:1:1702:G:H5'	1.81	0.62
51:1:1837:C:H2'	51:1:1899:A:H61	1.65	0.62
51:1:2126:A:H2'	51:1:2162:G:H21	1.65	0.62
18:R:28:ARG:HH22	18:R:61:LYS:HB2	1.64	0.62
53:3:545:C:O2'	53:3:549:C:H5''	2.00	0.62
53:3:999:C:H2'	53:3:1000:A:H8	1.64	0.62
58:B1:201:LEU:HB2	58:B1:221:ILE:HD13	1.80	0.62
27:b:137:GLY:HA3	53:3:712:A:H5'	1.82	0.62
51:1:1655:A:C2	51:1:2049:G:H4'	2.35	0.62
51:1:2248:C:H2'	51:1:2249:U:H5'	1.81	0.62
53:3:950:U:H2'	53:3:951:G:H8	1.65	0.62
40:p:52:ARG:HH22	51:1:2720:U:P	2.23	0.62
51:1:1533:C:H3'	51:1:1534:U:H5''	1.82	0.62
52:2:63:C:H2'	52:2:64:G:H8	1.64	0.62
55:8:3:DC:H2'	55:8:4:DT:C7	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:67:LEU:HD12	7:G:160:LEU:HD22	1.81	0.61
58:B1:111:THR:CG2	58:B1:300:GLN:NE2	2.63	0.61
4:D:21:ARG:NH1	51:1:466:A:H5'	2.14	0.61
8:H:18:ASN:ND2	19:S:89:ARG:O	2.33	0.61
53:3:422:C:H4'	53:3:423:G:C2	2.35	0.61
53:3:999:C:H2'	53:3:1000:A:C8	2.35	0.61
55:8:1:DC:H2''	55:8:2:DC:C5	2.35	0.61
51:1:2185:U:H2'	51:1:2186:G:H8	1.65	0.61
53:3:1241:G:H2'	53:3:1242:G:H8	1.65	0.61
53:3:1479:C:H2'	53:3:1480:A:H8	1.66	0.61
58:B1:395:LYS:HZ2	58:B1:399:LYS:HD3	1.65	0.61
9:I:151:GLN:NE2	53:3:437:U:H5''	2.14	0.61
33:i:89:SER:HB3	51:1:1063:G:C8	2.36	0.61
53:3:768:A:OP1	53:3:804:U:H4'	2.01	0.61
58:B1:1357:ILE:HD11	59:B2:1287:LEU:HD13	1.81	0.61
66:0:29:ARG:HD2	66:0:272:ASN:HD22	1.66	0.61
14:N:116:GLY:N	53:3:1367:C:OP1	2.32	0.61
21:U:11:ALA:HA	53:3:44:A:OP1	2.01	0.61
53:3:622:A:H2'	53:3:623:C:H5'	1.83	0.61
57:A1:211:ILE:HG12	57:A1:219:ARG:HH12	1.65	0.61
53:3:91:U:C3'	53:3:92:U:H5''	2.31	0.61
53:3:1497:G:H2'	53:3:1498:U:H5'	1.82	0.61
53:3:219:U:H2'	53:3:220:G:H8	1.65	0.61
55:8:13:DT:C7	58:B1:791:ALA:HB2	2.29	0.61
17:Q:30:ARG:HB3	53:3:363:A:OP2	2.00	0.61
53:3:530:G:H3'	53:3:531:U:C5'	2.31	0.61
29:d:53:THR:HG21	51:1:452:G:H8	1.66	0.61
41:q:23:TYR:CD1	51:1:533:G:H5'	2.35	0.61
51:1:1180:U:H3'	51:1:1181:U:H6	1.64	0.61
51:1:1827:U:C2'	51:1:1828:G:H5'	2.30	0.61
58:B1:68:TYR:HB3	58:B1:75:TYR:CZ	2.35	0.61
58:B1:154:LEU:HD21	58:B1:160:LEU:HD21	1.83	0.61
31:f:123:GLU:HG3	31:f:125:PRO:HD3	1.82	0.60
51:1:1807:G:H2'	51:1:1808:A:H5'	1.82	0.60
58:B1:395:LYS:NZ	58:B1:399:LYS:HD3	2.15	0.60
19:S:7:ALA:HB1	53:3:995:C:H5'	1.84	0.60
26:Z:49:ALA:HA	53:3:723:U:O4	2.01	0.60
51:1:1097:U:H2'	51:1:1098:A:O4'	2.00	0.60
51:1:2128:G:P	65:a:38:PHE:HB3	2.41	0.60
51:1:2245:U:H5''	51:1:2246:G:H5'	1.83	0.60
58:B1:770:LEU:HD13	59:B2:618:GLN:CG	2.30	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
65:a:50:ILE:HB	65:a:57:GLN:HB3	1.82	0.60
32:g:43:ASN:HA	32:g:46:PHE:HB2	1.83	0.60
51:1:2128:G:H21	51:1:2173:A:H1'	1.66	0.60
53:3:130:A:H1'	53:3:264:C:H5'	1.82	0.60
58:B1:342:LEU:HD23	58:B1:1352:ILE:HG23	1.83	0.60
59:B2:528:ARG:NH2	59:B2:576:SER:O	2.30	0.60
34:j:27:ARG:HD2	51:1:1143:A:H62	1.67	0.60
38:n:39:PRO:HG3	51:1:1651:G:H5'	1.82	0.60
46:v:9:ARG:HB3	46:v:41:GLU:HB2	1.82	0.60
51:1:1417:C:H4'	51:1:1587:G:H21	1.66	0.60
51:1:2061:G:H2'	51:1:2501:C:O2'	2.01	0.60
51:1:2661:G:H5''	66:0:19:ILE:HD11	1.83	0.60
58:B1:100:GLU:HA	59:B2:1328:LYS:HE2	1.82	0.60
9:I:120:LYS:HB3	9:I:130:ASN:HB3	1.84	0.60
11:K:3:HIS:HA	11:K:65:GLU:HA	1.82	0.60
52:2:11:C:H2'	52:2:12:C:O4'	2.02	0.60
53:3:397:A:H3'	53:3:397:A:N3	2.16	0.60
53:3:651:C:H2'	53:3:652:U:C6	2.35	0.60
18:R:27:THR:HG21	53:3:1328:C:H5''	1.83	0.60
51:1:2220:U:H2'	51:1:2221:G:H8	1.66	0.60
51:1:2267:A:H5''	51:1:2268:A:H5'	1.84	0.60
53:3:1060:U:H3	53:3:1197:A:H61	1.48	0.60
55:8:11:DC:H2'	55:8:12:DG:C8	2.37	0.60
42:r:35:PHE:HB2	42:r:59:ILE:HB	1.83	0.60
50:z:12:ALA:HB1	50:z:20:LYS:HG2	1.83	0.60
51:1:41:C:H2'	51:1:42:A:H5''	1.84	0.60
53:3:1016:A:H4'	53:3:1218:C:H4'	1.83	0.60
53:3:1304:G:H2'	53:3:1305:G:C1'	2.32	0.60
58:B1:926:PRO:HG2	58:B1:1248:ILE:HD11	1.84	0.60
66:0:470:VAL:HG13	66:0:481:ALA:HB3	1.82	0.60
9:I:37:PRO:HD2	9:I:41:GLY:HA3	1.83	0.60
51:1:2107:G:H2'	51:1:2108:A:C8	2.32	0.60
51:1:2343:U:H2'	51:1:2344:U:C6	2.37	0.60
57:A1:38:THR:HB	57:A2:45:ARG:HD3	1.82	0.60
6:F:4:ARG:HG2	51:1:2466:C:OP1	2.02	0.60
51:1:2371:G:O2'	51:1:2372:U:H5'	2.02	0.60
53:3:91:U:H3'	53:3:92:U:H5''	1.84	0.60
51:1:1906:G:H3'	51:1:1907:G:H5''	1.84	0.59
51:1:2183:A:H2'	51:1:2184:A:H5'	1.83	0.59
57:A1:112:ALA:HB3	57:A1:126:PRO:HA	1.83	0.59
58:B1:370:LYS:HG2	58:B1:441:LEU:HD23	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:633:ALA:HA	59:B2:806:PRO:O	2.01	0.59
24:X:51:HIS:HA	24:X:56:HIS:HA	1.83	0.59
28:c:135:GLY:HA2	51:1:743:A:OP1	2.02	0.59
52:2:95:U:H2'	52:2:96:G:C8	2.37	0.59
59:B2:1072:ASN:ND2	59:B2:1111:GLN:OE1	2.34	0.59
2:B:5:ASN:ND2	51:1:2020:A:H62	1.96	0.59
6:F:2:LYS:NZ	6:F:32:LYS:O	2.36	0.59
40:p:102:ARG:NH2	51:1:1754:A:O3'	2.35	0.59
51:1:1068:G:N3	51:1:1096:A:H5'	2.16	0.59
53:3:1241:G:H2'	53:3:1242:G:C8	2.36	0.59
53:3:1530:G:H2'	53:3:1531:A:C8	2.36	0.59
58:B1:99:ARG:NH1	58:B1:99:ARG:HG3	2.17	0.59
58:B1:223:LEU:HG	58:B1:223:LEU:O	2.00	0.59
58:B1:725:MET:SD	59:B2:1101:LEU:HD23	2.42	0.59
59:B2:55:SER:OG	59:B2:465:ARG:NH1	2.33	0.59
52:2:104:A:H2'	52:2:105:G:O4'	2.02	0.59
55:8:9:DG:H4'	58:B1:120:LEU:HG	1.84	0.59
58:B1:1161:GLY:HA3	58:B1:1179:PRO:HA	1.83	0.59
59:B2:918:LEU:O	59:B2:918:LEU:HD23	2.02	0.59
65:a:28:ALA:HA	65:a:31:LYS:HD3	1.85	0.59
6:F:11:CYS:SG	6:F:14:CYS:N	2.75	0.59
9:I:149:LYS:HG2	9:I:150:LYS:HG3	1.83	0.59
28:c:56:LYS:HE3	51:1:2830:C:H5''	1.85	0.59
43:s:59:GLU:HB3	43:s:66:ILE:HD11	1.82	0.59
51:1:629:G:H5''	51:1:650:C:O2'	2.03	0.59
51:1:1095:A:C2	66:0:632:ILE:HD13	2.37	0.59
63:5:26:A:H61	63:5:44:G:H22	1.50	0.59
8:H:106:ARG:HG3	8:H:107:LYS:HG3	1.84	0.59
51:1:869:G:H1	51:1:908:C:H42	1.50	0.59
53:3:123:U:H5''	53:3:311:C:O2'	2.03	0.59
53:3:328:C:H4'	53:3:329:A:H5'	1.84	0.59
53:3:1275:A:H2'	53:3:1276:G:O4'	2.03	0.59
59:B2:1142:ARG:NH1	59:B2:1161:LEU:O	2.36	0.59
27:b:228:ASP:CG	51:1:780:G:H1	2.10	0.59
51:1:937:C:H2'	51:1:938:G:C8	2.38	0.59
51:1:1064:C:C3'	51:1:1065:U:H5''	2.24	0.59
53:3:381:C:H2'	53:3:382:A:O4'	2.02	0.59
20:T:22:GLY:O	20:T:27:GLN:NE2	2.36	0.59
33:i:75:ALA:HB3	51:1:1060:U:OP1	2.02	0.59
51:1:1095:A:N3	66:0:632:ILE:HG21	2.18	0.59
51:1:2663:G:OP1	66:0:59:ARG:HD3	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2715:C:C3'	51:1:2716:C:H5''	2.33	0.59
53:3:210:C:H5'	53:3:211:G:C2	2.37	0.59
53:3:358:U:H2'	53:3:359:G:H8	1.66	0.59
58:B1:161:THR:HG23	58:B1:164:GLN:H	1.68	0.59
32:g:55:GLU:HA	32:g:58:LEU:HB2	1.85	0.59
51:1:876:C:C3'	51:1:877:A:H4'	2.33	0.59
53:3:1352:C:H2'	53:3:1353:G:C8	2.37	0.59
58:B1:951:GLN:NE2	58:B1:1014:GLY:O	2.35	0.59
59:B2:69:GLN:HE21	59:B2:101:ARG:HD2	1.67	0.59
66:0:415:VAL:HB	66:0:416:ILE:HD12	1.84	0.59
9:I:1:ALA:HB2	53:3:499:A:N6	2.18	0.59
14:N:8:THR:OG1	14:N:9:GLY:N	2.36	0.59
51:1:1509:A:H2'	51:1:1510:G:C8	2.38	0.59
53:3:1326:U:H2'	53:3:1327:C:C6	2.37	0.59
58:B1:275:ARG:NH1	58:B1:278:ARG:NH1	2.51	0.59
58:B1:412:LEU:HD22	58:B1:441:LEU:HD21	1.84	0.59
59:B2:707:ALA:O	59:B2:711:ASP:HB2	2.03	0.59
20:T:23:SER:HA	53:3:751:U:H4'	1.85	0.58
26:Z:39:LYS:NZ	53:3:1530:G:O6	2.36	0.58
51:1:96:C:H2'	51:1:97:C:H6	1.68	0.58
51:1:1434:A:H2'	51:1:1435:G:C8	2.38	0.58
52:2:30:C:C2'	52:2:31:C:H5'	2.33	0.58
53:3:410:G:H2'	53:3:429:U:C4	2.38	0.58
53:3:936:C:H2'	53:3:937:A:O4'	2.02	0.58
55:8:7:DC:H2''	55:8:8:DT:H71	1.84	0.58
58:B1:97:VAL:HG11	58:B1:101:ARG:NH2	2.18	0.58
15:O:8:ILE:HB	15:O:74:VAL:HB	1.85	0.58
51:1:2138:G:H2'	51:1:2139:U:H5'	1.84	0.58
17:Q:111:GLN:HB2	53:3:538:G:OP2	2.03	0.58
20:T:68:TYR:HB2	53:3:754:C:H4'	1.84	0.58
40:p:91:VAL:HG11	40:p:96:LEU:HD21	1.85	0.58
51:1:1697:G:C3'	51:1:1698:A:H5''	2.31	0.58
51:1:1810:A:H2'	51:1:1811:G:O4'	2.04	0.58
53:3:132:C:H5'	53:3:262:A:O2'	2.03	0.58
53:3:1218:C:H2'	53:3:1219:A:H8	1.67	0.58
57:A1:304:LYS:CB	61:NA:71:PRO:CB	2.81	0.58
58:B1:514:THR:HG21	58:B1:596:LEU:HD12	1.84	0.58
58:B1:750:PRO:CB	59:B2:549:ASP:OD2	2.45	0.58
23:W:28:LEU:HD21	23:W:58:ILE:HG12	1.85	0.58
30:e:38:GLY:HA3	51:1:2312:U:O2	2.03	0.58
42:r:61:ALA:HB2	42:r:98:ILE:HD13	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1443:U:H2'	51:1:1444:G:C8	2.38	0.58
52:2:3:C:H3'	52:2:4:C:H5''	1.85	0.58
58:B1:615:LYS:HG2	60:W0:5:THR:HG21	1.85	0.58
58:B1:638:SER:OG	58:B1:639:VAL:N	2.36	0.58
33:i:126:ARG:HA	33:i:129:GLU:HG3	1.86	0.58
53:3:76:G:C2'	53:3:77:A:H5'	2.34	0.58
53:3:813:U:H2'	53:3:814:A:C5'	2.32	0.58
53:3:1395:C:C6	53:3:1395:C:H5'	2.38	0.58
33:i:10:LEU:CG	51:1:1061:U:H1'	2.34	0.58
33:i:92:PRO:CB	51:1:1077:A:O4'	2.47	0.58
36:l:126:ARG:NH1	51:1:635:C:OP2	2.37	0.58
37:m:125:PRO:HB3	51:1:2485:G:O3'	2.04	0.58
48:x:25:LYS:HE2	51:1:189:G:OP2	2.03	0.58
51:1:940:G:C2'	51:1:941:A:H5''	2.34	0.58
51:1:2650:U:H2'	51:1:2651:C:C6	2.38	0.58
53:3:670:G:H2'	53:3:671:G:H5''	1.86	0.58
22:V:63:CYS:HG	22:V:73:THR:HG1	1.52	0.58
33:i:120:ASP:HB3	33:i:123:ALA:HB3	1.83	0.58
47:w:20:LYS:HG3	51:1:2355:G:H4'	1.85	0.58
51:1:472:A:H2'	51:1:473:G:H5'	1.85	0.58
51:1:572:A:H61	51:1:2029:G:N2	2.00	0.58
51:1:748:G:O2'	51:1:749:A:H3'	2.03	0.58
66:0:515:TYR:HB3	66:0:584:HIS:HB2	1.86	0.58
16:P:23:HIS:HB3	16:P:30:ILE:HG23	1.85	0.58
17:Q:28:GLN:HE22	53:3:33:A:H2	1.51	0.58
51:1:703:U:C2'	51:1:704:G:H5'	2.33	0.58
51:1:1846:G:H2'	51:1:1847:A:O4'	2.04	0.58
4:D:9:VAL:HG12	51:1:1309:G:OP1	2.03	0.58
27:b:79:ARG:NH1	27:b:81:GLU:OE2	2.36	0.58
29:d:163:ASN:HD21	51:1:322:A:H2'	1.68	0.58
51:1:917:A:H5''	51:1:2268:A:H61	1.69	0.58
53:3:427:U:H2'	53:3:428:G:C8	2.39	0.58
57:A2:82:LEU:HD11	57:A2:171:LEU:HD23	1.86	0.58
3:C:44:GLN:OE1	51:1:2371:G:H4'	2.04	0.58
25:Y:55:PRO:HB3	53:3:193:C:O3'	2.04	0.58
39:o:10:ARG:HD2	51:1:2294:G:P	2.44	0.58
51:1:553:G:H2'	51:1:554:U:O4'	2.04	0.58
53:3:219:U:H2'	53:3:220:G:C8	2.38	0.58
58:B1:201:LEU:HD11	58:B1:220:ARG:HH11	1.67	0.58
58:B1:438:GLU:HG3	58:B1:485:MET:HE1	1.85	0.58
1:A:64:PHE:HA	53:3:1011:C:C5'	2.33	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:97:ARG:HH12	53:3:1308:U:H5	1.52	0.57
51:1:1783:A:H5'	51:1:2608:G:H4'	1.86	0.57
51:1:2469:A:H8	51:1:2469:A:H5'	1.69	0.57
53:3:837:U:H2'	53:3:838:G:C8	2.38	0.57
53:3:1395:C:H5'	53:3:1395:C:H6	1.69	0.57
58:B1:42:GLU:HB3	58:B1:52:GLU:HG3	1.86	0.57
53:3:1060:U:H2'	53:3:1061:G:H8	1.68	0.57
51:1:760:G:H2'	51:1:761:A:C5'	2.35	0.57
51:1:832:U:H2'	51:1:833:A:C8	2.39	0.57
51:1:1111:A:C2	51:1:1112:G:H1'	2.39	0.57
51:1:1386:C:H2'	51:1:1387:A:H8	1.69	0.57
51:1:1801:A:H5''	51:1:2203:U:H2'	1.87	0.57
51:1:2248:C:C2'	51:1:2249:U:H5'	2.35	0.57
52:2:118:C:H2'	52:2:119:A:H4'	1.86	0.57
53:3:70:U:H5''	53:3:71:A:OP1	2.03	0.57
58:B1:510:LEU:HD22	58:B1:601:ILE:HD12	1.86	0.57
8:H:162:ALA:HB2	53:3:1056:U:H5'	1.85	0.57
30:e:41:GLU:HG3	30:e:44:ALA:HB3	1.87	0.57
36:l:30:THR:HG22	51:1:810:U:O4	2.04	0.57
42:r:6:GLN:HG2	42:r:11:GLN:HG2	1.84	0.57
51:1:2151:U:H2'	51:1:2152:G:C8	2.39	0.57
51:1:2584:U:H2'	51:1:2585:U:H2'	1.86	0.57
51:1:2682:A:H61	51:1:2728:U:C1'	2.06	0.57
53:3:1404:C:H2'	53:3:1405:G:C8	2.40	0.57
58:B1:198:CYS:HA	58:B1:221:ILE:HD11	1.86	0.57
8:H:174:LEU:HB2	53:3:1108:G:OP1	2.04	0.57
30:e:3:LEU:HA	30:e:6:TYR:HB3	1.86	0.57
53:3:1014:A:C2	53:3:1219:A:H1'	2.40	0.57
7:G:107:ARG:HH22	61:NA:218:GLU:HA	1.69	0.57
38:n:64:ARG:HH22	51:1:2852:G:H5'	1.68	0.57
58:B1:102:MET:HG2	58:B1:246:PRO:HG3	1.87	0.57
9:I:131:ILE:HD13	53:3:620:C:N3	2.19	0.57
51:1:729:G:H4'	51:1:763:G:C5'	2.34	0.57
51:1:1058:U:H5	51:1:1080:A:H61	1.50	0.57
51:1:2124:G:H2'	51:1:2125:G:O4'	2.05	0.57
58:B1:1046:ILE:HD12	58:B1:1059:LEU:HB3	1.86	0.57
59:B2:1122:LYS:NZ	59:B2:1126:ASP:OD1	2.38	0.57
66:O:492:GLU:HB2	66:O:571:VAL:HG22	1.85	0.57
22:V:67:SER:OG	22:V:68:LYS:N	2.37	0.57
43:s:18:ARG:NH1	43:s:76:VAL:O	2.37	0.57
51:1:32:C:H2'	51:1:33:C:C6	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1458:U:H4'	51:1:1459:G:C4	2.40	0.57
51:1:2156:G:C2'	51:1:2157:G:H5'	2.34	0.57
51:1:2398:U:H2'	51:1:2399:G:C8	2.39	0.57
51:1:2514:U:H2'	51:1:2515:C:C6	2.39	0.57
51:1:2743:U:H2'	51:1:2744:G:C5'	2.35	0.57
58:B1:1361:THR:HB	59:B2:1284:ALA:HB3	1.85	0.57
14:N:86:LEU:HB3	14:N:93:LEU:HD13	1.86	0.57
28:c:156:PHE:HB3	34:j:81:ILE:HG22	1.85	0.57
47:w:38:GLY:HA2	51:1:2330:G:N2	2.19	0.57
51:1:1109:C:H2'	51:1:1110:G:O4'	2.05	0.57
51:1:2117:A:H61	51:1:2170:A:H61	1.53	0.57
51:1:2732:G:O2'	51:1:2733:A:H5'	2.05	0.57
6:F:23:ILE:HD13	51:1:1032:A:H1'	1.87	0.57
14:N:90:ASP:O	14:N:92:SER:N	2.38	0.57
16:P:51:PHE:HB3	16:P:55:ARG:HG3	1.85	0.57
33:i:4:VAL:HA	33:i:7:TYR:HB3	1.87	0.57
34:j:27:ARG:NE	51:1:1143:A:N7	2.46	0.57
53:3:57:G:H5'	66:0:373:GLU:OE2	2.05	0.57
58:B1:130:MET:HE2	58:B1:135:ILE:HG12	1.87	0.57
59:B2:839:VAL:HG12	59:B2:1049:ILE:HG12	1.87	0.57
9:I:7:LYS:HE2	53:3:408:A:OP2	2.04	0.56
21:U:40:ASN:HB3	21:U:43:ALA:HB2	1.87	0.56
25:Y:79:THR:HG21	53:3:187:G:H5'	1.86	0.56
28:c:146:ILE:HG12	51:1:2051:A:H4'	1.87	0.56
51:1:2757:A:H2'	51:1:2758:A:H5''	1.87	0.56
53:3:280:C:H5''	53:3:281:G:OP2	2.04	0.56
59:B2:818:VAL:HG22	59:B2:1096:ILE:HG12	1.87	0.56
19:S:52:ARG:HG3	53:3:1317:C:N3	2.20	0.56
36:l:2:ARG:NH1	36:l:5:THR:OG1	2.39	0.56
51:1:668:A:H2'	51:1:670:A:H62	1.70	0.56
51:1:1506:U:H2'	51:1:1507:C:C6	2.40	0.56
51:1:1775:U:H2'	51:1:1776:G:O4'	2.05	0.56
51:1:1893:C:H2'	51:1:1894:C:H5'	1.87	0.56
58:B1:247:PRO:HA	58:B1:250:ARG:HG3	1.87	0.56
12:L:115:MET:HA	12:L:118:ARG:HE	1.70	0.56
29:d:27:LEU:HD13	51:1:600:G:H5'	1.88	0.56
35:k:63:VAL:HG12	35:k:107:LEU:HD21	1.87	0.56
51:1:11:C:H2'	51:1:12:U:H5''	1.87	0.56
51:1:1287:A:C2	51:1:1649:G:H4'	2.40	0.56
51:1:1550:C:H2'	51:1:1551:A:C8	2.40	0.56
51:1:1557:C:C3'	51:1:1558:C:H5''	2.28	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1638:C:H4'	51:1:2710:C:O2	2.06	0.56
53:3:1201:A:H4'	53:3:1202:U:H5''	1.86	0.56
53:3:1305:G:H22	53:3:1331:G:H2'	1.69	0.56
58:B1:99:ARG:CG	58:B1:99:ARG:HH11	2.18	0.56
58:B1:241:VAL:O	58:B1:241:VAL:HG12	2.04	0.56
58:B1:741:ALA:O	58:B1:762:ASN:ND2	2.38	0.56
59:B2:13:LYS:HB2	59:B2:1180:MET:HE2	1.86	0.56
59:B2:892:GLU:HA	59:B2:913:VAL:HG22	1.87	0.56
14:N:27:ILE:HG23	14:N:62:LEU:HB2	1.87	0.56
40:p:47:ILE:HD11	40:p:61:ARG:HB3	1.88	0.56
51:1:1133:A:H4'	51:1:1134:A:H5''	1.87	0.56
51:1:2127:G:O3'	65:a:38:PHE:HB3	2.05	0.56
53:3:427:U:H5''	53:3:542:G:OP1	2.06	0.56
53:3:458:U:H2'	53:3:459:A:C8	2.40	0.56
58:B1:1166:GLY:HA3	58:B1:1174:ARG:HB2	1.88	0.56
25:Y:73:ARG:CZ	53:3:261:U:H5	2.18	0.56
51:1:151:C:H2'	51:1:152:A:C8	2.40	0.56
51:1:2167:U:H3	51:1:2170:A:N6	2.03	0.56
58:B1:160:LEU:HD22	58:B1:164:GLN:HB3	1.86	0.56
10:J:80:LEU:HB2	10:J:97:PRO:HB3	1.87	0.56
51:1:1318:U:H2'	51:1:1319:C:C6	2.40	0.56
51:1:2556:C:H2'	51:1:2557:G:O4'	2.05	0.56
58:B1:39:LYS:O	58:B1:273:ILE:HG21	2.06	0.56
58:B1:1167:LYS:HZ2	58:B1:1170:LYS:HB2	1.70	0.56
66:0:107:ASP:OD2	66:0:337:ARG:NH2	2.38	0.56
51:1:814:C:C1'	51:1:1225:G:H21	2.06	0.56
51:1:972:A:OP2	51:1:974:G:H5'	2.06	0.56
51:1:2403:C:O2'	51:1:2404:U:H5'	2.05	0.56
53:3:603:U:H2'	53:3:604:G:C8	2.40	0.56
22:V:15:LYS:HB2	53:3:275:G:H5'	1.87	0.56
33:i:10:LEU:HD12	51:1:1061:U:H1'	1.86	0.56
33:i:78:LEU:HG	33:i:108:ILE:HD12	1.87	0.56
51:1:760:G:H5'	51:1:760:G:C8	2.37	0.56
51:1:2183:A:C2'	51:1:2184:A:H5'	2.36	0.56
51:1:2660:A:H2'	51:1:2661:G:O4'	2.05	0.56
52:2:97:C:C2'	52:2:98:G:H5'	2.35	0.56
53:3:235:C:H2'	53:3:236:A:H8	1.69	0.56
58:B1:804:ALA:HA	58:B1:1259:GLN:HG3	1.88	0.56
11:K:38:ARG:HH21	11:K:61:LEU:HD23	1.70	0.56
51:1:967:U:H2'	51:1:968:C:C6	2.41	0.56
51:1:2792:A:C2'	51:1:2793:C:H5''	2.36	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:1073:U:H2'	53:3:1074:G:C8	2.40	0.56
16:P:63:GLN:HG2	16:P:98:ALA:HB2	1.86	0.56
47:w:12:SER:HB3	51:1:2261:C:C5	2.41	0.56
58:B1:1175:LEU:HD22	58:B1:1190:ILE:HD11	1.88	0.56
50:z:37:ARG:NH2	51:1:929:U:H4'	2.21	0.55
51:1:296:U:H2'	51:1:297:G:C8	2.40	0.55
51:1:322:A:H5'	51:1:340:A:H1'	1.88	0.55
51:1:1062:G:O2'	51:1:1063:G:H4'	2.05	0.55
51:1:2113:U:H2'	51:1:2114:A:C8	2.41	0.55
53:3:1268:G:N2	53:3:1327:C:H1'	2.21	0.55
8:H:123:LEU:HD21	8:H:129:PHE:HB3	1.88	0.55
27:b:47:ARG:HD3	51:1:778:G:H5''	1.87	0.55
27:b:70:LYS:NZ	27:b:97:ASP:OD2	2.39	0.55
2:B:9:ARG:HG3	51:1:17:G:OP1	2.06	0.55
3:C:7:LYS:HA	3:C:23:THR:HA	1.88	0.55
7:G:45:THR:HG22	7:G:200:PRO:HB2	1.88	0.55
40:p:91:VAL:HG21	40:p:96:LEU:HD11	1.87	0.55
51:1:1386:C:H2'	51:1:1387:A:C8	2.42	0.55
52:2:97:C:H2'	52:2:98:G:H5'	1.87	0.55
53:3:211:G:H2'	53:3:212:G:H5'	1.88	0.55
53:3:570:G:H5'	53:3:820:U:O4'	2.07	0.55
59:B2:1142:ARG:NH2	59:B2:1166:ASP:OD1	2.38	0.55
12:L:36:SER:HB2	14:N:42:THR:HG22	1.87	0.55
22:V:67:SER:HB3	22:V:70:LYS:HB2	1.87	0.55
48:x:30:PRO:HG2	48:x:32:LEU:HD22	1.87	0.55
51:1:1258:U:H2'	51:1:1259:G:C8	2.42	0.55
51:1:1558:C:H4'	51:1:1559:U:H5'	1.88	0.55
51:1:1909:C:H2'	51:1:1910:G:C8	2.42	0.55
51:1:2169:A:H2'	51:1:2170:A:O4'	2.06	0.55
53:3:950:U:H2'	53:3:951:G:C8	2.41	0.55
53:3:994:A:H3'	53:3:994:A:OP2	2.06	0.55
8:H:161:ILE:HG22	53:3:1196:A:N1	2.22	0.55
13:M:52:GLY:HA3	13:M:56:PRO:HA	1.88	0.55
16:P:126:ARG:NH2	53:3:796:C:O3'	2.39	0.55
24:X:38:THR:HA	24:X:69:LYS:HA	1.89	0.55
26:Z:66:ARG:HH21	53:3:1099:G:H4'	1.71	0.55
51:1:1063:G:H5''	51:1:1064:C:H6	1.69	0.55
52:2:49:C:H2'	52:2:50:A:H8	1.70	0.55
53:3:82:G:H2'	53:3:83:C:H5'	1.88	0.55
14:N:4:GLN:NE2	53:3:1131:G:H5'	2.22	0.55
35:k:38:ILE:HG22	35:k:61:VAL:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1790:C:H2'	51:1:1791:A:C5	2.42	0.55
53:3:169:C:H2'	53:3:170:U:C6	2.42	0.55
15:O:59:LYS:HD2	53:3:972:C:O3'	2.07	0.55
34:j:27:ARG:NH2	51:1:1142:A:H4'	2.11	0.55
51:1:572:A:N6	51:1:2029:G:H21	2.05	0.55
51:1:1159:U:H2'	51:1:1160:G:H8	1.71	0.55
51:1:1877:A:H2'	51:1:1878:G:O4'	2.07	0.55
58:B1:508:LEU:HD22	59:B2:1101:LEU:HD21	1.88	0.55
58:B1:799:ARG:HG2	58:B1:1325:PHE:HZ	1.72	0.55
18:R:89:ARG:HB2	18:R:96:VAL:HG12	1.88	0.55
25:Y:4:LYS:HE2	53:3:332:G:OP1	2.06	0.55
34:j:65:THR:OG1	51:1:1141:U:OP2	2.22	0.55
40:p:94:ALA:HB2	51:1:2848:G:C8	2.42	0.55
51:1:2800:A:H3'	51:1:2801:G:H5'	1.88	0.55
58:B1:833:GLU:HB2	58:B1:1242:ARG:NH1	2.22	0.55
58:B1:1155:ILE:HG13	58:B1:1210:ILE:HB	1.89	0.55
13:M:19:ALA:HB2	53:3:827:U:O2'	2.07	0.55
19:S:58:ARG:NH1	53:3:979:C:O2	2.39	0.55
25:Y:81:GLN:HA	25:Y:84:LYS:HE3	1.88	0.55
33:i:105:LEU:HA	33:i:108:ILE:HG12	1.89	0.55
36:l:25:SER:HA	51:1:813:U:O4	2.07	0.55
51:1:96:C:H2'	51:1:97:C:C6	2.41	0.55
51:1:1045:C:H5'	51:1:1046:A:N7	2.21	0.55
1:A:64:PHE:HB2	53:3:1012:A:OP1	2.07	0.55
35:k:48:PRO:CB	53:3:1423:G:H5''	2.16	0.55
51:1:760:G:C2'	51:1:761:A:H5'	2.36	0.55
51:1:1437:C:H2'	51:1:1438:U:C6	2.41	0.55
51:1:1794:A:H2'	51:1:1795:C:C6	2.41	0.55
51:1:2636:C:H2'	51:1:2637:U:C6	2.42	0.55
53:3:918:A:H2'	53:3:919:A:O4'	2.06	0.55
58:B1:58:CYS:SG	58:B1:59:ALA:N	2.80	0.55
58:B1:145:VAL:HG23	58:B1:159:ILE:HG22	1.89	0.55
59:B2:633:LEU:HD13	59:B2:644:LEU:HD23	1.89	0.55
30:e:25:MET:HG2	52:2:57:A:C6	2.42	0.54
51:1:644:A:H2'	51:1:645:C:H5''	1.89	0.54
51:1:2151:U:H2'	51:1:2152:G:H8	1.73	0.54
51:1:2389:G:H5''	51:1:2390:U:O4'	2.07	0.54
51:1:2398:U:H2'	51:1:2399:G:H8	1.71	0.54
52:2:63:C:H2'	52:2:64:G:C8	2.41	0.54
57:A2:100:LEU:HD23	57:A2:115:ILE:HG21	1.89	0.54
59:B2:360:LEU:HD13	59:B2:378:ARG:HH11	1.72	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:U:18:GLN:HA	21:U:38:PHE:HA	1.90	0.54
51:1:296:U:H2'	51:1:297:G:H8	1.71	0.54
51:1:1909:C:H2'	51:1:1910:G:H8	1.72	0.54
58:B1:37:GLU:O	58:B1:61:ILE:CD1	2.52	0.54
58:B1:144:TYR:HE1	58:B1:162:GLU:CD	2.14	0.54
59:B2:917:SER:O	59:B2:919:ARG:HG3	2.07	0.54
8:H:171:ARG:HG2	53:3:1106:G:H5''	1.90	0.54
24:X:49:ALA:HA	24:X:58:PRO:HA	1.90	0.54
42:r:14:VAL:HG21	42:r:98:ILE:HG13	1.88	0.54
51:1:2026:U:H2'	51:1:2027:G:O4'	2.06	0.54
51:1:2428:G:H5''	51:1:2429:G:O5'	2.08	0.54
51:1:2602:A:H4'	51:1:2603:G:H5'	1.90	0.54
53:3:5:U:H4'	53:3:6:G:N7	2.23	0.54
53:3:1280:A:O2'	53:3:1281:C:H5'	2.07	0.54
62:NG:126:THR:CB	62:NG:175:PHE:C	2.80	0.54
8:H:45:GLU:HB3	8:H:46:LEU:HD12	1.89	0.54
22:V:45:VAL:HG22	22:V:72:TRP:HB2	1.90	0.54
24:X:77:ARG:HH22	53:3:1322:C:P	2.30	0.54
27:b:137:GLY:O	27:b:162:GLN:NE2	2.39	0.54
32:g:1:MET:N	32:g:21:VAL:O	2.41	0.54
34:j:125:TYR:HH	34:j:132:HIS:HE2	1.55	0.54
44:t:15:HIS:HE1	51:1:1339:G:OP2	1.91	0.54
46:v:47:VAL:HA	46:v:50:MET:HG2	1.89	0.54
65:a:33:LEU:HD22	65:a:216:THR:HB	1.89	0.54
7:G:175:ALA:HB1	7:G:180:ILE:HB	1.90	0.54
10:J:141:ASP:O	10:J:145:ASN:ND2	2.40	0.54
14:N:17:ARG:HH12	53:3:1129:C:C5'	2.21	0.54
15:O:10:LEU:HB2	15:O:72:ARG:HB2	1.88	0.54
30:e:162:ASP:OD1	30:e:162:ASP:N	2.41	0.54
51:1:554:U:H2'	51:1:555:G:O4'	2.08	0.54
53:3:256:U:H2'	53:3:257:G:C8	2.43	0.54
57:A1:47:LEU:HD23	57:A1:51:MET:HG3	1.89	0.54
59:B2:29:SER:O	59:B2:33:ASP:HB2	2.08	0.54
59:B2:243:PRO:HB2	59:B2:274:ILE:HG23	1.90	0.54
4:D:4:THR:O	51:1:687:C:H5''	2.07	0.54
11:K:10:VAL:HG12	11:K:84:VAL:HG12	1.88	0.54
35:k:3:GLN:HE21	51:1:1666:G:H1'	1.73	0.54
45:u:11:ILE:HG13	45:u:21:ARG:HB3	1.90	0.54
48:x:16:ASN:ND2	51:1:2081:U:H5''	2.23	0.54
51:1:1095:A:H1'	66:0:632:ILE:HG22	1.89	0.54
51:1:2215:C:H2'	51:1:2216:G:C8	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:235:GLU:HG2	51:1:2599:G:C8	2.42	0.54
51:1:320:A:H4'	51:1:322:A:N7	2.23	0.54
51:1:740:C:H5'	51:1:740:C:C6	2.34	0.54
51:1:2122:U:H2'	51:1:2123:G:C4'	2.38	0.54
53:3:575:G:O2'	53:3:821:G:H5'	2.08	0.54
58:B1:746:LEU:HG	58:B1:758:PRO:HG3	1.90	0.54
58:B1:759:ILE:HG23	58:B1:771:GLN:HB3	1.89	0.54
59:B2:103:VAL:HB	59:B2:114:VAL:HG11	1.89	0.54
59:B2:811:ASN:HA	59:B2:815:SER:HB2	1.90	0.54
64:6:48:C:H5'	64:6:50:U:OP1	2.08	0.54
66:0:164:ALA:HB1	66:0:262:ILE:HD11	1.89	0.54
66:0:617:MET:HE2	66:0:682:MET:HE3	1.89	0.54
33:i:80:LYS:HD3	33:i:86:LYS:HD2	1.88	0.54
33:i:131:THR:HG22	33:i:135:MET:HE2	1.88	0.54
43:s:60:HIS:ND1	43:s:61:ASN:OD1	2.41	0.54
51:1:226:A:H5''	51:1:257:C:O2'	2.08	0.54
51:1:455:C:H3'	51:1:456:C:C5'	2.38	0.54
51:1:886:A:N3	51:1:886:A:H2'	2.23	0.54
51:1:1564:C:H2'	51:1:1565:C:O4'	2.08	0.54
53:3:1342:C:H2'	53:3:1343:G:H8	1.73	0.54
53:3:1379:G:O2'	53:3:1380:U:H5'	2.07	0.54
59:B2:684:ASN:OD1	59:B2:687:ARG:NH2	2.41	0.54
64:6:19:G:H1'	64:6:57:A:C2	2.42	0.54
13:M:95:MET:HE2	13:M:129:ALA:HB1	1.90	0.54
18:R:88:LEU:HD13	18:R:91:ARG:HD2	1.90	0.54
29:d:53:THR:HG21	51:1:452:G:C8	2.43	0.54
33:i:97:VAL:HG23	33:i:137:LEU:HD23	1.89	0.54
40:p:96:LEU:HB3	40:p:99:LEU:HD13	1.90	0.54
51:1:918:A:H5''	52:2:97:C:O2'	2.07	0.54
52:2:29:A:H2'	52:2:30:C:C6	2.43	0.54
52:2:115:A:H2'	52:2:116:G:H8	1.72	0.54
53:3:1002:G:H2'	53:3:1003:G:O4'	2.07	0.54
58:B1:39:LYS:O	58:B1:273:ILE:HG23	2.08	0.54
66:0:105:VAL:O	66:0:337:ARG:NH1	2.41	0.54
15:O:53:ILE:HG12	53:3:1060:U:H5''	1.90	0.54
30:e:37:MET:HB2	30:e:56:LEU:HD11	1.90	0.54
35:k:25:LEU:HD22	51:1:2562:U:H4'	1.89	0.54
51:1:1753:G:N2	51:1:1755:A:H3'	2.23	0.54
53:3:231:U:H2'	53:3:232:G:H8	1.73	0.54
53:3:1273:C:H2'	53:3:1274:A:O4'	2.07	0.54
58:B1:30:ILE:HG21	58:B1:241:VAL:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:814:CYS:SG	58:B1:883:ARG:NH2	2.81	0.54
24:X:5:LYS:HG2	53:3:1313:U:OP2	2.07	0.53
51:1:1028:A:N6	51:1:1125:G:H2'	2.24	0.53
51:1:1558:C:H4'	51:1:1559:U:C5'	2.39	0.53
57:A2:43:LEU:HD13	57:A2:217:ILE:HD11	1.90	0.53
59:B2:985:GLU:HB3	59:B2:988:LYS:HB2	1.88	0.53
13:M:101:ALA:HB3	13:M:112:ASP:HB3	1.89	0.53
51:1:1018:U:O2'	51:1:1120:G:N2	2.41	0.53
51:1:2029:G:O6	51:1:2032:G:H5''	2.08	0.53
53:3:166:U:H2'	53:3:167:A:C8	2.43	0.53
64:6:62:C:H5'	65:a:53:ARG:HE	1.73	0.53
1:A:55:GLY:O	24:X:20:LYS:NZ	2.41	0.53
51:1:995:C:H6	51:1:995:C:H5'	1.72	0.53
51:1:1965:C:H5''	51:1:1966:A:H2'	1.89	0.53
51:1:2572:A:H5'	51:1:2574:G:H4'	1.90	0.53
53:3:112:G:N2	53:3:354:G:H5'	2.22	0.53
53:3:346:G:H2'	53:3:347:G:O4'	2.08	0.53
53:3:1506:U:O2'	53:3:1507:A:H5'	2.08	0.53
59:B2:628:HIS:HB3	59:B2:647:ARG:HH21	1.74	0.53
59:B2:1117:LEU:HD12	59:B2:1195:ILE:HG12	1.90	0.53
6:F:1:MET:HE3	51:1:2742:G:H5''	1.91	0.53
8:H:3:LYS:HA	53:3:1190:G:OP1	2.08	0.53
28:c:77:ARG:NH2	28:c:200:ASP:OD2	2.40	0.53
51:1:1172:C:H2'	51:1:1173:U:C6	2.43	0.53
53:3:1005:A:H2'	53:3:1006:G:H5'	1.90	0.53
57:A1:205:MET:HE3	57:A1:213:PRO:HB3	1.91	0.53
9:I:59:LYS:NZ	9:I:193:ASP:OD2	2.42	0.53
26:Z:38:GLU:HB2	53:3:1526:G:OP2	2.08	0.53
27:b:20:ASN:HB3	27:b:23:LEU:HD23	1.89	0.53
30:e:59:ILE:O	30:e:101:ARG:NH1	2.41	0.53
37:m:46:ILE:O	37:m:103:TYR:OH	2.27	0.53
46:v:14:LYS:HB2	52:2:98:G:H1	1.74	0.53
51:1:161:A:C3'	51:1:162:U:H5''	2.36	0.53
51:1:575:A:O2'	51:1:576:U:H5'	2.08	0.53
51:1:1123:C:H2'	51:1:1124:G:H8	1.73	0.53
51:1:1611:C:H6	51:1:1611:C:H5'	1.72	0.53
51:1:2257:U:O2'	51:1:2258:C:H5'	2.09	0.53
53:3:231:U:H2'	53:3:232:G:C8	2.43	0.53
58:B1:800:LEU:HB3	58:B1:920:ALA:HB1	1.89	0.53
59:B2:786:GLY:N	59:B2:789:THR:OG1	2.41	0.53
66:0:583:TYR:HB2	66:0:593:PHE:HZ	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:18:ASN:O	8:H:39:ARG:NH2	2.41	0.53
22:V:63:CYS:SG	22:V:73:THR:OG1	2.65	0.53
45:u:14:THR:OG1	45:u:68:ASN:ND2	2.41	0.53
51:1:186:G:H2'	51:1:187:G:H8	1.74	0.53
51:1:644:A:H2'	51:1:645:C:C5'	2.39	0.53
51:1:1726:C:H2'	51:1:1727:C:C6	2.44	0.53
53:3:166:U:H2'	53:3:167:A:H8	1.74	0.53
58:B1:78:LEU:O	58:B1:78:LEU:HD13	2.08	0.53
58:B1:111:THR:HG22	58:B1:300:GLN:NE2	2.23	0.53
58:B1:832:LYS:HB3	58:B1:1242:ARG:NH1	2.24	0.53
65:a:163:TYR:HB2	65:a:171:ILE:HD12	1.89	0.53
31:f:103:ASN:ND2	31:f:113:ASP:OD1	2.41	0.53
51:1:154:U:H2'	51:1:155:A:C8	2.44	0.53
51:1:1103:A:H3'	51:1:1104:C:H5''	1.91	0.53
51:1:1161:C:H2'	51:1:1162:G:H8	1.74	0.53
51:1:1161:C:H2'	51:1:1162:G:C8	2.43	0.53
51:1:2106:U:H2'	51:1:2107:G:H4'	1.90	0.53
53:3:1088:G:H21	53:3:1167:A:N6	2.03	0.53
58:B1:352:ARG:HD2	59:B2:1268:GLN:HE21	1.68	0.53
12:L:78:ARG:C	12:L:80:GLY:H	2.17	0.53
13:M:29:SER:HB3	53:3:589:U:H5''	1.90	0.53
28:c:24:VAL:HG21	28:c:188:LEU:HD23	1.91	0.53
28:c:56:LYS:CE	51:1:2830:C:H5''	2.39	0.53
48:x:17:ARG:CG	51:1:380:G:H5'	2.36	0.53
51:1:455:C:H3'	51:1:456:C:H5''	1.91	0.53
51:1:940:G:H2'	51:1:941:A:C5'	2.39	0.53
53:3:410:G:H2'	53:3:429:U:C5	2.44	0.53
53:3:1014:A:H2	53:3:1219:A:H1'	1.73	0.53
53:3:1042:A:H2'	53:3:1043:G:O4'	2.09	0.53
59:B2:246:LEU:HB3	59:B2:269:ILE:HD13	1.91	0.53
60:W0:3:ARG:NH1	60:W0:55:GLU:OE2	2.40	0.53
11:K:5:GLU:HB2	11:K:90:MET:HB2	1.90	0.53
20:T:43:ALA:O	20:T:46:LYS:NZ	2.42	0.53
29:d:119:ILE:HB	29:d:187:VAL:HG12	1.91	0.53
38:n:49:GLU:HB3	51:1:2839:G:H4'	1.91	0.53
46:v:35:GLU:OE2	46:v:93:ARG:NH1	2.42	0.53
49:y:21:LEU:HA	49:y:25:GLN:HB3	1.91	0.53
51:1:1141:U:H4'	51:1:1142:A:O4'	2.09	0.53
51:1:2024:G:OP2	51:1:2034:U:H4'	2.09	0.53
53:3:3:A:H5'	53:3:613:C:H4'	1.91	0.53
53:3:1176:A:H2'	53:3:1177:G:C8	2.44	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:68:TYR:CA	58:B1:75:TYR:HE2	2.22	0.53
22:V:8:GLN:NE2	22:V:59:GLU:OE2	2.42	0.53
29:d:68:ALA:HA	51:1:1255:U:C5	2.44	0.53
30:e:65:LEU:HD22	52:2:42:C:C4	2.44	0.53
44:t:31:VAL:HG12	44:t:84:TYR:HA	1.91	0.53
58:B1:785:ASP:O	58:B1:789:LYS:HB2	2.08	0.53
58:B1:850:LYS:HB2	58:B1:857:LEU:HB2	1.91	0.53
10:J:76:ASN:HB3	10:J:81:GLN:HG2	1.90	0.52
11:K:2:ARG:HH12	11:K:91:ARG:HB2	1.72	0.52
22:V:11:VAL:HG13	22:V:20:ILE:HD11	1.90	0.52
26:Z:25:ALA:HA	26:Z:28:LEU:HB2	1.90	0.52
36:l:47:ARG:NH2	51:1:251:A:H4'	2.24	0.52
45:u:86:PHE:HE1	45:u:91:LYS:HG3	1.74	0.52
51:1:1066:U:H2'	51:1:1068:G:OP2	2.08	0.52
51:1:1273:U:H4'	51:1:1275:A:OP1	2.08	0.52
51:1:2760:C:O2'	51:1:2761:A:H5'	2.08	0.52
53:3:1391:U:H2'	53:3:1392:G:C8	2.44	0.52
58:B1:205:LEU:HG	58:B1:217:LEU:HB3	1.90	0.52
58:B1:975:ILE:HD11	58:B1:1003:LEU:HD11	1.91	0.52
30:e:154:THR:HG21	51:1:2314:A:H1'	1.90	0.52
39:o:10:ARG:HD2	51:1:2294:G:OP1	2.09	0.52
51:1:1345:C:H6	51:1:1345:C:H5'	1.74	0.52
53:3:1054:C:H4'	53:3:1056:U:OP2	2.10	0.52
58:B1:290:ILE:HG21	62:NG:93:ILE:O	2.09	0.52
66:0:388:LEU:HD23	66:0:391:VAL:HG11	1.91	0.52
13:M:42:GLU:HG2	13:M:100:ILE:HD13	1.91	0.52
51:1:817:C:O2'	51:1:839:U:H5''	2.10	0.52
51:1:917:A:H2	52:2:79:G:N3	2.07	0.52
51:1:2869:G:H2'	51:1:2870:C:O4'	2.09	0.52
1:A:62:LYS:HG3	24:X:20:LYS:HB3	1.91	0.52
13:M:75:GLN:HB2	13:M:127:TYR:HB2	1.90	0.52
15:O:67:ILE:HG23	19:S:95:LEU:HD23	1.91	0.52
40:p:84:SER:OG	40:p:86:LYS:NZ	2.42	0.52
51:1:2625:G:H2'	51:1:2626:C:O4'	2.09	0.52
51:1:2720:U:H6	51:1:2720:U:H5'	1.73	0.52
66:0:91:GLY:N	70:0:802:PO4:O1	2.40	0.52
51:1:1672:A:C2	51:1:2582:G:H5'	2.44	0.52
53:3:608:A:H2'	53:3:609:A:O4'	2.08	0.52
53:3:1270:G:H2'	53:3:1271:A:H8	1.75	0.52
58:B1:215:LYS:HA	58:B1:218:THR:HG22	1.92	0.52
11:K:36:ILE:HG22	11:K:64:VAL:HG13	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:69:VAL:O	33:i:71:LYS:NZ	2.43	0.52
51:1:1869:G:H3'	51:1:1870:C:H5'	1.92	0.52
53:3:134:G:H2'	53:3:135:C:O4'	2.08	0.52
53:3:1412:C:H2'	53:3:1413:A:C8	2.45	0.52
53:3:1436:U:H2'	53:3:1437:A:C8	2.43	0.52
66:0:53:MET:HE1	66:0:472:ARG:HG3	1.91	0.52
