



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:44 AM UTC

PDB ID : 7QGH / pdb_00007qgh
EMDB ID : EMD-13955
Title : Structure of the E. coli disome - collided 70S ribosome
Authors : Kratzat, H.; Buschauer, R.; Berninghausen, O.; Beckmann, R.
Deposited on : 2021-12-08
Resolution : 4.48 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

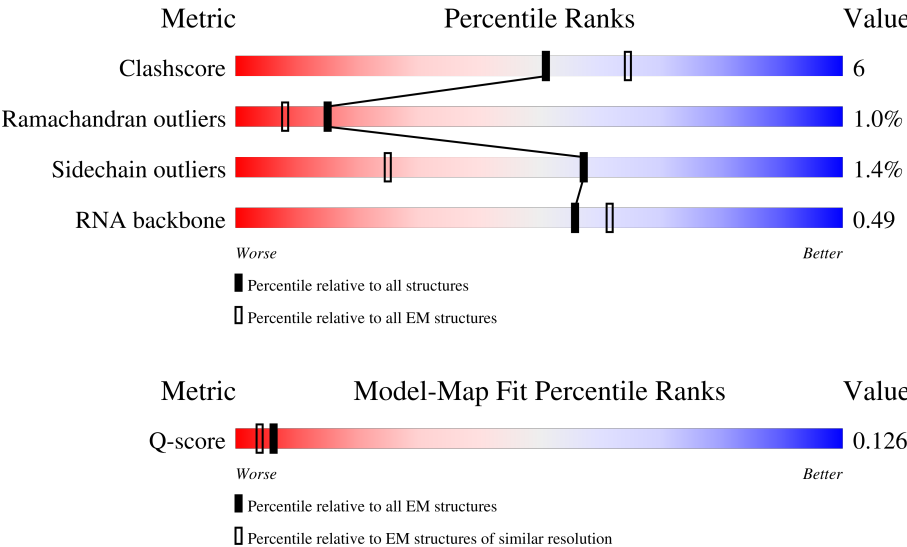
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 4.48 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.



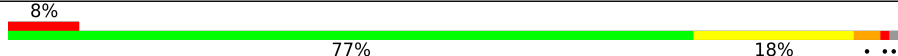
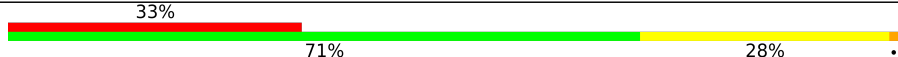
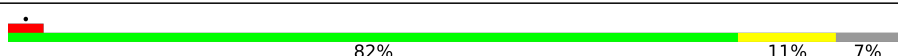
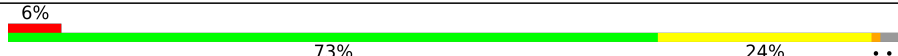
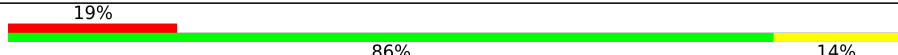
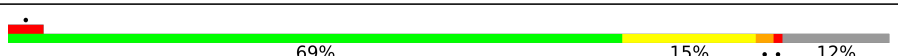
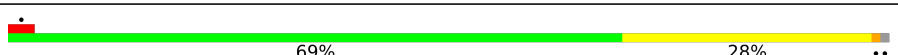
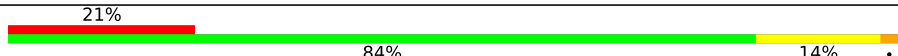
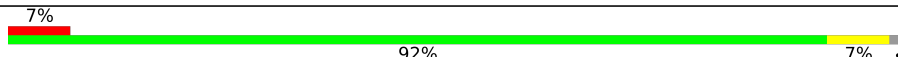
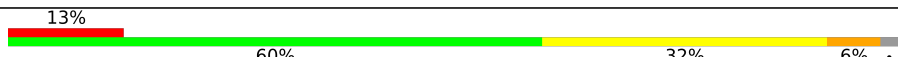
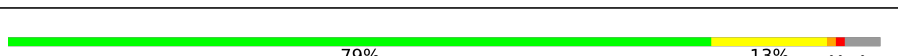
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2912 (3.99 - 4.98)

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

Mol	Chain	Length	Quality of chain
1	O	120	
2	P	275	
3	Q	209	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	R	201	
5	S	179	
6	T	177	
7	V	142	
8	W	142	
9	X	123	
10	Y	144	
11	Z	137	
12	a	127	
13	b	117	
14	c	115	
15	d	118	
16	e	103	
17	f	110	
18	g	100	
19	h	104	
20	i	94	
21	j	85	
22	k	78	
23	l	63	
24	m	59	
25	n	57	
26	o	55	
27	p	47	
28	q	67	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	r	55	
30	N	2903	
31	L	70	
32	C	223	
33	U	149	
34	M	75	
35	x	692	
36	0	1539	
37	1	244	
38	2	237	
39	3	206	
40	4	162	
41	5	131	
42	6	152	
43	7	130	
44	8	130	
45	9	110	
46	A	129	
47	B	124	
48	D	118	
49	E	101	
50	F	89	
51	G	100	
52	H	84	
53	I	75	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	J	92	25% 65% 16% • • 14%
55	K	87	8% 74% 22% • • •
56	s	88	15% 43% 13% • 42%
57	t	557	24% 24% • 74%
58	u	73	21% 67% 27% 5%

2 Entry composition [i](#)

There are 61 unique types of molecules in this entry. The entry contains 147973 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 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	118	Total	C	N	O	P	0	0
			2529	1126	464	821	118		

- Molecule 2 is a protein called 50S ribosomal protein L2.

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

- Molecule 3 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Q	209	Total	C	N	O	S	0	0
			1564	979	288	293	4		

- Molecule 4 is a protein called 50S ribosomal protein L4.

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

- Molecule 5 is a protein called 50S ribosomal protein L5.

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

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	176	Total	C	N	O	S	0	0
			1322	832	243	245	2		

- Molecule 7 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	V	141	Total	C	N	O	S	0	0
			1031	651	179	195	6		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	W	142	Total	C	N	O	S	0	0
			1128	714	212	198	4		

- Molecule 9 is a protein called 50S ribosomal protein L14.

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

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	Y	143	Total	C	N	O	S	0	0
			1044	649	206	188	1		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Z	136	Total	C	N	O	S	0	0
			1073	686	205	176	6		

- Molecule 12 is a protein called 50S ribosomal protein L17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	123	ALA	GLU	conflict	UNP P0AG44

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	b	116	Total	C	N	O	0	0
			891	552	178	161		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	c	114	Total	C	N	O	S	0	0
			915	573	179	162	1		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	d	117	Total	C	N	O	0	0
			946	604	192	150		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	e	103	Total	C	N	O	S	0	0
			815	516	153	144	2		

- Molecule 17 is a protein called 50S ribosomal protein L22.

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

- Molecule 18 is a protein called 50S ribosomal protein L23.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	98	SER	GLY	conflict	UNP P0ADZ0

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	h	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 20 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	i	94	Total	C	N	O	S	0	0
			752	479	137	133	3		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	j	75	Total	C	N	O	S	0	0
			568	353	113	101	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
j	3	UNK	HIS	conflict	UNP P0A7L8

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	k	77	Total	C	N	O	S	0	0
			624	388	129	105	2		

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	l	63	Total	C	N	O	S	0	0
			508	313	99	94	2		

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	m	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 25 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	n	56	Total	C	N	O	S	0	0
			443	269	94	79	1		

- Molecule 26 is a protein called 50S ribosomal protein L33.

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

- Molecule 27 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	p	46	Total	C	N	O	S	0	0
			376	228	90	56	2		

- Molecule 28 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	q	64	Total	C	N	O	S	0	0
			503	323	105	73	2		

- Molecule 29 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	r	38	Total	C	N	O	S	0	0
			301	185	65	47	4		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	N	2897	Total	C	N	O	P	1	0
			62215	27754	11448	20115	2898		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	52	Total	C	N	O	S	0	0
			404	250	73	75	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	68	SER	GLY	conflict	UNP P0A7M9

- Molecule 32 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	C	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	75	Total	C	N	O	P	0	0
			1594	711	281	527	75		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	x	14	Total	C	N	O	P	0	0
			294	132	51	97	14		

- Molecule 36 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	0	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 37 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 38 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	2	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 39 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	3	205	Total	C	N	O	S	0	0
			1642	1026	315	297	4		

- Molecule 40 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	4	150	Total	C	N	O	S	0	0
			1105	687	211	201	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	4	MET	ILE	conflict	UNP P0A7W1

- Molecule 41 is a protein called 30S ribosomal protein S6, non-modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	5	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	101	SER	PRO	conflict	UNP P02358

- Molecule 42 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 43 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	7	129	Total	C	N	O	S	0	0
			978	616	173	183	6		

- Molecule 44 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	8	127	Total	C	N	O	S	0	0
			1021	634	206	178	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
8	3	ASP	GLU	conflict	UNP P0A7X3

- Molecule 45 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	9	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 46 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	A	117	Total	C	N	O	S	0	0
			876	540	174	159	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	PRO	conflict	UNP P0A7R9

- Molecule 47 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	B	123	Total	C	N	O	S	0	0
			954	590	196	164	4		

- Molecule 48 is a protein called 30S ribosomal protein S13.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	MET	conflict	UNP P0A7S9

- Molecule 49 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	E	96	Total	C	N	O	S	0	0
			773	483	160	127	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	40	ALA	ASP	conflict	UNP P0AG59

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	F	88	Total	C	N	O	S	0	0
			709	437	143	128	1		

- Molecule 51 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	G	82	Total	C	N	O	S	0	0
			648	406	128	113	1		

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	2	ALA	THR	conflict	UNP P0AG63

- Molecule 53 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	I	55	Total	C	N	O	0	0
			455	288	86	81		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	15	THR	ALA	conflict	UNP P0A7T7
I	19	VAL	GLN	conflict	UNP P0A7T7

- Molecule 54 is a protein called 30S ribosomal protein S19.

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

- Molecule 55 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	K	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	LEU	MET	conflict	UNP P0A7U7

- Molecule 56 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	s	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

- Molecule 57 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	t	143	Total	C	N	O		0	0
			704	418	143	143			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	241	VAL	ILE	conflict	UNP P0AG67

- Molecule 58 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	u	73	Total	C	N	O	P	0	0
			1561	695	279	514	73		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	3	G	C	conflict	GB 1851743410
u	70	C	G	conflict	GB 1851743410

- Molecule 59 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	u	2	Total	Mg	0
			2	2	

- Molecule 60 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
60	u	1	Total	K	0
			1	1	

- Molecule 61 is water.

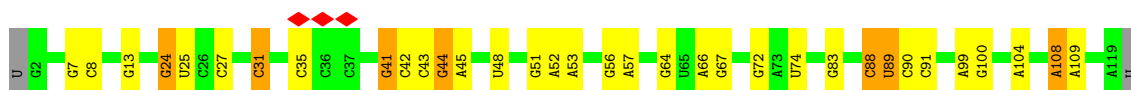
Mol	Chain	Residues	Atoms		AltConf
61	u	9	Total	O	0
			9	9	

3 Residue-property plots [i](#)

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.

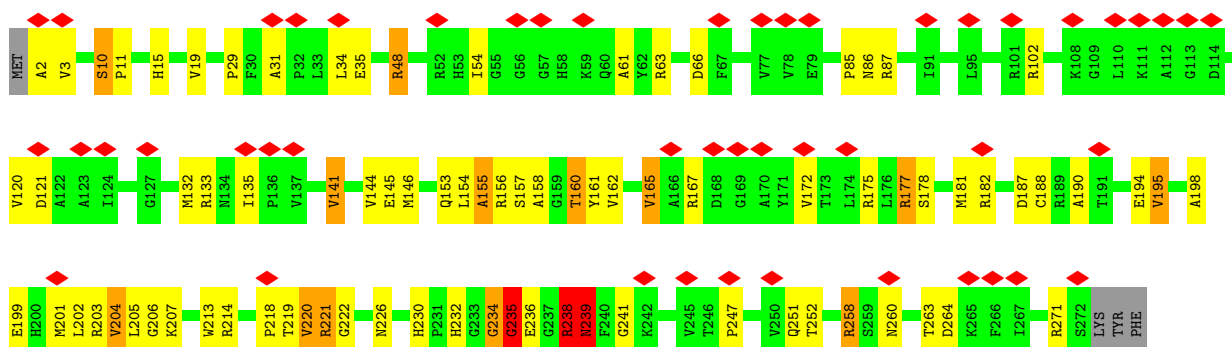
• Molecule 1: 5S rRNA

Chain O: 



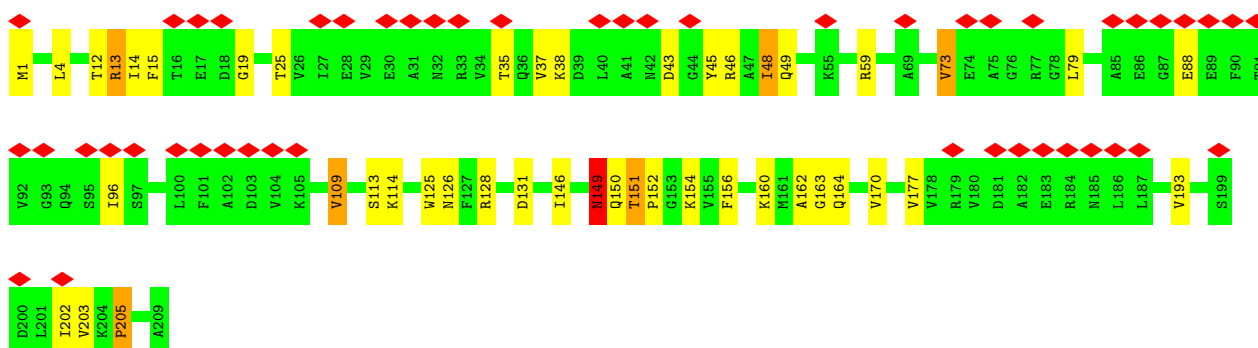
• Molecule 2: 50S ribosomal protein L2

Chain P: 

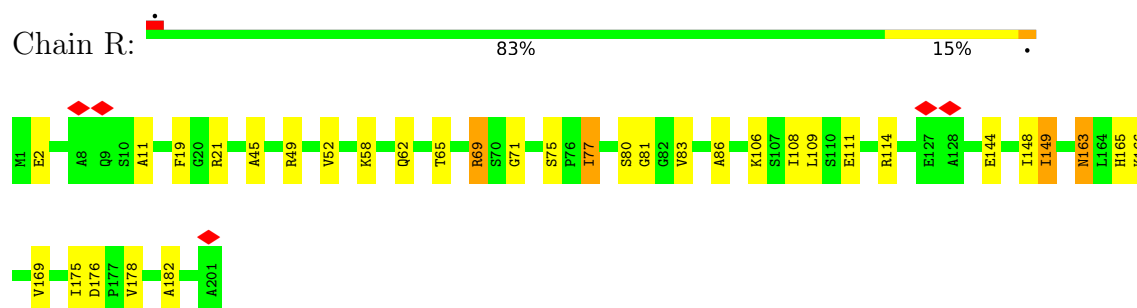


• Molecule 3: 50S ribosomal protein L3

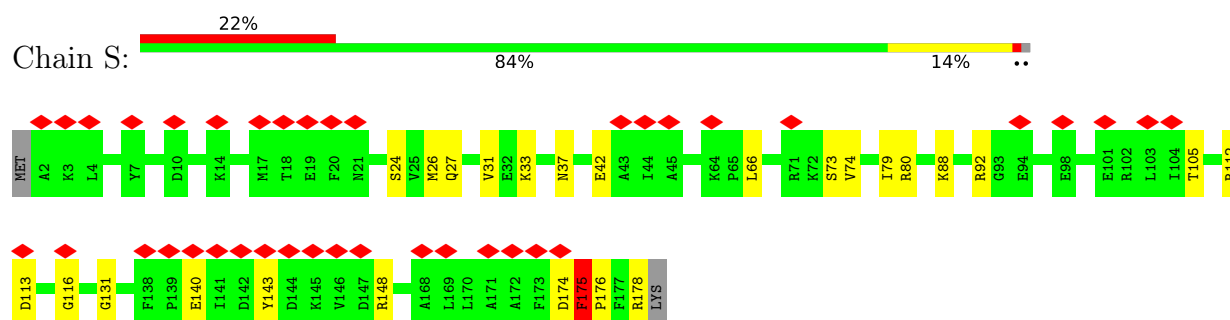
Chain Q: 



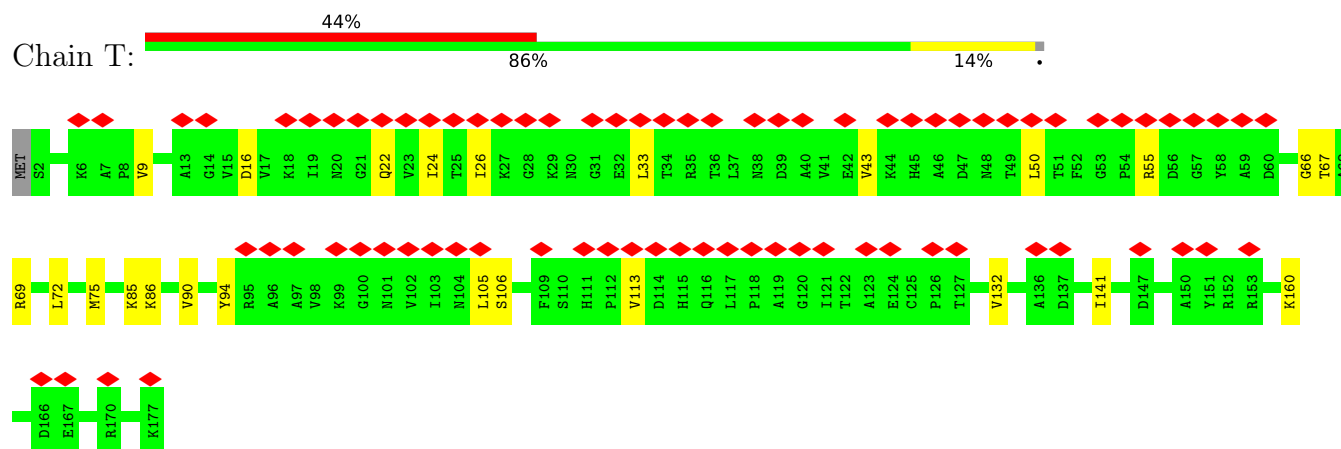
- Molecule 4: 50S ribosomal protein L4



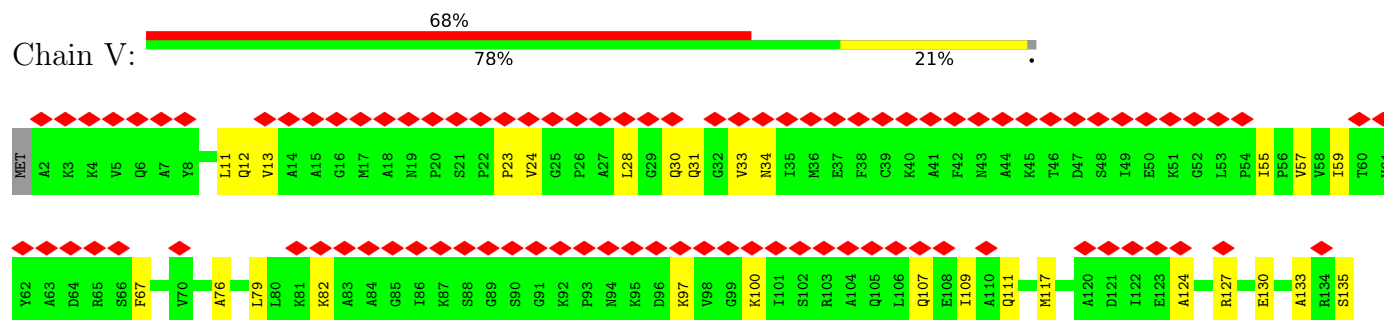
- Molecule 5: 50S ribosomal protein L5

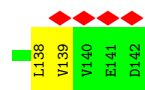


- Molecule 6: 50S ribosomal protein L6

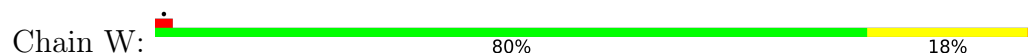


- Molecule 7: 50S ribosomal protein L11

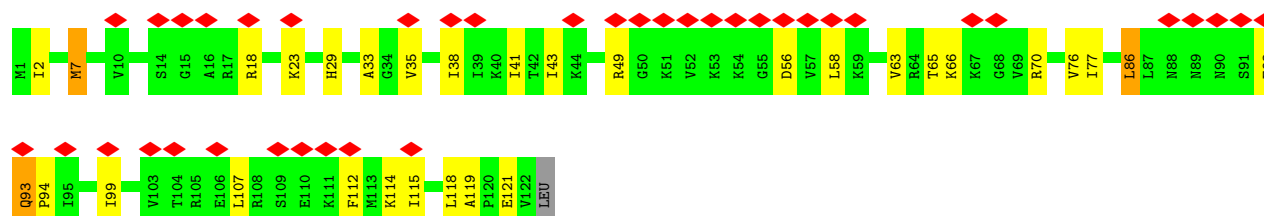
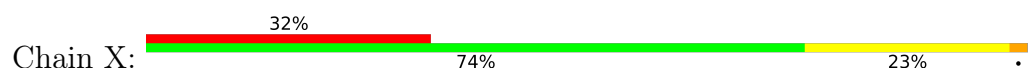




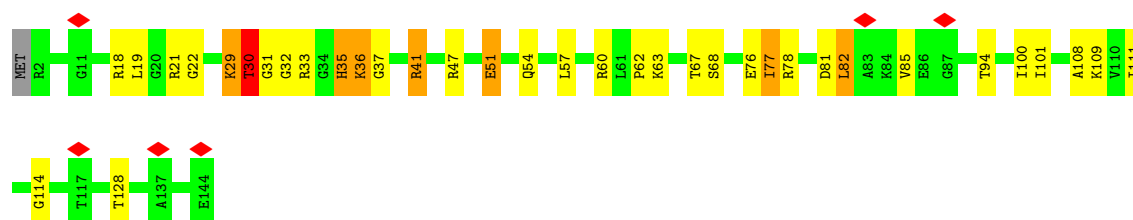
- Molecule 8: 50S ribosomal protein L13



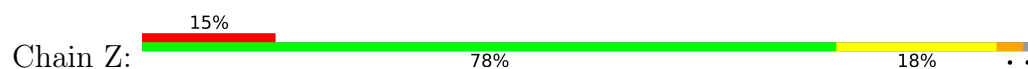
- Molecule 9: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L15

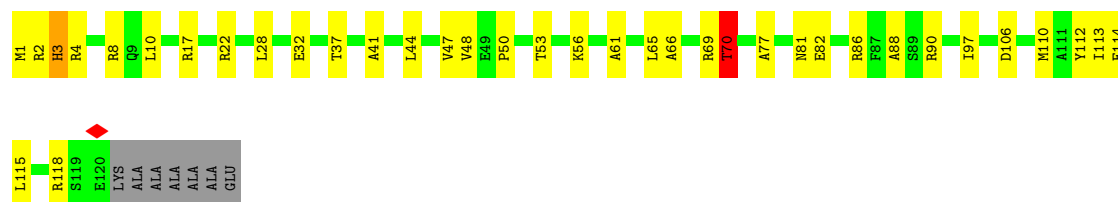


- Molecule 11: 50S ribosomal protein L16



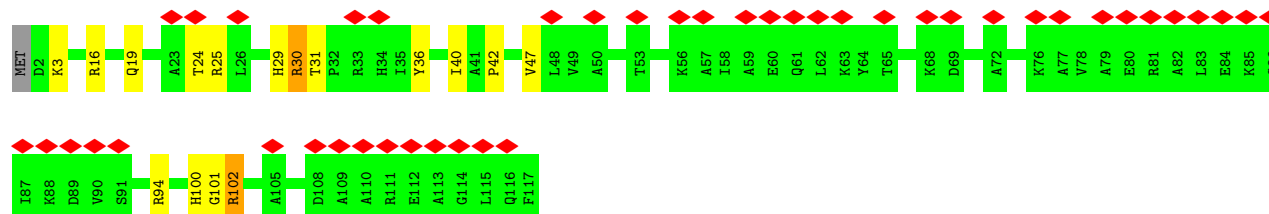
- Molecule 12: 50S ribosomal protein L17





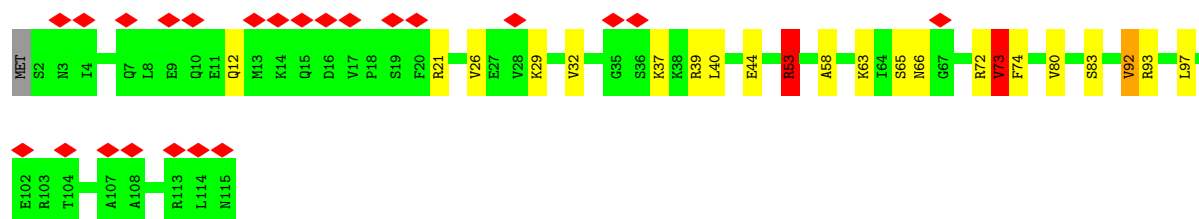
- Molecule 13: 50S ribosomal protein L18

Chain b: 38% 85% 12% ..



- Molecule 14: 50S ribosomal protein L19

Chain c: 20% 80% 17% ...



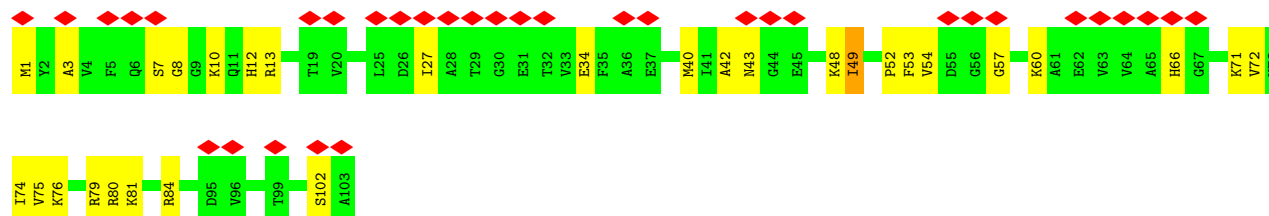
- Molecule 15: 50S ribosomal protein L20

Chain d: 8% 77% 18% ..

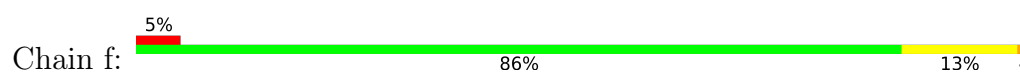


- Molecule 16: 50S ribosomal protein L21

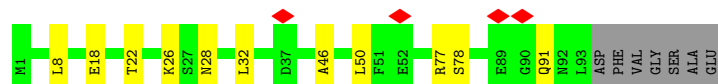
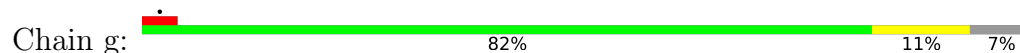
Chain e: 33% 71% 28% .



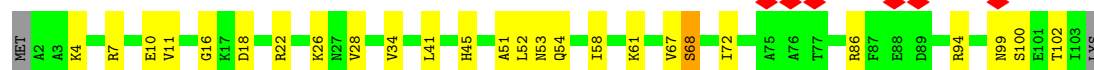
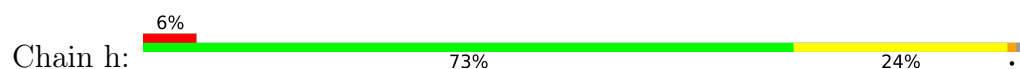
- Molecule 17: 50S ribosomal protein L22



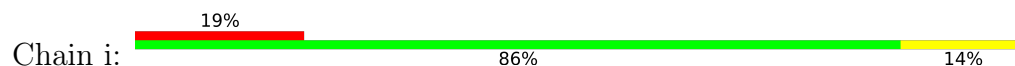
- Molecule 18: 50S ribosomal protein L23



- Molecule 19: 50S ribosomal protein L24



- Molecule 20: 50S ribosomal protein L25



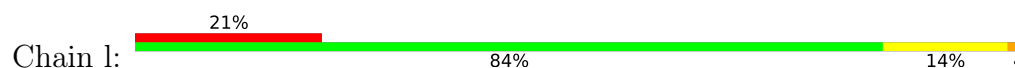
- Molecule 21: 50S ribosomal protein L27

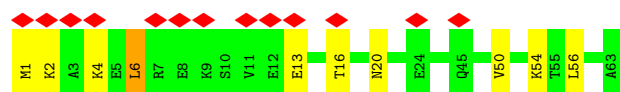


- Molecule 22: 50S ribosomal protein L28

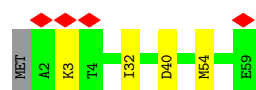


- Molecule 23: 50S ribosomal protein L29





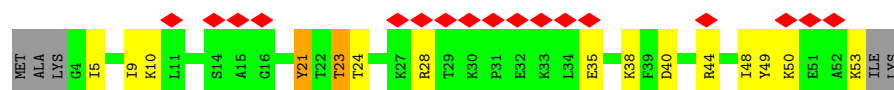
- Molecule 24: 50S ribosomal protein L30



- Molecule 25: 50S ribosomal protein L32



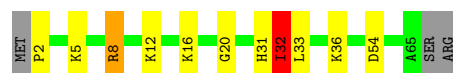
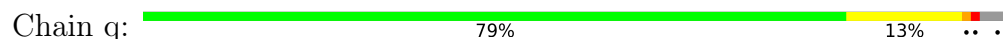
- Molecule 26: 50S ribosomal protein L33



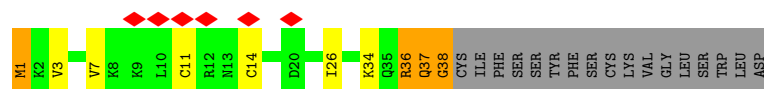
- Molecule 27: 50S ribosomal protein L34



