



## Full wwPDB EM Validation Report ⓘ

Jun 11, 2026 – 01:11 PM JST

PDB ID : 9XWO / pdb\_00009xwo  
EMDB ID : EMD-67339  
Title : Cryo-EM structure of SecM-arrested 70S ribosome (short SecM)  
Authors : Iso, K.; Ando, Y.; Taguchi, H.; Nureki, O.; Chadani, Y.; Itoh, Y.  
Deposited on : 2025-11-28  
Resolution : 2.89 Å(reported)  
Based on initial models : 8QOA, 9VVI

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

---

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

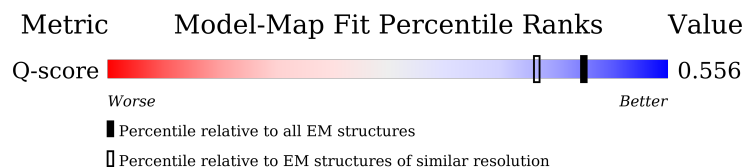
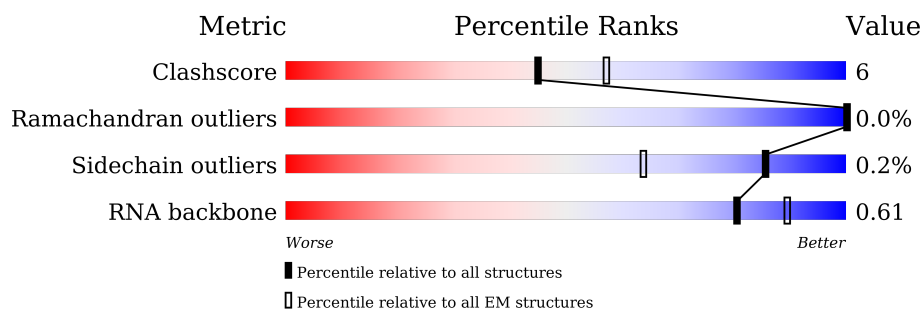
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.89 Å.

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









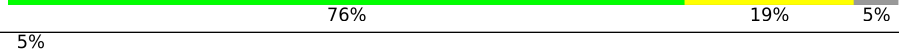
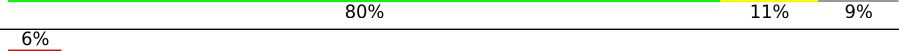
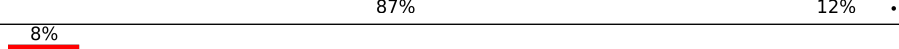
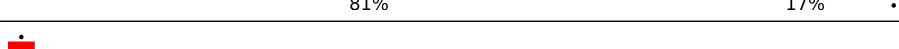
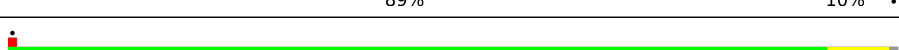
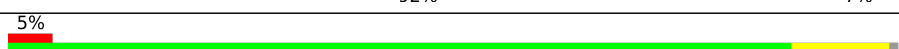
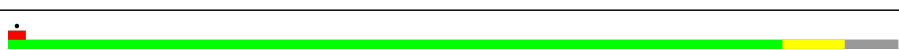

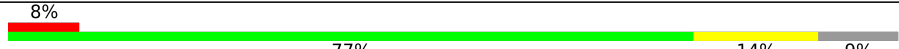





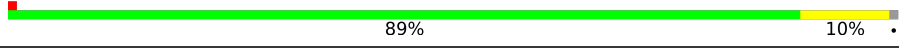
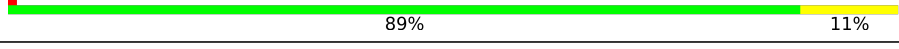



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12148 ( 2.39 - 3.39 )

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  $\geq 3$ , 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	1542	
2	B	241	
3	C	233	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	206	
5	E	167	
6	F	135	
7	G	179	
8	H	130	
9	I	130	
10	J	103	
11	K	129	
12	L	124	
13	M	118	
14	N	101	
15	O	89	
16	P	82	
17	Q	84	
18	R	75	
19	S	92	
20	T	87	
21	U	71	
22	a	2904	
23	b	119	
24	7	234	
25	c	273	
26	d	209	
27	e	201	
28	f	179	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	g	177	
30	h	149	
31	i	142	
32	j	123	
33	k	144	
34	l	136	
35	m	127	
36	n	117	
37	o	115	
38	p	118	
39	q	103	
40	r	110	
41	s	100	
42	t	104	
43	u	94	
44	v	85	
45	w	78	
46	x	63	
47	y	59	
48	4	70	
49	z	57	
50	0	55	
51	1	46	
52	2	65	
53	3	38	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	X	629	<div><div></div><div>97%</div></div>
55	Y	77	<div><div></div><div>57%</div><div>38%</div><div>5%</div></div>
56	Z	76	<div><div></div><div>5%</div><div>68%</div><div>30%</div><div></div></div>
57	5	76	<div><div></div><div>91%</div><div>38%</div><div>49%</div><div>11%</div><div></div></div>
58	6	165	<div><div></div><div>15%</div><div></div><div>82%</div></div>

## 2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 147950 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1525	Total	C	N	O	P	0	0
			32741	14609	6009	10598	1525		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	67	Total	C	N	O	S	0	0
			555	351	106	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

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



Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 22 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	a	2845	Total	C	N	O	P	0	0
			61098	27261	11245	19747	2845		

- Molecule 23 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	b	119	Total	C	N	O	P	0	0
			2550	1135	466	830	119		

- Molecule 24 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	7	153	Total	C	N	O	S	0	0
			1152	720	211	219	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 26 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 27 is a protein called 50S ribosomal protein L4.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 30 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	h	148	Total	C	N	O	S	0	0
			1101	694	196	210	1		

- Molecule 31 is a protein called 50S ribosomal protein L13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	136	Total	C	N	O	S	1	0
			1083	691	208	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 35 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	t	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	v	84	Total	C	N	O	S	0	0
			628	388	126	113	1		

- Molecule 45 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 46 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 48 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	48	Total	C	N	O	S	0	0
			373	232	66	69	6		

- Molecule 49 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 50 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
50	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 51 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 52 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 53 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 54 is a RNA chain called SecM mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	X	16	Total	C	N	O	P	0	0
			336	150	58	112	16		

- Molecule 55 is a RNA chain called A-site tRNA (prolyl-tRNA<sup>Pro</sup>).

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Y	77	Total	C	N	O	P	0	0
			1651	736	295	543	77		

- Molecule 56 is a RNA chain called P-site tRNA (tRNA<sup>Gly</sup>).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	Z	76	Total	C	N	O	P	S	0	0
			1624	724	287	536	76	1		

- Molecule 57 is a RNA chain called E-site tRNA (tRNA<sup>Ala</sup>).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	74	Total	C	N	O	P	0	0
			1589	708	284	523	74		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	34	CM0	U	conflict	GB 1845258627

- Molecule 58 is a protein called Secretion monitor.

Mol	Chain	Residues	Atoms				AltConf	Trace
58	6	30	Total	C	N	O	1	0
			245	159	44	42		

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
59	A	25	Total	K	0
			25	25	
59	a	86	Total	K	0
			86	86	
59	c	2	Total	K	0
			2	2	

*Continued on next page...*

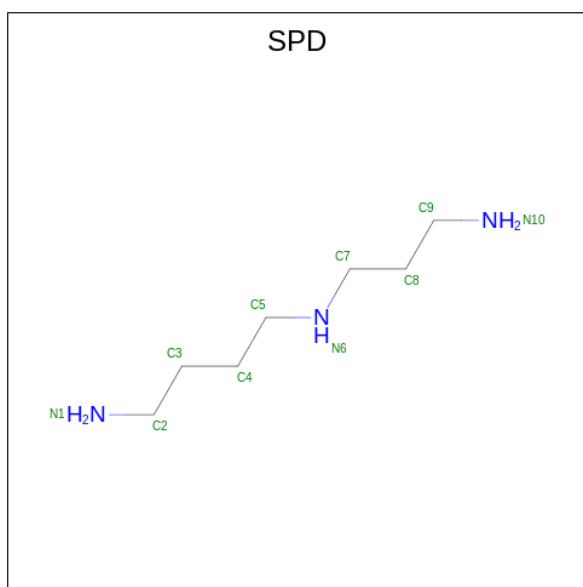
*Continued from previous page...*

Mol	Chain	Residues	Atoms		AltConf
59	e	1	Total 1	K 1	0
59	t	1	Total 1	K 1	0
59	Z	1	Total 1	K 1	0

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	70	Total 70	Mg 70	0
60	B	1	Total 1	Mg 1	0
60	a	199	Total 199	Mg 199	0
60	b	4	Total 4	Mg 4	0
60	c	1	Total 1	Mg 1	0
60	k	1	Total 1	Mg 1	0
60	z	1	Total 1	Mg 1	0
60	Y	1	Total 1	Mg 1	0
60	Z	1	Total 1	Mg 1	0

- Molecule 61 is SPERMIDINE (CCD ID: SPD) (formula: C<sub>7</sub>H<sub>19</sub>N<sub>3</sub>).



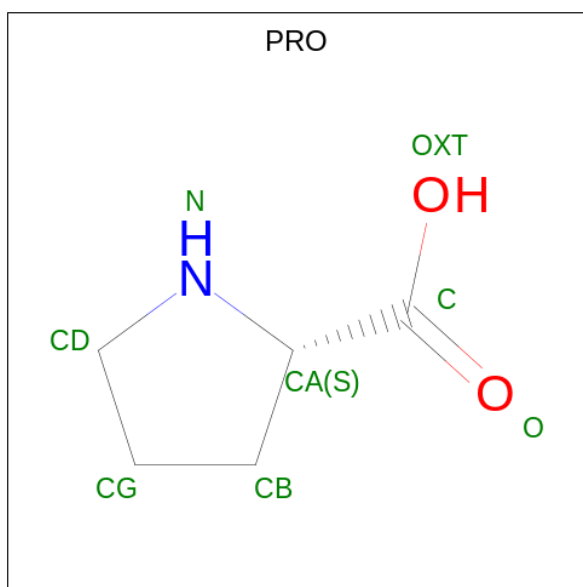
Mol	Chain	Residues	Atoms			AltConf
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	
61	a	1	Total	C	N	0
			10	7	3	

- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
62	4	1	Total	Zn	0
			1	1	
62	3	1	Total	Zn	0
			1	1	

- Molecule 63 is PROLINE (CCD ID: PRO) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



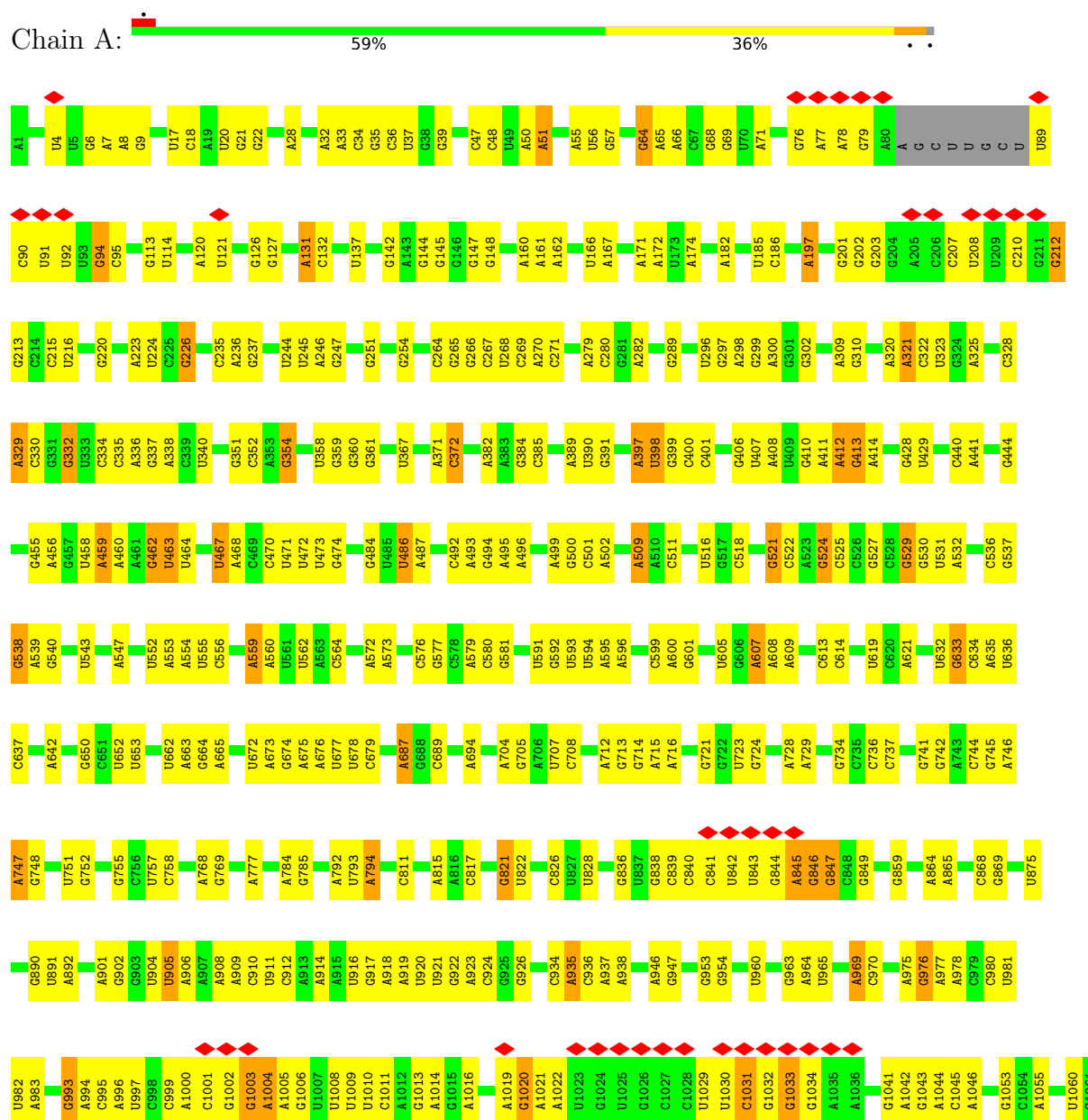


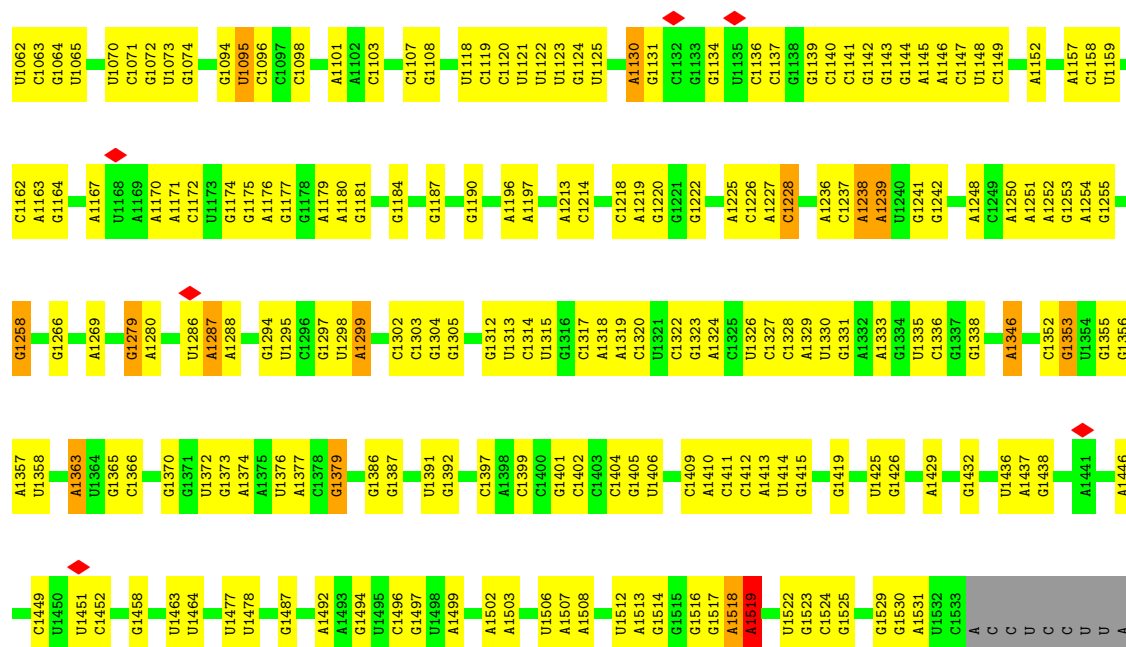
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
63	Y	1	7	5	1	1	0

### 3 Residue-property plots

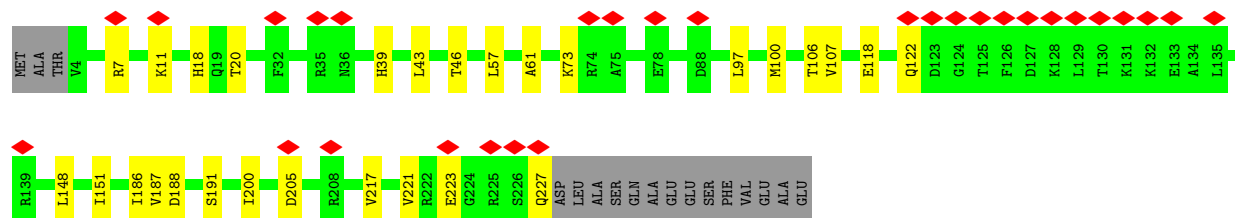
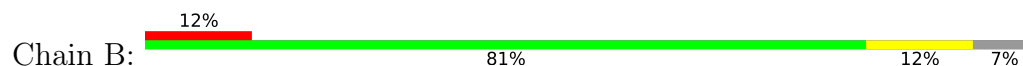
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S rRNA

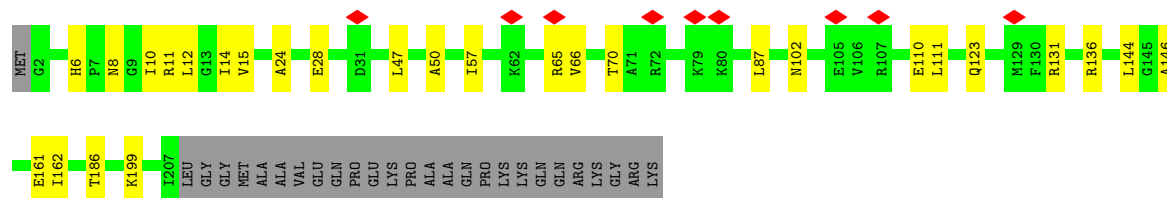
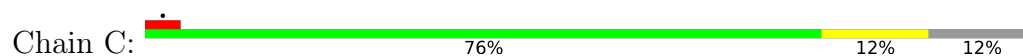




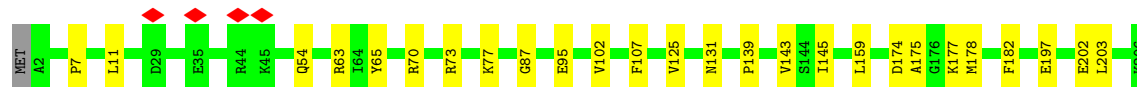
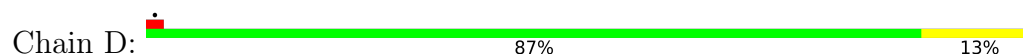
- Molecule 2: 30S ribosomal protein S2




- Molecule 3: 30S ribosomal protein S3

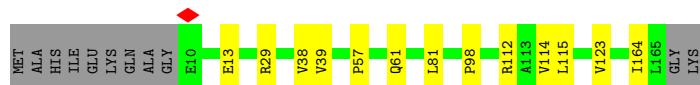


- Molecule 4: 30S ribosomal protein S4



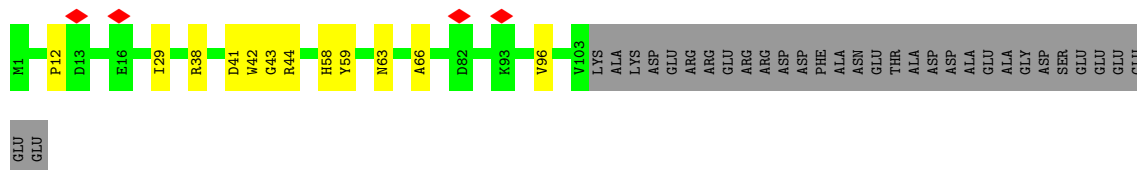
- Molecule 5: 30S ribosomal protein S5

Chain E:  86% 8% 7%



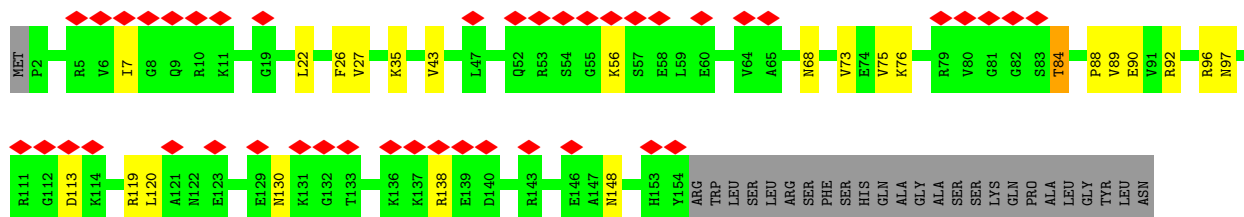
- Molecule 6: 30S ribosomal protein S6, fully modified isoform

Chain F:  67% 9% 24%




- Molecule 7: 30S ribosomal protein S7

Chain G:  24% 72% 13% 15%




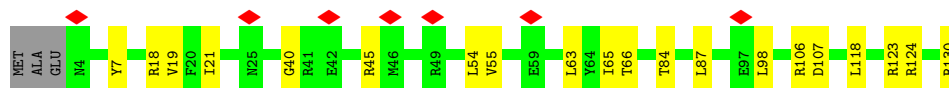
- Molecule 8: 30S ribosomal protein S8

Chain H:  85% 15%




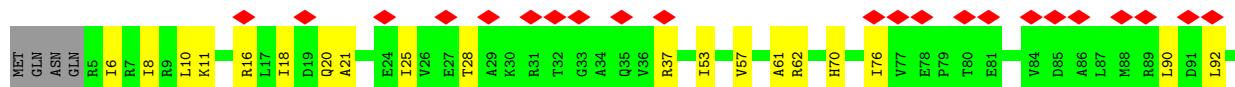
- Molecule 9: 30S ribosomal protein S9

Chain I:  5% 82% 15%



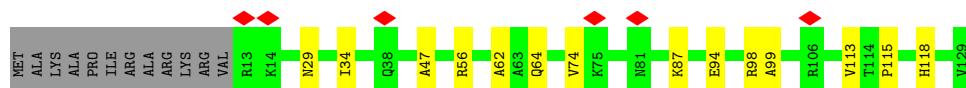
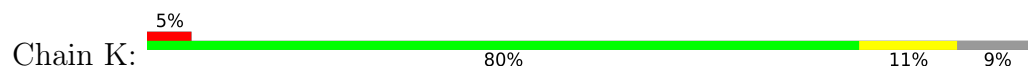
- Molecule 10: 30S ribosomal protein S10

Chain J:  22% 76% 19% 5%

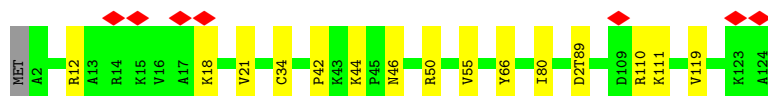
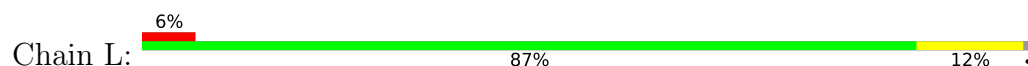




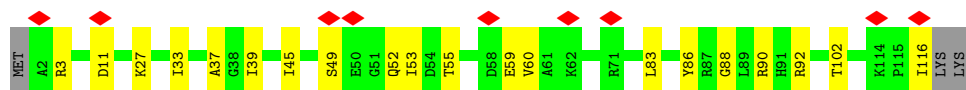
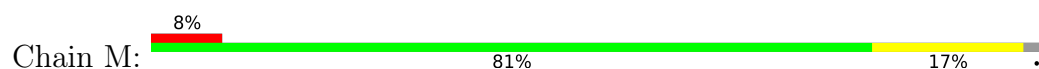
- Molecule 11: 30S ribosomal protein S11



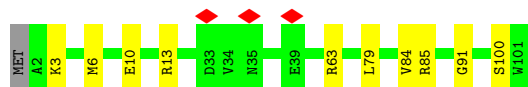
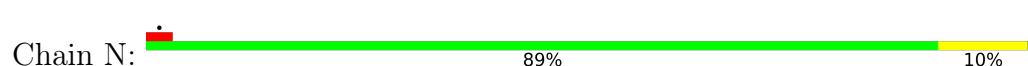
- Molecule 12: 30S ribosomal protein S12



- Molecule 13: 30S ribosomal protein S13



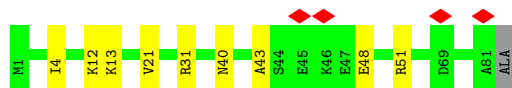
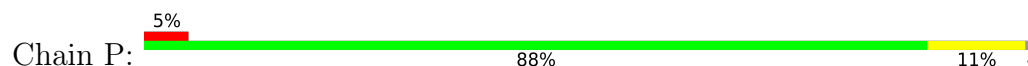
- Molecule 14: 30S ribosomal protein S14




- Molecule 15: 30S ribosomal protein S15

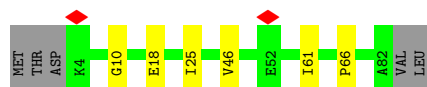


- Molecule 16: 30S ribosomal protein S16




- Molecule 17: 30S ribosomal protein S17

Chain Q:  87% 7% 6%




- Molecule 18: 30S ribosomal protein S18

Chain R:  5% 81% 8% 11%



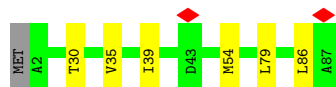
- Molecule 19: 30S ribosomal protein S19

Chain S:  8% 77% 14% 9%




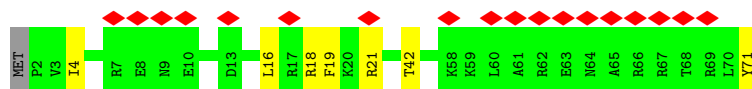
- Molecule 20: 30S ribosomal protein S20

Chain T:  92% 7% 1%



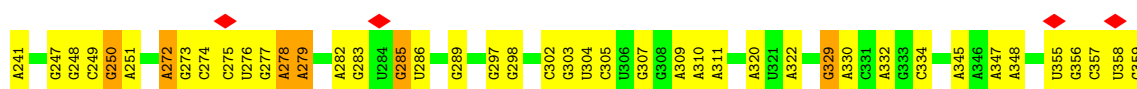
- Molecule 21: 30S ribosomal protein S21

Chain U:  25% 89% 10% 1%

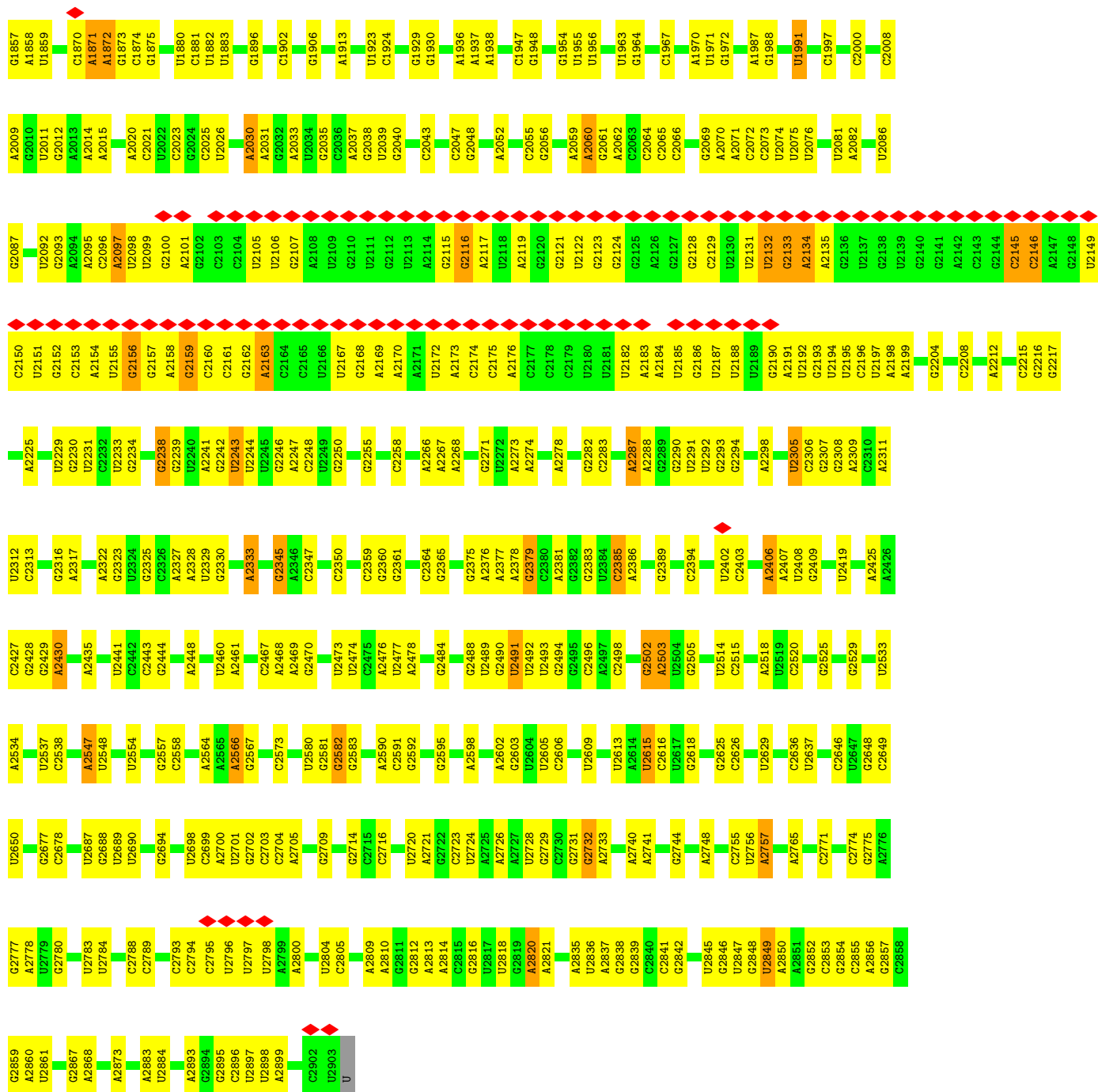


- Molecule 22: 23S rRNA

Chain a:  5% 61% 33% 1%

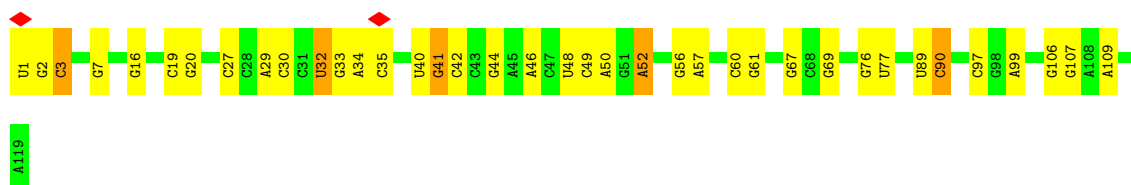






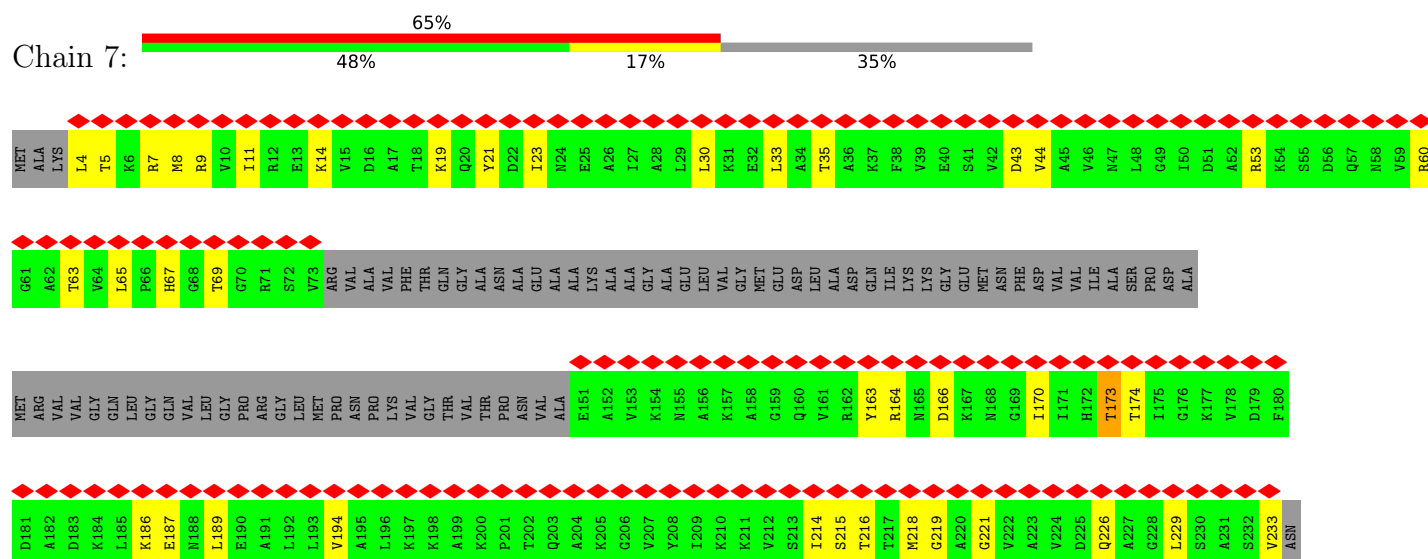
• Molecule 23: 5S rRNA

Chain b: 68% 28%

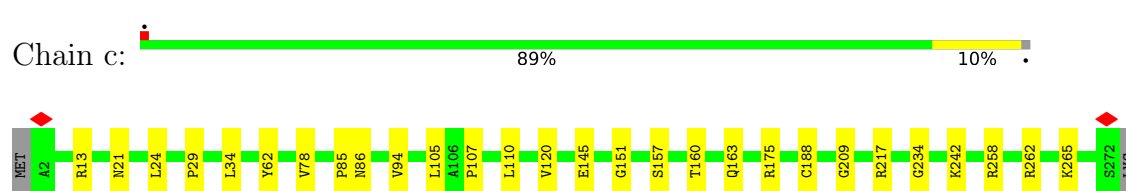




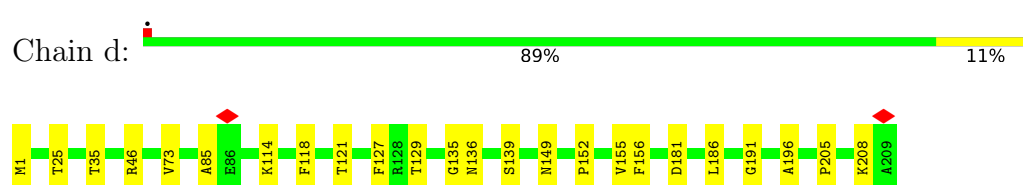
- Molecule 24: Large ribosomal subunit protein uL1