14:N:54:VAL:HG11	14:N:93:LEU:HD23	1.91	0.52
20:T:57:ARG:NH2	20:T:58:MET:SD	2.82	0.52
30:e:65:LEU:CD1	52:2:41:G:H2'	2.40	0.52
51:1:1637:A:H5'	51:1:1760:C:O2'	2.10	0.52
51:1:2114:A:C5	51:1:2115:G:H1'	2.45	0.52
53:3:235:C:H2'	53:3:236:A:C8	2.44	0.52
53:3:604:G:H2'	53:3:605:U:O4'	2.10	0.52
57:A2:140:ILE:HD12	57:A2:142:MET:HE3	1.92	0.52
58:B1:209:ASN:HA	58:B1:214:ARG:HH21	1.74	0.52
59:B2:714:VAL:HB	59:B2:787:PRO:HD2	1.92	0.52
59:B2:1070:HIS:NE2	59:B2:1114:GLU:OE1	2.36	0.52
12:L:91:ARG:NE	12:L:91:ARG:HA	2.25	0.52
34:j:118:MET:HA	34:j:121:LYS:HD3	1.91	0.52
51:1:118:A:OP2	51:1:119:A:H5''	2.10	0.52
51:1:1064:C:H2'	51:1:1065:U:C6	2.44	0.52
51:1:2628:C:H3'	51:1:2629:U:H5'	1.92	0.52
51:1:2800:A:C2	51:1:2895:G:H1'	2.45	0.52
51:1:2818:U:H2'	51:1:2819:G:H8	1.75	0.52
53:3:1353:G:O2'	53:3:1354:U:H5'	2.10	0.52
58:B1:144:TYR:CE1	58:B1:162:GLU:CD	2.88	0.52
9:I:53:GLN:HA	9:I:198:LEU:HD12	1.92	0.52
14:N:55:ASP:N	14:N:55:ASP:OD1	2.43	0.52
16:P:19:VAL:HG22	16:P:82:GLU:HB2	1.92	0.52
23:W:33:THR:OG1	23:W:34:GLU:N	2.43	0.52
39:o:51:ALA:HB3	39:o:78:VAL:HG12	1.92	0.52
51:1:519:U:H2'	51:1:520:G:C8	2.44	0.52
57:A1:100:LEU:HD21	57:A1:121:VAL:HG11	1.90	0.52
58:B1:770:LEU:CD1	59:B2:618:GLN:HG3	2.37	0.52
66:0:282:VAL:HA	66:0:286:LEU:HD12	1.91	0.52
17:Q:45:ASN:HB3	53:3:528:C:H41	1.75	0.52
27:b:140:VAL:HA	27:b:191:LEU:HA	1.91	0.52
32:g:84:ALA:HB2	32:g:148:ALA:HB1	1.90	0.52
51:1:154:U:H2'	51:1:155:A:H8	1.74	0.52
51:1:973:A:H5'	51:1:1188:U:H1'	1.92	0.52
51:1:1138:G:H2'	51:1:1139:G:O4'	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2650:U:H2'	51:1:2651:C:H6	1.74	0.52
53:3:210:C:H5'	53:3:211:G:N3	2.25	0.52
53:3:473:U:H2'	53:3:474:G:C8	2.45	0.52
59:B2:125:GLY:HA2	59:B2:499:SER:HB2	1.92	0.52
51:1:528:A:H2'	51:1:529:A:H5''	1.91	0.51
51:1:685:A:H5''	51:1:788:A:H62	1.74	0.51
51:1:857:G:H2'	51:1:858:G:O4'	2.10	0.51
53:3:123:U:OP1	53:3:312:C:H5'	2.10	0.51
53:3:1278:G:OP1	53:3:1279:G:H5'	2.10	0.51
58:B1:112:ALA:HA	58:B1:238:ILE:HA	1.91	0.51
58:B1:683:ILE:HD12	58:B1:754:ILE:HG21	1.93	0.51
25:Y:22:SER:HA	53:3:1458:G:O3'	2.11	0.51
41:q:54:ARG:NH2	51:1:1155:A:H4'	2.25	0.51
51:1:686:U:H3'	51:1:687:C:H5'	1.91	0.51
53:3:779:C:H2'	53:3:780:A:O4'	2.10	0.51
53:3:1042:A:H2'	53:3:1043:G:C1'	2.40	0.51
57:A1:16:ILE:HG23	57:A1:26:VAL:HG22	1.91	0.51
58:B1:390:LEU:N	58:B1:390:LEU:CD1	2.73	0.51
9:I:205:LYS:HE3	53:3:8:A:C5	2.45	0.51
48:x:7:THR:HG23	48:x:9:LYS:HG3	1.92	0.51
51:1:749:A:C2	51:1:1618:A:H2'	2.45	0.51
51:1:1447:C:H2'	51:1:1448:G:H8	1.75	0.51
53:3:1402:C:H2'	53:3:1403:C:O4'	2.10	0.51
53:3:1450:U:H1'	53:3:1454:G:N2	2.25	0.51
59:B2:524:ILE:HG21	59:B2:708:VAL:HG13	1.92	0.51
66:0:116:VAL:HG11	66:0:146:ARG:HD3	1.91	0.51
66:0:151:PHE:HE2	66:0:171:LEU:HG	1.75	0.51
11:K:38:ARG:NH1	11:K:40:GLU:OE1	2.43	0.51
29:d:58:LYS:NZ	29:d:62:GLN:OE1	2.43	0.51
29:d:63:LYS:HD3	51:1:2443:C:OP1	2.10	0.51
41:q:82:LEU:HD23	41:q:112:ALA:HB2	1.92	0.51
53:3:86:G:H4'	53:3:87:C:C5	2.44	0.51
53:3:1247:U:O2'	53:3:1248:A:H5'	2.10	0.51
53:3:1449:C:H2'	53:3:1450:U:O4'	2.10	0.51
53:3:1481:U:O2'	53:3:1482:G:H5'	2.09	0.51
8:H:13:ILE:HG13	8:H:14:VAL:HG23	1.91	0.51
23:W:41:SER:HB3	23:W:51:GLN:HE21	1.76	0.51
32:g:78:VAL:HG11	32:g:103:VAL:HG22	1.91	0.51
51:1:226:A:H2'	51:1:227:A:O4'	2.11	0.51
51:1:558:U:H2'	51:1:559:G:H8	1.76	0.51
51:1:1625:C:H2'	51:1:1626:A:O4'	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2165:C:H5''	51:1:2166:U:OP1	2.10	0.51
53:3:1411:C:H2'	53:3:1412:C:C6	2.45	0.51
59:B2:255:ILE:HB	59:B2:263:VAL:HB	1.93	0.51
66:0:97:ILE:HD11	66:0:443:PRO:HD2	1.92	0.51
66:0:105:VAL:HG22	66:0:337:ARG:HH11	1.75	0.51
66:0:342:VAL:HG12	66:0:378:ARG:HA	1.91	0.51
19:S:2:LYS:HG2	53:3:1048:G:H5''	1.92	0.51
27:b:106:PRO:HA	27:b:194:VAL:HA	1.92	0.51
31:f:40:VAL:O	31:f:54:ARG:NH2	2.43	0.51
36:l:108:ALA:HB3	36:l:125:LEU:HD11	1.92	0.51
39:o:21:LEU:HD11	51:1:2379:G:H4'	1.91	0.51
48:x:18:SER:HB2	51:1:2080:A:H5'	1.92	0.51
51:1:368:A:O2'	51:1:369:U:H5'	2.11	0.51
51:1:644:A:H2'	51:1:645:C:C4'	2.41	0.51
51:1:2432:A:H5'	64:6:76:A:O3'	2.09	0.51
53:3:1421:G:C5	53:3:1422:G:H1'	2.45	0.51
58:B1:99:ARG:HG3	58:B1:99:ARG:HH11	1.73	0.51
58:B1:201:LEU:HD12	58:B1:224:LEU:HD12	1.91	0.51
66:0:170:GLN:HE21	66:0:266:CYS:H	1.59	0.51
11:K:40:GLU:OE2	11:K:100:SER:OG	2.28	0.51
51:1:1068:G:O2'	51:1:1096:A:H4'	2.10	0.51
51:1:1669:A:O3'	51:1:2549:G:H5'	2.11	0.51
51:1:1906:G:H2'	51:1:1907:G:H5''	1.93	0.51
53:3:392:C:H2'	53:3:393:A:H8	1.75	0.51
53:3:701:U:C4'	53:3:703:G:H1'	2.41	0.51
55:8:13:DT:OP2	58:B1:791:ALA:CB	2.59	0.51
58:B1:99:ARG:HA	58:B1:248:ASP:HB2	1.92	0.51
4:D:8:SER:HA	51:1:1309:G:H5''	1.91	0.51
27:b:106:PRO:HD2	27:b:109:LEU:HD13	1.91	0.51
27:b:257:ARG:HH12	51:1:1799:G:H3'	1.75	0.51
29:d:145:ASP:HA	29:d:166:LYS:HB3	1.92	0.51
51:1:543:G:H3'	51:1:544:C:H5''	1.93	0.51
51:1:937:C:H2'	51:1:938:G:H8	1.74	0.51
53:3:184:G:H4'	53:3:224:U:O3'	2.11	0.51
53:3:757:U:H2'	53:3:758:C:O4'	2.10	0.51
23:W:70:THR:OG1	23:W:71:ASP:N	2.44	0.51
51:1:2104:C:H2'	51:1:2105:U:O4'	2.11	0.51
51:1:2586:U:H2'	51:1:2587:A:C8	2.46	0.51
53:3:406:G:O2'	53:3:407:U:H5'	2.11	0.51
53:3:1137:C:H4'	53:3:1138:G:C2	2.45	0.51
58:B1:375:GLU:HG2	59:B2:1245:ALA:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:437:PHE:HZ	58:B1:453:VAL:HG11	1.76	0.51
66:0:158:ILE:HG23	66:0:162:LEU:HD12	1.92	0.51
4:D:24:THR:O	4:D:28:ARG:NH1	2.44	0.51
9:I:73:ASN:OD1	9:I:76:LYS:NZ	2.44	0.51
9:I:82:LYS:O	9:I:88:ASN:ND2	2.36	0.51
16:P:121:ARG:HH22	53:3:1524:C:H5''	1.75	0.51
22:V:44:HIS:HB3	22:V:70:LYS:HG3	1.92	0.51
30:e:31:GLU:HB2	30:e:156:THR:HB	1.93	0.51
42:r:10:LYS:HE2	51:1:994:C:O2'	2.11	0.51
46:v:66:ASP:O	46:v:68:LYS:NZ	2.43	0.51
51:1:1645:G:H5''	51:1:1646:C:C5'	2.27	0.51
51:1:1907:G:H2'	51:1:1908:C:O4'	2.11	0.51
51:1:2743:U:C2'	51:1:2744:G:H5''	2.40	0.51
52:2:118:C:H2'	52:2:119:A:C4'	2.40	0.51
53:3:1138:G:H3'	53:3:1138:G:N3	2.25	0.51
58:B1:275:ARG:HH12	58:B1:278:ARG:NH1	2.09	0.51
20:T:13:GLU:O	20:T:83:ARG:NH2	2.42	0.50
33:i:91:LYS:HB2	33:i:94:LYS:HB2	1.92	0.50
37:m:17:ASN:ND2	37:m:97:GLN:OE1	2.36	0.50
51:1:878:A:H3'	51:1:879:G:H8	1.75	0.50
51:1:2186:G:H2'	51:1:2187:U:O4'	2.11	0.50
53:3:1206:G:H2'	53:3:1207:G:O4'	2.11	0.50
59:B2:93:SER:HA	59:B2:128:PRO:HA	1.93	0.50
59:B2:400:VAL:HG21	59:B2:452:ARG:HE	1.76	0.50
1:A:54:GLY:H	24:X:26:ASP:HA	1.76	0.50
7:G:103:TRP:HA	7:G:106:VAL:HG12	1.92	0.50
13:M:104:SER:O	53:3:642:A:H2	1.93	0.50
51:1:663:G:C3'	51:1:664:G:H5''	2.41	0.50
51:1:2881:U:H2'	51:1:2882:A:C8	2.46	0.50
53:3:407:U:H2'	53:3:408:A:C8	2.45	0.50
53:3:839:C:H2'	53:3:840:C:C6	2.46	0.50
66:0:158:ILE:HB	66:0:166:PRO:HG3	1.92	0.50
5:E:2:LYS:HG3	51:1:242:G:C8	2.46	0.50
9:I:104:MET:HG3	9:I:172:VAL:HG22	1.92	0.50
33:i:11:GLN:HB2	33:i:56:VAL:HG12	1.93	0.50
47:w:70:PRO:HD3	52:2:12:C:N4	2.26	0.50
53:3:35:G:H2'	53:3:36:C:C6	2.46	0.50
53:3:195:A:H2'	53:3:196:A:C8	2.47	0.50
59:B2:232:ILE:HG12	59:B2:237:LEU:HG	1.94	0.50
59:B2:400:VAL:HG11	59:B2:452:ARG:HD2	1.94	0.50
66:0:312:SER:OG	66:0:313:ASP:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:m:1:MET:HE1	63:5:63:G:O2'	2.11	0.50
51:1:859:G:HO2'	51:1:860:U:H6	1.58	0.50
51:1:1019:U:OP1	51:1:1035:U:O2'	2.29	0.50
51:1:1542:U:H2'	51:1:1543:G:O4'	2.10	0.50
51:1:2250:G:H21	51:1:2496:C:H5''	1.76	0.50
51:1:2266:A:H4'	51:1:2267:A:N3	2.26	0.50
51:1:2404:U:H2'	51:1:2405:G:O4'	2.10	0.50
53:3:91:U:H2'	53:3:92:U:H5''	1.93	0.50
53:3:458:U:H2'	53:3:459:A:H8	1.75	0.50
58:B1:395:LYS:NZ	58:B1:399:LYS:CD	2.74	0.50
58:B1:412:LEU:HD23	58:B1:416:ILE:HG13	1.92	0.50
66:0:94:ASP:HB3	66:0:465:HIS:HB2	1.93	0.50
14:N:27:ILE:HD12	14:N:34:LEU:HD22	1.93	0.50
27:b:59:GLN:HG2	27:b:84:PRO:HB2	1.93	0.50
33:i:8:VAL:HG11	33:i:26:ALA:HB1	1.93	0.50
33:i:14:ALA:HB1	33:i:45:THR:HG23	1.94	0.50
51:1:140:C:H2'	51:1:141:G:H4'	1.94	0.50
51:1:161:A:H3'	51:1:162:U:C5'	2.39	0.50
51:1:748:G:O2'	51:1:749:A:H5''	2.11	0.50
51:1:1159:U:H2'	51:1:1160:G:C8	2.46	0.50
51:1:2663:G:H8	51:1:2663:G:OP2	1.94	0.50
53:3:14:U:O2	53:3:17:U:H5	1.95	0.50
58:B1:749:LYS:HB3	58:B1:755:ILE:HD11	1.93	0.50
59:B2:974:ARG:HD2	59:B2:1014:LEU:HD21	1.92	0.50
65:a:12:ARG:HA	65:a:15:VAL:HB	1.92	0.50
66:0:139:ALA:N	66:0:263:LEU:O	2.43	0.50
4:D:10:LEU:HD23	51:1:770:G:H5''	1.94	0.50
33:i:92:PRO:HD2	51:1:1076:C:O2'	2.12	0.50
51:1:473:G:O2'	51:1:474:G:H5'	2.12	0.50
51:1:2041:U:H2'	51:1:2042:A:H8	1.77	0.50
51:1:2742:G:H1	51:1:2762:C:H42	1.60	0.50
53:3:267:C:O2	53:3:267:C:H2'	2.10	0.50
53:3:1441:A:H62	53:3:1461:G:H21	1.60	0.50
63:5:22:G:H2'	63:5:23:A:C8	2.47	0.50
63:5:23:A:H2'	63:5:24:G:C8	2.47	0.50
66:0:420:VAL:HG21	66:0:481:ALA:HB1	1.93	0.50
66:0:503:GLY:N	66:0:518:VAL:O	2.40	0.50
24:X:17:LYS:O	24:X:20:LYS:NZ	2.41	0.50
33:i:92:PRO:HB3	51:1:1077:A:H1'	1.92	0.50
51:1:1999:C:H5''	51:1:2723:C:O2'	2.12	0.50
51:1:2041:U:H2'	51:1:2042:A:C8	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:505:ASP:OD2	59:B2:812:PHE:HA	2.11	0.50
66:0:105:VAL:HG22	66:0:337:ARG:HD3	1.94	0.50
66:0:364:VAL:HG12	66:0:366:MET:H	1.77	0.50
67:h:6:5OH:N	67:h:6:5OH:CS	2.75	0.50
51:1:1536:C:H4'	51:1:1537:G:N2	2.27	0.50
58:B1:1371:ARG:HE	58:B1:1372:ARG:NH1	2.10	0.50
8:H:22:PHE:HE2	15:O:11:LYS:HD3	1.76	0.50
29:d:45:ALA:HB2	29:d:89:PRO:HD3	1.93	0.50
34:j:2:LYS:HA	51:1:995:C:N3	2.27	0.50
43:s:75:PHE:HE1	51:1:519:U:H1'	1.77	0.50
51:1:274:C:H2'	51:1:275:C:O4'	2.12	0.50
51:1:1434:A:H2'	51:1:1435:G:H8	1.77	0.50
51:1:1443:U:H2'	51:1:1444:G:H8	1.75	0.50
51:1:1472:C:H2'	51:1:1473:G:C8	2.47	0.50
53:3:1109:C:H2'	53:3:1110:A:O4'	2.12	0.50
57:A1:18:GLN:HA	57:A1:24:ALA:HA	1.94	0.50
62:NG:161:SER:HA	62:NG:170:PRO:HA	1.94	0.50
7:G:100:LEU:HB2	7:G:174:GLU:HG2	1.93	0.49
8:H:124:GLU:HG3	8:H:188:ALA:HB1	1.94	0.49
26:Z:32:ARG:HG3	26:Z:33:ARG:HG2	1.93	0.49
33:i:53:PRO:HD2	33:i:77:VAL:HB	1.94	0.49
51:1:355:U:H2'	51:1:356:G:C8	2.47	0.49
51:1:948:C:H2'	51:1:949:G:H8	1.77	0.49
51:1:2469:A:H2'	51:1:2470:G:O4'	2.12	0.49
53:3:38:G:H22	53:3:397:A:H5'	1.77	0.49
53:3:76:G:H2'	53:3:77:A:C5'	2.42	0.49
53:3:1386:G:H2'	53:3:1387:G:H8	1.77	0.49
25:Y:54:GLN:HE21	53:3:193:C:C1'	2.25	0.49
33:i:92:PRO:HB2	51:1:1077:A:C4'	2.42	0.49
46:v:45:ASP:N	46:v:45:ASP:OD1	2.44	0.49
51:1:864:G:H4'	52:2:101:A:H4'	1.94	0.49
51:1:948:C:H2'	51:1:949:G:C8	2.47	0.49
51:1:2811:G:H2'	51:1:2812:G:H8	1.77	0.49
53:3:89:U:H2'	53:3:90:C:O4'	2.12	0.49
53:3:599:C:H2'	53:3:600:A:C8	2.47	0.49
53:3:1013:G:N2	53:3:1015:G:H3'	2.27	0.49
54:4:44:G:OP1	59:B2:1073:LYS:NZ	2.37	0.49
58:B1:972:LYS:HD2	58:B1:1004:ALA:HA	1.93	0.49
59:B2:529:ARG:HH11	59:B2:572:ILE:HG22	1.77	0.49
65:a:166:ASP:OD2	65:a:172:HIS:ND1	2.45	0.49
10:J:37:VAL:HG11	10:J:113:VAL:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:127:ARG:HB2	53:3:796:C:OP1	2.12	0.49
27:b:201:LEU:CD2	53:3:773:G:H5''	2.42	0.49
34:j:45:THR:HB	34:j:48:VAL:HG22	1.93	0.49
40:p:61:ARG:NH2	40:p:99:LEU:O	2.44	0.49
53:3:359:G:H2'	53:3:360:G:O4'	2.13	0.49
53:3:781:A:OP1	53:3:1523:G:H5'	2.12	0.49
58:B1:1179:PRO:HD2	58:B1:1184:ASP:HA	1.93	0.49
31:f:28:LYS:N	31:f:78:VAL:O	2.46	0.49
47:w:12:SER:HB3	51:1:2261:C:C6	2.47	0.49
51:1:341:C:H2'	51:1:342:A:C8	2.47	0.49
51:1:934:U:H2'	51:1:935:C:C6	2.47	0.49
51:1:2208:C:H2'	51:1:2209:G:C8	2.47	0.49
53:3:1023:U:H2'	53:3:1024:G:C8	2.48	0.49
58:B1:145:VAL:HG12	58:B1:184:ALA:HB1	1.94	0.49
9:I:50:TYR:CD2	53:3:508:U:H4'	2.48	0.49
11:K:62:MET:HB3	11:K:64:VAL:HG23	1.93	0.49
28:c:4:LEU:HD23	28:c:29:VAL:HG11	1.94	0.49
28:c:45:TYR:CZ	51:1:2637:U:H5'	2.47	0.49
51:1:1735:A:H2'	51:1:1736:U:O4'	2.11	0.49
57:A1:100:LEU:HB2	57:A1:144:ILE:HG23	1.95	0.49
12:L:110:ARG:NH1	12:L:125:ASP:OD2	2.46	0.49
21:U:4:ILE:HG12	21:U:21:VAL:HG22	1.94	0.49
31:f:48:THR:OG1	31:f:49:LEU:N	2.45	0.49
38:n:49:GLU:CB	51:1:2839:G:H4'	2.42	0.49
53:3:70:U:H4'	53:3:71:A:H8	1.78	0.49
53:3:952:U:H2'	53:3:953:G:H8	1.78	0.49
53:3:1316:G:C2'	53:3:1317:C:H5''	2.40	0.49
59:B2:411:ARG:NH2	59:B2:427:ASP:OD2	2.44	0.49
59:B2:533:LEU:HD13	59:B2:540:ARG:HH21	1.77	0.49
63:5:51:U:H2'	63:5:52:G:C8	2.48	0.49
15:O:65:TYR:HB3	19:S:95:LEU:HD22	1.95	0.49
21:U:70:ARG:NH2	53:3:451:A:OP2	2.45	0.49
29:d:125:SER:O	29:d:137:LYS:NZ	2.39	0.49
38:n:22:ARG:HG3	38:n:70:THR:HA	1.93	0.49
43:s:18:ARG:NH1	51:1:518:G:H4'	2.28	0.49
53:3:745:G:OP1	53:3:852:G:H5'	2.13	0.49
53:3:1391:U:H2'	53:3:1392:G:H8	1.77	0.49
53:3:1491:G:H2'	67:h:6:5OH:O	2.11	0.49
66:0:433:LEU:O	66:0:437:ARG:N	2.45	0.49
32:g:7:ASP:HA	32:g:15:LEU:HD23	1.94	0.49
51:1:26:G:H1'	51:1:515:A:H61	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1597:A:H5''	51:1:1598:A:H5'	1.94	0.49
51:1:2104:C:H42	51:1:2185:U:H3	1.60	0.49
51:1:2220:U:H2'	51:1:2221:G:C8	2.47	0.49
53:3:1128:C:O2'	53:3:1129:C:H5'	2.13	0.49
53:3:1492:A:H1'	54:4:5:U:O2'	2.13	0.49
58:B1:421:VAL:O	58:B1:436:ALA:HA	2.12	0.49
59:B2:9:LYS:HG2	59:B2:1171:ARG:HH12	1.77	0.49
59:B2:562:GLU:OE1	59:B2:662:SER:OG	2.28	0.49
7:G:53:LEU:HD22	7:G:219:THR:HG21	1.95	0.49
24:X:54:ARG:HG3	24:X:55:GLN:HG2	1.95	0.49
28:c:56:LYS:HZ1	51:1:2830:C:H5''	1.78	0.49
44:t:64:LYS:HE2	51:1:1601:G:OP1	2.13	0.49
50:z:40:THR:HG22	50:z:43:ILE:HG12	1.94	0.49
51:1:1029:A:H2'	51:1:1030:C:O4'	2.13	0.49
53:3:253:A:H2'	53:3:254:G:C8	2.47	0.49
53:3:632:U:H3'	53:3:633:G:H5'	1.95	0.49
58:B1:124:ILE:HG23	58:B1:128:LEU:HD12	1.94	0.49
59:B2:857:VAL:HG13	59:B2:919:ARG:HH21	1.78	0.49
62:NG:126:THR:CB	62:NG:175:PHE:CA	2.90	0.49
14:N:121:ARG:HD2	53:3:1348:U:H4'	1.95	0.49
17:Q:71:HIS:HB2	17:Q:73:LEU:HD23	1.95	0.49
38:n:32:GLU:HG2	38:n:115:LEU:HD12	1.94	0.49
41:q:3:VAL:HG12	41:q:5:ARG:H	1.78	0.49
51:1:1111:A:H2'	51:1:1111:A:N3	2.28	0.49
51:1:1417:C:C4'	51:1:1587:G:H21	2.26	0.49
51:1:2122:U:H2'	51:1:2123:G:H4'	1.95	0.49
51:1:2792:A:C3'	51:1:2793:C:H5''	2.43	0.49
58:B1:220:ARG:HG2	58:B1:220:ARG:NH1	2.26	0.49
59:B2:18:ARG:HE	59:B2:620:ASN:HA	1.77	0.49
64:6:37:A:H2'	64:6:38:A:O4'	2.13	0.49
64:6:44:A:H3'	64:6:45:G:H5''	1.95	0.49
21:U:56:ARG:HA	21:U:59:HIS:HB3	1.95	0.48
29:d:94:GLN:CD	51:1:660:C:H5''	2.38	0.48
43:s:4:ILE:HG22	43:s:106:VAL:HG13	1.93	0.48
51:1:2128:G:H1	51:1:2160:C:H42	1.58	0.48
53:3:802:A:H2'	53:3:803:G:O4'	2.13	0.48
53:3:916:U:H2'	53:3:917:G:C8	2.47	0.48
55:8:14:DC:H2'	55:8:15:DC:C6	2.48	0.48
59:B2:732:ILE:HD11	59:B2:769:PRO:HB3	1.95	0.48
66:0:12:ASN:HA	66:0:85:ASN:HB2	1.94	0.48
66:0:127:TRP:O	66:0:131:ASN:ND2	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:O:289:PRO:HB3	66:O:337:ARG:HH21	1.78	0.48
9:I:73:ASN:HA	9:I:76:LYS:HD2	1.95	0.48
15:O:86:ALA:HA	15:O:90:LEU:HD12	1.95	0.48
30:e:128:SER:HB2	30:e:154:THR:HG23	1.95	0.48
47:w:20:LYS:HE3	51:1:2355:G:O2'	2.13	0.48
51:1:616:A:H2'	51:1:617:G:O4'	2.12	0.48
51:1:686:U:H6	51:1:788:A:N1	2.12	0.48
51:1:1180:U:H5''	51:1:1181:U:H5	1.78	0.48
51:1:1335:C:H2'	51:1:1336:A:C8	2.48	0.48
51:1:1474:U:H2'	51:1:1475:G:H5'	1.96	0.48
51:1:2176:A:H5'	65:a:219:GLY:C	2.38	0.48
51:1:2364:C:H2'	51:1:2365:G:O4'	2.13	0.48
51:1:2583:G:H2'	51:1:2584:U:O4'	2.13	0.48
52:2:101:A:H2'	52:2:102:G:O4'	2.13	0.48
53:3:530:G:H3'	53:3:531:U:H5'	1.95	0.48
53:3:701:U:H4'	53:3:703:G:H1'	1.93	0.48
58:B1:102:MET:HG2	58:B1:246:PRO:HD3	1.94	0.48
59:B2:554:HIS:HD2	59:B2:558:VAL:HB	1.77	0.48
65:a:46:VAL:HG13	65:a:212:VAL:HG22	1.95	0.48
16:P:27:ASN:ND2	53:3:692:U:H5	2.11	0.48
30:e:36:ASN:HB3	30:e:152:ASP:HB3	1.95	0.48
40:p:1:SER:N	51:1:2875:C:H4'	2.27	0.48
46:v:14:LYS:HB2	52:2:98:G:N1	2.28	0.48
51:1:2898:U:H2'	51:1:2899:A:H8	1.78	0.48
52:2:28:C:H2'	52:2:29:A:C8	2.48	0.48
53:3:17:U:H2'	53:3:18:C:C6	2.48	0.48
53:3:59:A:N6	53:3:331:G:H1'	2.28	0.48
62:NG:126:THR:CB	62:NG:175:PHE:CB	2.91	0.48
41:q:111:LYS:HD2	42:r:48:LYS:HD3	1.95	0.48
51:1:1326:U:H2'	51:1:1327:A:C8	2.41	0.48
51:1:1447:C:H2'	51:1:1448:G:C8	2.48	0.48
51:1:1753:G:H22	51:1:1755:A:H3'	1.79	0.48
51:1:2221:G:O2'	51:1:2222:C:H5'	2.13	0.48
51:1:2522:U:H2'	51:1:2523:G:H5'	1.96	0.48
51:1:2565:A:O2'	51:1:2566:A:H5'	2.13	0.48
53:3:207:C:C2'	53:3:208:U:H5''	2.42	0.48
57:A1:182:ARG:O	57:A1:205:MET:HA	2.14	0.48
58:B1:550:VAL:O	58:B1:569:LEU:HA	2.13	0.48
64:6:68:C:H2'	64:6:69:C:C6	2.48	0.48
7:G:165:ALA:HB1	7:G:172:ILE:HD13	1.96	0.48
15:O:7:ARG:HA	15:O:75:ASP:HA	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:92:PRO:CG	51:1:1077:A:H1'	2.44	0.48
52:2:32:U:H2'	52:2:33:G:O4'	2.14	0.48
53:3:1305:G:N2	53:3:1331:G:H2'	2.28	0.48
58:B1:1027:VAL:HB	58:B1:1121:LEU:HB2	1.95	0.48
8:H:152:VAL:HG12	8:H:197:VAL:HG13	1.96	0.48
9:I:96:ARG:HH21	9:I:114:ARG:HH12	1.62	0.48
12:L:96:ASN:N	12:L:96:ASN:OD1	2.46	0.48
17:Q:33:CYS:H	17:Q:54:VAL:HG13	1.78	0.48
29:d:2:GLU:HB3	29:d:11:ALA:HB1	1.96	0.48
39:o:104:GLN:NE2	39:o:108:ASP:OD2	2.47	0.48
42:r:9:GLY:O	51:1:996:A:H1'	2.13	0.48
48:x:5:GLN:O	48:x:73:ARG:NH2	2.45	0.48
51:1:248:G:O5'	51:1:249:C:H5''	2.14	0.48
51:1:1357:C:H2'	51:1:1358:G:O4'	2.14	0.48
51:1:2165:C:H41	51:1:2171:A:H61	1.60	0.48
51:1:2366:A:H2'	51:1:2367:G:O4'	2.13	0.48
53:3:141:G:H2'	53:3:142:G:O4'	2.13	0.48
53:3:591:U:H2'	53:3:592:G:C8	2.48	0.48
58:B1:633:ALA:HB2	59:B2:808:ASN:N	2.19	0.48
59:B2:836:LEU:HD13	59:B2:1054:LEU:HD13	1.95	0.48
64:6:59:A:H2'	64:6:60:U:H5'	1.96	0.48
4:D:12:ARG:HD3	51:1:686:U:O4	2.13	0.48
21:U:14:ARG:NH1	53:3:618:C:H1'	2.21	0.48
28:c:79:LEU:HD12	51:1:2635:A:H4'	1.96	0.48
40:p:61:ARG:HH21	40:p:99:LEU:HB3	1.79	0.48
48:x:57:VAL:HG22	51:1:372:G:H2'	1.96	0.48
51:1:639:U:H2'	51:1:640:C:C6	2.48	0.48
51:1:2637:U:H2'	51:1:2638:G:O4'	2.13	0.48
51:1:2644:G:O2'	51:1:2645:G:H5'	2.13	0.48
53:3:508:U:H1'	53:3:509:A:N7	2.29	0.48
53:3:591:U:H2'	53:3:592:G:H8	1.79	0.48
53:3:681:A:H2'	53:3:682:G:C8	2.48	0.48
53:3:714:G:H2'	53:3:715:A:O4'	2.13	0.48
53:3:1220:G:H2'	53:3:1221:G:O4'	2.13	0.48
55:8:3:DC:H2''	55:8:4:DT:C7	2.42	0.48
66:0:468:ILE:O	66:0:472:ARG:N	2.47	0.48
14:N:91:GLU:HA	14:N:94:ARG:HB2	1.94	0.48
51:1:281:C:H2'	51:1:282:A:C8	2.49	0.48
51:1:572:A:H2'	51:1:572:A:N3	2.29	0.48
51:1:704:G:H1'	51:1:726:G:N2	2.28	0.48
53:3:5:U:H4'	53:3:6:G:C8	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:513:C:H2'	53:3:514:C:C6	2.49	0.48
53:3:631:C:H3'	53:3:632:U:H5'	1.95	0.48
53:3:1005:A:H2'	53:3:1006:G:C5'	2.44	0.48
58:B1:108:ALA:HB1	58:B1:279:LEU:HD22	1.96	0.48
58:B1:809:VAL:HG21	58:B1:909:ILE:HG12	1.95	0.48
12:L:77:ARG:HD3	12:L:86:VAL:HG21	1.94	0.48
18:R:99:GLN:HB3	53:3:949:A:OP1	2.13	0.48
29:d:98:LYS:HG3	51:1:607:U:P	2.53	0.48
51:1:1701:A:C2'	51:1:1702:G:H5'	2.43	0.48
51:1:2860:A:H2'	51:1:2861:U:H5'	1.95	0.48
53:3:994:A:C8	53:3:1216:A:H4'	2.49	0.48
59:B2:565:GLU:HA	59:B2:569:ILE:HG12	1.95	0.48
51:1:174:U:H2'	51:1:175:G:C8	2.49	0.48
51:1:225:C:H2'	51:1:226:A:O4'	2.14	0.48
51:1:327:G:O2'	51:1:328:U:H5'	2.14	0.48
51:1:435:C:H2'	51:1:436:C:H5'	1.95	0.48
51:1:845:A:N3	51:1:845:A:H3'	2.29	0.48
51:1:941:A:H2'	51:1:942:G:O4'	2.14	0.48
51:1:1819:A:H4'	51:1:1820:U:H5'	1.96	0.48
51:1:2504:U:H2'	51:1:2505:G:H5'	1.95	0.48
59:B2:363:LEU:HB3	59:B2:381:ALA:HB1	1.96	0.48
59:B2:1314:GLN:HB2	60:W0:28:ARG:HH12	1.78	0.48
63:5:50:U:H2'	63:5:51:U:C6	2.49	0.48
66:0:553:VAL:HG11	66:0:578:LEU:HD22	1.96	0.48
16:P:121:ARG:NH2	53:3:1524:C:OP1	2.46	0.47
16:P:126:ARG:HH21	53:3:796:C:H4'	1.79	0.47
23:W:20:ILE:HD12	23:W:53:GLN:HB2	1.96	0.47
28:c:13:ARG:NH2	28:c:21:SER:OG	2.47	0.47
33:i:55:PRO:HG2	33:i:71:LYS:HG3	1.96	0.47
36:l:16:GLY:HA2	51:1:662:G:H5''	1.96	0.47
39:o:29:HIS:HB3	39:o:36:TYR:HB2	1.96	0.47
46:v:7:GLU:HA	46:v:65:VAL:HG23	1.96	0.47
51:1:100:U:H4'	51:1:101:A:O4'	2.14	0.47
51:1:1343:G:H1'	51:1:1597:A:C4	2.49	0.47
51:1:2534:A:H2'	51:1:2535:G:O4'	2.14	0.47
51:1:2762:C:H2'	51:1:2763:G:H5'	1.95	0.47
51:1:2818:U:H2'	51:1:2819:G:C8	2.49	0.47
52:2:5:U:H2'	52:2:6:G:H8	1.79	0.47
53:3:392:C:H2'	53:3:393:A:C8	2.49	0.47
58:B1:103:GLY:H	58:B1:244:VAL:HG22	1.79	0.47
66:0:502:GLU:HA	66:0:519:VAL:HA	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:VAL:HG22	30:e:139:GLU:HA	1.96	0.47
9:I:131:ILE:HG21	53:3:620:C:O2	2.14	0.47
16:P:80:ASN:HA	16:P:104:PHE:HB3	1.96	0.47
22:V:56:ASP:N	22:V:56:ASP:OD1	2.47	0.47
24:X:14:LEU:HA	24:X:17:LYS:HD2	1.96	0.47
31:f:44:HIS:HA	31:f:49:LEU:HD23	1.96	0.47
51:1:1018:U:H2'	51:1:1019:U:O4'	2.13	0.47
53:3:1500:A:H5''	53:3:1508:A:H5'	1.94	0.47
58:B1:255:LEU:HD23	58:B1:261:ALA:HB2	1.95	0.47
58:B1:891:ASP:OD2	58:B1:1290:ARG:NH2	2.47	0.47
58:B1:1146:GLU:OE2	58:B1:1310:THR:HG22	2.14	0.47
58:B1:1150:PRO:HG3	58:B1:1214:PRO:HB2	1.96	0.47
59:B2:318:SER:OG	59:B2:320:ASP:OD1	2.31	0.47
9:I:1:ALA:HB2	53:3:499:A:H61	1.79	0.47
20:T:45:HIS:O	20:T:47:LYS:N	2.47	0.47
25:Y:20:ASN:O	25:Y:24:ARG:N	2.46	0.47
27:b:247:TRP:CD2	51:1:1805:A:H5''	2.49	0.47
27:b:255:LYS:NZ	51:1:1844:C:H4'	2.28	0.47
29:d:109:LEU:HD13	29:d:112:LEU:HD12	1.97	0.47
33:i:133:ARG:HB3	51:1:1077:A:O2'	2.14	0.47
51:1:1123:C:H2'	51:1:1124:G:C8	2.49	0.47
51:1:2184:A:H2'	51:1:2185:U:O4'	2.13	0.47
52:2:5:U:H2'	52:2:6:G:C8	2.49	0.47
53:3:939:G:N3	53:3:1375:A:H2	2.12	0.47
53:3:1427:C:O2	53:3:1427:C:H2'	2.12	0.47
53:3:1527:U:O5'	53:3:1527:U:H6	1.97	0.47
58:B1:395:LYS:NZ	58:B1:399:LYS:CE	2.78	0.47
58:B1:1221:LEU:HD22	58:B1:1306:LEU:HB2	1.96	0.47
27:b:233:GLY:HA3	51:1:2598:A:H5''	1.96	0.47
33:i:124:MET:HE3	33:i:124:MET:HB3	1.70	0.47
51:1:157:C:H2'	51:1:158:U:O4'	2.13	0.47
51:1:419:U:H2'	51:1:420:C:C6	2.49	0.47
51:1:2185:U:H2'	51:1:2186:G:C8	2.48	0.47
51:1:2553:G:C3'	51:1:2554:U:H5''	2.41	0.47
51:1:2852:G:H2'	51:1:2853:C:O4'	2.14	0.47
53:3:1211:U:H4'	53:3:1213:A:C4	2.49	0.47
55:8:14:DC:H2'	55:8:15:DC:H6	1.79	0.47
58:B1:115:TRP:O	58:B1:1333:THR:HG21	2.13	0.47
58:B1:190:LYS:HB2	58:B1:190:LYS:HE3	1.41	0.47
58:B1:201:LEU:HD11	58:B1:220:ARG:HG2	1.95	0.47
59:B2:1286:THR:O	59:B2:1290:MET:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
62:NG:142:ALA:O	62:NG:143:ASP:CB	2.63	0.47
65:a:42:VAL:HB	65:a:175:ILE:HG22	1.96	0.47
14:N:4:GLN:HE22	53:3:1131:G:C5'	2.25	0.47
14:N:113:LYS:NZ	53:3:1367:C:C6	2.83	0.47
19:S:5:MET:SD	19:S:8:ARG:NH1	2.88	0.47
29:d:125:SER:OG	29:d:126:VAL:N	2.48	0.47
38:n:106:ASP:N	38:n:106:ASP:OD1	2.47	0.47
43:s:89:ALA:HB1	51:1:748:G:C8	2.49	0.47
49:y:31:GLN:HE21	49:y:36:GLN:HB2	1.80	0.47
51:1:118:A:H2'	51:1:120:U:O4	2.15	0.47
51:1:609:A:H2'	51:1:610:C:O4'	2.14	0.47
51:1:858:G:H5'	51:1:859:G:OP2	2.14	0.47
51:1:1182:G:H2'	51:1:1183:U:O4'	2.15	0.47
51:1:1533:C:C3'	51:1:1534:U:H5''	2.44	0.47
51:1:1932:A:H2'	51:1:1933:G:O4'	2.15	0.47
53:3:86:G:H4'	53:3:87:C:C6	2.50	0.47
53:3:110:C:H2'	53:3:111:G:O4'	2.13	0.47
66:0:557:ILE:HD13	66:0:576:ILE:HG12	1.96	0.47
9:I:80:ARG:NH1	53:3:613:C:OP2	2.47	0.47
46:v:21:ARG:NH2	52:2:76:G:O3'	2.47	0.47
48:x:22:ASN:HD22	51:1:200:U:H5'	1.79	0.47
51:1:41:C:C3'	51:1:42:A:H5''	2.44	0.47
51:1:282:A:H2'	51:1:283:G:C8	2.50	0.47
51:1:1018:U:H5''	51:1:1036:G:O2'	2.14	0.47
58:B1:29:MET:HG2	59:B2:1336:ASN:ND2	2.29	0.47
58:B1:120:LEU:HD22	58:B1:120:LEU:HA	1.77	0.47
59:B2:1311:GLY:O	60:W0:31:GLN:NE2	2.47	0.47
62:NG:161:SER:CA	62:NG:170:PRO:HA	2.44	0.47
8:H:17:TRP:O	8:H:53:ARG:NH2	2.47	0.47
18:R:102:LYS:HE2	53:3:952:U:O4	2.14	0.47
21:U:68:SER:OG	21:U:69:ASP:OD1	2.33	0.47
21:U:69:ASP:OD1	21:U:69:ASP:N	2.48	0.47
27:b:149:LYS:HG2	27:b:152:GLN:HE22	1.80	0.47
30:e:26:GLN:NE2	52:2:57:A:H4'	2.29	0.47
32:g:99:ILE:O	32:g:103:VAL:N	2.40	0.47
46:v:64:VAL:HA	46:v:69:GLU:HA	1.96	0.47
47:w:70:PRO:HB3	52:2:12:C:C5	2.50	0.47
51:1:395:U:H2'	51:1:396:G:C8	2.50	0.47
51:1:528:A:C2	51:1:2043:C:H4'	2.50	0.47
51:1:903:C:H2'	51:1:904:G:C8	2.49	0.47
51:1:1409:U:H2'	51:1:1410:G:C8	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1680:U:H2'	51:1:1681:G:O4'	2.15	0.47
51:1:1927:A:H2'	51:1:1928:A:C8	2.49	0.47
51:1:2146:C:H5''	51:1:2147:A:N7	2.30	0.47
51:1:2798:U:H4'	51:1:2799:A:C4	2.50	0.47
53:3:24:U:H2'	53:3:25:C:C6	2.50	0.47
53:3:110:C:H2'	53:3:111:G:C8	2.50	0.47
53:3:505:G:OP2	53:3:535:A:H5'	2.13	0.47
53:3:599:C:H2'	53:3:600:A:H8	1.80	0.47
53:3:946:A:H2'	53:3:947:G:C8	2.49	0.47
57:A2:102:LEU:HD12	57:A2:115:ILE:HG12	1.96	0.47
58:B1:198:CYS:HA	58:B1:221:ILE:CD1	2.45	0.47
58:B1:1036:ARG:HE	58:B1:1081:VAL:HG11	1.79	0.47
58:B1:1060:VAL:HG13	58:B1:1106:ILE:HG12	1.96	0.47
58:B1:1347:LEU:HG	58:B1:1357:ILE:HG23	1.96	0.47
58:B1:1361:THR:OG1	59:B2:1282:GLY:O	2.28	0.47
59:B2:689:ALA:HB2	59:B2:1233:LEU:HD23	1.97	0.47
63:5:26:A:N6	63:5:44:G:H1	2.13	0.47
66:0:176:GLU:O	66:0:179:PHE:N	2.47	0.47
10:J:18:ASN:OD1	10:J:33:THR:OG1	2.33	0.47
12:L:21:LEU:HD11	12:L:96:ASN:HD22	1.78	0.47
38:n:58:ASP:OD1	38:n:63:ARG:NH2	2.48	0.47
51:1:368:A:C2'	51:1:369:U:H5'	2.45	0.47
51:1:1409:U:H2'	51:1:1410:G:H8	1.80	0.47
51:1:1960:A:C2'	51:1:1961:C:H5''	2.44	0.47
51:1:2638:G:H1'	51:1:2778:A:N6	2.26	0.47
58:B1:526:VAL:HG12	58:B1:549:LYS:HB2	1.96	0.47
58:B1:1357:ILE:HD13	59:B2:1279:GLU:HG2	1.97	0.47
65:a:200:LYS:HD3	65:a:201:PRO:HD2	1.97	0.47
24:X:32:THR:HG1	24:X:34:SER:HG	1.62	0.47
35:k:66:LYS:HD2	51:1:1665:A:H5''	1.95	0.47
36:l:89:VAL:HA	36:l:121:THR:HB	1.97	0.47
39:o:67:ASN:HA	52:2:50:A:OP2	2.15	0.47
39:o:94:ARG:NH2	51:1:2293:G:H5''	2.30	0.47
42:r:78:ARG:NH1	51:1:990:A:H61	2.13	0.47
51:1:1387:A:H5'	51:1:1469:A:H1'	1.96	0.47
53:3:66:A:H5''	53:3:199:A:O2'	2.15	0.47
53:3:935:A:H2'	53:3:936:C:C6	2.50	0.47
53:3:987:G:H2'	53:3:988:G:H8	1.80	0.47
53:3:1223:C:H5	53:3:1224:U:H5	1.63	0.47
58:B1:128:LEU:HD21	58:B1:188:LEU:HB3	1.97	0.47
58:B1:968:ASN:HA	58:B1:1117:SER:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:1261:LEU:HD12	58:B1:1304:ARG:HH21	1.78	0.47
59:B2:400:VAL:HG22	59:B2:584:TYR:HB3	1.96	0.47
66:0:592:ALA:O	66:0:596:ALA:N	2.46	0.47
9:I:82:LYS:HE2	53:3:3:A:OP1	2.16	0.47
28:c:133:THR:HG22	28:c:134:HIS:H	1.80	0.47
41:q:105:PHE:HA	41:q:108:LEU:HD12	1.96	0.47
51:1:76:C:H2'	51:1:77:G:H8	1.80	0.47
51:1:552:U:H2'	51:1:553:G:H8	1.80	0.47
51:1:855:G:H3'	51:1:856:G:H5''	1.98	0.47
51:1:1175:A:H5'	51:1:1176:U:O4'	2.15	0.47
53:3:680:C:H2'	53:3:681:A:H8	1.80	0.47
57:A1:35:PHE:HA	57:A1:38:THR:HG22	1.97	0.47
58:B1:343:LEU:HD11	58:B1:1324:SER:HB3	1.97	0.47
58:B1:1219:ASP:O	58:B1:1223:LEU:HB2	2.15	0.47
59:B2:103:VAL:HG12	59:B2:117:ILE:HG22	1.97	0.47
59:B2:207:THR:OG1	59:B2:354:ASP:OD2	2.32	0.47
65:a:189:LEU:O	65:a:193:LEU:N	2.44	0.47
9:I:4:LEU:HD11	53:3:405:U:C6	2.50	0.46
15:O:42:LEU:HB3	15:O:71:LEU:HB2	1.96	0.46
29:d:155:GLU:HA	29:d:158:PHE:HB3	1.97	0.46
30:e:140:ILE:HG22	30:e:142:TYR:H	1.80	0.46
31:f:21:GLN:OE1	31:f:54:ARG:NH2	2.39	0.46
42:r:7:SER:OG	42:r:8:GLY:N	2.49	0.46
51:1:1906:G:C2'	51:1:1907:G:H5''	2.44	0.46
53:3:211:G:C2'	53:3:212:G:H5'	2.45	0.46
53:3:536:C:H2'	53:3:537:G:C8	2.49	0.46
58:B1:375:GLU:HB3	59:B2:1245:ALA:HB3	1.97	0.46
58:B1:833:GLU:N	58:B1:1242:ARG:HH12	2.12	0.46
63:5:8:U:H2'	63:5:13:C:N4	2.30	0.46
24:X:9:PHE:CE1	53:3:1318:A:H5'	2.50	0.46
39:o:13:ARG:HH21	39:o:17:LYS:HB2	1.80	0.46
50:z:17:PRO:HG3	51:1:969:G:OP1	2.14	0.46
51:1:311:A:H3'	51:1:312:G:C8	2.49	0.46
51:1:940:G:C3'	51:1:941:A:H5''	2.45	0.46
51:1:1017:G:H2'	51:1:1018:U:C6	2.50	0.46
51:1:1179:G:C4	51:1:1180:U:H1'	2.50	0.46
51:1:1300:G:H4'	51:1:1301:A:H5''	1.97	0.46
52:2:96:G:O2'	52:2:97:C:H5'	2.15	0.46
53:3:202:G:H2'	53:3:203:G:C8	2.50	0.46
53:3:479:U:H2'	53:3:480:U:H5'	1.96	0.46
53:3:1060:U:H2'	53:3:1061:G:C8	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:772:TYR:HE2	59:B2:561:ILE:HG21	1.81	0.46
59:B2:28:LEU:HD21	59:B2:524:ILE:HG13	1.98	0.46
12:L:71:THR:O	12:L:90:VAL:HG22	2.16	0.46
14:N:4:GLN:HE22	53:3:1131:G:C4'	2.28	0.46
17:Q:68:GLY:O	53:3:521:G:H5'	2.15	0.46
17:Q:109:ARG:HG3	53:3:538:G:OP1	2.15	0.46
21:U:68:SER:OG	21:U:69:ASP:N	2.47	0.46
51:1:610:C:H2'	51:1:611:C:H6	1.80	0.46
51:1:1023:U:H2'	51:1:1024:G:H5'	1.97	0.46
51:1:2467:C:H2'	51:1:2468:A:O4'	2.15	0.46
53:3:390:U:H2'	53:3:391:G:C8	2.50	0.46
53:3:629:A:H2'	53:3:630:A:O4'	2.15	0.46
53:3:1210:C:OP1	66:0:584:HIS:CG	2.68	0.46
53:3:1329:A:O2'	53:3:1330:U:H5'	2.16	0.46
53:3:1369:C:H2'	53:3:1370:G:C8	2.49	0.46
58:B1:385:LEU:HD23	58:B1:390:LEU:HB2	1.98	0.46
59:B2:230:PHE:HB2	59:B2:333:ILE:HB	1.97	0.46
59:B2:735:LYS:HA	59:B2:748:ILE:HG22	1.97	0.46
65:a:69:THR:HA	65:a:176:GLY:HA2	1.97	0.46
66:0:624:PRO:HA	66:0:651:GLY:HA2	1.97	0.46
9:I:61:ARG:HH12	9:I:68:GLU:N	2.13	0.46
12:L:26:VAL:HG22	12:L:42:VAL:HG21	1.98	0.46
19:S:51:PRO:O	19:S:54:SER:OG	2.31	0.46
25:Y:9:ARG:NH1	53:3:107:G:O6	2.49	0.46
25:Y:73:ARG:NE	53:3:261:U:H5	2.12	0.46
27:b:46:GLY:HA3	51:1:773:U:H4'	1.97	0.46
27:b:140:VAL:HG23	27:b:161:VAL:HG13	1.96	0.46
33:i:129:GLU:HB2	33:i:139:VAL:HG21	1.98	0.46
39:o:30:ARG:HH21	39:o:97:PHE:HB3	1.80	0.46