- Molecule 28: 50S ribosomal protein L35

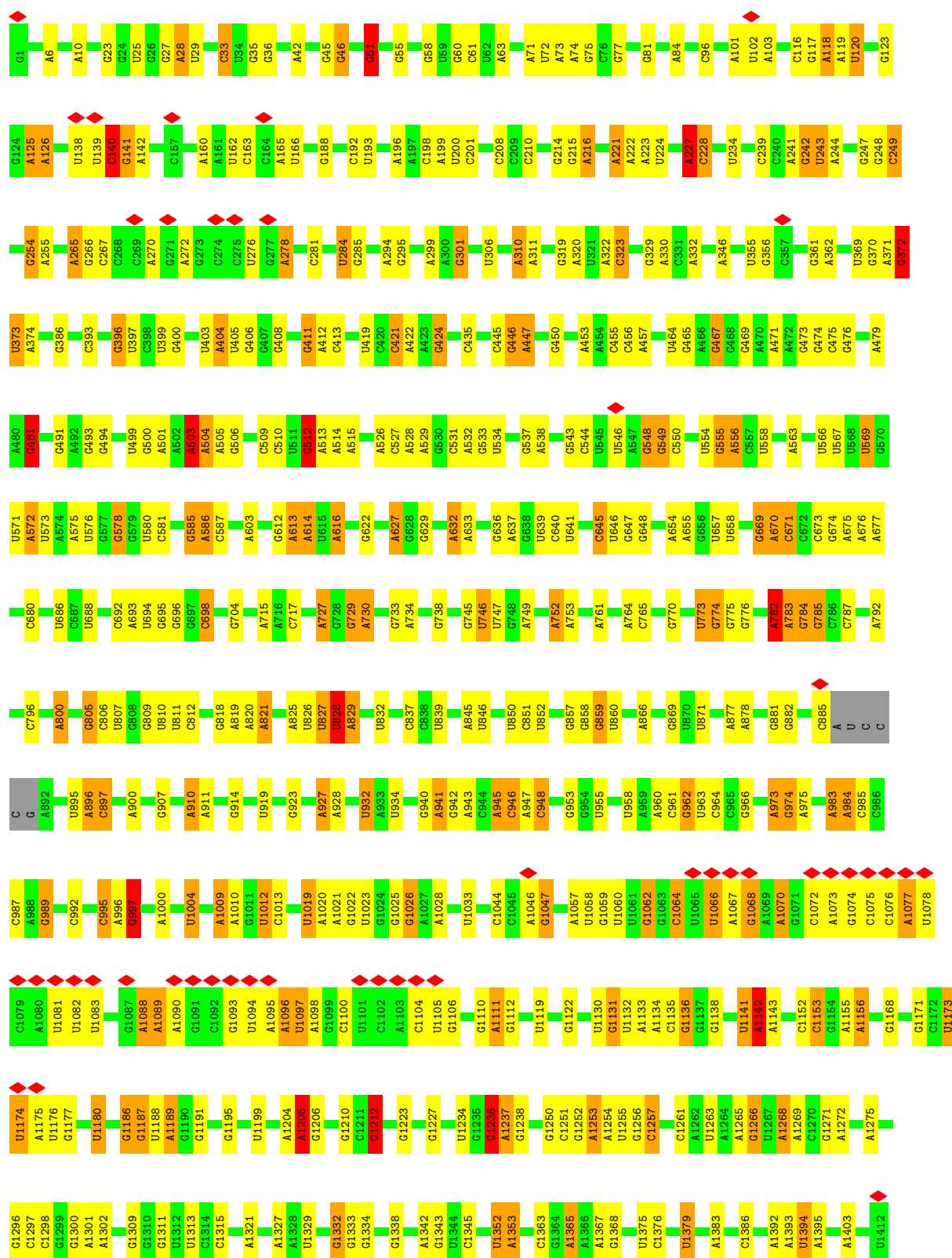


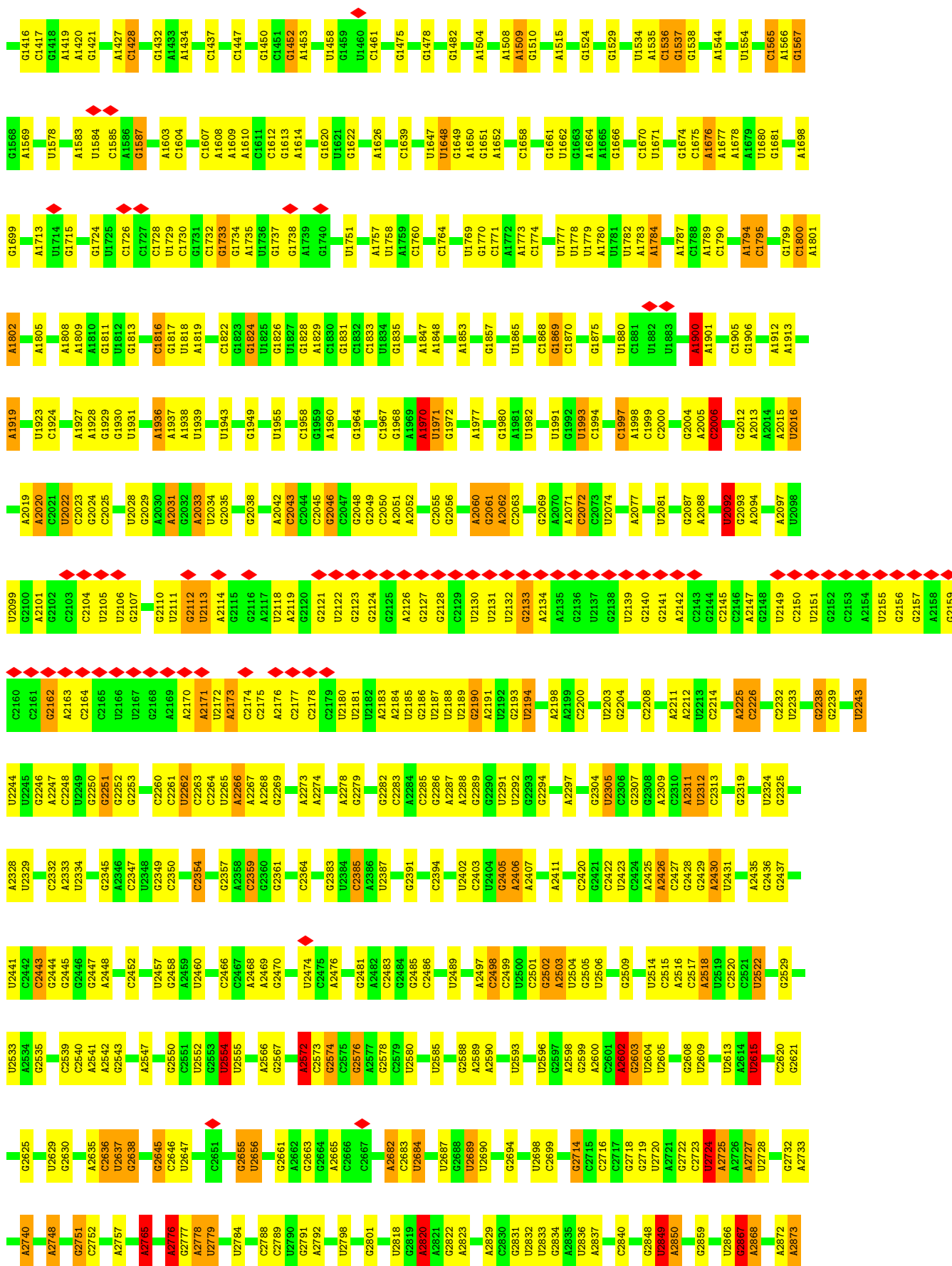
- Molecule 29: 50S ribosomal protein L36

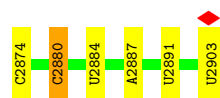


- Molecule 30: 23S rRNA

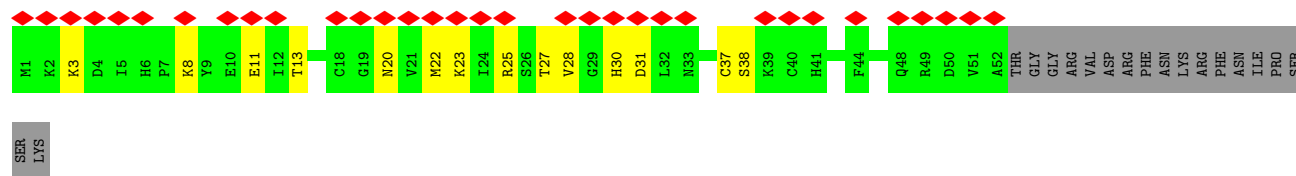
Chain N:  64% 28% 7%



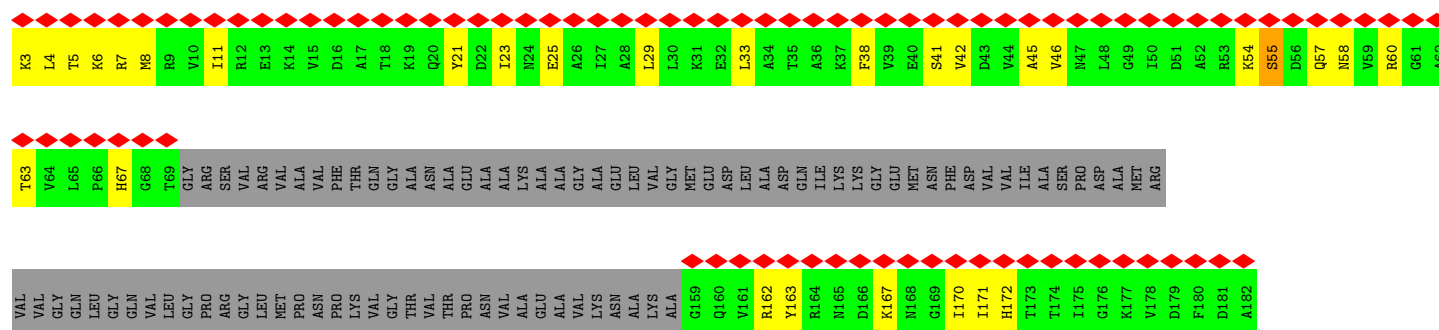




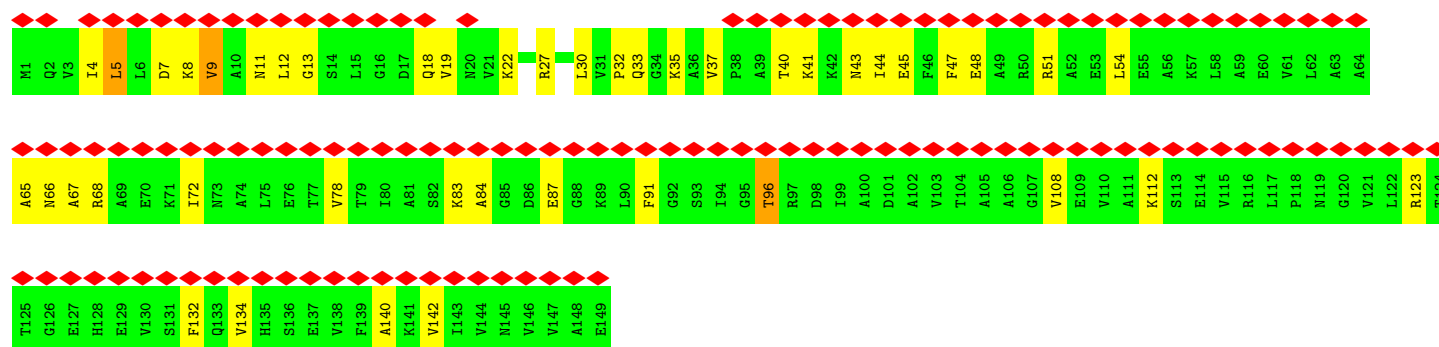
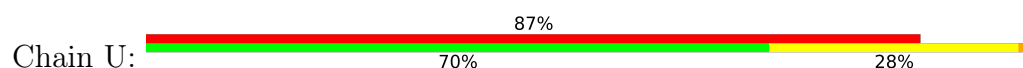
• Molecule 31: 50S ribosomal protein L31



• Molecule 32: 50S ribosomal protein L1

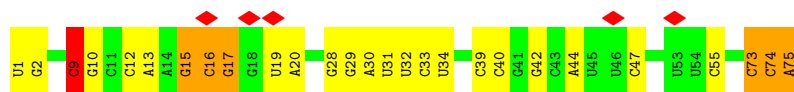


• Molecule 33: 50S ribosomal protein L9



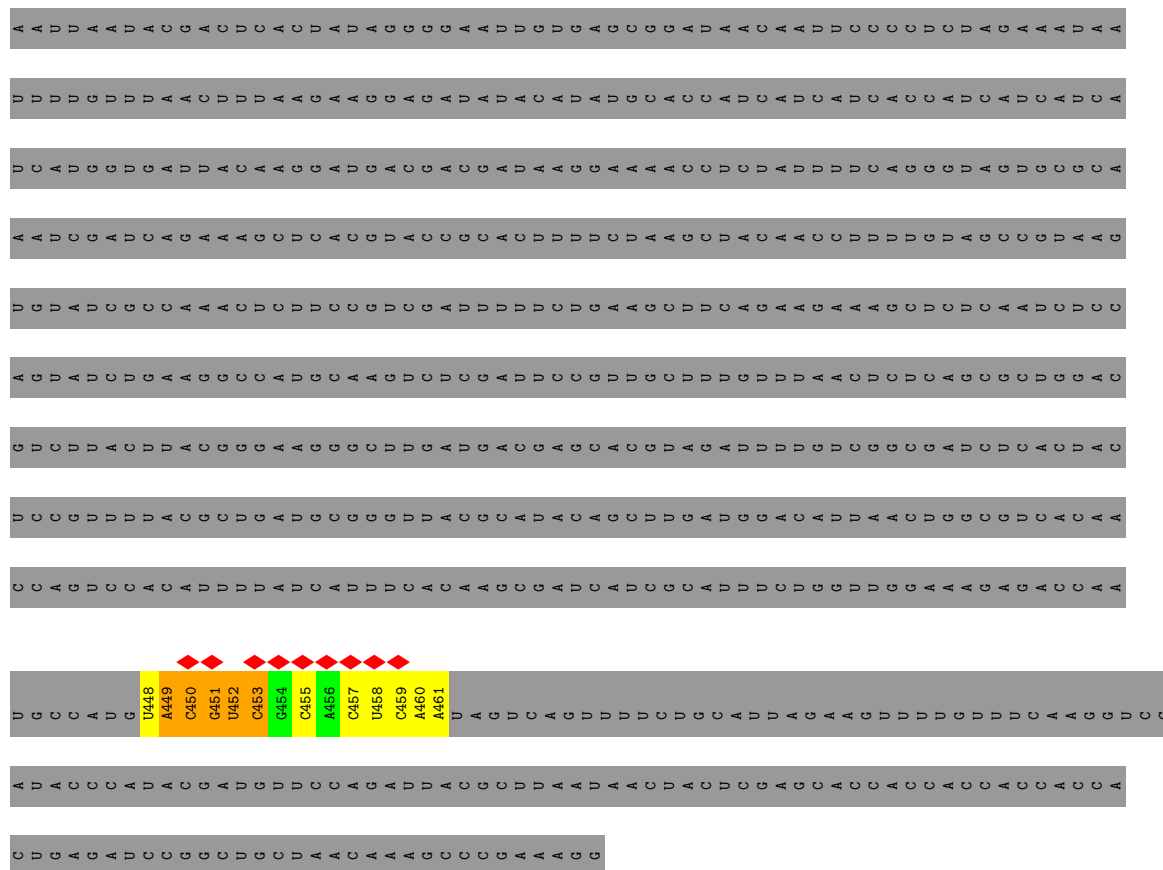
• Molecule 34: P-site tRNA





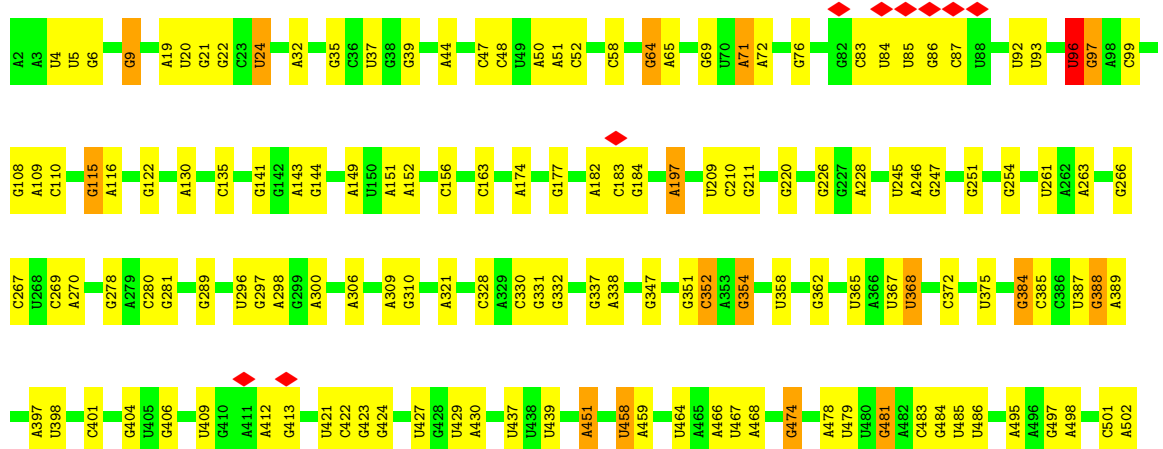
• Molecule 35: mRNA

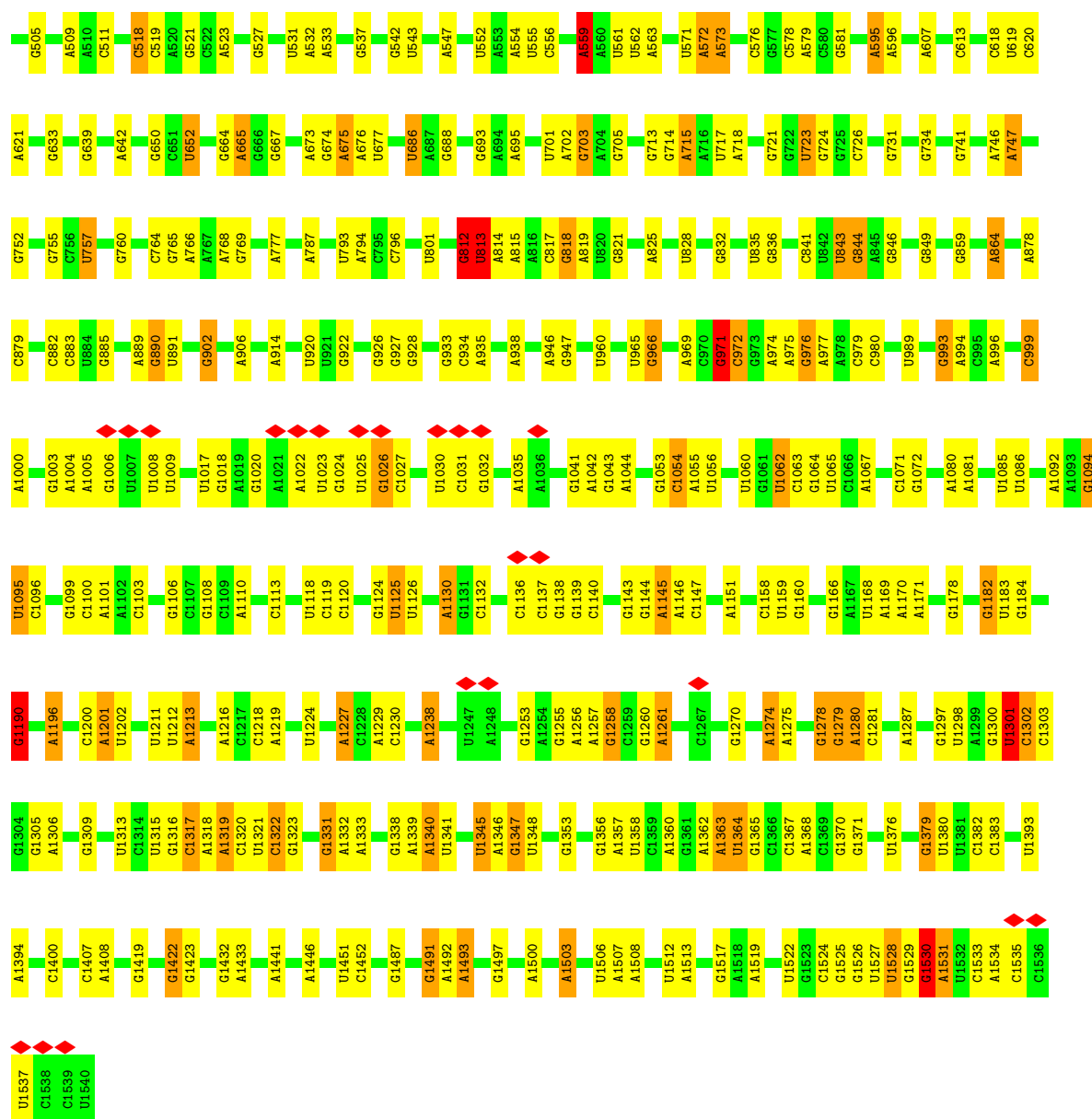
Chain x: 98%



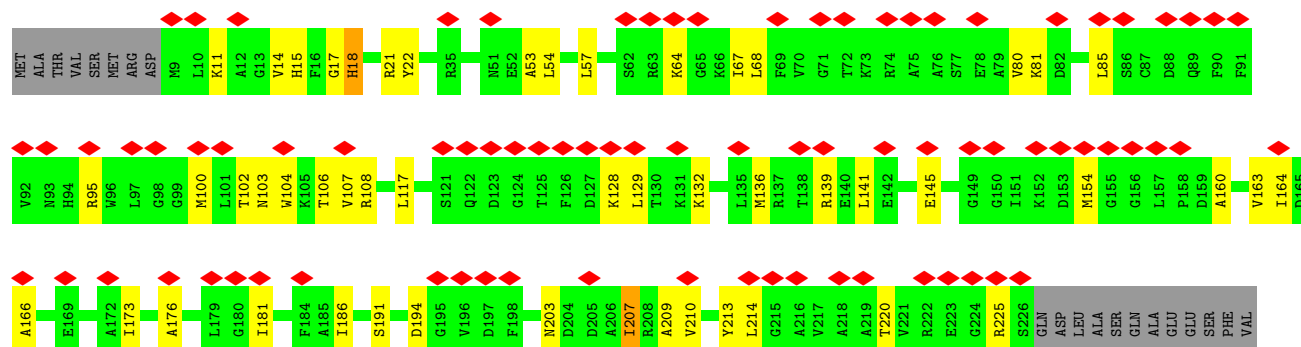
• Molecule 36: 16S rRNA

Chain 0: 68% 27% 5%



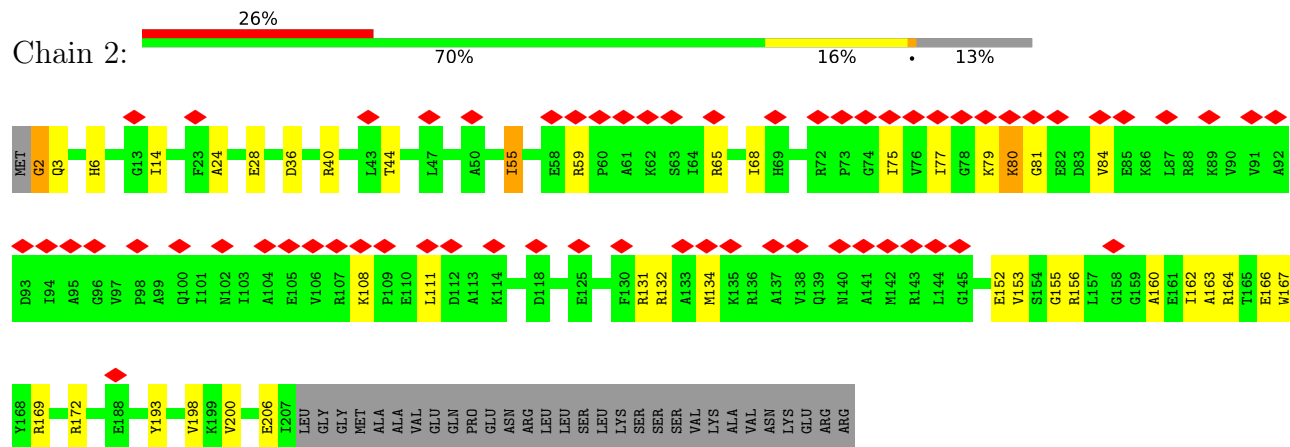


• Molecule 37: 30S ribosomal protein S2

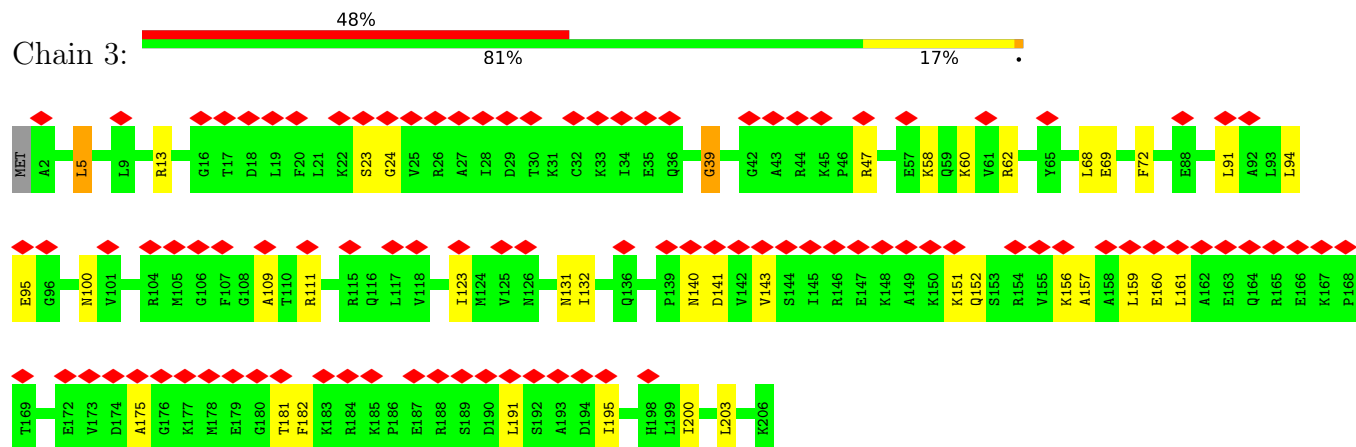


GLU
LEU
SER
ASN
LYS
ALA

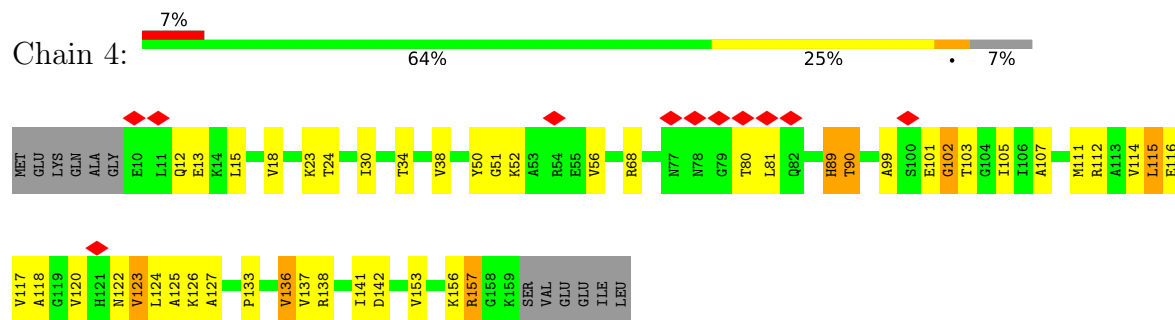
• Molecule 38: 30S ribosomal protein S3



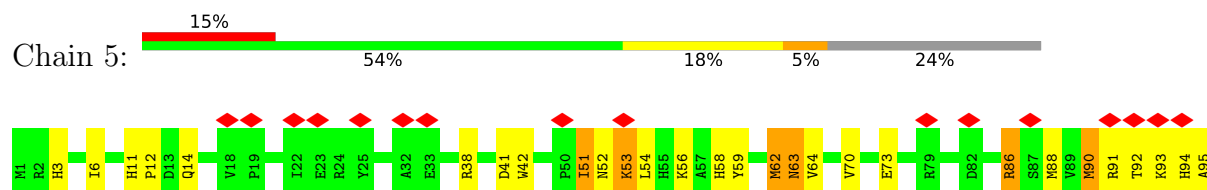
• Molecule 39: 30S ribosomal protein S4

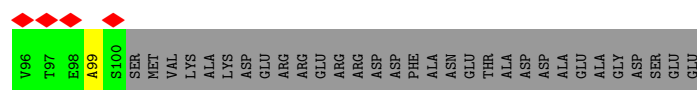


• Molecule 40: 30S ribosomal protein S5

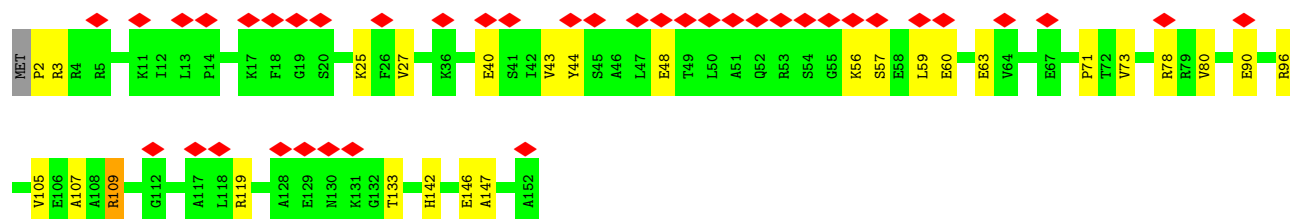
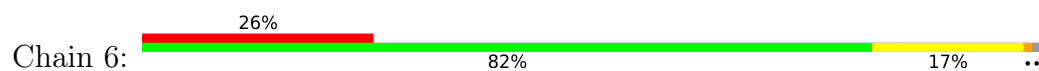


• Molecule 41: 30S ribosomal protein S6, non-modified isoform

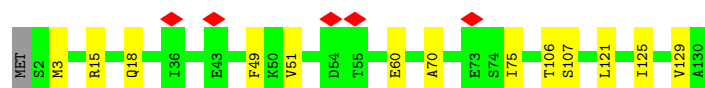
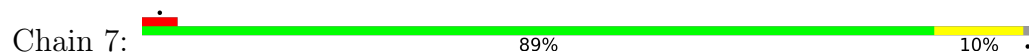




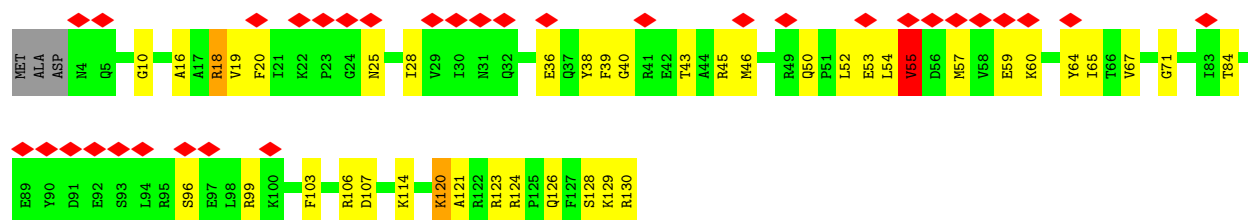
• Molecule 42: 30S ribosomal protein S7



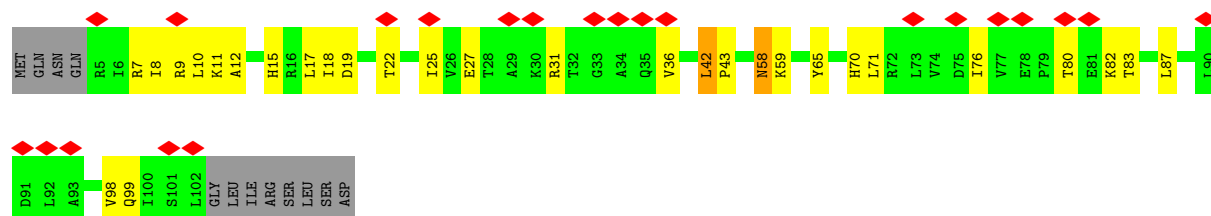
• Molecule 43: 30S ribosomal protein S8



• Molecule 44: 30S ribosomal protein S9

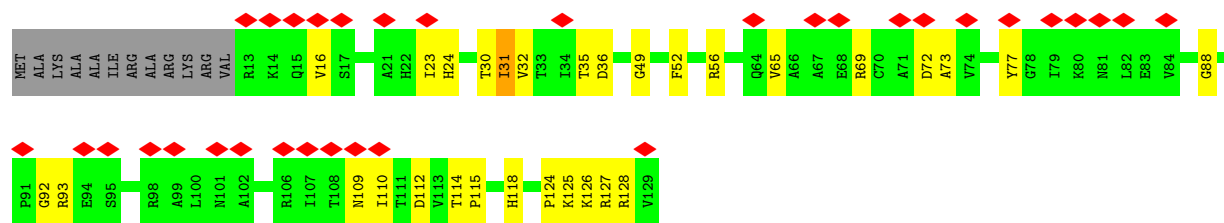


• Molecule 45: 30S ribosomal protein S10

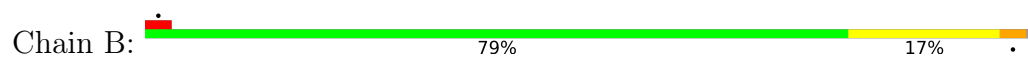


• Molecule 46: 30S ribosomal protein S11

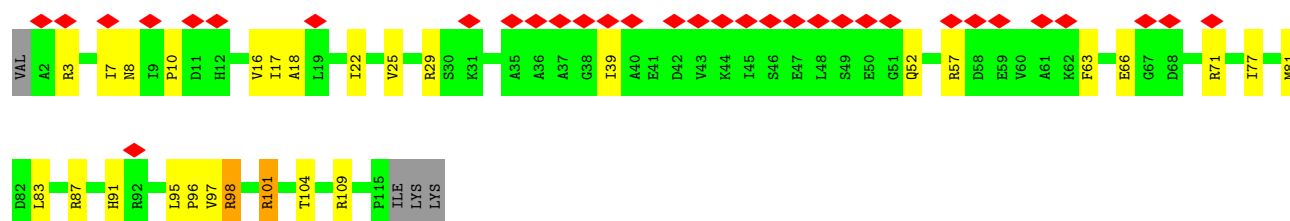
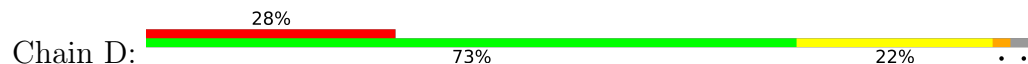




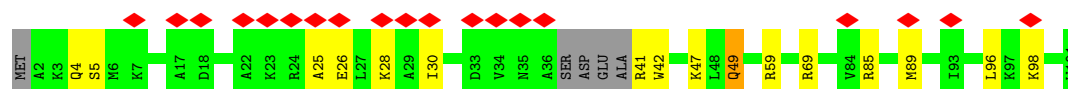
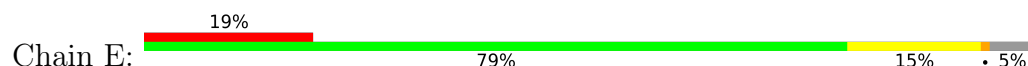
- Molecule 47: 30S ribosomal protein S12



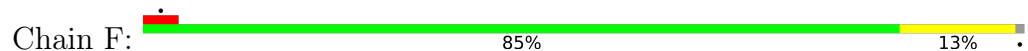
- Molecule 48: 30S ribosomal protein S13



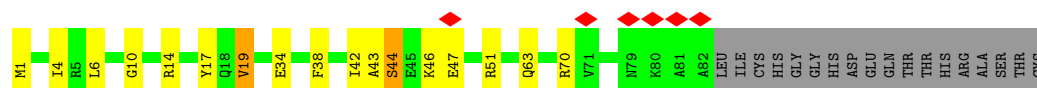
- Molecule 49: 30S ribosomal protein S14



- Molecule 50: 30S ribosomal protein S15



- Molecule 51: 30S ribosomal protein S16



- Molecule 52: 30S ribosomal protein S17

Chain H:  80% 13% .. 5%



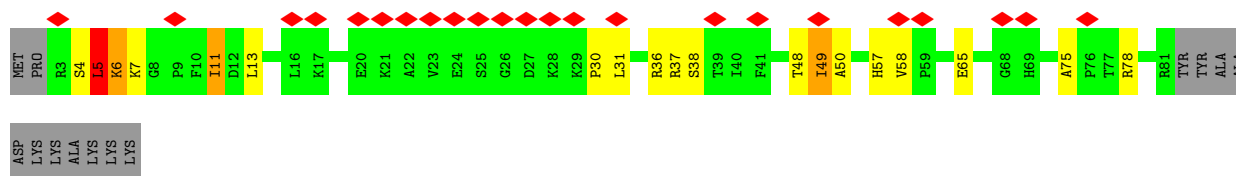
- Molecule 53: 30S ribosomal protein S18

Chain I:  45% 27% . 27%



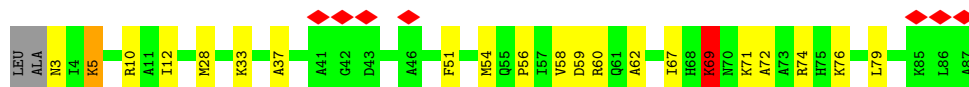
- Molecule 54: 30S ribosomal protein S19

Chain J:  25% 65% 16% . . 14%

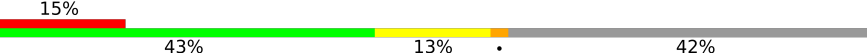


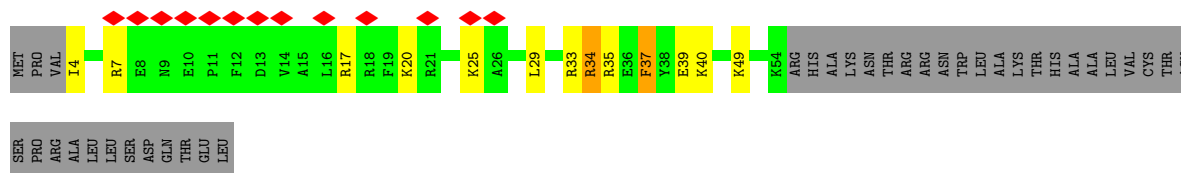
- Molecule 55: 30S ribosomal protein S20

Chain K:  8% 74% 22% . . .