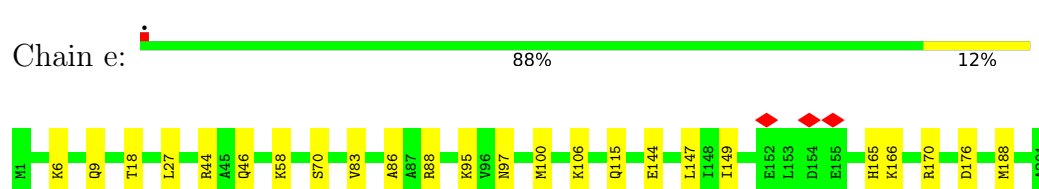
- Molecule 25: Large ribosomal subunit protein uL2



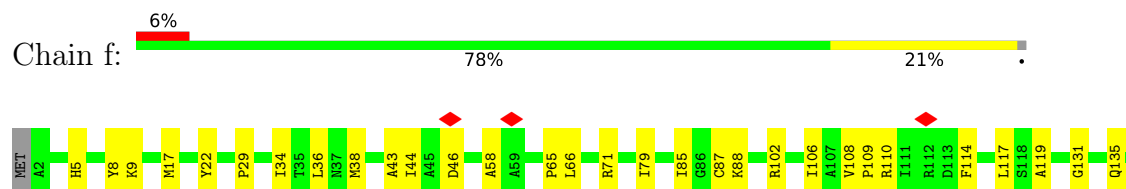
- Molecule 26: 50S ribosomal protein L3



- Molecule 27: 50S ribosomal protein L4

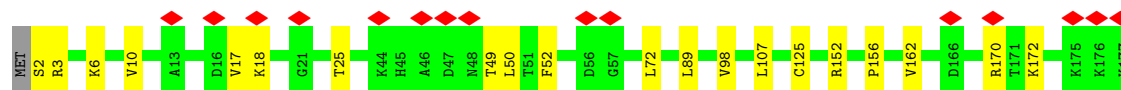
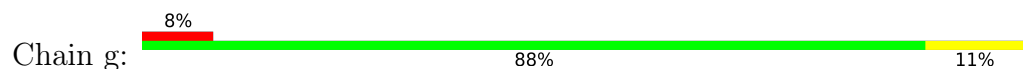


- Molecule 28: Large ribosomal subunit protein uL5

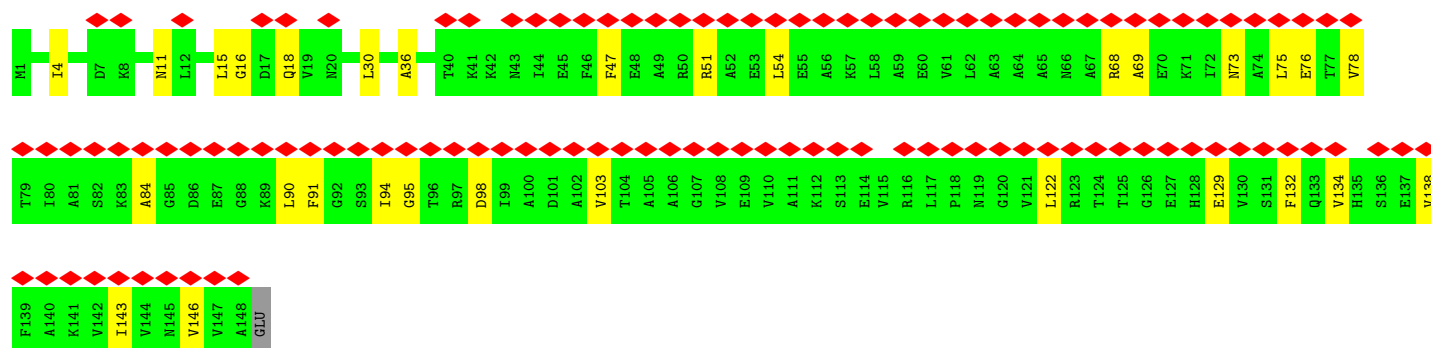
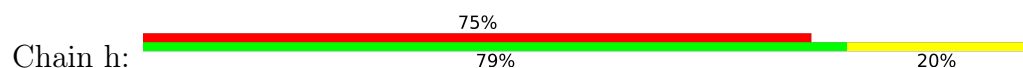




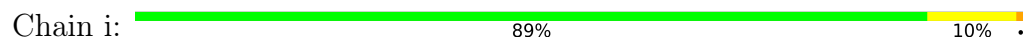
- Molecule 29: Large ribosomal subunit protein uL6



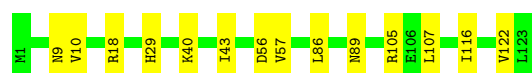
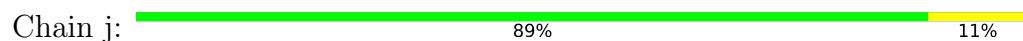
- Molecule 30: 50S ribosomal protein L9



- Molecule 31: 50S ribosomal protein L13




- Molecule 32: 50S ribosomal protein L14



- Molecule 33: 50S ribosomal protein L15




- Molecule 34: 50S ribosomal protein L16

Chain l:  81% 19%




- Molecule 35: Large ribosomal subunit protein bL17

Chain m:  83% 10% 7%




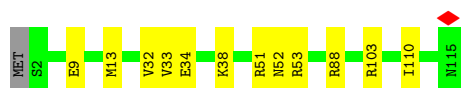
- Molecule 36: Large ribosomal subunit protein uL18

Chain n:  82% 17% .



- Molecule 37: Large ribosomal subunit protein bL19

Chain o:  89% 10% .



- Molecule 38: Large ribosomal subunit protein bL20

Chain p:  94% 5% .




- Molecule 39: 50S ribosomal protein L21

Chain q:  96% .




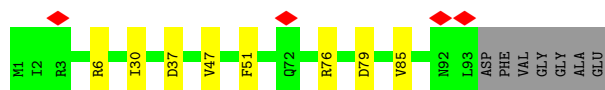
- Molecule 40: 50S ribosomal protein L22

Chain r:  87% 13%




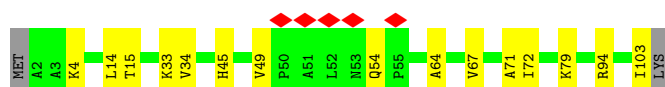
- Molecule 41: Large ribosomal subunit protein uL23

Chain s:  85% 8% 7%




- Molecule 42: 50S ribosomal protein L24

Chain t:  5% 84% 14%




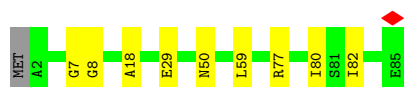
- Molecule 43: 50S ribosomal protein L25

Chain u:  87% 13%




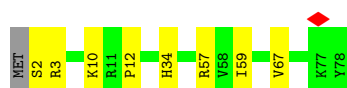
- Molecule 44: Large ribosomal subunit protein bL27

Chain v:  88% 11%



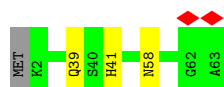
- Molecule 45: Large ribosomal subunit protein bL28

Chain w:  88% 10%

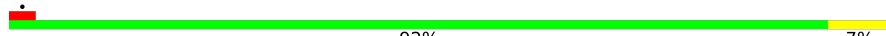


- Molecule 46: Large ribosomal subunit protein uL29

Chain x:  94% 5%

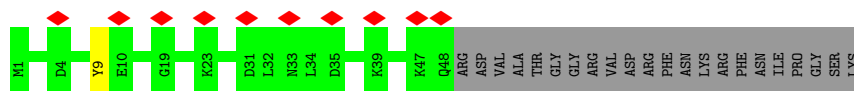


- Molecule 47: Large ribosomal subunit protein uL30

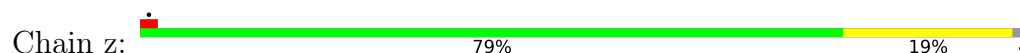
Chain y:  92% 7%



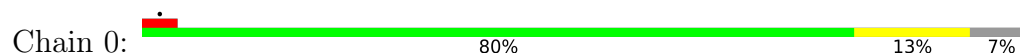
- Molecule 48: 50S ribosomal protein L31



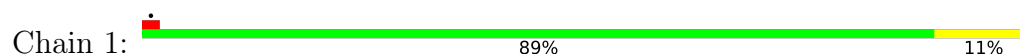
- Molecule 49: Large ribosomal subunit protein bL32



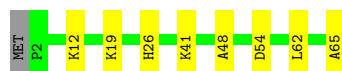
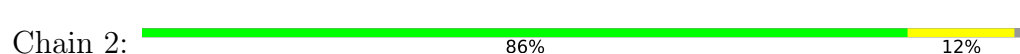
- Molecule 50: Large ribosomal subunit protein bL33



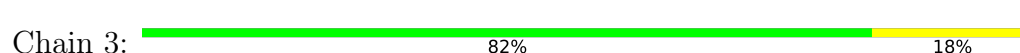
- Molecule 51: 50S ribosomal protein L34



- Molecule 52: Large ribosomal subunit protein bL35

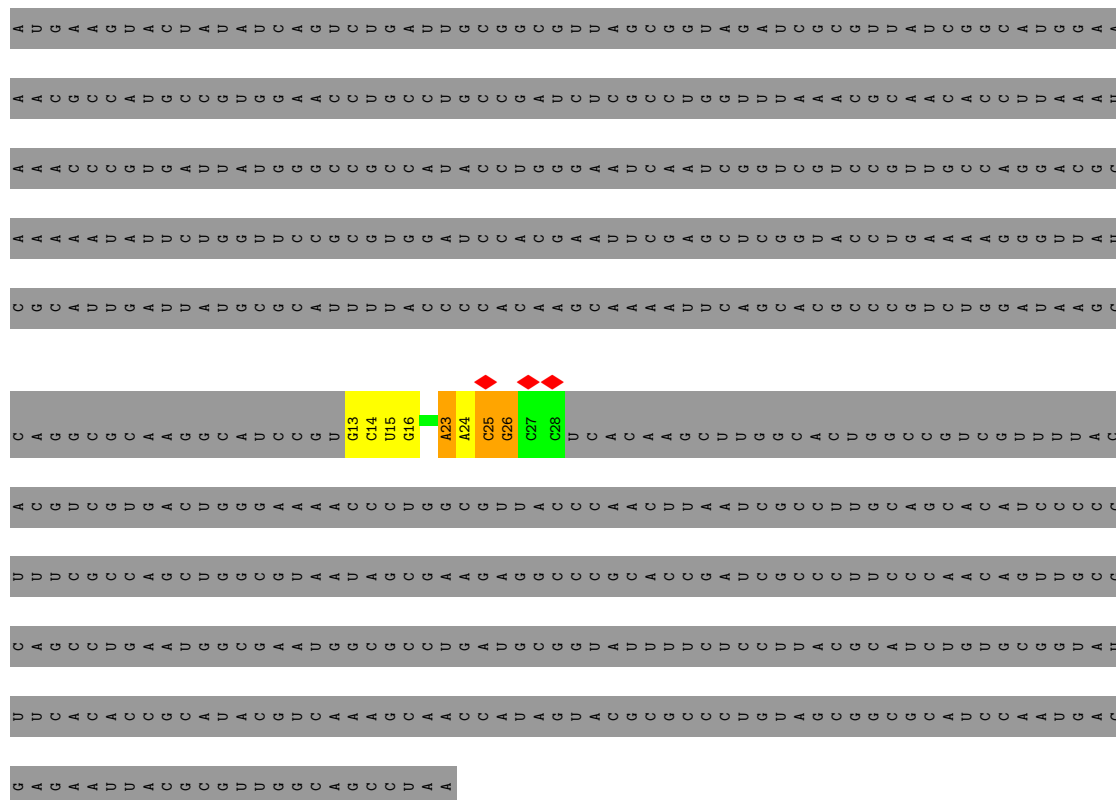


- Molecule 53: 50S ribosomal protein L36



- Molecule 54: SecM mRNA

Chain X:  97%



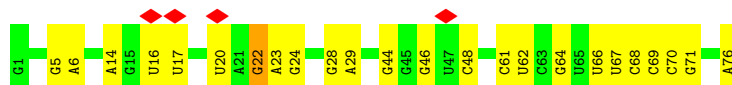
- Molecule 55: A-site tRNA (prolyl-tRNA<sup>Pro</sup>)

Chain Y:  57% 38% 5%




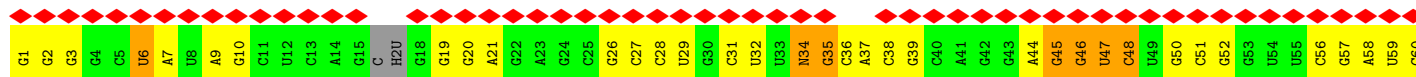
- Molecule 56: P-site tRNA (tRNA<sup>Gly</sup>)

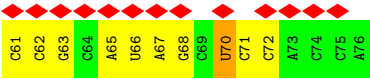
Chain Z:  5% 68% 30% .



- Molecule 57: E-site tRNA (tRNA<sup>Ala</sup>)

Chain 5:  38% 91% 49% 11% .





● Molecule 58: Secretion monitor



MET	SER	GLY	ILE	LEU	THR	ARG	TRP	ARG	GLN	PHE	GLY	LYS	ARG	TYR	PHE	TRP	PRO	HIS	LEU	LEU	GLY	MET	VAL	ALA	ALA	SER	LEU	GLY	LEU	PRO	ALA	ALA	ASN	SER	SER	ASN	ALA	ALA	PRO	ASN	ALA	ASN	PRO	ALA	LYS	ALA	THR	THR	ARG	ASN	HIS	GLU	SER	ALA	LYS	VAL	ASN	PHE	LEU	GLY
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

GLN	LEU	ALA	LEU	LEU	GLU	ALA	ASN	THR	ARG	ARG	PRO	ASN	SER	ASN	TYR	SER	VAL	ASP	TYR	TRP	HIS	GLN	HIS	ALA	ILE	ARG	THR	ILE	ARG	HIS	LEU	SER	PHE	ALA	MET	ALA	ALA	PRO	GLN	THR	LEU	PRO	VAL	ALA	GLU	GLU	SER	LEU	PRO	LEU	GLN	ALA	HIS	LEU	ALA	LEU	LEU	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

THR	LEU	SER	ALA	LEU	LEU	THR	GLN	GLU	GLY	THR	PRO	SER	GLU	LYS	G136	Y137	R138	Y141	A142	H143	P153	Y154	W155	Q158	G165
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	26202	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	165000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.727	Depositor
Minimum map value	-1.061	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	431.59802, 431.59802, 431.59802	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.71933, 0.71933, 0.71933	Depositor



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, D2T, CM0, OMU, 1MG, OMG, 6MZ, MG, UR3, MA6, IAS, H2U, OMC, 2MG, PSU, SPD, 4OC, 4D4, 3TD, K, MS6, 4SU, ZN, MEQ, G7M, 5MC, 5MU

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	0.11	0/36381	0.25	0/56747
2	B	0.12	0/1784	0.31	0/2403
3	C	0.12	0/1651	0.28	0/2225
4	D	0.10	0/1665	0.26	0/2227
5	E	0.13	0/1165	0.30	0/1568
6	F	0.12	0/858	0.28	0/1160
7	G	0.11	0/1219	0.28	0/1635
8	H	0.12	0/989	0.31	0/1326
9	I	0.11	0/1034	0.30	0/1375
10	J	0.13	0/796	0.30	0/1077
11	K	0.12	0/884	0.26	0/1191
12	L	0.13	0/960	0.30	0/1286
13	M	0.12	0/900	0.33	0/1204
14	N	0.11	0/817	0.24	0/1088
15	O	0.12	0/722	0.27	0/964
16	P	0.11	0/653	0.31	0/877
17	Q	0.11	0/650	0.28	0/871
18	R	0.11	0/564	0.24	0/756
19	S	0.10	0/685	0.25	0/922
20	T	0.14	0/676	0.24	0/895
21	U	0.12	0/597	0.29	0/792
22	a	0.12	0/67853	0.25	0/105848
23	b	0.10	0/2851	0.25	0/4444
24	7	0.12	0/1159	0.28	0/1557
25	c	0.14	0/2121	0.32	0/2852
26	d	0.15	0/1576	0.33	0/2119
27	e	0.13	0/1571	0.32	0/2113
28	f	0.13	0/1434	0.36	0/1926
29	g	0.12	0/1343	0.29	0/1816
30	h	0.13	0/1112	0.32	0/1503
31	i	0.11	0/1152	0.25	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	j	0.12	0/955	0.31	0/1279
33	k	0.12	0/1062	0.30	0/1413
34	l	0.12	0/1084	0.29	0/1447
35	m	0.13	0/958	0.32	0/1281
36	n	0.12	0/902	0.28	0/1209
37	o	0.12	0/929	0.30	0/1242
38	p	0.12	0/960	0.25	0/1278
39	q	0.12	0/829	0.31	0/1107
40	r	0.14	0/864	0.32	0/1156
41	s	0.10	0/744	0.26	0/994
42	t	0.10	0/787	0.26	0/1051
43	u	0.12	0/766	0.28	0/1025
44	v	0.12	0/636	0.29	0/841
45	w	0.14	0/635	0.31	0/848
46	x	0.10	0/502	0.21	0/667
47	y	0.11	0/453	0.24	0/605
48	4	0.13	0/380	0.37	0/508
49	z	0.10	0/450	0.26	0/599
50	0	0.11	0/424	0.26	0/565
51	1	0.13	0/380	0.34	0/498
52	2	0.13	0/513	0.31	0/676
53	3	0.11	0/303	0.27	0/397
54	X	0.09	0/373	0.23	0/578
55	Y	0.19	0/1723	0.24	0/2684
56	Z	0.20	1/1653 (0.1%)	0.24	0/2575
57	5	0.16	0/1673	0.28	0/2601
58	6	0.11	0/256	0.30	0/347
All	All	0.12	1/159016 (0.0%)	0.26	0/237789

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	Z	46	G7M	O3'-P	5.08	1.61	1.56

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32741	0	16491	387	0
2	B	1753	0	1780	16	0
3	C	1624	0	1696	16	0
4	D	1643	0	1707	17	0
5	E	1152	0	1196	8	0
6	F	839	0	833	7	0
7	G	1203	0	1254	16	0
8	H	979	0	1031	13	0
9	I	1022	0	1070	13	0
10	J	786	0	828	12	0
11	K	877	0	884	10	0
12	L	957	0	1017	11	0
13	M	891	0	952	14	0
14	N	805	0	844	7	0
15	O	714	0	734	4	0
16	P	643	0	661	5	0
17	Q	641	0	682	4	0
18	R	555	0	578	3	0
19	S	668	0	693	13	0
20	T	670	0	719	4	0
21	U	589	0	629	4	0
22	a	61098	0	30740	674	0
23	b	2550	0	1291	26	0
24	7	1152	0	1222	26	0
25	c	2082	0	2154	20	0
26	d	1566	0	1618	14	0
27	e	1552	0	1619	16	0
28	f	1410	0	1444	25	0
29	g	1323	0	1371	14	0
30	h	1101	0	1142	20	0
31	i	1129	0	1162	10	0
32	j	946	0	1023	8	0
33	k	1053	0	1129	6	0
34	l	1083	0	1158	17	0
35	m	945	0	989	7	0
36	n	892	0	923	15	0
37	o	917	0	962	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	p	947	0	1019	5	0
39	q	816	0	839	3	0
40	r	857	0	922	10	0
41	s	738	0	807	4	0
42	t	779	0	830	9	0
43	u	753	0	780	9	0
44	v	628	0	642	7	0
45	w	625	0	652	6	0
46	x	501	0	531	2	0
47	y	449	0	488	2	0
48	4	373	0	370	1	0
49	z	444	0	458	7	0
50	0	417	0	451	5	0
51	1	377	0	418	4	0
52	2	504	0	572	6	0
53	3	302	0	340	5	0
54	X	336	0	175	8	0
55	Y	1651	0	840	20	0
56	Z	1624	0	829	15	0
57	5	1589	0	808	36	0
58	6	245	0	236	4	0
59	A	25	0	0	0	0
59	Z	1	0	0	0	0
59	a	86	0	0	0	0
59	c	2	0	0	0	0
59	e	1	0	0	0	0
59	t	1	0	0	0	0
60	A	70	0	0	0	0
60	B	1	0	0	0	0
60	Y	1	0	0	0	0
60	Z	1	0	0	0	0
60	a	199	0	0	0	0
60	b	4	0	0	0	0
60	c	1	0	0	0	0
60	k	1	0	0	0	0
60	z	1	0	0	0	0
61	a	40	0	76	2	0
62	3	1	0	0	0	0
62	4	1	0	0	0	0
63	Y	7	0	7	0	0
All	All	147950	0	99316	1509	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 6.

All (1509) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:673:A:H2'	1:A:674:G:C8	2.20	0.76
1:A:1279:G:OP2	10:J:11:LYS:NZ	2.20	0.72
22:a:1779:U:OP2	22:a:1784:A:N6	2.21	0.71
1:A:674:G:H2'	1:A:675:A:H8	1.56	0.70
1:A:673:A:H2'	1:A:674:G:H8	1.56	0.69
1:A:826:C:O2	8:H:16:ASN:ND2	2.26	0.69
34:l:66:ARG:NH1	34:l:104:GLU:OE2	2.26	0.69
22:a:75:G:H22	22:a:111:A:H2	1.42	0.68
1:A:1071:C:H2'	1:A:1072:G:H8	1.55	0.68
7:G:113:ASP:HB2	7:G:119:ARG:HG3	1.76	0.68
22:a:1434:A:H2'	22:a:1435:G:H8	1.58	0.67
1:A:713:G:H2'	1:A:714:G:C8	2.30	0.67
22:a:1724:G:O6	22:a:1737:G:N2	2.27	0.67
28:f:158:THR:HG22	28:f:160:ALA:H	1.58	0.67
1:A:56:U:H2'	1:A:57:G:H8	1.60	0.67
61:a:3240:SPD:H42	40:r:87:PRO:HD2	1.76	0.67
4:D:11:LEU:HB3	4:D:63:ARG:HD3	1.77	0.67
30:h:84:ALA:HB2	30:h:90:LEU:HD23	1.76	0.67
2:B:97:LEU:H	2:B:100:MET:HE3	1.58	0.66
13:M:3:ARG:HH12	28:f:110:ARG:HG2	1.60	0.66
1:A:1497:G:H1'	1:A:1518:MA6:H2	1.77	0.66
22:a:1433:A:H2'	22:a:1434:A:C8	2.30	0.66
54:X:23:A:H2'	54:X:24:A:H8	1.60	0.66
22:a:411:G:OP2	22:a:2406:A:O2'	2.14	0.66
1:A:1187:G:N3	14:N:100:SER:OG	2.29	0.66
57:5:58:A:O2'	57:5:60:C:OP2	2.12	0.66
1:A:269:C:H2'	1:A:270:A:H8	1.59	0.65
22:a:2135:A:N6	22:a:2156:G:O2'	2.28	0.65
22:a:1607:C:N4	22:a:1622:G:OP2	2.29	0.65
1:A:1124:G:N2	1:A:1125:U:O4	2.30	0.65
22:a:514:A:N3	22:a:581:C:O2'	2.29	0.65
22:a:1007:C:OP1	31:i:37:ARG:NH1	2.30	0.65
1:A:401:C:O2'	1:A:621:A:N3	2.30	0.64
22:a:1434:A:H2'	22:a:1435:G:C8	2.33	0.64
22:a:581:C:H2'	22:a:582:A:H8	1.62	0.64
22:a:2298:A:OP1	28:f:71:ARG:NH1	2.30	0.64
1:A:1377:A:OP1	7:G:92:ARG:NH2	2.31	0.64
22:a:272:A:H2'	22:a:273:G:H8	1.63	0.64