51:1:562:U:O4'	51:1:2036:C:H5'	2.16	0.46
51:1:1557:C:H3'	51:1:1558:C:C5'	2.31	0.46
51:1:1717:A:H2'	51:1:1718:G:O4'	2.15	0.46
51:1:2126:A:C2'	51:1:2162:G:H21	2.29	0.46
53:3:82:G:C2'	53:3:83:C:H5'	2.45	0.46
53:3:1497:G:C2'	53:3:1498:U:H5'	2.46	0.46
58:B1:43:THR:HG22	58:B1:57:PHE:HE1	1.80	0.46
58:B1:111:THR:HG23	58:B1:300:GLN:NE2	2.24	0.46
58:B1:420:PRO:HA	58:B1:437:PHE:O	2.15	0.46
59:B2:800:MET:HB2	59:B2:800:MET:HE3	1.69	0.46
65:a:186:LYS:HA	65:a:189:LEU:HG	1.97	0.46
13:M:9:MET:HB2	13:M:32:LYS:HE2	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:70:GLY:O	14:N:74:GLN:N	2.41	0.46
14:N:128:LYS:HE3	64:6:34:C:OP2	2.16	0.46
27:b:48:ILE:HG22	51:1:779:U:P	2.55	0.46
27:b:200:MET:HE2	51:1:1820:U:C2	2.50	0.46
29:d:168:ASP:OD1	29:d:168:ASP:N	2.47	0.46
30:e:146:ASP:OD1	30:e:146:ASP:N	2.48	0.46
37:m:31:PHE:HB3	37:m:130:PHE:HE1	1.80	0.46
51:1:479:A:H4'	51:1:480:A:H5'	1.98	0.46
51:1:610:C:H2'	51:1:611:C:C6	2.50	0.46
51:1:1335:C:H2'	51:1:1336:A:H8	1.80	0.46
51:1:1709:U:H2'	51:1:1710:G:C8	2.50	0.46
51:1:1872:A:H2'	51:1:1873:G:O4'	2.15	0.46
51:1:2126:A:H5'	51:1:2127:G:O5'	2.16	0.46
51:1:2653:U:C3'	51:1:2654:A:H5''	2.38	0.46
51:1:2849:U:H4'	51:1:2868:A:C2	2.50	0.46
53:3:31:G:N2	53:3:47:C:H5''	2.31	0.46
53:3:177:G:O2'	53:3:1448:C:H4'	2.14	0.46
53:3:864:A:H2'	53:3:865:A:C8	2.50	0.46
58:B1:105:ILE:HD12	58:B1:242:LEU:CD2	2.44	0.46
58:B1:352:ARG:HB2	59:B2:1268:GLN:NE2	2.30	0.46
58:B1:847:ASP:N	58:B1:847:ASP:OD1	2.49	0.46
63:5:8:U:H2'	63:5:13:C:H41	1.80	0.46
1:A:53:THR:OG1	1:A:54:GLY:N	2.49	0.46
14:N:108:ARG:O	53:3:1347:G:H8	1.99	0.46
16:P:17:ASP:N	16:P:17:ASP:OD1	2.49	0.46
51:1:2644:G:C2'	51:1:2645:G:H5'	2.46	0.46
53:3:194:C:O2'	53:3:195:A:H5'	2.15	0.46
53:3:408:A:H2'	53:3:409:U:O4'	2.16	0.46
53:3:490:C:H2'	53:3:491:G:C8	2.50	0.46
53:3:1382:C:O2	53:3:1382:C:O4'	2.33	0.46
54:4:5:U:H2'	54:4:6:U:C6	2.50	0.46
58:B1:1167:LYS:NZ	58:B1:1170:LYS:HB2	2.30	0.46
66:0:20:ASP:HA	69:0:801:GDP:H5'	1.96	0.46
8:H:176:THR:HG22	8:H:179:ALA:H	1.81	0.46
21:U:5:ARG:HD2	53:3:376:G:H4'	1.97	0.46
32:g:103:VAL:O	32:g:107:GLY:N	2.49	0.46
41:q:92:LYS:NZ	51:1:995:C:O2'	2.44	0.46
51:1:1344:U:H3'	51:1:1345:C:H5'	1.96	0.46
51:1:1433:A:H2'	51:1:1434:A:O4'	2.16	0.46
51:1:1842:G:H2'	51:1:1843:C:O4'	2.16	0.46
53:3:51:A:H4'	53:3:52:C:H5''	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:A1:33:ARG:HE	57:A1:33:ARG:HB3	1.56	0.46
66:O:255:ARG:HD3	66:O:261:ILE:HB	1.97	0.46
12:L:87:PRO:HG3	12:L:148:LYS:HA	1.98	0.46
12:L:111:GLY:HA2	12:L:118:ARG:HD3	1.97	0.46
16:P:123:PRO:O	26:Z:34:ARG:N	2.40	0.46
17:Q:14:LYS:HE3	53:3:884:U:O2'	2.15	0.46
27:b:54:GLY:HA3	27:b:216:ARG:HG3	1.98	0.46
33:i:11:GLN:HG2	33:i:23:VAL:HG11	1.98	0.46
42:r:81:LYS:HD3	51:1:973:A:H5''	1.98	0.46
51:1:337:C:H2'	51:1:338:G:O4'	2.15	0.46
51:1:341:C:H2'	51:1:342:A:H8	1.80	0.46
51:1:621:A:H2'	51:1:622:G:O4'	2.15	0.46
51:1:1000:A:H2'	51:1:1001:A:C8	2.51	0.46
51:1:2670:A:H2'	51:1:2671:G:H8	1.81	0.46
51:1:2773:C:H2'	51:1:2774:C:C6	2.51	0.46
51:1:2898:U:H2'	51:1:2899:A:C8	2.51	0.46
53:3:70:U:H4'	53:3:71:A:C8	2.51	0.46
53:3:91:U:C2'	53:3:92:U:H5''	2.45	0.46
57:A1:29:GLU:HB3	57:A1:200:LYS:HG3	1.98	0.46
57:A2:294:ASN:HA	61:NA:464:ILE:N	2.28	0.46
62:NG:135:ARG:O	62:NG:178:VAL:HA	2.16	0.46
66:O:33:TYR:HE2	66:O:275:VAL:HB	1.81	0.46
1:A:63:ARG:HD2	53:3:1012:A:OP2	2.16	0.46
9:I:72:ARG:HG2	9:I:76:LYS:HE3	1.97	0.46
24:X:79:TYR:CZ	53:3:1226:C:H4'	2.51	0.46
27:b:200:MET:HE2	51:1:1820:U:N3	2.31	0.46
41:q:74:SER:OG	41:q:75:TYR:N	2.49	0.46
42:r:85:LYS:HA	51:1:814:C:OP1	2.16	0.46
47:w:38:GLY:CA	51:1:2330:G:H21	2.26	0.46
51:1:209:C:H4'	51:1:681:G:H4'	1.97	0.46
51:1:1015:U:H2'	51:1:1016:G:C8	2.51	0.46
51:1:1638:C:H5''	51:1:2710:C:O2'	2.16	0.46
51:1:2066:C:O2'	51:1:2067:G:H5'	2.16	0.46
51:1:2176:A:H5'	65:a:219:GLY:O	2.16	0.46
53:3:652:U:H2'	53:3:653:U:H5''	1.98	0.46
53:3:1414:U:H2'	53:3:1415:G:H8	1.81	0.46
60:W0:25:ARG:NH1	60:W0:61:ASN:OD1	2.49	0.46
63:5:70:G:H2'	63:5:71:G:C8	2.51	0.46
66:O:536:PHE:HD1	66:O:576:ILE:HG23	1.81	0.46
8:H:23:ALA:HB1	8:H:27:GLU:HG2	1.97	0.46
14:N:86:LEU:HD13	14:N:93:LEU:HD22	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:97:ARG:HG3	53:3:1308:U:OP2	2.16	0.46
34:j:80:HIS:CD2	51:1:2642:G:H5'	2.51	0.46
46:v:30:ILE:HG12	46:v:91:PHE:HB2	1.96	0.46
51:1:416:U:H3	51:1:2407:A:H61	1.63	0.46
51:1:878:A:H3'	51:1:879:G:C8	2.50	0.46
52:2:43:C:H2'	52:2:44:G:H5''	1.97	0.46
52:2:49:C:H2'	52:2:50:A:C8	2.49	0.46
53:3:312:C:H2'	53:3:313:A:C8	2.51	0.46
53:3:1268:G:H21	53:3:1327:C:H1'	1.80	0.46
55:8:20:DA:H4'	59:B2:143:ARG:NH1	2.31	0.46
57:A1:59:VAL:HG22	57:A1:144:ILE:HA	1.97	0.46
58:B1:109:SER:HB2	58:B1:296:LYS:HG2	1.98	0.46
66:0:515:TYR:HB3	66:0:584:HIS:CB	2.44	0.46
66:0:523:TYR:HD2	66:0:577:ARG:HH12	1.63	0.46
66:0:667:ALA:HB2	66:0:680:TYR:HE1	1.80	0.46
5:E:3:ILE:HD11	51:1:592:A:C2	2.51	0.45
24:X:36:ARG:HB3	53:3:1320:C:N4	2.30	0.45
27:b:141:HIS:ND1	27:b:192:GLY:O	2.37	0.45
38:n:64:ARG:HH11	51:1:2705:A:H2	1.62	0.45
44:t:2:ILE:HG13	44:t:5:GLU:HB3	1.98	0.45
51:1:863:A:H4'	52:2:100:G:N2	2.31	0.45
51:1:894:U:H2'	51:1:895:U:O4'	2.16	0.45
51:1:1758:U:C5	51:1:2696:U:H5'	2.51	0.45
51:1:1822:C:H2'	51:1:1823:G:H8	1.81	0.45
51:1:2211:A:H5'	51:1:2212:A:OP2	2.16	0.45
51:1:2573:C:H5''	51:1:2574:G:H5''	1.98	0.45
51:1:2649:C:H2'	51:1:2650:U:C6	2.51	0.45
51:1:2804:U:H2'	51:1:2805:C:C6	2.51	0.45
51:1:2811:G:H2'	51:1:2812:G:C8	2.51	0.45
52:2:66:A:N1	52:2:107:G:H2'	2.31	0.45
53:3:555:U:H2'	53:3:556:C:C6	2.52	0.45
53:3:1275:A:N1	53:3:1283:U:H5'	2.31	0.45
58:B1:209:ASN:HA	58:B1:214:ARG:NH2	2.30	0.45
58:B1:211:GLU:CG	58:B1:215:LYS:HE3	2.44	0.45
27:b:17:LYS:HE3	27:b:17:LYS:HB2	1.83	0.45
33:i:5:GLN:H	33:i:5:GLN:HG3	1.53	0.45
51:1:676:A:H62	51:1:802:A:H61	1.63	0.45
51:1:979:A:H2'	51:1:982:C:H42	1.81	0.45
51:1:1020:A:C1'	51:1:1021:A:OP2	2.60	0.45
51:1:1424:G:H2'	51:1:1425:G:O4'	2.17	0.45
51:1:2468:A:O2'	51:1:2469:A:H5'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2800:A:H3'	51:1:2801:G:C5'	2.45	0.45
53:3:253:A:H2'	53:3:254:G:H8	1.81	0.45
53:3:448:A:H3'	53:3:449:G:C8	2.51	0.45
53:3:1107:C:O2'	53:3:1191:A:H4'	2.16	0.45
53:3:1137:C:H5'	53:3:1138:G:H5'	1.97	0.45
53:3:1146:A:H2'	53:3:1147:C:H5'	1.97	0.45
53:3:1342:C:H2'	53:3:1343:G:C8	2.51	0.45
57:A2:64:VAL:HG11	57:A2:78:ILE:HG21	1.97	0.45
57:A2:80:GLU:HG3	59:B2:694:ARG:HH22	1.81	0.45
58:B1:202:ARG:HH11	58:B1:202:ARG:CG	2.14	0.45
58:B1:213:LYS:HA	58:B1:213:LYS:HE3	1.99	0.45
58:B1:842:ARG:HH22	58:B1:1250:ASP:HB2	1.80	0.45
59:B2:517:GLN:HB3	59:B2:760:ASN:H	1.79	0.45
66:0:131:ASN:OD1	66:0:137:ARG:NH2	2.50	0.45
9:I:173:ASP:HB3	9:I:178:GLU:H	1.82	0.45
15:O:6:ILE:HD12	15:O:102:LEU:HG	1.97	0.45
19:S:92:ILE:HD13	19:S:95:LEU:HD12	1.97	0.45
24:X:5:LYS:HG2	53:3:1313:U:P	2.56	0.45
25:Y:28:ARG:HD3	53:3:1438:G:OP1	2.16	0.45
25:Y:73:ARG:CZ	53:3:261:U:C5	2.98	0.45
30:e:12:VAL:HG13	30:e:27:VAL:HG11	1.98	0.45
39:o:24:THR:HB	39:o:42:PRO:HG3	1.97	0.45
39:o:27:VAL:HG12	39:o:93:ASP:HB3	1.98	0.45
43:s:33:LEU:O	43:s:37:THR:OG1	2.33	0.45
51:1:195:A:H3'	51:1:196:A:H4'	1.99	0.45
51:1:687:C:H2'	51:1:688:U:O4'	2.16	0.45
51:1:700:G:O2'	51:1:701:G:H5'	2.17	0.45
51:1:933:A:H5''	51:1:934:U:H5	1.81	0.45
51:1:999:U:O2'	51:1:1000:A:H5'	2.16	0.45
51:1:1112:G:O2'	51:1:1113:U:H5'	2.15	0.45
51:1:2146:C:H5''	51:1:2147:A:C8	2.51	0.45
51:1:2174:C:O2'	65:a:218:MET:HG2	2.17	0.45
51:1:2189:U:H2'	51:1:2190:G:C8	2.51	0.45
51:1:2385:C:H2'	51:1:2386:A:C8	2.51	0.45
53:3:405:U:C3'	53:3:406:G:H5'	2.40	0.45
53:3:1149:C:O2'	53:3:1150:A:H5'	2.17	0.45
58:B1:375:GLU:O	59:B2:1247:SER:HB3	2.16	0.45
58:B1:800:LEU:HD12	58:B1:800:LEU:HA	1.79	0.45
59:B2:1314:GLN:HA	60:W0:28:ARG:HH22	1.80	0.45
3:C:35:LEU:HD11	51:1:2286:G:N1	2.32	0.45
18:R:26:LYS:O	18:R:30:LYS:NZ	2.44	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:100:ARG:HH21	18:R:102:LYS:HD3	1.81	0.45
25:Y:2:ASN:N	53:3:332:G:OP2	2.50	0.45
50:z:40:THR:HG23	50:z:42:ALA:H	1.80	0.45
51:1:863:A:H2'	51:1:864:G:C8	2.51	0.45
51:1:1011:G:H1'	51:1:1013:C:O4'	2.16	0.45
51:1:2190:G:O2'	51:1:2191:A:H5'	2.16	0.45
51:1:2472:G:O6	51:1:2476:A:H4'	2.16	0.45
53:3:401:C:H2'	53:3:402:G:H8	1.81	0.45
66:0:305:THR:O	66:0:305:THR:OG1	2.34	0.45
11:K:49:TYR:HB3	23:W:73:HIS:CG	2.52	0.45
26:Z:66:ARG:HD2	53:3:1099:G:H4'	1.99	0.45
37:m:2:LEU:HD23	37:m:2:LEU:HA	1.85	0.45
51:1:677:A:O2'	51:1:2071:A:H5'	2.17	0.45
51:1:748:G:H2'	51:1:750:A:OP2	2.17	0.45
51:1:2843:G:O2'	51:1:2844:G:H5'	2.17	0.45
53:3:974:A:H5'	53:3:976:G:OP1	2.17	0.45
53:3:990:C:H2'	53:3:991:U:O4'	2.16	0.45
53:3:1005:A:C2'	53:3:1006:G:H5'	2.46	0.45
53:3:1202:U:H2'	53:3:1203:C:O4'	2.16	0.45
55:8:1:DC:H2''	55:8:2:DC:C6	2.51	0.45
55:8:13:DT:C6	58:B1:791:ALA:HA	2.51	0.45
58:B1:75:TYR:CD2	58:B1:75:TYR:O	2.70	0.45
58:B1:484:MET:CE	59:B2:1278:LEU:HD21	2.47	0.45
58:B1:926:PRO:HB2	58:B1:1241:TYR:HE1	1.82	0.45
63:5:6:G:H2'	63:5:7:A:C8	2.51	0.45
66:0:11:ARG:NH1	66:0:288:SER:OG	2.50	0.45
11:K:38:ARG:HB2	11:K:63:ASN:HB2	1.98	0.45
12:L:67:ASN:O	12:L:137:ARG:NH1	2.49	0.45
24:X:53:GLY:HA3	53:3:958:A:H61	1.81	0.45
38:n:21:PHE:HB3	38:n:47:VAL:HG21	1.99	0.45
40:p:27:VAL:HG13	40:p:42:PHE:HB3	1.98	0.45
50:z:27:GLY:HA3	50:z:37:ARG:HH21	1.81	0.45
51:1:2215:C:H2'	51:1:2216:G:H8	1.81	0.45
53:3:350:G:H2'	53:3:351:G:C8	2.52	0.45
53:3:423:G:H3'	53:3:423:G:N3	2.32	0.45
53:3:485:U:H5'	53:3:486:U:OP2	2.16	0.45
53:3:1005:A:H2'	53:3:1006:G:O4'	2.16	0.45
53:3:1306:A:C2	53:3:1332:A:H1'	2.51	0.45
57:A1:231:PHE:O	57:A2:218:ARG:NH1	2.49	0.45
58:B1:770:LEU:HD13	59:B2:618:GLN:CD	2.42	0.45
59:B2:893:THR:HB	59:B2:914:LYS:HA	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:107:GLY:CA	53:3:8:A:H1'	2.46	0.45
27:b:237:ARG:NH1	51:1:2590:A:O3'	2.49	0.45
38:n:39:PRO:HG3	51:1:1651:G:C5'	2.46	0.45
40:p:22:GLY:H	40:p:46:VAL:HG23	1.81	0.45
51:1:2332:C:H2'	51:1:2335:A:N3	2.31	0.45
52:2:97:C:H2'	52:2:98:G:C5'	2.46	0.45
53:3:315:A:H5''	53:3:317:U:OP2	2.17	0.45
53:3:820:U:H3'	53:3:821:G:C5'	2.47	0.45
58:B1:67:ASP:OD1	58:B1:67:ASP:O	2.35	0.45
58:B1:141:PHE:CE2	58:B1:296:LYS:CB	2.94	0.45
66:0:15:ILE:HG13	66:0:110:VAL:HB	1.99	0.45
5:E:34:LYS:HD2	51:1:2391:G:OP2	2.17	0.45
12:L:9:ARG:NH2	53:3:1346:A:C8	2.85	0.45
33:i:120:ASP:O	33:i:123:ALA:N	2.49	0.45
51:1:90:U:H2'	51:1:91:A:C8	2.51	0.45
51:1:503:A:H5''	51:1:505:A:OP1	2.17	0.45
51:1:634:C:H2'	51:1:635:C:C6	2.52	0.45
51:1:1528:A:H2'	51:1:1529:G:O4'	2.17	0.45
51:1:1725:U:H2'	51:1:1726:C:C6	2.51	0.45
51:1:1934:C:H4'	51:1:1974:C:O3'	2.17	0.45
57:A1:185:TYR:HA	57:A1:202:VAL:O	2.16	0.45
58:B1:33:TRP:HZ2	59:B2:1336:ASN:OD1	2.00	0.45
58:B1:213:LYS:HE3	58:B1:213:LYS:CA	2.47	0.45
58:B1:395:LYS:NZ	58:B1:399:LYS:HE2	2.32	0.45
63:5:33:U:H6	63:5:36:A:H8	1.65	0.45
63:5:69:G:H2'	63:5:70:G:C8	2.52	0.45
27:b:204:LEU:HD21	27:b:213:ARG:HH21	1.82	0.45
38:n:42:LYS:HG2	38:n:45:ARG:HH21	1.82	0.45
42:r:85:LYS:HE3	51:1:815:C:P	2.57	0.45
51:1:207:A:H2'	51:1:208:C:O4'	2.16	0.45
51:1:275:C:H2'	51:1:276:U:H4'	1.98	0.45
51:1:300:A:C5	51:1:334:C:H4'	2.52	0.45
51:1:519:U:H2'	51:1:520:G:H8	1.82	0.45
51:1:1045:C:C5'	51:1:1046:A:C8	2.94	0.45
51:1:1558:C:H6	51:1:1558:C:OP1	1.98	0.45
51:1:1697:G:H3'	51:1:1698:A:C5'	2.36	0.45
53:3:451:A:N6	53:3:480:U:H2'	2.32	0.45
53:3:556:C:H2'	53:3:557:G:O4'	2.17	0.45
53:3:819:A:H5'	53:3:820:U:H5	1.82	0.45
53:3:1261:A:H5''	53:3:1262:C:H5	1.82	0.45
59:B2:557:ARG:NH2	59:B2:607:SER:O	2.49	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
66:0:149:ALA:N	66:0:176:GLU:OE1	2.43	0.45
66:0:169:LEU:HG	66:0:263:LEU:HB3	1.99	0.45
6:F:29:ALA:O	31:f:169:ARG:NH1	2.44	0.45
28:c:103:ASP:OD1	28:c:103:ASP:N	2.49	0.45
30:e:70:ARG:HH12	30:e:71:LYS:HE3	1.82	0.45
31:f:120:ILE:HG22	31:f:134:GLY:HA3	1.99	0.45
51:1:322:A:H5'	51:1:340:A:C1'	2.46	0.45
51:1:1637:A:H4'	51:1:2711:A:O2'	2.16	0.45
51:1:2123:G:H2'	51:1:2124:G:C8	2.52	0.45
51:1:2177:C:H1'	65:a:172:HIS:NE2	2.32	0.45
51:1:2554:U:H2'	51:1:2555:U:C6	2.52	0.45
51:1:2646:C:H2'	51:1:2647:U:O4'	2.17	0.45
53:3:303:A:H2'	53:3:304:U:O4'	2.17	0.45
53:3:1449:C:O2'	53:3:1450:U:H5'	2.16	0.45
58:B1:506:VAL:HG23	58:B1:628:GLY:HA3	1.99	0.45
6:F:4:ARG:NH1	6:F:35:GLN:OE1	2.50	0.44
12:L:115:MET:HA	12:L:118:ARG:HB2	1.98	0.44
14:N:64:ILE:HG21	14:N:78:ILE:HG12	1.98	0.44
33:i:34:ILE:O	33:i:38:CYS:N	2.49	0.44
41:q:32:ARG:HB2	51:1:581:C:OP1	2.16	0.44
51:1:828:U:H2'	51:1:829:A:C8	2.51	0.44
51:1:942:G:H2'	51:1:943:A:O4'	2.16	0.44
51:1:2093:G:N7	51:1:2225:A:H2'	2.31	0.44
53:3:596:A:H5'	53:3:596:A:H8	1.82	0.44
53:3:1042:A:H2'	53:3:1043:G:H1'	1.99	0.44
53:3:1289:A:H2'	53:3:1290:G:H5'	1.99	0.44
58:B1:115:TRP:HB3	58:B1:1333:THR:CG2	2.46	0.44
59:B2:998:LEU:HG	59:B2:1011:LEU:HB3	1.99	0.44
59:B2:1246:ARG:HH11	59:B2:1266:GLY:HA2	1.82	0.44
66:0:514:GLN:HA	66:0:587:ASP:HB3	1.99	0.44
66:0:602:LYS:HD3	66:0:602:LYS:HA	1.82	0.44
9:I:24:VAL:H	53:3:409:U:H5''	1.82	0.44
9:I:141:VAL:HG23	9:I:180:THR:HG22	1.99	0.44
29:d:111:GLU:OE1	29:d:114:ARG:NH2	2.50	0.44
41:q:2:ARG:HH11	51:1:449:A:H4'	1.81	0.44
44:t:11:LEU:O	49:y:29:ARG:NH2	2.50	0.44
51:1:20:C:H2'	51:1:21:A:H8	1.81	0.44
51:1:311:A:H3'	51:1:312:G:H8	1.82	0.44
51:1:864:G:O2'	51:1:865:C:H5'	2.17	0.44
51:1:2157:G:H5''	51:1:2158:A:OP1	2.17	0.44
51:1:2206:C:H2'	51:1:2207:C:C6	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:29:U:H5'	53:3:296:U:OP1	2.17	0.44
53:3:169:C:H2'	53:3:170:U:C5	2.52	0.44
53:3:513:C:H2'	53:3:514:C:H6	1.82	0.44
53:3:884:U:H4'	53:3:885:G:C5'	2.43	0.44
53:3:1222:G:O2'	53:3:1223:C:H5'	2.17	0.44
53:3:1268:G:H21	53:3:1327:C:C1'	2.29	0.44
55:8:16:DT:H2'	55:8:17:DC:C6	2.52	0.44
56:9:12:DC:H3'	58:B1:47:ARG:HH12	1.82	0.44
58:B1:76:LYS:NZ	58:B1:76:LYS:HB3	2.32	0.44
58:B1:141:PHE:HE2	58:B1:296:LYS:CB	2.23	0.44
58:B1:175:GLU:H	58:B1:175:GLU:HG3	1.66	0.44
58:B1:1158:GLU:HA	58:B1:1223:LEU:HD21	1.99	0.44
59:B2:1002:LEU:HD21	59:B2:1007:LYS:HB2	1.98	0.44
63:5:13:C:H42	63:5:46:G:N2	2.15	0.44
66:0:498:VAL:HG11	66:0:522:MET:H	1.82	0.44
15:O:64:GLN:NE2	53:3:1368:A:OP1	2.51	0.44
16:P:117:HIS:CD2	53:3:675:A:H1'	2.53	0.44
20:T:49:HIS:CD2	53:3:764:C:H5''	2.52	0.44
27:b:46:GLY:HA3	51:1:773:U:H5'	2.00	0.44
28:c:109:VAL:HG11	28:c:193:VAL:HB	1.99	0.44
51:1:133:U:H2'	51:1:134:G:C8	2.52	0.44
51:1:1102:C:H2'	51:1:1103:A:O4'	2.17	0.44
51:1:1822:C:H2'	51:1:1823:G:C8	2.53	0.44
51:1:2457:U:O2'	51:1:2458:G:H5'	2.18	0.44
51:1:2654:A:H8	51:1:2654:A:OP1	2.01	0.44
51:1:2670:A:H2'	51:1:2671:G:C8	2.53	0.44
53:3:495:A:H4'	53:3:496:A:H5'	1.99	0.44
53:3:1209:C:H2'	53:3:1210:C:C6	2.52	0.44
58:B1:388:ARG:HG2	58:B1:388:ARG:NH1	2.32	0.44
58:B1:472:LEU:CD1	59:B2:1294:LYS:HG2	2.47	0.44
58:B1:978:ARG:HD3	58:B1:999:TYR:H	1.82	0.44
58:B1:1227:HIS:HA	58:B1:1230:THR:HG22	1.99	0.44
58:B1:1357:ILE:HG22	58:B1:1359:ALA:H	1.83	0.44
59:B2:176:ILE:HD11	59:B2:428:VAL:HG21	1.98	0.44
63:5:49:C:H2'	63:5:50:U:C6	2.52	0.44
1:A:46:GLY:HA2	1:A:49:ARG:HG2	1.98	0.44
28:c:32:ASN:O	28:c:96:ILE:N	2.50	0.44
28:c:109:VAL:HG13	28:c:201:LEU:HD13	2.00	0.44
35:k:97:THR:OG1	35:k:98:ARG:N	2.51	0.44
37:m:34:LYS:HE3	37:m:131:VAL:HG11	1.98	0.44
38:n:35:LYS:NZ	38:n:100:CYS:SG	2.91	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:25:ARG:HE	43:s:74:ILE:HG23	1.82	0.44
44:t:30:ILE:HG23	44:t:85:VAL:HB	1.99	0.44
51:1:892:A:O2'	51:1:893:C:H5'	2.17	0.44
51:1:1363:C:O2'	51:1:1364:G:H5'	2.18	0.44
51:1:1595:C:H2'	51:1:1596:A:C8	2.52	0.44
51:1:2443:C:O2'	51:1:2444:G:H5'	2.17	0.44
57:A1:192:VAL:HG12	57:A1:193:GLU:H	1.83	0.44
58:B1:731:ARG:HB3	59:B2:1105:SER:HB2	1.99	0.44
65:a:46:VAL:HG22	65:a:212:VAL:HG13	1.99	0.44
65:a:65:LEU:HD13	65:a:188:ASN:HD21	1.83	0.44
65:a:173:THR:HG22	65:a:174:THR:H	1.82	0.44
66:0:491:ARG:HD2	66:0:570:PRO:HB2	1.99	0.44
1:A:58:ASP:HB2	24:X:20:LYS:HB2	1.99	0.44
7:G:58:LYS:O	7:G:61:SER:OG	2.32	0.44
8:H:135:ARG:HH22	54:4:14:U:H1'	1.83	0.44
28:c:114:LYS:HD2	51:1:2820:A:O2'	2.17	0.44
31:f:41:GLU:HA	31:f:54:ARG:HH21	1.81	0.44
40:p:15:ASP:N	40:p:15:ASP:OD1	2.48	0.44
51:1:367:G:O2'	51:1:368:A:H5'	2.18	0.44
51:1:716:A:C2	51:1:717:C:H1'	2.52	0.44
51:1:861:A:H2'	51:1:862:G:O4'	2.18	0.44
51:1:1064:C:C3'	51:1:1065:U:C5'	2.91	0.44
51:1:2189:U:H2'	51:1:2190:G:H8	1.83	0.44
51:1:2515:C:H2'	51:1:2516:A:H8	1.81	0.44
53:3:288:A:H2'	53:3:289:G:H4'	1.99	0.44
53:3:667:G:H2'	53:3:668:G:H8	1.83	0.44
53:3:993:G:N3	53:3:993:G:H2'	2.32	0.44
60:W0:58:LEU:HD12	60:W0:59:ILE:HG12	2.00	0.44
66:0:70:ALA:O	66:0:84:ILE:N	2.46	0.44
3:C:29:LYS:HE2	51:1:2286:G:H3'	1.99	0.44
7:G:160:LEU:HD11	7:G:175:ALA:HB2	1.98	0.44
10:J:131:ASN:ND2	53:3:18:C:H5''	2.33	0.44
24:X:43:MET:HE2	24:X:43:MET:HB2	1.92	0.44
27:b:58:LYS:HB3	51:1:1568:G:H4'	1.98	0.44
30:e:39:VAL:HG12	30:e:41:GLU:H	1.82	0.44
34:j:6:ALA:HB3	34:j:48:VAL:HG21	1.99	0.44
41:q:5:ARG:HG3	51:1:584:C:OP2	2.17	0.44
45:u:81:ARG:HD3	51:1:335:C:H5''	1.98	0.44
51:1:19:A:O2'	51:1:553:G:H4'	2.18	0.44
51:1:598:U:H2'	51:1:599:A:H8	1.83	0.44
51:1:1716:U:H2'	51:1:1717:A:H8	1.81	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1748:C:H2'	51:1:1749:A:C8	2.52	0.44
51:1:2326:C:H4'	51:1:2327:A:OP1	2.18	0.44
51:1:2798:U:H4'	51:1:2799:A:C5	2.53	0.44
53:3:163:C:H2'	53:3:164:G:O4'	2.17	0.44
53:3:357:G:OP1	53:3:367:U:H2'	2.17	0.44
53:3:819:A:H5'	53:3:820:U:C5	2.53	0.44
58:B1:375:GLU:HB3	59:B2:1245:ALA:CB	2.48	0.44
2:B:42:ILE:HG12	38:n:100:CYS:HA	1.99	0.44
4:D:8:SER:OG	51:1:686:U:O2	2.36	0.44
7:G:87:ASP:OD1	7:G:87:ASP:N	2.51	0.44
7:G:218:ALA:HA	7:G:221:ARG:HD3	2.00	0.44
14:N:91:GLU:O	14:N:95:SER:N	2.48	0.44
15:O:71:LEU:O	15:O:72:ARG:NH1	2.40	0.44
17:Q:93:ARG:NH1	53:3:911:U:OP2	2.51	0.44
27:b:42:ARG:HH12	51:1:779:U:H5''	1.82	0.44
35:k:8:LEU:HD23	35:k:82:ASN:HB3	2.00	0.44
45:u:17:ASP:HB3	45:u:20:LYS:HD2	2.00	0.44
51:1:41:C:C2'	51:1:42:A:H5''	2.46	0.44
51:1:1319:C:O2'	51:1:1320:C:H5'	2.18	0.44
51:1:1468:U:H2'	51:1:1522:A:N6	2.33	0.44
51:1:2070:A:O2'	51:1:2071:A:H5'	2.17	0.44
51:1:2358:A:H2'	51:1:2359:C:O4'	2.18	0.44
53:3:1270:G:H2'	53:3:1271:A:C8	2.53	0.44
57:A1:68:TYR:HE1	57:A1:79:LEU:HD13	1.82	0.44
58:B1:201:LEU:CD1	58:B1:224:LEU:HD12	2.46	0.44
58:B1:478:LEU:HD21	60:W0:47:THR:HG23	1.99	0.44
58:B1:515:ARG:NH2	58:B1:718:SER:O	2.48	0.44
58:B1:804:ALA:HB2	58:B1:1256:ILE:CD1	2.47	0.44
66:0:99:VAL:HG11	66:0:126:VAL:HG12	1.99	0.44
66:0:309:ARG:NH1	66:0:315:GLU:OE1	2.50	0.44
7:G:15:PHE:HA	7:G:42:LEU:HD11	1.99	0.44
7:G:110:ILE:O	7:G:114:LYS:N	2.51	0.44
14:N:114:LYS:HB2	14:N:117:LEU:HB2	1.99	0.44
28:c:56:LYS:NZ	51:1:2830:C:H5''	2.33	0.44
36:l:110:VAL:HB	36:l:127:VAL:HG13	1.99	0.44
41:q:23:TYR:HB2	41:q:28:SER:HB3	1.98	0.44
43:s:77:ASP:OD1	43:s:77:ASP:N	2.48	0.44
51:1:816:C:H2'	51:1:817:C:C6	2.53	0.44
51:1:1292:G:H2'	51:1:1293:C:C6	2.53	0.44
51:1:1440:U:H2'	51:1:1441:G:C8	2.53	0.44
51:1:1469:A:H2'	51:1:1470:A:C8	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:2:75:G:H2'	52:2:76:G:O4'	2.18	0.44
53:3:16:A:O2'	53:3:17:U:H5'	2.18	0.44
59:B2:487:LEU:HD22	59:B2:487:LEU:HA	1.77	0.44
62:NG:161:SER:CB	62:NG:170:PRO:HA	2.48	0.44
66:0:360:PHE:HD1	66:0:360:PHE:HA	1.71	0.44
1:A:59:ARG:HD3	24:X:20:LYS:HE3	1.99	0.44
9:I:38:GLY:HA3	53:3:542:G:C5'	2.45	0.44
10:J:88:HIS:O	10:J:91:SER:OG	2.35	0.44
25:Y:25:SER:OG	53:3:1458:G:H5''	2.18	0.44
25:Y:34:VAL:HG11	25:Y:78:LEU:HD13	2.00	0.44
36:l:63:LYS:HE2	51:1:249:C:O2'	2.17	0.44
38:n:83:LEU:HG	38:n:86:ARG:HH21	1.83	0.44
51:1:48:G:O3'	51:1:51:G:H5'	2.17	0.44
53:3:410:G:C6	53:3:429:U:H1'	2.53	0.44
53:3:443:C:H2'	53:3:444:G:C8	2.53	0.44
53:3:1235:U:H2'	53:3:1236:A:O4'	2.18	0.44
54:4:4:U:H2'	54:4:5:U:C6	2.53	0.44
58:B1:111:THR:CG2	58:B1:300:GLN:HA	2.48	0.44
59:B2:24:VAL:HG11	59:B2:704:MET:HE1	1.99	0.44
59:B2:300:ASP:OD1	59:B2:313:ALA:N	2.51	0.44
59:B2:674:ASP:OD2	59:B2:1070:HIS:ND1	2.50	0.44
59:B2:811:ASN:ND2	59:B2:1098:LEU:O	2.51	0.44
65:a:9:ARG:HA	65:a:12:ARG:HB2	1.99	0.44
6:F:18:LYS:HE2	6:F:18:LYS:HB3	1.83	0.43
9:I:90:LEU:HD13	9:I:190:LEU:HD11	1.98	0.43
9:I:131:ILE:HD13	53:3:620:C:C2	2.52	0.43
10:J:75:LEU:HD13	10:J:119:VAL:HG13	2.00	0.43
12:L:91:ARG:HB3	12:L:92:PRO:HD2	1.99	0.43
22:V:18:LYS:HE2	53:3:255:G:H4'	1.99	0.43
23:W:11:ARG:HE	23:W:15:GLU:HB2	1.83	0.43
28:c:114:LYS:NZ	51:1:2723:C:OP1	2.52	0.43
36:l:28:GLY:H	36:l:31:GLY:HA2	1.82	0.43
40:p:52:ARG:HH21	51:1:2846:G:H5'	1.83	0.43
49:y:30:MET:SD	49:y:30:MET:N	2.91	0.43
51:1:196:A:N3	51:1:196:A:H2'	2.33	0.43
51:1:227:A:H1'	51:1:229:C:N4	2.34	0.43
51:1:596:U:H2'	51:1:597:G:H8	1.83	0.43
51:1:784:G:OP1	51:1:2588:G:H5''	2.18	0.43
51:1:941:A:O2'	51:1:1190:G:H4'	2.18	0.43
51:1:2039:U:H2'	51:1:2040:G:H8	1.83	0.43
53:3:212:G:H2'	53:3:213:G:O4'	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:961:U:H2'	53:3:962:C:O4'	2.18	0.43
57:A1:212:ASP:OD1	57:A1:212:ASP:N	2.48	0.43
58:B1:201:LEU:HD11	58:B1:220:ARG:NH1	2.32	0.43
58:B1:894:VAL:HG22	58:B1:1258:ARG:HH11	1.83	0.43
59:B2:11:ILE:HG22	59:B2:1172:LEU:HD11	1.99	0.43
59:B2:557:ARG:HB3	59:B2:587:LEU:HD13	2.00	0.43
59:B2:829:THR:HG23	59:B2:1059:ARG:HG2	2.00	0.43
66:0:537:ILE:HB	66:0:577:ARG:HG3	1.99	0.43
4:D:43:THR:HG23	4:D:44:VAL:H	1.83	0.43
10:J:146:MET:HE2	10:J:146:MET:HB3	1.90	0.43
22:V:15:LYS:CB	53:3:275:G:H5'	2.48	0.43
30:e:48:LEU:O	30:e:52:ALA:N	2.50	0.43
37:m:53:MET:HE1	37:m:103:TYR:HB3	1.99	0.43
39:o:26:LEU:HD13	39:o:39:VAL:HG22	2.00	0.43
42:r:102:SER:OG	42:r:103:ALA:N	2.51	0.43
47:w:33:ILE:HD11	47:w:78:ILE:HD11	2.00	0.43
48:x:36:ARG:HA	48:x:47:THR:HA	1.99	0.43
51:1:45:G:H5'	51:1:46:G:C5'	2.36	0.43
51:1:2888:C:H2'	51:1:2889:C:H6	1.82	0.43
53:3:1517:G:O2'	53:3:1518:A:H5'	2.19	0.43
58:B1:111:THR:HG21	58:B1:303:VAL:HB	2.00	0.43
58:B1:1033:GLY:HA3	58:B1:1081:VAL:O	2.18	0.43
59:B2:901:LEU:HD12	59:B2:901:LEU:HA	1.83	0.43
59:B2:1275:VAL:HG13	59:B2:1287:LEU:HD11	2.01	0.43
10:J:137:ARG:HH12	53:3:1078:U:H4'	1.83	0.43
22:V:24:ILE:HG23	22:V:41:THR:HB	1.99	0.43
24:X:4:LEU:HD23	24:X:9:PHE:HB2	2.01	0.43
33:i:72:THR:HB	33:i:115:ASP:HB2	2.01	0.43
37:m:74:THR:OG1	37:m:75:GLU:N	2.50	0.43
40:p:74:GLN:HB2	40:p:77:SER:HB3	2.00	0.43
51:1:121:G:H4'	51:1:149:A:H5'	2.00	0.43
51:1:532:A:H2'	51:1:532:A:N3	2.33	0.43
51:1:1156:A:H5'	51:1:1156:A:H8	1.82	0.43
51:1:2427:C:C5'	51:1:2429:G:H5'	2.47	0.43
59:B2:6:THR:OG1	59:B2:781:ASP:OD1	2.33	0.43
63:5:63:G:H2'	63:5:64:A:C8	2.53	0.43
66:0:75:MET:HE1	66:0:276:GLN:HB3	1.99	0.43
7:G:170:ILE:HA	7:G:173:LYS:HE2	1.99	0.43
8:H:110:LEU:HD22	8:H:145:ALA:HB2	1.99	0.43
12:L:65:LEU:O	12:L:69:ARG:HG3	2.18	0.43
28:c:53:GLY:HA3	28:c:77:ARG:HG2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:57:LYS:HB2	51:1:797:G:OP2	2.19	0.43
32:g:55:GLU:O	32:g:59:ALA:N	2.50	0.43
45:u:6:ARG:HB2	51:1:85:G:OP2	2.18	0.43
47:w:62:LYS:HE3	47:w:81:GLU:HG3	2.00	0.43
48:x:17:ARG:HD3	48:x:17:ARG:HA	1.80	0.43
51:1:285:G:O2'	51:1:286:U:H5'	2.18	0.43
51:1:1075:C:H3'	51:1:1076:C:C5'	2.40	0.43
51:1:1926:U:H2'	51:1:1927:A:H8	1.83	0.43
51:1:2250:G:N2	51:1:2496:C:H5''	2.33	0.43
51:1:2586:U:H2'	51:1:2587:A:H8	1.83	0.43
53:3:182:A:H2'	53:3:183:C:H5''	2.01	0.43
53:3:201:G:H21	53:3:469:C:H1'	1.83	0.43
53:3:1261:A:H5''	53:3:1262:C:C5	2.53	0.43
58:B1:161:THR:H	58:B1:164:GLN:HB2	1.82	0.43
58:B1:824:PRO:HD3	58:B1:835:LEU:HD12	2.00	0.43
66:0:617:MET:N	66:0:658:VAL:O	2.47	0.43
3:C:10:LEU:HD21	3:C:33:LEU:HD23	2.01	0.43
8:H:121:SER:HB2	8:H:125:ARG:HH12	1.82	0.43
9:I:115:GLN:HE22	53:3:406:G:H1'	1.84	0.43
16:P:24:ALA:HB2	16:P:29:THR:HG23	2.00	0.43
16:P:108:ASN:HB3	26:Z:6:ARG:HD3	1.99	0.43
19:S:70:HIS:HB3	53:3:974:A:H5'	2.00	0.43
19:S:74:ARG:NH2	53:3:1359:C:H3'	2.32	0.43
27:b:7:PRO:HA	27:b:13:ARG:HA	1.99	0.43
28:c:164:GLN:HE22	51:1:2822:G:H5''	1.83	0.43
35:k:2:ILE:HG13	35:k:62:VAL:HG11	1.99	0.43
51:1:566:U:O2'	51:1:567:U:H5'	2.18	0.43
51:1:752:A:O2'	51:1:1781:U:H5'	2.18	0.43
51:1:974:G:H1'	51:1:975:A:H8	1.77	0.43
51:1:1063:G:H5''	51:1:1064:C:C5	2.53	0.43
51:1:1117:C:H2'	51:1:1118:C:C6	2.54	0.43
51:1:1417:C:H2'	51:1:1418:G:O4'	2.19	0.43
51:1:1595:C:H2'	51:1:1596:A:H8	1.84	0.43
51:1:2122:U:H2'	51:1:2123:G:O4'	2.18	0.43
53:3:846:G:H2'	53:3:847:G:H8	1.83	0.43
58:B1:1079:LYS:HD3	58:B1:1098:GLN:HB3	1.99	0.43
5:E:40:LYS:HD3	51:1:2419:U:OP2	2.18	0.43
5:E:56:LEU:HD22	36:l:49:GLY:HA2	2.00	0.43
12:L:86:VAL:HG12	12:L:150:PHE:CZ	2.53	0.43
14:N:40:ARG:HD2	14:N:40:ARG:HA	1.78	0.43
25:Y:54:GLN:HE21	53:3:193:C:H1'	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:5:LEU:HD22	32:g:9:VAL:HG21	2.01	0.43
33:i:14:ALA:HB2	33:i:54:ILE:HG13	2.01	0.43
36:l:55:MET:HA	36:l:56:PRO:HD3	1.88	0.43
39:o:26:LEU:N	39:o:91:SER:O	2.48	0.43
41:q:30:VAL:HG13	51:1:580:U:O3'	2.19	0.43
44:t:34:VAL:HG21	44:t:43:ILE:HD11	1.99	0.43
51:1:1441:G:H4'	51:1:1628:G:C5'	2.49	0.43
51:1:1960:A:H2'	51:1:1961:C:C5'	2.47	0.43
51:1:2055:C:H5'	51:1:2056:G:O5'	2.18	0.43
51:1:2086:U:H2'	51:1:2087:G:C8	2.53	0.43
51:1:2303:G:O2'	51:1:2304:G:H5'	2.17	0.43
51:1:2529:G:H5''	51:1:2530:A:H5''	2.01	0.43
53:3:247:G:O2'	53:3:248:C:H5'	2.19	0.43
58:B1:40:LYS:HZ3	58:B1:40:LYS:HG2	1.74	0.43
58:B1:107:LEU:HA	58:B1:276:ASN:ND2	2.33	0.43
58:B1:128:LEU:CD2	58:B1:188:LEU:HB3	2.47	0.43
58:B1:1108:GLN:HG3	58:B1:1109:LEU:HD12	1.99	0.43
36:l:112:LEU:HD13	36:l:131:ALA:HA	2.00	0.43
39:o:15:ARG:CZ	52:2:8:C:H5''	2.49	0.43
51:1:1056:G:H21	51:1:1102:C:H5	1.65	0.43
51:1:1925:C:H2'	51:1:1926:U:O4'	2.18	0.43
53:3:556:C:O2'	53:3:557:G:H5'	2.19	0.43
53:3:650:G:O2'	53:3:651:C:H5'	2.17	0.43
53:3:839:C:H2'	53:3:840:C:H6	1.83	0.43
53:3:1352:C:H2'	53:3:1353:G:H8	1.83	0.43
58:B1:141:PHE:CD2	58:B1:297:ARG:HB2	2.54	0.43
58:B1:388:ARG:HG2	58:B1:388:ARG:HH11	1.84	0.43
58:B1:1024:THR:HG23	58:B1:1123:ARG:HA	2.00	0.43
65:a:47:ASN:HD22	65:a:170:ILE:HG13	1.84	0.43
66:0:491:ARG:O	66:0:613:LEU:N	2.45	0.43
66:0:505:HIS:N	66:0:516:GLY:O	2.43	0.43
7:G:123:GLY:HA3	7:G:127:LYS:HE2	2.00	0.43
10:J:111:ARG:O	10:J:115:GLU:N	2.51	0.43
19:S:58:ARG:HD2	53:3:980:C:H1'	2.01	0.43
20:T:17:ASP:OD1	20:T:17:ASP:N	2.51	0.43
44:t:7:LEU:HD22	44:t:46:ALA:HB2	1.99	0.43
51:1:20:C:H2'	51:1:21:A:C8	2.53	0.43
51:1:1091:G:O6	51:1:1099:G:O6	2.36	0.43
51:1:1808:A:H3'	51:1:1809:A:H8	1.82	0.43
51:1:2340:A:H2'	51:1:2341:G:H8	1.84	0.43
51:1:2461:A:H1'	51:1:2492:U:N3	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:52:C:H2'	53:3:53:A:C8	2.54	0.43
53:3:273:U:H2'	53:3:274:A:H5'	2.00	0.43
58:B1:242:LEU:C	58:B1:242:LEU:HD23	2.44	0.43
58:B1:434:ILE:HD11	59:B2:1274:GLU:HG3	2.00	0.43
58:B1:850:LYS:HB3	58:B1:855:ASP:HB2	2.00	0.43
65:a:216:THR:HG22	65:a:217:THR:H	1.83	0.43
66:0:70:ALA:N	66:0:84:ILE:O	2.48	0.43
66:0:520:ILE:HB	66:0:576:ILE:HD11	1.99	0.43
7:G:55:GLU:HB2	7:G:183:PHE:HZ	1.84	0.43
7:G:163:ILE:HD11	7:G:213:LEU:HD21	2.01	0.43
17:Q:86:VAL:HG22	17:Q:95:HIS:CE1	2.54	0.43
20:T:70:LYS:HE3	20:T:70:LYS:HB2	1.88	0.43
21:U:13:LYS:HE2	53:3:392:C:H5'	2.01	0.43
29:d:158:PHE:HA	29:d:169:VAL:HG21	2.00	0.43
37:m:64:TRP:NE1	51:1:873:C:H4'	2.33	0.43
37:m:109:PRO:HD2	37:m:112:LEU:HD11	2.00	0.43
50:z:10:ARG:NH1	51:1:1000:A:O2'	2.52	0.43
51:1:69:C:O2'	51:1:70:G:H5'	2.18	0.43
51:1:466:A:H2'	51:1:467:G:H5'	2.00	0.43
51:1:1343:G:N3	51:1:1343:G:H2'	2.34	0.43
51:1:2128:G:OP1	65:a:38:PHE:HB3	2.19	0.43
51:1:2724:U:H2'	51:1:2725:A:C8	2.54	0.43
53:3:605:U:O2'	53:3:606:G:H5'	2.19	0.43
53:3:865:A:H5'	53:3:1078:U:O4	2.18	0.43
55:8:2:DC:H6	55:8:2:DC:H2'	1.73	0.43
55:8:12:DG:OP1	58:B1:795:TYR:CE1	2.71	0.43
58:B1:45:ASN:HD22	58:B1:48:THR:H	1.65	0.43
58:B1:450:HIS:HA	58:B1:451:PRO:HD3	1.91	0.43
58:B1:568:SER:HB3	58:B1:570:LYS:NZ	2.34	0.43
58:B1:586:GLY:HA3	58:B1:612:LEU:HD11	2.01	0.43
58:B1:1026:PRO:HB2	58:B1:1028:ILE:HG23	2.00	0.43
4:D:21:ARG:NH2	51:1:684:G:OP1	2.52	0.43
8:H:113:LYS:HB2	8:H:184:ASN:HD22	1.84	0.43
8:H:172:VAL:HG23	53:3:1107:C:H5''	2.00	0.43
27:b:186:ASP:OD1	32:g:123:ARG:NH2	2.52	0.43
29:d:110:SER:O	29:d:114:ARG:NE	2.52	0.43
31:f:136:ASP:HB3	31:f:139:VAL:HG22	2.00	0.43
33:i:134:SER:HB2	51:1:1077:A:C2	2.54	0.43
51:1:1289:C:O2'	51:1:1330:C:H4'	2.19	0.43
51:1:1536:C:H4'	51:1:1537:G:C2	2.54	0.43
51:1:1786:A:H1'	51:1:1938:A:N6	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:2484:G:O2'	51:1:2485:G:H5'	2.19	0.43
53:3:220:G:O2'	53:3:221:C:H5'	2.18	0.43
58:B1:58:CYS:SG	58:B1:60:ARG:HG2	2.59	0.43
58:B1:201:LEU:CB	58:B1:221:ILE:HD13	2.47	0.43
58:B1:609:TYR:HD2	58:B1:610:ARG:NH1	2.17	0.43
58:B1:797:THR:HG22	58:B1:924:GLY:HA3	2.01	0.43
58:B1:950:ILE:HB	58:B1:1018:ALA:HB3	2.01	0.43
59:B2:616:ILE:HG13	59:B2:652:TYR:HB2	2.01	0.43
62:NG:135:ARG:O	62:NG:178:VAL:CA	2.67	0.43
64:6:69:C:H2'	64:6:70:G:C5'	2.39	0.43
65:a:51:ASP:HB3	65:a:54:LYS:HB3	2.01	0.43