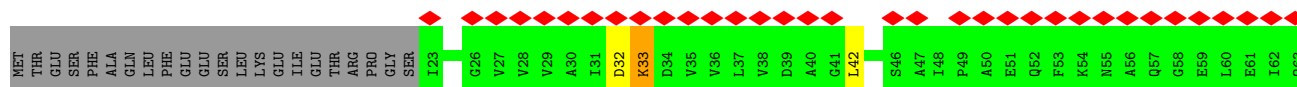
- Molecule 56: 30S ribosomal protein S21

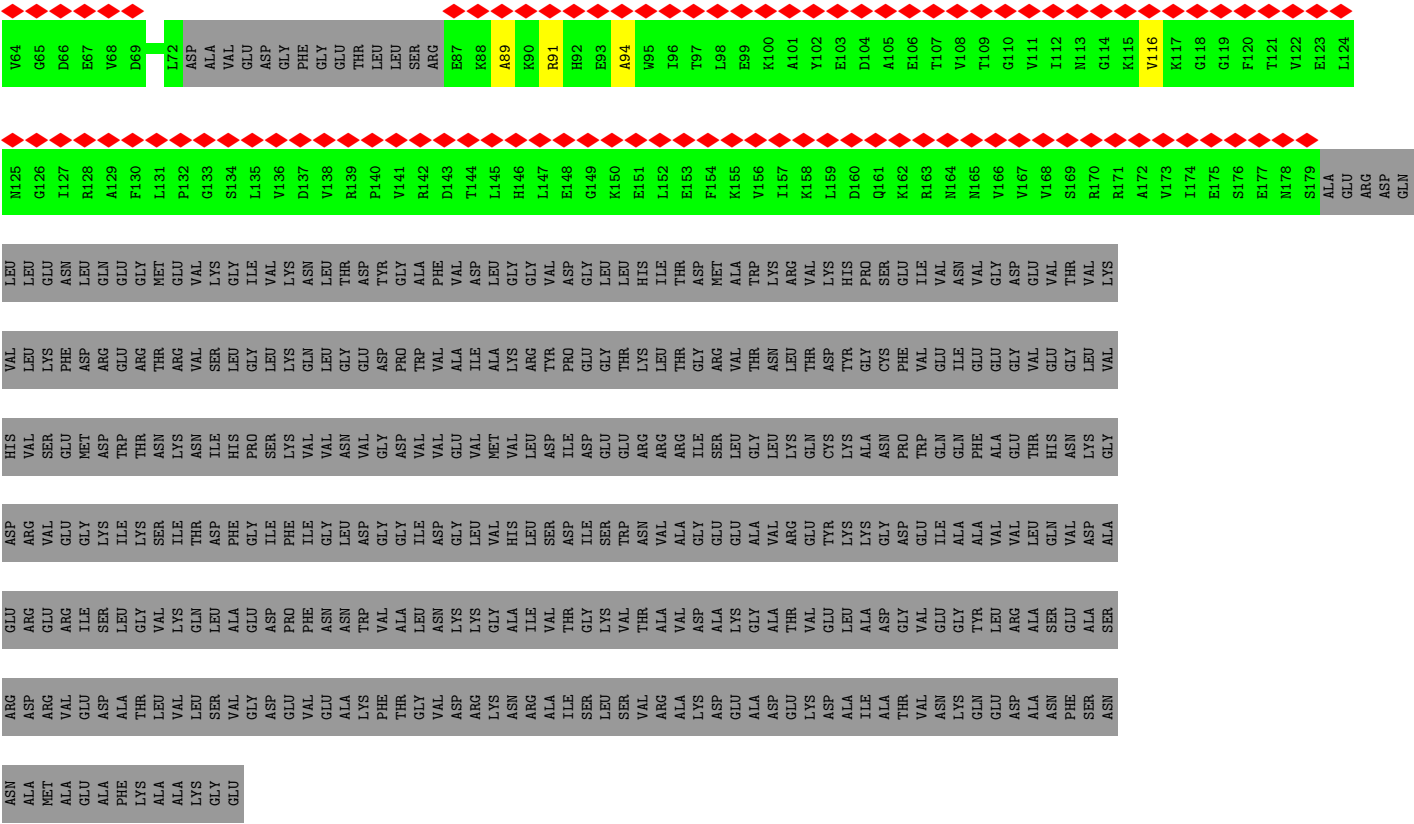
Chain s:  15% 43% 13% . 42%



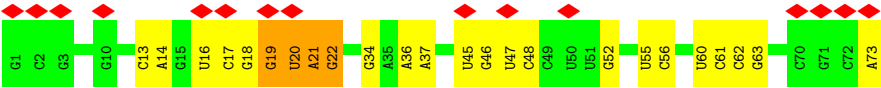
- Molecule 57: 30S ribosomal protein S1

Chain t:  24% 24% . 74%





• Molecule 58: A-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	75081	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	2.366	Depositor
Minimum map value	-0.728	Depositor
Average map value	-0.008	Depositor
Map value standard deviation	0.144	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	654.0, 654.0, 654.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.09, 1.09, 1.09	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	O	0.65	1/2828 (0.0%)	0.83	7/4410 (0.2%)
2	P	1.71	40/2121 (1.9%)	1.42	17/2852 (0.6%)
3	Q	1.54	14/1585 (0.9%)	1.29	10/2134 (0.5%)
4	R	1.21	8/1571 (0.5%)	1.09	5/2113 (0.2%)
5	S	0.84	0/1434	0.89	0/1926
6	T	0.83	0/1342	0.87	0/1816
7	V	0.77	0/1045	0.74	0/1410
8	W	1.42	10/1151 (0.9%)	1.10	0/1551
9	X	1.53	8/947 (0.8%)	1.27	4/1268 (0.3%)
10	Y	1.65	14/1053 (1.3%)	1.44	7/1403 (0.5%)
11	Z	1.42	4/1092 (0.4%)	1.20	2/1460 (0.1%)
12	a	1.65	10/973 (1.0%)	1.35	5/1301 (0.4%)
13	b	1.05	1/901 (0.1%)	1.04	5/1209 (0.4%)
14	c	1.38	4/927 (0.4%)	1.21	4/1240 (0.3%)
15	d	1.57	7/959 (0.7%)	1.33	8/1278 (0.6%)
16	e	1.40	6/828 (0.7%)	1.21	1/1107 (0.1%)
17	f	1.33	2/864 (0.2%)	1.14	1/1156 (0.1%)
18	g	1.22	0/744	1.11	0/994
19	h	1.01	1/787 (0.1%)	1.06	0/1051
20	i	0.96	0/765	0.90	0/1025
21	j	1.50	5/575 (0.9%)	1.38	6/762 (0.8%)
22	k	1.35	1/634 (0.2%)	1.16	2/848 (0.2%)
23	l	0.90	0/509	1.00	0/677
24	m	1.18	0/452	1.15	1/605 (0.2%)
25	n	1.48	2/449 (0.4%)	1.40	6/599 (1.0%)
26	o	1.44	5/416 (1.2%)	1.02	0/554
27	p	1.73	5/379 (1.3%)	1.61	5/498 (1.0%)
28	q	1.50	0/512	1.35	2/676 (0.3%)
29	r	1.43	3/302 (1.0%)	1.34	3/397 (0.8%)
30	N	0.95	272/69681 (0.4%)	0.95	167/108706 (0.2%)
31	L	0.74	0/411	0.84	0/550
32	C	0.32	0/1034	0.81	1/1387 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	U	0.33	0/1122	0.96	4/1515 (0.3%)
34	M	0.51	0/1779	0.77	3/2768 (0.1%)
35	x	0.41	0/327	0.69	0/506
36	0	0.76	33/36966 (0.1%)	0.85	49/57666 (0.1%)
37	1	1.00	1/1735 (0.1%)	0.98	2/2338 (0.1%)
38	2	1.08	4/1651 (0.2%)	0.97	3/2225 (0.1%)
39	3	0.97	2/1664 (0.1%)	1.03	2/2227 (0.1%)
40	4	1.53	6/1118 (0.5%)	1.35	7/1504 (0.5%)
41	5	1.16	5/835 (0.6%)	1.14	3/1128 (0.3%)
42	6	0.83	0/1195	0.86	1/1602 (0.1%)
43	7	1.15	1/988 (0.1%)	1.05	0/1326
44	8	1.09	1/1033 (0.1%)	1.13	2/1375 (0.1%)
45	9	0.95	1/796 (0.1%)	1.02	2/1077 (0.2%)
46	A	1.11	0/892	1.12	3/1205 (0.2%)
47	B	1.37	5/968 (0.5%)	1.24	3/1300 (0.2%)
48	D	1.09	1/892 (0.1%)	1.07	0/1193
49	E	1.10	0/784	1.14	1/1043 (0.1%)
50	F	1.20	2/717 (0.3%)	1.03	1/959 (0.1%)
51	G	1.18	3/658 (0.5%)	1.19	5/884 (0.6%)
52	H	1.08	1/657 (0.2%)	1.06	1/881 (0.1%)
53	I	1.20	0/462	1.15	1/621 (0.2%)
54	J	1.02	1/652 (0.2%)	1.00	1/877 (0.1%)
55	K	1.19	2/670 (0.3%)	1.20	2/888 (0.2%)
56	s	1.32	5/430 (1.2%)	1.22	1/570 (0.2%)
57	t	0.59	0/702	0.91	0/973
58	u	0.51	0/1744	0.72	0/2716
All	All	0.99	497/160708 (0.3%)	0.97	366/240330 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	P	0	3
3	Q	0	1
5	S	0	2
10	Y	0	2
11	Z	0	2
19	h	0	1
28	q	0	1
30	N	0	6

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
36	0	0	5
37	1	0	2
38	2	0	2
40	4	0	5
41	5	0	2
44	8	0	4
46	A	0	1
47	B	0	2
52	H	0	2
54	J	0	1
55	K	0	1
56	s	0	1
All	All	0	46

All (497) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	2502	G	P-OP2	14.13	1.77	1.49
30	N	1156	A	P-OP2	12.90	1.74	1.49
30	N	1333	G	P-OP2	10.90	1.70	1.49
30	N	783	A	P-OP2	10.79	1.70	1.49
40	4	127	ALA	C-O	-10.54	1.10	1.23
2	P	221	ARG	CA-C	-10.47	1.38	1.53
30	N	945	A	P-OP2	10.46	1.69	1.49
30	N	1639	C	P-OP1	10.31	1.69	1.49
10	Y	51	GLU	C-O	10.21	1.37	1.23
30	N	1664	A	P-OP2	10.12	1.69	1.49
30	N	945	A	P-OP1	10.05	1.69	1.49
2	P	219	THR	C-O	9.94	1.35	1.24
30	N	1670	C	P-OP1	9.83	1.68	1.49
47	B	23	ALA	N-CA	9.72	1.58	1.46
30	N	2074	U	P-OP1	9.70	1.68	1.49
2	P	213	TRP	CD2-CE2	9.65	1.57	1.41
12	a	2	ARG	C-O	-9.64	1.11	1.24
30	N	2588	G	P-OP1	9.39	1.67	1.49
41	5	63	ASN	C-O	-9.38	1.09	1.23
30	N	2005	A	P-OP1	9.11	1.67	1.49
30	N	827	U	P-OP1	9.03	1.67	1.49
30	N	450	G	P-OP2	9.02	1.67	1.49
55	K	5	LYS	C-O	-8.78	1.17	1.24
30	N	943	A	P-OP2	8.76	1.66	1.49
26	o	50	LYS	C-O	-8.71	1.15	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	828	U	O3'-P	-8.66	1.48	1.61
30	N	2349	G	O3'-P	-8.63	1.48	1.61
30	N	2025	C	P-OP2	8.58	1.66	1.49
36	0	578	C	P-OP1	8.56	1.66	1.49
30	N	2445	G	O3'-P	-8.53	1.48	1.61
30	N	800	A	P-OP1	8.53	1.66	1.49
2	P	213	TRP	CA-C	-8.51	1.39	1.52
30	N	567	U	P-OP1	8.43	1.65	1.49
30	N	2589	A	O3'-P	-8.35	1.48	1.61
30	N	963	U	O3'-P	-8.34	1.48	1.61
29	r	38	GLY	N-CA	8.31	1.58	1.45
30	N	1604	C	P-OP1	8.28	1.65	1.49
30	N	1777	U	O3'-P	-8.26	1.48	1.61
3	Q	162	ALA	CA-C	-8.26	1.41	1.52
2	P	48	ARG	C-O	-8.24	1.13	1.23
30	N	2615	U	P-OP1	8.24	1.65	1.49
30	N	1774	C	P-OP1	8.23	1.65	1.49
36	0	21	G	P-OP1	8.21	1.65	1.49
36	0	757	U	O3'-P	-8.17	1.48	1.61
30	N	2502	G	O5'-C5'	-8.13	1.30	1.42
39	3	39	GLY	N-CA	8.05	1.52	1.45
4	R	80	SER	C-O	-8.04	1.12	1.23
30	N	2060	A	O3'-P	-8.04	1.49	1.61
30	N	782	A	O3'-P	-7.96	1.49	1.61
10	Y	22	GLY	C-O	-7.94	1.11	1.23
2	P	238	ARG	C-O	7.94	1.33	1.24
30	N	1828	G	P-OP2	7.91	1.64	1.49
30	N	963	U	P-OP1	7.90	1.64	1.49
30	N	825	A	O3'-P	-7.89	1.49	1.61
2	P	204	VAL	CA-C	-7.88	1.42	1.52
30	N	692	C	O3'-P	-7.88	1.49	1.61
30	N	787	C	O3'-P	-7.88	1.49	1.61
10	Y	62	PRO	C-O	7.85	1.33	1.23
30	N	1968	G	O3'-P	-7.83	1.49	1.61
30	N	576	U	P-OP1	7.82	1.64	1.49
36	0	20	U	O3'-P	-7.78	1.49	1.61
30	N	2687	U	O3'-P	-7.78	1.49	1.61
30	N	1009	A	O3'-P	-7.76	1.49	1.61
2	P	230	HIS	CA-C	-7.75	1.43	1.52
30	N	1269	A	P-OP2	7.75	1.64	1.49
40	4	30	ILE	C-O	-7.75	1.16	1.24
30	N	585	G	O3'-P	-7.70	1.49	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Y	18	ARG	CZ-NH1	7.70	1.43	1.32
30	N	948	C	P-OP1	7.68	1.64	1.49
30	N	1257	C	O3'-P	-7.53	1.49	1.61
30	N	2019	A	O3'-P	-7.46	1.50	1.61
2	P	11	PRO	N-CA	7.43	1.56	1.47
30	N	2576	G	P-OP1	7.42	1.63	1.49
30	N	2543	G	P-OP1	7.39	1.63	1.49
30	N	2588	G	P-OP2	7.39	1.63	1.49
30	N	554	U	O3'-P	-7.38	1.50	1.61
30	N	2025	C	O3'-P	-7.38	1.50	1.61
30	N	445	C	O3'-P	-7.37	1.50	1.61
30	N	809	G	O3'-P	-7.37	1.50	1.61
30	N	116	C	O3'-P	-7.35	1.50	1.61
30	N	984	A	O3'-P	-7.35	1.50	1.61
30	N	2593	U	O3'-P	-7.34	1.50	1.61
30	N	2550	G	O3'-P	-7.30	1.50	1.61
14	c	93	ARG	CD-NE	-7.30	1.36	1.46
30	N	120	U	P-OP1	7.29	1.63	1.49
30	N	1664	A	P-OP1	7.28	1.63	1.49
8	W	97	PRO	C-O	7.22	1.33	1.24
27	p	38	GLY	CA-C	-7.22	1.41	1.51
10	Y	19	LEU	C-O	7.21	1.32	1.23
30	N	2714	G	P-OP2	7.21	1.63	1.49
36	0	667	G	O3'-P	-7.20	1.50	1.61
13	b	30	ARG	CZ-NH1	7.17	1.42	1.32
36	0	882	C	O3'-P	-7.17	1.50	1.61
2	P	213	TRP	CZ3-CH2	7.16	1.58	1.40
30	N	2050	C	O3'-P	-7.14	1.50	1.61
30	N	1152	C	O3'-P	-7.14	1.50	1.61
30	N	2588	G	O3'-P	-7.11	1.50	1.61
30	N	2873	A	C6-N1	-7.10	1.21	1.35
41	5	63	ASN	N-CA	7.08	1.55	1.46
30	N	2503	A	P-OP2	7.06	1.63	1.49
30	N	1375	U	O3'-P	-7.05	1.50	1.61
9	X	86	LEU	C-O	-7.02	1.15	1.24
4	R	77	ILE	CB-CG1	-7.01	1.39	1.53
30	N	397	U	O3'-P	-7.00	1.50	1.61
30	N	1780	A	P-OP1	7.00	1.62	1.49
30	N	673	C	O3'-P	-6.99	1.50	1.61
30	N	826	U	P-OP1	6.99	1.62	1.49
30	N	859	G	O3'-P	6.98	1.71	1.61
30	N	2498	C	P-OP2	6.96	1.62	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	j	14	ARG	C-O	-6.92	1.15	1.23
30	N	1019	U	O3'-P	-6.91	1.50	1.61
30	N	2052	A	O3'-P	-6.91	1.50	1.61
30	N	453	A	P-OP1	6.91	1.62	1.49
3	Q	125	TRP	CA-C	-6.90	1.44	1.52
12	a	47	VAL	C-O	-6.90	1.15	1.23
30	N	2022	U	P-OP1	6.89	1.62	1.49
30	N	1774	C	O3'-P	-6.88	1.50	1.61
25	n	11	SER	N-CA	-6.88	1.38	1.46
30	N	2635	A	O3'-P	-6.86	1.50	1.61
47	B	22	PRO	CA-C	6.86	1.62	1.52
30	N	2698	U	O3'-P	-6.80	1.50	1.61
30	N	1612	C	O3'-P	-6.79	1.50	1.61
2	P	221	ARG	C-O	-6.77	1.15	1.23
52	H	71	LYS	C-O	-6.75	1.15	1.24
12	a	66	ALA	CA-C	-6.74	1.43	1.52
30	N	1658	C	P-OP1	6.73	1.62	1.49
36	0	1500	A	O3'-P	-6.72	1.51	1.61
15	d	49	ASP	CA-C	-6.71	1.43	1.52
30	N	200	U	O3'-P	-6.71	1.51	1.61
2	P	222	GLY	C-O	-6.71	1.14	1.23
30	N	1658	C	O3'-P	-6.69	1.51	1.61
30	N	1782	U	P-OP1	6.68	1.62	1.49
30	N	1994	C	O3'-P	-6.68	1.51	1.61
8	W	81	ILE	C-O	6.67	1.32	1.24
19	h	68	SER	CB-OG	6.67	1.55	1.42
2	P	86	ASN	C-O	-6.67	1.15	1.24
30	N	2006	C	P-OP1	6.65	1.62	1.49
30	N	2466	C	O3'-P	-6.65	1.51	1.61
2	P	15	HIS	C-O	-6.64	1.14	1.24
30	N	1751	U	O3'-P	-6.64	1.51	1.61
15	d	49	ASP	C-O	6.62	1.32	1.24
30	N	955	U	O3'-P	-6.62	1.51	1.61
30	N	641	U	O3'-P	-6.60	1.51	1.61
30	N	1900	A	O3'-P	6.60	1.71	1.61
30	N	2062	A	P-OP2	6.58	1.62	1.49
30	N	192	C	P-OP1	6.57	1.62	1.49
30	N	2765	A	C6-N1	-6.57	1.22	1.35
30	N	1831	G	O3'-P	-6.55	1.51	1.61
30	N	1353	A	O3'-P	-6.54	1.51	1.61
25	n	10	ARG	CA-C	6.54	1.61	1.52
30	N	1268	A	P-OP1	6.54	1.62	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	2740	A	O3'-P	-6.53	1.51	1.61
36	O	812	G	O3'-P	6.53	1.71	1.61
30	N	2035	G	O5'-C5'	-6.52	1.33	1.42
12	a	2	ARG	C-N	-6.52	1.24	1.33
30	N	1993	U	O5'-C5'	-6.51	1.32	1.42
2	P	221	ARG	CB-CG	-6.50	1.32	1.52
14	c	21	ARG	C-O	-6.50	1.18	1.24
11	Z	39	GLY	C-O	-6.47	1.15	1.23
30	N	2518	A	P-OP2	6.46	1.61	1.49
9	X	66	LYS	CA-C	-6.46	1.44	1.52
16	e	79	ARG	C-O	6.45	1.31	1.23
30	N	1254	A	O3'-P	-6.45	1.51	1.61
30	N	810	U	P-OP1	6.43	1.61	1.49
2	P	213	TRP	CB-CG	-6.42	1.30	1.50
30	N	2264	C	O3'-P	-6.41	1.51	1.61
9	X	7	MET	N-CA	6.38	1.54	1.46
2	P	271	ARG	CZ-NH1	6.38	1.41	1.32
30	N	2605	U	O3'-P	-6.38	1.51	1.61
12	a	1	MET	C-O	6.37	1.36	1.23
30	N	2437	G	O3'-P	-6.37	1.51	1.61
30	N	2543	G	O5'-C5'	-6.37	1.32	1.42
30	N	1828	G	P-OP1	6.37	1.61	1.49
30	N	2031	A	P-OP1	-6.37	1.36	1.49
30	N	1970	A	P-OP2	6.36	1.61	1.49
30	N	1678	A	P-OP2	6.34	1.61	1.49
30	N	2489	U	O3'-P	-6.34	1.51	1.61
30	N	1813	G	O3'-P	-6.34	1.51	1.61
10	Y	62	PRO	CA-CB	-6.33	1.45	1.53
3	Q	163	GLY	N-CA	6.32	1.52	1.45
2	P	234	GLY	C-O	-6.32	1.15	1.23
3	Q	126	ASN	CA-C	-6.30	1.45	1.53
44	8	121	ALA	C-O	-6.30	1.16	1.24
30	N	975	A	P-OP2	6.29	1.61	1.49
30	N	2590	A	O3'-P	-6.28	1.51	1.61
30	N	839	U	O3'-P	-6.28	1.51	1.61
2	P	220	VAL	CA-CB	-6.27	1.46	1.54
2	P	204	VAL	N-CA	-6.26	1.39	1.46
47	B	114	ARG	C-O	-6.24	1.16	1.24
30	N	2572	A	O3'-P	-6.23	1.51	1.61
36	O	24	U	N3-C4	-6.23	1.25	1.38
14	c	53	ARG	N-CA	-6.23	1.36	1.46
27	p	39	ARG	NE-CZ	6.23	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	572	A	P-OP1	6.22	1.61	1.49
30	N	733	G	O3'-P	-6.21	1.51	1.61
30	N	2265	U	O3'-P	-6.20	1.51	1.61
36	0	726	C	O3'-P	-6.20	1.51	1.61
10	Y	41	ARG	CA-C	-6.18	1.45	1.52
30	N	192	C	O3'-P	-6.18	1.51	1.61
30	N	372	G	O3'-P	6.18	1.70	1.61
30	N	2447	G	O3'-P	-6.18	1.51	1.61
30	N	1794	A	O3'-P	-6.16	1.51	1.61
29	r	37	GLN	CA-C	-6.14	1.44	1.52
30	N	832	U	O3'-P	-6.14	1.51	1.61
15	d	10	ALA	C-O	6.13	1.31	1.24
12	a	112	TYR	CA-C	-6.12	1.45	1.52
30	N	1189	A	O3'-P	-6.11	1.51	1.61
30	N	515	A	O3'-P	-6.10	1.51	1.61
22	k	22	LEU	C-O	-6.10	1.15	1.23
40	4	24	THR	CA-C	-6.09	1.47	1.53
30	N	1771	C	O3'-P	-6.09	1.52	1.61
4	R	75	SER	CA-C	-6.08	1.46	1.53
30	N	997	G	O3'-P	-6.07	1.52	1.61
8	W	138	GLN	C-O	-6.06	1.16	1.23
26	o	10	LYS	C-O	-6.05	1.17	1.24
30	N	821	A	O3'-P	-6.05	1.52	1.61
40	4	24	THR	C-O	-6.05	1.14	1.23
41	5	51	ILE	C-O	-6.05	1.17	1.24
30	N	818	G	P-OP2	6.05	1.61	1.49
8	W	107	GLY	C-O	-6.04	1.17	1.24
30	N	569	U	O3'-P	-6.04	1.52	1.61
30	N	1778	U	O3'-P	-6.04	1.52	1.61
30	N	1790	C	O3'-P	-6.02	1.52	1.61
30	N	254	G	O3'-P	-6.01	1.52	1.61
38	2	3	GLN	N-CA	-5.99	1.39	1.46
8	W	98	GLU	N-CA	-5.99	1.39	1.46
30	N	2867	G	O3'-P	5.99	1.70	1.61
2	P	10	SER	CA-CB	5.99	1.62	1.53
56	s	34	ARG	CZ-NH1	5.99	1.41	1.32
30	N	2406	A	P-OP1	5.98	1.60	1.49
56	s	37	PHE	N-CA	5.98	1.53	1.46
30	N	2620	C	O3'-P	-5.98	1.52	1.61
30	N	671	C	P-OP2	5.97	1.60	1.49
30	N	2822	G	O3'-P	-5.97	1.52	1.61
30	N	676	A	O3'-P	-5.96	1.52	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	464	U	O3'-P	-5.96	1.52	1.61
36	0	1367	C	O3'-P	-5.96	1.52	1.61
8	W	84	ILE	CA-C	-5.95	1.46	1.53
10	Y	51	GLU	N-CA	-5.94	1.39	1.46
30	N	2025	C	O5'-C5'	-5.94	1.33	1.42
2	P	158	ALA	CA-C	-5.93	1.45	1.52
30	N	2625	G	O3'-P	-5.92	1.52	1.61
36	0	1393	U	O3'-P	-5.92	1.52	1.61
30	N	2061	G	C2'-O2'	5.92	1.51	1.42
2	P	214	ARG	CZ-NH1	5.91	1.41	1.32
10	Y	29	LYS	C-O	5.91	1.31	1.24
30	N	2072	C	O3'-P	-5.91	1.52	1.61
30	N	2385	C	P-OP1	5.91	1.60	1.49
10	Y	37	GLY	C-O	-5.90	1.16	1.23
47	B	23	ALA	C-O	-5.90	1.16	1.24
30	N	2081	U	O3'-P	-5.89	1.52	1.61
30	N	2247	A	O3'-P	-5.89	1.52	1.61
30	N	2637	U	O3'-P	-5.89	1.52	1.61
30	N	2072	C	O5'-C5'	-5.89	1.33	1.42
30	N	2499	C	P-OP2	5.88	1.60	1.49
30	N	730	A	P-OP2	5.88	1.60	1.49
30	N	2359	C	O3'-P	-5.87	1.52	1.61
36	0	980	C	P-OP1	5.87	1.60	1.49
30	N	566	U	O3'-P	-5.86	1.52	1.61
38	2	2	GLY	N-CA	5.85	1.54	1.45
51	G	4	ILE	C-O	-5.85	1.17	1.23
30	N	2444	G	O3'-P	-5.84	1.52	1.61
36	0	387	U	O3'-P	-5.84	1.52	1.61
30	N	198	C	O3'-P	-5.84	1.52	1.61
2	P	258	ARG	NE-CZ	-5.83	1.26	1.33
30	N	538	A	O3'-P	-5.83	1.52	1.61
12	a	106	ASP	N-CA	-5.83	1.40	1.46
30	N	1822	C	O3'-P	-5.82	1.52	1.61
30	N	2837	A	O3'-P	-5.82	1.52	1.61
2	P	235	GLY	C-N	-5.81	1.25	1.33
30	N	1824	G	P-OP2	5.79	1.60	1.49
30	N	2232	C	O3'-P	-5.79	1.52	1.61
30	N	2602	A	O3'-P	5.79	1.69	1.61
29	r	36	ARG	CD-NE	-5.79	1.38	1.46
45	9	58	ASN	CA-C	-5.78	1.45	1.52
40	4	50	TYR	C-O	5.78	1.31	1.24
54	J	6	LYS	N-CA	5.78	1.53	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	235	GLY	CA-C	-5.78	1.43	1.51
36	0	22	G	O3'-P	-5.77	1.52	1.61
2	P	160	THR	C-O	-5.77	1.16	1.24
30	N	2062	A	O5'-C5'	-5.77	1.34	1.42
30	N	2457	U	O3'-P	-5.75	1.52	1.61
2	P	204	VAL	C-N	-5.75	1.25	1.33
3	Q	164	GLN	C-O	5.75	1.30	1.24
4	R	62	GLN	N-CA	5.75	1.53	1.46
36	0	505	G	O3'-P	-5.75	1.52	1.61
26	o	23	THR	C-O	-5.74	1.19	1.24
8	W	30	THR	CB-CG2	-5.74	1.33	1.52
30	N	1261	C	O3'-P	-5.73	1.52	1.61
30	N	126	A	O3'-P	-5.73	1.52	1.61
30	N	2542	A	O3'-P	-5.72	1.52	1.61
30	N	2684	U	O3'-P	-5.72	1.52	1.61
26	o	48	ILE	C-O	-5.72	1.18	1.24
15	d	51	ARG	CA-CB	-5.72	1.44	1.53
30	N	783	A	C4'-O4'	5.72	1.54	1.45
30	N	2598	A	O3'-P	-5.71	1.52	1.61
30	N	1805	A	O3'-P	-5.71	1.52	1.61
30	N	2013	A	O3'-P	-5.71	1.52	1.61
30	N	2572	A	P-OP1	-5.71	1.37	1.49
30	N	1298	C	O3'-P	-5.70	1.52	1.61
30	N	966	G	O3'-P	-5.70	1.52	1.61
51	G	10	GLY	N-CA	5.70	1.51	1.45
9	X	41	ILE	C-O	-5.69	1.17	1.23
9	X	65	THR	C-O	-5.69	1.16	1.23
30	N	578	G	P-OP2	5.69	1.60	1.49
36	0	814	A	P-OP2	5.68	1.60	1.49
30	N	2049	G	O3'-P	-5.67	1.52	1.61
30	N	1795	C	O3'-P	-5.67	1.52	1.61
30	N	1662	U	P-OP2	5.66	1.60	1.49
4	R	81	GLY	C-N	-5.65	1.25	1.33
30	N	2268	A	P-OP1	5.65	1.60	1.49
30	N	29	U	O3'-P	-5.65	1.52	1.61
50	F	49	ASP	C-O	5.65	1.31	1.23
30	N	571	U	O3'-P	-5.64	1.52	1.61
41	5	99	ALA	CA-C	5.64	1.56	1.52
8	W	80	HIS	CA-C	-5.64	1.45	1.53
27	p	34	ARG	CG-CD	-5.64	1.35	1.52
9	X	23	LYS	CA-C	-5.63	1.45	1.52
1	O	83	G	O3'-P	-5.63	1.52	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	940	G	O3'-P	-5.63	1.52	1.61
30	N	25	U	O3'-P	-5.63	1.52	1.61
12	a	17	ARG	C-O	5.62	1.30	1.24
2	P	205	LEU	N-CA	5.60	1.53	1.46
30	N	1681	G	O3'-P	-5.60	1.52	1.61
50	F	51	HIS	C-O	5.60	1.30	1.24
11	Z	93	VAL	CA-CB	5.59	1.63	1.54
30	N	2499	C	P-OP1	5.59	1.60	1.49
30	N	680	C	O3'-P	-5.59	1.52	1.61
21	j	42	GLY	N-CA	5.58	1.55	1.45
30	N	1009	A	P-OP2	5.58	1.60	1.49
30	N	796	C	O3'-P	-5.58	1.52	1.61
30	N	393	C	P-OP1	5.57	1.60	1.49
30	N	2072	C	P-OP1	5.57	1.60	1.49
8	W	110	PRO	CA-C	-5.57	1.45	1.52
11	Z	11	LYS	C-O	-5.57	1.17	1.24
36	0	764	C	O3'-P	-5.57	1.52	1.61
3	Q	162	ALA	C-O	-5.56	1.17	1.23
30	N	2829	A	O3'-P	-5.56	1.52	1.61
30	N	2016	U	O3'-P	-5.56	1.52	1.61
30	N	1010	A	P-OP2	5.56	1.60	1.49
30	N	773	U	O3'-P	-5.54	1.52	1.61
36	0	765	G	O3'-P	-5.54	1.52	1.61
47	B	113	ALA	CA-C	-5.54	1.46	1.53
30	N	761	A	P-OP1	5.53	1.60	1.49
30	N	2248	C	P-OP2	5.53	1.60	1.49
30	N	784	G	O3'-P	5.53	1.69	1.61
30	N	2436	G	O3'-P	-5.52	1.52	1.61
3	Q	126	ASN	N-CA	5.51	1.54	1.46
30	N	1949	G	O3'-P	-5.50	1.52	1.61
9	X	114	LYS	C-O	-5.49	1.17	1.24
10	Y	35	HIS	CA-C	-5.48	1.45	1.53
30	N	1671	U	P-OP2	5.47	1.59	1.49
30	N	1186	G	P-OP2	5.46	1.59	1.49
30	N	419	U	O3'-P	-5.46	1.52	1.61
30	N	2332	C	O3'-P	-5.46	1.52	1.61
41	5	62	MET	C-N	-5.45	1.27	1.33
30	N	2051	A	O3'-P	5.45	1.69	1.61
30	N	688	U	O3'-P	-5.44	1.52	1.61
39	3	123	ILE	C-O	-5.44	1.18	1.24
15	d	32	TYR	C-N	-5.44	1.25	1.33
16	e	72	VAL	C-O	-5.44	1.18	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	p	34	ARG	C-O	-5.43	1.17	1.24
38	2	166	GLU	C-O	-5.43	1.17	1.24
3	Q	109	VAL	C-O	-5.43	1.18	1.24
21	j	15	ASP	N-CA	-5.43	1.39	1.45
2	P	239	ASN	CA-C	5.42	1.60	1.52
30	N	2516	A	O3'-P	-5.42	1.53	1.61
30	N	2243	U	P-OP1	5.41	1.59	1.49
56	s	40	LYS	CA-C	5.41	1.59	1.52
30	N	2260	C	O3'-P	-5.39	1.53	1.61
2	P	198	ALA	C-O	5.39	1.30	1.24
3	Q	126	ASN	C-O	-5.38	1.16	1.23
30	N	1026	G	P-OP2	-5.38	1.38	1.49
2	P	155	ALA	CA-C	-5.38	1.47	1.53
16	e	12	HIS	C-O	5.36	1.30	1.23
30	N	1255	U	O5'-C5'	-5.36	1.34	1.42
30	N	2048	G	O3'-P	-5.35	1.53	1.61
30	N	1394	U	O3'-P	-5.34	1.53	1.61
16	e	75	VAL	C-O	-5.34	1.18	1.24
30	N	2045	C	O3'-P	-5.34	1.53	1.61
30	N	1327	A	P-OP2	5.34	1.59	1.49
30	N	2285	C	O3'-P	-5.33	1.53	1.61
30	N	503	A	C6-N1	-5.33	1.24	1.35
9	X	35	VAL	C-O	5.33	1.29	1.24
30	N	411	G	P-OP1	5.33	1.59	1.49
30	N	239	C	O3'-P	-5.32	1.53	1.61
30	N	117	G	O3'-P	-5.32	1.53	1.61
30	N	1234	U	O3'-P	-5.31	1.53	1.61
4	R	81	GLY	N-CA	-5.31	1.37	1.45
4	R	45	ALA	N-CA	-5.30	1.40	1.46
30	N	2554	U	P-OP2	-5.29	1.38	1.49
2	P	156	ARG	CD-NE	-5.29	1.38	1.46
30	N	923	G	O3'-P	-5.29	1.53	1.61
30	N	1977	A	O3'-P	-5.29	1.53	1.61
2	P	54	ILE	N-CA	5.28	1.52	1.46
3	Q	149	ASN	CA-CB	-5.27	1.44	1.53
21	j	72	LYS	C-O	5.27	1.30	1.23
30	N	946	C	P-OP2	5.27	1.59	1.49
2	P	195	VAL	CB-CG1	-5.26	1.35	1.52
30	N	2694	G	O3'-P	-5.26	1.53	1.61
14	c	92	VAL	CA-C	-5.26	1.46	1.52
30	N	1960	A	O3'-P	-5.26	1.53	1.61
30	N	2074	U	O3'-P	-5.25	1.53	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	p	42	LEU	N-CA	-5.25	1.41	1.46
30	N	2452	C	O3'-P	-5.25	1.53	1.61
15	d	49	ASP	CB-CG	5.25	1.65	1.52
30	N	1782	U	O3'-P	-5.25	1.53	1.61
36	o	572	A	P-OP1	5.25	1.59	1.49
30	N	2426	A	O3'-P	-5.24	1.53	1.61
30	N	120	U	P-OP2	5.24	1.59	1.49
3	Q	12	THR	CA-CB	5.24	1.61	1.54
16	e	54	VAL	C-O	5.24	1.29	1.24
30	N	2289	G	O3'-P	-5.24	1.53	1.61
30	N	193	U	O3'-P	-5.23	1.53	1.61
12	a	8	ARG	NE-CZ	-5.23	1.27	1.33
30	N	698	C	O3'-P	-5.23	1.53	1.61
30	N	1342	A	P-OP2	5.23	1.59	1.49
30	N	2732	G	C3'-O3'	5.23	1.50	1.42
8	W	76	HIS	C-O	-5.23	1.17	1.23
16	e	43	ASN	CA-C	5.22	1.56	1.52
30	N	1968	G	P-OP1	5.22	1.59	1.49
30	N	1432	G	O3'-P	-5.22	1.53	1.61
51	G	34	GLU	CA-C	-5.22	1.46	1.52
30	N	1191	G	O3'-P	-5.21	1.53	1.61
17	f	96	ILE	N-CA	-5.21	1.39	1.46
30	N	960	A	O3'-P	-5.20	1.53	1.61
30	N	2028	U	O3'-P	-5.20	1.53	1.61
3	Q	170	VAL	CA-C	-5.20	1.46	1.52
30	N	1649	G	O3'-P	-5.20	1.53	1.61
36	o	1182	G	O3'-P	5.19	1.69	1.61
15	d	21	ALA	C-O	-5.19	1.16	1.23
10	Y	101	ILE	N-CA	-5.18	1.40	1.46
30	N	2723	C	O3'-P	-5.18	1.53	1.61
30	N	1296	G	O3'-P	-5.18	1.53	1.61
30	N	2682	A	P-OP2	5.18	1.59	1.49
38	2	152	GLU	CA-C	-5.18	1.47	1.53
36	o	1110	A	P-OP2	5.17	1.59	1.49
30	N	1153	C	P-OP2	5.17	1.59	1.49
26	o	21	TYR	CE2-CZ	-5.17	1.25	1.38
2	P	239	ASN	N-CA	-5.16	1.39	1.46
30	N	1680	U	O3'-P	-5.16	1.53	1.61
36	o	19	A	O3'-P	-5.15	1.53	1.61
56	s	35	ARG	CA-C	-5.15	1.46	1.52
30	N	1141	U	N3-C4	-5.14	1.28	1.38
30	N	1004	U	O3'-P	-5.13	1.53	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	N	694	U	O3'-P	-5.13	1.53	1.61
30	N	1648	U	P-OP2	5.13	1.59	1.49
30	N	2727	A	O3'-P	-5.13	1.53	1.61
10	Y	62	PRO	N-CA	-5.13	1.41	1.46
30	N	208	C	O3'-P	-5.13	1.53	1.61
17	f	85	ILE	C-O	-5.12	1.18	1.24
2	P	195	VAL	C-O	-5.12	1.17	1.24
12	a	10	LEU	CA-C	-5.12	1.45	1.53
36	0	559	A	N1-C2	5.12	1.44	1.34
43	7	106	THR	CA-C	-5.12	1.46	1.53
4	R	52	VAL	C-O	-5.12	1.18	1.24
30	N	1652	A	O3'-P	-5.12	1.53	1.61
21	j	45	PHE	CA-CB	-5.11	1.45	1.53
30	N	234	U	N3-C4	-5.11	1.28	1.38
48	D	101	ARG	CZ-NH1	5.11	1.40	1.32
30	N	963	U	P-OP2	5.11	1.59	1.49
3	Q	150	GLN	N-CA	5.11	1.52	1.46
30	N	2262	U	O3'-P	-5.11	1.53	1.61
56	s	34	ARG	CA-C	5.11	1.59	1.52
40	4	50	TYR	CA-C	-5.10	1.46	1.52
11	Z	73	ILE	C-O	-5.10	1.18	1.24
30	N	2699	C	O3'-P	-5.10	1.53	1.61
2	P	213	TRP	CD1-NE1	5.09	1.48	1.37
30	N	2503	A	P-OP1	5.09	1.59	1.49
2	P	175	ARG	CA-C	-5.08	1.46	1.52
30	N	632	A	O3'-P	-5.08	1.53	1.61
30	N	2502	G	O3'-P	-5.08	1.53	1.61
30	N	1142	A	O3'-P	5.08	1.68	1.61
30	N	408	G	O3'-P	-5.08	1.53	1.61
30	N	745	G	O3'-P	-5.08	1.53	1.61
30	N	1677	A	O3'-P	-5.08	1.53	1.61
30	N	1186	G	O3'-P	-5.07	1.53	1.61
30	N	727	A	P-OP1	5.07	1.59	1.49
30	N	1650	A	O3'-P	-5.06	1.53	1.61
36	0	715	A	O3'-P	-5.06	1.53	1.61
10	Y	63	LYS	N-CA	-5.05	1.39	1.46
30	N	1334	G	O3'-P	-5.05	1.53	1.61
36	0	1062	U	O3'-P	-5.05	1.53	1.61
30	N	1367	A	O3'-P	-5.04	1.53	1.61
3	Q	131	ASP	C-O	-5.04	1.17	1.23
30	N	2000	C	O3'-P	-5.04	1.53	1.61
36	0	581	G	O3'-P	-5.03	1.53	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	1	18	HIS	C-O	-5.03	1.20	1.24
36	0	787	A	O3'-P	-5.03	1.53	1.61
30	N	1187	G	P-OP2	5.03	1.59	1.49
36	0	1054	C	P-OP2	5.03	1.59	1.49
36	0	37	U	N3-C4	-5.02	1.28	1.38
36	0	368	U	N3-C4	-5.02	1.28	1.38
2	P	177	ARG	C-O	-5.01	1.17	1.24
36	0	613	C	O3'-P	-5.01	1.53	1.61
36	0	920	U	O3'-P	-5.01	1.53	1.61
55	K	10	ARG	CD-NE	-5.00	1.39	1.46