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2848:G:O2'	22:a:2867:G:N2	2.30	0.64
9:I:106:ARG:NH1	9:I:107:ASP:O	2.30	0.64
25:c:107:PRO:HD2	25:c:110:LEU:HD22	1.78	0.64
22:a:460:A:N3	58:6:138:ARG:NH2	2.46	0.64
22:a:1536:C:O2'	22:a:1537:G:N2	2.31	0.64
1:A:890:G:O2'	1:A:906:A:N6	2.31	0.63
1:A:714:G:H2'	1:A:715:A:C8	2.33	0.63
24:7:166:ASP:OD1	24:7:170:ILE:N	2.31	0.63
30:h:16:GLY:HA2	30:h:47:PHE:HE2	1.63	0.63
1:A:946:A:O2'	1:A:1333:A:N3	2.30	0.63
22:a:475:C:O2	22:a:479:A:N6	2.27	0.63
1:A:664:G:H22	1:A:741:G:H1	1.47	0.63
1:A:1356:G:H2'	1:A:1357:A:C8	2.33	0.63
7:G:75:VAL:HA	7:G:88:PRO:HA	1.81	0.63
24:7:60:ARG:HD2	24:7:164:ARG:HD3	1.80	0.63
1:A:694:A:O2'	57:5:37:A:O2'	2.17	0.63
22:a:2728:U:HO2'	22:a:2729:G:H8	1.45	0.63
3:C:131:ARG:NH2	54:X:26:G:OP1	2.32	0.63
5:E:115:LEU:HD13	5:E:123:VAL:HG11	1.81	0.63
22:a:1432:G:H2'	22:a:1433:A:C8	2.34	0.63
22:a:2153:C:H2'	22:a:2154:A:C8	2.34	0.63
23:b:77:U:OP1	43:u:21:ARG:NH1	2.32	0.63
1:A:744:C:H2'	1:A:745:G:H8	1.64	0.62
57:5:70:U:H2'	57:5:71:C:C6	2.34	0.62
22:a:832:U:H2'	22:a:833:A:H8	1.64	0.62
1:A:269:C:H2'	1:A:270:A:C8	2.35	0.62
22:a:2305:U:H5''	28:f:131:GLY:HA3	1.82	0.62
27:e:46:GLN:O	27:e:88:ARG:NH2	2.33	0.62
22:a:1796:U:H2'	22:a:1797:G:H8	1.65	0.61
22:a:210:C:OP1	51:1:29:GLN:NE2	2.32	0.61
22:a:568:U:H1'	22:a:2030:6MZ:H9C1	1.81	0.61
1:A:875:U:O2'	8:H:15:ARG:NH1	2.33	0.61
1:A:1152:A:OP1	10:J:70:HIS:ND1	2.31	0.61
22:a:2175:C:O2'	24:7:219:GLY:O	2.17	0.61
3:C:110:GLU:HB2	3:C:144:LEU:HD12	1.82	0.61
24:7:14:LYS:HD2	24:7:33:LEU:HD21	1.82	0.61
54:X:13:G:H1	57:5:35:G:H22	1.46	0.61
1:A:662:U:O2'	1:A:836:G:OP1	2.19	0.61
34:l:42:THR:HG22	34:l:93:VAL:HG12	1.82	0.61
1:A:910:C:OP2	12:L:18:LYS:NZ	2.34	0.61
1:A:938:A:N3	1:A:1376:U:O2'	2.25	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:39:ILE:HD11	13:M:52:GLN:HB3	1.81	0.61
34:l:77:PRO:HG2	34:l:80:VAL:HG21	1.81	0.61
56:Z:22:G:H2'	56:Z:23:A:H8	1.66	0.61
1:A:1055:A:O2'	3:C:161:GLU:O	2.17	0.61
1:A:1218:C:H2'	1:A:1219:A:C8	2.36	0.61
22:a:2192:U:H2'	22:a:2193:G:H8	1.65	0.61
1:A:337:G:H2'	1:A:338:A:C8	2.36	0.61
11:K:34:ILE:HB	11:K:74:VAL:HG11	1.82	0.61
22:a:1509:A:H2'	22:a:1510:G:C8	2.36	0.61
34:l:84:LYS:HG3	44:v:7:GLY:HA3	1.83	0.61
22:a:581:C:H2'	22:a:582:A:C8	2.35	0.60
55:Y:24:C:H2'	55:Y:25:G:H8	1.66	0.60
56:Z:28:G:H2'	56:Z:29:A:H8	1.66	0.60
22:a:894:U:H2'	22:a:895:U:O4'	2.01	0.60
45:w:59:ILE:HG12	45:w:67:VAL:HG21	1.83	0.60
1:A:147:G:H2'	1:A:148:G:C8	2.37	0.60
22:a:880:G:C2	22:a:881:G:H1'	2.37	0.60
22:a:2153:C:H2'	22:a:2154:A:H8	1.67	0.60
53:3:16:ILE:HG12	53:3:25:VAL:HG22	1.83	0.60
9:I:123:ARG:NH1	9:I:124:ARG:O	2.34	0.60
22:a:249:C:O2	52:2:12:LYS:NZ	2.34	0.60
22:a:2134:A:N3	22:a:2159:G:O2'	2.35	0.60
28:f:108:VAL:HG11	28:f:176:PRO:HG3	1.83	0.60
30:h:16:GLY:HA2	30:h:47:PHE:CE2	2.36	0.60
16:P:4:ILE:HG12	16:P:21:VAL:HG22	1.84	0.60
1:A:1226:C:OP2	13:M:102:THR:OG1	2.15	0.59
30:h:94:ILE:HB	30:h:122:LEU:HB2	1.84	0.59
1:A:1004:A:H2'	1:A:1005:A:O4'	2.02	0.59
22:a:2591:C:H2'	22:a:2592:G:C8	2.36	0.59
1:A:509:A:N3	1:A:543:U:O2'	2.35	0.59
1:A:1522:U:H2'	1:A:1523:G:H8	1.67	0.59
22:a:856:G:H2'	22:a:857:G:C8	2.37	0.59
22:a:1406:U:H2'	22:a:1407:G:H8	1.68	0.59
24:7:7:ARG:NH1	24:7:35:THR:O	2.36	0.59
35:m:79:LEU:HD23	35:m:83:LEU:HD12	1.83	0.59
57:5:46:G7M:O2'	57:5:48:C:OP2	2.20	0.59
22:a:639:U:H2'	22:a:640:C:C6	2.38	0.59
22:a:2591:C:H2'	22:a:2592:G:H8	1.68	0.59
1:A:1143:G:H2'	1:A:1144:G:H8	1.66	0.59
5:E:38:VAL:HG11	5:E:114:VAL:HG22	1.85	0.59
1:A:335:C:H2'	1:A:336:A:H8	1.68	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:C:H2'	1:A:1163:A:H8	1.68	0.59
22:a:527:C:N4	22:a:2777:G:O2'	2.28	0.59
22:a:1129:A:N6	22:a:2491:U:OP1	2.35	0.59
1:A:946:A:H2'	1:A:947:G:C8	2.37	0.59
1:A:1314:C:H2'	1:A:1315:U:H6	1.68	0.59
1:A:1513:A:H2'	1:A:1514:G:C8	2.38	0.59
22:a:1847:A:H4'	22:a:1848:A:H8	1.67	0.59
34:l:21:ALA:HB2	34:l:97:GLN:HB2	1.84	0.59
1:A:993:G:O2'	1:A:994:A:N7	2.35	0.58
27:e:83:VAL:HB	27:e:86:ALA:HB2	1.85	0.58
30:h:129:GLU:HG2	30:h:143:ILE:HG12	1.85	0.58
57:5:67:A:H2'	57:5:68:G:C8	2.38	0.58
1:A:492:C:H2'	1:A:493:A:C8	2.38	0.58
22:a:891:G:H2'	22:a:892:A:H8	1.68	0.58
22:a:2071:A:H2'	22:a:2072:C:C6	2.38	0.58
35:m:24:MET:HE1	35:m:40:LYS:HD3	1.85	0.58
9:I:118:LEU:HD22	9:I:124:ARG:HG2	1.84	0.58
22:a:698:C:O2'	22:a:734:A:N6	2.36	0.58
1:A:337:G:H2'	1:A:338:A:H8	1.68	0.58
12:L:55:VAL:HG11	12:L:80:ILE:HD11	1.85	0.58
1:A:8:A:N6	4:D:202:GLU:O	2.34	0.58
1:A:197:A:N1	1:A:220:G:O2'	2.29	0.58
22:a:1509:A:H2'	22:a:1510:G:H8	1.69	0.58
31:i:125:TYR:OH	31:i:132:HIS:NE2	2.33	0.58
1:A:662:U:H2'	1:A:663:A:C8	2.38	0.58
1:A:17:U:H2'	1:A:18:C:C6	2.38	0.58
7:G:90:GLU:OE2	7:G:96:ARG:NH2	2.37	0.58
22:a:2096:C:H2'	22:a:2097:A:H8	1.68	0.58
34:l:20:LEU:HD13	43:u:81:PRO:HG2	1.85	0.58
57:5:67:A:H2'	57:5:68:G:H8	1.69	0.58
1:A:539:A:H2'	1:A:540:G:C8	2.39	0.58
22:a:1443:U:H2'	22:a:1444:G:H8	1.68	0.58
22:a:1802:A:H2'	22:a:1803:A:C8	2.38	0.58
22:a:2859:G:H2'	22:a:2860:A:C8	2.39	0.58
1:A:34:C:H2'	1:A:35:G:H8	1.69	0.58
12:L:110:ARG:HB3	12:L:119:VAL:HG21	1.86	0.57
22:a:2469:A:H4'	34:l:55[B]:ARG:HD2	1.86	0.57
23:b:2:G:O2'	23:b:3:C:OP1	2.21	0.57
18:R:36:SER:HA	18:R:72:ASP:HB2	1.86	0.57
22:a:272:A:H2'	22:a:273:G:C8	2.39	0.57
22:a:1315:C:O2'	22:a:1392:A:N3	2.34	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
61:a:3239:SPD:N1	26:d:135:GLY:O	2.36	0.57
22:a:151:C:H2'	22:a:152:A:H8	1.69	0.57
25:c:29:PRO:HG2	25:c:34:LEU:HD11	1.85	0.57
1:A:1071:C:H2'	1:A:1072:G:C8	2.38	0.57
8:H:11:LEU:HD22	8:H:75:ILE:HD11	1.85	0.57
22:a:307:G:N1	22:a:310:A:OP2	2.29	0.57
22:a:1013:C:H2'	22:a:1014:A:H8	1.70	0.57
22:a:2469:A:H2'	22:a:2470:G:O4'	2.04	0.57
19:S:50:ALA:HB1	19:S:57:HIS:HB3	1.86	0.57
22:a:2502:G:H5''	22:a:2503:2MA:H5''	1.86	0.57
22:a:5:A:H2'	22:a:6:A:C8	2.40	0.57
22:a:219:A:N3	22:a:234:U:O2'	2.32	0.57
22:a:1296:G:OP1	22:a:2709:G:O2'	2.17	0.57
57:5:1:G:H2'	57:5:2:G:C8	2.40	0.57
1:A:963:G:C2	1:A:964:A:C8	2.92	0.57
22:a:555:G:HO2'	22:a:556:A:H8	1.53	0.57
22:a:1386:C:H2'	22:a:1387:A:C8	2.39	0.57
22:a:2129:C:H5''	24:7:5:THR:HB	1.86	0.57
57:5:66:U:H2'	57:5:67:A:H8	1.70	0.57
1:A:78:A:H2'	1:A:79:G:C8	2.40	0.57
1:A:212:G:H2'	1:A:213:G:H8	1.69	0.57
1:A:1355:G:H2'	1:A:1356:G:H8	1.69	0.57
2:B:7:ARG:O	2:B:11:LYS:HG2	2.05	0.57
22:a:1808:A:H3'	22:a:1809:A:C8	2.40	0.57
27:e:170:ARG:NH1	27:e:176:ASP:OD1	2.37	0.57
55:Y:64:U:H2'	55:Y:65:C:H6	1.68	0.57
1:A:412:A:O2'	1:A:413:G:H4'	2.05	0.56
22:a:365:U:H2'	22:a:366:C:C6	2.40	0.56
22:a:1386:C:H2'	22:a:1387:A:H8	1.69	0.56
22:a:1667:G:O2'	22:a:1991:U:O4	2.22	0.56
22:a:2187:U:H2'	22:a:2188:U:C6	2.40	0.56
28:f:17:MET:HG3	28:f:22:TYR:HB2	1.85	0.56
1:A:28:A:O2'	1:A:296:U:OP1	2.21	0.56
22:a:891:G:H2'	22:a:892:A:C8	2.41	0.56
36:n:51:ALA:HB3	36:n:78:VAL:HG23	1.86	0.56
1:A:674:G:H2'	1:A:675:A:C8	2.38	0.56
22:a:247:G:OP2	22:a:249:C:N4	2.30	0.56
22:a:2182:U:H2'	22:a:2183:A:C8	2.40	0.56
22:a:2857:G:N2	22:a:2860:A:OP2	2.33	0.56
29:g:50:LEU:HD13	29:g:72:LEU:HD13	1.87	0.56
35:m:28:LEU:HD23	35:m:48:VAL:HG21	1.86	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:C:O2	1:A:212:G:N2	2.38	0.56
1:A:1144:G:N2	1:A:1146:A:H62	2.02	0.56
22:a:993:G:OP2	38:p:51:ARG:NH2	2.39	0.56
22:a:1796:U:H2'	22:a:1797:G:C8	2.40	0.56
1:A:56:U:H2'	1:A:57:G:C8	2.41	0.56
1:A:1323:G:H2'	1:A:1324:A:C8	2.40	0.56
22:a:832:U:H2'	22:a:833:A:C8	2.40	0.56
22:a:2788:C:H2'	22:a:2789:C:C6	2.40	0.56
22:a:742:A:H2'	22:a:743:A:C8	2.41	0.56
22:a:5:A:H2'	22:a:6:A:H8	1.70	0.56
22:a:876:C:H2'	22:a:877:A:O4'	2.05	0.56
22:a:1746:A:H2'	22:a:1747:U:C6	2.41	0.56
1:A:473:U:H2'	1:A:474:G:H8	1.69	0.56
3:C:57:ILE:HG12	3:C:66:VAL:HG22	1.88	0.56
22:a:309:A:N3	22:a:329:G:O2'	2.37	0.56
22:a:1720:U:H2'	22:a:1721:G:O4'	2.06	0.56
22:a:2086:U:H2'	22:a:2087:G:C8	2.40	0.56
22:a:2618:G:H21	26:d:155:VAL:HG21	1.71	0.56
22:a:2850:A:N7	22:a:2868:A:O2'	2.28	0.56
1:A:471:U:H2'	1:A:472:U:C6	2.41	0.55
22:a:476:G:N1	22:a:479:A:OP2	2.36	0.55
55:Y:30:U:H2'	55:Y:31:G:H8	1.70	0.55
1:A:113:G:H1'	1:A:354:G:H5'	1.89	0.55
1:A:1266:G:N2	1:A:1269:A:OP2	2.34	0.55
11:K:87:LYS:HB2	11:K:113:VAL:HG23	1.87	0.55
22:a:249:C:OP2	22:a:2394:C:O2'	2.23	0.55
22:a:577:G:O2'	22:a:1254:A:OP1	2.24	0.55
22:a:2328:A:H2'	22:a:2329:U:C6	2.41	0.55
1:A:1314:C:H2'	1:A:1315:U:C6	2.41	0.55
24:7:63:THR:HG22	24:7:163:TYR:HE2	1.70	0.55
1:A:980:C:O2'	14:N:13:ARG:NH1	2.39	0.55
22:a:1443:U:H2'	22:a:1444:G:C8	2.41	0.55
22:a:2183:A:H2'	22:a:2184:A:C8	2.41	0.55
22:a:2514:U:H2'	22:a:2515:C:C6	2.42	0.55
19:S:3:ARG:HH21	19:S:7:LYS:HB3	1.72	0.55
22:a:2547:A:H2'	22:a:2548:U:C6	2.42	0.55
1:A:1253:G:H2'	1:A:1254:A:H8	1.72	0.55
22:a:414:C:H2'	22:a:415:A:H8	1.71	0.55
37:o:88:ARG:NH2	37:o:110:ILE:O	2.35	0.55
1:A:552:U:H2'	1:A:553:A:H8	1.71	0.55
1:A:923:A:O2'	1:A:1399:C:OP2	2.25	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:881:G:N2	22:a:896:A:N7	2.55	0.55
22:a:1997:C:OP2	26:d:129:THR:OG1	2.20	0.55
2:B:43:LEU:HA	2:B:46:THR:HB	1.88	0.55
1:A:1513:A:H2'	1:A:1514:G:H8	1.72	0.55
2:B:18:HIS:CD2	2:B:188:ASP:OD2	2.59	0.55
22:a:1278:C:H2'	22:a:1279:G:H8	1.72	0.55
22:a:2106:U:H2'	22:a:2107:G:H8	1.72	0.55
55:Y:64:U:H2'	55:Y:65:C:C6	2.42	0.55
57:5:50:G:H2'	57:5:51:C:C6	2.41	0.55
1:A:1001:C:H2'	1:A:1002:G:C8	2.42	0.54
1:A:1413:A:H2	1:A:1487:G:H22	1.53	0.54
2:B:73:LYS:NZ	2:B:205:ASP:OD1	2.40	0.54
22:a:2135:A:H4'	22:a:2160:C:H4'	1.88	0.54
57:5:1:G:H2'	57:5:2:G:H8	1.70	0.54
1:A:89:U:H2'	1:A:90:C:C6	2.42	0.54
9:I:21:ILE:HG12	9:I:63:LEU:HG	1.90	0.54
22:a:1528:A:OP2	22:a:1543:G:N2	2.32	0.54
43:u:64:VAL:HG22	43:u:69:GLU:HG2	1.89	0.54
1:A:689:C:OP1	11:K:29:ASN:ND2	2.39	0.54
1:A:996:A:H2'	1:A:997:U:C6	2.42	0.54
1:A:1239:A:H62	1:A:1299:A:H62	1.55	0.54
2:B:61:ALA:HB2	2:B:221:VAL:HG23	1.88	0.54
22:a:84:A:N1	22:a:98:G:O2'	2.37	0.54
22:a:358:U:H2'	22:a:359:G:H8	1.70	0.54
22:a:833:A:H2'	22:a:834:G:C8	2.42	0.54
22:a:1746:A:H2'	22:a:1747:U:H6	1.72	0.54
22:a:2185:U:H2'	22:a:2186:G:H8	1.71	0.54
22:a:2096:C:H2'	22:a:2097:A:C8	2.43	0.54
1:A:78:A:H2'	1:A:79:G:H8	1.72	0.54
22:a:948:C:H2'	22:a:949:G:H8	1.71	0.54
23:b:7:G:H1'	36:n:38:GLN:HE22	1.71	0.54
24:7:226:GLN:HA	24:7:229:LEU:HD12	1.88	0.54
29:g:156:PRO:O	29:g:172:LYS:N	2.39	0.54
56:Z:23:A:H2'	56:Z:24:G:C8	2.43	0.54
7:G:75:VAL:HG21	7:G:148:ASN:HD22	1.71	0.54
7:G:76:LYS:HE2	7:G:89:VAL:HG21	1.89	0.54
22:a:576:U:H2'	22:a:577:G:C8	2.42	0.54
27:e:147:LEU:HD11	27:e:170:ARG:HG3	1.90	0.54
1:A:390:U:H2'	1:A:391:G:C8	2.43	0.54
1:A:1238:A:H2	1:A:1241:G:N3	2.04	0.54
1:A:1253:G:H2'	1:A:1254:A:C8	2.43	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:721:A:H2'	22:a:722:A:C8	2.43	0.54
22:a:2070:A:H2'	22:a:2071:A:C8	2.43	0.54
22:a:2233:U:H2'	22:a:2234:G:C8	2.43	0.54
1:A:1524:C:H2'	1:A:1525:G:C8	2.42	0.54
22:a:554:U:H2'	22:a:555:G:O4'	2.08	0.54
22:a:1311:G:OP2	22:a:1311:G:N2	2.27	0.54
1:A:1412:C:H2'	1:A:1413:A:C8	2.43	0.54
36:n:37:ALA:HB3	36:n:78:VAL:HG21	1.89	0.54
21:U:4:ILE:HG13	21:U:19:PHE:HA	1.89	0.53
22:a:864:G:O2'	22:a:914:G:O6	2.26	0.53
22:a:2246:G:H2'	22:a:2247:A:C8	2.43	0.53
22:a:2329:U:H2'	22:a:2330:G:C8	2.43	0.53
7:G:22:LEU:HD11	7:G:97:ASN:HD22	1.74	0.53
22:a:494:G:H4'	40:r:6:LYS:HB2	1.89	0.53
22:a:2376:A:N3	36:n:111:ARG:NH2	2.46	0.53
28:f:58:ALA:HB2	28:f:65:PRO:HD3	1.90	0.53
55:Y:24:C:H2'	55:Y:25:G:C8	2.43	0.53
1:A:745:G:H2'	1:A:746:A:H8	1.72	0.53
1:A:811:C:O2'	1:A:901:A:N1	2.41	0.53
1:A:1120:C:H2'	1:A:1121:U:H6	1.74	0.53
55:Y:27:A:H61	55:Y:45:G:H1	1.55	0.53
1:A:1507:A:H2'	1:A:1508:A:C8	2.43	0.53
22:a:282:A:H2'	22:a:283:G:H8	1.74	0.53
22:a:1654:A:O2'	26:d:118:PHE:O	2.22	0.53
22:a:720:U:H2'	22:a:721:A:C8	2.44	0.53
22:a:2246:G:H2'	22:a:2247:A:H8	1.73	0.53
22:a:2795:C:H2'	22:a:2796:U:C6	2.44	0.53
30:h:16:GLY:HA3	30:h:51:ARG:HH21	1.72	0.53
22:a:282:A:H2'	22:a:283:G:C8	2.44	0.53
22:a:755:U:H2'	22:a:756:A:C8	2.44	0.53
22:a:2898:U:H2'	22:a:2899:A:H8	1.73	0.53
27:e:6:LYS:O	27:e:9:GLN:NE2	2.42	0.53
1:A:746:A:H2'	1:A:747:A:C8	2.43	0.53
1:A:1496:C:H2'	1:A:1497:G:C8	2.43	0.53
7:G:68:ASN:ND2	7:G:130:ASN:OD1	2.41	0.53
22:a:463:G:N2	22:a:466:A:OP2	2.30	0.53
22:a:64:A:H2'	22:a:65:U:C6	2.44	0.53
22:a:1141:U:H4'	22:a:1142:A:O4'	2.09	0.53
22:a:2419:U:H4'	50:0:22:THR:HG21	1.90	0.53
1:A:715:A:H2'	1:A:716:A:C8	2.44	0.53
1:A:970:C:N4	9:I:130:ARG:O	2.42	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1636:U:H2'	22:a:1637:A:C8	2.43	0.53
22:a:2097:A:H2'	22:a:2098:U:C6	2.44	0.53
1:A:236:A:H2'	1:A:237:G:C8	2.44	0.52
22:a:414:C:H2'	22:a:415:A:C8	2.44	0.52
22:a:1009:A:N3	22:a:1153:C:O2'	2.42	0.52
24:7:4:LEU:HB2	24:7:9:ARG:HE	1.74	0.52
25:c:262:ARG:O	25:c:265:LYS:NZ	2.42	0.52
1:A:1376:U:H2'	1:A:1377:A:C8	2.44	0.52
22:a:691:C:OP1	25:c:217:ARG:NH1	2.42	0.52
22:a:1353:A:H2'	22:a:1354:A:C8	2.44	0.52
24:7:163:TYR:HB3	24:7:173:THR:HG21	1.90	0.52
1:A:539:A:H2'	1:A:540:G:H8	1.74	0.52
2:B:148:LEU:HD22	2:B:151:ILE:HD11	1.92	0.52
22:a:279:A:N6	22:a:361:G:H1'	2.25	0.52
22:a:365:U:H2'	22:a:366:C:H6	1.74	0.52
31:i:114:LEU:HG	31:i:118:MET:HE3	1.91	0.52
1:A:559:A:H4'	1:A:560:A:H3'	1.92	0.52
4:D:54:GLN:HB3	4:D:203:LEU:HB2	1.91	0.52
22:a:1440:U:H2'	22:a:1441:G:C8	2.44	0.52
22:a:2025:C:H2'	22:a:2026:U:C6	2.44	0.52
22:a:593:U:H2'	22:a:594:U:C6	2.45	0.52
22:a:729:G:H5''	22:a:730:A:H5''	1.90	0.52
22:a:1682:G:H2'	22:a:1683:U:C6	2.44	0.52
22:a:2241:A:H2'	22:a:2242:G:C8	2.45	0.52
27:e:176:ASP:OD1	27:e:176:ASP:N	2.42	0.52
1:A:37:U:H5	1:A:397:A:C2	2.28	0.52
1:A:922:G:H2'	1:A:923:A:C8	2.44	0.52
25:c:62:TYR:HA	25:c:86:ASN:HD21	1.74	0.52
43:u:4:ILE:HG12	43:u:50:MET:HE1	1.92	0.52
22:a:580:U:H2'	22:a:581:C:C6	2.45	0.52
22:a:645:C:H2'	22:a:647:G:N7	2.25	0.52
22:a:2258:C:O2'	22:a:2427:C:OP2	2.28	0.52
22:a:2845:U:H5''	37:o:52:ASN:O	2.10	0.52
29:g:170:ARG:NH2	53:3:29:ALA:O	2.43	0.52
1:A:1062:U:H2'	1:A:1063:C:C6	2.45	0.52
22:a:171:U:H2'	22:a:172:A:H8	1.74	0.52
22:a:2145:C:H3'	22:a:2146:C:H6	1.75	0.52
1:A:1143:G:H2'	1:A:1144:G:C8	2.45	0.52
5:E:81:LEU:HB2	5:E:98:PRO:HG3	1.92	0.52
22:a:582:A:H2'	22:a:583:G:H8	1.75	0.52
22:a:1405:U:H2'	22:a:1406:U:C6	2.44	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2064:C:H2'	22:a:2065:C:H6	1.73	0.52
22:a:2467:C:O2	34:l:123:LYS:NZ	2.33	0.52
28:f:102:ARG:NH1	48:4:9:TYR:OH	2.43	0.52
57:5:47:U:H2'	57:5:50:G:OP1	2.09	0.52
22:a:1406:U:H2'	22:a:1407:G:C8	2.45	0.52
26:d:152:PRO:HG3	26:d:156:PHE:CZ	2.45	0.52
1:A:846:G:H2'	1:A:847:G:C8	2.45	0.51
22:a:580:U:H2'	22:a:581:C:H6	1.74	0.51
22:a:2105:U:H2'	22:a:2106:U:C6	2.45	0.51
22:a:2537:U:H2'	22:a:2538:C:C6	2.45	0.51
1:A:212:G:H2'	1:A:213:G:C8	2.44	0.51
1:A:473:U:H2'	1:A:474:G:C8	2.45	0.51
1:A:652:U:O4	1:A:752:G:O2'	2.22	0.51
6:F:43:GLY:HA2	6:F:58:HIS:CE1	2.44	0.51
7:G:68:ASN:O	7:G:138:ARG:NE	2.43	0.51
10:J:21:ALA:HB1	10:J:92:LEU:HD13	1.92	0.51
56:Z:70:C:H2'	56:Z:71:G:H8	1.75	0.51
1:A:77:A:H2'	1:A:78:A:C8	2.45	0.51
16:P:12:LYS:HG2	16:P:13:LYS:HG2	1.92	0.51
1:A:501:C:H2'	1:A:502:A:H8	1.74	0.51
3:C:162:ILE:HD12	54:X:24:A:H1'	1.91	0.51
24:7:67:HIS:NE2	24:7:187:GLU:OE1	2.41	0.51
24:7:215:SER:HB3	24:7:221:GLY:HA2	1.92	0.51
1:A:1355:G:H2'	1:A:1356:G:C8	2.45	0.51
22:a:1357:C:H2'	22:a:1358:G:O4'	2.10	0.51
22:a:2192:U:H2'	22:a:2193:G:C8	2.45	0.51
22:a:2804:U:H2'	22:a:2805:C:H6	1.75	0.51
1:A:555:U:H2'	1:A:556:C:C6	2.46	0.51
1:A:1287:A:H2'	1:A:1288:A:C8	2.45	0.51
1:A:1391:U:H2'	1:A:1392:G:C8	2.44	0.51
22:a:907:G:O2'	34:l:100:LYS:NZ	2.40	0.51
22:a:910:A:H2'	22:a:911:A:C8	2.44	0.51
22:a:2070:A:H2'	22:a:2071:A:H8	1.76	0.51
27:e:18:THR:HG23	27:e:106:LYS:HG2	1.93	0.51
55:Y:48:U:H4'	55:Y:49:C:H5'	1.93	0.51
1:A:1218:C:H2'	1:A:1219:A:H8	1.73	0.51
19:S:70:LYS:HB2	19:S:73:GLU:HG3	1.91	0.51
1:A:838:G:H2'	1:A:839:C:C6	2.45	0.51
14:N:79:LEU:HB2	14:N:84:VAL:HG23	1.92	0.51
22:a:2059:A:H1'	58:6:153:PRO:HB3	1.92	0.51
22:a:2229:U:H2'	22:a:2230:G:H8	1.75	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1179:A:H2'	1:A:1180:A:O4'	2.10	0.51
3:C:111:LEU:HD22	3:C:146:ALA:HB2	1.93	0.51
10:J:25:ILE:HD13	10:J:90:LEU:HD23	1.93	0.51
22:a:1417:C:O2'	22:a:1587:G:O2'	2.19	0.51
22:a:2185:U:H2'	22:a:2186:G:C8	2.46	0.51
22:a:2537:U:H2'	22:a:2538:C:H6	1.73	0.51
22:a:2788:C:O2'	22:a:2809:A:N3	2.40	0.51
24:7:189:LEU:HD22	24:7:214:ILE:HD11	1.93	0.51
43:u:31:TYR:HE2	43:u:90:ASP:HB3	1.75	0.51
22:a:1000:A:H2'	22:a:1001:A:C8	2.46	0.51
22:a:1442:U:H2'	22:a:1443:U:C6	2.46	0.51
22:a:2595:G:N2	22:a:2598:A:OP2	2.34	0.51
49:z:54:VAL:HG23	49:z:55:ILE:HG13	1.92	0.51
58:6:155:TRP:HE3	58:6:158:GLN:HE21	1.58	0.51
22:a:764:A:H5'	25:c:209:GLY:HA2	1.92	0.50
22:a:2175:C:H2'	22:a:2176:A:H8	1.75	0.50
24:7:8:MET:HA	24:7:11:ILE:HG12	1.93	0.50
1:A:538:G:H5'	12:L:111:LYS:HB2	1.94	0.50
22:a:1405:U:H2'	22:a:1406:U:H6	1.77	0.50
50:0:11:LEU:HB3	50:0:49:TYR:HB3	1.94	0.50
56:Z:70:C:H2'	56:Z:71:G:C8	2.46	0.50
57:5:71:C:H2'	57:5:72:C:C6	2.46	0.50
22:a:745:1MG:O2'	22:a:748:G:O2'	2.27	0.50
22:a:859:G:O2'	22:a:916:G:O6	2.26	0.50
22:a:2014:A:H2'	22:a:2015:A:C8	2.46	0.50
22:a:2106:U:H2'	22:a:2107:G:C8	2.45	0.50
57:5:28:C:H2'	57:5:29:U:H6	1.77	0.50
1:A:995:C:N3	1:A:1046:A:O2'	2.44	0.50
22:a:155:A:H2'	22:a:156:A:C8	2.47	0.50
22:a:582:A:H2'	22:a:583:G:C8	2.47	0.50
57:5:28:C:H2'	57:5:29:U:C6	2.46	0.50
1:A:1118:U:H2'	1:A:1119:C:H6	1.76	0.50
13:M:55:THR:O	13:M:59:GLU:HG2	2.11	0.50
1:A:736:C:H2'	1:A:737:C:H6	1.77	0.50
1:A:744:C:H2'	1:A:745:G:C8	2.46	0.50
1:A:1524:C:H2'	1:A:1525:G:H8	1.76	0.50
22:a:1306:C:H2'	22:a:1307:A:H8	1.77	0.50
22:a:2064:C:H2'	22:a:2065:C:C6	2.46	0.50
22:a:2243:U:H2'	22:a:2244:U:C6	2.47	0.50
23:b:48:U:H4'	36:n:100:HIS:HD2	1.77	0.50
29:g:52:PHE:HE1	29:g:72:LEU:HD12	1.77	0.50

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:h:15:LEU:O	30:h:51:ARG:NH2	2.44	0.50
1:A:77:A:H2'	1:A:78:A:H8	1.76	0.50
1:A:493:A:H2'	1:A:494:G:C8	2.47	0.50
1:A:1163:A:H2'	1:A:1164:G:H8	1.76	0.50
4:D:174:ASP:OD2	4:D:177:LYS:NZ	2.44	0.50
22:a:347:A:H2'	22:a:348:A:C8	2.47	0.50
22:a:589:U:H2'	22:a:590:A:C8	2.47	0.50
22:a:1590:A:H2'	22:a:1591:A:C8	2.47	0.50
22:a:2795:C:H2'	22:a:2796:U:H6	1.77	0.50
22:a:2804:U:H2'	22:a:2805:C:C6	2.46	0.50
1:A:131:A:H2'	1:A:132:C:C6	2.46	0.50
1:A:1118:U:H1'	1:A:1179:A:C5	2.46	0.50
12:L:34:CYS:HA	12:L:55:VAL:HG12	1.93	0.50
22:a:813:U:H2'	22:a:814:C:H6	1.77	0.50
22:a:1149:G:H2'	22:a:1150:C:C6	2.47	0.50
24:7:11:ILE:HG22	24:7:33:LEU:HD22	1.93	0.50
28:f:44:ILE:HG21	28:f:79:ILE:HG22	1.94	0.50
34:l:75:GLU:HB2	34:l:90:GLU:HG3	1.93	0.50
1:A:335:C:H2'	1:A:336:A:C8	2.47	0.50
3:C:10:ILE:HG23	3:C:11:ARG:HG3	1.93	0.50
22:a:1529:G:H2'	22:a:1530:G:H8	1.77	0.50
32:j:40:LYS:HE3	32:j:57:VAL:HG12	1.93	0.50
1:A:21:G:H2'	1:A:22:G:C8	2.46	0.49
1:A:501:C:H2'	1:A:502:A:C8	2.46	0.49
22:a:1:G:H2'	22:a:2:G:C8	2.47	0.49
22:a:624:C:O2'	22:a:657:U:OP1	2.30	0.49
22:a:1429:G:H2'	22:a:1430:G:H8	1.75	0.49
41:s:76:ARG:NH1	41:s:79:ASP:OD1	2.39	0.49
22:a:871:U:H2'	22:a:872:U:C6	2.46	0.49
22:a:1506:U:H2'	22:a:1507:C:C6	2.47	0.49
22:a:1614:A:N6	40:r:92:ARG:O	2.42	0.49
22:a:1672:A:C2	22:a:2582:G:H5'	2.46	0.49
26:d:136:ASN:ND2	26:d:139:SER:O	2.45	0.49
1:A:310:G:H5''	16:P:31:ARG:HB2	1.94	0.49
1:A:1013:G:N2	1:A:1016:A:OP2	2.33	0.49
13:M:33:ILE:HD13	13:M:60:VAL:HG22	1.94	0.49
22:a:17:G:H2'	22:a:18:U:C6	2.48	0.49
22:a:820:A:H4'	22:a:836:G:H22	1.77	0.49
22:a:1858:A:H2'	22:a:1859:U:O4'	2.12	0.49
22:a:2184:A:H2'	22:a:2185:U:C6	2.47	0.49
22:a:2731:G:H2'	22:a:2732:G:C8	2.47	0.49