66:0:245:GLU:HA	66:0:248:ILE:HD12	2.01	0.43
3:C:20:TYR:OH	51:1:2348:U:H5'	2.19	0.42
5:E:4:LYS:O	36:l:48:ARG:NH1	2.43	0.42
9:I:23:GLY:HA3	53:3:409:U:OP1	2.19	0.42
10:J:73:VAL:HG23	10:J:75:LEU:HG	2.00	0.42
12:L:86:VAL:HG12	12:L:150:PHE:CE2	2.53	0.42
51:1:919:U:H2'	51:1:920:A:O4'	2.19	0.42
51:1:1278:C:H2'	51:1:1279:G:C8	2.54	0.42
51:1:1539:U:H2'	51:1:1540:G:H8	1.84	0.42
51:1:1557:C:C5	51:1:1558:C:H2'	2.54	0.42
51:1:2170:A:C4	51:1:2171:A:H8	2.37	0.42
58:B1:903:LEU:HD12	58:B1:903:LEU:HA	1.77	0.42
66:0:69:THR:OG1	66:0:367:HIS:NE2	2.34	0.42
10:J:12:GLU:HA	10:J:38:VAL:HG12	2.00	0.42
10:J:137:ARG:NH1	53:3:1078:U:H4'	2.34	0.42
16:P:34:THR:HA	16:P:40:ALA:HA	2.00	0.42
18:R:6:ILE:HG13	18:R:7:ASN:H	1.84	0.42
19:S:81:ILE:HG21	53:3:1202:U:C2	2.55	0.42
21:U:20:VAL:HG12	21:U:35:ARG:HA	2.01	0.42
30:e:84:ILE:HG21	51:1:2312:U:C4'	2.48	0.42
31:f:70:LEU:HD11	51:1:2758:A:N1	2.34	0.42
33:i:27:LEU:HD11	33:i:34:ILE:HD13	2.00	0.42
41:q:24:TYR:CE1	51:1:17:G:H4'	2.54	0.42
51:1:792:A:H3'	51:1:793:A:H5'	2.00	0.42
51:1:1132:U:H2'	51:1:1133:A:C8	2.54	0.42
51:1:1645:G:C5'	51:1:1646:C:H5'	2.31	0.42
51:1:1923:U:H2'	51:1:1924:C:C6	2.54	0.42
53:3:613:C:H2'	53:3:614:C:C6	2.53	0.42
53:3:1211:U:H4'	53:3:1213:A:N3	2.34	0.42
53:3:1517:G:C2'	53:3:1518:A:H5'	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:8:3:DC:N1	55:8:4:DT:H72	2.34	0.42
58:B1:62:PHE:N	58:B1:62:PHE:CD1	2.86	0.42
58:B1:137:ARG:HA	58:B1:142:GLU:HG2	2.02	0.42
58:B1:139:LEU:HD23	58:B1:139:LEU:HA	1.89	0.42
58:B1:515:ARG:HH12	58:B1:724:MET:HG2	1.84	0.42
66:0:170:GLN:NE2	66:0:266:CYS:H	2.18	0.42
4:D:25:LYS:HE2	4:D:25:LYS:HB2	1.89	0.42
14:N:17:ARG:HH12	53:3:1129:C:H5'	1.84	0.42
18:R:47:LEU:HD22	18:R:51:GLN:HE21	1.83	0.42
35:k:22:ILE:HD12	51:1:1952:A:C2	2.55	0.42
36:l:19:LEU:HD23	51:1:587:C:O2	2.18	0.42
51:1:186:G:O2'	51:1:187:G:H5'	2.19	0.42
51:1:467:G:O2'	51:1:468:G:H5'	2.20	0.42
51:1:1726:C:H2'	51:1:1727:C:H6	1.82	0.42
58:B1:24:LEU:HD21	58:B1:116:PHE:CE2	2.54	0.42
58:B1:1046:ILE:HG22	58:B1:1061:VAL:HA	2.00	0.42
59:B2:125:GLY:H	59:B2:495:ALA:HB1	1.84	0.42
59:B2:1157:GLN:HG3	59:B2:1159:VAL:HG13	2.00	0.42
59:B2:1313:HIS:CD2	60:W0:31:GLN:HE22	2.37	0.42
62:NG:130:PRO:HA	62:NG:148:VAL:O	2.19	0.42
63:5:25:C:H2'	63:5:26:A:H8	1.84	0.42
7:G:134:LEU:O	7:G:137:THR:OG1	2.38	0.42
12:L:115:MET:HB3	53:3:1240:U:OP2	2.20	0.42
15:O:47:GLU:HG3	53:3:1254:A:OP1	2.19	0.42
16:P:121:ARG:HA	16:P:122:PRO:HD3	1.82	0.42
17:Q:109:ARG:CZ	53:3:537:G:H5''	2.50	0.42
18:R:96:VAL:HG22	53:3:1308:U:OP1	2.20	0.42
18:R:107:THR:HG21	53:3:1306:A:N3	2.33	0.42
20:T:80:LEU:HD12	20:T:80:LEU:HA	1.90	0.42
34:j:60:ASP:HA	34:j:93:ILE:HD11	1.99	0.42
37:m:19:GLY:O	37:m:38:ARG:NH1	2.44	0.42
37:m:57:VAL:HB	37:m:60:GLN:HB3	2.01	0.42
50:z:13:ILE:H	50:z:13:ILE:HG13	1.70	0.42
51:1:526:A:N6	51:1:2626:C:H4'	2.35	0.42
51:1:1047:G:H2'	51:1:1110:G:N2	2.34	0.42
51:1:1278:C:H2'	51:1:1279:G:H8	1.84	0.42
51:1:1837:C:H2'	51:1:1899:A:N6	2.32	0.42
51:1:2314:A:H2'	51:1:2315:G:C8	2.54	0.42
51:1:2332:C:H2'	51:1:2335:A:C2	2.55	0.42
51:1:2425:A:H4'	51:1:2426:A:C5'	2.49	0.42
51:1:2881:U:H2'	51:1:2882:A:H8	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:794:A:H4'	53:3:1521:C:O2'	2.19	0.42
53:3:1062:U:H2'	53:3:1063:C:C6	2.54	0.42
53:3:1065:U:P	53:3:1190:G:H22	2.42	0.42
53:3:1479:C:H2'	53:3:1480:A:C8	2.51	0.42
54:4:43:G:H5'	59:B2:688:GLN:HE22	1.84	0.42
57:A1:78:ILE:HA	57:A1:81:ILE:HG22	2.00	0.42
58:B1:362:ARG:HB2	58:B1:364:HIS:HD2	1.83	0.42
59:B2:444:ASP:OD1	59:B2:444:ASP:N	2.51	0.42
59:B2:699:LEU:HG	59:B2:799:ASN:HD22	1.85	0.42
2:B:37:HIS:ND1	2:B:38:LEU:O	2.41	0.42
13:M:31:LEU:HD22	53:3:643:C:H5''	2.01	0.42
14:N:122:ARG:HG3	53:3:1343:G:O2'	2.18	0.42
18:R:111:PRO:HB2	18:R:113:LYS:HG3	2.02	0.42
21:U:21:VAL:HG12	21:U:33:ILE:HB	2.01	0.42
28:c:148:GLN:HB2	28:c:152:PRO:HG3	2.01	0.42
33:i:67:THR:HG22	33:i:68:PHE:H	1.85	0.42
36:l:78:ARG:CZ	51:1:626:A:H2'	2.49	0.42
51:1:2323:G:O2'	51:1:2324:U:H5'	2.19	0.42
51:1:2720:U:H5'	51:1:2720:U:C6	2.53	0.42
55:8:15:DC:H5'	59:B2:1269:ARG:HD3	2.00	0.42
58:B1:96:LYS:NZ	59:B2:1298:VAL:HG11	2.34	0.42
58:B1:244:VAL:HA	58:B1:269:TYR:OH	2.19	0.42
59:B2:469:VAL:HA	59:B2:472:GLU:HG2	2.02	0.42
8:H:15:LYS:HD2	8:H:15:LYS:HA	1.81	0.42
9:I:40:HIS:HB3	9:I:43:ARG:HH21	1.85	0.42
27:b:200:MET:HG3	51:1:1820:U:C2	2.54	0.42
28:c:118:PHE:HE1	51:1:2048:G:H21	1.66	0.42
36:l:90:VAL:N	36:l:121:THR:O	2.52	0.42
37:m:1:MET:SD	37:m:1:MET:N	2.88	0.42
37:m:112:LEU:HA	37:m:115:GLU:HB3	2.00	0.42
40:p:2:ASN:ND2	51:1:2876:G:H4'	2.32	0.42
41:q:92:LYS:HZ2	51:1:995:C:HO2'	1.64	0.42
51:1:123:G:H5''	51:1:1375:U:O2'	2.20	0.42
51:1:1545:A:H2'	51:1:1546:G:O4'	2.19	0.42
51:1:1916:A:N1	53:3:1409:C:H5'	2.34	0.42
51:1:1922:G:H2'	51:1:1923:U:O4'	2.19	0.42
51:1:2039:U:H2'	51:1:2040:G:C8	2.55	0.42
51:1:2138:G:C2'	51:1:2139:U:H5'	2.49	0.42
51:1:2743:U:H2'	51:1:2744:G:C4'	2.48	0.42
51:1:2788:C:H2'	51:1:2789:C:C6	2.53	0.42
53:3:505:G:O5'	53:3:505:G:H8	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:3:879:C:H2'	53:3:880:C:C6	2.54	0.42
53:3:1163:A:H2'	53:3:1164:G:C8	2.55	0.42
53:3:1330:U:H2'	53:3:1331:G:O4'	2.19	0.42
58:B1:848:VAL:HB	58:B1:858:VAL:HG22	2.02	0.42
59:B2:646:SER:OG	59:B2:647:ARG:N	2.52	0.42
63:5:4:C:H2'	63:5:5:G:C8	2.55	0.42
64:6:17(A):U:O2'	64:6:18:G:H5''	2.19	0.42
66:0:34:THR:OG1	66:0:71:PHE:O	2.37	0.42
13:M:91:LEU:HD23	13:M:91:LEU:HA	1.86	0.42
15:O:100:ILE:HB	62:NG:170:PRO:O	2.19	0.42
28:c:123:LYS:HE2	38:n:1:MET:HE1	2.01	0.42
32:g:11:ASN:ND2	51:1:2095:A:O5'	2.53	0.42
32:g:118:PRO:HD2	32:g:130:VAL:HG13	2.01	0.42
48:x:22:ASN:HD22	48:x:22:ASN:HA	1.65	0.42
51:1:234:U:O2'	51:1:235:U:H5'	2.19	0.42
51:1:288:U:H2'	51:1:289:G:H8	1.83	0.42
51:1:744:U:H4'	51:1:1658:C:H4'	2.02	0.42
51:1:970:U:H2'	51:1:971:G:C8	2.55	0.42
51:1:1071:G:H5''	51:1:1072:C:H5	1.84	0.42
51:1:1201:U:H2'	51:1:1202:G:C8	2.54	0.42
51:1:1649:G:H2'	51:1:1650:A:H8	1.84	0.42
51:1:2240:U:H2'	51:1:2241:A:H8	1.85	0.42
53:3:97:G:H2'	53:3:98:A:O4'	2.20	0.42
53:3:216:U:H2'	53:3:217:C:C6	2.55	0.42
58:B1:102:MET:HG2	58:B1:246:PRO:CG	2.49	0.42
59:B2:998:LEU:HD21	59:B2:1015:ALA:HB2	2.02	0.42
66:0:148:GLY:N	66:0:176:GLU:OE1	2.52	0.42
66:0:487:GLN:HB3	66:0:488:VAL:H	1.70	0.42
66:0:665:GLY:O	66:0:668:THR:OG1	2.37	0.42
3:C:35:LEU:HD13	3:C:37:LYS:HE2	2.01	0.42
14:N:17:ARG:HH12	53:3:1129:C:H4'	1.85	0.42
18:R:16:ILE:O	18:R:19:THR:OG1	2.33	0.42
20:T:47:LYS:O	20:T:49:HIS:ND1	2.53	0.42
28:c:12:THR:OG1	28:c:13:ARG:N	2.51	0.42
33:i:131:THR:HG22	33:i:135:MET:CE	2.50	0.42
34:j:104:ALA:CB	51:1:1139:G:H5'	2.50	0.42
46:v:42:LEU:HD12	46:v:47:VAL:HG11	2.02	0.42
51:1:239:C:H2'	51:1:240:C:O4'	2.20	0.42
51:1:436:C:H2'	51:1:437:U:C6	2.55	0.42
51:1:627:A:H8	51:1:627:A:OP1	2.03	0.42
51:1:1120:G:H2'	51:1:1121:C:O4'	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:1258:U:H2'	51:1:1259:G:H8	1.85	0.42
51:1:2233:U:H2'	51:1:2234:G:C8	2.54	0.42
51:1:2432:A:H1'	64:6:75:C:O4'	2.20	0.42
51:1:2736:A:H2'	51:1:2737:G:H8	1.85	0.42
53:3:34:C:H2'	53:3:35:G:C8	2.54	0.42
53:3:66:A:H5'	53:3:173:U:C4	2.55	0.42
53:3:521:G:O2'	53:3:522:C:H5'	2.19	0.42
53:3:1306:A:H2'	53:3:1307:U:O4'	2.20	0.42
59:B2:538:LEU:HD13	59:B2:543:ALA:HB2	2.00	0.42
66:0:505:HIS:CE1	66:0:595:LEU:HB3	2.55	0.42
1:A:37:CYS:H	1:A:40:CYS:HB3	1.85	0.42
5:E:15:LYS:HB2	5:E:64:ALA:HB1	2.02	0.42
5:E:54:LEU:HD12	5:E:54:LEU:HA	1.90	0.42
14:N:95:SER:OG	14:N:96:GLU:N	2.53	0.42
15:O:25:ILE:HD12	15:O:25:ILE:HA	1.95	0.42
21:U:79:ASN:N	21:U:79:ASN:OD1	2.53	0.42
22:V:30:HIS:HD2	22:V:33:TYR:H	1.66	0.42
27:b:258:SER:O	27:b:258:SER:OG	2.34	0.42
34:j:27:ARG:HD2	51:1:1143:A:N6	2.34	0.42
36:l:51:GLU:OE1	36:l:60:ARG:NH1	2.52	0.42
38:n:64:ARG:NH2	51:1:2852:G:H5'	2.34	0.42
41:q:73:ILE:HD11	41:q:77:LYS:HB3	2.01	0.42
43:s:97:LEU:HD23	43:s:97:LEU:HA	1.91	0.42
51:1:198:C:O5'	51:1:198:C:H6	2.03	0.42
51:1:1068:G:H21	51:1:1096:A:H5'	1.85	0.42
51:1:1318:U:H2'	51:1:1319:C:H6	1.83	0.42
51:1:1449:G:O2'	51:1:1450:G:H5'	2.20	0.42
51:1:2533:U:H2'	51:1:2534:A:O4'	2.19	0.42
51:1:2534:A:H2'	51:1:2535:G:H5''	2.02	0.42
51:1:2685:G:H2'	51:1:2686:G:H8	1.84	0.42
51:1:2802:G:H2'	51:1:2803:G:O4'	2.20	0.42
51:1:2834:G:H2'	51:1:2879:A:H61	1.84	0.42
53:3:146:G:O2'	53:3:147:G:H5'	2.20	0.42
53:3:749:A:H2'	53:3:750:C:O4'	2.20	0.42
53:3:1428:A:OP2	53:3:1428:A:O4'	2.37	0.42
57:A1:51:MET:HA	57:A1:52:PRO:HD3	1.93	0.42
58:B1:385:LEU:CD2	58:B1:390:LEU:HB2	2.50	0.42
58:B1:390:LEU:N	58:B1:390:LEU:HD13	2.35	0.42
58:B1:434:ILE:HD11	59:B2:1274:GLU:CG	2.49	0.42
58:B1:930:LEU:HA	58:B1:1244:GLN:HG3	2.02	0.42
59:B2:50:GLU:HG2	59:B2:73:TYR:HE1	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:B2:524:ILE:HD12	59:B2:712:SER:HB2	2.02	0.42
66:0:210:ASP:OD1	66:0:210:ASP:N	2.51	0.42
7:G:66:ILE:HB	7:G:88:GLN:HG3	2.02	0.42
9:I:184:LYS:HB3	9:I:184:LYS:HE3	1.77	0.42
28:c:35:THR:OG1	28:c:49:GLN:O	2.36	0.42
41:q:84:LYS:HB3	41:q:115:ALA:HB1	2.02	0.42
42:r:80:ARG:N	51:1:565:C:OP2	2.51	0.42
43:s:28:LYS:O	43:s:32:ALA:N	2.50	0.42
47:w:14:ALA:HB1	51:1:2271:G:OP1	2.20	0.42
48:x:60:LYS:NZ	51:1:372:G:O4'	2.49	0.42
50:z:10:ARG:HB2	50:z:53:MET:CB	2.50	0.42
51:1:2689:U:O2	51:1:2713:U:H5''	2.19	0.42
51:1:2704:C:H2'	51:1:2705:A:O4'	2.20	0.42
53:3:768:A:H2'	53:3:769:G:O4'	2.20	0.42
53:3:1037:C:H2'	53:3:1038:C:C6	2.54	0.42
53:3:1341:U:O2'	53:3:1342:C:H5'	2.20	0.42
53:3:1494:G:H8	53:3:1494:G:OP2	2.03	0.42
58:B1:144:TYR:N	58:B1:144:TYR:CD1	2.88	0.42
58:B1:394:ILE:O	58:B1:394:ILE:HG13	2.19	0.42
58:B1:1272:SER:OG	58:B1:1273:ASP:N	2.53	0.42
7:G:70:GLY:HA3	7:G:163:ILE:HB	2.02	0.41
8:H:156:LEU:H	8:H:156:LEU:HG	1.67	0.41
11:K:49:TYR:OH	23:W:62:ARG:O	2.30	0.41
16:P:118:ASN:HB2	53:3:718:A:H5'	2.02	0.41
17:Q:88:ASP:HB3	53:3:523:A:H61	1.84	0.41
18:R:7:ASN:HD21	18:R:18:LEU:HD13	1.84	0.41
21:U:6:LEU:HD11	21:U:70:ARG:HD2	2.01	0.41
22:V:70:LYS:HD3	53:3:254:G:H5''	2.02	0.41
27:b:110:LYS:N	27:b:113:ASP:OD2	2.51	0.41
28:c:173:GLN:NE2	51:1:2771:C:O2'	2.50	0.41
30:e:133:GLU:HG3	30:e:135:ILE:H	1.85	0.41
31:f:28:LYS:HE2	31:f:28:LYS:HB2	1.92	0.41
34:j:44:TYR:O	41:q:63:ARG:NE	2.53	0.41
47:w:18:GLY:N	47:w:35:ARG:O	2.52	0.41
47:w:58:LYS:HE2	51:1:2366:A:H4'	2.01	0.41
51:1:353:C:H2'	51:1:354:A:H8	1.85	0.41
51:1:1017:G:C6	51:1:1018:U:O4	2.73	0.41
51:1:1275:A:N6	51:1:1296:G:H4'	2.35	0.41
51:1:1472:C:H2'	51:1:1473:G:H8	1.85	0.41
51:1:1882:U:H2'	51:1:1883:U:C6	2.54	0.41
52:2:78:A:H2'	52:2:79:G:O4'	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:B1:1289:ASN:O	58:B1:1293:GLU:HB2	2.20	0.41
65:a:200:LYS:HB2	65:a:200:LYS:HE2	1.87	0.41
67:h:2:DPP:NG	67:h:3:SER:N	2.65	0.41
8:H:19:SER:OG	19:S:91:GLU:O	2.30	0.41
15:O:102:LEU:HD13	62:NG:172:GLU:H	1.85	0.41
16:P:52:ARG:NH1	53:3:689:C:OP2	2.51	0.41
18:R:106:ARG:HB3	53:3:947:G:OP1	2.20	0.41
25:Y:55:PRO:HA	53:3:194:C:H5'	2.02	0.41
27:b:167:ASP:OD2	53:3:682:G:H5'	2.19	0.41
27:b:253:GLY:HA2	51:1:1797:G:H5'	2.01	0.41
29:d:130:LYS:HA	51:1:321:U:OP2	2.19	0.41
36:l:95:LEU:HD22	36:l:100:ILE:HD11	2.01	0.41
51:1:479:A:H1'	51:1:481:G:H5''	2.02	0.41
51:1:524:G:H5'	51:1:539:G:N2	2.35	0.41
51:1:974:G:N3	51:1:974:G:H2'	2.35	0.41
51:1:1069:A:H2	51:1:1096:A:OP1	2.02	0.41
51:1:1494:A:H2'	51:1:1495:A:O4'	2.20	0.41
51:1:2480:C:OP2	51:1:2537:U:H4'	2.20	0.41
51:1:2547:A:H2'	51:1:2548:U:C6	2.55	0.41
51:1:2692:G:H1'	51:1:2847:U:H1'	2.02	0.41
51:1:2773:C:H2'	51:1:2774:C:H6	1.86	0.41
53:3:114:U:O2'	53:3:115:G:H5'	2.20	0.41
53:3:834:U:H2'	53:3:835:U:C6	2.55	0.41
53:3:1049:U:H4'	53:3:1050:G:H5''	2.02	0.41
53:3:1223:C:C5	53:3:1224:U:H5	2.38	0.41
58:B1:243:PRO:HG2	59:B2:1332:SER:C	2.44	0.41
59:B2:22:LEU:HD22	59:B2:603:ILE:HG21	2.02	0.41
6:F:1:MET:HE2	6:F:1:MET:HB2	1.89	0.41
11:K:9:MET:HE3	11:K:86:ARG:HB3	2.03	0.41
23:W:11:ARG:NH2	53:3:845:A:H4'	2.36	0.41
27:b:143:VAL:HB	27:b:153:LEU:HD22	2.01	0.41
28:c:149:ASN:HB2	51:1:2574:G:O2'	2.20	0.41
31:f:71:LEU:HD23	31:f:71:LEU:HA	1.84	0.41
32:g:43:ASN:O	32:g:47:PHE:N	2.54	0.41
33:i:123:ALA:CB	51:1:1081:U:H4'	2.33	0.41
36:l:2:ARG:NH1	36:l:2:ARG:O	2.45	0.41
36:l:59:ARG:HD2	51:1:250:G:H4'	2.03	0.41
41:q:90:ASP:OD2	51:1:996:A:H4'	2.19	0.41
49:y:41:HIS:CD2	51:1:96:C:H4'	2.55	0.41
51:1:214:G:H1'	51:1:217:A:H5'	2.02	0.41
51:1:278:A:H2'	51:1:278:A:N3	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:596:U:H2'	51:1:597:G:C8	2.55	0.41
51:1:1062:G:O2'	51:1:1063:G:C4'	2.69	0.41
51:1:1872:A:H2'	51:1:1873:G:H5'	2.02	0.41
53:3:675:A:H2'	53:3:676:A:O4'	2.19	0.41
53:3:947:G:H4'	53:3:1332:A:H2	1.86	0.41
53:3:1129:C:H42	53:3:1143:G:H1	1.66	0.41
53:3:1311:A:H2'	53:3:1312:G:O4'	2.20	0.41
53:3:1499:A:O2'	53:3:1520:C:H5'	2.19	0.41
57:A1:205:MET:HE1	57:A1:217:ILE:HG13	2.02	0.41
58:B1:144:TYR:CE1	58:B1:162:GLU:OE1	2.73	0.41
58:B1:559:ALA:HB3	58:B1:562:GLU:HB3	2.01	0.41
59:B2:22:LEU:HB3	59:B2:655:VAL:HG11	2.01	0.41
62:NG:175:PHE:O	62:NG:178:VAL:O	2.38	0.41
63:5:17:C:H6	63:5:17:C:H2'	1.69	0.41
13:M:12:ARG:HD2	13:M:26:MET:HE2	2.02	0.41
16:P:38:GLY:HA2	53:3:708:C:O4'	2.19	0.41
22:V:57:VAL:HG13	22:V:78:VAL:HB	2.03	0.41
34:j:108:MET:HB3	51:1:1006:C:O2'	2.20	0.41
51:1:181:A:H2'	51:1:182:A:C8	2.55	0.41
51:1:1916:A:H2'	51:1:1917:U:O4'	2.20	0.41
51:1:2472:G:H2'	51:1:2475:C:H42	1.84	0.41
53:3:47:C:H4'	53:3:48:C:O5'	2.20	0.41
53:3:226:G:O2'	53:3:227:G:H5'	2.21	0.41
53:3:938:A:H1'	53:3:1376:U:O2'	2.21	0.41
53:3:1479:C:C4	53:3:1480:A:N7	2.89	0.41
57:A1:76:GLU:HB3	57:A1:80:GLU:HB3	2.01	0.41
58:B1:71:LEU:HB2	58:B1:90:VAL:HG11	2.03	0.41
58:B1:647:PRO:HG3	58:B1:697:MET:HB3	2.01	0.41
59:B2:478:ARG:HD2	59:B2:492:MET:HA	2.02	0.41
8:H:5:HIS:HA	8:H:6:PRO:HD3	1.94	0.41
8:H:162:ALA:HB2	53:3:1056:U:C5'	2.48	0.41
9:I:32:LYS:HA	9:I:32:LYS:HD3	1.67	0.41
9:I:66:VAL:HB	9:I:71:PHE:HD2	1.84	0.41
17:Q:29:LYS:HD2	17:Q:29:LYS:HA	1.79	0.41
23:W:11:ARG:NH1	53:3:845:A:H5'	2.35	0.41
25:Y:56:ILE:HD13	25:Y:59:ARG:HH22	1.84	0.41
27:b:55:GLY:HA2	51:1:692:C:OP1	2.21	0.41
28:c:130:GLN:HE22	51:1:2578:G:H21	1.69	0.41
32:g:116:ARG:HA	32:g:116:ARG:HD3	1.82	0.41
35:k:17:ARG:NH1	53:3:1471:U:OP1	2.53	0.41
41:q:23:TYR:CE1	51:1:533:G:H5'	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:t:23:ALA:HB1	44:t:29:THR:HB	2.02	0.41
51:1:373:U:H2'	51:1:374:A:H8	1.85	0.41
51:1:2259:U:H2'	51:1:2260:C:H6	1.85	0.41
51:1:2427:C:H5''	51:1:2429:G:H5'	2.02	0.41
51:1:2701:U:H3'	51:1:2702:G:H5''	2.02	0.41
53:3:627:G:H2'	53:3:628:G:O4'	2.21	0.41
53:3:817:C:H4'	53:3:818:G:H5''	2.03	0.41
59:B2:902:LEU:HD11	59:B2:908:GLU:HB2	2.02	0.41
66:0:438:LEU:HD11	66:0:472:ARG:HD3	2.03	0.41
66:0:513:GLY:O	66:0:584:HIS:CD2	2.74	0.41
5:E:27:ASN:O	5:E:35:LYS:NZ	2.47	0.41
9:I:50:TYR:HD2	53:3:509:A:H5''	1.84	0.41
18:R:7:ASN:O	18:R:9:PRO:HD3	2.20	0.41
18:R:13:HIS:CE1	53:3:1296:C:H5'	2.55	0.41
38:n:49:GLU:O	38:n:53:THR:OG1	2.32	0.41
38:n:92:GLY:HA3	51:1:2880:C:H1'	2.03	0.41
51:1:690:G:H2'	51:1:691:C:O4'	2.19	0.41
51:1:799:G:H5''	51:1:800:A:H2'	2.02	0.41
51:1:910:A:N1	51:1:2277:G:H1'	2.36	0.41
51:1:1917:U:O2'	51:1:1918:A:H5'	2.20	0.41
51:1:2361:G:O2'	51:1:2362:C:H5'	2.20	0.41
51:1:2385:C:H2'	51:1:2386:A:H8	1.86	0.41
51:1:2528:U:H2'	51:1:2530:A:O5'	2.20	0.41
51:1:2564:A:OP1	51:1:2648:G:H4'	2.21	0.41
51:1:2646:C:O5'	51:1:2646:C:H6	2.03	0.41
51:1:2698:U:H2'	51:1:2699:C:C6	2.55	0.41
51:1:2799:A:C2'	51:1:2800:A:H5'	2.43	0.41
53:3:215:C:H2'	53:3:216:U:C6	2.56	0.41
58:B1:59:ALA:HB1	58:B1:90:VAL:HG23	2.01	0.41
58:B1:513:MET:HG3	58:B1:544:LEU:HD11	2.01	0.41
58:B1:576:ARG:HD3	58:B1:593:ASN:HA	2.03	0.41
58:B1:820:ILE:HG12	58:B1:884:SER:HB2	2.01	0.41
59:B2:687:ARG:HH11	59:B2:687:ARG:HD3	1.75	0.41
66:0:504:LYS:HE2	66:0:504:LYS:HB2	1.82	0.41
1:A:1:MET:HE2	1:A:1:MET:HB3	1.74	0.41
15:O:61:ALA:HB2	53:3:1061:G:H5''	2.03	0.41
15:O:92:LEU:HB3	15:O:93:ALA:H	1.69	0.41
22:V:9:GLY:H	22:V:24:ILE:HD13	1.86	0.41
27:b:209:ALA:HA	27:b:212:TRP:CE2	2.55	0.41
28:c:16:THR:OG1	28:c:18:ASP:OD1	2.35	0.41
28:c:133:THR:HG21	51:1:1676:A:H1'	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:133:ARG:HD2	33:i:133:ARG:HA	1.82	0.41
36:l:57:LEU:HD12	36:l:57:LEU:HA	1.93	0.41
41:q:4:LYS:HB3	41:q:4:LYS:HE2	1.92	0.41
42:r:85:LYS:HE3	51:1:815:C:OP2	2.20	0.41
44:t:38:ALA:O	44:t:81:LYS:NZ	2.39	0.41
47:w:47:VAL:HG21	47:w:76:ILE:HG22	2.02	0.41
49:y:19:LEU:HA	49:y:23:ARG:HH21	1.86	0.41
51:1:671:C:H2'	51:1:672:C:C6	2.56	0.41
51:1:1636:U:H2'	51:1:1637:A:C8	2.55	0.41
51:1:1748:C:H2'	51:1:1749:A:H8	1.84	0.41
51:1:2096:C:H2'	51:1:2097:A:C8	2.55	0.41
53:3:842:U:H2'	53:3:844:G:H5'	2.02	0.41
57:A2:28:LEU:HB2	57:A2:201:LEU:HB3	2.02	0.41
58:B1:144:TYR:OH	58:B1:162:GLU:OE1	2.34	0.41
58:B1:1350:ASN:HA	58:B1:1353:VAL:HG12	2.02	0.41
59:B2:27:LEU:O	59:B2:528:ARG:NH1	2.43	0.41
59:B2:886:LYS:HE2	59:B2:918:LEU:HD13	2.03	0.41
64:6:53:G:H1'	65:a:55:SER:OG	2.21	0.41
9:I:80:ARG:HG3	53:3:613:C:OP1	2.21	0.41
9:I:205:LYS:NZ	53:3:26:A:H2	2.19	0.41
12:L:83:THR:O	12:L:83:THR:HG22	2.21	0.41
14:N:18:VAL:HG22	14:N:64:ILE:HG23	2.02	0.41
17:Q:101:LEU:O	17:Q:103:CYS:N	2.54	0.41
31:f:148:ARG:HA	31:f:161:VAL:HB	2.03	0.41
32:g:2:GLN:HE21	32:g:20:ASN:HB2	1.85	0.41
33:i:94:LYS:NZ	51:1:1076:C:H4'	2.36	0.41
33:i:100:ILE:HB	33:i:139:VAL:HG12	2.02	0.41
51:1:1091:G:H2'	51:1:1092:C:C6	2.56	0.41
53:3:78:A:H61	53:3:91:U:H3	1.69	0.41
53:3:1201:A:H4'	53:3:1202:U:C5'	2.49	0.41
53:3:1230:C:O2'	53:3:1231:G:H5'	2.20	0.41
53:3:1255:G:H2'	53:3:1279:G:H1	1.85	0.41
58:B1:839:VAL:HG12	58:B1:864:LEU:HD12	2.02	0.41
58:B1:1050:THR:HG23	58:B1:1057:SER:HB3	2.03	0.41
59:B2:746:ALA:O	59:B2:974:ARG:NH2	2.45	0.41
1:A:1:MET:HB2	52:2:43:C:OP1	2.20	0.41
1:A:64:PHE:HA	53:3:1011:C:H5'	2.03	0.41
2:B:7:PRO:HD2	51:1:1263:U:O2'	2.21	0.41
9:I:145:ARG:HH22	9:I:147:LYS:HD2	1.86	0.41
11:K:44:ARG:HA	11:K:58:HIS:HA	2.03	0.41
17:Q:114:SER:N	53:3:502:A:OP1	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:86:ALA:HB1	19:S:91:GLU:HB2	2.03	0.41
25:Y:66:ILE:HG23	25:Y:70:LYS:HD3	2.01	0.41
30:e:65:LEU:HD11	52:2:41:G:H2'	2.02	0.41
33:i:135:MET:SD	51:1:1063:G:H1'	2.60	0.41
36:l:99:ASN:ND2	51:1:621:A:OP2	2.54	0.41
44:t:8:LEU:O	49:y:29:ARG:NH1	2.53	0.41
47:w:19:VAL:HG13	47:w:34:VAL:HG22	2.03	0.41
51:1:610:C:O5'	51:1:610:C:H6	2.03	0.41
51:1:732:C:H2'	51:1:733:G:O4'	2.21	0.41
51:1:1137:G:H2'	51:1:1138:G:H8	1.85	0.41
51:1:1341:G:H5''	51:1:1397:U:O2	2.21	0.41
51:1:1429:G:H2'	51:1:1430:G:H8	1.85	0.41
51:1:2700:A:H2'	51:1:2701:U:C6	2.56	0.41
51:1:2739:U:O2'	51:1:2740:A:H5'	2.21	0.41
53:3:20:U:H2'	53:3:21:G:O4'	2.20	0.41
53:3:55:A:C4	66:0:329:PHE:HB3	2.56	0.41
53:3:244:U:O4	53:3:906:A:H1'	2.20	0.41
53:3:987:G:H2'	53:3:988:G:C8	2.55	0.41
53:3:1448:C:H2'	53:3:1449:C:C6	2.56	0.41
55:8:14:DC:C2	55:8:15:DC:C5	3.09	0.41
58:B1:239:LEU:N	58:B1:239:LEU:HD23	2.36	0.41
58:B1:245:LEU:CG	58:B1:246:PRO:HD2	2.47	0.41
58:B1:279:LEU:HD13	58:B1:299:LEU:HD13	2.02	0.41
58:B1:616:PRO:HA	58:B1:619:ILE:HG22	2.02	0.41
58:B1:1177:ILE:HD12	58:B1:1186:TYR:HE2	1.85	0.41
59:B2:310:ILE:HG21	59:B2:325:LEU:HB3	2.03	0.41
59:B2:590:PRO:HB2	59:B2:655:VAL:HG21	2.01	0.41
59:B2:657:THR:HG21	59:B2:1188:ASP:HB2	2.03	0.41
66:0:145:ASP:CG	69:0:801:GDP:HN21	2.29	0.41
66:0:162:LEU:HD23	66:0:162:LEU:HA	1.94	0.41
66:0:200:VAL:HG23	66:0:201:THR:HG23	2.02	0.41
66:0:521:ASP:HB2	66:0:579:HIS:HD2	1.86	0.41
15:O:15:HIS:HD2	53:3:1152:A:H5'	1.86	0.41
27:b:179:GLU:HB2	27:b:270:ARG:HB3	2.02	0.41
28:c:47:ALA:HA	28:c:84:LEU:HG	2.04	0.41
29:d:131:THR:HG23	51:1:321:U:H5''	2.03	0.41
29:d:163:ASN:HD21	51:1:322:A:C2'	2.32	0.41
32:g:14:SER:O	32:g:14:SER:OG	2.36	0.41
34:j:132:HIS:ND1	51:1:7:G:H5'	2.36	0.41
37:m:88:ASN:OD1	37:m:88:ASN:N	2.52	0.41
41:q:24:TYR:HE1	51:1:17:G:H4'	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:4:U:H2'	51:1:5:A:C8	2.56	0.41
51:1:399:U:OP1	51:1:2090:A:H5''	2.21	0.41
51:1:535:G:H2'	51:1:536:G:O4'	2.20	0.41
51:1:1944:U:O2'	51:1:1945:G:H5''	2.21	0.41
51:1:2360:G:H2'	51:1:2361:G:O4'	2.21	0.41
53:3:26:A:H61	53:3:558:G:H1'	1.86	0.41
53:3:346:G:H3'	53:3:346:G:N3	2.36	0.41
53:3:619:U:H3'	53:3:619:U:H6	1.86	0.41
55:8:2:DC:C6	55:8:2:DC:H5'	2.56	0.41
57:A1:48:LEU:HA	57:A1:48:LEU:HD12	1.78	0.41
58:B1:233:LYS:HA	58:B1:234:PRO:HD3	1.89	0.41
58:B1:777:HIS:CD2	59:B2:550:VAL:HG13	2.56	0.41
58:B1:1263:LYS:NZ	58:B1:1315:ALA:O	2.49	0.41
59:B2:854:ILE:HG21	59:B2:917:SER:CB	2.39	0.41
27:b:129:LEU:HD12	27:b:133:ASN:HB2	2.03	0.40
28:c:29:VAL:HB	28:c:98:VAL:HG22	2.02	0.40
31:f:159:LYS:NZ	51:1:2657:A:O2'	2.53	0.40
43:s:42:LYS:CB	51:1:2010:G:H5''	2.47	0.40
49:y:32:ALA:HB2	49:y:37:LEU:HD23	2.03	0.40
51:1:284:U:H2'	51:1:285:G:C8	2.55	0.40
51:1:1130:U:O2'	51:1:1131:G:OP1	2.35	0.40
51:1:2004:G:H2'	51:1:2005:A:O4'	2.21	0.40
51:1:2548:U:C4	51:1:2549:G:N7	2.88	0.40
53:3:471:U:H2'	53:3:472:U:C6	2.56	0.40
53:3:546:A:H4'	53:3:548:G:O3'	2.20	0.40
53:3:623:C:H2'	53:3:624:C:C6	2.56	0.40
53:3:1097:C:H2'	53:3:1098:C:C6	2.56	0.40
57:A2:42:ALA:HB1	57:A2:224:LEU:HD11	2.03	0.40
58:B1:68:TYR:CB	58:B1:75:TYR:HE2	2.34	0.40
66:0:352:SER:OG	66:0:396:THR:O	2.33	0.40
1:A:27:THR:OG1	30:e:58:ALA:O	2.37	0.40
12:L:65:LEU:HA	12:L:68:VAL:HG12	2.03	0.40
19:S:50:LEU:HD23	19:S:50:LEU:HA	1.85	0.40
19:S:97:LYS:HB3	19:S:97:LYS:HE2	1.86	0.40
27:b:144:GLU:OE1	27:b:150:GLY:N	2.55	0.40
27:b:211:ARG:HG3	51:1:764:A:N3	2.36	0.40
42:r:16:GLU:HG2	42:r:101:ILE:HG12	2.04	0.40
45:u:48:VAL:HA	45:u:49:PRO:HD3	1.96	0.40
51:1:94:A:H2'	51:1:95:A:O4'	2.21	0.40
51:1:179:C:O2'	51:1:180:G:H5'	2.21	0.40
51:1:227:A:H1'	51:1:229:C:H41	1.86	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1:272:A:H2'	51:1:273:G:H8	1.86	0.40
51:1:631:A:H1'	51:1:2415:G:O2'	2.21	0.40
51:1:917:A:C2	52:2:79:G:N3	2.88	0.40
51:1:1380:G:C8	51:1:1380:G:O5'	2.74	0.40
51:1:1508:A:H2'	51:1:1509:A:O4'	2.21	0.40
51:1:1757:A:O5'	51:1:1757:A:H8	2.04	0.40
51:1:2441:U:H2'	51:1:2442:C:H6	1.87	0.40
53:3:401:C:H2'	53:3:402:G:C8	2.56	0.40
53:3:812:G:OP1	53:3:903:G:H1'	2.21	0.40
53:3:876:C:H2'	53:3:877:G:H8	1.86	0.40
57:A2:104:LYS:O	57:A2:139:SER:OG	2.36	0.40
58:B1:1361:THR:N	59:B2:1282:GLY:O	2.53	0.40
59:B2:861:ALA:HB1	59:B2:882:ILE:HD13	2.01	0.40
66:0:176:GLU:O	66:0:178:HIS:N	2.54	0.40
66:0:197:ASP:C	66:0:199:GLY:H	2.29	0.40
66:0:230:SER:HB2	66:0:233:LEU:HB3	2.03	0.40
4:D:19:ARG:NH2	51:1:124:G:C5	2.89	0.40
12:L:78:ARG:HA	12:L:78:ARG:HD3	1.81	0.40
20:T:11:VAL:HG23	20:T:26:VAL:HG11	2.04	0.40
21:U:4:ILE:HD12	21:U:67:ILE:HG13	2.03	0.40
33:i:73:PRO:HA	33:i:74:PRO:HD3	1.94	0.40
36:l:62:PRO:HG3	51:1:2393:U:H5''	2.04	0.40
48:x:9:LYS:HZ2	48:x:9:LYS:HG2	1.75	0.40
51:1:118:A:N3	51:1:178:G:H1'	2.36	0.40
51:1:123:G:H4'	51:1:1376:C:O5'	2.21	0.40
51:1:606:U:H4'	51:1:658:U:HO2'	1.86	0.40
51:1:935:C:H2'	51:1:936:A:H8	1.87	0.40
51:1:1507:C:H2'	51:1:1508:A:O4'	2.21	0.40
51:1:1747:U:H2'	51:1:1748:C:C6	2.56	0.40
51:1:1808:A:H3'	51:1:1809:A:C8	2.56	0.40
51:1:1913:A:O2'	67:h:4:SER:HA	2.22	0.40
53:3:78:A:H8	53:3:78:A:O5'	2.05	0.40
53:3:1100:C:C2	53:3:1102:A:H5'	2.57	0.40
58:B1:111:THR:HG23	58:B1:300:GLN:HA	2.03	0.40
58:B1:390:LEU:HD13	58:B1:390:LEU:H	1.86	0.40
58:B1:472:LEU:HD11	59:B2:1294:LYS:HG2	2.03	0.40
58:B1:515:ARG:HG2	58:B1:516:ASP:H	1.85	0.40
59:B2:741:MET:HE3	59:B2:974:ARG:HH12	1.85	0.40
59:B2:870:ILE:HB	59:B2:944:ARG:HD3	2.02	0.40
59:B2:912:ASP:HB3	59:B2:913:VAL:H	1.72	0.40
63:5:17:C:H2'	63:5:18:G:C8	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
63:5:37:A:H3'	63:5:38:A:C8	2.56	0.40
65:a:167:LYS:HE2	65:a:167:LYS:HB2	1.76	0.40
7:G:203:ASP:OD1	7:G:203:ASP:N	2.54	0.40
10:J:24:VAL:HG12	10:J:25:LYS:H	1.87	0.40
12:L:3:ARG:HB3	12:L:4:ARG:HH11	1.87	0.40
17:Q:40:THR:HG21	67:h:6:5OH:OS	2.21	0.40
18:R:97:ARG:NH1	53:3:1308:U:H5	2.19	0.40
19:S:63:CYS:SG	19:S:64:ARG:N	2.94	0.40
24:X:79:TYR:CE1	53:3:1226:C:H4'	2.57	0.40
27:b:68:ARG:O	27:b:188:ARG:NH2	2.55	0.40
44:t:1:MET:HE2	51:1:136:G:H21	1.85	0.40
46:v:80:HIS:H	46:v:86:LEU:HA	1.86	0.40
51:1:1461:C:O5'	51:1:1461:C:H6	2.05	0.40
51:1:2011:U:H2'	51:1:2012:G:O4'	2.22	0.40
51:1:2853:C:H2'	51:1:2854:G:H8	1.86	0.40
53:3:216:U:O3'	53:3:464:U:H4'	2.21	0.40
53:3:404:G:H2'	53:3:405:U:C6	2.55	0.40
53:3:702:A:H2'	53:3:702:A:N3	2.37	0.40
58:B1:109:SER:CB	58:B1:296:LYS:HG2	2.51	0.40
58:B1:182:ALA:HB1	58:B1:238:ILE:CG2	2.52	0.40
58:B1:820:ILE:HD11	58:B1:822:MET:HE2	2.02	0.40
59:B2:805:MET:HB2	59:B2:805:MET:HE3	1.86	0.40
65:a:6:LYS:HA	65:a:9:ARG:HG2	2.03	0.40
7:G:155:GLY:HA3	61:NA:219:GLU:CB	2.50	0.40
14:N:104:THR:HG22	14:N:106:ASP:H	1.86	0.40
17:Q:58:ASN:OD1	17:Q:58:ASN:N	2.52	0.40
23:W:47:ARG:H	23:W:47:ARG:HG2	1.60	0.40
26:Z:7:GLU:HG3	26:Z:15:LEU:HB2	2.02	0.40
29:d:148:ILE:HB	29:d:169:VAL:HG12	2.04	0.40
32:g:8:LYS:HG3	32:g:14:SER:HA	2.04	0.40
36:l:63:LYS:HE3	51:1:2394:C:H5''	2.03	0.40
46:v:26:PHE:HE2	46:v:89:ILE:HG13	1.87	0.40
51:1:859:G:O2'	51:1:860:U:H6	2.04	0.40
51:1:987:C:H2'	51:1:988:A:O4'	2.21	0.40
51:1:2701:U:H3'	51:1:2702:G:C5'	2.51	0.40
51:1:2722:G:H8	51:1:2722:G:O5'	2.05	0.40
53:3:26:A:N6	53:3:558:G:H1'	2.36	0.40
58:B1:349:TYR:HA	59:B2:1246:ARG:O	2.22	0.40
59:B2:159:SER:HB2	59:B2:442:VAL:HG11	2.04	0.40
66:0:68:THR:HG22	66:0:69:THR:H	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	
1	A	64/70 (91%)	54 (84%)	10 (16%)	0	100	100
2	B	54/57 (95%)	49 (91%)	5 (9%)	0	100	100
3	C	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
4	D	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
5	E	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	8	37
6	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	G	216/241 (90%)	186 (86%)	29 (13%)	1 (0%)	25	64
8	H	204/233 (88%)	184 (90%)	19 (9%)	1 (0%)	25	64
9	I	203/206 (98%)	178 (88%)	24 (12%)	1 (0%)	25	64
10	J	155/167 (93%)	131 (84%)	22 (14%)	2 (1%)	10	42
11	K	98/135 (73%)	83 (85%)	14 (14%)	1 (1%)	13	49
12	L	149/179 (83%)	129 (87%)	18 (12%)	2 (1%)	10	42
13	M	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
14	N	125/130 (96%)	95 (76%)	25 (20%)	5 (4%)	2	18
15	O	96/103 (93%)	77 (80%)	18 (19%)	1 (1%)	13	49
16	P	114/129 (88%)	90 (79%)	22 (19%)	2 (2%)	7	34
17	Q	121/124 (98%)	97 (80%)	18 (15%)	6 (5%)	1	16
18	R	112/118 (95%)	99 (88%)	12 (11%)	1 (1%)	14	51
19	S	98/101 (97%)	80 (82%)	15 (15%)	3 (3%)	3	22
20	T	86/89 (97%)	77 (90%)	8 (9%)	1 (1%)	11	44
21	U	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	10	42
22	V	78/84 (93%)	67 (86%)	10 (13%)	1 (1%)	10	42
23	W	63/75 (84%)	59 (94%)	4 (6%)	0	100	100
24	X	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
25	Y	83/87 (95%)	80 (96%)	3 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	Z	63/71 (89%)	45 (71%)	18 (29%)	0	100	100
27	b	269/273 (98%)	233 (87%)	31 (12%)	5 (2%)	6	33
28	c	207/209 (99%)	181 (87%)	25 (12%)	1 (0%)	25	64
29	d	199/201 (99%)	186 (94%)	13 (6%)	0	100	100
30	e	175/179 (98%)	155 (89%)	18 (10%)	2 (1%)	12	46
31	f	174/177 (98%)	152 (87%)	19 (11%)	3 (2%)	7	36
32	g	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	19	56
33	i	139/142 (98%)	116 (84%)	22 (16%)	1 (1%)	19	56
34	j	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	19	56
35	k	120/123 (98%)	99 (82%)	19 (16%)	2 (2%)	7	36
36	l	141/144 (98%)	121 (86%)	20 (14%)	0	100	100
37	m	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
38	n	118/127 (93%)	101 (86%)	17 (14%)	0	100	100
39	o	114/117 (97%)	103 (90%)	10 (9%)	1 (1%)	14	51
40	p	112/115 (97%)	102 (91%)	10 (9%)	0	100	100
41	q	115/118 (98%)	111 (96%)	3 (3%)	1 (1%)	14	51
42	r	101/103 (98%)	86 (85%)	14 (14%)	1 (1%)	13	49
43	s	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
44	t	91/100 (91%)	78 (86%)	13 (14%)	0	100	100
45	u	100/104 (96%)	81 (81%)	18 (18%)	1 (1%)	13	49
46	v	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
47	w	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
48	x	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
49	y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	8	37
50	z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
57	A1	295/329 (90%)	276 (94%)	19 (6%)	0	100	100
57	A2	282/329 (86%)	271 (96%)	11 (4%)	0	100	100
58	B1	1329/1407 (94%)	1205 (91%)	119 (9%)	5 (0%)	30	68
59	B2	1338/1342 (100%)	1206 (90%)	128 (10%)	4 (0%)	37	72
60	W0	80/91 (88%)	77 (96%)	3 (4%)	0	100	100
61	NA	490/495 (99%)	482 (98%)	8 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
62	NG	150/181 (83%)	135 (90%)	11 (7%)	4 (3%)	4	26
65	a	130/234 (56%)	112 (86%)	18 (14%)	0	100	100
66	0	695/716 (97%)	621 (89%)	71 (10%)	3 (0%)	30	68
67	h	2/6 (33%)	1 (50%)	1 (50%)	0	100	100
All	All	10508/11185 (94%)	9407 (90%)	1034 (10%)	67 (1%)	24	60