All (366) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	M	73	C	O3'-P-O5'	18.22	131.33	104.00
3	Q	151	THR	CA-C-N	12.71	134.22	119.47
3	Q	151	THR	C-N-CA	12.71	134.22	119.47
30	N	1936	A	C4'-C3'-O3'	-11.05	96.43	113.00
30	N	2725	A	C3'-C2'-O2'	-10.61	94.78	110.70
30	N	242	G	C4'-C3'-O3'	9.96	124.35	109.40
55	K	10	ARG	CB-CG-CD	-9.43	89.62	111.30
30	N	774	G	C1'-C2'-O2'	-9.42	94.27	108.40
30	N	2251	G	C3'-C2'-O2'	9.29	124.63	110.70
30	N	774	G	C4'-C3'-O3'	-9.29	99.07	113.00
36	0	561	U	C4'-C3'-O3'	-9.23	99.16	113.00
30	N	995	C	C4'-C3'-O3'	-8.78	96.23	109.40
30	N	2776	A	C2'-C3'-O3'	8.71	122.57	109.50
30	N	670	A	C2'-C3'-O3'	8.63	122.45	109.50
2	P	204	VAL	N-CA-C	8.55	120.29	112.43
30	N	2732	G	C4'-C3'-O3'	-8.48	100.28	113.00
36	0	1528	U	C1'-C2'-O2'	-8.42	99.18	111.80
30	N	1937	A	C4'-C3'-O3'	-8.38	100.43	113.00
36	0	1347	G	C4'-C3'-O3'	8.29	121.83	109.40
30	N	2060	A	O3'-P-O5'	8.25	116.37	104.00
30	N	1136	G	P-O5'-C5'	-8.20	108.60	120.90
30	N	784	G	C2'-C3'-O3'	8.18	125.97	113.70
30	N	1236	G	C4'-C3'-O3'	-8.03	100.96	113.00
36	0	717	U	C4'-C3'-O3'	-8.03	100.96	113.00
30	N	2324	U	C4'-C3'-O3'	-8.00	101.00	113.00
36	0	1345	U	C4'-C3'-O3'	7.98	121.37	109.40
2	P	221	ARG	CG-CD-NE	-7.95	94.52	112.00
2	P	232	HIS	O-C-N	-7.92	113.77	123.04

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	746	U	C4'-C3'-O3'	-7.90	101.15	113.00
30	N	1141	U	C2'-C3'-O3'	7.80	121.20	109.50
9	X	94	PRO	N-CA-C	7.71	122.82	110.40
30	N	2266	A	C4'-C3'-O3'	-7.61	97.98	109.40
41	5	90	MET	CA-C-N	7.60	136.05	121.54
41	5	90	MET	C-N-CA	7.60	136.05	121.54
1	O	44	G	C4'-C3'-O3'	-7.56	101.66	113.00
30	N	2406	A	C2'-C3'-O3'	-7.51	102.44	113.70
33	U	30	LEU	N-CA-C	7.49	119.13	110.97
36	0	115	G	C2'-C3'-O3'	7.47	120.71	109.50
9	X	35	VAL	O-C-N	7.44	129.90	121.94
30	N	1142	A	C2'-C3'-O3'	7.41	120.62	109.50
28	q	8	ARG	CD-NE-CZ	-7.37	114.08	124.40
36	0	518	C	C4'-C3'-O3'	7.37	120.45	109.40
4	R	81	GLY	O-C-N	-7.35	113.15	122.70
36	0	1278	G	C4'-C3'-O3'	-7.31	102.04	113.00
54	J	5	LEU	CB-CG-CD2	7.26	132.48	110.70
30	N	2543	G	P-O5'-C5'	-7.24	110.04	120.90
13	b	101	GLY	O-C-N	7.24	125.90	121.85
4	R	81	GLY	CA-C-N	-7.18	107.34	121.41
4	R	81	GLY	C-N-CA	-7.18	107.34	121.41
30	N	2497	A	C5'-C4'-C3'	-7.17	104.44	115.20
36	0	752	G	C4'-C3'-O3'	-7.14	102.30	113.00
30	N	2225	A	C2'-C3'-O3'	7.10	120.14	109.50
30	N	33	C	C4'-C3'-O3'	-7.06	102.41	113.00
2	P	239	ASN	N-CA-C	7.05	125.83	110.80
36	0	1362	A	C4'-C3'-O3'	-7.05	102.43	113.00
30	N	227	A	C4'-C3'-O3'	-7.03	102.45	113.00
36	0	878	A	C3'-C2'-O2'	7.01	121.22	110.70
27	p	39	ARG	NE-CZ-NH2	-7.01	112.89	119.20
30	N	2732	G	C1'-C2'-O2'	-7.00	97.91	108.40
30	N	1648	U	P-O5'-C5'	-6.98	110.42	120.90
46	A	126	LYS	N-CA-C	6.98	120.67	109.79
40	4	111	MET	CG-SD-CE	-6.96	85.60	100.90
21	j	14	ARG	CG-CD-NE	-6.94	96.72	112.00
36	0	1279	G	N9-C1'-C2'	6.93	122.40	112.00
2	P	157	SER	N-CA-C	-6.92	100.55	110.59
30	N	1993	U	C3'-C2'-O2'	-6.91	100.33	110.70
15	d	6	ARG	NE-CZ-NH2	6.87	125.39	119.20
30	N	1666	G	C3'-C2'-O2'	6.86	120.99	110.70
3	Q	13	ARG	NE-CZ-NH2	6.85	125.36	119.20
34	M	73	C	OP1-P-O3'	-6.83	87.51	108.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	p	39	ARG	NE-CZ-NH1	6.82	128.32	121.50
30	N	995	C	C2'-C3'-O3'	6.82	119.72	109.50
30	N	1865	U	C4'-C3'-O3'	-6.81	102.78	113.00
30	N	989	G	C4'-C3'-O3'	-6.79	102.82	113.00
15	d	22	LYS	N-CA-C	-6.78	100.44	110.48
36	0	1190	G	C1'-C2'-O2'	-6.77	101.64	111.80
2	P	241	GLY	N-CA-C	6.74	124.66	114.61
30	N	2238	G	C2'-C3'-O3'	6.71	119.57	109.50
42	6	109	ARG	CG-CD-NE	-6.71	97.24	112.00
4	R	65	THR	O-C-N	-6.70	114.56	122.81
30	N	2061	G	C4'-C3'-O3'	-6.70	102.94	113.00
30	N	2832	U	C4'-C3'-O3'	-6.70	102.94	113.00
27	p	34	ARG	NE-CZ-NH1	-6.70	114.80	121.50
30	N	1313	U	N1-C1'-C2'	6.70	122.05	112.00
30	N	974	G	N9-C1'-C2'	6.67	124.01	114.00
14	c	93	ARG	CG-CD-NE	-6.63	97.42	112.00
1	O	108	A	C2'-C3'-O3'	-6.58	103.84	113.70
30	N	2509	G	C3'-C2'-O2'	6.56	120.54	110.70
13	b	102	ARG	NE-CZ-NH2	6.54	125.09	119.20
44	8	18	ARG	CB-CG-CD	-6.53	96.29	111.30
30	N	2071	A	C3'-C2'-O2'	6.52	120.48	110.70
36	0	1190	G	C4'-C3'-O3'	-6.52	99.62	109.40
36	0	665	A	C2'-C3'-O3'	-6.52	103.92	113.70
30	N	421	C	C2'-C3'-O3'	6.52	119.28	109.50
30	N	1666	G	O4'-C4'-C3'	-6.51	97.49	104.00
36	0	1145	A	C4'-C3'-O3'	-6.50	103.25	113.00
36	0	388	G	C2'-C3'-O3'	6.47	119.20	109.50
36	0	1301	U	N1-C1'-C2'	6.45	121.67	112.00
55	K	69	LYS	N-CA-C	6.45	124.53	110.80
10	Y	30	THR	N-CA-CB	6.44	121.37	110.49
36	0	1151	A	C4'-C3'-O3'	-6.43	103.35	113.00
30	N	1452	G	C4'-C3'-O3'	-6.42	103.38	113.00
36	0	1491	G	C2'-C3'-O3'	-6.39	104.12	113.70
10	Y	68	SER	N-CA-C	6.38	118.32	111.36
10	Y	47	ARG	NE-CZ-NH2	6.38	124.94	119.20
14	c	73	VAL	N-CA-CB	6.37	117.67	110.72
30	N	404	A	C4'-C3'-O3'	6.37	118.96	109.40
30	N	1212	G	C4'-C3'-O3'	-6.35	103.47	113.00
36	0	818	G	C4'-C3'-O3'	-6.35	103.47	113.00
53	I	57	ARG	CA-CB-CG	6.34	126.79	114.10
30	N	2443	C	O4'-C4'-C3'	-6.32	97.68	104.00
51	G	43	ALA	CA-C-N	6.31	133.59	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	G	43	ALA	C-N-CA	6.31	133.59	121.54
40	4	127	ALA	N-CA-C	6.30	119.51	110.24
25	n	25	VAL	CA-C-N	6.29	133.03	121.70
25	n	25	VAL	C-N-CA	6.29	133.03	121.70
36	0	1213	A	C4'-C3'-O3'	-6.29	103.57	113.00
1	O	44	G	N9-C1'-C2'	6.29	121.43	112.00
22	k	57	ARG	NE-CZ-NH2	6.28	124.85	119.20
2	P	11	PRO	CB-CA-C	-6.27	103.37	111.39
21	j	41	ARG	CD-NE-CZ	6.26	133.17	124.40
33	U	67	ALA	N-CA-C	-6.25	105.15	112.89
38	2	167	TRP	N-CA-C	6.24	119.72	110.48
30	N	2728	U	C2'-C3'-O3'	-6.22	104.36	113.70
30	N	859	G	C1'-C2'-O2'	-6.20	102.49	111.80
30	N	2364	C	O4'-C4'-C3'	-6.20	97.80	104.00
30	N	2501	C	C4'-C3'-O3'	-6.15	103.78	113.00
30	N	446	G	C2'-C3'-O3'	6.14	118.71	109.50
36	0	1201	A	C2'-C3'-O3'	6.14	118.71	109.50
21	j	41	ARG	CB-CG-CD	6.12	125.39	111.30
30	N	2728	U	C4'-C3'-O3'	-6.09	103.86	113.00
36	0	818	G	N9-C1'-C2'	6.08	121.11	112.00
30	N	1352	U	O4'-C1'-C2'	-6.07	101.53	107.60
40	4	138	ARG	N-CA-CB	6.07	120.75	110.49
47	B	44	LYS	N-CA-C	6.06	120.47	112.35
2	P	221	ARG	N-CA-CB	6.06	120.15	110.46
12	a	69	ARG	NE-CZ-NH2	6.03	124.63	119.20
27	p	12	ARG	CA-CB-CG	6.03	126.16	114.10
30	N	2725	A	C1'-C2'-O2'	-6.02	99.37	108.40
46	A	124	PRO	CA-C-N	6.02	128.95	120.28
46	A	124	PRO	C-N-CA	6.02	128.95	120.28
10	Y	78	ARG	NE-CZ-NH2	6.01	124.61	119.20
51	G	44	SER	N-CA-C	-6.01	98.00	110.80
47	B	22	PRO	O-C-N	-6.01	114.53	122.64
30	N	2319	G	C4'-C3'-O3'	-6.00	104.00	113.00
12	a	70	THR	N-CA-C	5.98	123.53	110.80
24	m	32	ILE	N-CA-CB	5.97	117.03	110.53
36	0	64	G	C2'-C3'-O3'	-5.95	104.77	113.70
30	N	827	U	C2'-C3'-O3'	-5.94	104.80	113.70
21	j	19	LYS	N-CA-C	5.93	120.52	113.16
30	N	1567	G	C1'-C2'-O2'	-5.93	102.90	111.80
30	N	2034	U	C4'-C3'-O3'	-5.93	104.11	113.00
30	N	1626	A	C2'-C3'-O3'	-5.91	104.83	113.70
29	r	36	ARG	NE-CZ-NH1	-5.90	115.60	121.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	820	A	O4'-C4'-C3'	-5.90	98.10	104.00
30	N	782	A	C4'-C3'-O3'	-5.90	100.55	109.40
30	N	974	G	C4'-C3'-O3'	-5.90	100.56	109.40
30	N	2468	A	C4'-C3'-O3'	-5.89	104.17	113.00
30	N	2035	G	C4'-C3'-O3'	-5.89	100.57	109.40
30	N	2518	A	C1'-C2'-O2'	-5.88	102.98	111.80
3	Q	113	SER	N-CA-C	5.88	117.64	110.41
21	j	41	ARG	N-CA-C	5.86	120.73	112.93
30	N	1254	A	C4'-C3'-O3'	-5.86	104.21	113.00
30	N	2543	G	C5'-C4'-C3'	-5.86	107.22	116.00
36	0	330	C	P-O5'-C5'	-5.85	112.13	120.90
30	N	301	G	C4'-C3'-O3'	-5.84	104.24	113.00
30	N	871	U	P-O5'-C5'	-5.84	112.14	120.90
30	N	2246	G	O4'-C4'-C3'	-5.83	98.17	104.00
30	N	2873	A	P-O5'-C5'	-5.80	112.20	120.90
25	n	25	VAL	N-CA-C	5.80	116.44	110.82
40	4	38	VAL	CG1-CB-CG2	-5.79	98.07	110.80
3	Q	151	THR	O-C-N	-5.79	114.95	121.43
30	N	140	C	N1-C1'-C2'	5.77	120.66	112.00
30	N	974	G	C2'-C3'-O3'	5.77	118.16	109.50
2	P	258	ARG	NE-CZ-NH1	-5.76	115.74	121.50
2	P	31	ALA	CA-C-N	-5.76	114.96	120.83
2	P	31	ALA	C-N-CA	-5.76	114.96	120.83
30	N	2447	G	P-O3'-C3'	5.76	128.84	120.20
2	P	177	ARG	CG-CD-NE	-5.76	99.33	112.00
2	P	238	ARG	N-CA-C	5.75	123.05	110.80
30	N	512	G	P-O3'-C3'	5.75	128.83	120.20
15	d	33	ARG	CB-CG-CD	-5.74	98.09	111.30
30	N	782	A	C2'-C3'-O3'	5.73	118.10	109.50
16	e	79	ARG	CD-NE-CZ	-5.73	116.37	124.40
30	N	1970	A	C2'-C3'-O3'	5.73	118.10	109.50
30	N	2035	G	C1'-C2'-O2'	-5.73	103.20	111.80
36	0	971	G	C2'-C3'-O3'	-5.71	105.14	113.70
30	N	2267	A	N9-C1'-C2'	5.71	120.56	112.00
30	N	2049	G	C3'-C2'-O2'	5.70	119.25	110.70
13	b	102	ARG	NE-CZ-NH1	-5.69	115.81	121.50
36	0	1280	A	C4'-C3'-O3'	-5.69	104.47	113.00
30	N	2543	G	O5'-C5'-C4'	5.69	120.03	111.50
2	P	156	ARG	CB-CG-CD	-5.69	98.22	111.30
40	4	24	THR	N-CA-C	5.68	117.56	110.91
1	O	88	C	C4'-C3'-O3'	-5.67	104.49	113.00
38	2	3	GLN	N-CA-C	5.67	122.14	113.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	0	96	U	C2'-C3'-O3'	5.66	122.19	113.70
13	b	100	HIS	CA-C-N	-5.66	115.46	123.95
13	b	100	HIS	C-N-CA	-5.66	115.46	123.95
30	N	555	G	C4'-C3'-O3'	-5.66	104.51	113.00
15	d	13	ARG	NE-CZ-NH2	5.65	124.29	119.20
25	n	7	LYS	CD-CE-NZ	5.65	129.99	111.90
44	8	126	GLN	CA-C-O	-5.65	114.83	121.16
14	c	53	ARG	CB-CG-CD	-5.65	98.31	111.30
30	N	2776	A	C8-N9-C1'	-5.63	110.80	127.70
30	N	301	G	N9-C1'-C2'	5.62	120.43	112.00
36	0	1196	A	C4'-C3'-O3'	-5.61	104.58	113.00
30	N	1900	A	P-O3'-C3'	5.61	128.62	120.20
30	N	2019	A	C3'-C2'-O2'	5.61	119.11	110.70
38	2	6	HIS	N-CA-C	-5.61	102.58	109.65
30	N	2776	A	C4-N9-C1'	5.61	143.12	126.30
30	N	1205	A	C4'-C3'-O3'	5.60	117.80	109.40
30	N	1661	G	C3'-C2'-O2'	5.60	119.11	110.70
12	a	69	ARG	CG-CD-NE	5.60	124.32	112.00
30	N	2517	C	O3'-P-O5'	-5.59	95.61	104.00
30	N	1261	C	O4'-C4'-C3'	-5.58	98.42	104.00
25	n	55	ILE	N-CA-C	5.57	120.93	109.34
30	N	752	A	N9-C1'-C2'	5.57	122.35	114.00
33	U	5	LEU	N-CA-C	5.57	118.76	110.52
28	q	8	ARG	CG-CD-NE	5.56	124.24	112.00
36	0	1432	G	C4'-C3'-O3'	-5.56	104.66	113.00
1	O	24	G	C2'-C3'-O3'	-5.56	105.36	113.70
30	N	1565	C	C5'-C4'-C3'	-5.55	106.87	115.20
36	0	665	A	C3'-C2'-O2'	5.55	119.03	110.70
30	N	2034	U	O3'-P-O5'	-5.55	95.67	104.00
30	N	784	G	P-O3'-C3'	5.55	128.53	120.20
36	0	686	U	C4'-C3'-O3'	-5.54	104.69	113.00
30	N	1565	C	C2'-C3'-O3'	5.53	117.80	109.50
30	N	2645	G	C5'-C4'-C3'	-5.53	106.91	115.20
37	1	17	GLY	CA-C-O	-5.51	117.82	122.29
14	c	21	ARG	NE-CZ-NH1	-5.51	115.99	121.50
30	N	727	A	N9-C1'-C2'	5.50	120.26	112.00
30	N	372	G	C1'-C2'-O2'	-5.50	103.55	111.80
30	N	2751	G	C2'-C3'-O3'	-5.50	105.45	113.70
30	N	1428	C	C2'-C3'-O3'	-5.48	105.48	113.70
30	N	1012	U	C2'-C3'-O3'	-5.48	105.48	113.70
36	0	1125	U	N1-C1'-C2'	5.48	120.22	112.00
3	Q	160	LYS	CG-CD-CE	5.47	123.89	111.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	2724	U	C2'-C3'-O3'	-5.47	105.50	113.70
30	N	947	A	C3'-C2'-O2'	-5.47	102.50	110.70
30	N	2645	G	P-O5'-C5'	-5.46	112.70	120.90
36	0	813	U	C4'-C3'-O3'	-5.46	104.81	113.00
41	5	63	ASN	N-CA-C	5.45	117.29	110.91
30	N	645	C	N1-C1'-C2'	5.45	120.18	112.00
30	N	962	G	C3'-C2'-O2'	5.45	118.87	110.70
40	4	157	ARG	NE-CZ-NH1	-5.43	116.07	121.50
30	N	983	A	C5'-C4'-O4'	-5.42	101.66	109.80
30	N	923	G	C3'-C2'-O2'	5.42	118.82	110.70
25	n	7	LYS	CG-CD-CE	-5.41	98.85	111.30
30	N	2038	G	C3'-C2'-O2'	5.41	118.82	110.70
30	N	2497	A	C2'-C3'-O3'	5.40	117.60	109.50
29	r	1	MET	CB-CG-SD	-5.39	96.53	112.70
36	0	563	A	N9-C1'-C2'	5.39	120.09	112.00
30	N	51	G	C4'-C3'-O3'	-5.38	104.92	113.00
30	N	2820	A	C4'-C3'-O3'	-5.38	104.93	113.00
36	0	1211	U	C2'-C3'-O3'	-5.38	105.63	113.70
36	0	5	U	C2'-C3'-O3'	-5.38	105.63	113.70
52	H	71	LYS	N-CA-C	5.38	122.25	110.80
21	j	41	ARG	NH1-CZ-NH2	-5.36	112.34	119.30
30	N	1819	A	C1'-C2'-O2'	-5.34	103.79	111.80
30	N	2354	C	C5'-C4'-C3'	-5.34	107.99	116.00
30	N	1937	A	N9-C1'-C2'	5.33	120.00	112.00
30	N	783	A	O4'-C1'-C2'	-5.33	102.27	107.60
30	N	1236	G	P-O3'-C3'	5.33	128.19	120.20
45	9	42	LEU	CA-C-N	5.32	126.50	119.84
45	9	42	LEU	C-N-CA	5.32	126.50	119.84
10	Y	18	ARG	NE-CZ-NH2	-5.32	114.41	119.20
30	N	2645	G	C2'-C3'-O3'	5.32	117.47	109.50
36	0	388	G	O3'-P-O5'	-5.31	96.03	104.00
10	Y	29	LYS	CD-CE-NZ	-5.31	94.91	111.90
30	N	1620	G	C3'-C2'-O2'	5.30	118.66	110.70
36	0	1094	G	C4'-C3'-O3'	-5.30	105.06	113.00
22	k	28	ARG	NE-CZ-NH2	-5.29	114.44	119.20
30	N	1977	A	C2'-C3'-O3'	-5.29	105.77	113.70
30	N	2552	U	C3'-C2'-O2'	5.28	118.62	110.70
27	p	12	ARG	CB-CG-CD	-5.27	99.17	111.30
30	N	2092	U	P-O5'-C5'	-5.27	112.99	120.90
30	N	1650	A	C3'-C2'-O2'	5.27	118.60	110.70
30	N	1770	G	C3'-C2'-O2'	5.27	118.60	110.70
30	N	2498	C	C3'-C2'-O2'	5.27	118.61	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	310	A	C1'-C2'-O2'	-5.26	100.51	108.40
50	F	64	ARG	CG-CD-NE	-5.26	100.43	112.00
30	N	2849	U	P-O5'-C5'	5.25	128.78	120.90
11	Z	118	LYS	CB-CG-CD	-5.24	99.25	111.30
30	N	785	G	P-O5'-C5'	-5.24	113.04	120.90
39	3	5	LEU	CB-CA-C	-5.24	104.46	112.11
30	N	372	G	C2'-C3'-O3'	5.23	117.35	109.50
30	N	2430	A	C3'-C2'-O2'	5.23	118.54	110.70
30	N	2867	G	C4'-C3'-O3'	5.23	117.24	109.40
30	N	669	G	N9-C1'-C2'	5.22	119.83	112.00
30	N	2394	C	O4'-C4'-C3'	-5.22	98.78	104.00
30	N	2497	A	C4'-C3'-O3'	-5.22	101.57	109.40
9	X	29	HIS	CB-CA-C	-5.22	103.47	111.66
3	Q	114	LYS	CA-CB-CG	5.21	124.53	114.10
30	N	278	A	N9-C1'-C2'	5.21	119.81	112.00
36	0	1530	G	C4'-C3'-O3'	-5.21	105.19	113.00
30	N	2049	G	O4'-C4'-C3'	-5.21	98.80	104.00
2	P	226	ASN	CA-C-N	-5.20	114.30	119.56
2	P	226	ASN	C-N-CA	-5.20	114.30	119.56
3	Q	12	THR	N-CA-C	-5.20	101.48	108.19
1	O	41	G	C4'-C3'-O3'	-5.20	105.20	113.00
2	P	156	ARG	CG-CD-NE	5.20	123.44	112.00
36	0	1303	C	N1-C1'-C2'	5.20	119.80	112.00
30	N	2502	G	C3'-C2'-O2'	-5.20	102.91	110.70
36	0	652	U	C2'-C3'-O3'	-5.20	105.91	113.70
30	N	2596	U	C2'-C3'-O3'	-5.19	105.91	113.70
30	N	2638	G	C4'-C3'-O3'	-5.19	105.21	113.00
32	C	55	SER	N-CA-C	5.19	116.94	111.28
30	N	2311	A	P-O3'-C3'	5.19	127.98	120.20
47	B	12	ARG	NE-CZ-NH1	-5.18	116.32	121.50
36	0	812	G	C1'-C2'-O2'	-5.17	100.64	108.40
4	R	49	ARG	NE-CZ-NH1	-5.17	116.33	121.50
30	N	1998	A	O4'-C4'-C3'	-5.17	98.83	104.00
30	N	421	C	C4'-C3'-O3'	5.17	117.15	109.40
30	N	2580	U	N1-C1'-C2'	5.17	119.75	112.00
30	N	2474	U	N1-C1'-C2'	5.16	119.74	112.00
30	N	1676	A	C3'-C2'-O2'	5.15	118.43	110.70
49	E	49	GLN	N-CA-C	-5.15	104.28	110.88
17	f	11	ARG	N-CA-CB	5.15	118.00	110.58
30	N	2238	G	C4'-C3'-O3'	-5.15	101.67	109.40
30	N	481	G	C2'-C3'-O3'	-5.15	105.98	113.70
30	N	1343	G	N9-C1'-C2'	5.15	119.72	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	X	35	VAL	CA-C-O	-5.14	115.22	121.18
30	N	2621	G	C3'-C2'-O2'	5.13	118.40	110.70
56	s	33	ARG	CA-CB-CG	5.13	124.37	114.10
30	N	2035	G	C2'-C3'-O3'	5.13	117.19	109.50
3	Q	128	ARG	CA-C-N	5.13	127.99	120.71
3	Q	128	ARG	C-N-CA	5.13	127.99	120.71
12	a	69	ARG	N-CA-C	-5.13	103.27	110.50
30	N	27	G	C5'-C4'-O4'	-5.12	102.12	109.80
30	N	2062	A	O4'-C4'-C3'	-5.11	100.99	106.10
1	O	100	G	C3'-C2'-O2'	5.11	118.36	110.70
30	N	2019	A	C2'-C3'-O3'	-5.11	106.04	113.70
39	3	23	SER	O-C-N	5.11	128.03	122.11
33	U	96	THR	N-CA-C	-5.11	106.90	113.23
10	Y	41	ARG	CA-CB-CG	-5.10	103.90	114.10
30	N	2732	G	C3'-C2'-O2'	-5.10	103.05	110.70
51	G	42	ILE	CA-C-N	5.10	131.27	121.54
51	G	42	ILE	C-N-CA	5.10	131.27	121.54
30	N	123	G	C3'-C2'-O2'	5.08	118.32	110.70
34	M	9	C	C2'-C3'-O3'	-5.08	106.08	113.70
15	d	32	TYR	CA-C-O	5.08	125.84	120.10
29	r	36	ARG	CG-CD-NE	-5.08	100.83	112.00
30	N	1180	U	N1-C1'-C2'	5.07	119.61	112.00
30	N	1253	A	C2'-C3'-O3'	5.07	117.11	109.50
40	4	30	ILE	CB-CA-C	5.06	117.72	110.33
30	N	1928	A	C3'-C2'-O2'	5.06	118.29	110.70
30	N	820	A	O4'-C1'-C2'	-5.06	102.54	107.60
15	d	3	ARG	NE-CZ-NH1	-5.06	116.44	121.50
30	N	1131	G	O3'-P-O5'	-5.06	96.42	104.00
30	N	566	U	C2'-C3'-O3'	-5.05	106.12	113.70
36	0	812	G	P-O3'-C3'	5.05	127.78	120.20
36	0	595	A	C4'-C3'-O3'	5.04	116.96	109.40
36	0	971	G	P-O5'-C5'	-5.04	113.35	120.90
37	1	103	ASN	N-CA-CB	5.03	119.92	110.56
30	N	995	C	C1'-C2'-O2'	-5.03	104.26	111.80
11	Z	8	LYS	CB-CG-CD	-5.03	99.74	111.30
12	a	1	MET	CB-CG-SD	-5.02	97.63	112.70
36	0	801	U	C2'-C3'-O3'	-5.02	106.17	113.70
30	N	1937	A	P-O5'-C5'	-5.02	113.37	120.90
30	N	2049	G	C2'-C3'-O3'	-5.02	106.17	113.70
30	N	2502	G	P-O5'-C5'	5.02	128.43	120.90
15	d	53	ARG	NE-CZ-NH1	5.02	126.52	121.50
36	0	1145	A	N9-C1'-C2'	5.01	119.52	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	N	1997	C	O4'-C4'-C3'	-5.00	99.00	104.00
15	d	9	ILE	N-CA-C	5.00	117.34	111.09