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2853:C:H2'	22:a:2854:G:H8	1.77	0.49
1:A:464:U:N3	1:A:467:U:OP2	2.33	0.49
1:A:1401:G:H2'	1:A:1402:4OC:O4'	2.13	0.49
22:a:2047:C:H2'	22:a:2048:G:H8	1.74	0.49
22:a:2728:U:O2'	22:a:2729:G:H8	1.95	0.49
1:A:384:G:H2'	1:A:385:C:C6	2.48	0.49
22:a:1570:A:H2'	22:a:1571:A:C8	2.48	0.49
22:a:1794:A:H2'	22:a:1795:C:C6	2.47	0.49
22:a:1873:G:H2'	22:a:1874:C:C6	2.48	0.49
57:5:50:G:H2'	57:5:51:C:H6	1.78	0.49
1:A:579:A:O2'	15:O:54:ARG:NH1	2.45	0.49
1:A:1409:C:H2'	1:A:1410:A:H8	1.76	0.49
22:a:909:A:H2'	22:a:912:C:H5	1.78	0.49
22:a:1441:G:H2'	22:a:1442:U:C6	2.47	0.49
26:d:1:MET:HB3	26:d:205:PRO:HG2	1.94	0.49
56:Z:23:A:H2'	56:Z:24:G:H8	1.78	0.49
9:I:84:THR:HG23	9:I:98:LEU:HD13	1.94	0.49
22:a:2065:C:H2'	22:a:2066:C:H6	1.77	0.49
25:c:145:GLU:HB2	25:c:188:CYS:HB3	1.94	0.49
26:d:46:ARG:NH1	26:d:85:ALA:O	2.34	0.49
1:A:472:U:H2'	1:A:473:U:C6	2.48	0.49
1:A:1219:A:H2'	1:A:1220:G:C8	2.48	0.49
13:M:11:ASP:HA	13:M:45:ILE:HB	1.95	0.49
13:M:86:TYR:O	13:M:90:ARG:HG2	2.12	0.49
22:a:1:G:H2'	22:a:2:G:H8	1.78	0.49
22:a:1440:U:H2'	22:a:1441:G:H8	1.78	0.49
22:a:2072:C:H2'	22:a:2073:C:H6	1.78	0.49
22:a:2408:U:H2'	22:a:2409:G:H8	1.78	0.49
22:a:2809:A:H2'	22:a:2810:A:C8	2.47	0.49
31:i:31:GLU:OE2	31:i:34:ARG:NH1	2.46	0.49
42:t:14:LEU:HD11	42:t:71:ALA:HB2	1.94	0.49
1:A:202:G:H2'	1:A:203:G:H8	1.78	0.49
22:a:358:U:H2'	22:a:359:G:C8	2.47	0.49
22:a:2099:U:H3	22:a:2190:G:H1	1.61	0.49
27:e:144:GLU:OE2	27:e:166:LYS:NZ	2.42	0.49
29:g:18:LYS:HB3	29:g:25:THR:HB	1.94	0.49
2:B:187:VAL:HG13	2:B:191:SER:HB2	1.94	0.49
6:F:41:ASP:OD1	6:F:58:HIS:NE2	2.46	0.49
8:H:29:SER:HB3	8:H:57:PRO:HB2	1.95	0.49
8:H:77:ARG:NH1	8:H:79:SER:O	2.45	0.49
22:a:2145:C:H5''	22:a:2146:C:H5	1.78	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2705:A:O2'	22:a:2852:G:OP1	2.24	0.49
23:b:1:U:H2'	23:b:2:G:H8	1.78	0.49
1:A:64:G:H4'	1:A:65:A:H3'	1.95	0.48
22:a:813:U:H2'	22:a:814:C:C6	2.48	0.48
22:a:1548:A:H2'	22:a:1549:A:C8	2.48	0.48
28:f:8:TYR:HB2	28:f:173:PHE:CZ	2.48	0.48
1:A:34:C:H2'	1:A:35:G:C8	2.47	0.48
1:A:37:U:H5	1:A:397:A:H2	1.61	0.48
1:A:728:A:H2'	1:A:729:A:C8	2.48	0.48
3:C:12:LEU:HD11	14:N:91:GLY:HA2	1.95	0.48
22:a:1019:U:OP1	22:a:1035:U:O2'	2.23	0.48
22:a:1038:G:H2'	22:a:1039:A:C8	2.48	0.48
22:a:2816:G:N3	22:a:2883:A:O2'	2.44	0.48
1:A:35:G:H2'	1:A:36:C:C6	2.47	0.48
1:A:384:G:H2'	1:A:385:C:H6	1.78	0.48
1:A:522:C:H41	12:L:50:ARG:NH2	2.11	0.48
1:A:634:C:H2'	1:A:635:A:H8	1.77	0.48
1:A:676:A:H5''	11:K:115:PRO:HB3	1.95	0.48
1:A:1437:A:H2'	1:A:1438:G:H8	1.78	0.48
6:F:38:ARG:HB3	6:F:63:ASN:HB2	1.94	0.48
38:p:86:ALA:HB2	38:p:116:ALA:HB2	1.94	0.48
55:Y:30:U:H2'	55:Y:31:G:C8	2.49	0.48
1:A:166:U:H2'	1:A:167:A:H8	1.76	0.48
1:A:235:C:H2'	1:A:236:A:H8	1.78	0.48
1:A:458:U:H2'	1:A:459:A:C8	2.48	0.48
1:A:1162:C:H2'	1:A:1163:A:C8	2.47	0.48
22:a:598:U:H2'	22:a:599:A:H8	1.77	0.48
22:a:632:A:H2'	22:a:633:A:C8	2.48	0.48
22:a:657:U:H2'	22:a:658:U:C6	2.48	0.48
22:a:875:G:H2'	22:a:876:C:C6	2.49	0.48
22:a:1683:U:H2'	22:a:1684:G:H8	1.79	0.48
22:a:1721:G:O2'	22:a:1739:A:N6	2.46	0.48
31:i:34:ARG:HG3	31:i:39:LYS:HB2	1.94	0.48
1:A:642:A:N7	8:H:107:SER:HA	2.29	0.48
2:B:100:MET:HA	2:B:107:VAL:HG21	1.95	0.48
14:N:3:LYS:HB2	14:N:6:MET:HG2	1.94	0.48
17:Q:46:VAL:HG21	17:Q:61:ILE:HG21	1.95	0.48
22:a:703:U:H2'	22:a:704:G:O4'	2.13	0.48
22:a:1586:A:H3'	22:a:1587:G:H8	1.78	0.48
43:u:6:ALA:HB3	43:u:65:VAL:HG22	1.95	0.48
56:Z:28:G:H2'	56:Z:29:A:C8	2.46	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1041:G:H2'	1:A:1042:A:C8	2.49	0.48
22:a:1223:G:OP1	39:q:68:ARG:NH1	2.47	0.48
22:a:2123:G:H2'	22:a:2124:G:H8	1.79	0.48
22:a:2291:U:H2'	22:a:2292:U:C6	2.49	0.48
22:a:2470:G:OP1	34:l:55[A]:ARG:NH2	2.46	0.48
30:h:68:ARG:HD2	30:h:134:VAL:HG11	1.96	0.48
1:A:50:A:O2'	1:A:360:G:N2	2.46	0.48
1:A:94:G:H5''	1:A:95:C:H5	1.79	0.48
1:A:999:C:H2'	1:A:1000:A:H8	1.79	0.48
22:a:304:U:H2'	22:a:305:C:C6	2.49	0.48
22:a:672:C:OP2	33:k:42:SER:OG	2.28	0.48
22:a:784:G:H5'	22:a:785:G:OP1	2.13	0.48
22:a:1183:U:H2'	22:a:1184:U:C6	2.49	0.48
22:a:1278:C:H2'	22:a:1279:G:C8	2.48	0.48
22:a:1361:G:H2'	22:a:1362:C:C6	2.48	0.48
22:a:1564:C:H2'	22:a:1565:C:C6	2.49	0.48
22:a:1771:C:H2'	22:a:1772:A:C8	2.49	0.48
22:a:2467:C:H2'	22:a:2468:A:O4'	2.14	0.48
22:a:2590:A:H2'	22:a:2591:C:H6	1.78	0.48
23:b:16:G:N2	23:b:69:G:H1'	2.29	0.48
30:h:78:VAL:HG21	30:h:103:VAL:HG22	1.95	0.48
41:s:30:ILE:HG13	41:s:85:VAL:HB	1.96	0.48
54:X:24:A:H2'	54:X:25:C:H5'	1.96	0.48
1:A:751:U:H2'	1:A:752:G:O4'	2.13	0.48
1:A:1010:U:H2'	1:A:1011:C:C6	2.49	0.48
5:E:57:PRO:O	5:E:61:GLN:HG2	2.13	0.48
22:a:1264:A:OP2	22:a:1265:A:O2'	2.26	0.48
22:a:1882:U:C2	22:a:1883:U:C5	3.02	0.48
23:b:106:G:H2'	23:b:107:G:O4'	2.14	0.48
28:f:135:GLN:HG2	28:f:141:ILE:HG21	1.95	0.48
29:g:2:SER:O	29:g:6:LYS:HG2	2.13	0.48
1:A:401:C:OP2	4:D:70:ARG:NH1	2.47	0.48
1:A:407:U:H2'	1:A:408:A:H8	1.79	0.48
1:A:745:G:H2'	1:A:746:A:C8	2.48	0.48
3:C:24:ALA:HB1	3:C:28:GLU:HG2	1.96	0.48
22:a:755:U:H2'	22:a:756:A:H8	1.79	0.48
22:a:1231:U:H2'	22:a:1232:G:H8	1.79	0.48
22:a:1444:G:H2'	22:a:1445:G:H8	1.78	0.48
22:a:1585:C:H2'	22:a:1586:A:O4'	2.14	0.48
28:f:29:PRO:HB3	28:f:160:ALA:HB2	1.96	0.48
1:A:1222:G:OP2	1:A:1322:C:N4	2.45	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:16:ARG:O	10:J:20:GLN:HG2	2.13	0.48
13:M:83:LEU:HD11	19:S:65:GLU:HB3	1.95	0.48
22:a:1198:U:H2'	22:a:1199:U:C6	2.49	0.48
22:a:2646:C:OP2	22:a:2732:G:O2'	2.32	0.48
1:A:358:U:H2'	1:A:359:G:H8	1.79	0.47
22:a:20:C:H2'	22:a:21:A:H8	1.78	0.47
22:a:160:A:N3	22:a:2208:C:O2'	2.42	0.47
22:a:310:A:H5''	42:t:15:THR:HG23	1.96	0.47
22:a:851:C:H2'	22:a:852:U:C6	2.48	0.47
22:a:1563:U:H2'	22:a:1564:C:C6	2.48	0.47
22:a:2598:A:H5''	25:c:234:GLY:HA3	1.96	0.47
1:A:1512:U:H2'	1:A:1513:A:C8	2.49	0.47
22:a:2074:U:H2'	22:a:2075:U:C6	2.49	0.47
30:h:73:ASN:O	30:h:76:GLU:HG3	2.14	0.47
37:o:33:VAL:HG22	37:o:38:LYS:HG3	1.96	0.47
42:t:34:VAL:HG13	42:t:67:VAL:HG12	1.95	0.47
22:a:589:U:H2'	22:a:590:A:H8	1.80	0.47
24:7:19:LYS:HD3	24:7:21:TYR:CE1	2.49	0.47
49:z:38:HIS:HB3	49:z:44:THR:HG22	1.96	0.47
53:3:2:LYS:NZ	53:3:32:LYS:O	2.33	0.47
1:A:978:A:C2	1:A:1319:A:C4	3.02	0.47
22:a:172:A:H2'	22:a:173:A:H8	1.80	0.47
1:A:33:A:H2'	1:A:34:C:C6	2.49	0.47
1:A:215:C:H2'	1:A:216:U:C6	2.50	0.47
1:A:591:U:H2'	1:A:592:G:H8	1.79	0.47
1:A:636:U:H2'	1:A:637:C:C6	2.50	0.47
1:A:1120:C:C2	1:A:1121:U:C5	3.03	0.47
9:I:55:VAL:HG21	9:I:87:LEU:HD13	1.95	0.47
22:a:150:U:H2'	22:a:151:C:H6	1.79	0.47
22:a:172:A:H2'	22:a:173:A:C8	2.49	0.47
22:a:1248:G:OP1	27:e:44:ARG:NH1	2.39	0.47
22:a:1636:U:H2'	22:a:1637:A:H8	1.79	0.47
22:a:2175:C:H2'	22:a:2176:A:C8	2.48	0.47
50:0:10:LYS:HE3	50:0:54:ILE:HA	1.96	0.47
1:A:839:C:H2'	1:A:840:C:C6	2.49	0.47
1:A:936:C:C2	1:A:937:A:C8	3.02	0.47
1:A:1372:U:H2'	1:A:1373:G:O4'	2.15	0.47
4:D:102:VAL:HG13	4:D:107:PHE:HB2	1.96	0.47
12:L:42:PRO:HG3	12:L:50:ARG:HG3	1.97	0.47
22:a:69:C:O2	22:a:73:A:O2'	2.29	0.47
22:a:659:G:O2'	27:e:95:LYS:O	2.24	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:848:C:H2'	22:a:849:A:H8	1.79	0.47
22:a:871:U:H2'	22:a:872:U:H6	1.79	0.47
22:a:947:A:H2'	22:a:948:C:C6	2.49	0.47
22:a:1366:A:OP1	45:w:2:SER:OG	2.25	0.47
22:a:2174:C:H1'	24:7:218:MET:HE1	1.97	0.47
22:a:2812:G:H2'	22:a:2813:A:C8	2.50	0.47
55:Y:44:U:H2'	55:Y:45:G:C8	2.49	0.47
1:A:246:A:C2	1:A:282:A:C5	3.02	0.47
1:A:996:A:H2'	1:A:997:U:H6	1.77	0.47
1:A:1120:C:H2'	1:A:1121:U:C6	2.49	0.47
1:A:1404:C:H2'	1:A:1405:G:C8	2.49	0.47
22:a:6:A:H2'	22:a:7:G:H8	1.79	0.47
22:a:704:G:H1'	22:a:727:A:N6	2.29	0.47
22:a:714:U:H1'	22:a:717:C:H5	1.78	0.47
22:a:1571:A:H2'	22:a:1572:A:H8	1.80	0.47
22:a:1987:A:H2'	22:a:1988:G:H8	1.79	0.47
22:a:2564:A:OP1	22:a:2648:G:O2'	2.27	0.47
23:b:49:C:H2'	23:b:50:A:C8	2.50	0.47
1:A:254:G:O2'	17:Q:18:GLU:O	2.32	0.47
1:A:672:U:H2'	1:A:673:A:C8	2.50	0.47
1:A:1238:A:OP1	1:A:1335:U:O2'	2.22	0.47
13:M:37:ALA:HB2	13:M:59:GLU:HG3	1.95	0.47
22:a:72:U:O4	46:x:58:ASN:ND2	2.48	0.47
22:a:828:U:H2'	22:a:829:A:C8	2.50	0.47
22:a:2625:G:H2'	22:a:2626:C:C6	2.50	0.47
1:A:674:G:H21	11:K:118:HIS:HB2	1.79	0.47
1:A:1312:G:H5'	19:S:5:LEU:HD11	1.96	0.47
15:O:25:THR:HG21	15:O:70:LEU:HB2	1.96	0.47
22:a:598:U:H2'	22:a:599:A:C8	2.50	0.47
22:a:1021:A:H61	22:a:1142:A:N6	2.13	0.47
22:a:1839:G:C2	22:a:1840:G:C8	3.03	0.47
22:a:2229:U:O2	45:w:34:HIS:HE1	1.98	0.47
22:a:2581:G:OP2	22:a:2581:G:N2	2.42	0.47
23:b:52:A:N7	36:n:64:TYR:OH	2.38	0.47
41:s:47:VAL:HG13	41:s:51:PHE:HD2	1.80	0.47
1:A:712:A:H2'	1:A:713:G:C8	2.49	0.47
1:A:1098:C:O2'	21:U:71:TYR:O	2.32	0.47
22:a:29:U:H2'	22:a:30:G:C8	2.49	0.47
22:a:151:C:H2'	22:a:152:A:C8	2.49	0.47
22:a:634:C:H2'	22:a:635:C:C6	2.50	0.47
22:a:936:A:H2'	22:a:937:C:C6	2.50	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2771:C:O2'	26:d:208:LYS:NZ	2.38	0.47
25:c:163:GLN:OE1	25:c:175:ARG:NH1	2.48	0.47
29:g:2:SER:OG	29:g:3:ARG:N	2.49	0.47
57:5:31:C:H2'	57:5:32:U:C6	2.50	0.47
1:A:440:C:C2	1:A:441:A:C8	3.03	0.46
1:A:920:U:H2'	1:A:921:U:C6	2.50	0.46
1:A:1477:U:H2'	1:A:1478:U:C6	2.49	0.46
4:D:145:ILE:HD12	4:D:178:MET:HB3	1.97	0.46
10:J:28:THR:HG21	10:J:90:LEU:HD22	1.97	0.46
22:a:117:G:OP2	22:a:119:A:O2'	2.24	0.46
22:a:927:A:H2'	22:a:928:A:C8	2.50	0.46
22:a:1529:G:H2'	22:a:1530:G:C8	2.50	0.46
22:a:1704:C:H2'	22:a:1705:A:C8	2.50	0.46
22:a:2419:U:OP1	52:2:41:LYS:NZ	2.34	0.46
23:b:76:G:OP1	43:u:9:ARG:NH1	2.42	0.46
55:Y:74:A:H5'	55:Y:75:C:OP1	2.15	0.46
1:A:202:G:H2'	1:A:203:G:C8	2.49	0.46
1:A:462:G:O2'	1:A:463:U:O5'	2.31	0.46
1:A:1163:A:H2'	1:A:1164:G:C8	2.51	0.46
1:A:1463:U:H2'	1:A:1464:U:C6	2.50	0.46
22:a:1050:A:H2'	22:a:1051:G:C8	2.49	0.46
22:a:1410:G:H2'	22:a:1411:U:C6	2.50	0.46
22:a:2698:U:H2'	22:a:2699:C:C6	2.50	0.46
40:r:20:VAL:HG11	40:r:44:ALA:HA	1.96	0.46
57:5:2:G:H2'	57:5:3:G:H8	1.81	0.46
1:A:1414:U:H2'	1:A:1415:G:H8	1.80	0.46
22:a:18:U:H2'	22:a:19:A:C8	2.50	0.46
22:a:274:C:H2'	22:a:275:C:O4'	2.15	0.46
22:a:1179:G:H2'	22:a:1180:U:C6	2.51	0.46
22:a:1755:A:N6	22:a:2694:G:O2'	2.48	0.46
22:a:2408:U:H2'	22:a:2409:G:C8	2.51	0.46
22:a:2477:U:O2	53:3:4:ARG:NH1	2.47	0.46
22:a:2687:U:H2'	22:a:2688:G:O4'	2.15	0.46
25:c:78:VAL:HA	25:c:94:VAL:HG12	1.96	0.46
30:h:90:LEU:HD11	30:h:146:VAL:HG11	1.98	0.46
57:5:3:G:H1	57:5:70:U:H3	1.63	0.46
1:A:1095:U:H2'	1:A:1096:C:C6	2.51	0.46
6:F:63:ASN:HD22	6:F:96:VAL:HB	1.79	0.46
8:H:114:ARG:O	8:H:118:GLN:HG2	2.16	0.46
22:a:1336:A:H2'	22:a:1337:G:C8	2.50	0.46
22:a:1683:U:H2'	22:a:1684:G:C8	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2898:U:H2'	22:a:2899:A:C8	2.51	0.46
27:e:27:LEU:HD11	27:e:100:MET:HB3	1.97	0.46
29:g:107:LEU:O	29:g:152:ARG:NH2	2.45	0.46
1:A:1175:G:H2'	1:A:1176:A:H8	1.79	0.46
1:A:1241:G:OP1	7:G:35:LYS:NZ	2.45	0.46
1:A:1319:A:C8	1:A:1323:G:C5	3.03	0.46
5:E:13:GLU:HG2	5:E:39:VAL:HG12	1.96	0.46
8:H:49:PHE:HB2	8:H:59:LEU:HD11	1.96	0.46
22:a:6:A:H2'	22:a:7:G:C8	2.50	0.46
22:a:24:G:O2'	40:r:78:GLU:O	2.29	0.46
22:a:651:G:H5'	52:2:19:LYS:HG3	1.97	0.46
22:a:1412:U:H2'	22:a:1413:A:C8	2.50	0.46
22:a:1442:U:H2'	22:a:1443:U:H6	1.81	0.46
22:a:1819:A:H5''	25:c:160:THR:HG21	1.97	0.46
22:a:1853:A:H2'	22:a:1854:A:C8	2.50	0.46
22:a:2116:G:H2'	22:a:2117:A:C5	2.50	0.46
22:a:2216:G:H2'	22:a:2217:G:H8	1.80	0.46
1:A:613:C:H2'	1:A:614:C:C6	2.50	0.46
1:A:946:A:H2'	1:A:947:G:H8	1.79	0.46
1:A:1239:A:H62	1:A:1299:A:N6	2.13	0.46
22:a:279:A:C2	22:a:362:A:H4'	2.51	0.46
22:a:1794:A:H2'	22:a:1795:C:H6	1.80	0.46
22:a:2215:C:H2'	22:a:2216:G:C8	2.50	0.46
24:7:53:ARG:HB3	57:5:62:C:H4'	1.97	0.46
40:r:72:THR:HG21	40:r:108:SER:HB3	1.96	0.46
1:A:677:U:H3	1:A:713:G:H22	1.64	0.46
22:a:64:A:H2'	22:a:65:U:H6	1.80	0.46
22:a:1499:C:C2	22:a:1500:G:C8	3.04	0.46
22:a:1709:U:H2'	22:a:1710:G:H8	1.80	0.46
22:a:2756:U:OP2	53:3:19:ARG:NE	2.48	0.46
22:a:2849:U:H4'	22:a:2868:A:C2	2.51	0.46
30:h:4:ILE:HG12	30:h:18:GLN:HG2	1.97	0.46
52:2:62:LEU:HB3	52:2:65:ALA:HB2	1.98	0.46
57:5:70:U:H2'	57:5:71:C:H6	1.77	0.46
1:A:600:A:H2'	1:A:601:G:H8	1.81	0.46
1:A:634:C:H2'	1:A:635:A:C8	2.51	0.46
1:A:1002:G:H2'	1:A:1003:G:O4'	2.15	0.46
1:A:1327:C:H2'	1:A:1328:C:C6	2.51	0.46
22:a:843:G:H2'	22:a:844:A:C8	2.50	0.46
22:a:1013:C:H2'	22:a:1014:A:C8	2.51	0.46
22:a:1197:G:H2'	22:a:1198:U:H6	1.81	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1224:U:H2'	22:a:1225:G:C8	2.51	0.46
22:a:1353:A:H2'	22:a:1354:A:H8	1.81	0.46
22:a:1534:U:H4'	22:a:1535:A:C8	2.51	0.46
22:a:2233:U:H2'	22:a:2234:G:H8	1.80	0.46
23:b:60:C:H2'	23:b:61:G:H8	1.80	0.46
46:x:39:GLN:HB3	46:x:41:HIS:CE1	2.50	0.46
1:A:236:A:H2'	1:A:237:G:H8	1.81	0.46
1:A:470:C:H2'	1:A:471:U:C6	2.50	0.46
1:A:672:U:H2'	1:A:673:A:H8	1.81	0.46
1:A:1060:U:OP1	14:N:85:ARG:NH2	2.46	0.46
1:A:1363:A:O2'	1:A:1365:G:N7	2.38	0.46
22:a:20:C:H2'	22:a:21:A:C8	2.51	0.46
22:a:608:A:H2'	22:a:609:A:C8	2.51	0.46
22:a:710:U:H2'	22:a:711:G:H8	1.80	0.46
22:a:1703:G:H2'	22:a:1704:C:C6	2.51	0.46
22:a:2557:G:H2'	22:a:2558:C:C6	2.51	0.46
23:b:49:C:H2'	23:b:50:A:H8	1.81	0.46
34:l:76:LYS:NZ	34:l:85:GLY:O	2.47	0.46
57:5:66:U:H2'	57:5:67:A:C8	2.50	0.46
1:A:235:C:H2'	1:A:236:A:C8	2.50	0.46
1:A:1147:C:H2'	1:A:1148:U:C6	2.51	0.46
9:I:54:LEU:HD23	9:I:98:LEU:HD23	1.98	0.46
12:L:44:LYS:HA	12:L:46:ASN:H	1.81	0.46
22:a:363:G:H2'	22:a:364:C:C6	2.51	0.46
22:a:796:C:H2'	22:a:797:G:C8	2.51	0.46
22:a:922:C:O2'	44:v:29:GLU:OE2	2.33	0.46
22:a:1856:U:H2'	22:a:1857:G:O4'	2.16	0.46
22:a:2375:G:N2	22:a:2378:A:OP2	2.34	0.46
22:a:2836:U:H2'	22:a:2837:A:C8	2.51	0.46
23:b:30:C:H1'	23:b:57:A:H61	1.81	0.46
26:d:35:THR:HG22	26:d:73:VAL:HG21	1.98	0.46
31:i:9:GLU:HG2	31:i:10:THR:HG23	1.97	0.46
31:i:76:HIS:CE1	31:i:85:LYS:HB2	2.50	0.46
56:Z:22:G:H2'	56:Z:23:A:C8	2.50	0.46
1:A:845:A:H2'	1:A:846:G:O4'	2.16	0.45
15:O:36:ILE:O	15:O:40:GLN:HG2	2.16	0.45
22:a:191:A:H2'	22:a:192:C:C6	2.51	0.45
22:a:1360:G:N7	22:a:1361:G:C8	2.84	0.45
22:a:2187:U:H2'	22:a:2188:U:H6	1.80	0.45
22:a:2273:A:H2'	22:a:2274:A:C8	2.52	0.45
24:7:23:ILE:HD12	24:7:23:ILE:H	1.81	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:C:H2'	1:A:581:G:O4'	2.17	0.45
1:A:769:G:H4'	1:A:1513:A:H4'	1.97	0.45
1:A:821:G:H2'	1:A:822:U:C6	2.52	0.45
1:A:953:G:H2'	1:A:954:G:O4'	2.15	0.45
1:A:1225:A:H2'	1:A:1225:A:N3	2.31	0.45
22:a:935:C:H2'	22:a:936:A:H8	1.82	0.45
22:a:1409:U:H2'	22:a:1410:G:H8	1.81	0.45
22:a:1447:C:H2'	22:a:1448:G:H8	1.81	0.45
22:a:1530:G:H2'	22:a:1531:C:C6	2.51	0.45
22:a:1571:A:H2'	22:a:1572:A:C8	2.51	0.45
24:7:4:LEU:O	24:7:9:ARG:NH2	2.49	0.45
55:Y:2:G:H2'	55:Y:3:G:H8	1.80	0.45
1:A:76:G:H2'	1:A:77:A:C8	2.52	0.45
1:A:524:G:H2'	1:A:525:C:C6	2.50	0.45
1:A:529:G:H5'	1:A:530:G:OP2	2.16	0.45
22:a:18:U:H2'	22:a:19:A:H8	1.81	0.45
22:a:742:A:H2'	22:a:743:A:H8	1.81	0.45
22:a:1447:C:O2'	22:a:1544:A:N3	2.41	0.45
22:a:2364:C:H2'	22:a:2365:G:O4'	2.15	0.45
23:b:42:C:C5	28:f:66:LEU:HD22	2.52	0.45
30:h:95:GLY:N	30:h:98:ASP:OD2	2.48	0.45
1:A:1029:U:C4	1:A:1031:C:H1'	2.51	0.45
1:A:1410:A:H2'	1:A:1411:C:C6	2.51	0.45
22:a:1874:C:H2'	22:a:1875:G:O4'	2.16	0.45
22:a:2312:U:H5'	28:f:85:ILE:HD11	1.98	0.45
22:a:2329:U:H2'	22:a:2330:G:H8	1.80	0.45
24:7:23:ILE:HD13	24:7:186:LYS:HE3	1.99	0.45
29:g:10:VAL:HA	29:g:49:THR:HG22	1.98	0.45
29:g:89:LEU:HD22	29:g:162:VAL:HG22	1.96	0.45
32:j:105:ARG:HG2	32:j:122:VAL:HG12	1.99	0.45
42:t:49:VAL:HB	42:t:54:GLN:HB2	1.97	0.45
55:Y:4:C:H2'	55:Y:5:G:H8	1.81	0.45
1:A:126:G:OP1	1:A:605:U:O2'	2.26	0.45
1:A:144:G:H2'	1:A:145:G:C8	2.51	0.45
1:A:390:U:H2'	1:A:391:G:H8	1.80	0.45
1:A:1130:A:H2'	1:A:1131:G:O4'	2.17	0.45
14:N:10:GLU:HG3	14:N:63:ARG:HD2	1.99	0.45
22:a:48:G:N1	22:a:177:G:OP2	2.48	0.45
22:a:228:C:N4	22:a:2407:A:N3	2.64	0.45
22:a:969:G:H2'	22:a:970:U:C6	2.51	0.45
22:a:1645:G:H5''	22:a:1646:C:H5'	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2000:C:OP1	35:m:5:LYS:NZ	2.43	0.45
22:a:2460:U:C2	22:a:2461:A:C8	3.04	0.45
22:a:2783:U:H2'	22:a:2784:U:H6	1.81	0.45
23:b:32:U:C2	23:b:33:G:C8	3.04	0.45
24:7:44:VAL:HG22	24:7:214:ILE:HG12	1.98	0.45
28:f:114:PHE:HE1	28:f:117:LEU:HG	1.82	0.45
35:m:36:THR:OG1	35:m:37:THR:N	2.50	0.45
37:o:32:VAL:HG12	37:o:34:GLU:HG3	1.99	0.45
40:r:2:GLU:HG2	40:r:108:SER:HB2	1.97	0.45
54:X:24:A:C2'	54:X:25:C:H5'	2.46	0.45
55:Y:2:G:H2'	55:Y:3:G:C8	2.52	0.45
1:A:911:U:H2'	1:A:912:C:C6	2.52	0.45
1:A:1009:U:H3	1:A:1020:G:H1	1.65	0.45
1:A:1326:U:H2'	1:A:1327:C:C6	2.52	0.45
13:M:33:ILE:HG23	13:M:59:GLU:HB2	1.97	0.45
22:a:682:G:H5'	51:1:26:ASN:CG	2.41	0.45
22:a:1435:G:H2'	22:a:1436:G:C8	2.51	0.45
22:a:1536:C:H4'	22:a:1537:G:C4	2.52	0.45
22:a:1754:A:O3'	37:o:103:ARG:NH2	2.47	0.45
22:a:2377:A:H2'	22:a:2378:A:C8	2.51	0.45
57:5:37:A:H2'	57:5:38:C:O4'	2.17	0.45
1:A:768:A:H4'	1:A:1523:G:N2	2.31	0.45
1:A:908:A:H2'	1:A:909:A:H8	1.82	0.45
1:A:1397:C:P	5:E:29:ARG:HH22	2.40	0.45
12:L:50:ARG:HB3	12:L:66:TYR:HE1	1.82	0.45
22:a:372:G:O2'	22:a:400:G:O6	2.26	0.45
22:a:572:A:OP2	39:q:80:ARG:NH1	2.47	0.45
22:a:1704:C:H2'	22:a:1705:A:H8	1.81	0.45
22:a:1880:U:H2'	22:a:1881:C:C6	2.52	0.45
22:a:2096:C:O2'	22:a:2097:A:OP1	2.31	0.45
1:A:322:C:H2'	1:A:323:U:C6	2.52	0.45
1:A:1352:C:H2'	1:A:1353:G:C8	2.52	0.45
1:A:1356:G:H2'	1:A:1357:A:H8	1.77	0.45
10:J:6:ILE:HB	10:J:76:ILE:HB	1.99	0.45
22:a:171:U:H2'	22:a:172:A:C8	2.52	0.45
22:a:285:G:C6	22:a:356:G:C6	3.04	0.45
22:a:363:G:H2'	22:a:364:C:H6	1.82	0.45
22:a:729:G:OP1	25:c:13:ARG:HG2	2.17	0.45
22:a:1407:G:H2'	22:a:1408:G:H8	1.81	0.45
22:a:2215:C:H2'	22:a:2216:G:H8	1.81	0.45
22:a:2359:C:H2'	22:a:2360:G:C8	2.52	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:c:157:SER:O	25:c:160:THR:OG1	2.29	0.45
30:h:69:ALA:HB2	30:h:138:VAL:HG13	1.99	0.45
33:k:108:ALA:HB3	33:k:125:LEU:HD22	1.98	0.45
20:T:39:ILE:HA	20:T:86:LEU:HD11	1.99	0.45
22:a:848:C:H2'	22:a:849:A:C8	2.51	0.45
22:a:1490:A:O2'	22:a:1491:G:H5'	2.17	0.45
22:a:2151:U:H2'	22:a:2152:G:H8	1.80	0.45
22:a:2649:C:H2'	22:a:2650:U:H6	1.81	0.45
22:a:2855:C:H2'	22:a:2856:A:H8	1.82	0.45
1:A:1123:U:O2'	1:A:1124:G:H5'	2.16	0.45
1:A:1386:G:H2'	1:A:1387:G:H8	1.80	0.45
6:F:12:PRO:O	6:F:44:ARG:NH2	2.50	0.45
13:M:88:GLY:O	13:M:92:ARG:HG3	2.17	0.45
22:a:1505:A:H2'	22:a:1506:U:C6	2.51	0.45
22:a:2123:G:H2'	22:a:2124:G:C8	2.52	0.45
32:j:107:LEU:HB2	32:j:116:ILE:HD11	1.98	0.45
1:A:1238:A:N7	1:A:1303:C:H1'	2.32	0.44
1:A:1255:G:O2'	1:A:1258:G:N3	2.45	0.44
7:G:56:LYS:HE2	7:G:56:LYS:HB2	1.89	0.44
22:a:630:G:N2	22:a:633:A:OP2	2.38	0.44
22:a:667:U:H2'	22:a:668:A:O4'	2.17	0.44
22:a:1027:A:C2	22:a:2488:G:H5'	2.52	0.44
22:a:1530:G:H2'	22:a:1531:C:H6	1.82	0.44
22:a:1532:A:C6	22:a:1540:G:C6	3.05	0.44
22:a:1532:A:H2'	22:a:1533:C:H6	1.83	0.44
22:a:2190:G:H2'	22:a:2191:A:C8	2.52	0.44
23:b:41:G:H5''	28:f:66:LEU:HD13	1.99	0.44
24:7:194:VAL:HG13	24:7:233:VAL:HG22	2.00	0.44
1:A:264:C:O2'	17:Q:66:PRO:O	2.35	0.44
1:A:500:G:H2'	1:A:501:C:C6	2.51	0.44
1:A:1014:A:C2	1:A:1219:A:H1'	2.53	0.44
1:A:1141:C:H2'	1:A:1142:G:H8	1.83	0.44
22:a:297:G:H2'	22:a:298:G:O4'	2.18	0.44
22:a:882:G:N2	22:a:896:A:OP1	2.50	0.44
22:a:1873:G:H2'	22:a:1874:C:H6	1.80	0.44
22:a:2489:U:H2'	22:a:2490:G:O4'	2.17	0.44
35:m:44:LEU:HD23	35:m:113:ILE:HD13	1.98	0.44
49:z:52:ARG:CZ	49:z:54:VAL:HG12	2.47	0.44
55:Y:19:G:O2'	55:Y:58:G:N2	2.47	0.44
1:A:1121:U:H2'	1:A:1122:U:H6	1.82	0.44
4:D:107:PHE:CG	4:D:145:ILE:HD11	2.52	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1469:A:H2'	22:a:1470:A:C8	2.53	0.44
22:a:1747:U:H2'	22:a:1748:C:C6	2.53	0.44
22:a:1923:U:H2'	22:a:1924:C:C6	2.51	0.44
22:a:2194:U:H2'	22:a:2195:U:H6	1.81	0.44
22:a:2345:G:N3	22:a:2381:A:H2'	2.31	0.44
22:a:2837:A:H2'	22:a:2838:G:H8	1.81	0.44
22:a:2854:G:H2'	22:a:2855:C:H6	1.82	0.44
24:7:30:LEU:HB3	24:7:216:THR:HG23	1.99	0.44
55:Y:26:C:N3	55:Y:27:A:C8	2.85	0.44
1:A:399:G:H2'	1:A:400:C:C6	2.53	0.44
1:A:592:G:H2'	1:A:593:U:H6	1.82	0.44
1:A:592:G:H2'	1:A:593:U:C6	2.52	0.44
1:A:1010:U:H2'	1:A:1011:C:H6	1.83	0.44
1:A:1319:A:C8	1:A:1323:G:C6	3.06	0.44
4:D:202:GLU:OE1	5:E:112:ARG:NH1	2.50	0.44
7:G:26:PHE:HZ	7:G:120:LEU:HD11	1.82	0.44
11:K:94:GLU:HG3	21:U:16:LEU:HD21	1.99	0.44
19:S:3:ARG:HH11	19:S:10:PHE:HB2	1.82	0.44
22:a:282:A:N6	22:a:359:G:O6	2.50	0.44
22:a:366:C:C2	22:a:367:G:C8	3.05	0.44
22:a:1019:U:O2'	22:a:1021:A:N7	2.44	0.44
22:a:2154:A:H2'	22:a:2155:U:O4'	2.16	0.44
22:a:2255:G:N2	44:v:8:GLY:O	2.50	0.44
22:a:2895:G:H2'	22:a:2896:C:C6	2.53	0.44
35:m:56:LYS:NZ	35:m:90:ARG:O	2.48	0.44
40:r:4:ILE:HG12	40:r:106:VAL:HG22	2.00	0.44
1:A:90:C:H2'	1:A:91:U:C6	2.53	0.44
1:A:358:U:H2'	1:A:359:G:C8	2.53	0.44
1:A:599:C:H2'	1:A:600:A:H8	1.82	0.44
1:A:757:U:OP1	1:A:822:U:O2'	2.32	0.44
1:A:918:A:H2'	1:A:919:A:C8	2.53	0.44
1:A:1064:G:H21	1:A:1190:G:H1'	1.82	0.44
1:A:1147:C:H4'	9:I:7:TYR:CE2	2.53	0.44
1:A:1171:A:H2'	1:A:1172:C:C6	2.51	0.44
1:A:1236:A:H2'	1:A:1237:C:C6	2.52	0.44
1:A:1250:A:H2'	1:A:1251:A:C8	2.52	0.44
4:D:65:TYR:OH	4:D:95:GLU:OE2	2.32	0.44
11:K:64:GLN:HG3	11:K:99:ALA:HB2	1.98	0.44
22:a:128:C:H2'	22:a:129:C:H6	1.83	0.44
22:a:146:A:H2'	22:a:147:C:C6	2.53	0.44
22:a:155:A:H2'	22:a:156:A:H8	1.82	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:177:G:H3'	22:a:178:G:H8	1.82	0.44
22:a:181:A:H2'	22:a:182:A:H8	1.83	0.44
22:a:320:A:H4'	22:a:322:A:N7	2.32	0.44
22:a:391:A:H1'	22:a:411:G:O4'	2.18	0.44
22:a:639:U:H2'	22:a:640:C:H6	1.80	0.44
22:a:2095:A:H5''	30:h:11:ASN:HD22	1.82	0.44
40:r:24:ILE:HD13	40:r:36:LEU:HD11	2.00	0.44
56:Z:66:U:H2'	56:Z:67:U:C6	2.51	0.44
1:A:268:U:H2'	1:A:269:C:H6	1.83	0.44
1:A:1330:U:C4	1:A:1331:G:C6	3.06	0.44
22:a:825:A:H4'	22:a:2428:G:C5	2.52	0.44
22:a:1747:U:H2'	22:a:1748:C:H6	1.83	0.44
22:a:2327:A:H2'	22:a:2328:A:C8	2.53	0.44
22:a:2677:G:H2'	22:a:2678:C:C6	2.53	0.44
36:n:12:THR:O	36:n:16:ARG:HG2	2.18	0.44
56:Z:68:C:H2'	56:Z:69:C:H6	1.83	0.44
57:5:36:C:H2'	57:5:37:A:O4'	2.17	0.44
1:A:335:C:C2	1:A:336:A:C8	3.06	0.44
22:a:364:C:H2'	22:a:365:U:C6	2.53	0.44
22:a:1361:G:H2'	22:a:1362:C:H6	1.83	0.44
22:a:2162:G:C4	22:a:2163:A:C8	3.06	0.44
23:b:40:U:N3	23:b:44:G:OP2	2.42	0.44
1:A:212:G:C4	1:A:213:G:C8	3.05	0.44
1:A:398:U:H2'	1:A:399:G:H8	1.83	0.44
1:A:745:G:C2	1:A:746:A:C5	3.06	0.44
1:A:976:G:OP2	1:A:1358:U:O2'	2.36	0.44
1:A:1399:C:O2	1:A:1502:A:N6	2.51	0.44
3:C:14:ILE:HG22	3:C:15:VAL:HG13	2.00	0.44
4:D:125:VAL:HG22	4:D:143:VAL:HG22	1.99	0.44
8:H:43:GLU:HG3	8:H:101:ILE:HD13	1.99	0.44
22:a:197:A:N6	22:a:2430:A:H2'	2.33	0.44
22:a:302:C:H2'	22:a:303:G:H8	1.82	0.44
22:a:543:G:H2'	22:a:544:C:C6	2.53	0.44
22:a:851:C:H2'	22:a:852:U:H6	1.83	0.44
22:a:884:U:H2'	22:a:885:C:C6	2.53	0.44
22:a:1398:C:C2	22:a:1399:C:C5	3.06	0.44
22:a:1771:C:H2'	22:a:1772:A:H8	1.82	0.44
22:a:2011:U:H2'	22:a:2012:G:O4'	2.18	0.44
22:a:2230:G:H2'	22:a:2231:U:C6	2.52	0.44
26:d:114:LYS:HE3	26:d:196:ALA:HB2	1.98	0.44
22:a:541:A:H2'	22:a:542:C:C6	2.53	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2008:C:H2'	22:a:2009:A:H8	1.83	0.44
22:a:2196:C:H2'	22:a:2197:U:C6	2.53	0.44
22:a:2247:A:H2'	22:a:2248:C:H6	1.83	0.44
49:z:43:ILE:HG22	49:z:49:TYR:HB2	2.00	0.44
1:A:562:U:H1'	12:L:12:ARG:HD2	1.99	0.43
1:A:792:A:H1'	1:A:794:A:N7	2.32	0.43
2:B:57:LEU:HD13	2:B:217:VAL:HG13	1.99	0.43
22:a:364:C:H2'	22:a:365:U:H6	1.82	0.43
22:a:858:G:N3	22:a:2268:A:H2'	2.33	0.43
22:a:935:C:H2'	22:a:936:A:C8	2.53	0.43
22:a:1048:A:C8	22:a:1111:A:C6	3.06	0.43
22:a:1532:A:H2'	22:a:1533:C:C6	2.53	0.43
22:a:2039:U:H2'	22:a:2040:G:C8	2.53	0.43
22:a:2385:C:H2'	22:a:2386:A:C8	2.53	0.43
22:a:2533:U:H2'	22:a:2534:A:O4'	2.18	0.43
23:b:29:A:H2'	23:b:30:C:O4'	2.17	0.43
27:e:58:LYS:NZ	27:e:70:SER:O	2.46	0.43
52:2:26:HIS:NE2	52:2:48:ALA:HB2	2.33	0.43
57:5:10:G:N2	57:5:26:G:H1'	2.32	0.43
1:A:521:G:O2'	1:A:536:C:O2'	2.33	0.43
22:a:223:A:N1	22:a:407:G:O2'	2.48	0.43
22:a:1435:G:H2'	22:a:1436:G:H8	1.83	0.43
22:a:2097:A:H2'	22:a:2098:U:H6	1.83	0.43
22:a:2615:U:C2	49:z:4:GLN:HA	2.53	0.43
23:b:2:G:HO2'	23:b:3:C:P	2.38	0.43
28:f:5:HIS:CE1	28:f:9:LYS:HE3	2.53	0.43
28:f:36:LEU:HD22	28:f:154:ILE:HG12	2.00	0.43
1:A:608:A:H2'	1:A:609:A:O4'	2.19	0.43
1:A:632:U:H5''	1:A:633:G:C8	2.53	0.43
1:A:859:G:OP2	1:A:869:G:N1	2.32	0.43
1:A:1063:C:OP2	1:A:1064:G:O2'	2.35	0.43
1:A:1228:C:H1'	13:M:116:ILE:HD11	1.99	0.43
22:a:743:A:O2'	22:a:1659:G:OP1	2.36	0.43
22:a:1019:U:H2'	22:a:1020:A:C8	2.53	0.43
22:a:1196:C:C2	22:a:1197:G:C8	3.06	0.43
22:a:2086:U:H2'	22:a:2087:G:H8	1.83	0.43
22:a:2473:U:O2	22:a:2473:U:H2'	2.17	0.43
27:e:165:HIS:CD2	27:e:166:LYS:HG3	2.53	0.43
1:A:91:U:H2'	1:A:92:U:C6	2.53	0.43
1:A:161:A:H2'	1:A:162:A:C8	2.53	0.43
1:A:360:G:H2'	1:A:361:G:C8	2.53	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:G:O2'	1:A:463:U:H6	2.00	0.43
1:A:923:A:H2'	1:A:924:C:C6	2.54	0.43
1:A:1073:U:C2	1:A:1074:G:C8	3.06	0.43
1:A:1312:G:H2'	1:A:1313:U:C6	2.53	0.43
1:A:1330:U:H2'	1:A:1331:G:O4'	2.18	0.43
7:G:27:VAL:HG22	7:G:43:VAL:HG21	1.99	0.43
11:K:47:ALA:HB1	11:K:62:ALA:HB1	2.00	0.43
22:a:150:U:H2'	22:a:151:C:C6	2.53	0.43
22:a:967:U:H2'	22:a:968:C:C6	2.52	0.43
22:a:1028:A:N6	22:a:1125:G:H2'	2.33	0.43
22:a:1709:U:H2'	22:a:1710:G:C8	2.54	0.43
22:a:2100:G:C6	22:a:2190:G:C6	3.06	0.43
22:a:2287:A:OP1	50:0:30:LYS:NZ	2.52	0.43
42:t:4:LYS:O	42:t:94:ARG:NH1	2.51	0.43
1:A:371:A:H2'	1:A:372:C:O4'	2.18	0.43
1:A:676:A:H2'	1:A:677:U:H6	1.82	0.43
1:A:1377:A:C6	7:G:7:ILE:HG21	2.53	0.43
4:D:73:ARG:HG3	4:D:77:LYS:HE3	1.99	0.43
7:G:84:THR:OG1	57:5:34:CM0:O8	2.25	0.43
22:a:181:A:H2'	22:a:182:A:C8	2.52	0.43
22:a:400:G:N7	45:w:57:ARG:NH2	2.64	0.43
22:a:721:A:H2'	22:a:722:A:H8	1.81	0.43
22:a:2149:U:H2'	22:a:2150:C:C6	2.53	0.43
23:b:19:C:H2'	23:b:20:G:H8	1.82	0.43
23:b:48:U:P	36:n:30:ARG:HH22	2.41	0.43
26:d:121:THR:HB	26:d:127:PHE:CD2	2.53	0.43
1:A:593:U:H2'	1:A:594:U:H6	1.83	0.43
9:I:18:ARG:NH1	9:I:66:THR:OG1	2.47	0.43
18:R:21:ILE:HD13	18:R:55:LEU:HG	2.01	0.43
22:a:500:G:N1	22:a:503:A:OP2	2.48	0.43
22:a:546:U:H5'	22:a:547:A:N3	2.33	0.43
22:a:1462:C:O2'	22:a:2702:G:O2'	2.32	0.43
28:f:34:ILE:HG12	28:f:156:ILE:HG12	1.99	0.43
1:A:309:A:H2'	1:A:310:G:H8	1.84	0.43
1:A:334:C:H2'	1:A:335:C:H6	1.83	0.43
1:A:579:A:H2'	1:A:580:C:C6	2.53	0.43
1:A:964:A:H2	1:A:969:A:N3	2.16	0.43
5:E:164:ILE:O	8:H:114:ARG:NH2	2.51	0.43
22:a:78:U:H2'	22:a:79:C:C6	2.53	0.43
22:a:438:G:H2'	22:a:439:A:C8	2.54	0.43
22:a:534:U:O2'	38:p:49:ASP:OD2	2.34	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:689:A:H2'	22:a:690:G:C8	2.53	0.43
22:a:709:U:H2'	22:a:710:U:C6	2.54	0.43
22:a:2037:A:H2'	22:a:2038:G:C8	2.54	0.43
22:a:2163:A:N3	22:a:2163:A:H2'	2.34	0.43
22:a:2266:A:H4'	22:a:2267:A:N3	2.34	0.43
22:a:2292:U:H2'	22:a:2293:G:C8	2.54	0.43
22:a:2375:G:N2	22:a:2377:A:H3'	2.32	0.43
22:a:2780:G:OP2	31:i:120:ARG:HD3	2.19	0.43
24:7:65:LEU:HD12	24:7:69:THR:HG22	2.00	0.43
32:j:10:VAL:HG13	32:j:86:LEU:HD13	2.00	0.43
44:v:50:ASN:HB2	44:v:82:ILE:HB	2.00	0.43
55:Y:5:G:H2'	55:Y:6:A:H8	1.84	0.43
56:Z:66:U:H2'	56:Z:67:U:H6	1.83	0.43
1:A:412:A:O2'	1:A:414:A:H5'	2.18	0.43
1:A:1005:A:C2	1:A:1006:G:H1'	2.54	0.43
1:A:1130:A:C2	1:A:1146:A:C6	3.07	0.43
1:A:1171:A:H2'	1:A:1172:C:H6	1.84	0.43
1:A:1366:C:O2'	10:J:62:ARG:NH1	2.51	0.43
1:A:1458:G:OP1	20:T:30:THR:OG1	2.27	0.43
1:A:1516:2MG:H2'	1:A:1518:MA6:OP2	2.19	0.43
22:a:1597:A:H5''	22:a:1598:A:H5'	1.99	0.43
22:a:2615:U:H2'	22:a:2616:C:H6	1.83	0.43
22:a:2841:C:H2'	22:a:2842:G:C8	2.54	0.43
55:Y:21:H2U:H2'	55:Y:21:H2U:H62	1.72	0.43
1:A:554:A:H2'	1:A:555:U:C6	2.54	0.43
22:a:355:U:H2'	22:a:356:G:H8	1.84	0.43
22:a:754:U:H2'	22:a:755:U:C6	2.53	0.43
22:a:1223:G:N2	22:a:1226:A:OP2	2.44	0.43
22:a:1844:C:H2'	22:a:1845:G:H8	1.84	0.43
22:a:2038:G:H2'	22:a:2039:U:O4'	2.19	0.43
22:a:2290:G:H2'	22:a:2291:U:C6	2.54	0.43
22:a:2756:U:H1'	22:a:2757:A:H5''	2.00	0.43
23:b:27:C:OP1	36:n:34:HIS:NE2	2.47	0.43
1:A:299:G:H2'	1:A:300:A:C8	2.54	0.43
1:A:486:U:H2'	1:A:487:A:H8	1.84	0.43
1:A:1070:U:H2'	1:A:1071:C:C6	2.54	0.43
22:a:1281:G:H2'	22:a:1282:U:C6	2.54	0.43
22:a:2700:A:H2'	22:a:2701:U:C6	2.54	0.43
31:i:131:ASN:N	31:i:131:ASN:OD1	2.52	0.43
44:v:59:LEU:HD12	44:v:80:ILE:HD12	2.00	0.43
1:A:329:A:O2'	1:A:332:G:N7	2.46	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:704:A:C4	1:A:705:G:C8	3.07	0.42
1:A:1294:G:H2'	1:A:1295:U:C6	2.54	0.42
2:B:186:ILE:HD13	2:B:200:ILE:HB	2.01	0.42
22:a:3:U:H2'	22:a:4:U:C6	2.54	0.42
22:a:30:G:O2'	22:a:1214:A:N3	2.44	0.42
22:a:357:C:H2'	22:a:358:U:C6	2.54	0.42
22:a:1198:U:H2'	22:a:1199:U:H6	1.83	0.42
22:a:1641:A:H2'	22:a:1642:G:O4'	2.18	0.42
22:a:2169:A:H2'	22:a:2170:A:C8	2.54	0.42
22:a:2794:C:H2'	22:a:2795:C:C6	2.54	0.42
28:f:119:ALA:O	28:f:167:ARG:NH1	2.52	0.42
30:h:75:LEU:HD23	30:h:75:LEU:HA	1.88	0.42
1:A:17:U:H2'	1:A:18:C:H6	1.81	0.42
1:A:1236:A:H4'	1:A:1304:G:H4'	2.01	0.42
1:A:1312:G:H2'	1:A:1313:U:H6	1.83	0.42
1:A:1425:U:H2'	1:A:1426:G:H8	1.84	0.42
3:C:50:ALA:O	3:C:70:THR:OG1	2.33	0.42
3:C:186:THR:HG22	3:C:199:LYS:HG2	2.01	0.42
9:I:7:TYR:HE1	9:I:18:ARG:HB3	1.84	0.42
22:a:586:A:N1	22:a:809:G:O2'	2.48	0.42
22:a:644:A:H2'	22:a:645:C:O4'	2.19	0.42
22:a:686:U:H6	22:a:788:A:N1	2.17	0.42
22:a:1515:A:H3'	22:a:1516:G:H8	1.83	0.42
22:a:2636:C:H2'	22:a:2637:U:C6	2.54	0.42
22:a:2896:C:H2'	22:a:2897:U:C6	2.54	0.42
34:l:53:MET:HE1	34:l:103:TYR:CD1	2.55	0.42
36:n:49:VAL:HG21	36:n:82:ALA:HA	2.01	0.42
1:A:320:A:H2'	1:A:321:A:C8	2.55	0.42
1:A:389:A:H3'	1:A:390:U:H6	1.84	0.42
2:B:118:GLU:O	2:B:122:GLN:HG2	2.19	0.42
3:C:47:LEU:HD21	3:C:87:LEU:HD11	2.01	0.42
22:a:1409:U:H2'	22:a:1410:G:C8	2.54	0.42
22:a:1947:C:C2	22:a:1948:G:C8	3.07	0.42
22:a:2115:G:O6	22:a:2117:A:O2'	2.37	0.42
22:a:2250:G:O2'	22:a:2496:C:OP1	2.37	0.42
22:a:2774:C:H2'	22:a:2775:G:O4'	2.18	0.42
22:a:2812:G:H2'	22:a:2813:A:H8	1.83	0.42
25:c:21:ASN:HB3	25:c:24:LEU:HG	2.01	0.42
26:d:181:ASP:HB3	26:d:186:LEU:HB2	2.01	0.42
55:Y:14:A:H2'	55:Y:15:G:O4'	2.20	0.42
1:A:707:U:H2'	1:A:708:C:H6	1.84	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:821:G:H2'	1:A:822:U:H6	1.84	0.42
1:A:868:C:H2'	1:A:869:G:O4'	2.20	0.42
1:A:1118:U:H2'	1:A:1119:C:C6	2.53	0.42
1:A:1124:G:H3'	10:J:37:ARG:HE	1.84	0.42
1:A:1297:G:H1'	1:A:1298:U:H5	1.84	0.42
1:A:1377:A:O2'	1:A:1379:G:N7	2.52	0.42
7:G:26:PHE:HE2	7:G:120:LEU:HD21	1.85	0.42
8:H:7:ILE:O	8:H:11:LEU:HG	2.20	0.42
10:J:8:ILE:HG12	10:J:100:ILE:HG12	2.02	0.42
17:Q:10:GLY:HA3	17:Q:25:ILE:HD13	2.01	0.42
19:S:11:ILE:HB	19:S:41:PHE:HE1	1.84	0.42
22:a:240:C:OP2	22:a:241:A:O2'	2.36	0.42
22:a:549:G:H2'	22:a:550:C:C6	2.54	0.42
22:a:594:U:H2'	22:a:595:C:C6	2.54	0.42
22:a:1028:A:H2'	22:a:1029:A:C8	2.55	0.42
22:a:1292:G:H2'	22:a:1293:C:C6	2.55	0.42
22:a:2305:U:H2'	22:a:2306:C:C6	2.54	0.42
22:a:2783:U:H2'	22:a:2784:U:C6	2.54	0.42
22:a:2841:C:H2'	22:a:2842:G:H8	1.84	0.42
29:g:17:VAL:HG11	29:g:50:LEU:HD21	2.01	0.42
1:A:999:C:H2'	1:A:1000:A:C8	2.54	0.42
1:A:1107:C:C4	1:A:1108:G:C8	3.07	0.42
13:M:49:SER:O	13:M:53:ILE:HG12	2.19	0.42
19:S:3:ARG:NH2	19:S:7:LYS:HE2	2.34	0.42
22:a:227:A:C2	22:a:2407:A:H1'	2.55	0.42
22:a:687:C:H1'	51:1:4:THR:HG22	2.02	0.42
22:a:807:U:O2'	22:a:2060:A:N1	2.47	0.42
22:a:1954:G:O2'	22:a:1956:U:O4	2.33	0.42
22:a:2076:U:OP2	22:a:2238:G:N2	2.38	0.42
22:a:2514:U:H2'	22:a:2515:C:H6	1.82	0.42
22:a:2838:G:C4	22:a:2839:G:C8	3.07	0.42
32:j:40:LYS:NZ	32:j:89:ASN:OD1	2.53	0.42
45:w:3:ARG:O	45:w:12:PRO:HD3	2.19	0.42
54:X:15:U:H2'	54:X:16:G:C8	2.55	0.42
57:5:37:A:C2	57:5:38:C:H1'	2.54	0.42
1:A:1405:G:H2'	1:A:1406:U:H6	1.84	0.42
1:A:1507:A:H2'	1:A:1508:A:H8	1.85	0.42
22:a:27:G:O2'	22:a:28:A:OP2	2.33	0.42
22:a:303:G:H2'	22:a:304:U:C6	2.54	0.42
22:a:1287:A:H3'	22:a:1288:G:N2	2.35	0.42
22:a:1604:C:H2'	22:a:1605:C:C6	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:2121:G:H2'	22:a:2122:U:C6	2.54	0.42
22:a:2720:U:C2	22:a:2721:A:C8	3.07	0.42
22:a:2847:U:H2'	22:a:2848:G:O4'	2.20	0.42
1:A:297:G:N2	1:A:300:A:OP2	2.38	0.42
1:A:1103:C:O2	2:B:106:THR:HG21	2.20	0.42
1:A:1299:A:N3	1:A:1299:A:H2'	2.35	0.42
1:A:1318:A:O2'	19:S:37:ARG:HD2	2.20	0.42
6:F:42:TRP:HB2	6:F:59:TYR:HB2	2.02	0.42
22:a:635:C:OP2	33:k:109:LYS:NZ	2.49	0.42
22:a:814:C:H1'	22:a:1225:G:N2	2.35	0.42
22:a:1026:G:C2	22:a:1027:A:C8	3.08	0.42
22:a:1182:G:H2'	22:a:1183:U:O4'	2.19	0.42
22:a:1496:A:H2'	22:a:1498:C:C5	2.54	0.42
22:a:2492:U:H2'	22:a:2493:U:C6	2.55	0.42
22:a:2605:PSU:H2'	22:a:2606:C:C6	2.55	0.42
22:a:2740:A:H2'	22:a:2741:A:C8	2.55	0.42
57:5:6:U:O4	57:5:7:A:N6	2.53	0.42
57:5:71:C:H2'	57:5:72:C:H6	1.84	0.42
1:A:736:C:H2'	1:A:737:C:C6	2.54	0.42
22:a:273:G:H2'	22:a:274:C:C6	2.54	0.42
22:a:498:G:O2'	42:t:45:HIS:NE2	2.42	0.42
22:a:1412:U:H2'	22:a:1413:A:H8	1.85	0.42
22:a:1536:C:H4'	22:a:1537:G:N3	2.35	0.42
22:a:2443:C:H2'	22:a:2444:G:H8	1.85	0.42
22:a:2547:A:H5''	22:a:2566:A:C2	2.55	0.42
22:a:2836:U:H2'	22:a:2837:A:H8	1.84	0.42
29:g:52:PHE:CE1	29:g:72:LEU:HD12	2.55	0.42
36:n:83:LEU:HD11	36:n:114:GLY:HA3	2.01	0.42
56:Z:67:U:H2'	56:Z:68:C:H6	1.83	0.42
57:5:62:C:H2'	57:5:63:G:C8	2.55	0.42
1:A:20:U:H2'	1:A:21:G:O4'	2.20	0.42
1:A:207:C:H2'	1:A:208:U:C6	2.54	0.42
1:A:223:A:H2'	1:A:224:U:C6	2.55	0.42
1:A:270:A:H2'	1:A:271:C:H6	1.84	0.42
1:A:1251:A:H2'	1:A:1252:A:C8	2.55	0.42
16:P:40:ASN:HB3	16:P:43:ALA:HB2	2.00	0.42
22:a:499:U:H2'	22:a:500:G:O4'	2.19	0.42
22:a:666:A:H2'	22:a:667:U:C6	2.55	0.42
22:a:1567:G:H3'	25:c:85:PRO:HG3	2.00	0.42
22:a:2820:A:N3	22:a:2820:A:H2'	2.34	0.42
22:a:2898:U:O2	31:i:134:ALA:HB1	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:b:46:A:H5''	36:n:3:LYS:HE2	2.02	0.42
1:A:51:A:N7	1:A:114:U:O2'	2.49	0.42
1:A:428:G:OP2	4:D:7:PRO:HG2	2.20	0.42
1:A:455:G:H2'	1:A:456:A:H8	1.84	0.42
1:A:494:G:O2'	1:A:496:A:H1'	2.19	0.42
1:A:600:A:H2'	1:A:601:G:C8	2.55	0.42
1:A:1096:C:O2	1:A:1170:A:O2'	2.36	0.42
1:A:1241:G:H2'	1:A:1242:G:H8	1.84	0.42
4:D:159:LEU:HD13	4:D:175:ALA:HB1	2.02	0.42
22:a:75:G:H2'	22:a:75:G:N3	2.35	0.42
22:a:588:U:H2'	22:a:589:U:C6	2.55	0.42
22:a:1190:G:H2'	22:a:1191:G:H8	1.85	0.42
22:a:1441:G:H2'	22:a:1442:U:H6	1.85	0.42
22:a:1469:A:H2'	22:a:1470:A:H8	1.85	0.42
22:a:1799:G:OP1	25:c:258:ARG:NH1	2.39	0.42
22:a:2294:G:H5'	36:n:98:GLN:HE22	1.84	0.42
26:d:25:THR:OG1	26:d:191:GLY:O	2.30	0.42
32:j:43:ILE:HD12	32:j:56:ASP:HB2	2.01	0.42
34:l:41:LEU:HG	34:l:96:ILE:HG13	2.02	0.42
37:o:9:GLU:O	37:o:13:MET:HG3	2.20	0.42
1:A:6:G:H4'	1:A:298:A:H4'	2.02	0.41
1:A:160:A:H2'	1:A:161:A:C8	2.54	0.41
1:A:1031:C:H4'	1:A:1032:G:C2	2.55	0.41
1:A:1033:G:C4	1:A:1034:G:C8	3.08	0.41
22:a:491:G:O6	40:r:49:LYS:NZ	2.46	0.41
22:a:753:A:H2'	22:a:754:U:H6	1.85	0.41
22:a:1125:G:OP2	22:a:1126:A:O2'	2.23	0.41
22:a:1190:G:H2'	22:a:1191:G:C8	2.55	0.41
22:a:1327:A:H2'	22:a:1328:A:O4'	2.20	0.41
22:a:2216:G:H2'	22:a:2217:G:C8	2.55	0.41
22:a:2241:A:H2'	22:a:2242:G:H8	1.85	0.41
22:a:2282:G:H4'	22:a:2389:G:O2'	2.20	0.41
22:a:2316:G:C2	22:a:2317:A:C8	3.07	0.41
22:a:2328:A:H2'	22:a:2329:U:H6	1.84	0.41
22:a:2547:A:H4'	32:j:29:HIS:CE1	2.55	0.41
22:a:2590:A:H2'	22:a:2591:C:C6	2.55	0.41
22:a:2649:C:H2'	22:a:2650:U:C6	2.55	0.41
24:7:44:VAL:HG22	24:7:214:ILE:HG23	2.01	0.41
32:j:9:ASN:OD1	32:j:18:ARG:NH1	2.48	0.41
33:k:57:LEU:HD22	52:2:54:ASP:HB3	2.02	0.41
1:A:455:G:H2'	1:A:456:A:C8	2.55	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:A:H2'	1:A:909:A:C8	2.55	0.41
1:A:1329:A:C5	1:A:1330:U:C5	3.08	0.41
19:S:3:ARG:HE	19:S:7:LYS:HB2	1.85	0.41
21:U:18:ARG:HG2	21:U:21:ARG:HH21	1.85	0.41
22:a:640:C:H2'	22:a:641:U:C6	2.55	0.41
22:a:1677:A:H2'	22:a:1678:A:H8	1.84	0.41
22:a:2020:A:H5'	49:z:9:THR:CG2	2.50	0.41
22:a:2794:C:H2'	22:a:2795:C:H6	1.86	0.41
39:q:61:ALA:HB2	39:q:98:ILE:HD13	2.02	0.41
56:Z:5:G:H2'	56:Z:6:A:H8	1.85	0.41
57:5:10:G:N3	57:5:10:G:H2'	2.35	0.41
57:5:27:C:H2'	57:5:28:C:H6	1.85	0.41
1:A:935:A:H2'	1:A:936:C:H6	1.84	0.41
1:A:982:U:H4'	1:A:983:A:O4'	2.21	0.41
1:A:1176:A:H2'	1:A:1177:G:C8	2.55	0.41
1:A:1314:C:OP2	19:S:4:SER:OG	2.29	0.41
1:A:1436:U:H2'	1:A:1437:A:H8	1.85	0.41
8:H:90:ASP:N	8:H:90:ASP:OD1	2.52	0.41
19:S:3:ARG:HH21	19:S:7:LYS:HE2	1.86	0.41
22:a:732:C:H2'	22:a:733:G:O4'	2.20	0.41
22:a:1198:U:C2	22:a:1199:U:C5	3.09	0.41
22:a:1880:U:H2'	22:a:1881:C:H6	1.84	0.41
22:a:2081:U:H2'	22:a:2082:A:H8	1.85	0.41
22:a:2092:U:OP1	22:a:2199:A:O2'	2.32	0.41
22:a:2636:C:H2'	22:a:2637:U:H6	1.85	0.41
57:5:59:U:H2'	57:5:60:C:O4'	2.20	0.41
1:A:171:A:H2'	1:A:172:A:C8	2.55	0.41
22:a:215:G:H4'	22:a:216:A:H4'	2.02	0.41
22:a:819:A:H5''	22:a:973:A:N1	2.36	0.41
22:a:1289:C:C2	22:a:1290:C:C5	3.09	0.41
22:a:2703:C:C2	22:a:2704:C:C5	3.09	0.41
34:l:53:MET:HE1	34:l:103:TYR:CG	2.56	0.41
47:y:10:THR:HG21	47:y:56:LYS:HG3	2.02	0.41
1:A:264:C:H2'	1:A:265:G:O4'	2.21	0.41
1:A:397:A:O2'	1:A:398:U:OP2	2.35	0.41
1:A:537:G:H2'	1:A:538:G:H8	1.86	0.41
1:A:742:G:H5''	15:O:58:ARG:NH2	2.36	0.41
1:A:891:U:H2'	1:A:892:A:H8	1.86	0.41
13:M:27:LYS:HE3	13:M:27:LYS:HB2	1.95	0.41
22:a:1153:C:H5''	38:p:62:ILE:HD13	2.02	0.41
22:a:1219:U:H2'	22:a:1220:G:H8	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:l:110:GLU:O	34:l:114:ARG:HG3	2.20	0.41
42:t:72:ILE:HD13	42:t:103:ILE:HD13	2.01	0.41
58:6:141:TYR:CE2	58:6:143:HIS:HB2	2.56	0.41
1:A:137:U:H3	1:A:226:G:H1	1.69	0.41
1:A:613:C:H2'	1:A:614:C:H6	1.85	0.41
1:A:678:U:H2'	1:A:679:C:C6	2.56	0.41
1:A:1157:A:C2	1:A:1181:G:C4	3.09	0.41
2:B:217:VAL:O	2:B:221:VAL:HG12	2.20	0.41
2:B:223:GLU:O	2:B:227:GLN:HG3	2.21	0.41
4:D:139:PRO:HA	4:D:182:PHE:HD1	1.85	0.41
22:a:279:A:H61	22:a:361:G:H1'	1.86	0.41
22:a:1216:G:OP1	38:p:11:ARG:NH1	2.54	0.41
22:a:1689:A:H2'	22:a:1690:A:C8	2.56	0.41
22:a:1734:G:H2'	22:a:1735:A:H8	1.85	0.41
22:a:2190:G:H2'	22:a:2191:A:H8	1.86	0.41
28:f:43:ALA:HA	28:f:46:ASP:O	2.20	0.41
37:o:51:ARG:CZ	37:o:53:ARG:HG3	2.51	0.41
47:y:47:MET:O	47:y:51:VAL:HG22	2.21	0.41
56:Z:67:U:H2'	56:Z:68:C:C6	2.55	0.41
1:A:553:A:H5''	12:L:21:VAL:HG21	2.02	0.41
1:A:1516:2MG:N2	1:A:1519:MA6:OP2	2.54	0.41
9:I:19:VAL:HG13	9:I:65:ILE:HG12	2.01	0.41
20:T:54:MET:HE3	20:T:54:MET:HB3	1.87	0.41
22:a:729:G:O2'	22:a:763:G:H4'	2.21	0.41
22:a:1429:G:H2'	22:a:1430:G:C8	2.54	0.41
22:a:1433:A:H2'	22:a:1434:A:H8	1.79	0.41
22:a:2160:C:H2'	22:a:2161:C:H6	1.83	0.41
22:a:2167:U:H2'	22:a:2168:G:C8	2.56	0.41
22:a:2313:C:H5''	28:f:88:LYS:HD3	2.02	0.41
22:a:2700:A:H2'	22:a:2701:U:H6	1.86	0.41
22:a:2813:A:H2'	22:a:2814:A:H8	1.85	0.41
30:h:30:LEU:HB3	30:h:36:ALA:HB3	2.01	0.41
43:u:21:ARG:HA	43:u:25:LYS:O	2.20	0.41
49:z:46:ASP:O	49:z:53:LYS:NZ	2.49	0.41
57:5:56:C:H2'	57:5:57:G:C8	2.56	0.41
1:A:89:U:H2'	1:A:90:C:H6	1.85	0.41
1:A:707:U:H2'	1:A:708:C:C6	2.55	0.41
1:A:757:U:H2'	1:A:758:C:O4'	2.21	0.41
3:C:123:GLN:OE1	3:C:136:ARG:NH2	2.50	0.41
4:D:87:GLY:HA3	4:D:197:GLU:HG3	2.02	0.41
10:J:53:ILE:HG12	10:J:61:ALA:O	2.21	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:396:G:OP2	45:w:10:LYS:NZ	2.52	0.41
22:a:1629:U:O2'	22:a:2698:U:OP1	2.33	0.41
22:a:2311:A:H3'	22:a:2312:U:C6	2.56	0.41
22:a:2333:A:OP2	44:v:77:ARG:NH2	2.44	0.41
23:b:40:U:H3'	23:b:41:G:H4'	2.03	0.41
30:h:47:PHE:HE1	30:h:54:LEU:HD12	1.86	0.41
33:k:132:ARG:HG3	33:k:142:ILE:HD12	2.03	0.41
55:Y:76:C:H2'	55:Y:77:A:C8	2.56	0.41
56:Z:61:C:H2'	56:Z:62:U:C6	2.56	0.41
1:A:591:U:H2'	1:A:592:G:C8	2.55	0.41
1:A:593:U:H2'	1:A:594:U:C6	2.56	0.41
1:A:619:U:N3	4:D:131:ASN:OD1	2.49	0.41
1:A:784:A:H2'	1:A:785:G:C8	2.56	0.41
1:A:1157:A:N7	1:A:1180:A:N6	2.68	0.41
1:A:1225:A:H5''	1:A:1226:C:OP2	2.21	0.41
2:B:20:THR:HG22	2:B:39:HIS:CG	2.56	0.41
3:C:6:HIS:CE1	3:C:8:ASN:HB3	2.55	0.41
20:T:35:VAL:HG11	20:T:79:LEU:HD13	2.03	0.41
22:a:332:A:O2'	22:a:334:C:OP2	2.36	0.41
22:a:754:U:H2'	22:a:755:U:H6	1.86	0.41
22:a:833:A:H2'	22:a:834:G:H8	1.84	0.41
22:a:880:G:C2	22:a:898:C:C2	3.09	0.41
22:a:1604:C:H2'	22:a:1605:C:H6	1.85	0.41
22:a:1871:A:H2'	22:a:1872:A:C8	2.56	0.41
22:a:2132:U:O2'	22:a:2133:G:N7	2.46	0.41
22:a:2193:G:H2'	22:a:2194:U:H6	1.86	0.41
22:a:2723:C:H2'	22:a:2724:U:O4'	2.21	0.41
25:c:145:GLU:HG2	25:c:151:GLY:C	2.46	0.41
30:h:103:VAL:HG21	30:h:132:PHE:CE2	2.56	0.41
51:1:30:VAL:HG22	51:1:33:ARG:NH2	2.36	0.41
1:A:309:A:O2'	1:A:607:A:N1	2.48	0.41
1:A:407:U:H2'	1:A:408:A:C8	2.56	0.41
1:A:594:U:H2'	1:A:595:A:O4'	2.21	0.41
1:A:864:A:H2'	1:A:865:A:C8	2.56	0.41
8:H:64:LYS:HE2	8:H:71:VAL:HG21	2.02	0.41
10:J:10:LEU:O	10:J:18:ILE:HD11	2.21	0.41
11:K:94:GLU:OE2	11:K:98:ARG:NH2	2.43	0.41
22:a:1045:C:H1'	22:a:1047:G:N3	2.36	0.41
22:a:1204:A:O4'	22:a:1206:G:C8	2.74	0.41
22:a:1335:C:H2'	22:a:1336:A:C8	2.56	0.41
22:a:1349:C:C2	22:a:1350:C:C5	3.10	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:a:1538:G:H2'	22:a:1539:U:C6	2.56	0.41
27:e:115:GLN:HE22	33:k:1:MET:N	2.19	0.41
42:t:33:LYS:HB3	42:t:64:ALA:HB1	2.03	0.41
1:A:268:U:C2	1:A:269:C:C5	3.08	0.40
1:A:687:A:C2	1:A:704:A:C5	3.08	0.40
6:F:29:ILE:HG23	6:F:66:ALA:HB2	2.03	0.40
18:R:23:TYR:HA	18:R:29:LEU:HD11	2.03	0.40
22:a:70:G:H5'	22:a:112:U:O2	2.21	0.40
22:a:488:G:N2	22:a:491:G:H5''	2.37	0.40
22:a:608:A:H2'	22:a:609:A:H8	1.85	0.40
22:a:863:A:H2'	22:a:864:G:C8	2.55	0.40
22:a:1773:A:N7	22:a:1829:A:H1'	2.36	0.40
22:a:1987:A:H2'	22:a:1988:G:C8	2.57	0.40
22:a:2243:U:H2'	22:a:2244:U:H6	1.85	0.40
22:a:2271:G:OP1	44:v:18:ALA:HB1	2.21	0.40
25:c:120:VAL:HB	30:h:91:PHE:HB3	2.03	0.40
41:s:6:ARG:HH22	41:s:37:ASP:CG	2.29	0.40
42:t:79:LYS:HE3	42:t:79:LYS:HB2	1.92	0.40
50:0:10:LYS:HG3	50:0:52:ALA:HB3	2.03	0.40
1:A:916:U:H2'	1:A:917:G:H8	1.87	0.40
1:A:1147:C:H2'	1:A:1148:U:H6	1.86	0.40
22:a:78:U:H2'	22:a:79:C:H6	1.85	0.40
22:a:128:C:H2'	22:a:129:C:C6	2.57	0.40
22:a:250:G:H2'	22:a:251:A:C8	2.56	0.40
22:a:278:A:N1	22:a:361:G:O2'	2.43	0.40
22:a:457:A:N1	22:a:470:A:H5''	2.37	0.40
22:a:593:U:H2'	22:a:594:U:H6	1.86	0.40
22:a:863:A:H2'	22:a:864:G:H8	1.86	0.40
22:a:987:C:H2'	22:a:988:A:O4'	2.21	0.40
22:a:1336:A:H2'	22:a:1337:G:H8	1.86	0.40
22:a:1370:C:H2'	22:a:1371:G:O4'	2.20	0.40
22:a:1703:G:H2'	22:a:1704:C:H6	1.85	0.40
22:a:1853:A:N1	22:a:2087:G:H1'	2.36	0.40
22:a:1902:C:H4'	25:c:242:LYS:O	2.21	0.40
22:a:2065:C:H2'	22:a:2066:C:C6	2.56	0.40
22:a:2379:G:H4'	36:n:21:LEU:HD11	2.03	0.40
22:a:2583:G:O2'	55:Y:77:A:N1	2.49	0.40
23:b:90:C:H5'	34:l:18:ARG:HG2	2.03	0.40
36:n:60:GLU:HG3	36:n:61:GLN:HG3	2.03	0.40
1:A:185:U:H2'	1:A:186:C:C6	2.56	0.40
1:A:207:C:C2	1:A:212:G:N2	2.88	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:U:H2'	1:A:982:U:C5	2.56	0.40
1:A:1319:A:O2'	1:A:1323:G:N7	2.48	0.40
1:A:1346:A:N1	1:A:1374:A:H5''	2.36	0.40
3:C:65:ARG:HD2	3:C:102:ASN:HD21	1.87	0.40
19:S:3:ARG:NH1	19:S:10:PHE:HB2	2.36	0.40
22:a:95:A:H2'	22:a:96:C:O4'	2.21	0.40
22:a:577:G:H2'	22:a:578:G:C8	2.56	0.40
22:a:1292:G:H2'	22:a:1293:C:H6	1.87	0.40
25:c:105:LEU:O	25:c:107:PRO:HD3	2.22	0.40
27:e:97:ASN:HB2	27:e:100:MET:HG3	2.02	0.40
27:e:149:ILE:HB	27:e:188:MET:HG2	2.03	0.40
28:f:106:ILE:C	28:f:109:PRO:HD2	2.46	0.40
1:A:904:U:H2'	1:A:905:U:C6	2.56	0.40
1:A:1148:U:H2'	1:A:1149:C:O4'	2.21	0.40
16:P:48:GLU:OE1	16:P:51:ARG:NH2	2.39	0.40
22:a:404:A:H1'	22:a:405:U:OP2	2.21	0.40
22:a:532:A:H4'	22:a:533:G:C8	2.56	0.40
22:a:1518:C:H2'	22:a:1519:G:H8	1.86	0.40
22:a:1744:A:H3'	22:a:1745:A:H8	1.85	0.40
22:a:2100:G:H2'	22:a:2101:A:H8	1.87	0.40
22:a:2443:C:H2'	22:a:2444:G:C8	2.56	0.40
28:f:8:TYR:HB2	28:f:173:PHE:HZ	1.86	0.40
43:u:31:TYR:CE2	43:u:90:ASP:HB3	2.56	0.40
57:5:9:A:O3'	57:5:45:G:O2'	2.35	0.40
9:I:40:GLY:HA2	9:I:45:ARG:HH21	1.87	0.40
11:K:56:ARG:HH11	57:5:39:G:H5''	1.86	0.40
22:a:30:G:H2'	22:a:31:C:C6	2.56	0.40
22:a:918:A:H5''	23:b:97:C:O2'	2.22	0.40
22:a:1494:A:H2'	22:a:1495:A:C8	2.57	0.40
22:a:1831:G:H2'	22:a:1832:C:C6	2.56	0.40
22:a:2793:C:H2'	22:a:2794:C:H6	1.87	0.40
22:a:2845:U:H2'	22:a:2846:G:C8	2.57	0.40
28:f:38:MET:HB2	28:f:87:CYS:SG	2.62	0.40
29:g:72:LEU:HD23	29:g:72:LEU:HA	1.85	0.40
29:g:98:VAL:HG23	29:g:125:CYS:SG	2.61	0.40
54:X:15:U:H2'	54:X:16:G:H8	1.87	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	222/241 (92%)	214 (96%)	8 (4%)	0	100	100
3	C	204/233 (88%)	198 (97%)	6 (3%)	0	100	100
4	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
5	E	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
7	G	151/179 (84%)	150 (99%)	1 (1%)	0	100	100
8	H	127/130 (98%)	127 (100%)	0	0	100	100
9	I	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	J	96/103 (93%)	94 (98%)	1 (1%)	1 (1%)	12	39
11	K	113/129 (88%)	111 (98%)	2 (2%)	0	100	100
12	L	120/124 (97%)	117 (98%)	3 (2%)	0	100	100
13	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
14	N	98/101 (97%)	98 (100%)	0	0	100	100
15	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	P	79/82 (96%)	78 (99%)	1 (1%)	0	100	100
17	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
18	R	65/75 (87%)	65 (100%)	0	0	100	100
19	S	82/92 (89%)	82 (100%)	0	0	100	100
20	T	84/87 (97%)	84 (100%)	0	0	100	100
21	U	68/71 (96%)	68 (100%)	0	0	100	100
24	7	149/234 (64%)	145 (97%)	4 (3%)	0	100	100
25	c	269/273 (98%)	267 (99%)	2 (1%)	0	100	100
26	d	206/209 (99%)	202 (98%)	3 (2%)	1 (0%)	24	54
27	e	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
28	f	175/179 (98%)	169 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	g	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
30	h	146/149 (98%)	145 (99%)	1 (1%)	0	100	100
31	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
32	j	121/123 (98%)	121 (100%)	0	0	100	100
33	k	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
34	l	133/136 (98%)	133 (100%)	0	0	100	100
35	m	116/127 (91%)	113 (97%)	3 (3%)	0	100	100
36	n	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
37	o	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
38	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
39	q	101/103 (98%)	101 (100%)	0	0	100	100
40	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	s	91/100 (91%)	91 (100%)	0	0	100	100
42	t	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
43	u	92/94 (98%)	92 (100%)	0	0	100	100
44	v	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
45	w	75/78 (96%)	75 (100%)	0	0	100	100
46	x	60/63 (95%)	60 (100%)	0	0	100	100
47	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
48	4	46/70 (66%)	45 (98%)	1 (2%)	0	100	100
49	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
50	0	49/55 (89%)	49 (100%)	0	0	100	100
51	1	44/46 (96%)	44 (100%)	0	0	100	100
52	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
53	3	36/38 (95%)	36 (100%)	0	0	100	100
58	6	29/165 (18%)	28 (97%)	1 (3%)	0	100	100
All	All	5764/6312 (91%)	5681 (99%)	81 (1%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	d	149	ASN
10	J	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	
2	B	186/199 (94%)	186 (100%)	0	100	100
3	C	170/190 (90%)	170 (100%)	0	100	100
4	D	172/173 (99%)	172 (100%)	0	100	100
5	E	119/126 (94%)	119 (100%)	0	100	100
6	F	90/116 (78%)	90 (100%)	0	100	100
7	G	126/147 (86%)	124 (98%)	2 (2%)	55	83
8	H	104/105 (99%)	104 (100%)	0	100	100
9	I	105/107 (98%)	105 (100%)	0	100	100
10	J	86/90 (96%)	86 (100%)	0	100	100
11	K	89/98 (91%)	89 (100%)	0	100	100
12	L	102/103 (99%)	102 (100%)	0	100	100
13	M	93/96 (97%)	93 (100%)	0	100	100
14	N	83/84 (99%)	83 (100%)	0	100	100
15	O	76/77 (99%)	76 (100%)	0	100	100
16	P	65/65 (100%)	65 (100%)	0	100	100
17	Q	73/78 (94%)	73 (100%)	0	100	100
18	R	58/65 (89%)	58 (100%)	0	100	100
19	S	72/79 (91%)	72 (100%)	0	100	100
20	T	65/66 (98%)	65 (100%)	0	100	100
21	U	60/61 (98%)	59 (98%)	1 (2%)	53	82
24	7	122/181 (67%)	119 (98%)	3 (2%)	42	74
25	c	216/218 (99%)	216 (100%)	0	100	100
26	d	163/163 (100%)	163 (100%)	0	100	100
27	e	165/165 (100%)	165 (100%)	0	100	100
28	f	148/150 (99%)	148 (100%)	0	100	100
29	g	137/138 (99%)	137 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	h	113/114 (99%)	113 (100%)	0	100	100
31	i	116/116 (100%)	115 (99%)	1 (1%)	70	90
32	j	104/104 (100%)	104 (100%)	0	100	100
33	k	103/103 (100%)	103 (100%)	0	100	100
34	l	108/107 (101%)	107 (99%)	1 (1%)	70	90
35	m	98/103 (95%)	98 (100%)	0	100	100
36	n	86/87 (99%)	86 (100%)	0	100	100
37	o	99/100 (99%)	99 (100%)	0	100	100
38	p	89/90 (99%)	89 (100%)	0	100	100
39	q	84/84 (100%)	84 (100%)	0	100	100
40	r	93/93 (100%)	93 (100%)	0	100	100
41	s	80/84 (95%)	80 (100%)	0	100	100
42	t	83/85 (98%)	83 (100%)	0	100	100
43	u	78/78 (100%)	78 (100%)	0	100	100
44	v	61/63 (97%)	61 (100%)	0	100	100
45	w	67/68 (98%)	67 (100%)	0	100	100
46	x	54/55 (98%)	54 (100%)	0	100	100
47	y	48/49 (98%)	48 (100%)	0	100	100
48	4	44/62 (71%)	44 (100%)	0	100	100
49	z	47/48 (98%)	47 (100%)	0	100	100
50	0	46/49 (94%)	46 (100%)	0	100	100
51	1	38/38 (100%)	38 (100%)	0	100	100
52	2	51/52 (98%)	51 (100%)	0	100	100
53	3	34/34 (100%)	34 (100%)	0	100	100
58	6	24/134 (18%)	24 (100%)	0	100	100
All	All	4793/5140 (93%)	4785 (100%)	8 (0%)	85	96