All (67) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	31	ILE
9	I	29	THR
14	N	57	VAL
14	N	90	ASP
14	N	91	GLU
17	Q	87	LYS
20	T	46	LYS
30	e	175	PRO
31	f	45	ALA
32	g	136	SER
35	k	92	GLU
42	r	54	VAL
49	y	24	GLU
58	B1	121	PRO
10	J	75	LEU
11	K	56	LYS
17	Q	3	VAL
17	Q	24	GLU
17	Q	102	ASP
19	S	60	ARG
21	U	45	GLU
27	b	46	GLY
28	c	197	THR
33	i	121	ILE
59	B2	43	PRO
59	B2	918	LEU
62	NG	102	PRO
66	0	176	GLU
66	0	177	GLU
12	L	6	ILE
17	Q	101	LEU
17	Q	108	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	S	61	ASN
27	b	205	GLY
39	o	34	HIS
41	q	5	ARG
58	B1	904	ALA
59	B2	888	THR
62	NG	124	PRO
7	G	20	ARG
14	N	23	GLY
16	P	89	GLY
22	V	50	ASN
31	f	44	HIS
58	B1	43	THR
58	B1	193	ASP
14	N	102	PHE
27	b	255	LYS
30	e	174	PHE
31	f	174	LYS
35	k	93	GLN
45	u	6	ARG
58	B1	1325	PHE
66	0	198	GLN
16	P	88	PRO
18	R	7	ASN
19	S	35	ALA
62	NG	129	GLU
34	j	110	PRO
27	b	232	GLY
8	H	12	GLY
12	L	79	VAL
27	b	240	GLY
59	B2	1317	PRO
62	NG	122	PRO
10	J	97	PRO
15	O	57	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	
1	A	59/62 (95%)	56 (95%)	3 (5%)	20	42
2	B	47/48 (98%)	44 (94%)	3 (6%)	14	36
3	C	45/49 (92%)	45 (100%)	0	100	100
4	D	38/38 (100%)	37 (97%)	1 (3%)	41	61
5	E	51/52 (98%)	51 (100%)	0	100	100
6	F	34/34 (100%)	34 (100%)	0	100	100
7	G	180/199 (90%)	175 (97%)	5 (3%)	38	59
8	H	169/190 (89%)	165 (98%)	4 (2%)	44	63
9	I	172/173 (99%)	169 (98%)	3 (2%)	56	72
10	J	118/126 (94%)	115 (98%)	3 (2%)	42	62
11	K	87/116 (75%)	83 (95%)	4 (5%)	23	45
12	L	124/147 (84%)	122 (98%)	2 (2%)	58	74
13	M	104/105 (99%)	104 (100%)	0	100	100
14	N	105/107 (98%)	102 (97%)	3 (3%)	37	58
15	O	86/90 (96%)	80 (93%)	6 (7%)	12	33
16	P	89/99 (90%)	88 (99%)	1 (1%)	70	80
17	Q	103/104 (99%)	98 (95%)	5 (5%)	21	43
18	R	92/96 (96%)	91 (99%)	1 (1%)	70	80
19	S	83/84 (99%)	82 (99%)	1 (1%)	67	79
20	T	76/77 (99%)	75 (99%)	1 (1%)	65	77
21	U	65/65 (100%)	64 (98%)	1 (2%)	60	75
22	V	74/78 (95%)	73 (99%)	1 (1%)	62	75
23	W	56/65 (86%)	54 (96%)	2 (4%)	30	52
24	X	70/79 (89%)	69 (99%)	1 (1%)	62	75
25	Y	65/66 (98%)	65 (100%)	0	100	100
26	Z	55/61 (90%)	52 (94%)	3 (6%)	18	40
27	b	216/218 (99%)	212 (98%)	4 (2%)	52	69
28	c	164/164 (100%)	162 (99%)	2 (1%)	67	79
29	d	165/165 (100%)	163 (99%)	2 (1%)	67	79
30	e	148/150 (99%)	147 (99%)	1 (1%)	81	87
31	f	137/138 (99%)	137 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	g	114/114 (100%)	112 (98%)	2 (2%)	54	71
33	i	109/110 (99%)	95 (87%)	14 (13%)	3	15
34	j	116/116 (100%)	115 (99%)	1 (1%)	75	83
35	k	103/104 (99%)	100 (97%)	3 (3%)	37	58
36	l	102/103 (99%)	100 (98%)	2 (2%)	50	68
37	m	109/109 (100%)	109 (100%)	0	100	100
38	n	100/103 (97%)	99 (99%)	1 (1%)	73	81
39	o	86/87 (99%)	86 (100%)	0	100	100
40	p	99/100 (99%)	97 (98%)	2 (2%)	50	68
41	q	89/90 (99%)	86 (97%)	3 (3%)	32	53
42	r	84/84 (100%)	81 (96%)	3 (4%)	30	52
43	s	93/93 (100%)	93 (100%)	0	100	100
44	t	80/84 (95%)	79 (99%)	1 (1%)	65	77
45	u	82/85 (96%)	81 (99%)	1 (1%)	67	79
46	v	78/78 (100%)	77 (99%)	1 (1%)	65	77
47	w	57/63 (90%)	56 (98%)	1 (2%)	54	71
48	x	67/68 (98%)	67 (100%)	0	100	100
49	y	55/55 (100%)	55 (100%)	0	100	100
50	z	48/49 (98%)	46 (96%)	2 (4%)	25	47
57	A1	185/286 (65%)	174 (94%)	11 (6%)	16	38
57	A2	186/286 (65%)	185 (100%)	1 (0%)	86	89
58	B1	1110/1168 (95%)	1021 (92%)	89 (8%)	10	29
59	B2	1150/1157 (99%)	1119 (97%)	31 (3%)	40	60
60	W0	70/75 (93%)	69 (99%)	1 (1%)	62	75
65	a	110/181 (61%)	110 (100%)	0	100	100
66	0	574/588 (98%)	546 (95%)	28 (5%)	21	43
67	h	2/2 (100%)	2 (100%)	0	100	100
All	All	8135/8683 (94%)	7874 (97%)	261 (3%)	36	55