There are no chirality outliers.

All (46) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
36	0	24	U	Sidechain
36	0	368	U	Sidechain
36	0	559	A	Sidechain
36	0	571	U	Sidechain
36	0	864	A	Sidechain
37	1	102	THR	Peptide
37	1	14	VAL	Peptide
38	2	79	LYS	Peptide
38	2	80	LYS	Peptide
40	4	102	GLY	Peptide
40	4	136	VAL	Peptide
40	4	137	VAL	Peptide
40	4	142	ASP	Peptide
40	4	89	HIS	Peptide
41	5	52	ASN	Peptide
41	5	93	LYS	Peptide
44	8	128	SER	Peptide
44	8	53	GLU	Peptide
44	8	54	LEU	Peptide
44	8	55	VAL	Peptide
46	A	125	LYS	Peptide
47	B	22	PRO	Peptide
47	B	77	HIS	Peptide
52	H	17	MET	Peptide
52	H	69	LYS	Peptide
54	J	37	ARG	Peptide
55	K	3	ASN	Peptide
30	N	1802	A	Sidechain
30	N	2522	U	Sidechain
30	N	2765	A	Sidechain
30	N	586	A	Sidechain
30	N	850	U	Sidechain
30	N	927	A	Sidechain
2	P	195	VAL	Peptide
2	P	234	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	P	238	ARG	Peptide
3	Q	151	THR	Peptide
5	S	174	ASP	Peptide
5	S	175	PHE	Peptide
10	Y	114	GLY	Peptide
10	Y	82	LEU	Peptide
11	Z	57	VAL	Peptide,Mainchain
19	h	52	LEU	Peptide
28	q	31	HIS	Peptide
56	s	34	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	2529	0	1281	11	0
2	P	2082	0	2154	55	0
3	Q	1564	0	1616	24	0
4	R	1552	0	1619	18	0
5	S	1410	0	1443	33	0
6	T	1322	0	1371	14	0
7	V	1031	0	1085	21	0
8	W	1128	0	1162	15	0
9	X	938	0	1012	19	0
10	Y	1044	0	1117	18	0
11	Z	1073	0	1157	17	0
12	a	960	0	1000	15	0
13	b	891	0	923	9	0
14	c	915	0	958	14	0
15	d	946	0	1019	21	0
16	e	815	0	839	19	0
17	f	857	0	922	10	0
18	g	738	0	807	5	0
19	h	779	0	831	11	0
20	i	752	0	780	9	0
21	j	568	0	581	10	0
22	k	624	0	652	15	0
23	l	508	0	543	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	m	448	0	488	2	0
25	n	443	0	458	13	0
26	o	409	0	440	6	0
27	p	376	0	418	16	0
28	q	503	0	572	12	0
29	r	301	0	341	7	0
30	N	62215	0	31274	421	0
31	L	404	0	405	11	0
32	C	1027	0	1091	43	0
33	U	1111	0	1148	52	0
34	M	1594	0	809	110	0
35	x	294	0	150	38	0
36	0	33015	0	16607	244	0
37	1	1704	0	1731	39	0
38	2	1624	0	1696	48	0
39	3	1642	0	1704	31	0
40	4	1105	0	1148	21	0
41	5	817	0	808	17	0
42	6	1181	0	1238	17	0
43	7	978	0	1031	6	0
44	8	1021	0	1070	36	0
45	9	786	0	828	19	0
46	A	876	0	887	23	0
47	B	954	0	1016	18	0
48	D	883	0	939	24	0
49	E	773	0	824	12	0
50	F	709	0	728	16	0
51	G	648	0	666	9	0
52	H	648	0	691	6	0
53	I	455	0	478	13	0
54	J	637	0	665	10	0
55	K	664	0	714	17	0
56	s	425	0	449	13	0
57	t	704	0	327	3	0
58	u	1561	0	785	44	0
59	u	2	0	0	0	0
60	u	1	0	0	0	0
61	u	9	0	0	0	0
All	All	147973	0	99496	1314	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 (1314) 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)
35:x:448:U:C6	38:2:162:ILE:HD11	1.46	1.47
30:N:306:U:H3	30:N:310:A:N6	1.15	1.41
35:x:451:G:N3	39:3:47:ARG:HD3	1.35	1.39
2:P:133:ARG:CD	33:U:123:ARG:NH1	1.86	1.37
35:x:448:U:C5	38:2:162:ILE:HD11	1.60	1.37
36:0:1493:A:C2	58:u:37:A:O2'	1.79	1.35
30:N:2251:G:O6	34:M:75:A:N1	1.63	1.32
36:0:1160:G:OP1	37:1:132:LYS:NZ	1.60	1.32
36:0:1238:A:N6	36:0:1301:U:H3	1.22	1.32
30:N:2253:G:H1	34:M:73:C:N4	1.33	1.26
22:k:60:ASP:OD2	33:U:27:ARG:NH2	1.68	1.25
34:M:31:U:H5'	36:0:1340:A:O2'	1.29	1.25
34:M:33:C:OP2	44:8:130:ARG:HG3	1.36	1.25
2:P:133:ARG:HD3	33:U:123:ARG:NH1	1.41	1.24
36:0:1493:A:N1	58:u:37:A:O2'	1.66	1.24
30:N:499:U:H3	30:N:503:A:N6	1.39	1.21
5:S:112:ARG:CG	48:D:71:ARG:HH22	1.54	1.21
30:N:882:G:C4'	58:u:19:G:N2	1.94	1.20
30:N:882:G:C4'	58:u:19:G:H22	1.47	1.18
34:M:29:G:OP1	36:0:1229:A:O2'	1.60	1.18
34:M:40:C:O2	36:0:1338:G:N2	1.79	1.14
30:N:1924:C:H4'	34:M:13:A:C4'	1.77	1.14
30:N:1924:C:C4'	34:M:13:A:H4'	1.78	1.12
36:0:1103:C:O2'	37:1:106:THR:CG2	1.99	1.11
5:S:143:TYR:CE2	48:D:7:ILE:O	2.04	1.10
30:N:2253:G:N1	34:M:73:C:N4	1.99	1.10
2:P:133:ARG:HD2	33:U:123:ARG:HH11	0.96	1.10
30:N:1924:C:H4'	34:M:13:A:H4'	1.11	1.09
5:S:112:ARG:HG2	48:D:71:ARG:NH2	1.66	1.09
35:x:448:U:C5	38:2:162:ILE:CD1	2.34	1.08
30:N:882:G:O4'	58:u:56:C:N3	1.88	1.07
30:N:715:A:C6	50:F:53:ARG:NH1	2.23	1.07
30:N:882:G:H4'	58:u:19:G:N2	1.24	1.07
35:x:448:U:C6	38:2:162:ILE:CD1	2.37	1.06
36:0:1103:C:O2'	37:1:106:THR:HG21	1.52	1.06
35:x:451:G:N3	39:3:47:ARG:CD	2.19	1.06
30:N:1924:C:H4'	34:M:13:A:C5'	1.87	1.04
30:N:306:U:N3	30:N:310:A:N6	1.86	1.03
5:S:112:ARG:HG2	48:D:71:ARG:HH22	0.87	1.02
34:M:34:U:OP2	44:8:129:LYS:NZ	1.90	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:882:G:O2'	58:u:56:C:O2	1.76	1.01
30:N:1923:U:H4'	34:M:12:C:H1'	1.41	1.01
34:M:32:U:C5	44:8:129:LYS:NZ	2.29	1.00
5:S:112:ARG:CG	48:D:71:ARG:NH2	2.20	1.00
30:N:1924:C:C5'	34:M:13:A:H4'	1.91	0.99
34:M:30:A:H1'	36:0:1339:A:C2	1.97	0.99
35:x:451:G:C2	39:3:47:ARG:HD3	1.97	0.98
34:M:30:A:C1'	36:0:1339:A:C2	2.47	0.98
2:P:133:ARG:HD2	33:U:123:ARG:NH1	1.64	0.97
35:x:450:C:H42	38:2:164:ARG:NH1	1.63	0.96
34:M:15:G:H5''	34:M:15:G:C8	2.03	0.93
34:M:29:G:OP1	36:0:1229:A:O3'	1.87	0.93
30:N:2251:G:C6	34:M:75:A:N1	2.35	0.93
34:M:15:G:H5''	34:M:15:G:H8	1.31	0.93
36:0:1493:A:C2	58:u:37:A:H1'	2.04	0.93
34:M:33:C:OP2	44:8:130:ARG:CG	2.15	0.92
2:P:133:ARG:CD	33:U:123:ARG:HH11	1.60	0.92
34:M:40:C:O2'	36:0:1338:G:H1'	1.69	0.92
34:M:28:G:O3'	36:0:1229:A:H4'	1.70	0.91
5:S:143:TYR:HE2	48:D:7:ILE:O	1.45	0.91
35:x:448:U:H5	38:2:162:ILE:CD1	1.82	0.89
2:P:133:ARG:HD3	33:U:123:ARG:HH12	1.38	0.89
36:0:1060:U:C5	38:2:2:GLY:HA3	2.07	0.89
2:P:187:ASP:OD1	33:U:123:ARG:NH2	2.06	0.89
35:x:449:A:H62	38:2:164:ARG:HD3	1.34	0.88
30:N:2304:G:H22	30:N:2312:U:H3	1.23	0.87
30:N:897:C:H5'	58:u:56:C:C5'	1.93	0.87
34:M:31:U:C5'	36:0:1340:A:O2'	2.21	0.86
35:x:448:U:H6	38:2:162:ILE:HD11	1.11	0.86
34:M:30:A:O4'	36:0:1339:A:C2	2.28	0.86
2:P:121:ASP:CG	33:U:91:PHE:CE1	2.53	0.86
9:X:49:ARG:HH22	36:0:1423:G:P	1.97	0.86
30:N:882:G:C1'	58:u:56:C:C2	2.59	0.86
30:N:715:A:C1'	50:F:40:GLN:HE22	1.89	0.85
30:N:2177:C:O3'	32:C:211:LYS:HE2	1.76	0.85
34:M:29:G:OP1	36:0:1229:A:C3'	2.24	0.85
5:S:80:ARG:HD3	34:M:55:C:N1	1.87	0.85
36:0:1103:C:O2'	37:1:106:THR:HG22	1.77	0.84
30:N:2251:G:N1	34:M:75:A:C2	2.45	0.84
2:P:35:GLU:OE2	30:N:1816:C:N4	2.10	0.84
34:M:40:C:H4'	36:0:1338:G:O2'	1.77	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:0:1054:C:C4	58:u:34:G:C8	2.67	0.82
2:P:121:ASP:CG	33:U:91:PHE:HE1	1.87	0.82
36:0:1493:A:N1	58:u:37:A:C2'	2.42	0.81
35:x:448:U:H6	38:2:162:ILE:CD1	1.85	0.81
45:9:83:THR:O	45:9:87:LEU:HB2	1.79	0.81
34:M:15:G:H5'	34:M:16:C:OP2	1.81	0.81
5:S:143:TYR:CD2	48:D:7:ILE:O	2.32	0.81
36:0:1100:C:OP2	37:1:95:ARG:HD3	1.81	0.81
30:N:882:G:O4'	58:u:56:C:C2	2.34	0.80
34:M:31:U:H5''	36:0:1341:U:H5'	1.62	0.80
34:M:29:G:OP1	36:0:1229:A:C2'	2.29	0.80
46:A:109:ASN:OD1	56:s:7:ARG:HG2	1.80	0.80
30:N:2251:G:C6	34:M:75:A:C2	2.71	0.79
36:0:1493:A:H2	58:u:37:A:H1'	1.47	0.79
35:x:449:A:H62	38:2:164:ARG:CD	1.95	0.79
36:0:1493:A:C2	58:u:37:A:C2'	2.66	0.78
30:N:284:U:H3	30:N:356:G:H1	1.30	0.78
30:N:882:G:H1'	58:u:56:C:C2	2.19	0.78
30:N:2253:G:N1	34:M:73:C:C4	2.47	0.78
34:M:34:U:OP1	44:8:129:LYS:HD3	1.83	0.78
12:a:53:THR:HG21	30:N:2840:C:H5''	1.66	0.77
5:S:112:ARG:HG3	48:D:71:ARG:NH2	2.00	0.77
36:0:1493:A:N1	58:u:37:A:C1'	2.46	0.77
29:r:3:VAL:HG21	30:N:2539:C:H5'	1.67	0.77
48:D:101:ARG:NH1	48:D:104:THR:OG1	2.16	0.77
33:U:40:THR:HB	33:U:43:ASN:HD22	1.49	0.76
36:0:1238:A:N7	36:0:1301:U:O4	2.17	0.76
36:0:1279:G:OP1	45:9:9:ARG:NH2	2.18	0.76
9:X:49:ARG:NH2	36:0:1422:G:O3'	2.18	0.76
2:P:121:ASP:OD2	33:U:91:PHE:CE1	2.39	0.76
32:C:3:LYS:HG3	32:C:4:LEU:H	1.50	0.76
5:S:80:ARG:CD	34:M:55:C:C6	2.68	0.75
9:X:49:ARG:NH2	36:0:1423:G:OP1	2.18	0.75
34:M:16:C:H3'	34:M:17:G:H5'	1.68	0.75
36:0:1100:C:OP2	37:1:95:ARG:CD	2.33	0.75
35:x:449:A:N6	38:2:164:ARG:HD3	2.02	0.75
30:N:306:U:C2	30:N:310:A:N6	2.54	0.75
2:P:221:ARG:NH1	30:N:1789:A:OP2	2.20	0.74
34:M:29:G:P	36:0:1229:A:H4'	2.26	0.74
34:M:34:U:P	44:8:129:LYS:NZ	2.61	0.74
3:Q:14:ILE:HA	14:c:12:GLN:HE22	1.52	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:1093:G:N2	30:N:1098:A:H62	1.85	0.74
45:9:65:TYR:HB3	49:E:96:LEU:HD11	1.69	0.74
48:D:87:ARG:O	48:D:91:HIS:HB2	1.87	0.74
30:N:896:A:C4	58:u:56:C:H5'	2.23	0.74
30:N:499:U:N3	30:N:503:A:N6	2.11	0.74
30:N:882:G:C4'	58:u:56:C:N3	2.51	0.74
36:0:673:A:O3'	41:5:86:ARG:NH2	2.20	0.73
36:0:1493:A:C2	58:u:37:A:C1'	2.69	0.73
40:4:101:GLU:OE2	40:4:103:THR:OG1	2.05	0.73
2:P:121:ASP:OD1	33:U:91:PHE:HE1	1.69	0.73
30:N:2112:G:H2'	30:N:2113:U:H5'	1.69	0.73
30:N:882:G:C3'	58:u:19:G:N2	2.52	0.73
30:N:2093:G:H5'	33:U:22:LYS:HD3	1.71	0.73
36:0:1238:A:N6	36:0:1301:U:N3	2.01	0.73
30:N:1924:C:H5'	34:M:13:A:H4'	1.68	0.72
36:0:1527:U:OP2	56:s:39:GLU:OE1	2.07	0.72
54:J:30:PRO:HA	54:J:48:THR:O	1.88	0.72
36:0:1147:C:O2	44:8:18:ARG:NH2	2.22	0.72
30:N:1924:C:C5'	34:M:13:A:C4'	2.67	0.72
40:4:81:LEU:HD13	40:4:123:VAL:HG11	1.72	0.72
5:S:80:ARG:HD2	34:M:55:C:C6	2.25	0.72
30:N:1093:G:H21	30:N:1098:A:N6	1.87	0.72
54:J:6:LYS:HG3	54:J:7:LYS:HG2	1.70	0.71
30:N:2251:G:N1	34:M:75:A:H2	1.85	0.71
12:a:77:ALA:O	12:a:81:ASN:HB2	1.90	0.71
34:M:34:U:P	44:8:129:LYS:HZ3	2.11	0.71
34:M:16:C:C3'	34:M:17:G:H5'	2.20	0.71
30:N:2177:C:H4'	32:C:211:LYS:HZ1	1.56	0.71
28:q:8:ARG:NH2	30:N:243:U:OP1	2.24	0.71
36:0:1081:A:OP2	40:4:52:LYS:NZ	2.23	0.70
5:S:37:ASN:ND2	30:N:2312:U:O2	2.24	0.70
49:E:47:LYS:HB3	54:J:13:LEU:HD12	1.72	0.70
30:N:2637:U:N3	30:N:2776:A:N6	2.40	0.70
30:N:715:A:C5	50:F:53:ARG:NH1	2.59	0.70
36:0:404:G:O2'	36:0:498:A:N1	2.23	0.70
2:P:258:ARG:NH1	2:P:264:ASP:OD1	2.23	0.70
4:R:163:ASN:ND2	30:N:323:C:H2'	2.07	0.70
35:x:450:C:N4	38:2:164:ARG:NH1	2.39	0.70
30:N:2128:G:H21	30:N:2173:A:H1'	1.57	0.69
36:0:664:G:H22	36:0:741:G:H1	1.37	0.69
5:S:80:ARG:HD3	34:M:55:C:C6	2.27	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:f:15:GLN:HE22	30:N:1266:G:H5''	1.56	0.69
30:N:1919:A:H1'	36:O:1407:C:O2'	1.92	0.69
35:x:448:U:H5	38:2:162:ILE:HD13	1.57	0.69
36:O:1309:G:OP2	48:D:98:ARG:NH1	2.25	0.69
22:k:60:ASP:OD2	33:U:27:ARG:CZ	2.41	0.69
30:N:613:A:N7	30:N:616:A:N1	2.41	0.68
1:O:48:U:OP1	13:b:30:ARG:NH2	2.26	0.68
2:P:133:ARG:CD	33:U:123:ARG:CZ	2.71	0.68
36:O:501:C:OP1	47:B:114:ARG:NH2	2.26	0.68
2:P:87:ARG:NH2	30:N:1817:G:OP1	2.26	0.68
37:1:209:ALA:O	37:1:213:TYR:HB2	1.94	0.68
18:g:46:ALA:O	18:g:50:LEU:HB2	1.94	0.68
36:O:1054:C:N4	58:u:34:G:N7	2.41	0.68
8:W:113:PRO:HD2	30:N:558:U:OP1	1.94	0.67
30:N:2107:G:OP1	32:C:3:LYS:HE3	1.94	0.67
30:N:2134:A:N6	30:N:2157:G:H4'	2.09	0.67
36:O:1493:A:H61	58:u:37:A:H4'	1.58	0.67
30:N:962:G:H21	30:N:2250:G:H1	1.41	0.67
34:M:28:G:O3'	36:O:1229:A:C4'	2.43	0.67
34:M:29:G:P	36:O:1229:A:O3'	2.52	0.67
49:E:26:GLU:HG2	49:E:30:ILE:HD12	1.77	0.67
44:8:84:THR:HG21	44:8:103:PHE:HB3	1.75	0.67
34:M:30:A:O4'	36:O:1339:A:N1	2.27	0.67
36:O:1064:G:N2	36:O:1190:G:O2'	2.28	0.67
6:T:67:THR:HG21	30:N:2757:A:N1	2.11	0.66
30:N:1912:A:N1	36:O:1408:A:H4'	2.11	0.66
48:D:29:ARG:HH21	48:D:63:PHE:HB2	1.59	0.66
30:N:2156:G:H2'	30:N:2157:G:H5'	1.78	0.66
30:N:882:G:C1'	58:u:56:C:O2	2.42	0.66
30:N:499:U:C2	30:N:503:A:N6	2.63	0.66
36:O:427:U:OP1	39:3:13:ARG:NH2	2.28	0.66
36:O:458:U:H3	36:O:474:G:H1	1.44	0.66
46:A:24:HIS:HB3	46:A:31:ILE:HG23	1.78	0.66
58:u:21:A:H4'	58:u:22:G:OP1	1.96	0.66
30:N:2121:G:H4'	32:C:167:LYS:HD3	1.79	0.65
34:M:74:C:H2'	34:M:75:A:H1'	1.78	0.65
34:M:33:C:P	44:8:130:ARG:HG3	2.36	0.65
28:q:8:ARG:NH2	30:N:243:U:P	2.69	0.65
36:O:554:A:H5'	47:B:26:ALA:HB1	1.78	0.65
30:N:1311:G:H21	30:N:1603:A:H62	1.45	0.65
33:U:87:GLU:OE2	41:5:14:GLN:NE2	2.30	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:x:450:C:H42	38:2:164:ARG:HH11	1.38	0.65
22:k:39:TRP:CD1	33:U:32:PRO:HA	2.32	0.65
30:N:715:A:C1'	50:F:40:GLN:NE2	2.60	0.65
36:0:974:A:OP1	49:E:69:ARG:NH2	2.30	0.65
36:0:1060:U:OP1	49:E:85:ARG:NH2	2.30	0.64
2:P:121:ASP:CG	33:U:91:PHE:CD1	2.75	0.64
27:p:37:LYS:HE2	30:N:469:G:O6	1.97	0.64
36:0:437:U:OP1	39:3:152:GLN:NE2	2.30	0.64
30:N:2637:U:H3	30:N:2776:A:N6	1.96	0.64
34:M:34:U:OP1	44:8:129:LYS:CD	2.45	0.64
3:Q:38:LYS:O	3:Q:46:ARG:HA	1.97	0.64
30:N:1019:U:H3	30:N:1142:A:N6	1.95	0.64
43:7:75:ILE:HD13	43:7:129:VAL:HG22	1.79	0.64
30:N:2405:G:O2'	30:N:2411:A:N6	2.30	0.64
35:x:449:A:N7	38:2:164:ARG:HD3	2.12	0.64
2:P:29:PRO:HG2	2:P:34:LEU:HD11	1.78	0.64
5:S:88:LYS:HD3	30:N:2313:C:H5''	1.80	0.64
30:N:140:C:OP1	30:N:141:G:N2	2.30	0.64
30:N:2178:C:P	32:C:211:LYS:HE2	2.37	0.64
44:8:123:ARG:NH1	44:8:124:ARG:O	2.31	0.64
1:O:31:C:H4'	5:S:26:MET:HE1	1.79	0.64
30:N:882:G:O3'	58:u:19:G:N2	2.31	0.64
9:X:2:ILE:HB	9:X:33:ALA:HB3	1.80	0.63
9:X:92:GLU:O	9:X:93:GLN:HB2	1.98	0.63
15:d:6:ARG:NH1	30:N:585:G:N7	2.47	0.63
33:U:84:ALA:HA	33:U:91:PHE:H	1.62	0.63
43:7:15:ARG:NH1	43:7:75:ILE:O	2.30	0.63
36:0:972:C:OP2	45:9:59:LYS:HD3	1.98	0.63
18:g:28:ASN:OD1	18:g:91:GLN:NE2	2.31	0.63
52:H:9:GLN:HG2	52:H:60:GLU:HG2	1.81	0.63
6:T:86:LYS:HG3	6:T:132:VAL:HG22	1.81	0.63
11:Z:55:ARG:NH2	30:N:2469:A:O2'	2.32	0.63
30:N:1105:U:H2'	30:N:1106:G:H8	1.64	0.63
34:M:33:C:OP2	44:8:130:ARG:CD	2.46	0.63
44:8:25:ASN:HA	44:8:59:GLU:HG3	1.81	0.63
44:8:46:MET:HE2	44:8:50:GLN:HE21	1.63	0.63
27:p:44:VAL:HG13	27:p:44:VAL:O	1.99	0.62
36:0:1160:G:P	37:1:132:LYS:NZ	2.71	0.62
9:X:49:ARG:NH2	36:0:1423:G:P	2.71	0.62
36:0:1086:U:H3	36:0:1099:G:H22	1.46	0.62
42:6:147:ALA:O	46:A:56:ARG:NH2	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:2141:G:H2'	30:N:2142:A:H8	1.63	0.62
36:0:1054:C:N4	58:u:34:G:C8	2.66	0.62
30:N:1066:U:O2'	30:N:1074:G:N2	2.32	0.62
54:J:11:ILE:HG22	54:J:38:SER:HB3	1.81	0.62
3:Q:45:TYR:HH	30:N:2636:C:HO2'	1.42	0.62
11:Z:20:LEU:HD13	20:i:81:PRO:HG2	1.82	0.62
56:s:4:ILE:O	56:s:20:LYS:NZ	2.33	0.62
36:0:1527:U:OP2	56:s:39:GLU:CD	2.42	0.62
30:N:1924:C:C4'	34:M:13:A:C5'	2.73	0.61
30:N:1093:G:H21	30:N:1098:A:H62	1.46	0.61
30:N:2849:U:O2'	30:N:2866:U:O2	2.15	0.61
31:L:20:ASN:ND2	31:L:37:CYS:SG	2.73	0.61
36:0:1238:A:N6	36:0:1301:U:C2	2.68	0.61
20:i:51:GLN:HE22	20:i:86:LEU:HD21	1.65	0.61
22:k:16:ASN:HA	22:k:25:THR:O	2.01	0.61
30:N:1779:U:H5	30:N:1784:A:N7	1.99	0.61
44:8:52:LEU:HB3	44:8:57:MET:HB3	1.81	0.61
35:x:450:C:C2	38:2:131:ARG:NH2	2.68	0.61
33:U:7:ASP:HB3	33:U:9:VAL:HG23	1.83	0.61
34:M:30:A:H1'	36:0:1339:A:N3	2.16	0.61
17:f:15:GLN:NE2	30:N:1266:G:H5''	2.16	0.61
30:N:2127:G:H4'	32:C:38:PHE:CD1	2.36	0.61
35:x:452:U:C2	38:2:132:ARG:NH2	2.69	0.61
36:0:1055:A:H1'	38:2:156:ARG:HH21	1.66	0.61
3:Q:49:GLN:HE21	3:Q:79:LEU:HB3	1.64	0.60
36:0:1493:A:N1	58:u:37:A:H1'	2.13	0.60
45:9:19:ASP:HA	45:9:22:THR:HG22	1.83	0.60
1:O:24:G:O2'	1:O:27:C:N4	2.34	0.60
22:k:12:PRO:HB3	22:k:30:LEU:HD23	1.82	0.60
36:0:812:G:OP1	36:0:902:G:N2	2.34	0.60
35:x:450:C:H42	38:2:164:ARG:HH12	1.49	0.60
30:N:693:A:O2'	30:N:1353:A:N3	2.33	0.60
36:0:933:G:N7	42:6:3:ARG:NH1	2.49	0.60
30:N:475:C:O2	30:N:479:A:N6	2.33	0.60
30:N:882:G:C2'	58:u:56:C:O2	2.49	0.60
38:2:36:ASP:OD1	38:2:59:ARG:NH2	2.34	0.60
33:U:9:VAL:HB	33:U:13:GLY:HA3	1.83	0.60
34:M:40:C:O2'	36:0:1338:G:C1'	2.46	0.60
7:V:31:GLN:NE2	30:N:1097:U:O4	2.34	0.60
3:Q:156:PHE:CE1	8:W:81:ILE:HD12	2.37	0.60
27:p:9:VAL:HG23	30:N:1309:G:OP1	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:j:18:ALA:O	21:j:20:ARG:NH1	2.35	0.59
28:q:12:LYS:NZ	30:N:249:C:O2	2.33	0.59
30:N:613:A:H62	30:N:616:A:H61	1.49	0.59
28:q:16:LYS:HE2	28:q:20:GLY:HA2	1.84	0.59
21:j:15:ASP:OD1	30:N:2263:C:N4	2.35	0.59
2:P:236:GLU:HG2	30:N:2600:A:N7	2.18	0.59
34:M:30:A:O2'	36:0:1340:A:H1'	2.02	0.59
46:A:112:ASP:HB3	56:s:20:LYS:HE2	1.84	0.59
13:b:16:ARG:NH2	13:b:19:GLN:OE1	2.33	0.59
34:M:29:G:H5''	36:0:1230:C:C5'	2.31	0.59
36:0:1526:G:H3'	56:s:39:GLU:OE1	2.03	0.59
7:V:135:SER:OG	30:N:1062:G:N3	2.34	0.59
33:U:72:ILE:HB	33:U:108:VAL:HG12	1.84	0.59
54:J:31:LEU:HB2	54:J:49:ILE:HG22	1.84	0.59
1:O:43:C:O2	5:S:92:ARG:NH2	2.36	0.59
33:U:96:THR:HG23	33:U:112:LYS:HE2	1.85	0.59
53:I:26:ILE:O	53:I:30:LYS:HB2	2.02	0.59
15:d:88:VAL:HA	16:e:49:ILE:HD12	1.85	0.59
30:N:2128:G:H4'	32:C:218:MET:HE1	1.85	0.59
36:0:946:A:H2'	36:0:947:G:C8	2.38	0.59
36:0:1224:U:O2'	36:0:1322:C:OP1	2.21	0.59
37:1:141:LEU:O	37:1:145:GLU:HB2	2.03	0.59
38:2:40:ARG:NH1	38:2:55:ILE:O	2.36	0.59
30:N:2251:G:O6	34:M:75:A:C6	2.50	0.59
36:0:693:G:OP1	46:A:127:ARG:NH2	2.36	0.59
41:5:38:ARG:HG2	41:5:63:ASN:HB2	1.85	0.59
30:N:1068:G:N1	30:N:1073:A:N6	2.50	0.59
30:N:1315:C:O2'	30:N:1392:A:N3	2.30	0.59
36:0:579:A:O2'	50:F:54:ARG:NH1	2.36	0.59
30:N:896:A:C4	58:u:56:C:C5'	2.79	0.58
30:N:1019:U:N3	30:N:1142:A:N6	2.50	0.58
36:0:1261:A:N6	36:0:1274:A:O2'	2.34	0.58
30:N:1726:C:N4	30:N:1735:A:N6	2.51	0.58
32:C:54:LYS:HD2	32:C:57:GLN:HG3	1.85	0.58
35:x:451:G:OP2	40:4:56:VAL:HG11	2.02	0.58
48:D:83:LEU:HD21	54:J:65:GLU:HG2	1.85	0.58
34:M:29:G:N3	36:0:1339:A:H2	2.01	0.58
47:B:50:ARG:NH1	47:B:89:ASP:OD2	2.35	0.58
15:d:92:ARG:HG2	30:N:997:G:OP1	2.03	0.58
30:N:1212:G:O2'	30:N:1237:A:N6	2.36	0.58
45:9:27:GLU:O	45:9:31:ARG:HB2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:A:93:ARG:HH12	56:s:25:LYS:HD3	1.68	0.58
28:q:32:ILE:O	28:q:36:LYS:NZ	2.36	0.58
32:C:201:PRO:HB2	32:C:204:ALA:HB2	1.86	0.58
3:Q:46:ARG:NH2	3:Q:88:GLU:O	2.36	0.58
30:N:1019:U:C4	30:N:1142:A:N6	2.72	0.58
36:0:675:A:H1'	46:A:118:HIS:CD2	2.38	0.58
36:0:890:G:O2'	36:0:906:A:N6	2.36	0.58
39:3:60:LYS:HE3	39:3:195:ILE:HG22	1.84	0.58
36:0:1302:C:C5	48:D:17:ILE:HD13	2.38	0.58
28:q:5:LYS:HE2	30:N:254:G:N7	2.19	0.58
39:3:91:LEU:HD13	39:3:191:LEU:HD11	1.86	0.58
7:V:34:ASN:H	7:V:67:PHE:HE2	1.52	0.58
32:C:213:SER:C	32:C:214:ILE:HD12	2.29	0.58
36:0:927:G:O2'	36:0:1503:A:N7	2.35	0.58
2:P:121:ASP:OD2	33:U:91:PHE:CD1	2.57	0.57
9:X:70:ARG:NH1	30:N:2684:U:O4'	2.37	0.57
11:Z:45:GLN:NE2	30:N:2485:G:OP1	2.34	0.57
36:0:979:C:O2	49:E:59:ARG:NH1	2.35	0.57
37:1:81:LYS:O	37:1:85:LEU:HB2	2.04	0.57
11:Z:66:ARG:NH1	11:Z:104:GLU:OE2	2.36	0.57
30:N:715:A:C4'	50:F:40:GLN:HE22	2.18	0.57
36:0:769:G:H4'	36:0:1513:A:H4'	1.84	0.57
27:p:34:ARG:HD3	30:N:467:G:OP2	2.05	0.57
34:M:40:C:O2'	36:0:1338:G:O2'	2.19	0.57
38:2:156:ARG:HD3	38:2:193:TYR:HB3	1.86	0.57
30:N:2176:A:H5''	32:C:221:GLY:N	2.20	0.57
36:0:1368:A:OP2	44:8:114:LYS:HD3	2.05	0.57
50:F:46:HIS:O	50:F:48:LYS:N	2.36	0.57
22:k:6:GLN:O	22:k:74:ARG:NH1	2.37	0.57
20:i:62:THR:HG22	20:i:71:LYS:HG2	1.86	0.57
36:0:796:C:O3'	46:A:127:ARG:NH1	2.38	0.57
47:B:68:GLY:O	47:B:99:ARG:NH1	2.36	0.57
2:P:144:VAL:HB	2:P:154:LEU:HB2	1.86	0.57
10:Y:111:ILE:HD12	10:Y:111:ILE:H	1.70	0.57
4:R:69:ARG:HG3	30:N:674:G:O2'	2.05	0.56
32:C:63:THR:HG22	32:C:163:TYR:HE1	1.69	0.56
35:x:451:G:C4	39:3:47:ARG:CD	2.87	0.56
30:N:481:G:O2'	30:N:506:G:N2	2.37	0.56
34:M:30:A:C4'	36:0:1339:A:N1	2.68	0.56
36:0:1316:G:H22	36:0:1319:A:H5''	1.69	0.56
10:Y:76:GLU:OE2	30:N:627:A:O2'	2.23	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:k:72:ARG:NH2	22:k:78:TYR:OH	2.33	0.56
30:N:1924:C:H4'	34:M:13:A:H5'	1.83	0.56
44:8:36:GLU:HA	44:8:40:GLY:HA3	1.88	0.56
21:j:23:VAL:HG22	21:j:38:VAL:HG22	1.87	0.56
30:N:897:C:H1'	58:u:56:C:H5	1.71	0.56
22:k:10:LYS:NZ	30:N:396:G:OP2	2.37	0.56
30:N:805:G:N2	30:N:829:A:OP1	2.38	0.56
2:P:133:ARG:HE	33:U:123:ARG:HD3	1.70	0.56
8:W:32:LEU:HD22	8:W:54:ILE:HG21	1.85	0.56
8:W:135:GLN:NE2	30:N:6:A:N3	2.53	0.56
22:k:45:ARG:HH21	22:k:47:VAL:HG22	1.71	0.56
33:U:132:PHE:HB2	33:U:140:ALA:HB3	1.87	0.56
6:T:24:ILE:HD11	6:T:43:VAL:HG11	1.87	0.56
30:N:1726:C:H42	30:N:1735:A:N6	2.04	0.56
34:M:39:C:O2'	36:0:1339:A:H4'	2.06	0.56
4:R:149:ILE:HD12	4:R:175:ILE:HG21	1.88	0.56
7:V:97:LYS:HD2	7:V:139:VAL:HG21	1.87	0.56
30:N:715:A:H1'	50:F:40:GLN:NE2	2.20	0.56
30:N:897:C:H1'	58:u:56:C:C5	2.41	0.56
36:0:451:A:H61	36:0:481:G:H5'	1.70	0.56
36:0:1067:A:N1	36:0:1108:G:O2'	2.35	0.56
36:0:1270:G:HO2'	36:0:1313:U:HO2'	1.53	0.56
46:A:93:ARG:NH2	46:A:112:ASP:OD1	2.39	0.56
35:x:451:G:C4	39:3:47:ARG:NE	2.71	0.56
30:N:413:C:HO2'	30:N:1880:U:HO2'	1.53	0.56
1:O:42:C:C5	5:S:66:LEU:HD22	2.40	0.55
12:a:53:THR:HA	12:a:56:LYS:HD3	1.88	0.55
30:N:2156:G:C2'	30:N:2157:G:H5'	2.36	0.55
30:N:2163:A:H2'	30:N:2164:C:H5'	1.88	0.55
55:K:59:ASP:OD1	55:K:76:LYS:NZ	2.33	0.55
27:p:31:LEU:HD22	27:p:42:LEU:HD23	1.88	0.55
30:N:837:C:N3	30:N:941:A:N6	2.54	0.55
11:Z:50:ARG:HD3	11:Z:65:ILE:HD11	1.88	0.55
32:C:54:LYS:HD2	32:C:57:GLN:HE21	1.70	0.55
36:0:246:A:N1	36:0:278:G:O2'	2.35	0.55
36:0:409:U:OP1	39:3:24:GLY:HA3	2.06	0.55
30:N:1724:G:O6	30:N:1737:G:C2	2.59	0.55
32:C:67:HIS:HB2	32:C:188:ASN:HD21	1.71	0.55
40:4:13:GLU:OE1	40:4:68:ARG:NH2	2.39	0.55
42:6:40:GLU:OE2	44:8:43:THR:HG23	2.06	0.55
2:P:2:ALA:N	2:P:199:GLU:OE1	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:235:GLY:O	2:P:239:ASN:ND2	2.39	0.55
5:S:140:GLU:OE2	31:L:27:THR:HG23	2.07	0.55
16:e:49:ILE:HB	16:e:52:PRO:HA	1.89	0.55
29:r:36:ARG:HD2	29:r:37:GLN:HB2	1.88	0.55
36:0:768:A:N3	36:0:1512:U:O2'	2.40	0.55
1:O:72:G:H21	1:O:104:A:H62	1.55	0.55
6:T:33:LEU:HD22	6:T:75:MET:HG2	1.89	0.54
30:N:1070:A:N7	30:N:1096:A:O2'	2.36	0.54
30:N:1980:G:O2'	30:N:1982:U:OP2	2.22	0.54
37:1:117:LEU:HB3	37:1:141:LEU:HD11	1.89	0.54
11:Z:74:THR:HA	11:Z:88:ASN:O	2.07	0.54