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	73	VAL
7	G	84	THR
21	U	42	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
24	7	43	ASP
24	7	173	THR
24	7	174	THR
31	i	131	ASN
34	l	36	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	36	ASN
3	C	8	ASN
3	C	100	GLN
3	C	102	ASN
6	F	3	HIS
6	F	94	HIS
7	G	9	GLN
7	G	148	ASN
8	H	38	ASN
11	K	40	ASN
11	K	81	ASN
14	N	49	GLN
15	O	35	GLN
15	O	50	HIS
16	P	63	GLN
20	T	3	ASN
20	T	48	GLN
20	T	61	GLN
20	T	82	GLN
24	7	20	GLN
24	7	168	ASN
25	c	86	ASN
25	c	243	HIS
27	e	9	GLN
27	e	115	GLN
29	g	38	ASN
31	i	58	ASN
31	i	76	HIS
31	i	80	HIS
32	j	3	GLN
33	k	99	ASN
36	n	29	HIS
36	n	38	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
36	n	98	GLN
37	o	52	ASN
46	x	45	GLN
53	3	13	ASN
58	6	147	GLN
58	6	158	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1523/1542 (98%)	201 (13%)	0
22	a	2842/2904 (97%)	316 (11%)	0
23	b	118/119 (99%)	12 (10%)	0
54	X	15/629 (2%)	4 (26%)	0
55	Y	76/77 (98%)	11 (14%)	0
56	Z	75/76 (98%)	8 (10%)	0
57	5	72/76 (94%)	15 (20%)	0
All	All	4721/5423 (87%)	567 (12%)	0