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	35	ASP
1	A	57	VAL
2	B	2	VAL
2	B	21	LEU
2	B	24	VAL
4	D	43	THR
7	G	17	HIS
7	G	20	ARG
7	G	46	VAL
7	G	48	MET
7	G	160	LEU
8	H	62	SER
8	H	63	ILE
8	H	156	LEU
8	H	172	VAL
9	I	32	LYS
9	I	33	ILE
9	I	170	LEU
10	J	120	HIS
10	J	121	ASN
10	J	123	LEU
11	K	47	LEU
11	K	53	LYS
11	K	92	THR
11	K	93	LYS
12	L	29	LEU
12	L	134	VAL
14	N	20	ILE
14	N	21	LYS
14	N	24	ASN
15	O	83	THR
15	O	84	VAL
15	O	87	LEU
15	O	89	ARG
15	O	99	GLN
15	O	102	LEU
16	P	15	VAL
17	Q	20	VAL
17	Q	42	LYS
17	Q	43	LYS
17	Q	45	ASN
17	Q	97	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	R	82	LEU
19	S	78	LEU
20	T	55	LEU
21	U	19	VAL
22	V	40	THR
23	W	28	LEU
23	W	47	ARG
24	X	38	THR
26	Z	24	LYS
26	Z	35	GLU
26	Z	40	PRO
27	b	12	ARG
27	b	18	VAL
27	b	171	VAL
27	b	194	VAL
28	c	79	LEU
28	c	98	VAL
29	d	79	ARG
29	d	80	SER
30	e	108	PRO
32	g	5	LEU
32	g	143	ILE
33	i	2	LYS
33	i	3	LYS
33	i	5	GLN
33	i	18	ASN
33	i	23	VAL
33	i	27	LEU
33	i	29	GLN
33	i	67	THR
33	i	72	THR
33	i	117	THR
33	i	124	MET
33	i	131	THR
33	i	134	SER
33	i	135	MET
34	j	10	THR
35	k	61	VAL
35	k	85	VAL
35	k	86	LEU
36	l	85	VAL
36	l	127	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	n	50	PRO
40	p	32	VAL
40	p	109	ILE
41	q	82	LEU
41	q	84	LYS
41	q	86	SER
42	r	48	LYS
42	r	49	ILE
42	r	51	VAL
44	t	67	VAL
45	u	27	VAL
46	v	70	ILE
47	w	19	VAL
50	z	10	ARG
50	z	15	ARG
57	A1	9	LEU
57	A1	12	ARG
57	A1	13	LEU
57	A1	18	GLN
57	A1	19	VAL
57	A1	22	THR
57	A1	27	THR
57	A1	28	LEU
57	A1	33	ARG
57	A1	46	ILE
57	A1	48	LEU
57	A2	74	VAL
58	B1	24	LEU
58	B1	40	LYS
58	B1	42	GLU
58	B1	44	ILE
58	B1	47	ARG
58	B1	49	PHE
58	B1	50	LYS
58	B1	60	ARG
58	B1	66	LYS
58	B1	69	GLU
58	B1	71	LEU
58	B1	74	LYS
58	B1	76	LYS
58	B1	78	LEU
58	B1	80	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	B1	81	ARG
58	B1	87	LYS
58	B1	91	GLU
58	B1	93	THR
58	B1	94	GLN
58	B1	95	THR
58	B1	96	LYS
58	B1	99	ARG
58	B1	100	GLU
58	B1	114	ILE
58	B1	117	LEU
58	B1	120	LEU
58	B1	126	LEU
58	B1	132	LEU
58	B1	135	ILE
58	B1	142	GLU
58	B1	144	TYR
58	B1	145	VAL
58	B1	146	VAL
58	B1	147	ILE
58	B1	152	THR
58	B1	154	LEU
58	B1	157	GLN
58	B1	159	ILE
58	B1	172	PHE
58	B1	174	ASP
58	B1	175	GLU
58	B1	180	MET
58	B1	190	LYS
58	B1	193	ASP
58	B1	196	GLN
58	B1	210	SER
58	B1	212	THR
58	B1	216	LYS
58	B1	222	LYS
58	B1	223	LEU
58	B1	227	PHE
58	B1	233	LYS
58	B1	237	MET
58	B1	238	ILE
58	B1	239	LEU
58	B1	240	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	B1	244	VAL
58	B1	255	LEU
58	B1	256	ASP
58	B1	259	ARG
58	B1	317	THR
58	B1	322	ARG
58	B1	324	LEU
58	B1	363	LEU
58	B1	385	LEU
58	B1	386	GLU
58	B1	387	LEU
58	B1	390	LEU
58	B1	393	THR
58	B1	394	ILE
58	B1	395	LYS
58	B1	416	ILE
58	B1	417	ARG
58	B1	425	ARG
58	B1	506	VAL
58	B1	514	THR
58	B1	800	LEU
58	B1	807	LEU
58	B1	839	VAL
58	B1	901	ARG
58	B1	903	LEU
58	B1	1172	LYS
58	B1	1181	ASP
58	B1	1233	ILE
58	B1	1327	GLU
58	B1	1328	THR
58	B1	1331	VAL
58	B1	1332	LEU
59	B2	4	SER
59	B2	44	GLU
59	B2	49	LEU
59	B2	56	VAL
59	B2	146	VAL
59	B2	483	ASP
59	B2	487	LEU
59	B2	516	ASP
59	B2	538	LEU
59	B2	540	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
59	B2	545	PHE
59	B2	546	GLU
59	B2	615	VAL
59	B2	857	VAL
59	B2	859	GLU
59	B2	887	VAL
59	B2	890	LYS
59	B2	893	THR
59	B2	894	GLN
59	B2	895	LEU
59	B2	900	LYS
59	B2	901	LEU
59	B2	902	LEU
59	B2	903	ARG
59	B2	905	ILE
59	B2	912	ASP
59	B2	918	LEU
59	B2	920	VAL
59	B2	922	ASN
59	B2	1076	ILE
59	B2	1151	LEU
60	W0	63	ILE
66	0	31	LEU
66	0	97	ILE
66	0	214	LEU
66	0	360	PHE
66	0	415	VAL
66	0	418	ILE
66	0	483	VAL
66	0	485	LYS
66	0	488	VAL
66	0	507	LYS
66	0	512	ARG
66	0	519	VAL
66	0	522	MET
66	0	525	LEU
66	0	526	GLU
66	0	551	PRO
66	0	584	HIS
66	0	626	GLU
66	0	627	ASN
66	0	628	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
66	0	630	ASP
66	0	636	SER
66	0	638	ARG
66	0	642	LEU
66	0	643	LYS
66	0	646	GLU
66	0	648	GLU
66	0	649	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	HIS
2	B	5	ASN
4	D	26	ASN
7	G	17	HIS
7	G	57	ASN
7	G	93	HIS
7	G	176	ASN
8	H	138	GLN
8	H	139	ASN
9	I	53	GLN
9	I	58	GLN
9	I	84	ASN
10	J	81	GLN
10	J	88	HIS
10	J	131	ASN
10	J	145	ASN
10	J	147	ASN
12	L	121	ASN
12	L	147	ASN
13	M	66	GLN
14	N	4	GLN
14	N	24	ASN
14	N	30	ASN
15	O	15	HIS
15	O	35	GLN
16	P	27	ASN
16	P	37	GLN
16	P	39	ASN
16	P	63	GLN
16	P	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	Q	45	ASN
17	Q	76	HIS
17	Q	95	HIS
17	Q	111	GLN
18	R	13	HIS
19	S	48	GLN
20	T	27	GLN
21	U	26	ASN
21	U	63	GLN
23	W	51	GLN
25	Y	54	GLN
25	Y	67	HIS
25	Y	69	ASN
25	Y	74	HIS
26	Z	63	ASN
27	b	24	HIS
27	b	52	HIS
27	b	57	HIS
27	b	114	GLN
27	b	152	GLN
28	c	42	ASN
28	c	49	GLN
28	c	58	ASN
28	c	136	ASN
28	c	164	GLN
29	d	94	GLN
29	d	97	ASN
29	d	163	ASN
30	e	26	GLN
31	f	63	GLN
31	f	87	GLN
31	f	103	ASN
31	f	110	HIS
31	f	142	GLN
32	g	11	ASN
32	g	73	ASN
32	g	135	HIS
33	i	110	GLN
34	j	40	HIS
34	j	135	GLN
35	k	3	GLN
35	k	9	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	l	99	ASN
37	m	3	GLN
37	m	17	ASN
37	m	97	GLN
38	n	9	GLN
38	n	73	ASN
38	n	81	ASN
39	o	61	GLN
39	o	98	GLN
40	p	55	HIS
40	p	74	GLN
41	q	70	GLN
42	r	11	GLN
43	s	57	ASN
44	t	15	HIS
44	t	48	GLN
44	t	59	ASN
45	u	68	ASN
46	v	49	ASN
46	v	78	GLN
47	w	8	ASN
47	w	53	HIS
48	x	22	ASN
48	x	35	HIS
49	y	20	ASN
49	y	25	GLN
49	y	31	GLN
50	z	8	GLN
57	A1	66	HIS
57	A1	84	ASN
57	A1	117	HIS
57	A1	128	HIS
57	A1	227	GLN
57	A2	23	HIS
57	A2	227	GLN
58	B1	45	ASN
58	B1	196	GLN
58	B1	364	HIS
58	B1	424	ASN
58	B1	450	HIS
58	B1	469	HIS
58	B1	805	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
58	B1	817	HIS
58	B1	865	HIS
58	B1	1195	GLN
58	B1	1238	GLN
58	B1	1259	GLN
59	B2	69	GLN
59	B2	314	ASN
59	B2	330	HIS
59	B2	343	HIS
59	B2	518	ASN
59	B2	554	HIS
59	B2	580	GLN
59	B2	688	GLN
59	B2	762	ASN
59	B2	808	ASN
59	B2	965	GLN
59	B2	1237	HIS
59	B2	1268	GLN
59	B2	1313	HIS
60	W0	7	GLN
60	W0	31	GLN
60	W0	62	GLN
65	a	24	ASN
65	a	47	ASN
66	0	44	HIS
66	0	85	ASN
66	0	157	GLN
66	0	272	ASN
66	0	296	ASN
66	0	344	ASN
66	0	365	GLN
66	0	428	GLN
66	0	487	GLN
66	0	505	HIS
66	0	517	HIS
66	0	530	ASN
66	0	579	HIS