34:M:74:C:H2'	34:M:75:A:C1'	2.38	0.54
36:0:673:A:H2'	36:0:674:G:C8	2.42	0.54
36:0:993:G:O2'	36:0:994:A:N7	2.40	0.54
41:5:41:ASP:OD1	41:5:58:HIS:NE2	2.41	0.54
30:N:306:U:O4	30:N:310:A:N7	2.41	0.54
30:N:2850:A:N7	30:N:2868:A:O2'	2.35	0.54
34:M:16:C:O2	34:M:16:C:H5''	2.07	0.54
35:x:448:U:C6	38:2:162:ILE:CG1	2.91	0.54
49:E:41:ARG:NH1	49:E:42:TRP:O	2.41	0.54
2:P:121:ASP:OD1	33:U:91:PHE:CE1	2.53	0.54
4:R:178:VAL:O	4:R:182:ALA:HB2	2.08	0.54
8:W:56:VAL:HB	8:W:124:VAL:HG12	1.88	0.54
30:N:1536:C:O2	30:N:1537:G:N2	2.41	0.54
29:r:3:VAL:HG12	29:r:36:ARG:HE	1.73	0.54
30:N:1332:G:N7	30:N:1609:A:O2'	2.37	0.54
45:9:10:LEU:HG	45:9:98:VAL:HG12	1.88	0.54
7:V:100:LYS:HA	7:V:139:VAL:O	2.08	0.54
9:X:43:ILE:HD12	9:X:56:ASP:HB2	1.90	0.54
25:n:53:LYS:HE2	25:n:56:ALA:HB2	1.89	0.54
34:M:33:C:H4'	36:0:966:G:N3	2.22	0.54
35:x:450:C:N3	38:2:131:ARG:NH2	2.56	0.54
36:0:676:A:H5''	46:A:115:PRO:HB3	1.90	0.54
25:n:43:ILE:HG22	25:n:49:TYR:HB2	1.89	0.54
36:0:1003:G:H21	36:0:1005:A:H5'	1.73	0.54
41:5:11:HIS:HD2	41:5:12:PRO:HD2	1.72	0.54
30:N:370:G:O2'	30:N:424:G:OP1	2.22	0.54
30:N:1450:G:N2	30:N:1452:G:O6	2.41	0.54
34:M:29:G:OP1	36:0:1229:A:C4'	2.55	0.54
35:x:450:C:O2	38:2:131:ARG:NH1	2.39	0.54
17:f:73:LYS:HB2	17:f:106:VAL:HB	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:2848:G:O2'	30:N:2867:G:N2	2.36	0.53
36:0:1006:G:O6	36:0:1023:U:O2	2.27	0.53
36:0:1522:U:OP1	46:A:128:ARG:NH1	2.40	0.53
48:D:3:ARG:O	48:D:57:ARG:NH1	2.38	0.53
30:N:2506[A]:U:OP2	30:N:2576:G:N1	2.33	0.53
34:M:29:G:OP1	36:0:1229:A:H4'	2.08	0.53
37:1:67:ILE:HD12	37:1:160:ALA:HB3	1.91	0.53
48:D:39:ILE:HD12	48:D:52:GLN:HE21	1.73	0.53
3:Q:13:ARG:NH1	30:N:2683:C:H4'	2.22	0.53
12:a:22:ARG:HG3	12:a:70:THR:HA	1.91	0.53
30:N:1936:A:H2	30:N:1943:U:H3	1.56	0.53
34:M:29:G:N3	36:0:1339:A:C2	2.77	0.53
45:9:8:ILE:HA	45:9:99:GLN:O	2.08	0.53
46:A:30:THR:HG21	46:A:92:GLY:HA3	1.89	0.53
16:e:1:MET:HA	16:e:42:ALA:O	2.07	0.53
30:N:2162:G:H2'	30:N:2163:A:H8	1.73	0.53
33:U:33:GLN:HB3	33:U:35:LYS:HE2	1.89	0.53
48:D:77:ILE:HG22	48:D:81:MET:HE2	1.90	0.53
33:U:7:ASP:OD2	33:U:35:LYS:HD2	2.09	0.53
36:0:1103:C:HO2'	37:1:106:THR:CG2	2.17	0.53
7:V:12:GLN:HE21	7:V:55:ILE:H	1.57	0.53
9:X:77:ILE:HG12	14:c:72:ARG:HD2	1.90	0.53
12:a:114:GLU:OE1	12:a:118:ARG:NH2	2.42	0.53
2:P:204:VAL:O	2:P:206:GLY:N	2.40	0.53
30:N:1417:C:HO2'	30:N:1587:G:HO2'	1.55	0.53
30:N:2177:C:O3'	32:C:211:LYS:CE	2.53	0.53
36:0:76:G:H1	36:0:93:U:H3	1.56	0.53
37:1:80:VAL:HG12	37:1:214:LEU:HD21	1.91	0.53
15:d:88:VAL:HG22	16:e:49:ILE:O	2.09	0.53
30:N:987:C:O2'	30:N:1000:A:N3	2.36	0.53
36:0:263:A:OP2	55:K:74:ARG:NH1	2.42	0.53
36:0:1166:G:N1	36:0:1169:A:OP2	2.40	0.53
45:9:80:THR:HG22	45:9:82:LYS:H	1.74	0.53
4:R:176:ASP:OD1	4:R:176:ASP:N	2.40	0.53
6:T:24:ILE:HG21	6:T:72:LEU:HD21	1.91	0.53
15:d:37:GLN:HE21	30:N:1252:G:H1	1.55	0.53
19:h:86:ARG:NH2	19:h:102:THR:OG1	2.42	0.53
34:M:15:G:C8	34:M:15:G:C5'	2.86	0.53
40:4:99:ALA:O	40:4:102:GLY:N	2.39	0.53
5:S:116:GLY:HA3	5:S:178:ARG:HB3	1.91	0.52
30:N:1924:C:C4'	34:M:13:A:O5'	2.56	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:J:36:ARG:NH2	54:J:75:ALA:O	2.42	0.52
7:V:76:ALA:HA	7:V:79:LEU:HB3	1.91	0.52
10:Y:21:ARG:HA	30:N:811:U:H2'	1.91	0.52
27:p:12:ARG:NH1	30:N:465:G:OP1	2.42	0.52
30:N:28:A:N6	30:N:512:G:H1'	2.24	0.52
30:N:1028:A:N3	30:N:2486:C:O2'	2.42	0.52
35:x:453:C:H41	38:2:132:ARG:HE	1.56	0.52
25:n:17:ARG:NE	30:N:1266:G:OP2	2.40	0.52
36:0:502:A:OP1	47:B:115:SER:HB3	2.09	0.52
47:B:34:CYS:SG	47:B:78:SER:OG	2.67	0.52
30:N:51:G:O2'	30:N:118:A:N6	2.42	0.52
33:U:83:LYS:HG3	33:U:91:PHE:HB3	1.92	0.52
4:R:19:PHE:HE1	4:R:109:LEU:HD13	1.75	0.52
16:e:74:ILE:HD13	30:N:992:C:H4'	1.90	0.52
18:g:8:LEU:HD23	18:g:50:LEU:HD21	1.91	0.52
21:j:41:ARG:HH11	30:N:2387:U:H1'	1.74	0.52
35:x:451:G:C2	39:3:47:ARG:CD	2.82	0.52
38:2:55:ILE:HG22	38:2:68:ILE:HG12	1.92	0.52
50:F:46:HIS:C	50:F:48:LYS:H	2.17	0.52
58:u:20:U:O2'	58:u:21:A:P	2.68	0.52
2:P:133:ARG:HD3	33:U:123:ARG:CZ	2.28	0.52
2:P:160:THR:HG23	2:P:177:ARG:HG2	1.91	0.52
30:N:1070:A:H2'	30:N:1097:U:H4'	1.92	0.52
36:0:1493:A:N6	58:u:37:A:H4'	2.24	0.52
10:Y:76:GLU:HG3	10:Y:111:ILE:HD13	1.91	0.52
30:N:1924:C:C4'	34:M:13:A:C4'	2.58	0.52
38:2:156:ARG:NH1	38:2:160:ALA:O	2.43	0.52
1:O:89:U:H6	30:N:958:U:H2'	1.74	0.52
14:c:37:LYS:HD2	14:c:39:ARG:HH11	1.75	0.52
19:h:86:ARG:NH1	19:h:100:SER:OG	2.42	0.52
30:N:948:C:O2	30:N:984:A:O2'	2.28	0.52
41:5:90:MET:SD	53:I:61:ARG:NH1	2.83	0.52
55:K:28:MET:HE1	55:K:67:ILE:HG12	1.91	0.52
2:P:133:ARG:NE	33:U:123:ARG:HD3	2.24	0.52
16:e:57:GLY:HA2	16:e:102:SER:O	2.10	0.52
30:N:877:A:O2'	30:N:900:A:N6	2.43	0.52
34:M:28:G:N2	36:0:1338:G:H22	2.07	0.52
52:H:17:MET:HG3	52:H:20:SER:HB3	1.91	0.52
30:N:639:U:H2'	30:N:640:C:C6	2.45	0.51
30:N:1266:G:O2'	30:N:2012:G:O6	2.22	0.51
30:N:1726:C:N4	30:N:1735:A:H61	2.06	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:2:GLU:HB3	4:R:11:ALA:HB1	1.92	0.51
19:h:34:VAL:HG13	19:h:67:VAL:HG22	1.93	0.51
37:1:68:LEU:HD12	37:1:154:MET:HE1	1.92	0.51
38:2:77:ILE:HA	38:2:84:VAL:HG23	1.92	0.51
57:t:91:ARG:HA	57:t:94:ALA:HB3	1.93	0.51
2:P:48:ARG:HD3	30:N:773:U:O2'	2.09	0.51
23:l:6:LEU:HD13	23:l:56:LEU:HD22	1.93	0.51
36:0:843:U:OP1	36:0:844:G:N2	2.43	0.51
25:n:4:GLN:HA	30:N:2615:U:C2	2.45	0.51
30:N:698:C:O2'	30:N:734:A:N6	2.44	0.51
30:N:2638:G:O2'	30:N:2778:A:N6	2.44	0.51
2:P:220:VAL:HG21	30:N:782:A:N7	2.26	0.51
4:R:144:GLU:HG2	4:R:166:LYS:HD2	1.92	0.51
9:X:76:VAL:HG12	14:c:73:VAL:HG22	1.92	0.51
16:e:76:LYS:O	16:e:84:ARG:HA	2.11	0.51
21:j:19:LYS:NZ	30:N:2261:C:OP1	2.33	0.51
30:N:612:G:N2	30:N:614:A:O2'	2.44	0.51
45:9:15:HIS:HA	45:9:18:ILE:HG22	1.93	0.51
52:H:59:VAL:HG21	52:H:75:LEU:HD22	1.92	0.51
9:X:99:ILE:HD12	9:X:118:LEU:HB2	1.93	0.51
30:N:2533:U:OP1	30:N:2665:A:O2'	2.29	0.51
53:I:32:TYR:HB3	53:I:55:LEU:HD21	1.93	0.51
34:M:16:C:H4'	34:M:17:G:OP2	2.10	0.51
39:3:58:LYS:NZ	39:3:69:GLU:OE1	2.44	0.51
42:6:109:ARG:O	42:6:119:ARG:NH2	2.44	0.51
46:A:35:THR:OG1	46:A:36:ASP:N	2.44	0.51
9:X:77:ILE:HG12	14:c:72:ARG:CD	2.41	0.51
23:l:54:LYS:HE3	30:N:72:U:OP2	2.11	0.51
28:q:8:ARG:NH2	30:N:243:U:OP2	2.44	0.51
30:N:1939:U:OP1	30:N:2604:U:O2'	2.27	0.51
30:N:2114:A:N3	30:N:2114:A:H2'	2.25	0.51
34:M:28:G:H22	36:0:1338:G:N2	2.09	0.51
37:1:54:LEU:HG	37:1:220:THR:HG21	1.92	0.51
44:8:19:VAL:HA	44:8:65:ILE:HG22	1.92	0.51
53:I:42:SER:HB3	53:I:52:GLN:HE21	1.75	0.51
4:R:163:ASN:HD21	30:N:323:C:H2'	1.74	0.51
12:a:41:ALA:HB1	12:a:97:ILE:HD12	1.92	0.51
7:V:117:MET:HA	30:N:1058:U:O2'	2.11	0.50
12:a:32:GLU:HG2	12:a:115:LEU:HD12	1.93	0.50
2:P:165:VAL:HG21	2:P:181:MET:HE1	1.93	0.50
35:x:450:C:N4	38:2:164:ARG:HH11	2.02	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:VAL:HG12	2:P:19:VAL:HG22	1.92	0.50
19:h:11:VAL:HG12	19:h:72:ILE:HG22	1.93	0.50
30:N:1093:G:N2	30:N:1098:A:N6	2.48	0.50
36:O:1527:U:OP2	56:s:39:GLU:OE2	2.28	0.50
38:2:172:ARG:NH2	38:2:206:GLU:OE2	2.44	0.50
19:h:51:ALA:O	19:h:54:GLN:NE2	2.44	0.50
30:N:2105:U:H2'	30:N:2106:U:O4'	2.12	0.50
30:N:2185:U:H2'	30:N:2186:G:C8	2.47	0.50
32:C:183:ASP:O	32:C:187:GLU:HG2	2.12	0.50
34:M:16:C:O2	34:M:16:C:H2'	2.11	0.50
30:N:897:C:H5'	58:u:56:C:H5'	1.86	0.50
30:N:2602:A:OP1	34:M:75:A:OP2	2.29	0.50
34:M:28:G:N2	36:O:1338:G:N2	2.59	0.50
55:K:54:MET:HE3	55:K:58:VAL:HG21	1.94	0.50
34:M:33:C:C4'	36:O:966:G:N3	2.74	0.50
36:O:401:C:O2'	36:O:621:A:N3	2.39	0.50
55:K:69:LYS:O	55:K:72:ALA:HB3	2.12	0.50
46:A:72:ASP:O	46:A:73:ALA:HB3	2.11	0.50
15:d:49:ASP:OD2	30:N:534:U:O2'	2.21	0.50
16:e:7:SER:OG	16:e:8:GLY:N	2.45	0.50
19:h:7:ARG:NH2	19:h:26:LYS:O	2.45	0.50
27:p:29:GLN:NE2	30:N:210:C:OP1	2.40	0.50
39:3:141:ASP:O	39:3:181:THR:HA	2.12	0.50
7:V:124:ALA:HB1	30:N:1081:U:H4'	1.93	0.49
7:V:127:ARG:HA	7:V:130:GLU:HB2	1.94	0.49
30:N:527:C:N4	30:N:2779:U:OP2	2.44	0.49
44:8:120:LYS:HG2	44:8:123:ARG:HB3	1.94	0.49
25:n:16:ARG:NE	30:N:1266:G:OP1	2.37	0.49
30:N:2106:U:H2'	30:N:2107:G:C8	2.48	0.49
35:x:449:A:C5	38:2:164:ARG:HD3	2.47	0.49
36:O:1103:C:C2'	37:1:106:THR:HG21	2.39	0.49
7:V:55:ILE:HG22	7:V:57:VAL:HB	1.94	0.49
24:m:3:LYS:HE2	24:m:40:ASP:HB3	1.93	0.49
34:M:33:C:OP2	44:8:130:ARG:NE	2.46	0.49
36:O:976:G:OP2	36:O:1358:U:O2'	2.29	0.49
40:4:122:ASN:N	40:4:122:ASN:OD1	2.42	0.49
42:6:57:SER:HB3	42:6:60:GLU:HG2	1.93	0.49
45:9:11:LYS:HA	45:9:70:HIS:O	2.12	0.49
46:A:110:ILE:HG22	56:s:17:ARG:NH1	2.27	0.49
13:b:40:ILE:HG12	13:b:47:VAL:HG12	1.94	0.49
28:q:8:ARG:HH21	30:N:243:U:P	2.33	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:372:G:HO2'	30:N:400:G:H1	1.61	0.49
31:L:37:CYS:SG	31:L:38:SER:N	2.85	0.49
32:C:23:ILE:HG12	32:C:224:VAL:HB	1.93	0.49
36:O:542:G:H5'	39:3:39:GLY:HA3	1.94	0.49
20:i:6:ALA:HB1	20:i:40:ILE:HG23	1.95	0.49
30:N:897:C:O2'	58:u:55:U:O3'	2.30	0.49
30:N:1047:G:O2'	30:N:1111:A:N6	2.46	0.49
34:M:16:C:H3'	34:M:17:G:C5'	2.40	0.49
36:O:552:U:H5'	47:B:83:ARG:HH11	1.76	0.49
37:1:141:LEU:O	37:1:145:GLU:CB	2.61	0.49
52:H:31:HIS:HD2	52:H:34:TYR:H	1.59	0.49
30:N:715:A:H1'	50:F:40:GLN:HE22	1.72	0.49
30:N:2113:U:H2'	30:N:2114:A:H8	1.77	0.49
48:D:10:PRO:HB2	48:D:18:ALA:HB1	1.94	0.49
4:R:83:VAL:HB	4:R:86:ALA:HB2	1.95	0.49
15:d:4:VAL:HG22	30:N:1199:U:H1'	1.95	0.49
16:e:71:LYS:NZ	30:N:1223:G:N7	2.61	0.49
30:N:2149:U:H2'	30:N:2150:C:O4'	2.13	0.49
12:a:61:ALA:O	12:a:65:LEU:HB2	2.13	0.49
27:p:18:PHE:HA	27:p:43:THR:HG21	1.95	0.49
30:N:503:A:O2'	30:N:506:G:OP2	2.28	0.49
30:N:1724:G:C6	30:N:1737:G:N2	2.81	0.49
30:N:2540:C:O2'	30:N:2740:A:N3	2.42	0.49
51:G:6:LEU:HG	51:G:17:TYR:HB3	1.94	0.49
4:R:21:ARG:HD3	4:R:106:LYS:HB3	1.93	0.49
30:N:715:A:C4'	50:F:40:GLN:NE2	2.76	0.49
36:O:757:U:O2'	36:O:879:C:O2	2.31	0.49
40:4:99:ALA:HB2	40:4:124:LEU:HG	1.93	0.49
42:6:142:HIS:O	42:6:146:GLU:HB2	2.13	0.49
1:O:74:U:O2	20:i:29:ILE:HD13	2.13	0.49
8:W:13:ARG:NH1	8:W:49:ASP:O	2.39	0.49
23:l:2:LYS:HD3	30:N:77:G:OP1	2.13	0.49
37:1:176:ALA:HB1	37:1:181:ILE:HB	1.94	0.49
6:T:67:THR:HG22	30:N:2748:A:H1'	1.95	0.48
10:Y:67:THR:HG21	30:N:244:A:H5''	1.95	0.48
26:o:35:GLU:HA	26:o:49:TYR:O	2.13	0.48
30:N:1853:A:N3	30:N:2233:U:O2'	2.43	0.48
30:N:2150:C:H2'	30:N:2151:U:O4'	2.13	0.48
36:O:972:C:P	45:9:59:LYS:HD3	2.53	0.48
8:W:108:MET:HE2	30:N:1138:G:N3	2.27	0.48
30:N:355:U:H2'	30:N:356:G:H8	1.78	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:1297:C:O2'	30:N:1302:A:N1	2.39	0.48
30:N:1783:A:H5'	30:N:2608:G:H4'	1.95	0.48
47:B:64:THR:HG23	47:B:93:VAL:HG12	1.95	0.48
49:E:89:MET:HE1	49:E:98:LYS:HD3	1.95	0.48
4:R:58:LYS:HG3	4:R:71:GLY:HA2	1.95	0.48
30:N:1924:C:H4'	34:M:13:A:O5'	2.13	0.48
32:C:3:LYS:HG3	32:C:4:LEU:N	2.25	0.48
34:M:30:A:P	36:0:1230:C:H5''	2.52	0.48
35:x:449:A:H62	38:2:164:ARG:CG	2.25	0.48
33:U:5:LEU:HD12	33:U:5:LEU:N	2.29	0.48
36:0:812:G:O2'	36:0:813:U:H6	1.96	0.48
37:1:207:ILE:HA	37:1:210:VAL:HG22	1.95	0.48
2:P:207:LYS:HB2	30:N:729:G:C6	2.48	0.48
15:d:51:ARG:HG2	30:N:1156:A:C8	2.48	0.48
16:e:27:ILE:O	16:e:66:HIS:NE2	2.42	0.48
30:N:1868:C:N4	30:N:1869:G:O6	2.46	0.48
30:N:33:C:O2	30:N:447:A:N6	2.47	0.48
30:N:1724:G:O6	30:N:1737:G:N2	2.47	0.48
40:4:153:VAL:HG12	40:4:156:LYS:HZ1	1.77	0.48
46:A:16:VAL:HG12	46:A:77:TYR:HB3	1.96	0.48
10:Y:57:LEU:HD22	28:q:54:ASP:HB3	1.96	0.48
18:g:18:GLU:OE2	30:N:1392:A:N6	2.43	0.48
25:n:3:VAL:HG23	30:N:2015:A:C6	2.48	0.48
30:N:1534:U:O2'	30:N:1537:G:O6	2.29	0.48
32:C:25:GLU:O	32:C:29:LEU:HG	2.13	0.48
36:0:705:G:H21	46:A:31:ILE:HD11	1.78	0.48
44:8:28:ILE:HD11	44:8:57:MET:HE1	1.95	0.48
44:8:55:VAL:O	44:8:60:LYS:NZ	2.43	0.48
45:9:27:GLU:O	45:9:31:ARG:CB	2.61	0.48
12:a:82:GLU:OE2	12:a:86:ARG:NH2	2.47	0.48
14:c:26:VAL:O	14:c:44:GLU:HA	2.14	0.48
27:p:33:ARG:NH2	30:N:467:G:OP1	2.46	0.48
30:N:882:G:H1'	58:u:56:C:O2	2.11	0.48
30:N:2139:U:H2'	30:N:2140:G:C8	2.49	0.48
32:C:212:VAL:HG23	32:C:224:VAL:HG23	1.95	0.48
33:U:68:ARG:C	33:U:68:ARG:HD2	2.38	0.48
34:M:28:G:O3'	36:0:1229:A:C5'	2.62	0.48
36:0:642:A:C5	43:7:107:SER:HA	2.49	0.48
36:0:1130:A:H61	36:0:1144:G:H1'	1.79	0.48
37:1:104:TRP:O	37:1:108:ARG:N	2.46	0.48
2:P:167:ARG:HG2	2:P:172:VAL:HG12	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:W:81:ILE:O	30:N:1131:G:OP1	2.32	0.48
27:p:1:MET:SD	30:N:752:A:H3'	2.53	0.48
30:N:1363:C:O2'	30:N:1809:A:N3	2.41	0.48
33:U:51:ARG:HG3	33:U:51:ARG:HH11	1.79	0.48
51:G:46:LYS:HG3	51:G:47:GLU:H	1.79	0.48
53:I:34:THR:HG23	53:I:36:SER:H	1.79	0.48
13:b:31:THR:O	13:b:102:ARG:NH1	2.41	0.48
34:M:1:U:H2'	34:M:2:G:H8	1.78	0.48
36:0:197:A:N1	36:0:220:G:O2'	2.45	0.48
2:P:235:GLY:O	30:N:2599:G:N7	2.47	0.47
19:h:45:HIS:HB3	19:h:58:ILE:HG12	1.95	0.47
33:U:40:THR:HB	33:U:43:ASN:ND2	2.22	0.47
37:1:136:MET:SD	37:1:139:ARG:NH2	2.87	0.47
48:D:8:ASN:HD22	48:D:22:ILE:HG13	1.78	0.47
2:P:66:ASP:OD2	2:P:102:ARG:NH1	2.46	0.47
41:5:88:MET:HE3	53:I:64:TYR:CD2	2.49	0.47
56:s:37:PHE:HB3	56:s:39:GLU:H	1.79	0.47
2:P:120:VAL:HG11	33:U:91:PHE:O	2.14	0.47
3:Q:35:THR:HG22	3:Q:73:VAL:HG11	1.96	0.47
11:Z:33:LEU:HD13	11:Z:117:PHE:HB3	1.95	0.47
30:N:299:A:N3	30:N:319:G:O2'	2.37	0.47
34:M:40:C:O2'	36:0:1338:G:C2'	2.61	0.47
36:0:677:U:H3	36:0:713:G:H22	1.62	0.47
17:f:90:LYS:NZ	30:N:746:U:O2'	2.47	0.47
18:g:22:THR:O	18:g:26:LYS:HB3	2.15	0.47
30:N:160:A:N3	30:N:2208:C:O2'	2.44	0.47
30:N:1187:G:N2	30:N:1188:U:O4	2.47	0.47
30:N:1475:G:H1'	30:N:1732:C:H41	1.79	0.47
57:t:32:ASP:O	57:t:33:LYS:C	2.56	0.47
4:R:77:ILE:HD13	4:R:77:ILE:HG21	1.25	0.47
7:V:30:GLN:OE1	30:N:1095:A:N6	2.48	0.47
8:W:114:LEU:HG	8:W:118:MET:HE3	1.97	0.47
11:Z:42:THR:HG22	11:Z:93:VAL:HG12	1.97	0.47
27:p:19:ARG:HG2	30:N:126:A:O5'	2.14	0.47
10:Y:81:ASP:HB2	10:Y:100:ILE:HD11	1.95	0.47
30:N:284:U:O4	30:N:356:G:O6	2.33	0.47
30:N:2776:A:O5'	30:N:2776:A:H8	1.97	0.47
36:0:254:G:O3'	52:H:71:LYS:NZ	2.47	0.47
36:0:618:C:O2'	51:G:14:ARG:NH2	2.47	0.47
44:8:38:TYR:HD2	44:8:39:PHE:HD1	1.61	0.47
53:I:51:TYR:O	53:I:55:LEU:HB2	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:S:42:GLU:OE1	5:S:148:ARG:NH1	2.48	0.47
10:Y:51:GLU:OE1	10:Y:60:ARG:NH1	2.46	0.47
11:Z:57:VAL:HG13	11:Z:116:ALA:HB2	1.96	0.47
11:Z:136:MET:HE3	20:i:57:TYR:HB3	1.96	0.47
15:d:11:ARG:HA	15:d:11:ARG:HD2	1.81	0.47
15:d:97:ASP:OD2	16:e:13:ARG:NE	2.47	0.47
30:N:548:G:H5''	30:N:549:G:H5'	1.97	0.47
30:N:910:A:H2'	30:N:911:A:C8	2.50	0.47
30:N:1847:A:O2'	30:N:1848:A:H8	1.98	0.47
30:N:2176:A:H2'	30:N:2177:C:C6	2.49	0.47
36:0:261:U:OP2	55:K:74:ARG:NH2	2.47	0.47
36:0:674:G:P	41:5:86:ARG:HH22	2.38	0.47
36:0:1100:C:OP2	37:1:95:ARG:HD2	2.13	0.47
37:1:81:LYS:O	37:1:85:LEU:CB	2.62	0.47
39:3:95:GLU:HA	39:3:100:ASN:ND2	2.29	0.47
2:P:155:ALA:HB2	2:P:162:VAL:HG23	1.97	0.47
5:S:80:ARG:HA	34:M:55:C:H4'	1.97	0.47
11:Z:118:LYS:HE3	11:Z:118:LYS:HB3	1.84	0.47
25:n:6:ASN:ND2	30:N:2020:A:H62	2.12	0.47
51:G:70:ARG:HD2	51:G:70:ARG:HA	1.62	0.47
10:Y:41:ARG:NH1	30:N:807:U:OP2	2.48	0.47
30:N:528:A:C2	30:N:2042:A:H2'	2.50	0.47
30:N:2243:U:H2'	30:N:2244:U:C6	2.50	0.47
30:N:2252:G:N2	34:M:74:C:C2	2.83	0.47
32:C:55:SER:O	32:C:58:ASN:ND2	2.48	0.47
36:0:1006:G:C6	36:0:1023:U:O2	2.68	0.47
14:c:29:LYS:HD3	14:c:40:LEU:HD21	1.97	0.47
15:d:16:LYS:NZ	30:N:1227:G:OP2	2.48	0.47
19:h:41:LEU:HA	19:h:61:LYS:O	2.15	0.47
21:j:41:ARG:NH1	30:N:2262:U:OP1	2.47	0.47
21:j:65:GLY:HA3	21:j:83:GLU:O	2.14	0.47
30:N:2177:C:H4'	32:C:211:LYS:NZ	2.26	0.47
30:N:2273:A:H2'	30:N:2274:A:C8	2.50	0.47
32:C:163:TYR:HD2	32:C:171:ILE:HD11	1.80	0.47
32:C:171:ILE:HD13	32:C:196:LEU:HD11	1.96	0.47
2:P:260:ASN:ND2	2:P:263:THR:OG1	2.48	0.46
10:Y:111:ILE:HD11	30:N:636:G:C6	2.49	0.46
11:Z:9:PHE:HZ	30:N:911:A:H2'	1.80	0.46
28:q:54:ASP:OD2	30:N:2359:C:O2'	2.29	0.46
30:N:499:U:H3	30:N:503:A:H62	0.55	0.46
30:N:2189:U:H2'	30:N:2190:G:C8	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:0:999:C:N3	36:0:1042:A:N6	2.63	0.46
25:n:25:VAL:HG21	25:n:28:LEU:HD23	1.97	0.46
30:N:1999:C:O3'	30:N:2722:G:N2	2.48	0.46
36:0:1006:G:O6	36:0:1023:U:C2	2.67	0.46
36:0:1218:C:H2'	36:0:1219:A:C8	2.51	0.46
46:A:23:ILE:HG22	46:A:32:VAL:HG13	1.96	0.46
5:S:24:SER:HB3	5:S:27:GLN:HB2	1.97	0.46
7:V:107:GLN:O	7:V:111:GLN:HB2	2.15	0.46
30:N:1509:A:H2'	30:N:1510:G:C8	2.50	0.46
30:N:2183:A:H2'	30:N:2184:A:C8	2.51	0.46
32:C:163:TYR:HB2	32:C:171:ILE:HD11	1.97	0.46
36:0:1113:C:H4'	38:2:14:ILE:HD12	1.97	0.46
47:B:38:TYR:HB2	47:B:52:VAL:O	2.15	0.46
2:P:153:GLN:O	30:N:1818:U:O2'	2.31	0.46
29:r:11:CYS:SG	29:r:14:CYS:N	2.88	0.46
30:N:882:G:H4'	58:u:19:G:H22	0.53	0.46
36:0:296:U:O2'	36:0:556:C:O2	2.33	0.46
30:N:81:G:HO2'	30:N:295:G:HO2'	1.62	0.46
30:N:500:G:N1	30:N:503:A:OP2	2.42	0.46
30:N:2180:U:H2'	30:N:2181:U:O4'	2.16	0.46
32:C:163:TYR:CD2	32:C:171:ILE:HD11	2.50	0.46
45:9:83:THR:O	45:9:87:LEU:CB	2.58	0.46
2:P:182:ARG:NH1	30:N:1800:C:OP2	2.49	0.46
15:d:37:GLN:NE2	30:N:1252:G:H22	2.14	0.46
2:P:132:MET:HG2	2:P:135:ILE:HD12	1.96	0.46
29:r:1:MET:HE2	29:r:34:LYS:HD3	1.98	0.46
30:N:503:A:H4'	30:N:504:A:H5'	1.96	0.46
30:N:2104:C:H2'	30:N:2105:U:C6	2.51	0.46
30:N:2514:U:H2'	30:N:2515:C:C6	2.51	0.46
35:x:449:A:C6	38:2:164:ARG:HD3	2.51	0.46
37:1:53:ALA:O	37:1:57:LEU:HB2	2.16	0.46
45:9:10:LEU:O	45:9:71:LEU:HA	2.15	0.46
5:S:74:VAL:HG22	5:S:79:ILE:HD11	1.97	0.46
5:S:140:GLU:CD	31:L:27:THR:HG23	2.41	0.46
17:f:38:TYR:CD2	25:n:28:LEU:HD22	2.50	0.46
34:M:30:A:HO2'	36:0:1340:A:H1'	1.81	0.46
36:0:523:A:N1	47:B:89:ASP:HB2	2.30	0.46
38:2:108:LYS:HD3	38:2:111:LEU:HD12	1.96	0.46
40:4:105:ILE:HD11	40:4:115:LEU:HD23	1.96	0.46
44:8:129:LYS:HB2	44:8:129:LYS:HE3	1.70	0.46
11:Z:55:ARG:NH2	30:N:2469:A:O3'	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:i:48:MET:SD	20:i:51:GLN:NE2	2.89	0.46
30:N:45:G:H5''	30:N:46:G:H5'	1.97	0.46
30:N:499:U:O4	30:N:503:A:N7	2.49	0.46
31:L:13:THR:HA	31:L:23:LYS:HA	1.97	0.46
36:0:928:G:O2'	36:0:1533:C:OP1	2.34	0.46
36:0:938:A:N3	36:0:1376:U:O2'	2.40	0.46
36:0:1227:A:OP2	48:D:95:LEU:HD21	2.15	0.46
36:0:1356:G:H2'	36:0:1357:A:C8	2.51	0.46
38:2:65:ARG:O	38:2:65:ARG:HG3	2.16	0.46
1:O:7:G:H5'	13:b:29:HIS:CE1	2.51	0.46
7:V:33:VAL:HG13	7:V:59:ILE:HG21	1.97	0.46
14:c:29:LYS:HB2	14:c:83:SER:HB2	1.98	0.46
30:N:2126:A:H2'	30:N:2162:G:C2	2.50	0.46
34:M:29:G:N2	36:0:1339:A:C2	2.84	0.46
36:0:1103:C:HO2'	37:1:106:THR:HG21	1.72	0.46
36:0:1106:G:O2'	38:2:169:ARG:NH1	2.49	0.46
8:W:31:GLU:HG2	8:W:142:ILE:HG12	1.97	0.45
25:n:4:GLN:NE2	30:N:2016:U:O2	2.49	0.45
28:q:5:LYS:CE	30:N:254:G:N7	2.79	0.45
30:N:299:A:N1	30:N:322:A:O2'	2.46	0.45
30:N:1236:G:HO2'	30:N:1237:A:P	2.39	0.45
30:N:1900:A:H1'	30:N:1970:A:H2'	1.98	0.45
30:N:2177:C:O2'	32:C:170:ILE:HG12	2.15	0.45
36:0:1126:U:OP1	45:9:7:ARG:NH2	2.49	0.45
38:2:55:ILE:HD13	38:2:55:ILE:HG21	1.65	0.45
4:R:148:ILE:HB	4:R:169:VAL:HG22	1.98	0.45
7:V:11:LEU:HD23	30:N:1097:U:O2	2.16	0.45
27:p:12:ARG:CZ	27:p:44:VAL:HG21	2.45	0.45
30:N:270:A:N1	30:N:369:U:O2'	2.38	0.45
30:N:675:A:N3	30:N:2443:C:O2'	2.47	0.45
30:N:857:G:N2	30:N:2269:G:O4'	2.49	0.45
30:N:2006:C:O2'	30:N:2823:A:N3	2.48	0.45
30:N:2506[A]:U:OP2	30:N:2576:G:N2	2.47	0.45
33:U:41:LYS:HD3	33:U:44:ILE:HD12	1.98	0.45
34:M:39:C:H1'	36:0:1339:A:O2'	2.17	0.45
35:x:449:A:N7	38:2:164:ARG:NH1	2.65	0.45
36:0:766:A:OP2	36:0:812:G:N2	2.50	0.45
40:4:133:PRO:HA	40:4:136:VAL:HG12	1.97	0.45
55:K:79:LEU:HA	55:K:79:LEU:HD23	1.83	0.45
2:P:251:GLN:NE2	2:P:252:THR:O	2.48	0.45
22:k:37:ARG:HG2	22:k:46:PHE:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:N:749:A:N1	30:N:753:A:O2'	2.43	0.45
30:N:1447:C:O2'	30:N:1544:A:N3	2.39	0.45
30:N:2186:G:H2'	30:N:2187:U:O4'	2.17	0.45
34:M:28:G:H4'	36:O:1229:A:C5'	2.45	0.45
36:O:1302:C:C6	48:D:17:ILE:HD13	2.50	0.45
40:4:18:VAL:HA	40:4:34:THR:O	2.16	0.45
15:d:37:GLN:HE21	30:N:1252:G:H22	1.62	0.45
30:N:1064:C:N4	30:N:1070:A:OP2	2.49	0.45
33:U:4:ILE:HG22	33:U:37:VAL:O	2.16	0.45
54:J:50:ALA:HB1	54:J:57:HIS:HB3	1.97	0.45
2:P:19:VAL:HG23	2:P:203:ARG:HB3	1.99	0.45
10:Y:100:ILE:HD13	10:Y:100:ILE:HG21	1.75	0.45
16:e:34:GLU:HG2	16:e:60:LYS:HG2	1.98	0.45
30:N:1019:U:H3	30:N:1142:A:H61	1.61	0.45
30:N:1176:U:H2'	30:N:1177:G:C8	2.51	0.45
30:N:1733:G:H2'	30:N:1734:G:C8	2.51	0.45
30:N:1794:A:H2'	30:N:1795:C:C6	2.52	0.45
34:M:28:G:O3'	36:O:1229:A:H5''	2.16	0.45
37:1:100:MET:HA	37:1:107:VAL:HG21	1.99	0.45
7:V:11:LEU:HD11	7:V:28:LEU:HB3	1.99	0.45
11:Z:123:LYS:HE3	30:N:2483:C:N3	2.32	0.45
12:a:44:LEU:HD23	12:a:113:ILE:HD13	1.98	0.45
25:n:16:ARG:HA	30:N:2046:G:H5'	1.99	0.45
35:x:451:G:N3	39:3:47:ARG:NE	2.64	0.45
38:2:155:GLY:HA2	38:2:163:ALA:HB1	1.98	0.45
39:3:58:LYS:HD3	39:3:203:LEU:HD23	1.98	0.45
40:4:89:HIS:CD2	40:4:90:THR:H	2.33	0.45
44:8:106:ARG:NH1	44:8:107:ASP:O	2.50	0.45
9:X:99:ILE:HD13	9:X:115:ILE:HG23	1.99	0.45
15:d:88:VAL:HA	16:e:49:ILE:CD1	2.47	0.45
27:p:35:ARG:HG3	27:p:42:LEU:HD21	1.98	0.45
41:5:62:MET:HG2	41:5:64:VAL:HG23	1.97	0.45
5:S:131:GLY:HA3	30:N:2305:U:H5''	1.98	0.45
10:Y:54:GLN:HE21	30:N:2428:G:N2	2.14	0.45
29:r:7:VAL:HG22	29:r:38:GLY:HA3	1.99	0.45
30:N:715:A:N1	50:F:53:ARG:NH1	2.59	0.45
30:N:2458:G:O2'	30:N:2460:U:O4	2.34	0.45
35:x:449:A:N6	38:2:164:ARG:CD	2.69	0.45