All (567) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	4	U
1	A	7	A
1	A	9	G
1	A	32	A
1	A	39	G
1	A	47	C
1	A	48	C
1	A	51	A
1	A	55	A
1	A	64	G
1	A	66	A
1	A	68	G
1	A	69	G
1	A	71	A
1	A	94	G
1	A	120	A
1	A	121	U
1	A	127	G
1	A	131	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	142	G
1	A	174	A
1	A	182	A
1	A	197	A
1	A	201	G
1	A	210	C
1	A	212	G
1	A	226	G
1	A	244	U
1	A	245	U
1	A	247	G
1	A	251	G
1	A	266	G
1	A	267	C
1	A	279	A
1	A	280	C
1	A	289	G
1	A	302	G
1	A	321	A
1	A	325	A
1	A	328	C
1	A	329	A
1	A	330	C
1	A	332	G
1	A	340	U
1	A	351	G
1	A	352	C
1	A	354	G
1	A	367	U
1	A	372	C
1	A	382	A
1	A	397	A
1	A	398	U
1	A	406	G
1	A	410	G
1	A	411	A
1	A	412	A
1	A	413	G
1	A	429	U
1	A	444	G
1	A	459	A
1	A	460	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	A	462	G
1	A	463	U
1	A	467	U
1	A	468	A
1	A	484	G
1	A	486	U
1	A	495	A
1	A	499	A
1	A	509	A
1	A	511	C
1	A	518	C
1	A	521	G
1	A	524	G
1	A	527	G7M
1	A	529	G
1	A	531	U
1	A	532	A
1	A	538	G
1	A	547	A
1	A	559	A
1	A	564	C
1	A	572	A
1	A	573	A
1	A	576	C
1	A	577	G
1	A	596	A
1	A	607	A
1	A	633	G
1	A	650	G
1	A	653	U
1	A	665	A
1	A	687	A
1	A	721	G
1	A	723	U
1	A	724	G
1	A	734	G
1	A	747	A
1	A	748	G
1	A	755	G
1	A	777	A
1	A	793	U
1	A	794	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	815	A
1	A	817	C
1	A	821	G
1	A	828	U
1	A	841	C
1	A	842	U
1	A	843	U
1	A	844	G
1	A	845	A
1	A	846	G
1	A	847	G
1	A	849	G
1	A	902	G
1	A	905	U
1	A	914	A
1	A	926	G
1	A	934	C
1	A	935	A
1	A	960	U
1	A	965	U
1	A	969	A
1	A	975	A
1	A	976	G
1	A	977	A
1	A	993	G
1	A	1003	G
1	A	1004	A
1	A	1008	U
1	A	1019	A
1	A	1020	G
1	A	1021	A
1	A	1022	A
1	A	1030	U
1	A	1031	C
1	A	1033	G
1	A	1043	G
1	A	1044	A
1	A	1045	C
1	A	1053	G
1	A	1065	U
1	A	1094	G
1	A	1095	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1101	A
1	A	1130	A
1	A	1134	G
1	A	1136	C
1	A	1137	C
1	A	1139	G
1	A	1140	C
1	A	1145	A
1	A	1158	C
1	A	1159	U
1	A	1167	A
1	A	1174	G
1	A	1184	G
1	A	1196	A
1	A	1197	A
1	A	1213	A
1	A	1214	C
1	A	1227	A
1	A	1228	C
1	A	1238	A
1	A	1239	A
1	A	1248	A
1	A	1258	G
1	A	1279	G
1	A	1280	A
1	A	1286	U
1	A	1287	A
1	A	1299	A
1	A	1302	C
1	A	1305	G
1	A	1317	C
1	A	1320	C
1	A	1336	C
1	A	1338	G
1	A	1346	A
1	A	1353	G
1	A	1363	A
1	A	1370	G
1	A	1379	G
1	A	1419	G
1	A	1429	A
1	A	1432	G

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	1446	A
1	A	1449	C
1	A	1451	U
1	A	1452	C
1	A	1492	A
1	A	1494	G
1	A	1499	A
1	A	1503	A
1	A	1506	U
1	A	1517	G
1	A	1519	MA6
1	A	1529	G
1	A	1530	G
1	A	1531	A
22	a	2	G
22	a	10	A
22	a	15	G
22	a	27	G
22	a	34	U
22	a	51	G
22	a	71	A
22	a	74	A
22	a	75	G
22	a	84	A
22	a	96	C
22	a	101	A
22	a	118	A
22	a	119	A
22	a	120	U
22	a	131	A
22	a	139	U
22	a	142	A
22	a	163	C
22	a	196	A
22	a	199	A
22	a	216	A
22	a	222	A
22	a	223	A
22	a	248	G
22	a	250	G
22	a	272	A
22	a	276	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	a	277	G
22	a	278	A
22	a	279	A
22	a	285	G
22	a	286	U
22	a	289	G
22	a	311	A
22	a	329	G
22	a	330	A
22	a	345	A
22	a	361	G
22	a	386	G
22	a	396	G
22	a	405	U
22	a	406	G
22	a	411	G
22	a	412	A
22	a	481	G
22	a	491	G
22	a	504	A
22	a	505	A
22	a	509	C
22	a	532	A
22	a	545	U
22	a	546	U
22	a	547	A
22	a	549	G
22	a	563	A
22	a	573	U
22	a	575	A
22	a	603	A
22	a	615	U
22	a	627	A
22	a	637	A
22	a	645	C
22	a	646	U
22	a	647	G
22	a	653	U
22	a	654	A
22	a	655	A
22	a	668	A
22	a	685	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	a	686	U
22	a	717	C
22	a	726	G
22	a	730	A
22	a	747	5MU
22	a	764	A
22	a	775	G
22	a	776	G
22	a	782	A
22	a	784	G
22	a	785	G
22	a	789	A
22	a	805	G
22	a	812	C
22	a	827	U
22	a	828	U
22	a	846	U
22	a	859	G
22	a	881	G
22	a	884	U
22	a	888	C
22	a	890	C
22	a	891	G
22	a	893	C
22	a	895	U
22	a	896	A
22	a	897	C
22	a	910	A
22	a	931	U
22	a	946	C
22	a	961	C
22	a	973	A
22	a	974	G
22	a	980	A
22	a	983	A
22	a	990	A
22	a	996	A
22	a	1005	C
22	a	1012	U
22	a	1013	C
22	a	1026	G
22	a	1033	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	a	1041	G
22	a	1045	C
22	a	1047	G
22	a	1110	G
22	a	1111	A
22	a	1112	G
22	a	1130	U
22	a	1132	U
22	a	1133	A
22	a	1135	C
22	a	1142	A
22	a	1236	G
22	a	1250	G
22	a	1253	A
22	a	1255	U
22	a	1256	G
22	a	1271	G
22	a	1272	A
22	a	1300	G
22	a	1301	A
22	a	1329	U
22	a	1352	U
22	a	1365	A
22	a	1379	U
22	a	1383	A
22	a	1386	C
22	a	1416	G
22	a	1419	A
22	a	1428	C
22	a	1452	G
22	a	1460	U
22	a	1482	G
22	a	1493	C
22	a	1497	U
22	a	1508	A
22	a	1515	A
22	a	1534	U
22	a	1535	A
22	a	1536	C
22	a	1537	G
22	a	1539	U
22	a	1566	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	a	1567	G
22	a	1569	A
22	a	1578	U
22	a	1584	U
22	a	1585	C
22	a	1608	A
22	a	1639	C
22	a	1646	C
22	a	1647	U
22	a	1648	U
22	a	1649	G
22	a	1674	G
22	a	1715	G
22	a	1729	U
22	a	1730	C
22	a	1738	G
22	a	1758	U
22	a	1764	C
22	a	1772	A
22	a	1773	A
22	a	1800	C
22	a	1801	A
22	a	1808	A
22	a	1816	C
22	a	1829	A
22	a	1848	A
22	a	1870	C
22	a	1871	A
22	a	1872	A
22	a	1896	G
22	a	1906	G
22	a	1913	A
22	a	1929	G
22	a	1930	G
22	a	1936	A
22	a	1937	A
22	a	1938	A
22	a	1955	U
22	a	1963	U
22	a	1964	G
22	a	1967	C
22	a	1970	A

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
22	a	1971	U
22	a	1972	G
22	a	1991	U
22	a	2021	C
22	a	2023	C
22	a	2030	6MZ
22	a	2031	A
22	a	2033	A
22	a	2035	G
22	a	2043	C
22	a	2052	A
22	a	2055	C
22	a	2056	G
22	a	2060	A
22	a	2061	G
22	a	2062	A
22	a	2069	G7M
22	a	2093	G
22	a	2097	A
22	a	2116	G
22	a	2119	A
22	a	2128	G
22	a	2131	U
22	a	2132	U
22	a	2133	G
22	a	2134	A
22	a	2145	C
22	a	2146	C
22	a	2156	G
22	a	2157	G
22	a	2158	A
22	a	2159	G
22	a	2163	A
22	a	2172	U
22	a	2173	A
22	a	2198	A
22	a	2204	G
22	a	2212	A
22	a	2225	A
22	a	2238	G
22	a	2239	G
22	a	2243	U