5.3.3 RNA ⓘ

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
51	1	2902/2904 (99%)	420 (14%)	10 (0%)
52	2	119/120 (99%)	12 (10%)	1 (0%)
53	3	1538/1542 (99%)	181 (11%)	6 (0%)
54	4	28/44 (63%)	13 (46%)	3 (10%)
63	5	75/76 (98%)	38 (50%)	7 (9%)
64	6	76/77 (98%)	18 (23%)	0
All	All	4738/4763 (99%)	682 (14%)	27 (0%)

All (682) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
51	1	10	A
51	1	12	U
51	1	35	G
51	1	42	A
51	1	46	G
51	1	51	G
51	1	63	A
51	1	71	A
51	1	74	A
51	1	75	G
51	1	98	G
51	1	102	U
51	1	103	A
51	1	119	A
51	1	120	U
51	1	139	U
51	1	140	C
51	1	141	G
51	1	142	A
51	1	149	A
51	1	162	U
51	1	163	C
51	1	181	A
51	1	196	A
51	1	215	G
51	1	216	A
51	1	219	A
51	1	221	A
51	1	222	A
51	1	228	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	229	C
51	1	232	G
51	1	233	A
51	1	248	G
51	1	255	A
51	1	266	G
51	1	276	U
51	1	278	A
51	1	281	C
51	1	285	G
51	1	294	A
51	1	311	A
51	1	323	C
51	1	324	A
51	1	329	G
51	1	330	A
51	1	346	A
51	1	353	C
51	1	361	G
51	1	362	A
51	1	371	A
51	1	372	G
51	1	386	G
51	1	387	U
51	1	404	A
51	1	405	U
51	1	411	G
51	1	412	A
51	1	424	G
51	1	451	U
51	1	455	C
51	1	456	C
51	1	481	G
51	1	491	G
51	1	504	A
51	1	508	A
51	1	528	A
51	1	531	C
51	1	532	A
51	1	533	G
51	1	544	C
51	1	545	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	563	A
51	1	572	A
51	1	573	U
51	1	586	A
51	1	588	U
51	1	603	A
51	1	614	A
51	1	627	A
51	1	637	A
51	1	646	U
51	1	654	A
51	1	655	A
51	1	664	G
51	1	686	U
51	1	687	C
51	1	695	G
51	1	717	C
51	1	730	A
51	1	740	C
51	1	747	C
51	1	748	G
51	1	749	A
51	1	760	G
51	1	764	A
51	1	774	G
51	1	776	G
51	1	782	A
51	1	784	G
51	1	785	G
51	1	803	U
51	1	805	G
51	1	812	C
51	1	819	A
51	1	827	U
51	1	828	U
51	1	830	G
51	1	845	A
51	1	846	U
51	1	856	G
51	1	858	G
51	1	860	U
51	1	869	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	871	U
51	1	872	U
51	1	877	A
51	1	878	A
51	1	885	C
51	1	887	U
51	1	896	A
51	1	897	C
51	1	907	G
51	1	910	A
51	1	914	G
51	1	915	C
51	1	932	U
51	1	934	U
51	1	941	A
51	1	946	C
51	1	961	C
51	1	974	G
51	1	975	A
51	1	983	A
51	1	985	C
51	1	995	C
51	1	1012	U
51	1	1013	C
51	1	1021	A
51	1	1022	G
51	1	1023	U
51	1	1026	G
51	1	1033	U
51	1	1034	G
51	1	1045	C
51	1	1046	A
51	1	1047	G
51	1	1053	C
51	1	1055	G
51	1	1057	A
51	1	1058	U
51	1	1059	G
51	1	1062	G
51	1	1064	C
51	1	1065	U
51	1	1066	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	1069	A
51	1	1070	A
51	1	1071	G
51	1	1072	C
51	1	1073	A
51	1	1076	C
51	1	1078	U
51	1	1080	A
51	1	1081	U
51	1	1082	U
51	1	1083	U
51	1	1084	A
51	1	1085	A
51	1	1086	A
51	1	1087	G
51	1	1088	A
51	1	1092	C
51	1	1104	C
51	1	1105	U
51	1	1106	G
51	1	1111	A
51	1	1131	G
51	1	1132	U
51	1	1133	A
51	1	1135	C
51	1	1143	A
51	1	1157	G
51	1	1172	C
51	1	1173	U
51	1	1175	A
51	1	1177	G
51	1	1179	G
51	1	1180	U
51	1	1211	C
51	1	1212	G
51	1	1221	C
51	1	1248	G
51	1	1249	U
51	1	1253	A
51	1	1256	G
51	1	1271	G
51	1	1272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	1273	U
51	1	1275	A
51	1	1289	C
51	1	1300	G
51	1	1301	A
51	1	1341	G
51	1	1345	C
51	1	1352	U
51	1	1365	A
51	1	1378	A
51	1	1379	U
51	1	1383	A
51	1	1398	C
51	1	1416	G
51	1	1419	A
51	1	1420	A
51	1	1427	A
51	1	1428	C
51	1	1458	U
51	1	1478	G
51	1	1482	G
51	1	1490	A
51	1	1491	G
51	1	1493	C
51	1	1504	A
51	1	1515	A
51	1	1524	G
51	1	1533	C
51	1	1534	U
51	1	1535	A
51	1	1536	C
51	1	1537	G
51	1	1555	G
51	1	1558	C
51	1	1559	U
51	1	1560	G
51	1	1569	A
51	1	1578	U
51	1	1584	U
51	1	1608	A
51	1	1611	C
51	1	1616	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	1618	A
51	1	1647	U
51	1	1648	U
51	1	1654	A
51	1	1674	G
51	1	1682	G
51	1	1698	A
51	1	1715	G
51	1	1729	U
51	1	1730	C
51	1	1732	C
51	1	1733	G
51	1	1738	G
51	1	1758	U
51	1	1764	C
51	1	1773	A
51	1	1780	A
51	1	1785	A
51	1	1791	A
51	1	1800	C
51	1	1801	A
51	1	1808	A
51	1	1816	C
51	1	1820	U
51	1	1821	A
51	1	1829	A
51	1	1839	G
51	1	1857	G
51	1	1869	G
51	1	1870	C
51	1	1871	A
51	1	1901	A
51	1	1906	G
51	1	1907	G
51	1	1912	A
51	1	1913	A
51	1	1914	C
51	1	1925	C
51	1	1929	G
51	1	1930	G
51	1	1937	A
51	1	1938	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	1944	U
51	1	1955	U
51	1	1961	C
51	1	1963	U
51	1	1967	C
51	1	1970	A
51	1	1971	U
51	1	1972	G
51	1	1991	U
51	1	1992	G
51	1	1993	U
51	1	1996	C
51	1	1997	C
51	1	2022	U
51	1	2023	C
51	1	2030	A
51	1	2031	A
51	1	2043	C
51	1	2055	C
51	1	2056	G
51	1	2060	A
51	1	2061	G
51	1	2062	A
51	1	2069	G
51	1	2072	C
51	1	2077	A
51	1	2092	U
51	1	2095	A
51	1	2096	C
51	1	2100	G
51	1	2106	U
51	1	2111	U
51	1	2112	G
51	1	2114	A
51	1	2118	U
51	1	2119	A
51	1	2120	G
51	1	2122	U
51	1	2125	G
51	1	2128	G
51	1	2132	U
51	1	2133	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	2134	A
51	1	2138	G
51	1	2141	G
51	1	2145	C
51	1	2153	C
51	1	2158	A
51	1	2162	G
51	1	2166	U
51	1	2172	U
51	1	2173	A
51	1	2178	C
51	1	2182	U
51	1	2184	A
51	1	2192	U
51	1	2198	A
51	1	2203	U
51	1	2204	G
51	1	2211	A
51	1	2225	A
51	1	2239	G
51	1	2278	A
51	1	2283	C
51	1	2287	A
51	1	2297	A
51	1	2305	U
51	1	2309	A
51	1	2325	G
51	1	2327	A
51	1	2333	A
51	1	2337	G
51	1	2350	C
51	1	2385	C
51	1	2402	U
51	1	2406	A
51	1	2423	U
51	1	2425	A
51	1	2426	A
51	1	2427	C
51	1	2428	G
51	1	2429	G
51	1	2430	A
51	1	2435	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	2441	U
51	1	2447	G
51	1	2448	A
51	1	2469	A
51	1	2474	U
51	1	2476	A
51	1	2480	C
51	1	2491	U
51	1	2502	G
51	1	2505	G
51	1	2518	A
51	1	2529	G
51	1	2535	G
51	1	2547	A
51	1	2554	U
51	1	2566	A
51	1	2567	G
51	1	2572	A
51	1	2602	A
51	1	2603	G
51	1	2609	U
51	1	2613	U
51	1	2615	U
51	1	2636	C
51	1	2646	C
51	1	2654	A
51	1	2689	U
51	1	2690	U
51	1	2714	G
51	1	2716	C
51	1	2720	U
51	1	2724	U
51	1	2733	A
51	1	2744	G
51	1	2748	A
51	1	2757	A
51	1	2758	A
51	1	2764	A
51	1	2765	A
51	1	2778	A
51	1	2779	U
51	1	2791	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
51	1	2793	C
51	1	2798	U
51	1	2800	A
51	1	2801	G
51	1	2820	A
51	1	2821	A
51	1	2867	G
51	1	2868	A
51	1	2872	A
51	1	2880	C
51	1	2884	U
51	1	2893	A
52	2	2	G
52	2	4	C
52	2	13	G
52	2	35	C
52	2	53	A
52	2	56	G
52	2	67	G
52	2	88	C
52	2	89	U
52	2	90	C
52	2	108	A
52	2	109	A
53	3	6	G
53	3	9	G
53	3	22	G
53	3	32	A
53	3	39	G
53	3	44	A
53	3	48	C
53	3	50	A
53	3	51	A
53	3	54	C
53	3	71	A
53	3	78	A
53	3	84	U
53	3	85	U
53	3	87	C
53	3	92	U
53	3	94	G
53	3	100	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	3	101	A
53	3	110	C
53	3	121	U
53	3	130	A
53	3	144	G
53	3	173	U
53	3	183	C
53	3	197	A
53	3	208	U
53	3	210	C
53	3	211	G
53	3	247	G
53	3	251	G
53	3	253	A
53	3	266	G
53	3	267	C
53	3	280	C
53	3	281	G
53	3	289	G
53	3	328	C
53	3	352	C
53	3	354	G
53	3	367	U
53	3	369	G
53	3	372	C
53	3	397	A
53	3	413	G
53	3	414	A
53	3	419	C
53	3	422	C
53	3	423	G
53	3	429	U
53	3	467	U
53	3	468	A
53	3	474	G
53	3	479	U
53	3	480	U
53	3	485	U
53	3	486	U
53	3	495	A
53	3	496	A
53	3	497	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	3	509	A
53	3	531	U
53	3	532	A
53	3	547	A
53	3	559	A
53	3	561	U
53	3	566	G
53	3	572	A
53	3	573	A
53	3	575	G
53	3	576	C
53	3	577	G
53	3	596	A
53	3	633	G
53	3	653	U
53	3	665	A
53	3	671	G
53	3	686	U
53	3	687	A
53	3	688	G
53	3	703	G
53	3	724	G
53	3	731	G
53	3	733	G
53	3	755	G
53	3	777	A
53	3	793	U
53	3	794	A
53	3	814	A
53	3	817	C
53	3	818	G
53	3	819	A
53	3	821	G
53	3	842	U
53	3	843	U
53	3	844	G
53	3	846	G
53	3	887	G
53	3	902	G
53	3	934	C
53	3	935	A
53	3	938	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	3	943	U
53	3	960	U
53	3	963	G
53	3	966	G
53	3	969	A
53	3	975	A
53	3	976	G
53	3	977	A
53	3	992	U
53	3	993	G
53	3	994	A
53	3	1004	A
53	3	1012	A
53	3	1026	G
53	3	1029	U
53	3	1031	C
53	3	1032	G
53	3	1033	G
53	3	1053	G
53	3	1054	C
53	3	1055	A
53	3	1086	U
53	3	1094	G
53	3	1096	C
53	3	1101	A
53	3	1130	A
53	3	1133	G
53	3	1136	C
53	3	1137	C
53	3	1138	G
53	3	1139	G
53	3	1146	A
53	3	1159	U
53	3	1168	U
53	3	1182	G
53	3	1184	G
53	3	1196	A
53	3	1212	U
53	3	1225	A
53	3	1238	A
53	3	1241	G
53	3	1275	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	3	1278	G
53	3	1280	A
53	3	1282	C
53	3	1286	U
53	3	1287	A
53	3	1290	G
53	3	1299	A
53	3	1300	G
53	3	1301	U
53	3	1302	C
53	3	1305	G
53	3	1317	C
53	3	1320	C
53	3	1363	A
53	3	1378	C
53	3	1381	U
53	3	1394	A
53	3	1395	C
53	3	1398	A
53	3	1419	G
53	3	1422	G
53	3	1428	A
53	3	1431	A
53	3	1446	A
53	3	1448	C
53	3	1452	C
53	3	1453	G
53	3	1492	A
53	3	1497	G
53	3	1499	A
53	3	1503	A
53	3	1505	G
53	3	1506	U
53	3	1508	A
53	3	1517	G
53	3	1529	G
53	3	1530	G
54	4	4	U
54	4	8	U
54	4	9	U
54	4	10	C
54	4	12	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	4	13	U
54	4	14	U
54	4	15	U
54	4	16	U
54	4	17	U
54	4	18	U
54	4	19	U
54	4	20	U
63	5	2	C
63	5	7	A
63	5	8	U
63	5	9	A
63	5	11	C
63	5	13	C
63	5	15	G
63	5	17	C
63	5	18	G
63	5	19	G
63	5	20	U
63	5	21	A
63	5	26	A
63	5	32	U
63	5	33	U
63	5	35	A
63	5	36	A
63	5	38	A
63	5	39	U
63	5	43	C
63	5	44	G
63	5	46	G
63	5	47	U
63	5	48	C
63	5	49	C
63	5	52	G
63	5	53	G
63	5	55	U
63	5	56	C
63	5	57	G
63	5	58	A
63	5	59	U
63	5	60	U
63	5	61	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
63	5	66	U
63	5	73	A
63	5	74	C
63	5	76	A
64	6	5	G
64	6	7	G
64	6	9	G
64	6	10	G
64	6	14	A
64	6	18	G
64	6	19	G
64	6	21	A
64	6	22	G
64	6	27	U
64	6	43	A
64	6	44	A
64	6	45	G
64	6	47	U
64	6	48	C
64	6	49	G
64	6	59	A
64	6	70	G

All (27) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
51	1	227	A
51	1	490	C
51	1	784	G
51	1	859	G
51	1	1020	A
51	1	1130	U
51	1	2296	U
51	1	2326	C
51	1	2756	U
51	1	2873	A
52	2	88	C
53	3	70	U
53	3	413	G
53	3	1012	A
53	3	1054	C
53	3	1301	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
53	3	1395	C
54	4	13	U
54	4	18	U
54	4	19	U
63	5	7	A
63	5	35	A
63	5	48	C
63	5	57	G
63	5	60	U
63	5	73	A
63	5	75	C

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

4 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	$\# Z > 2$
67	UAL	h	5	67	7,8,9	2.29	3 (42%)	5,9,11	2.92	2 (40%)
67	5OH	h	6	67	8,12,13	0.79	0	3,16,18	1.51	1 (33%)
67	KBE	h	1	67	8,8,9	0.61	0	7,8,10	1.20	1 (14%)
67	DPP	h	2	67	3,5,6	0.56	0	1,5,7	0.08	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
67	UAL	h	5	67	-	0/3/7/9	-
67	5OH	h	6	67	-	0/2/18/20	0/1/1/1
67	KBE	h	1	67	-	0/7/7/8	-
67	DPP	h	2	67	-	0/2/4/6	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
67	h	5	UAL	C1-N1	-4.83	1.32	1.40
67	h	5	UAL	C-CA	-2.88	1.40	1.45
67	h	5	UAL	CA-N	2.02	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
67	h	5	UAL	CA-CB-N1	-5.30	115.60	125.60
67	h	5	UAL	O-C-CA	-3.26	121.25	125.39
67	h	6	5OH	CR-CB-CA	-2.36	110.06	112.61
67	h	1	KBE	CB-CA-C	-2.05	109.24	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
67	h	5	UAL	1	0
67	h	6	5OH	4	0
67	h	2	DPP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is 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
70	PO4	0	802	-	4,4,4	1.11	0	6,6,6	0.69	0
69	GDP	0	801	-	24,30,30	0.93	1 (4%)	30,47,47	1.45	5 (16%)

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
69	GDP	0	801	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	0	801	GDP	C6-N1	-2.44	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	0	801	GDP	PA-O3A-PB	-4.36	117.85	132.83
69	0	801	GDP	C3'-C2'-C1'	2.57	104.85	100.98
69	0	801	GDP	C5-C6-N1	2.34	118.09	113.95
69	0	801	GDP	C8-N7-C5	2.22	107.23	102.99
69	0	801	GDP	O6-C6-C5	-2.07	120.33	124.37

There are no chirality outliers.

There are no torsion outliers.

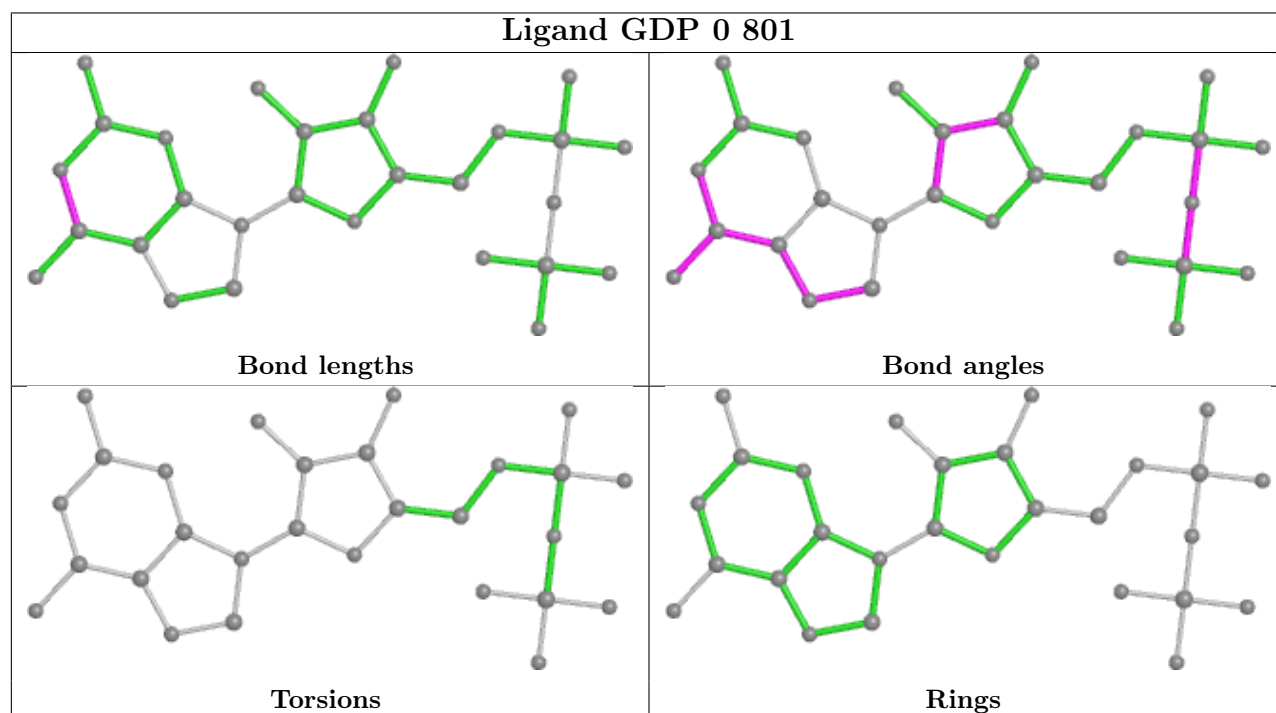
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
70	0	802	PO4	1	0
69	0	801	GDP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

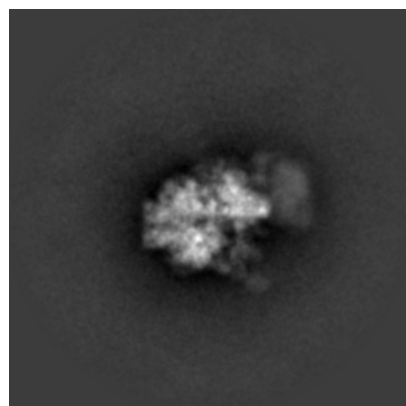
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38942. These allow visual inspection of the internal detail of the map and identification of artifacts.

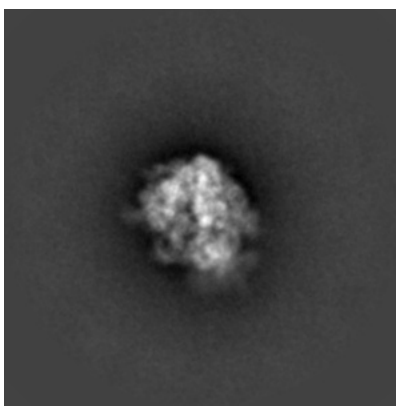
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

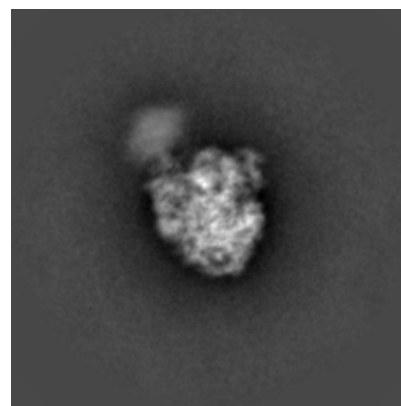
6.1.1 Primary map



X

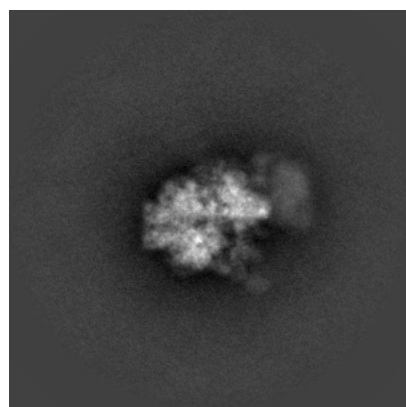


Y

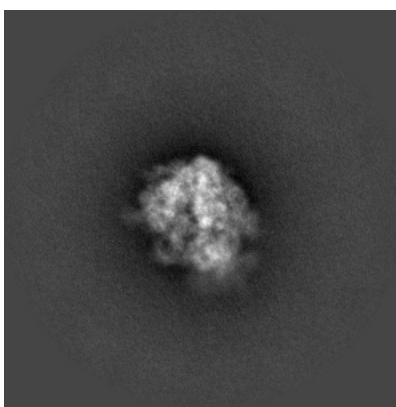


Z

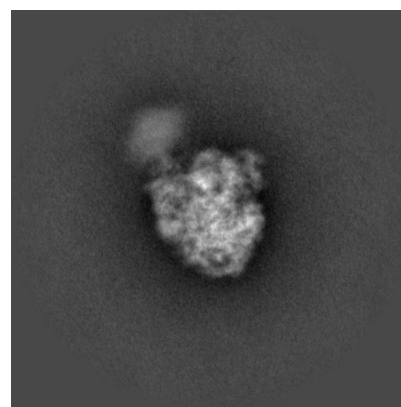
6.1.2 Raw map



X



Y

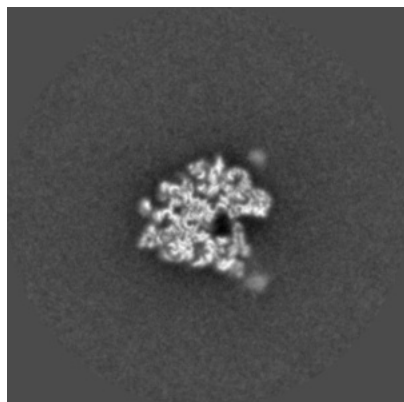


Z

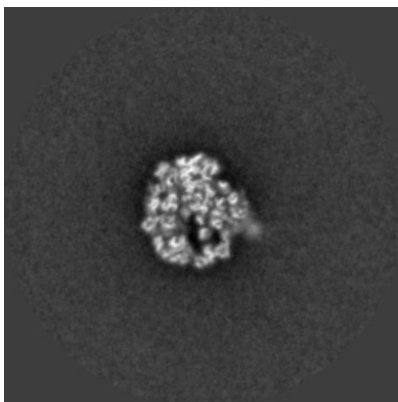
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

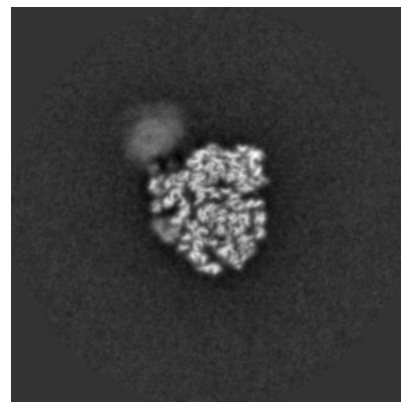
6.2.1 Primary map



X Index: 240

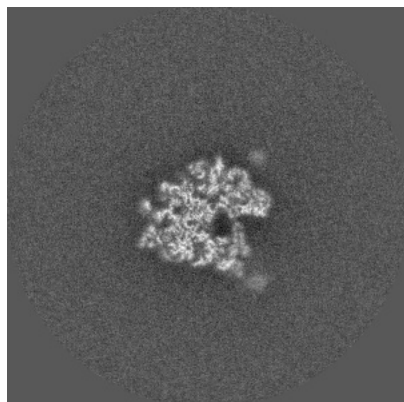


Y Index: 240

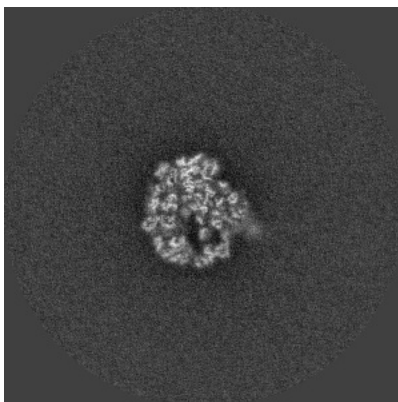


Z Index: 240

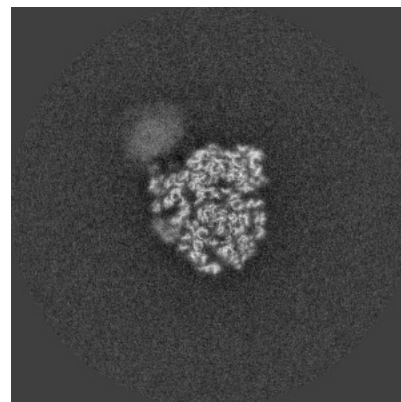
6.2.2 Raw map



X Index: 240



Y Index: 240

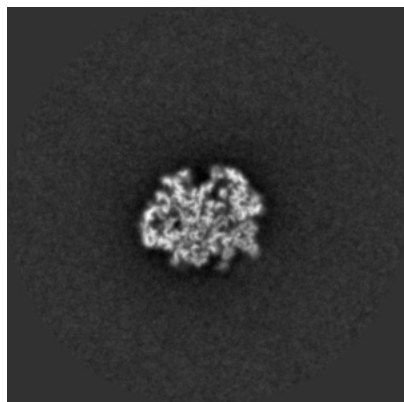


Z Index: 240

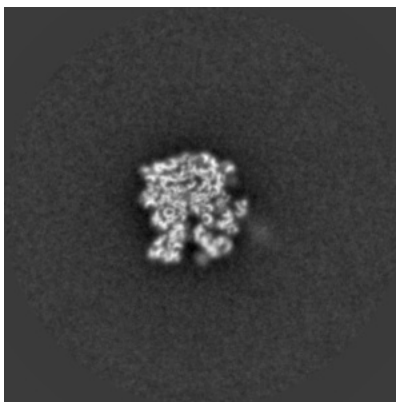
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