36:O:309:A:H2'	36:O:310:G:H8	1.81	0.45
39:3:140:ASN:N	39:3:182:PHE:O	2.49	0.45
41:5:70:VAL:HA	41:5:73:GLU:HG2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:R:165:HIS:CD2	30:N:1205:A:C6	3.05	0.45
8:W:82:GLY:HA2	30:N:1131:G:OP1	2.17	0.45
34:M:32:U:C6	44:8:129:LYS:NZ	2.75	0.45
37:1:53:ALA:O	37:1:57:LEU:CB	2.65	0.45
46:A:49:GLY:O	46:A:69:ARG:NH1	2.50	0.45
2:P:141:VAL:HG13	2:P:190:ALA:HB1	1.99	0.45
33:U:12:LEU:HD22	33:U:19:VAL:HG11	1.99	0.45
36:0:971:G:O6	36:0:1364:U:O2'	2.35	0.45
36:0:1379:G:O6	42:6:2:PRO:HB2	2.17	0.45
10:Y:82:LEU:HA	10:Y:85:VAL:HG13	1.99	0.44
14:c:63:LYS:HE3	14:c:65:SER:HB2	1.99	0.44
14:c:92:VAL:HG21	14:c:97:LEU:HD21	1.98	0.44
23:l:13:GLU:HA	23:l:16:THR:HG22	1.99	0.44
30:N:569:U:H5''	30:N:821:A:C2	2.52	0.44
30:N:2123:G:H2'	30:N:2124:G:C8	2.52	0.44
32:C:184:LYS:O	32:C:188:ASN:ND2	2.50	0.44
36:0:835:U:OP1	53:I:53:ARG:NH2	2.32	0.44
42:6:56:LYS:HE3	42:6:60:GLU:HG3	1.98	0.44
47:B:114:ARG:HG2	47:B:119:VAL:HB	1.99	0.44
11:Z:9:PHE:CZ	30:N:911:A:H2'	2.52	0.44
15:d:31:VAL:HG13	30:N:580:U:O3'	2.17	0.44
26:o:40:ASP:O	26:o:44:ARG:N	2.50	0.44
30:N:514:A:N3	30:N:581:C:O2'	2.44	0.44
30:N:881:G:N2	30:N:895:U:O2	2.49	0.44
30:N:1072:C:H42	30:N:1098:A:N6	2.16	0.44
30:N:2029:G:N1	30:N:2033:A:OP2	2.34	0.44
33:U:18:GLN:HE22	33:U:44:ILE:HD13	1.83	0.44
36:0:362:G:N1	36:0:365:U:OP2	2.43	0.44
36:0:946:A:O2'	36:0:1333:A:N3	2.45	0.44
2:P:145:GLU:HB2	2:P:188:CYS:HB3	1.98	0.44
3:Q:146:ILE:HG21	3:Q:146:ILE:HD13	1.62	0.44
32:C:45:ALA:HA	32:C:172:HIS:CD2	2.52	0.44
34:M:28:G:H4'	36:0:1229:A:H5''	1.98	0.44
36:0:71:A:H61	36:0:99:C:H1'	1.83	0.44
36:0:825:A:H4'	43:7:3:MET:HE2	1.99	0.44
36:0:1317:C:H4'	49:E:49:GLN:HE21	1.83	0.44
40:4:80:THR:OG1	40:4:81:LEU:N	2.50	0.44
40:4:107:ALA:HA	40:4:125:ALA:HB3	1.99	0.44
42:6:73:VAL:HG12	42:6:90:GLU:HA	1.99	0.44
46:A:31:ILE:HD13	46:A:31:ILE:HG21	1.70	0.44
3:Q:37:VAL:HG22	3:Q:48:ILE:HG22	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:149:ASN:HD22	30:N:2572:A:H2'	1.81	0.44
12:a:3:HIS:O	12:a:4:ARG:HB2	2.17	0.44
30:N:613:A:N7	30:N:616:A:C6	2.85	0.44
30:N:897:C:O2'	58:u:55:U:H4'	2.17	0.44
30:N:2141:G:H2'	30:N:2142:A:C8	2.48	0.44
36:0:35:G:O2'	47:B:115:SER:O	2.31	0.44
37:1:163:VAL:HG21	37:1:173:ILE:HD11	1.98	0.44
37:1:166:ALA:HB3	37:1:191:SER:HB3	2.00	0.44
39:3:100:ASN:OD1	39:3:111:ARG:NH1	2.51	0.44
45:9:12:ALA:HB3	45:9:18:ILE:HB	1.98	0.44
6:T:9:VAL:HB	6:T:50:LEU:HB2	2.00	0.44
8:W:113:PRO:HD2	30:N:558:U:P	2.58	0.44
16:e:49:ILE:H	16:e:49:ILE:HG13	1.70	0.44
23:l:1:MET:HG2	23:l:4:LYS:HD3	2.00	0.44
30:N:1077:A:N6	30:N:1089:A:OP1	2.46	0.44
36:0:9:G:OP2	40:4:126:LYS:HD2	2.18	0.44
36:0:481:G:O2'	36:0:483:C:N4	2.50	0.44
36:0:552:U:H5'	47:B:83:ARG:NH1	2.32	0.44
7:V:79:LEU:HD21	7:V:109:ILE:HG21	1.99	0.44
30:N:1875:G:O3'	32:C:205:LYS:HE3	2.13	0.44
34:M:30:A:C2'	36:0:1340:A:HO2'	2.22	0.44
34:M:40:C:HO2'	36:0:1338:G:H1'	1.75	0.44
36:0:1096:C:O2	36:0:1170:A:O2'	2.34	0.44
36:0:1178:G:C5	44:8:99:ARG:NH2	2.86	0.44
36:0:1321:U:O2'	54:J:78:ARG:NH1	2.51	0.44
44:8:16:ALA:O	44:8:67:VAL:HA	2.17	0.44
53:I:33:ILE:HG21	53:I:33:ILE:HD13	1.68	0.44
3:Q:4:LEU:HD21	3:Q:96:ILE:HG22	1.99	0.44
15:d:113:ALA:O	15:d:117:LEU:HB2	2.18	0.44
23:l:20:ASN:HB3	23:l:50:VAL:HG22	2.00	0.44
32:C:5:THR:OG1	32:C:6:LYS:N	2.49	0.44
32:C:211:LYS:HE3	32:C:211:LYS:HB3	1.83	0.44
36:0:573:A:N3	36:0:883:C:O2'	2.47	0.44
36:0:1060:U:P	49:E:85:ARG:HH22	2.41	0.44
36:0:1080:A:OP1	40:4:52:LYS:HD2	2.18	0.44
7:V:24:VAL:HG12	30:N:1070:A:H61	1.83	0.44
12:a:90:ARG:HD2	30:N:2880:C:O2'	2.18	0.44
30:N:2130:U:H5'	30:N:2159:G:N2	2.33	0.44
22:k:17:ASN:HB2	22:k:25:THR:HB	1.99	0.44
30:N:1044:C:O2'	30:N:1111:A:N1	2.48	0.44
33:U:45:GLU:HA	33:U:48:GLU:HG2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:U:47:PHE:HA	33:U:51:ARG:HB2	2.00	0.44
36:0:1062:U:H2'	36:0:1063:C:C6	2.52	0.44
42:6:107:ALA:HB1	42:6:133:THR:HB	2.00	0.44
3:Q:25:THR:HG21	3:Q:193:VAL:HG22	2.00	0.43
3:Q:43:ASP:OD1	30:N:2784:U:H4'	2.17	0.43
6:T:66:GLY:O	6:T:69:ARG:HB3	2.17	0.43
53:I:71:THR:HG23	53:I:73:ARG:H	1.82	0.43
9:X:70:ARG:NH2	30:N:2683:C:O2	2.52	0.43
14:c:53:ARG:NH2	30:N:2720:U:OP1	2.51	0.43
30:N:897:C:C5'	58:u:56:C:C5'	2.74	0.43
30:N:2251:G:O6	34:M:75:A:C2	2.51	0.43
36:0:620:C:C2	39:3:132:ILE:HD13	2.53	0.43
36:0:1026:G:C6	36:0:1035:A:C6	3.06	0.43
36:0:1143:G:H2'	36:0:1144:G:H8	1.83	0.43
51:G:6:LEU:HD12	51:G:19:VAL:HB	1.99	0.43
51:G:38:PHE:CE1	51:G:51:ARG:HG2	2.52	0.43
3:Q:13:ARG:HD2	3:Q:15:PHE:CZ	2.53	0.43
4:R:165:HIS:CD2	30:N:1205:A:C5	3.06	0.43
16:e:3:ALA:HA	16:e:40:MET:O	2.17	0.43
17:f:77:ASP:HB2	17:f:102:HIS:HB2	2.00	0.43
21:j:33:ALA:N	21:j:64:ASP:OD1	2.51	0.43
36:0:1493:A:C6	58:u:37:A:O2'	2.40	0.43
2:P:85:PRO:HG3	30:N:1567:G:H2'	2.00	0.43
23:l:56:LEU:HD23	23:l:56:LEU:HA	1.86	0.43
24:m:54:MET:HB2	24:m:54:MET:HE3	1.75	0.43
30:N:285:G:O6	30:N:355:U:O2	2.36	0.43
30:N:2128:G:N2	30:N:2173:A:H1'	2.27	0.43
36:0:1064:G:O2'	36:0:1190:G:N2	2.51	0.43
42:6:105:VAL:O	42:6:109:ARG:HG2	2.19	0.43
3:Q:109:VAL:HG22	3:Q:203:VAL:HG22	2.00	0.43
7:V:133:ALA:O	7:V:138:LEU:N	2.51	0.43
30:N:1338:G:O2'	30:N:1393:A:N1	2.49	0.43
30:N:2170:A:H2'	30:N:2171:A:O4'	2.19	0.43
31:L:11:GLU:HA	31:L:25:ARG:HA	2.01	0.43
36:0:71:A:N1	36:0:99:C:O2'	2.47	0.43
36:0:714:G:H2'	36:0:715:A:C8	2.53	0.43
42:6:59:LEU:O	42:6:63:GLU:HB2	2.18	0.43
6:T:85:LYS:HG2	6:T:141:ILE:HD12	1.99	0.43
10:Y:77:ILE:CD1	10:Y:108:ALA:HB1	2.48	0.43
21:j:37:ILE:HG22	21:j:38:VAL:HG23	2.01	0.43
30:N:526:A:O2'	30:N:2043:C:O2	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1:15:HIS:HB2	37:1:203:ASN:HD22	1.84	0.43
2:P:161:TYR:HB3	2:P:194:GLU:HB3	2.01	0.43
3:Q:19:GLY:HA3	14:c:80:VAL:HG23	2.00	0.43
3:Q:45:TYR:OH	30:N:2636:C:O2'	2.07	0.43
6:T:94:TYR:HA	6:T:106:SER:O	2.19	0.43
11:Z:40:ARG:HD3	11:Z:93:VAL:HG21	2.00	0.43
26:o:21:TYR:HE2	26:o:38:LYS:HB3	1.83	0.43
34:M:34:U:OP2	44:8:129:LYS:CE	2.64	0.43
36:0:269:C:H2'	36:0:270:A:C8	2.54	0.43
37:1:186:ILE:HB	37:1:213:TYR:CZ	2.54	0.43
38:2:40:ARG:O	38:2:44:THR:OG1	2.34	0.43
48:D:16:VAL:HG23	48:D:17:ILE:HG13	2.00	0.43
55:K:67:ILE:HG13	55:K:71:LYS:HD3	2.00	0.43
15:d:112:LYS:HG3	16:e:48:LYS:HE2	2.01	0.43
28:q:33:LEU:HB2	30:N:2420:C:OP2	2.19	0.43
30:N:221:A:N1	30:N:265:A:O2'	2.51	0.43
36:0:297:G:N2	36:0:300:A:OP2	2.48	0.43
36:0:723:U:C5'	56:s:49:LYS:HE2	2.48	0.43
38:2:153:VAL:HG12	38:2:198:VAL:HG22	2.01	0.43
39:3:62:ARG:HH21	39:3:68:LEU:HA	1.82	0.43
39:3:95:GLU:HG3	39:3:191:LEU:HD22	2.00	0.43
39:3:109:ALA:HA	39:3:161:LEU:HD11	2.00	0.43
40:4:114:VAL:O	40:4:118:ALA:HB2	2.18	0.43
42:6:71:PRO:O	42:6:96:ARG:NH1	2.51	0.43
5:S:37:ASN:ND2	30:N:2313:C:O4'	2.52	0.43
25:n:8:PRO:HD2	30:N:1263:U:O2'	2.19	0.43
26:o:23:THR:OG1	26:o:24:THR:N	2.52	0.43
30:N:1924:C:O4'	34:M:13:A:O5'	2.37	0.43
36:0:1507:A:H2'	36:0:1508:A:C8	2.53	0.43
9:X:63:VAL:HG12	9:X:107:LEU:HD21	2.00	0.43
10:Y:30:THR:O	10:Y:32:GLY:N	2.52	0.43
10:Y:33:ARG:NH1	30:N:587:C:O2	2.46	0.43
26:o:9:ILE:HG22	26:o:53:LYS:HB2	2.00	0.43
30:N:897:C:H5'	58:u:56:C:H5''	1.92	0.43
30:N:1779:U:OP2	30:N:1784:A:N6	2.50	0.43
31:L:30:HIS:ND1	31:L:31:ASP:O	2.52	0.43
33:U:66:ASN:ND2	33:U:134:VAL:O	2.51	0.43
36:0:723:U:H5''	56:s:49:LYS:HE2	2.01	0.43
38:2:134:MET:HE2	38:2:134:MET:HB3	1.91	0.43
48:D:96:PRO:HA	48:D:109:ARG:HG2	2.01	0.43
3:Q:156:PHE:CD1	8:W:81:ILE:HD12	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:b:29:HIS:HB3	13:b:36:TYR:HB2	2.00	0.42
17:f:85:ILE:HA	17:f:94:ASP:O	2.19	0.42
22:k:31:PRO:HG2	22:k:33:LEU:HD13	2.01	0.42
30:N:373:U:H2'	30:N:374:A:H8	1.84	0.42
30:N:828:U:H2'	30:N:829:A:C8	2.53	0.42
30:N:1078:U:O2'	30:N:1088:A:OP1	2.34	0.42
30:N:2174:C:O2'	30:N:2175:C:H5'	2.19	0.42
32:C:7:ARG:O	32:C:11:ILE:HG12	2.19	0.42
36:0:537:G:H5''	47:B:110:ARG:HH12	1.84	0.42
36:0:1530:G:H2'	36:0:1531:A:C8	2.54	0.42
39:3:159:LEU:HD13	39:3:175:ALA:HB1	2.01	0.42
50:F:35:GLN:HE21	50:F:39:LEU:HD13	1.84	0.42
55:K:33:LYS:O	55:K:37:ALA:HB3	2.19	0.42
3:Q:59:ARG:NH1	30:N:2831:G:OP2	2.41	0.42
5:S:105:THR:HG21	31:L:22:MET:SD	2.59	0.42
5:S:140:GLU:HA	31:L:28:VAL:HG22	2.01	0.42
12:a:37:THR:HG22	12:a:110:MET:HE1	2.00	0.42
30:N:537:G:O2'	30:N:556:A:N6	2.50	0.42
32:C:42:VAL:HG12	32:C:216:THR:HG22	2.00	0.42
34:M:9:C:O2'	34:M:44:A:O2'	2.33	0.42
37:1:18:HIS:CE1	57:t:42:LEU:O	2.66	0.42
37:1:128:LYS:HG3	37:1:129:LEU:HG	2.01	0.42
30:N:320:A:H4'	30:N:322:A:C8	2.54	0.42
30:N:2602:A:H4'	30:N:2603:G:H5'	2.00	0.42
35:x:448:U:H6	38:2:162:ILE:CG1	2.29	0.42
36:0:1380:U:C5	42:6:3:ARG:HA	2.54	0.42
43:7:49:PHE:HA	43:7:60:GLU:O	2.19	0.42
53:I:21:ILE:HD12	53:I:22:ASP:HB2	2.01	0.42
2:P:201:MET:HG3	2:P:202:LEU:HD12	2.01	0.42
12:a:3:HIS:CD2	30:N:2820:A:H4'	2.54	0.42
20:i:75:GLN:HB2	20:i:92:VAL:HG23	2.01	0.42
34:M:33:C:H5'	36:0:966:G:N2	2.35	0.42
36:0:96:U:H2'	36:0:97:G:C8	2.54	0.42
36:0:1315:U:O2'	36:0:1360:A:N3	2.47	0.42
58:u:20:U:HO2'	58:u:21:A:P	2.41	0.42
16:e:81:LYS:HD2	30:N:973:A:OP2	2.20	0.42
17:f:93:ALA:HB2	30:N:1614:A:C2	2.55	0.42
30:N:2155:U:H2'	30:N:2156:G:H5'	2.01	0.42
32:C:46:VAL:HG13	32:C:212:VAL:HG12	2.01	0.42
32:C:63:THR:HG22	32:C:163:TYR:CE1	2.53	0.42
39:3:157:ALA:O	39:3:160:GLU:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:5:51:ILE:HD13	41:5:51:ILE:HG21	1.64	0.42
2:P:61:ALA:O	2:P:63:ARG:NH2	2.51	0.42
3:Q:154:LYS:HE2	30:N:2024:G:O3'	2.20	0.42
6:T:16:ASP:O	6:T:26:ILE:HA	2.20	0.42
16:e:80:ARG:NH2	30:N:572:A:OP2	2.47	0.42
30:N:2469:A:N6	30:N:2481:G:O2'	2.50	0.42
30:N:2522:U:O2'	30:N:2647:U:OP1	2.35	0.42
36:0:228:A:H5'	51:G:63:GLN:NE2	2.34	0.42
36:0:713:G:H2'	36:0:714:G:C8	2.54	0.42
3:Q:1:MET:HG2	3:Q:205:PRO:HG2	2.01	0.42
3:Q:149:ASN:ND2	30:N:2572:A:H2'	2.35	0.42
8:W:96:ARG:HH21	8:W:99:ARG:HG2	1.85	0.42
30:N:476:G:N1	30:N:479:A:OP2	2.46	0.42
30:N:2092:U:N3	30:N:2226:C:OP2	2.44	0.42
30:N:2291:U:H2'	30:N:2292:U:C6	2.54	0.42
33:U:8:LYS:O	33:U:9:VAL:O	2.38	0.42
33:U:78:VAL:HG23	33:U:142:VAL:HG11	2.01	0.42
36:0:135:C:O2	51:G:1:MET:HB2	2.20	0.42
36:0:352:C:O2'	36:0:354:G:OP1	2.32	0.42
37:1:64:LYS:HD2	37:1:64:LYS:HA	1.92	0.42
39:3:95:GLU:HA	39:3:100:ASN:HD22	1.84	0.42
47:B:34:CYS:HA	47:B:55:VAL:HA	2.01	0.42
53:I:26:ILE:HG21	53:I:67:LEU:HB3	2.01	0.42
55:K:56:PRO:O	55:K:60:ARG:HB2	2.20	0.42
6:T:22:GLN:HE22	6:T:55:ARG:HH21	1.66	0.42
30:N:2175:C:OP1	32:C:8:MET:HG2	2.20	0.42
30:N:2328:A:H2'	30:N:2329:U:C6	2.55	0.42
30:N:2689:U:OP2	30:N:2719:G:N2	2.38	0.42
36:0:1118:U:H2'	36:0:1119:C:C6	2.54	0.42
36:0:1363:A:O2'	36:0:1365:G:N7	2.42	0.42
40:4:112:ARG:O	40:4:116:GLU:HB2	2.20	0.42
41:5:51:ILE:N	41:5:53:LYS:O	2.52	0.42
44:8:40:GLY:O	44:8:45:ARG:NH2	2.36	0.42
54:J:4:SER:HB3	54:J:5:LEU:HD12	2.00	0.42
55:K:33:LYS:O	55:K:37:ALA:CB	2.68	0.42
2:P:236:GLU:HB3	30:N:2599:G:N7	2.35	0.42
5:S:33:LYS:HD3	5:S:92:ARG:NH1	2.35	0.42
7:V:79:LEU:O	7:V:82:LYS:NZ	2.52	0.42
30:N:1769:U:O2'	30:N:1958:C:OP1	2.36	0.42
33:U:51:ARG:HG3	33:U:51:ARG:NH1	2.35	0.42
34:M:30:A:O2'	36:0:1340:A:C1'	2.67	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:0:746:A:H2'	36:0:747:A:C8	2.55	0.42
37:1:21:ARG:HG3	37:1:22:TYR:CD2	2.55	0.42
3:Q:152:PRO:HG2	3:Q:156:PHE:CZ	2.55	0.42
30:N:1173:U:H3'	30:N:1174:U:H4'	2.02	0.42
32:C:195:ALA:O	32:C:198:LYS:HB2	2.20	0.42
36:0:1041:G:H2'	36:0:1042:A:C8	2.54	0.42
36:0:1118:U:H2'	36:0:1119:C:H6	1.85	0.42
1:O:72:G:N2	1:O:104:A:H62	2.17	0.41
2:P:146:MET:HE1	30:N:1800:C:C5'	2.50	0.41
2:P:247:PRO:HD3	30:N:1824:G:O3'	2.20	0.41
8:W:110:PRO:O	8:W:115:GLY:HA3	2.20	0.41
12:a:28:LEU:HD23	12:a:48:VAL:HG21	2.01	0.41
15:d:24:TYR:CD1	30:N:533:G:H5'	2.55	0.41
15:d:48:ARG:NE	15:d:49:ASP:OD1	2.49	0.41
30:N:58:G:O2'	30:N:73:A:N1	2.46	0.41
30:N:247:G:OP2	30:N:249:C:N4	2.47	0.41
30:N:2124:G:O2'	32:C:41:SER:HB3	2.20	0.41
34:M:34:U:P	44:8:129:LYS:CE	3.07	0.41
36:0:509:A:N3	36:0:543:U:O2'	2.49	0.41
36:0:812:G:HO2'	36:0:813:U:P	2.43	0.41
36:0:1081:A:H5'	40:4:23:LYS:HG3	2.01	0.41
36:0:1380:U:O2	36:0:1382:C:N4	2.49	0.41
44:8:20:PHE:HB2	44:8:64:TYR:O	2.20	0.41
55:K:28:MET:HE3	55:K:58:VAL:HG22	2.02	0.41
30:N:942:G:O2'	30:N:1189:A:N3	2.52	0.41
38:2:24:ALA:HB1	38:2:28:GLU:HG2	2.03	0.41
45:9:22:THR:HA	45:9:25:ILE:HG22	2.02	0.41
47:B:82:ILE:HD13	47:B:82:ILE:HG21	1.88	0.41
55:K:12:ILE:HD13	55:K:12:ILE:HG21	1.72	0.41
55:K:51:PHE:HA	55:K:54:MET:HG2	2.01	0.41
55:K:62:ALA:HA	55:K:67:ILE:HG22	2.02	0.41
9:X:38:ILE:HD11	9:X:112:PHE:HZ	1.84	0.41
27:p:19:ARG:NH2	30:N:125:A:OP2	2.53	0.41
30:N:1058:U:H2'	30:N:1059:G:C8	2.55	0.41
30:N:2541:A:HO2'	30:N:2765:A:H2	1.68	0.41
33:U:54:LEU:HD23	33:U:54:LEU:C	2.45	0.41
36:0:254:G:H5''	52:H:71:LYS:HE3	2.02	0.41
36:0:946:A:H2'	36:0:947:G:H8	1.85	0.41
36:0:1216:A:H5''	49:E:5:SER:HB2	2.02	0.41
36:0:1306:A:N6	36:0:1331:G:H1'	2.35	0.41
5:S:175:PHE:HA	5:S:176:PRO:HD3	1.95	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:j:41:ARG:HH12	30:N:2262:U:H5''	1.84	0.41
30:N:629:G:N3	30:N:639:U:O2'	2.52	0.41
30:N:1075:C:H2'	30:N:1076:C:C6	2.54	0.41
30:N:1826:G:O2'	30:N:1971:U:OP2	2.35	0.41
30:N:2193:G:H2'	30:N:2194:U:C6	2.56	0.41
30:N:2788:C:H2'	30:N:2789:C:C6	2.56	0.41
35:x:451:G:N3	39:3:47:ARG:NH1	2.69	0.41
36:0:228:A:C4'	51:G:63:GLN:HE21	2.32	0.41
36:0:555:U:H2'	36:0:556:C:C6	2.55	0.41
5:S:112:ARG:NH2	5:S:113:ASP:OD2	2.53	0.41
14:c:58:ALA:HA	14:c:74:PHE:O	2.20	0.41
25:n:43:ILE:HG21	25:n:43:ILE:HD13	1.78	0.41
30:N:214:G:N2	30:N:216:A:N3	2.68	0.41
30:N:227:A:O2'	30:N:228:C:O5'	2.38	0.41
30:N:493:G:H2'	30:N:494:G:O4'	2.21	0.41
34:M:40:C:C4'	36:0:1338:G:O2'	2.59	0.41
36:0:337:G:H2'	36:0:338:A:C8	2.56	0.41
47:B:50:ARG:HG3	47:B:90:LEU:HD11	2.01	0.41
50:F:26:GLU:OE2	50:F:77:ARG:NE	2.53	0.41
4:R:111:GLU:OE2	4:R:114:ARG:NH1	2.49	0.41
30:N:2176:A:H4'	32:C:215:SER:CB	2.50	0.41
36:0:1119:C:H2'	36:0:1120:C:H6	1.84	0.41
39:3:72:PHE:HE1	39:3:94:LEU:HD11	1.84	0.41
39:3:200:ILE:HD13	39:3:200:ILE:HG21	1.76	0.41
41:5:6:ILE:HB	41:5:62:MET:HB3	2.02	0.41
42:6:78:ARG:HB3	42:6:80:VAL:HG23	2.01	0.41
48:D:87:ARG:HG3	48:D:97:VAL:HG13	2.03	0.41
27:p:24:THR:HG23	27:p:27:GLY:H	1.86	0.41
30:N:1212:G:H2'	30:N:1236:G:H22	1.85	0.41
30:N:1912:A:N1	36:0:1408:A:C4'	2.81	0.41
33:U:65:ALA:O	33:U:68:ARG:HB3	2.20	0.41
36:0:1071:C:H2'	36:0:1072:G:H8	1.86	0.41
44:8:96:SER:O	44:8:99:ARG:HB3	2.21	0.41
49:E:25:ALA:O	49:E:28:LYS:HG2	2.21	0.41
9:X:121:GLU:HG3	14:c:66:ASN:HD21	1.85	0.41
10:Y:109:LYS:HE2	10:Y:128:THR:HG22	2.03	0.41
30:N:2122:U:H2'	30:N:2123:G:O4'	2.21	0.41
30:N:2554:U:H2'	30:N:2555:U:C6	2.55	0.41
30:N:2572:A:OP1	30:N:2574:G:H4'	2.20	0.41
5:S:140:GLU:OE1	31:L:27:THR:HG23	2.21	0.41
11:Z:136:MET:SD	20:i:75:GLN:O	2.78	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:e:10:LYS:HE3	16:e:10:LYS:HB3	1.92	0.41
19:h:4:LYS:O	19:h:94:ARG:NH2	2.50	0.41
19:h:16:GLY:C	19:h:18:ASP:H	2.28	0.41
30:N:372:G:H1'	30:N:373:U:H5	1.85	0.41
30:N:715:A:H1'	50:F:40:GLN:CD	2.46	0.41
30:N:715:A:N6	50:F:53:ARG:NH1	2.66	0.41
30:N:932:U:O2'	30:N:934:U:O4	2.36	0.41
30:N:1509:A:H2'	30:N:1510:G:H8	1.84	0.41
30:N:2087:G:H2'	30:N:2088:A:H8	1.86	0.41
30:N:2131:U:O5'	30:N:2133:G:H4'	2.21	0.41
30:N:2724:U:H2'	30:N:2725:A:C8	2.56	0.41
31:L:8:LYS:HD3	31:L:8:LYS:HA	1.82	0.41
36:0:109:A:H5'	36:0:110:C:C5	2.56	0.41
36:0:331:G:H2'	55:K:5:LYS:NZ	2.35	0.41
36:0:384:G:H2'	36:0:385:C:C6	2.56	0.41
36:0:1524:C:H2'	36:0:1525:G:C8	2.56	0.41
37:1:164:ILE:HD11	37:1:210:VAL:HB	2.02	0.41
39:3:151:LYS:HA	39:3:156:LYS:HE3	2.03	0.41
42:6:44:TYR:O	42:6:48:GLU:HB2	2.21	0.41
45:9:36:VAL:HG22	45:9:76:ILE:HG12	2.03	0.41
55:K:5:LYS:HE3	55:K:5:LYS:HB2	1.90	0.41
5:S:73:SER:OG	34:M:55:C:H4'	2.21	0.41
9:X:77:ILE:HG21	9:X:77:ILE:HD13	1.75	0.41
30:N:373:U:H2'	30:N:374:A:C8	2.56	0.41
30:N:2866:U:H4'	30:N:2867:G:H5'	2.02	0.41
32:C:21:TYR:CD2	32:C:222:VAL:HG23	2.56	0.41
34:M:1:U:H2'	34:M:2:G:C8	2.54	0.41
36:0:151:A:H3'	36:0:152:A:H8	1.86	0.41
37:1:225:ARG:H	37:1:225:ARG:HG3	1.66	0.41
1:O:8:C:O3'	13:b:25:ARG:NH1	2.54	0.40
4:R:108:ILE:HD13	4:R:108:ILE:HG21	1.72	0.40
7:V:13:VAL:HG21	7:V:23:PRO:HG2	2.02	0.40
9:X:7:MET:HB3	9:X:18:ARG:HD2	2.02	0.40
13:b:24:THR:HG22	13:b:42:PRO:HD3	2.03	0.40
17:f:24:ILE:HD13	17:f:36:LEU:HD11	2.02	0.40
17:f:85:ILE:HG23	17:f:93:ALA:HB1	2.03	0.40
27:p:34:ARG:CD	30:N:467:G:OP2	2.69	0.40
30:N:927:A:H2'	30:N:928:A:C8	2.56	0.40
32:C:60:ARG:HE	32:C:162:ARG:HH11	1.68	0.40
36:0:501:C:H2'	36:0:502:A:C8	2.56	0.40
36:0:552:U:O2'	47:B:83:ARG:O	2.39	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:0:686:U:O4	36:0:703:G:O2'	2.32	0.40
36:0:1371:G:O3'	44:8:71:GLY:HA3	2.21	0.40
42:6:27:VAL:HG12	42:6:43:VAL:HG21	2.02	0.40
43:7:18:GLN:NE2	43:7:70:ALA:HB1	2.35	0.40
2:P:178:SER:HB2	30:N:1799:G:N7	2.36	0.40
15:d:33:ARG:HG2	30:N:1252:G:N3	2.35	0.40
19:h:10:GLU:OE2	19:h:22:ARG:NH2	2.48	0.40
22:k:39:TRP:CB	33:U:32:PRO:HB3	2.51	0.40
30:N:1394:U:H4'	30:N:1603:A:H4'	2.02	0.40
30:N:2602:A:C6	34:M:75:A:H5''	2.57	0.40
36:0:464:U:O2'	36:0:466:A:N7	2.49	0.40
36:0:619:U:H3	39:3:131:ASN:HB3	1.87	0.40
46:A:110:ILE:HG22	56:s:17:ARG:CZ	2.51	0.40
6:T:90:VAL:O	6:T:160:LYS:HA	2.21	0.40
22:k:3:ARG:HD3	30:N:1365:A:OP1	2.21	0.40
29:r:3:VAL:HG12	29:r:36:ARG:HB3	2.02	0.40
30:N:632:A:H2'	30:N:633:A:C8	2.56	0.40
30:N:704:G:H1'	30:N:727:A:N6	2.37	0.40
30:N:851:C:H2'	30:N:852:U:C6	2.57	0.40
30:N:2101:A:H61	30:N:2188:U:H3	1.69	0.40
30:N:2655:G:O2'	30:N:2656:U:O5'	2.38	0.40
36:0:1095:U:P	36:0:1108:G:H1	2.45	0.40
36:0:1255:G:O2'	36:0:1258:G:N3	2.46	0.40
40:4:12:GLN:HG3	40:4:117:VAL:HG12	2.04	0.40
41:5:3:HIS:CE1	41:5:95:ALA:HB2	2.56	0.40
41:5:42:TRP:HB2	41:5:59:TYR:HB2	2.01	0.40
41:5:90:MET:HE1	53:I:23:TYR:CE1	2.56	0.40
10:Y:35:HIS:O	10:Y:36:LYS:O	2.39	0.40
13:b:94:ARG:HH12	30:N:2294:G:P	2.43	0.40
15:d:15:LYS:HE2	15:d:15:LYS:HB2	1.80	0.40
22:k:37:ARG:HG3	22:k:48:THR:HB	2.02	0.40
30:N:475:C:H4'	30:N:510:C:H5'	2.04	0.40
30:N:770:G:H1'	30:N:1379:U:C4	2.57	0.40
30:N:964:C:O2'	30:N:2273:A:N3	2.49	0.40
46:A:52:PHE:HZ	46:A:65:VAL:HG11	1.87	0.40
6:T:105:LEU:HB2	6:T:113:VAL:HB	2.04	0.40
26:o:5:ILE:HG21	26:o:28:ARG:HH12	1.86	0.40
30:N:657:U:H2'	30:N:658:U:C6	2.56	0.40
30:N:1009:A:N3	30:N:1153:C:O2'	2.53	0.40
33:U:12:LEU:HD12	33:U:13:GLY:N	2.36	0.40
36:0:1160:G:OP1	37:1:132:LYS:CE	2.58	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:5:3:HIS:HB2	41:5:92:THR:HA	2.04	0.40
46:A:88:GLY:N	46:A:114:THR:HG22	2.37	0.40
58:u:20:U:O2'	58:u:21:A:OP1	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	P	269/275 (98%)	247 (92%)	18 (7%)	4 (2%)	8	38
3	Q	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	24	63
4	R	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
5	S	175/179 (98%)	163 (93%)	11 (6%)	1 (1%)	21	59
6	T	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
7	V	139/142 (98%)	112 (81%)	27 (19%)	0	100	100
8	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
9	X	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	7	35
10	Y	141/144 (98%)	121 (86%)	16 (11%)	4 (3%)	4	24
11	Z	134/137 (98%)	118 (88%)	11 (8%)	5 (4%)	2	20
12	a	118/127 (93%)	103 (87%)	13 (11%)	2 (2%)	7	35
13	b	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
14	c	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
15	d	115/118 (98%)	115 (100%)	0	0	100	100
16	e	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	12	47
17	f	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14	50
18	g	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	h	100/104 (96%)	84 (84%)	14 (14%)	2 (2%)	6	31
20	i	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
21	j	73/85 (86%)	71 (97%)	2 (3%)	0	100	100
22	k	75/78 (96%)	71 (95%)	3 (4%)	1 (1%)	9	41
23	l	61/63 (97%)	56 (92%)	5 (8%)	0	100	100
24	m	56/59 (95%)	52 (93%)	4 (7%)	0	100	100
25	n	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6	32
26	o	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
27	p	44/47 (94%)	40 (91%)	4 (9%)	0	100	100
28	q	62/67 (92%)	56 (90%)	5 (8%)	1 (2%)	7	37
29	r	36/55 (66%)	35 (97%)	1 (3%)	0	100	100
31	L	50/70 (71%)	44 (88%)	5 (10%)	1 (2%)	6	31
32	C	130/223 (58%)	123 (95%)	7 (5%)	0	100	100
33	U	147/149 (99%)	124 (84%)	21 (14%)	2 (1%)	9	39
37	1	216/244 (88%)	188 (87%)	27 (12%)	1 (0%)	24	63
38	2	204/237 (86%)	186 (91%)	16 (8%)	2 (1%)	12	47
39	3	203/206 (98%)	182 (90%)	21 (10%)	0	100	100
40	4	148/162 (91%)	116 (78%)	30 (20%)	2 (1%)	9	39
41	5	98/131 (75%)	81 (83%)	11 (11%)	6 (6%)	1	13
42	6	149/152 (98%)	139 (93%)	10 (7%)	0	100	100
43	7	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
44	8	125/130 (96%)	103 (82%)	20 (16%)	2 (2%)	7	37
45	9	96/110 (87%)	84 (88%)	9 (9%)	3 (3%)	3	22
46	A	115/129 (89%)	102 (89%)	13 (11%)	0	100	100
47	B	121/124 (98%)	104 (86%)	15 (12%)	2 (2%)	7	35
48	D	112/118 (95%)	103 (92%)	8 (7%)	1 (1%)	14	50
49	E	92/101 (91%)	78 (85%)	13 (14%)	1 (1%)	11	45
50	F	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
51	G	80/100 (80%)	69 (86%)	10 (12%)	1 (1%)	9	41
52	H	78/84 (93%)	66 (85%)	9 (12%)	3 (4%)	2	19
53	I	53/75 (71%)	49 (92%)	3 (6%)	1 (2%)	6	32