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	a	2278	A
22	a	2283	C
22	a	2287	A
22	a	2288	A
22	a	2305	U
22	a	2307	G
22	a	2308	G
22	a	2309	A
22	a	2322	A
22	a	2323	G
22	a	2325	G
22	a	2333	A
22	a	2345	G
22	a	2347	C
22	a	2350	C
22	a	2361	G
22	a	2379	G
22	a	2383	G
22	a	2385	C
22	a	2402	U
22	a	2403	C
22	a	2406	A
22	a	2425	A
22	a	2429	G
22	a	2430	A
22	a	2435	A
22	a	2441	U
22	a	2448	A
22	a	2474	U
22	a	2476	A
22	a	2478	A
22	a	2484	G
22	a	2491	U
22	a	2494	G
22	a	2498	OMC
22	a	2502	G
22	a	2505	G
22	a	2518	A
22	a	2520	C
22	a	2525	G
22	a	2529	G
22	a	2547	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
22	a	2554	U
22	a	2566	A
22	a	2567	G
22	a	2573	C
22	a	2582	G
22	a	2602	A
22	a	2603	G
22	a	2609	U
22	a	2613	U
22	a	2615	U
22	a	2629	U
22	a	2689	U
22	a	2690	U
22	a	2714	G
22	a	2716	C
22	a	2726	A
22	a	2732	G
22	a	2733	A
22	a	2744	G
22	a	2748	A
22	a	2755	C
22	a	2757	A
22	a	2765	A
22	a	2778	A
22	a	2797	U
22	a	2798	U
22	a	2800	A
22	a	2818	U
22	a	2820	A
22	a	2821	A
22	a	2835	A
22	a	2849	U
22	a	2861	U
22	a	2873	A
22	a	2884	U
22	a	2893	A
23	b	3	C
23	b	32	U
23	b	34	A
23	b	35	C
23	b	41	G
23	b	52	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
23	b	56	G
23	b	67	G
23	b	89	U
23	b	90	C
23	b	99	A
23	b	109	A
54	X	14	C
54	X	23	A
54	X	25	C
54	X	26	G
55	Y	3	G
55	Y	9	A
55	Y	10	G
55	Y	16	C
55	Y	18	U
55	Y	19	G
55	Y	20	G
55	Y	21	H2U
55	Y	22	A
55	Y	73	G
55	Y	75	C
56	Z	14	A
56	Z	16	H2U
56	Z	17	H2U
56	Z	22	G
56	Z	44	G
56	Z	48	C
56	Z	64	G
56	Z	76	A
57	5	6	U
57	5	19	G
57	5	20	G
57	5	21	A
57	5	34	CM0
57	5	35	G
57	5	44	A
57	5	45	G
57	5	46	G7M
57	5	47	U
57	5	48	C
57	5	52	G
57	5	61	C

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
57	5	65	A
57	5	70	U

There are no RNA pucker outliers to report.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	MA6	A	1519	1	23,26,27	0.31	0	34,38,41	0.64	1 (2%)
56	PSU	Z	55	56	18,21,22	0.48	0	22,30,33	0.59	0
56	H2U	Z	16	56	18,21,22	0.38	0	21,30,33	0.44	0
22	6MZ	a	1618	22	22,25,26	0.34	0	30,36,39	0.48	0
22	6MZ	a	2030	22	22,25,26	0.32	0	30,36,39	0.52	0
22	PSU	a	2504	22,59	18,21,22	0.51	0	22,30,33	0.56	0
55	1MG	Y	38	55	22,26,27	0.42	0	33,39,42	0.46	0
22	2MA	a	2503	22,59,60	22,25,26	0.97	2 (9%)	33,37,40	1.40	3 (9%)
22	PSU	a	746	22,60	18,21,22	0.54	0	22,30,33	0.39	0
56	H2U	Z	20	56	18,21,22	0.31	0	21,30,33	0.75	1 (4%)
22	5MU	a	747	22	19,22,23	0.30	0	28,32,35	0.34	0
22	PSU	a	2457	22	18,21,22	0.49	0	22,30,33	0.58	0
22	3TD	a	1915	22	18,22,23	0.15	0	22,32,35	0.31	0
12	D2T	L	89	12	7,9,10	0.89	0	6,11,13	1.69	2 (33%)
22	PSU	a	2580	22	18,21,22	0.51	0	22,30,33	0.62	1 (4%)
55	5MU	Y	55	55	19,22,23	0.29	0	28,32,35	0.32	0
22	PSU	a	955	22,59	18,21,22	0.50	0	22,30,33	0.57	0
22	2MG	a	2445	22	23,26,27	0.32	0	32,38,41	0.33	0
1	G7M	A	527	1	23,26,27	0.32	0	35,39,42	0.49	0
55	H2U	Y	21	55	18,21,22	0.27	0	21,30,33	0.57	0
22	5MC	a	1962	22,59	18,22,23	0.30	0	26,32,35	0.45	0
22	PSU	a	1911	22	18,21,22	0.48	0	22,30,33	0.58	0
1	UR3	A	1498	1	19,22,23	0.28	0	26,32,35	0.35	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	PSU	a	2605	22	18,21,22	0.49	0	22,30,33	0.60	0
56	G7M	Z	46	56	23,26,27	0.30	0	35,39,42	0.47	0
34	MS6	l	82	34	5,7,8	0.32	0	2,7,9	0.09	0
56	5MU	Z	54	56	19,22,23	0.29	0	28,32,35	0.31	0
11	IAS	K	119	11	6,7,8	0.90	0	6,8,10	0.93	0
56	4SU	Z	8	56	18,21,22	0.30	0	26,30,33	0.34	0
57	G7M	5	46	57	23,26,27	0.30	0	35,39,42	0.48	0
22	2MG	a	1835	22	23,26,27	0.29	0	32,38,41	0.32	0
1	5MC	A	967	1	18,22,23	0.30	0	26,32,35	0.44	0
22	OMC	a	2498	22,60	19,22,23	0.30	0	26,31,34	0.39	0
22	OMU	a	2552	22	19,22,23	0.28	0	26,31,34	0.44	0
22	G7M	a	2069	22,59	23,26,27	0.34	0	35,39,42	0.48	0
22	OMG	a	2251	22,56,59	23,26,27	0.30	0	33,38,41	0.36	0
22	1MG	a	745	22	22,26,27	0.43	0	33,39,42	0.49	0
1	MA6	A	1518	1	23,26,27	0.42	0	34,38,41	0.73	1 (2%)
34	4D4	l	81	34	9,11,12	0.77	0	8,13,15	1.96	3 (37%)
57	CM0	5	34	57	22,26,27	0.48	0	28,37,40	0.42	0
57	PSU	5	55	57	18,21,22	0.49	0	22,30,33	0.56	0
22	5MU	a	1939	22,59	19,22,23	0.28	0	28,32,35	0.38	0
22	PSU	a	2604	22	18,21,22	0.53	0	22,30,33	0.57	0
1	4OC	A	1402	1	20,23,24	0.32	0	26,32,35	0.47	0
1	2MG	A	1516	1	23,26,27	0.30	0	32,38,41	0.39	0
1	5MC	A	1407	1	18,22,23	0.34	0	26,32,35	0.48	0
1	2MG	A	1207	59,1	23,26,27	0.29	0	32,38,41	0.35	0
1	PSU	A	516	60,1	18,21,22	0.49	0	22,30,33	0.60	1 (4%)
55	PSU	Y	56	55	18,21,22	0.47	0	22,30,33	0.58	0
56	H2U	Z	17	56	18,21,22	0.38	0	21,30,33	0.42	0
57	5MU	5	54	57	19,22,23	0.27	0	28,32,35	0.32	0
22	H2U	a	2449	22	18,21,22	0.30	0	21,30,33	0.45	0
22	PSU	a	1917	22	18,21,22	0.52	0	22,30,33	0.56	0
55	G7M	Y	47	55	23,26,27	0.32	0	35,39,42	0.47	0
26	MEQ	d	150	26	8,9,10	0.51	0	5,10,12	0.21	0
1	2MG	A	966	1	23,26,27	0.30	0	32,38,41	0.40	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	MA6	A	1519	1	-	4/11/29/30	0/3/3/3
56	PSU	Z	55	56	-	1/7/25/26	0/2/2/2

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
56	H2U	Z	16	56	-	6/7/38/39	0/2/2/2
22	6MZ	a	1618	22	-	0/9/27/28	0/3/3/3
22	6MZ	a	2030	22	-	2/9/27/28	0/3/3/3
22	PSU	a	2504	22,59	-	2/7/25/26	0/2/2/2
55	1MG	Y	38	55	-	0/7/25/26	0/3/3/3
22	2MA	a	2503	22,59,60	-	1/7/25/26	0/3/3/3
22	PSU	a	746	22,60	-	3/7/25/26	0/2/2/2
56	H2U	Z	20	56	-	2/7/38/39	0/2/2/2
22	5MU	a	747	22	-	0/7/25/26	0/2/2/2
22	PSU	a	2457	22	-	0/7/25/26	0/2/2/2
22	3TD	a	1915	22	-	0/7/25/26	0/2/2/2
12	D2T	L	89	12	-	2/7/12/14	-
22	PSU	a	2580	22	-	0/7/25/26	0/2/2/2
55	5MU	Y	55	55	-	0/7/25/26	0/2/2/2
22	PSU	a	955	22,59	-	0/7/25/26	0/2/2/2
22	2MG	a	2445	22	-	0/9/27/28	0/3/3/3
1	G7M	A	527	1	-	2/7/25/26	0/3/3/3
55	H2U	Y	21	55	-	7/7/38/39	0/2/2/2
22	5MC	a	1962	22,59	-	0/7/25/26	0/2/2/2
22	PSU	a	1911	22	-	0/7/25/26	0/2/2/2
1	UR3	A	1498	1	-	0/7/25/26	0/2/2/2
22	PSU	a	2605	22	-	0/7/25/26	0/2/2/2
56	G7M	Z	46	56	-	0/7/25/26	0/3/3/3
34	MS6	l	82	34	-	1/4/6/8	-
56	5MU	Z	54	56	-	0/7/25/26	0/2/2/2
11	IAS	K	119	11	-	0/7/7/8	-
56	4SU	Z	8	56	-	0/7/25/26	0/2/2/2
57	G7M	5	46	57	-	1/7/25/26	0/3/3/3
22	2MG	a	1835	22	-	0/9/27/28	0/3/3/3
1	5MC	A	967	1	-	0/7/25/26	0/2/2/2
22	OMC	a	2498	22,60	-	0/9/27/28	0/2/2/2
22	OMU	a	2552	22	-	0/9/27/28	0/2/2/2
22	G7M	a	2069	22,59	-	1/7/25/26	0/3/3/3
22	OMG	a	2251	22,56,59	-	1/9/27/28	0/3/3/3
22	1MG	a	745	22	-	0/7/25/26	0/3/3/3
1	MA6	A	1518	1	-	0/11/29/30	0/3/3/3
34	4D4	l	81	34	-	1/11/12/14	-
57	CM0	5	34	57	-	5/12/30/31	0/2/2/2
57	PSU	5	55	57	-	1/7/25/26	0/2/2/2
22	5MU	a	1939	22,59	-	0/7/25/26	0/2/2/2

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	a	2604	22	-	1/7/25/26	0/2/2/2
1	4OC	A	1402	1	-	0/9/29/30	0/2/2/2
1	2MG	A	1516	1	-	0/9/27/28	0/3/3/3
1	5MC	A	1407	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1207	59,1	-	0/9/27/28	0/3/3/3
1	PSU	A	516	60,1	-	0/7/25/26	0/2/2/2
55	PSU	Y	56	55	-	0/7/25/26	0/2/2/2
56	H2U	Z	17	56	-	5/7/38/39	0/2/2/2
57	5MU	5	54	57	-	0/7/25/26	0/2/2/2
22	H2U	a	2449	22	-	0/7/38/39	0/2/2/2
22	PSU	a	1917	22	-	0/7/25/26	0/2/2/2
55	G7M	Y	47	55	-	0/7/25/26	0/3/3/3
26	MEQ	d	150	26	-	3/8/9/11	-
1	2MG	A	966	1	-	0/9/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	a	2503	2MA	C6-N6	-3.13	1.26	1.34
22	a	2503	2MA	C6-N1	2.02	1.37	1.35

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	a	2503	2MA	N6-C6-N1	4.76	123.77	117.03
34	l	81	4D4	NE-CZ-NH2	4.01	127.75	120.70
22	a	2503	2MA	C2-N1-C6	3.93	124.20	118.08
22	a	2503	2MA	C5-C6-N1	-3.86	112.34	119.01
12	L	89	D2T	O-C-CA	-2.79	117.47	124.78
34	l	81	4D4	NH1-CZ-NE	-2.68	113.01	119.19
34	l	81	4D4	O-C-CA	-2.64	117.86	124.78
56	Z	20	H2U	C4-N3-C2	-2.64	123.60	125.79
1	A	1518	MA6	C2-N1-C6	2.41	117.45	111.75
12	L	89	D2T	OD1-CG-CB	-2.36	117.50	122.44
1	A	1519	MA6	C2-N1-C6	2.35	117.30	111.75
22	a	2580	PSU	O4'-C1'-C2'	2.16	108.19	105.14
1	A	516	PSU	O4'-C1'-C2'	2.05	108.03	105.14

There are no chirality outliers.

All (52) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
12	L	89	D2T	O-C-CA-CB
26	d	150	MEQ	O-C-CA-CB
55	Y	21	H2U	C3'-C4'-C5'-O5'
55	Y	21	H2U	O4'-C1'-N1-C6
55	Y	21	H2U	C2'-C1'-N1-C6
56	Z	16	H2U	O4'-C4'-C5'-O5'
56	Z	16	H2U	C3'-C4'-C5'-O5'
56	Z	16	H2U	O4'-C1'-N1-C6
56	Z	17	H2U	O4'-C1'-N1-C6
56	Z	17	H2U	C2'-C1'-N1-C6
57	5	46	G7M	C4'-C5'-O5'-P
22	a	746	PSU	C2'-C1'-C5-C4
22	a	746	PSU	C2'-C1'-C5-C6
22	a	2251	OMG	C1'-C2'-O2'-CM2
55	Y	21	H2U	C2'-C1'-N1-C2
56	Z	17	H2U	C2'-C1'-N1-C2
1	A	1519	MA6	O4'-C4'-C5'-O5'
22	a	2030	6MZ	O4'-C4'-C5'-O5'
1	A	527	G7M	O4'-C4'-C5'-O5'
1	A	527	G7M	C3'-C4'-C5'-O5'
1	A	1519	MA6	C3'-C4'-C5'-O5'
55	Y	21	H2U	O4'-C4'-C5'-O5'
22	a	2030	6MZ	C3'-C4'-C5'-O5'
22	a	2504	PSU	O4'-C4'-C5'-O5'
26	d	150	MEQ	OE1-CD-CG-CB
56	Z	16	H2U	C2'-C1'-N1-C6
26	d	150	MEQ	NE2-CD-CG-CB
57	5	34	CM0	O4'-C4'-C5'-O5'
34	l	82	MS6	CB-CG-SD-CE
1	A	1519	MA6	C5-C6-N6-C10
55	Y	21	H2U	C4'-C5'-O5'-P
57	5	34	CM0	C3'-C4'-C5'-O5'
56	Z	16	H2U	C2'-C1'-N1-C2
12	L	89	D2T	CG-CB-SB-CB1
56	Z	16	H2U	O4'-C1'-N1-C2
22	a	2504	PSU	C3'-C4'-C5'-O5'
55	Y	21	H2U	O4'-C1'-N1-C2
1	A	1519	MA6	C5-C6-N6-C9
56	Z	17	H2U	O4'-C1'-N1-C2
22	a	2503	2MA	O4'-C4'-C5'-O5'
22	a	2069	G7M	O4'-C4'-C5'-O5'
57	5	55	PSU	O4'-C1'-C5-C4
22	a	746	PSU	O4'-C1'-C5-C4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
57	5	34	CM0	C4-C5-O5-C7
57	5	34	CM0	C6-C5-O5-C7
56	Z	17	H2U	C4'-C5'-O5'-P
56	Z	20	H2U	C2'-C1'-N1-C6
56	Z	55	PSU	O4'-C1'-C5-C6
22	a	2604	PSU	C3'-C4'-C5'-O5'
56	Z	20	H2U	C2'-C1'-N1-C2
34	1	81	4D4	O-C-CA-CB
57	5	34	CM0	C2'-C1'-N1-C2

There are no ring outliers.

11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	1519	MA6	1	0
22	a	2030	6MZ	1	0
22	a	2503	2MA	1	0
55	Y	21	H2U	1	0
22	a	2605	PSU	1	0
57	5	46	G7M	1	0
22	a	745	1MG	1	0
1	A	1518	MA6	2	0
57	5	34	CM0	1	0
1	A	1402	4OC	1	0
1	A	1516	2MG	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 397 are monoatomic - leaving 5 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
61	SPD	a	3239	-	9,9,9	0.23	0	8,8,8	0.85	0
61	SPD	a	3240	-	9,9,9	0.23	0	8,8,8	0.89	0
61	SPD	a	3237	-	9,9,9	0.19	0	8,8,8	0.85	0
61	SPD	a	3238	-	9,9,9	0.25	0	8,8,8	0.85	0
63	PRO	Y	101	55	5,7,8	0.54	0	7,8,10	1.29	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
61	SPD	a	3239	-	-	0/7/7/7	-
61	SPD	a	3240	-	-	0/7/7/7	-
61	SPD	a	3237	-	-	0/7/7/7	-
61	SPD	a	3238	-	-	0/7/7/7	-
63	PRO	Y	101	55	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

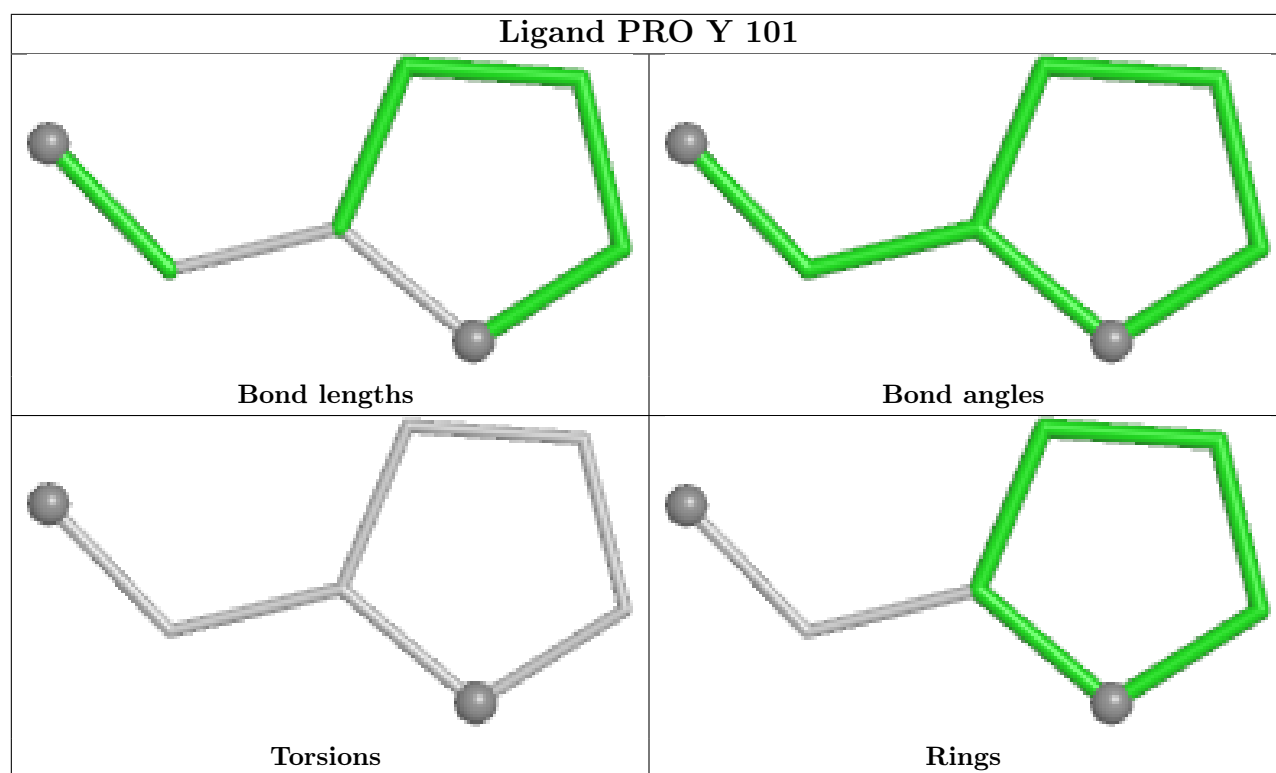
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	a	3239	SPD	1	0
61	a	3240	SPD	1	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.

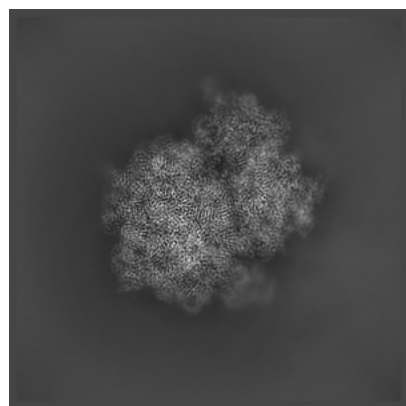
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-67339. These allow visual inspection of the internal detail of the map and identification of artifacts.

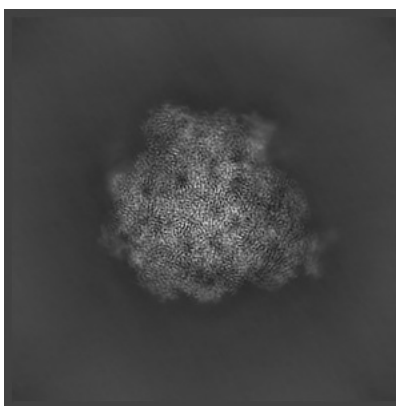
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

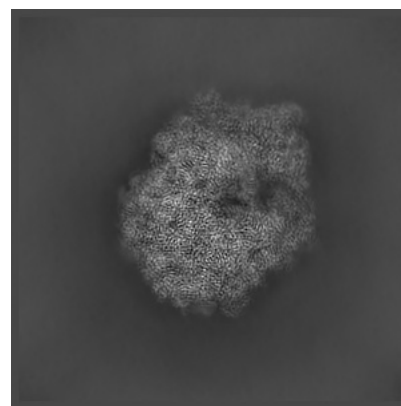
#### 6.1.1 Primary map



X

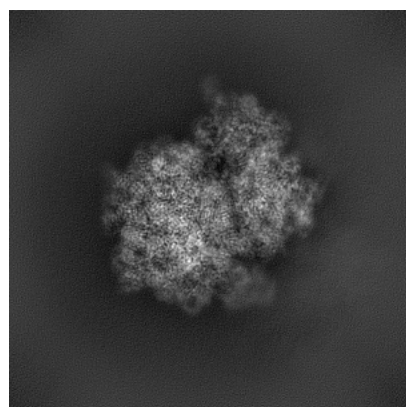


Y

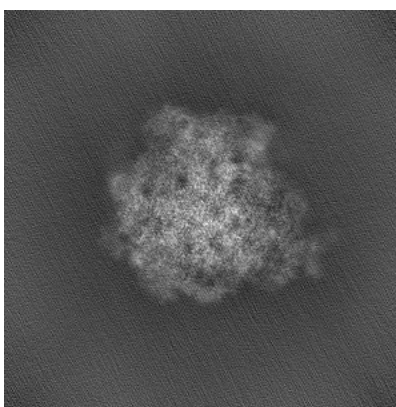


Z

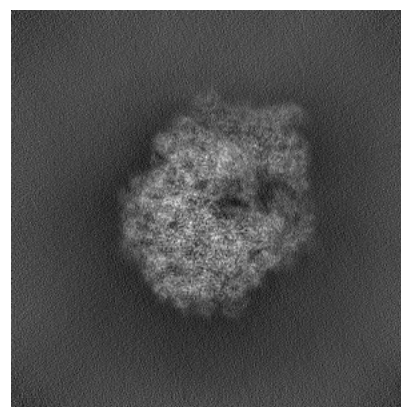
#### 6.1.2 Raw map



X



Y

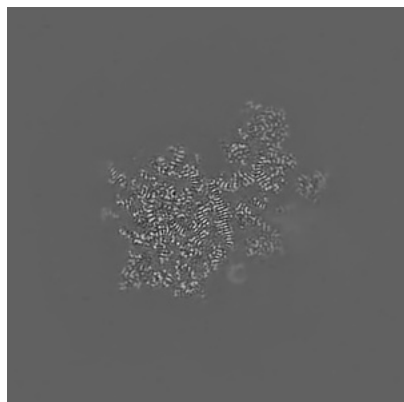


Z

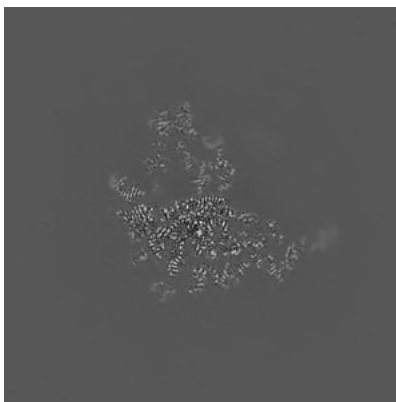
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

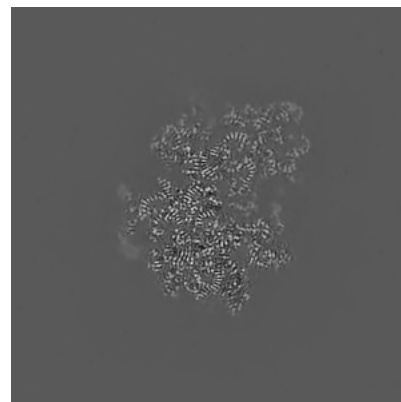
### 6.2.1 Primary map



X Index: 300

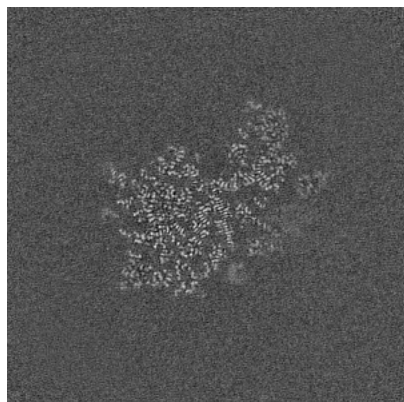


Y Index: 300

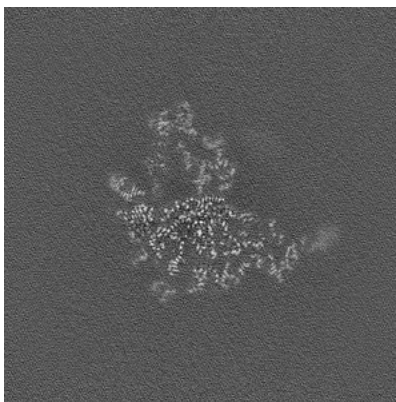


Z Index: 300

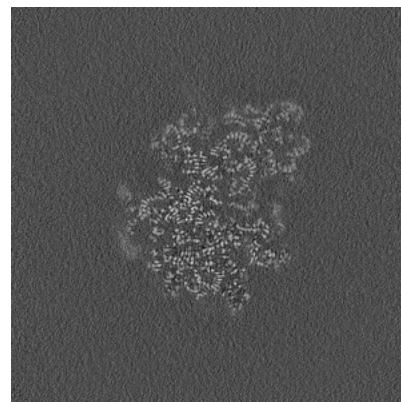
### 6.2.2 Raw map



X Index: 200



Y Index: 200



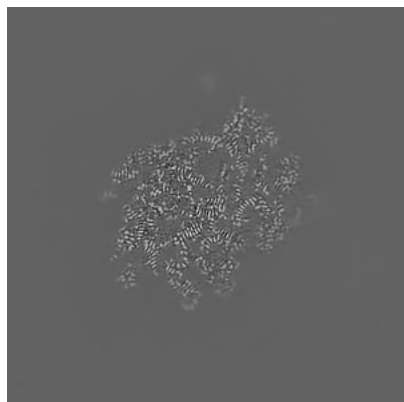
Z Index: 200

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

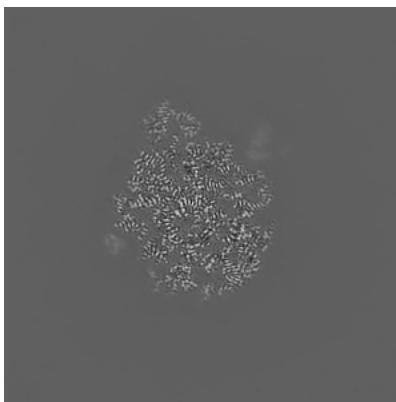


## 6.3 Largest variance slices [i](#)

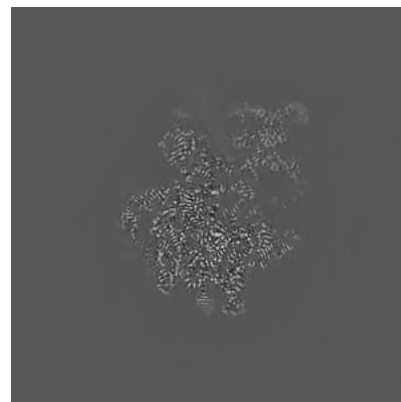
### 6.3.1 Primary map



X Index: 266

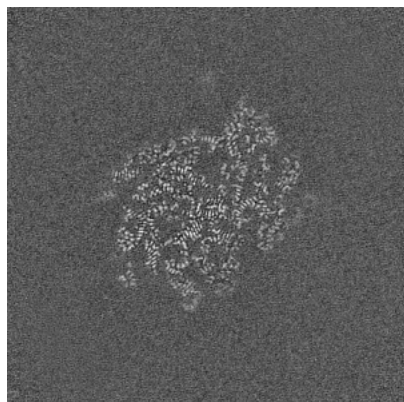


Y Index: 258

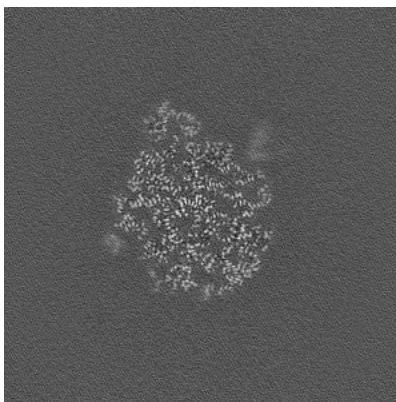


Z Index: 288

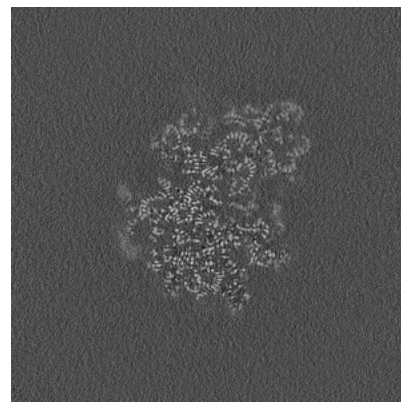
### 6.3.2 Raw map



X Index: 178



Y Index: 172

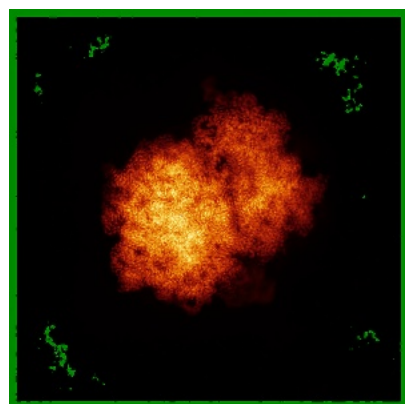


Z Index: 200

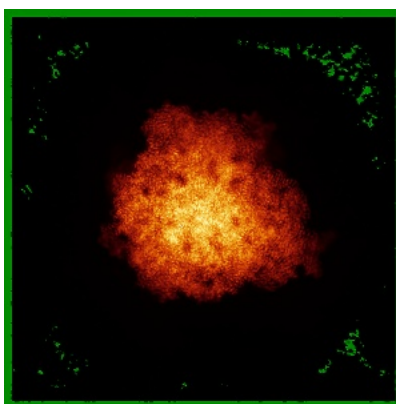
The images above show the largest variance slices of the map in three orthogonal directions.