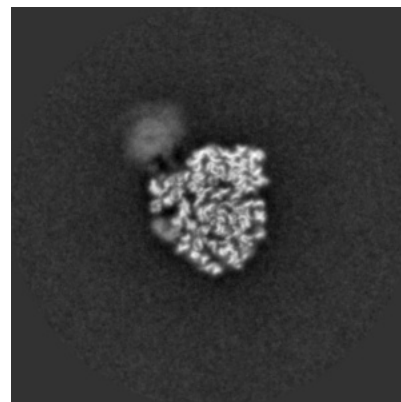
6.3.1 Primary map



X Index: 264

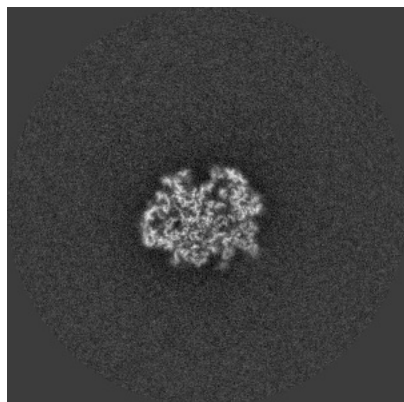


Y Index: 223

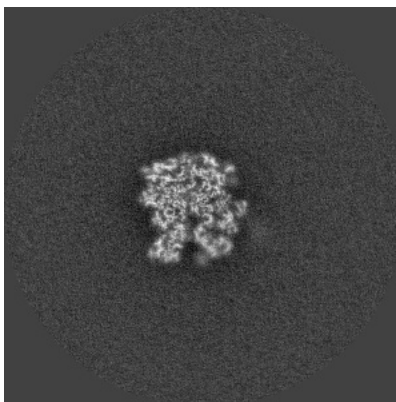


Z Index: 238

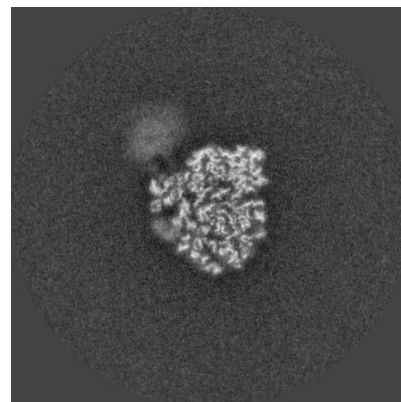
6.3.2 Raw map



X Index: 264



Y Index: 222



Z Index: 238

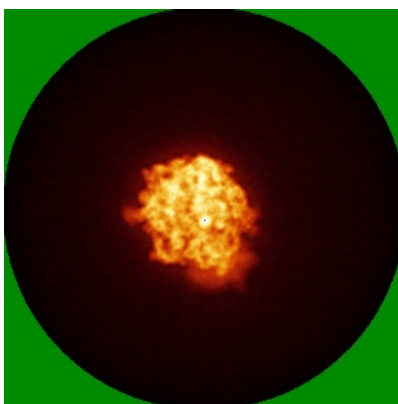
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X

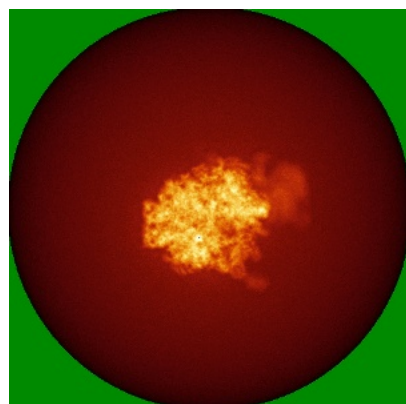


Y

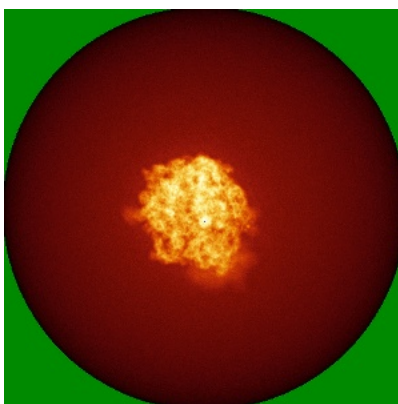


Z

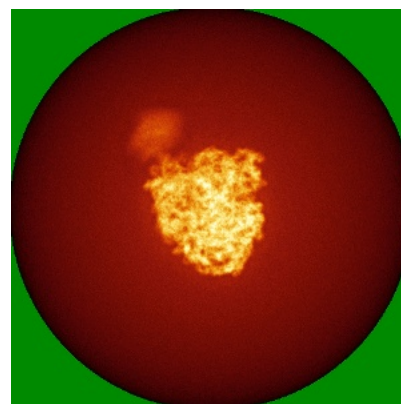
6.4.2 Raw map



X



Y

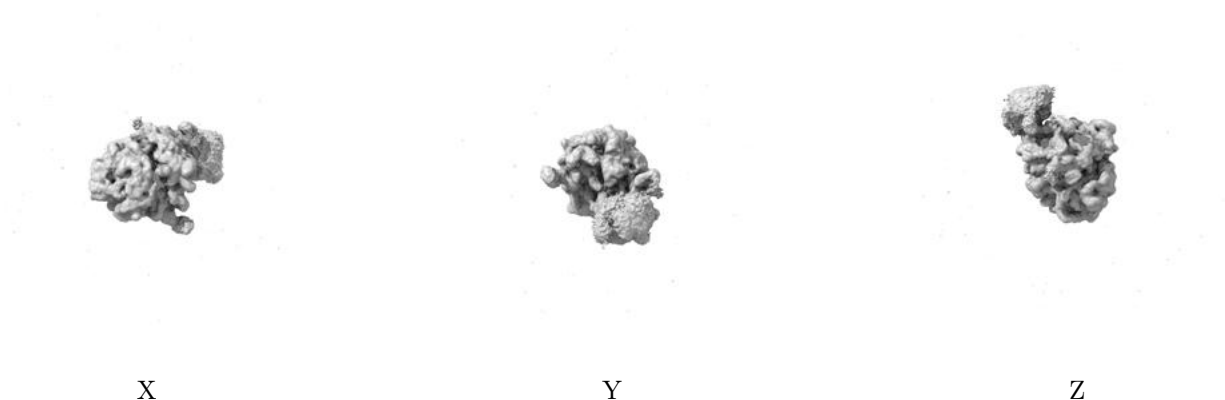


Z

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

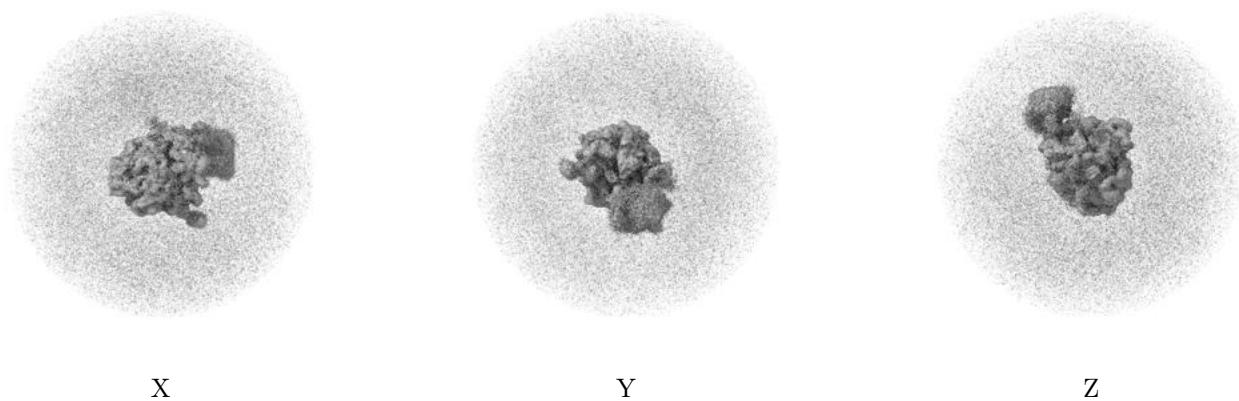
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

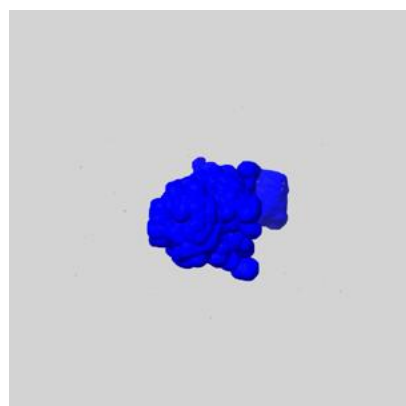
6.6 Mask visualisation [i](#)

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

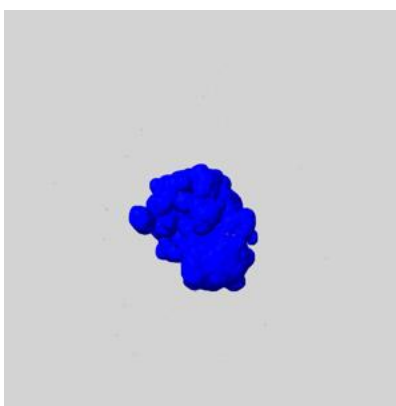
A mask typically either:

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

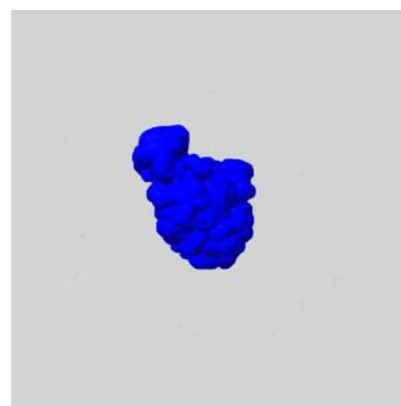
6.6.1 emd_38942_msk_1.map [i](#)



X



Y

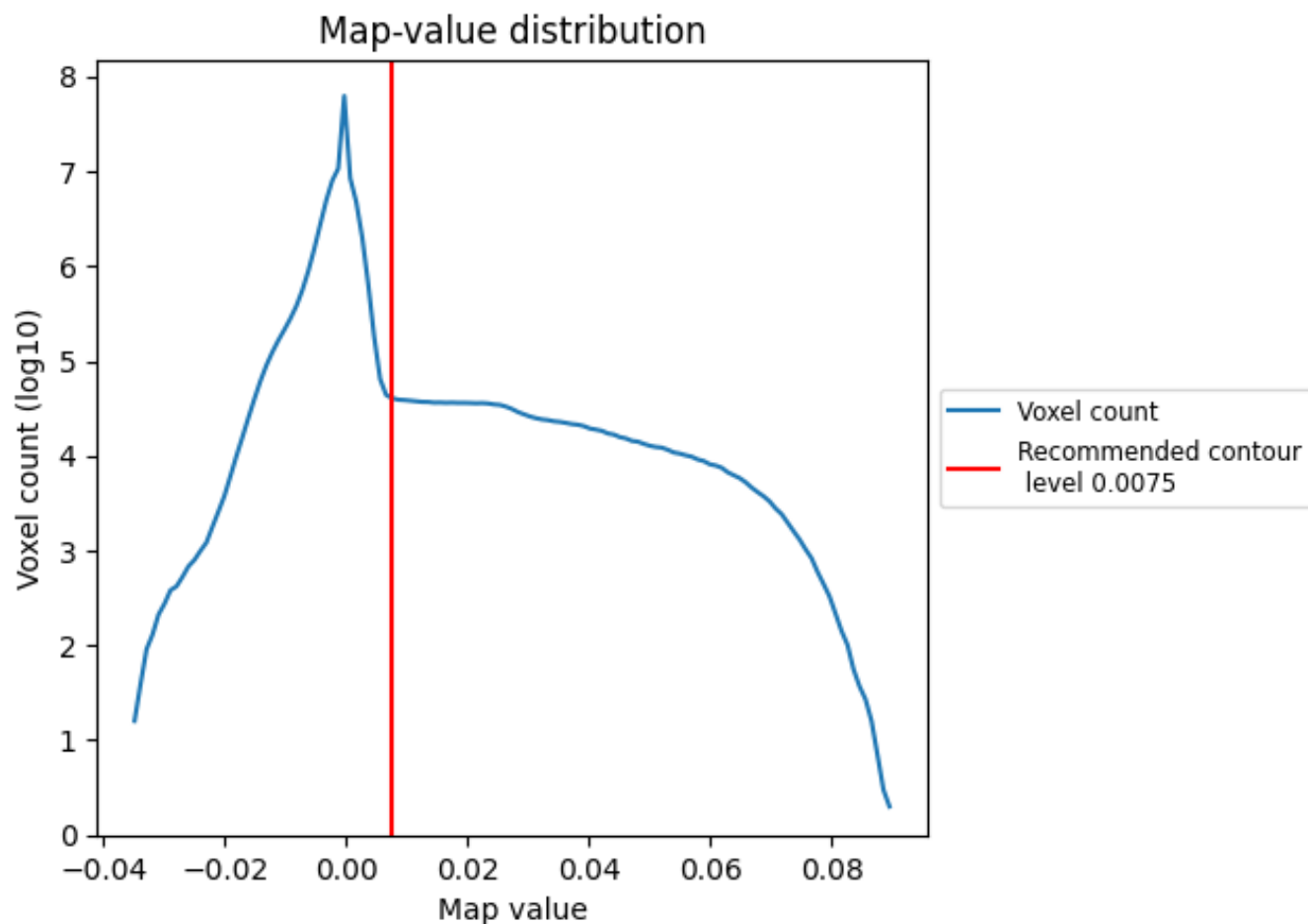


Z

7 Map analysis [i](#)

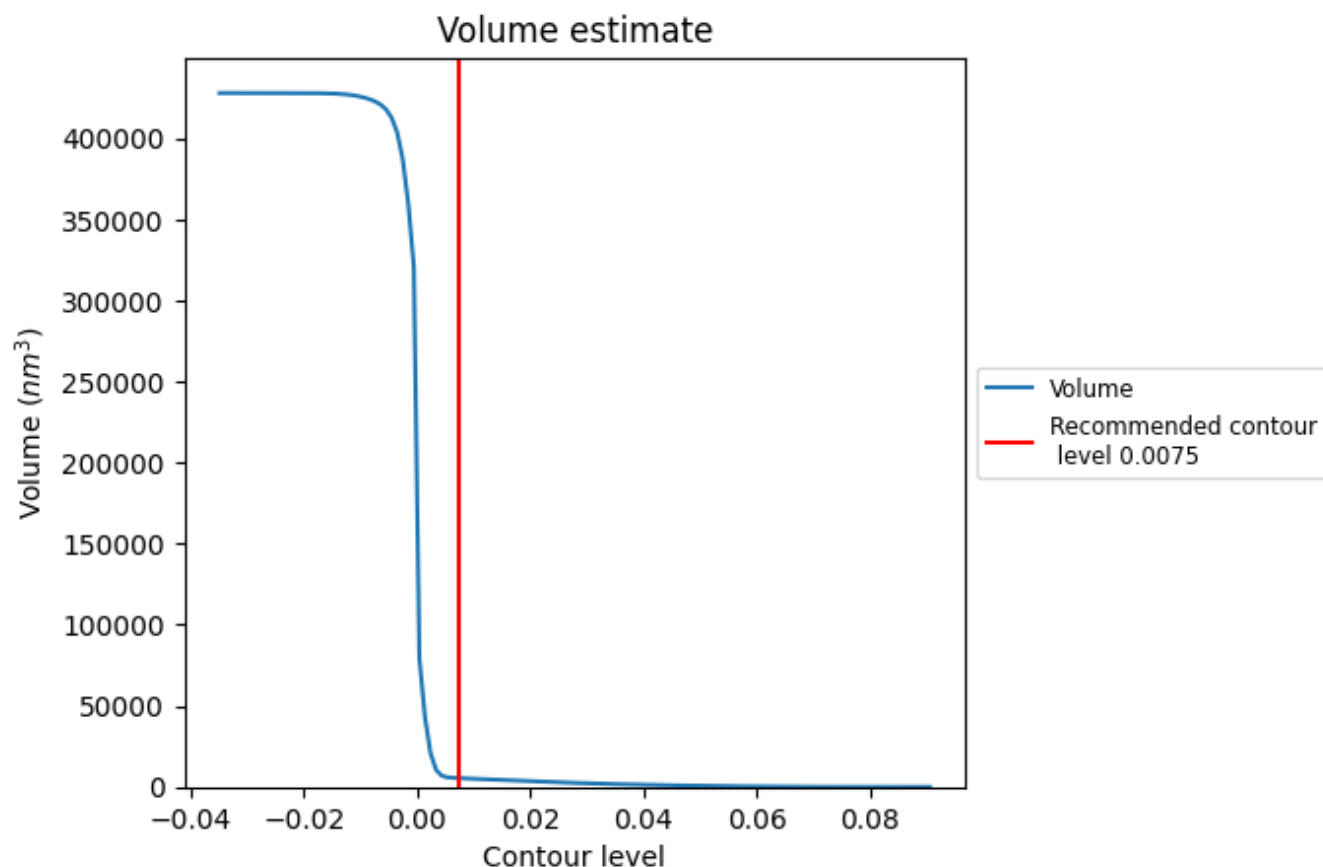
This section contains the results of statistical analysis of the map.

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.

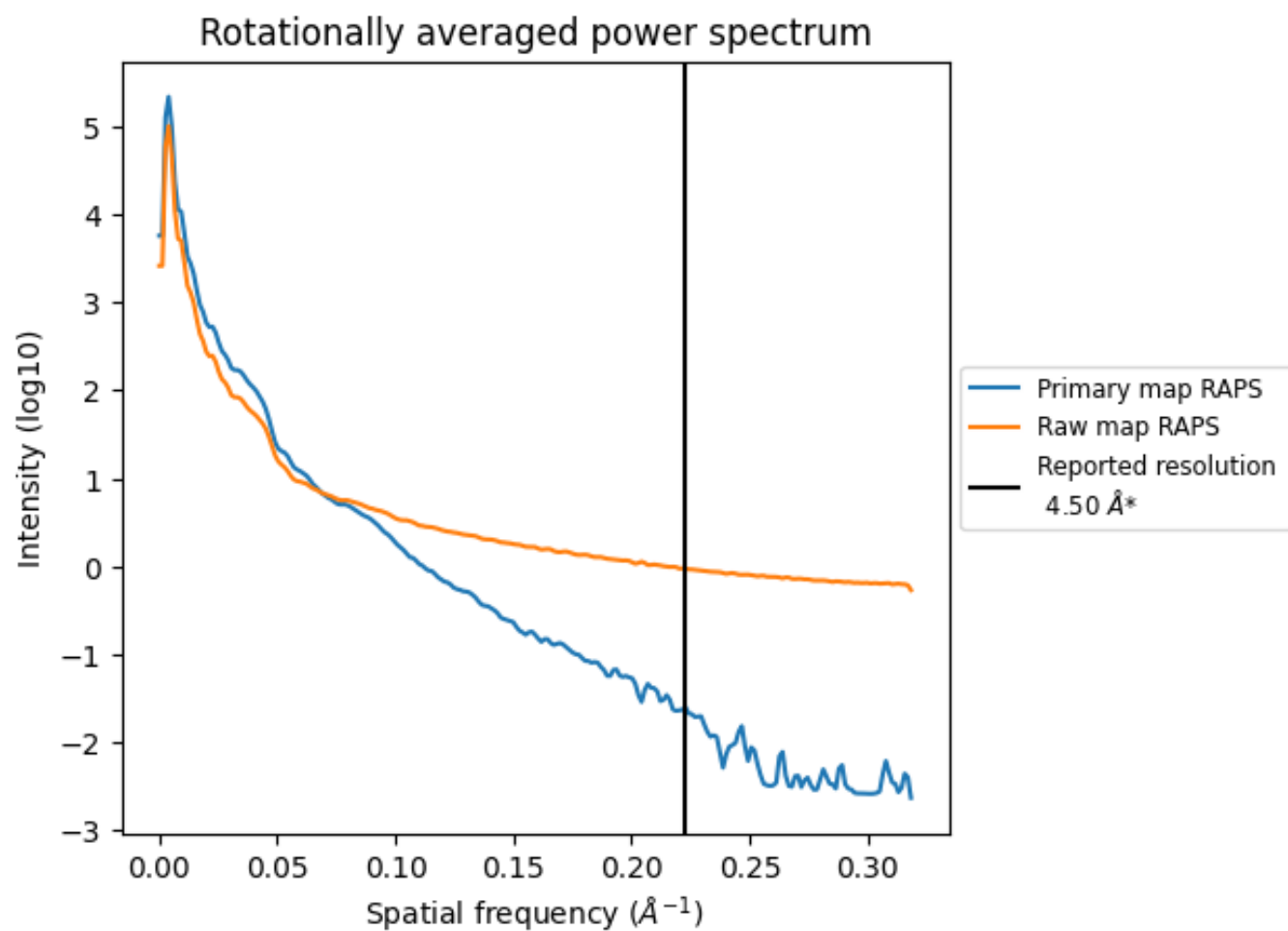
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5419 nm^3 ; this corresponds to an approximate mass of 4895 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 ⓘ

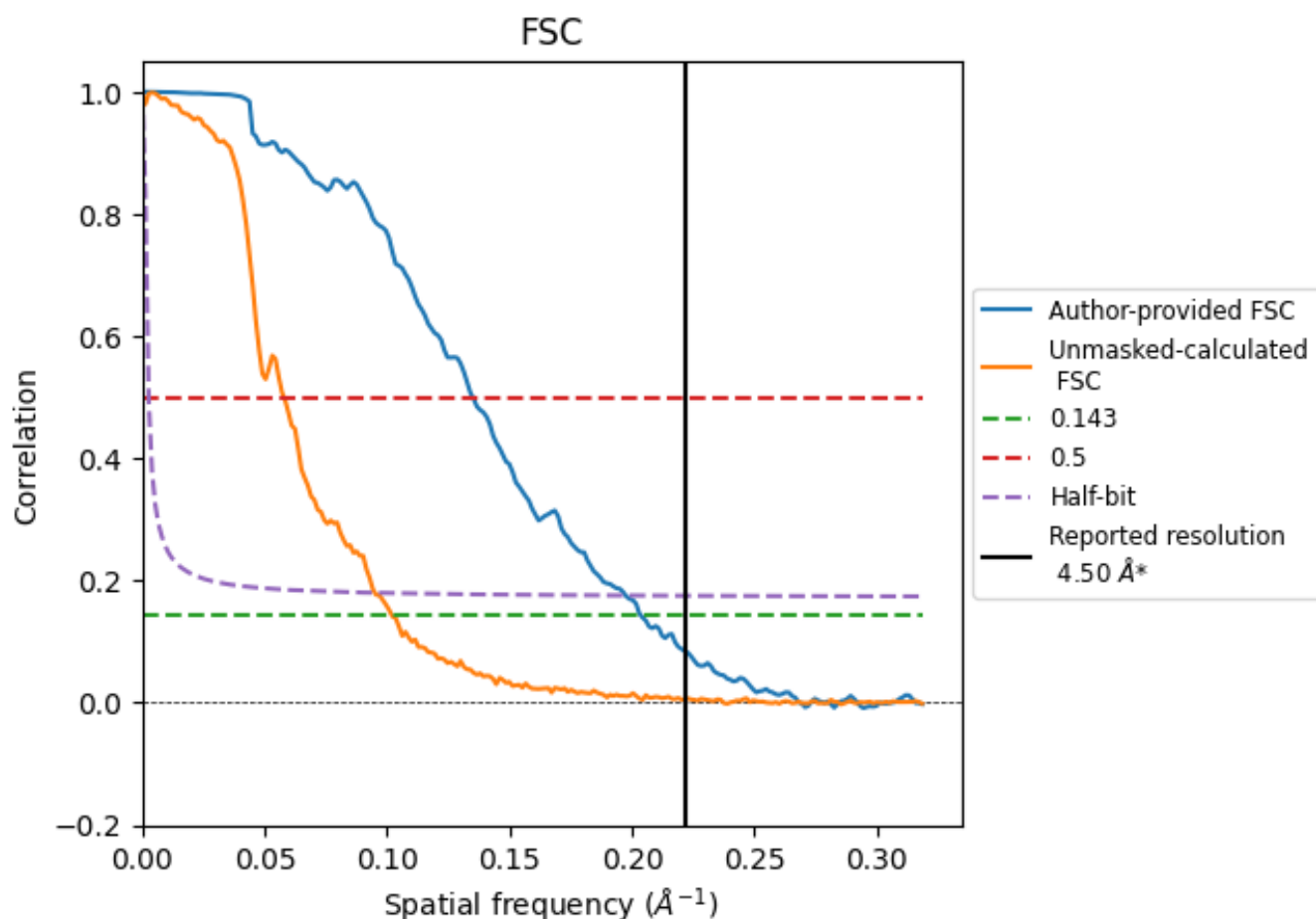


*Reported resolution corresponds to spatial frequency of 0.222 Å⁻¹

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 0.222 Å⁻¹

8.2 Resolution estimates [i](#)

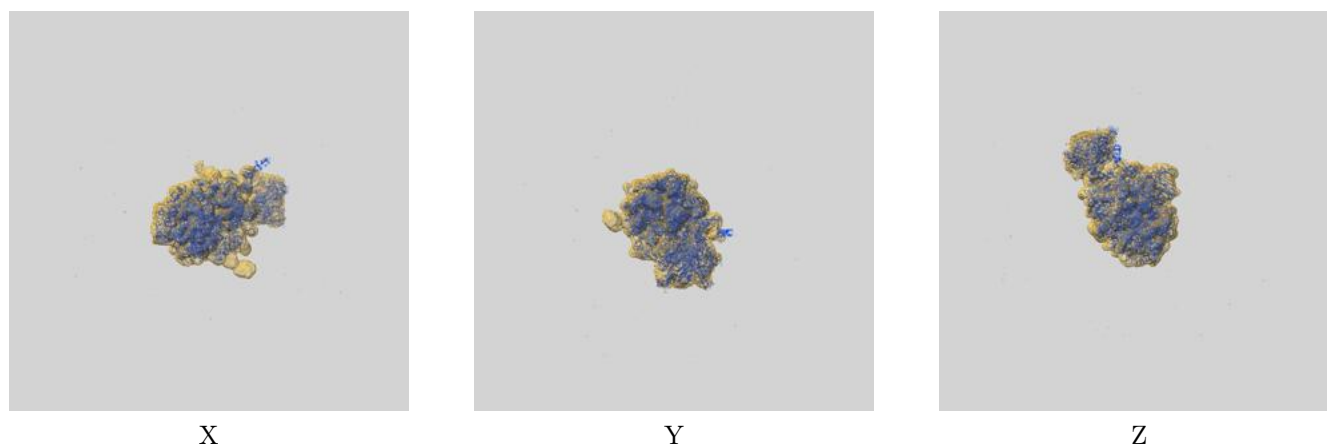
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.50	-	-
Author-provided FSC curve	4.91	7.41	5.07
Unmasked-calculated*	9.81	17.30	10.52

*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 9.81 differs from the reported value 4.5 by more than 10 %

9 Map-model fit [i](#)

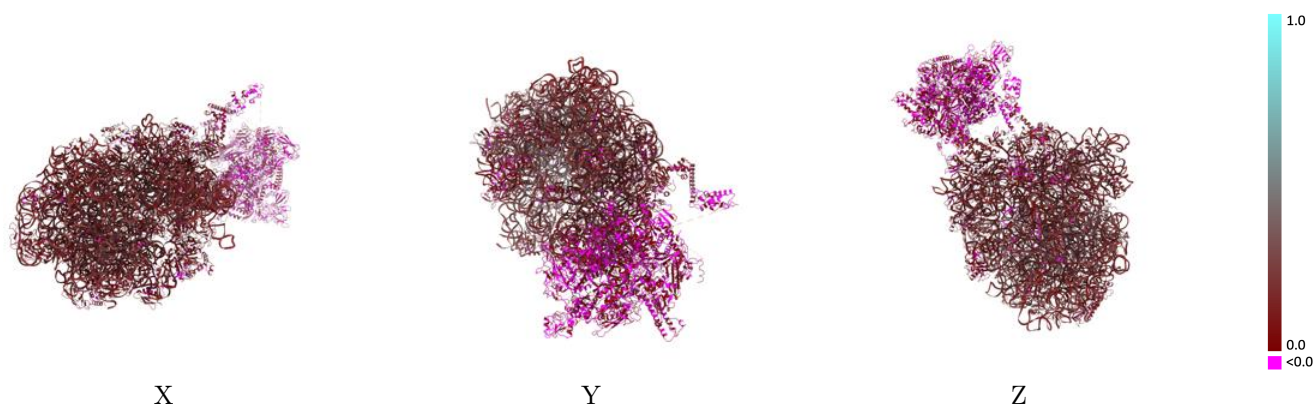
This section contains information regarding the fit between EMDB map EMD-38942 and PDB model 8Y5M. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



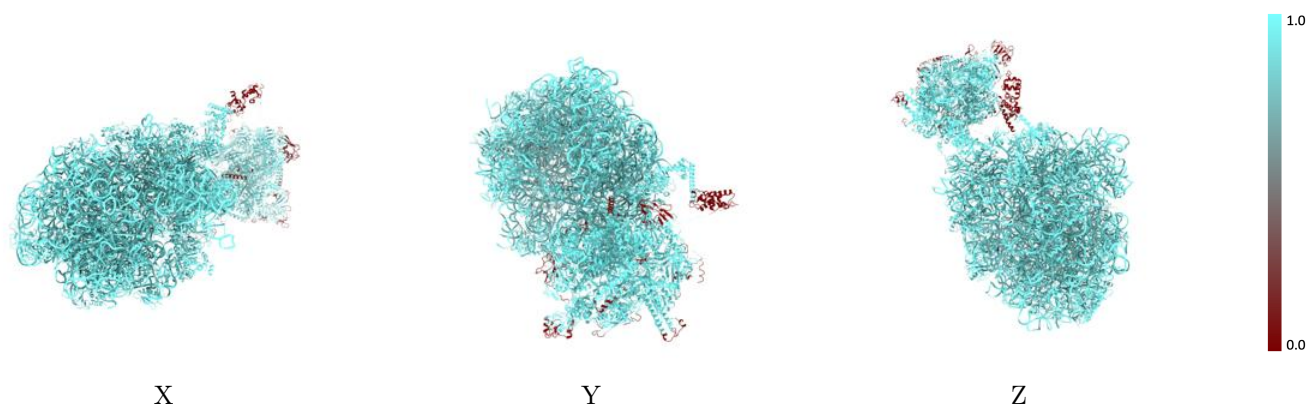
The images above show the 3D surface view of the map at the recommended contour level 0.0075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



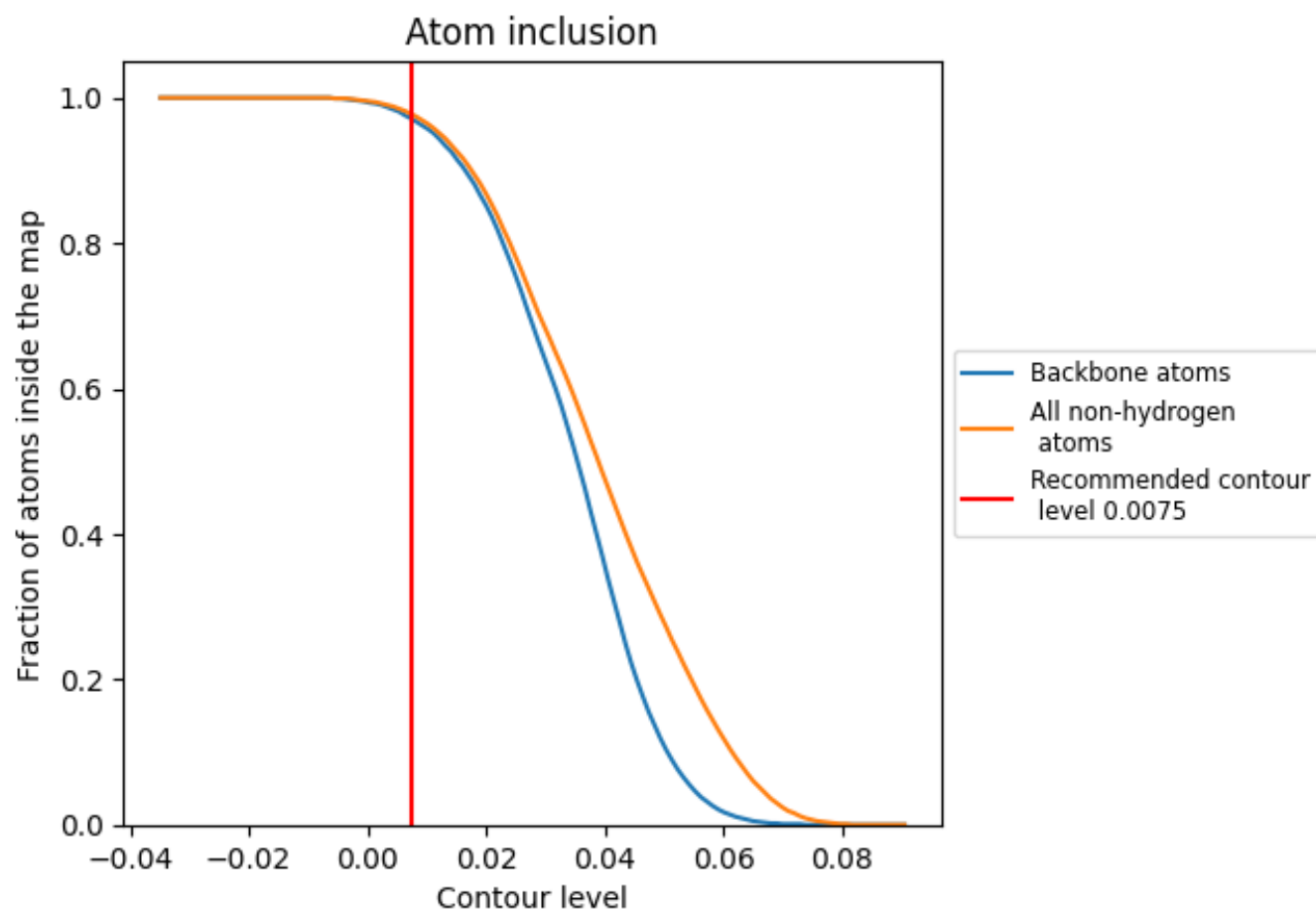
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0075).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 98% 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 (0.0075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9770	 0.1550
0	 0.9680	 0.1420
1	 1.0000	 0.2040
2	 1.0000	 0.1720
3	 1.0000	 0.1910
4	 0.9750	 0.0940
5	 0.9950	 0.1250
6	 0.9950	 0.1820
8	 1.0000	 0.0050
9	 1.0000	 0.0520
A	 0.9260	 0.0890
A1	 0.6540	 0.0140
A2	 0.8070	 0.0190
B	 0.9980	 0.1500
B1	 0.9130	 0.0230
B2	 0.9190	 0.0300
C	 0.9880	 0.1570
D	 0.9750	 0.1320
E	 1.0000	 0.1560
F	 1.0000	 0.0960
G	 0.9920	 0.1230
H	 0.9890	 0.1510
I	 0.9990	 0.1330
J	 0.9930	 0.1430
K	 0.9840	 0.1350
L	 0.9780	 0.1450
M	 0.9740	 0.1270
N	 0.9990	 0.1190
NA	 0.8830	 0.1380
NG	 0.9660	 0.0530
O	 0.9960	 0.1270
P	 0.9960	 0.1510
Q	 0.9570	 0.1600
R	 0.9910	 0.1590
S	 0.9990	 0.1480



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
T	 0.9930	 0.1370
U	 0.9970	 0.1330
V	 0.9910	 0.1450
W	 1.0000	 0.1240
W0	 0.5980	 -0.0110
X	 1.0000	 0.1500
Y	 0.9890	 0.1540
Z	 0.9790	 0.1320
a	 0.9950	 0.0760
b	 0.9920	 0.1670
c	 0.9940	 0.1590
d	 0.9950	 0.1600
e	 0.9800	 0.1280
f	 0.9920	 0.1440
g	 0.9090	 0.1210
h	 1.0000	 0.1620
i	 0.9800	 0.0990
j	 0.9960	 0.1460
k	 0.9810	 0.2100
l	 0.9970	 0.1540
m	 0.9920	 0.1580
n	 0.9980	 0.1480
o	 1.0000	 0.1230
p	 0.9930	 0.1850
q	 0.9990	 0.1340
r	 0.9990	 0.1460
s	 0.9920	 0.1640
t	 0.9900	 0.1180
u	 0.9950	 0.1290
v	 0.9960	 0.1260
w	 1.0000	 0.1280
x	 0.9970	 0.1560
y	 0.9960	 0.1260
z	 0.9950	 0.1560