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

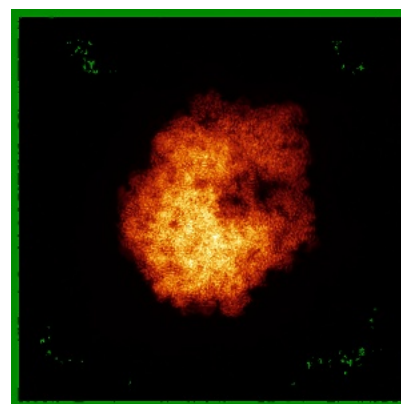
### 6.4.1 Primary map



X

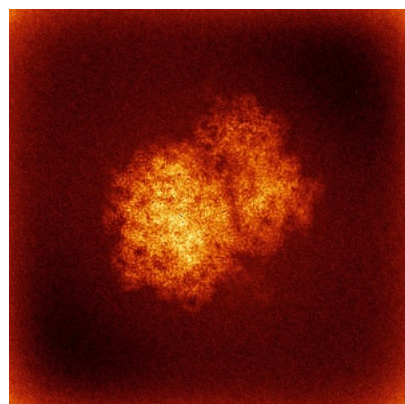


Y

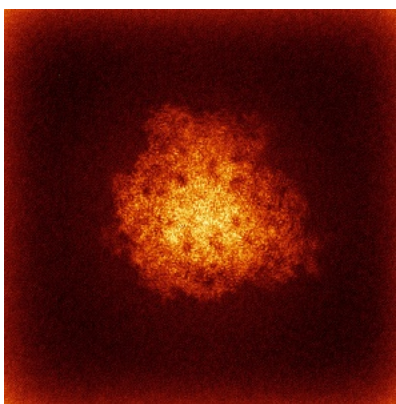


Z

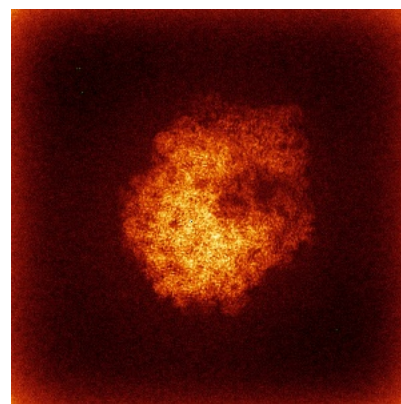
### 6.4.2 Raw map



X



Y



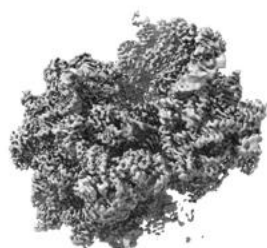
Z

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



## 6.5 Orthogonal surface views [i](#)

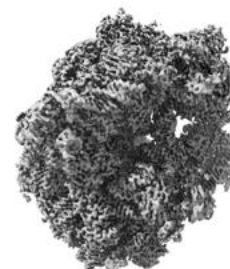
### 6.5.1 Primary map



X



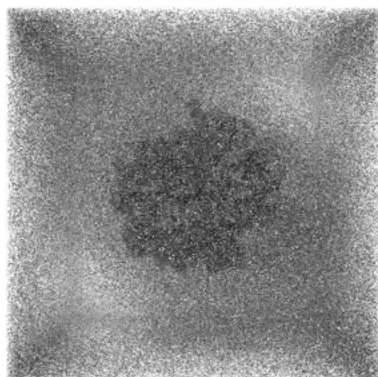
Y



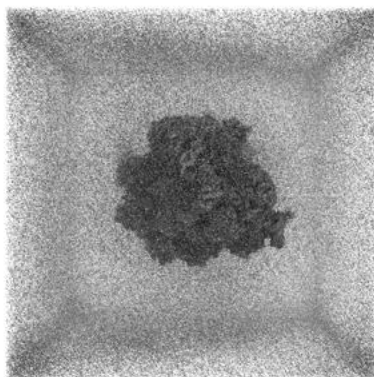
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

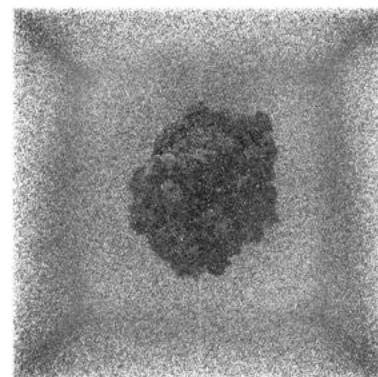
### 6.5.2 Raw map



X



Y



Z

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

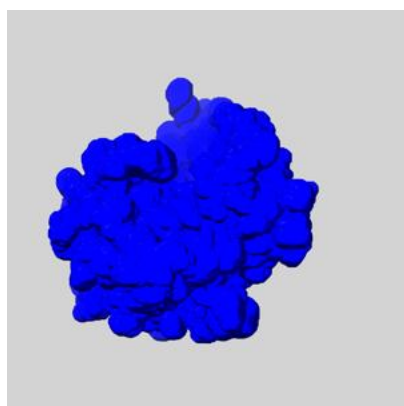
## 6.6 Mask visualisation [i](#)

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

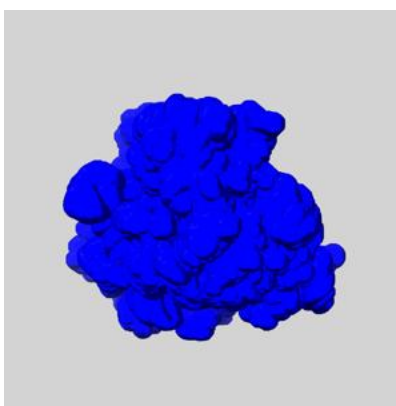
A mask typically either:

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

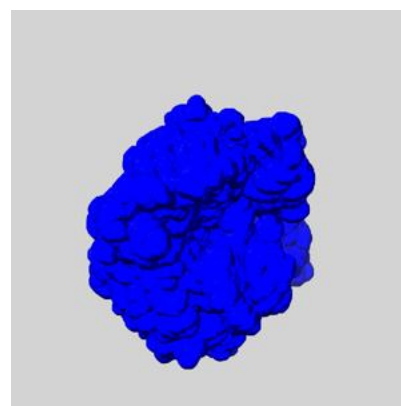
### 6.6.1 emd\_67339\_msk\_1.map [i](#)



X



Y

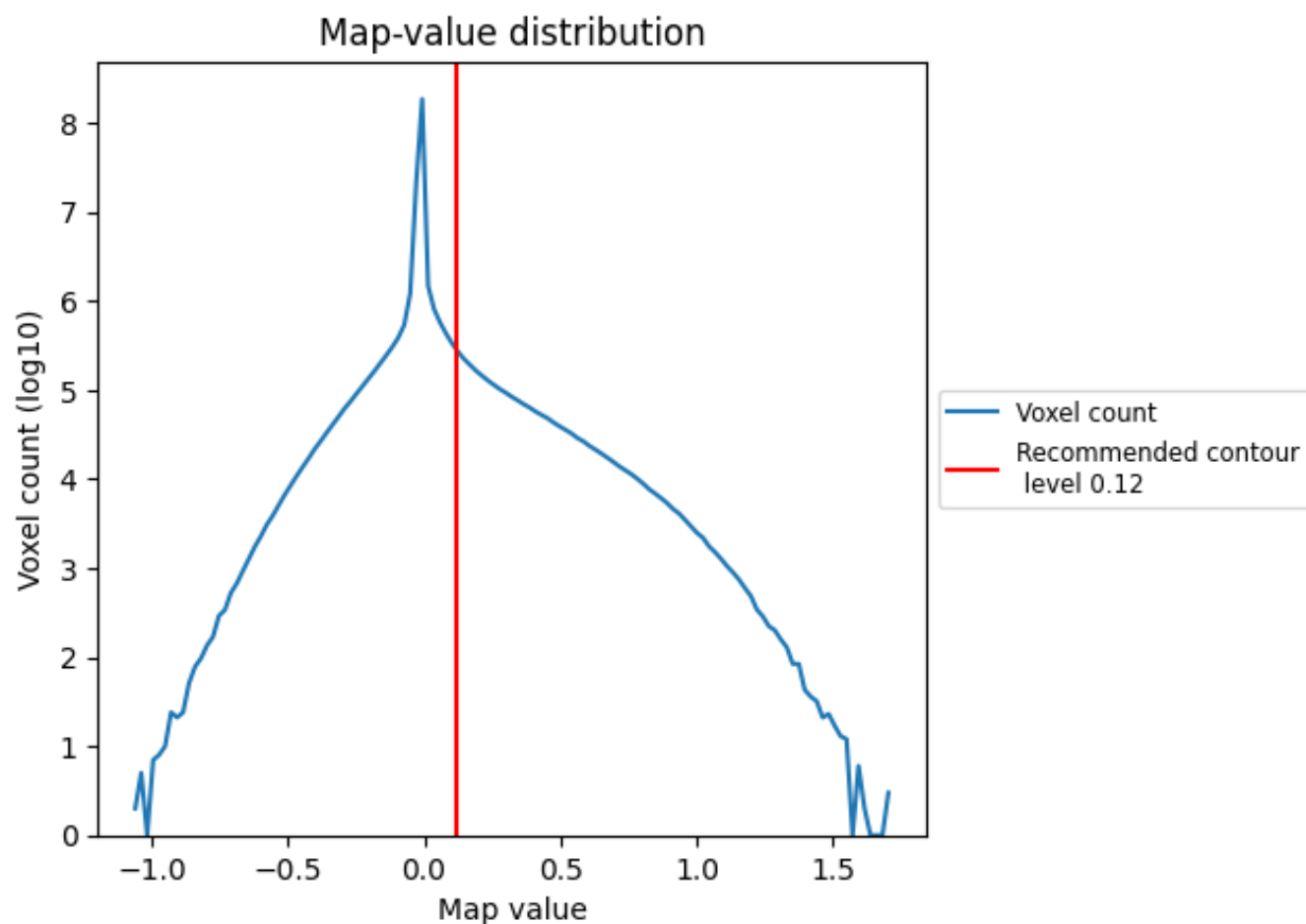


Z

## 7 Map analysis [i](#)

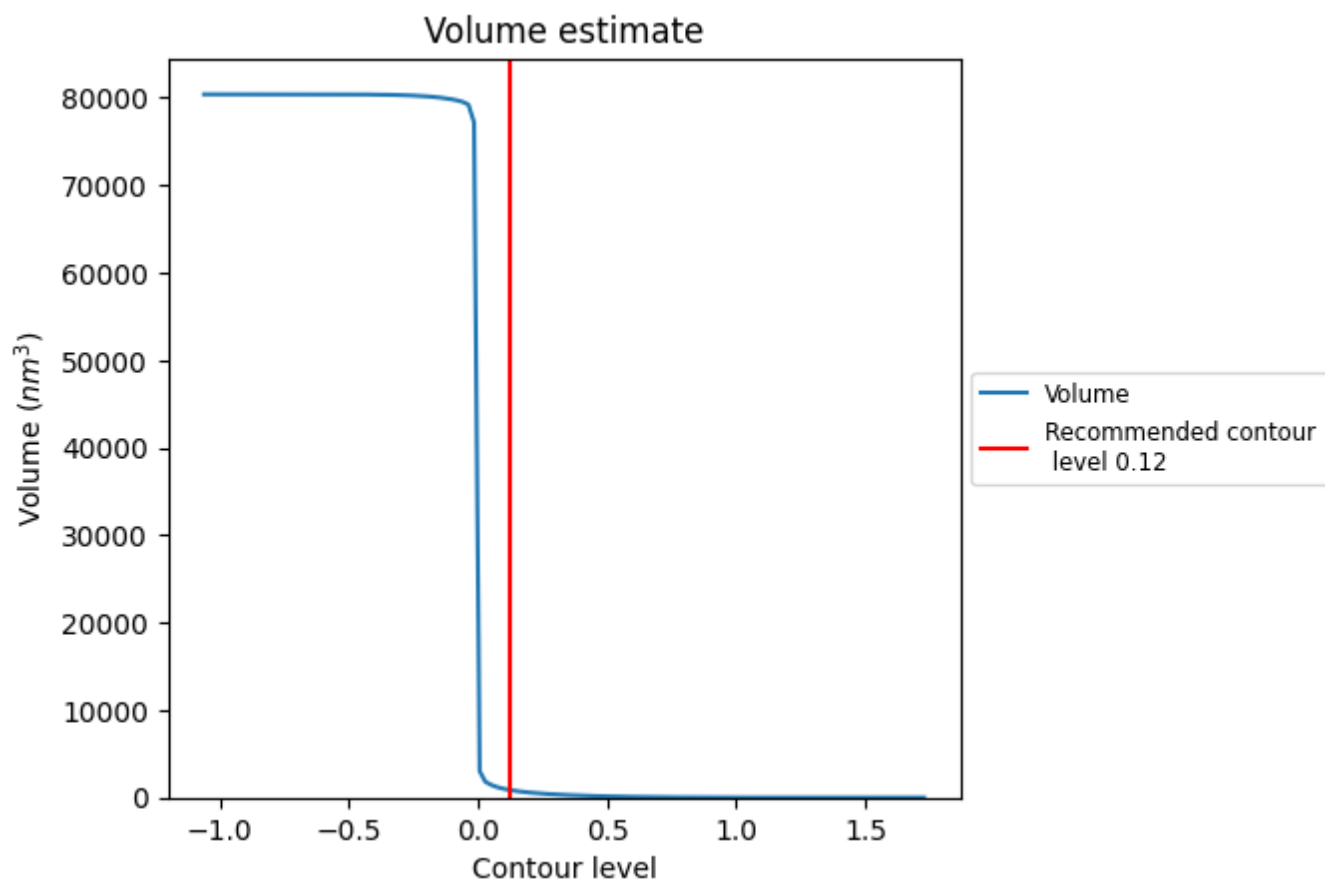
This section contains the results of statistical analysis of the map.

### 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.

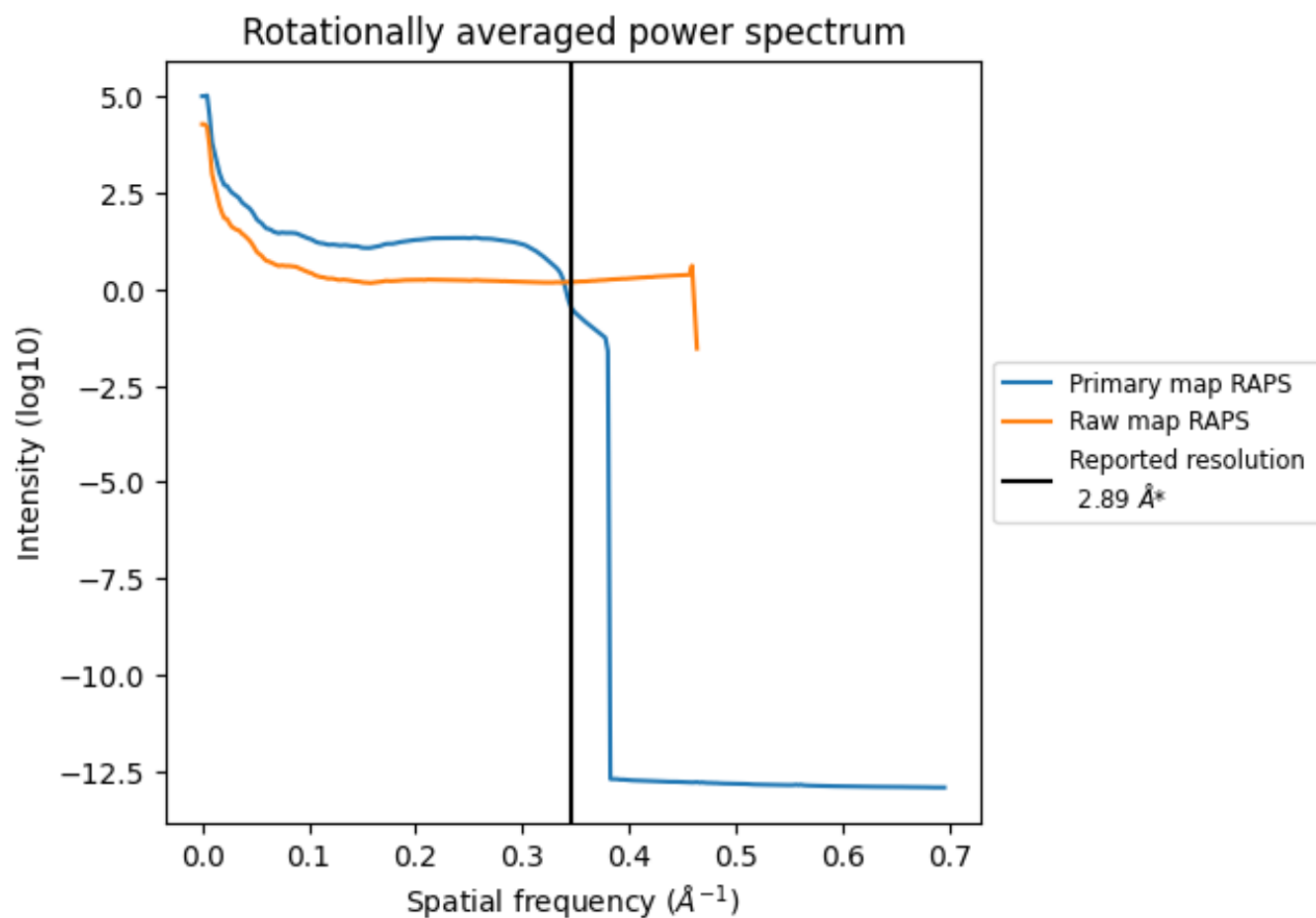
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 880  $\text{nm}^3$ ; this corresponds to an approximate mass of 795 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 ⓘ

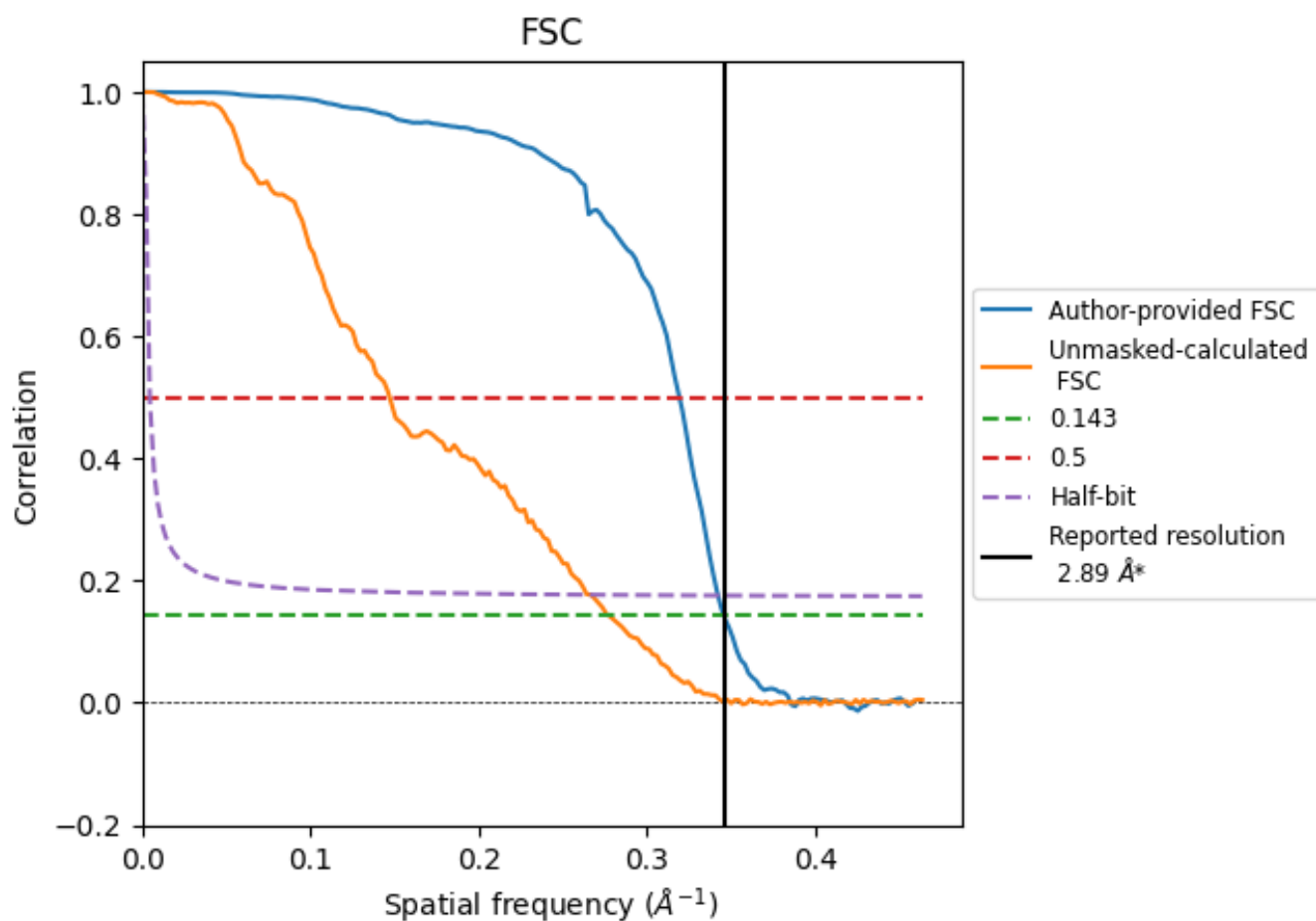


\*Reported resolution corresponds to spatial frequency of 0.346 Å<sup>-1</sup>

## 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 0.346  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

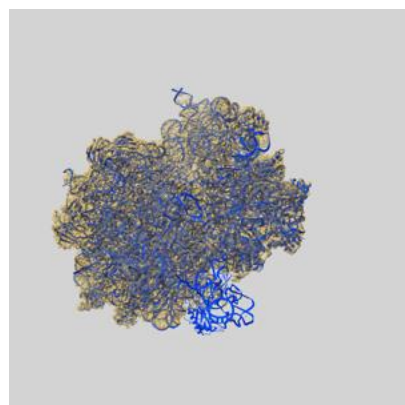
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.89	-	-
Author-provided FSC curve	2.89	3.13	2.92
Unmasked-calculated*	3.61	6.80	3.75

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.61 differs from the reported value 2.89 by more than 10 %

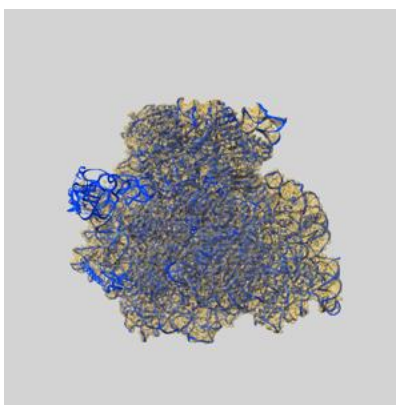
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-67339 and PDB model 9XWO. Per-residue inclusion information can be found in section [3](#) on page [18](#).

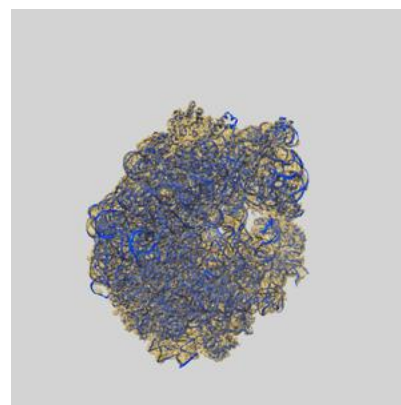
### 9.1 Map-model overlay [i](#)



X



Y

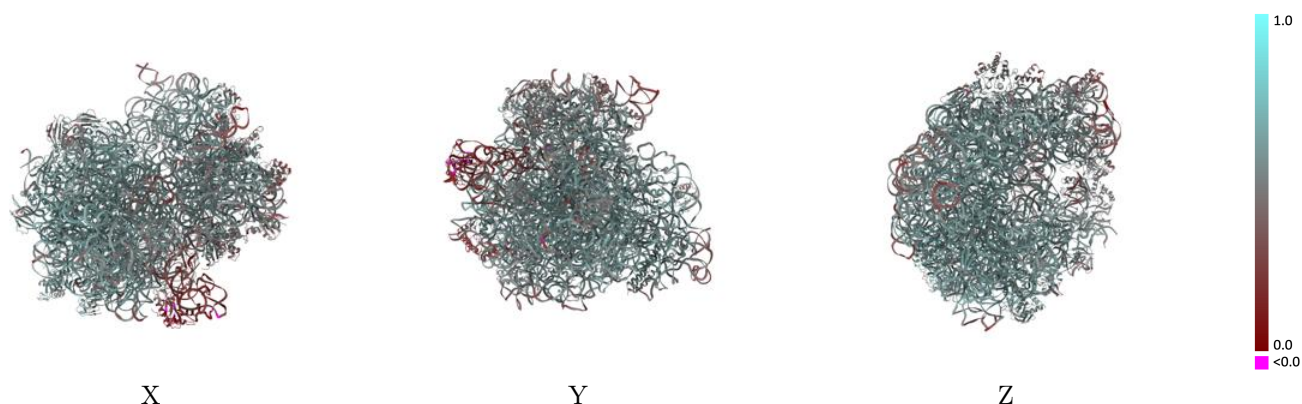


Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 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.

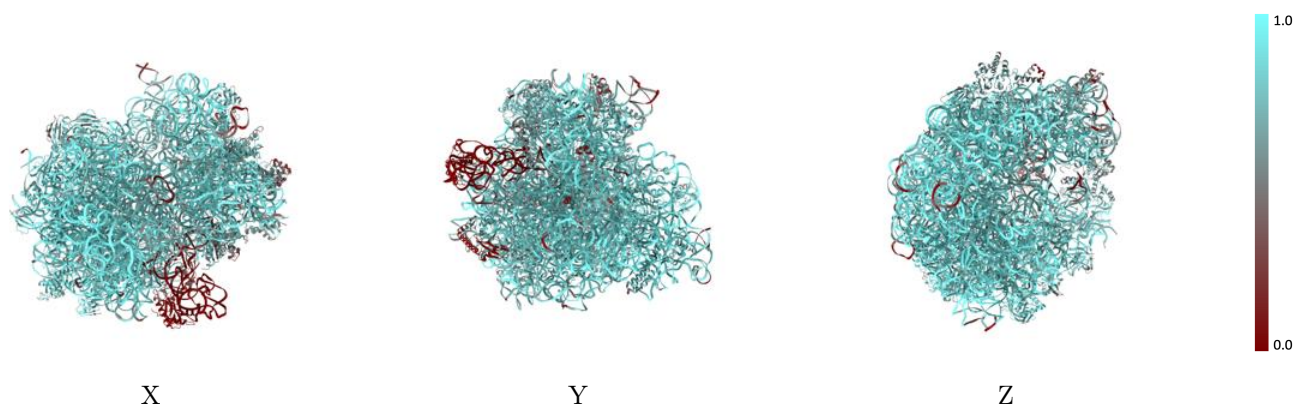


## 9.2 Q-score mapped to coordinate model [i](#)



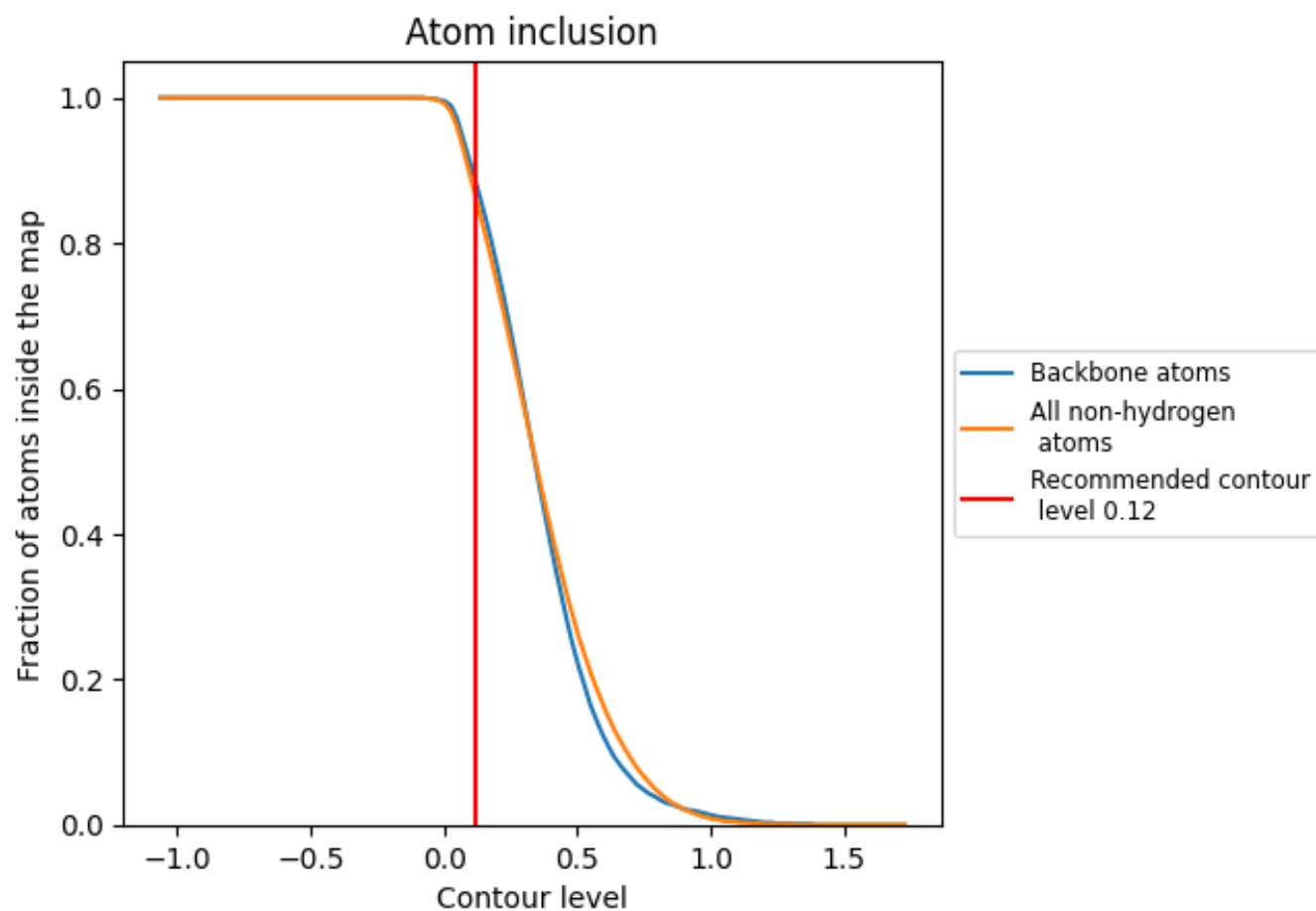
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 86% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8640	 0.5560
0	 0.8260	 0.5500
1	 0.9440	 0.6180
2	 0.9470	 0.6180
3	 0.8770	 0.5800
4	 0.5800	 0.4270
5	 0.0910	 0.2750
6	 0.8970	 0.5900
7	 0.0010	 0.1710
A	 0.9120	 0.5580
B	 0.6300	 0.4650
C	 0.7650	 0.5210
D	 0.7940	 0.5350
E	 0.8500	 0.5630
F	 0.7260	 0.4980
G	 0.5390	 0.4320
H	 0.8660	 0.5690
I	 0.7140	 0.4780
J	 0.6240	 0.4560
K	 0.7710	 0.5270
L	 0.8190	 0.5600
M	 0.7060	 0.4880
N	 0.7750	 0.5090
O	 0.8230	 0.5510
P	 0.8410	 0.5620
Q	 0.8000	 0.5350
R	 0.7590	 0.5180
S	 0.6960	 0.4940
T	 0.8030	 0.5370
U	 0.5370	 0.4320
X	 0.6840	 0.4870
Y	 0.9080	 0.5570
Z	 0.8680	 0.5480
a	 0.9210	 0.5820
b	 0.9150	 0.5450



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
c	 0.9200	 0.6020
d	 0.9100	 0.5910
e	 0.8550	 0.5720
f	 0.7220	 0.4950
g	 0.7140	 0.4900
h	 0.2250	 0.3470
i	 0.9070	 0.5930
j	 0.8980	 0.5930
k	 0.9100	 0.5950
l	 0.8990	 0.5950
m	 0.9340	 0.6000
n	 0.8050	 0.5200
o	 0.8760	 0.5800
p	 0.9370	 0.6110
q	 0.8830	 0.5830
r	 0.8960	 0.5920
s	 0.8210	 0.5430
t	 0.8090	 0.5420
u	 0.8030	 0.5420
v	 0.9320	 0.6040
w	 0.8850	 0.5860
x	 0.7610	 0.5090
y	 0.8580	 0.5820
z	 0.8900	 0.5910