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	J	77/92 (84%)	73 (95%)	4 (5%)	0	100	100
55	K	83/87 (95%)	78 (94%)	4 (5%)	1 (1%)	10	43
56	s	49/88 (56%)	40 (82%)	9 (18%)	0	100	100
57	t	139/557 (25%)	115 (83%)	21 (15%)	3 (2%)	5	29
All	All	5936/6871 (86%)	5354 (90%)	522 (9%)	60 (1%)	15	47

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	P	239	ASN
10	Y	36	LYS
11	Z	58	LYS
16	e	53	PHE
25	n	55	ILE
28	q	32	ILE
33	U	9	VAL
41	5	53	LYS
45	9	58	ASN
51	G	44	SER
52	H	70	THR
11	Z	59	ARG
12	a	3	HIS
33	U	11	ASN
38	2	81	GLY
41	5	56	LYS
41	5	91	ARG
44	8	55	VAL
47	B	23	ALA
52	H	18	GLU
55	K	69	LYS
57	t	33	LYS
2	P	235	GLY
11	Z	39	GLY
18	g	77	ARG
18	g	78	SER
19	h	99	ASN
22	k	3	ARG
38	2	80	LYS
41	5	54	LEU
41	5	94	HIS
45	9	43	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	B	78	SER
52	H	71	LYS
53	I	48	ARG
2	P	10	SER
2	P	238	ARG
3	Q	149	ASN
5	S	175	PHE
9	X	93	GLN
10	Y	29	LYS
10	Y	30	THR
10	Y	31	GLY
11	Z	69	PRO
31	L	3	LYS
40	4	51	GLY
41	5	86	ARG
48	D	66	GLU
57	t	116	VAL
12	a	88	ALA
17	f	64	ALA
19	h	53	ASN
37	1	194	ASP
40	4	90	THR
49	E	4	GLN
57	t	89	ALA
11	Z	87	GLY
45	9	42	LEU
9	X	119	ALA
44	8	10	GLY

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	P	216/220 (98%)	213 (99%)	3 (1%)	59	71
3	Q	164/164 (100%)	159 (97%)	5 (3%)	36	56
4	R	165/165 (100%)	162 (98%)	3 (2%)	51	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	S	148/150 (99%)	147 (99%)	1 (1%)	76	79
6	T	137/138 (99%)	137 (100%)	0	100	100
7	V	109/110 (99%)	109 (100%)	0	100	100
8	W	116/116 (100%)	115 (99%)	1 (1%)	70	76
9	X	103/104 (99%)	101 (98%)	2 (2%)	50	66
10	Y	102/103 (99%)	100 (98%)	2 (2%)	48	65
11	Z	109/110 (99%)	108 (99%)	1 (1%)	70	76
12	a	100/102 (98%)	98 (98%)	2 (2%)	48	65
13	b	86/87 (99%)	85 (99%)	1 (1%)	63	73
14	c	98/100 (98%)	95 (97%)	3 (3%)	35	56
15	d	89/90 (99%)	87 (98%)	2 (2%)	45	64
16	e	84/84 (100%)	83 (99%)	1 (1%)	63	73
17	f	93/93 (100%)	93 (100%)	0	100	100
18	g	80/85 (94%)	79 (99%)	1 (1%)	61	72
19	h	83/85 (98%)	81 (98%)	2 (2%)	43	63
20	i	78/78 (100%)	77 (99%)	1 (1%)	61	72
21	j	56/62 (90%)	55 (98%)	1 (2%)	51	66
22	k	67/68 (98%)	67 (100%)	0	100	100
23	l	55/55 (100%)	54 (98%)	1 (2%)	51	66
24	m	48/49 (98%)	48 (100%)	0	100	100
25	n	47/48 (98%)	46 (98%)	1 (2%)	47	65
26	o	45/49 (92%)	45 (100%)	0	100	100
27	p	38/39 (97%)	38 (100%)	0	100	100
28	q	51/54 (94%)	49 (96%)	2 (4%)	28	50
29	r	34/50 (68%)	33 (97%)	1 (3%)	37	57
31	L	47/63 (75%)	47 (100%)	0	100	100
32	C	110/174 (63%)	109 (99%)	1 (1%)	70	76
33	U	114/114 (100%)	114 (100%)	0	100	100
37	1	180/202 (89%)	178 (99%)	2 (1%)	65	74
38	2	170/196 (87%)	167 (98%)	3 (2%)	51	66
39	3	172/173 (99%)	170 (99%)	2 (1%)	63	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	4	113/123 (92%)	107 (95%)	6 (5%)	20	42
41	5	87/112 (78%)	87 (100%)	0	100	100
42	6	124/125 (99%)	123 (99%)	1 (1%)	73	77
43	7	104/105 (99%)	101 (97%)	3 (3%)	37	57
44	8	105/107 (98%)	104 (99%)	1 (1%)	68	76
45	9	86/97 (89%)	85 (99%)	1 (1%)	63	73
46	A	90/98 (92%)	89 (99%)	1 (1%)	65	74
47	B	103/104 (99%)	103 (100%)	0	100	100
48	D	92/96 (96%)	90 (98%)	2 (2%)	45	64
49	E	79/83 (95%)	79 (100%)	0	100	100
50	F	75/77 (97%)	75 (100%)	0	100	100
51	G	65/80 (81%)	64 (98%)	1 (2%)	57	70
52	H	74/77 (96%)	73 (99%)	1 (1%)	59	71
53	I	48/66 (73%)	47 (98%)	1 (2%)	47	65
54	J	70/80 (88%)	66 (94%)	4 (6%)	18	41
55	K	65/66 (98%)	65 (100%)	0	100	100
56	s	44/76 (58%)	43 (98%)	1 (2%)	44	63
All	All	4818/5152 (94%)	4750 (99%)	68 (1%)	57	71

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	P	141	VAL
2	P	165	VAL
2	P	218	PRO
3	Q	48	ILE
3	Q	73	VAL
3	Q	177	VAL
3	Q	202	ILE
3	Q	205	PRO
4	R	69	ARG
4	R	149	ILE
4	R	163	ASN
5	S	31	VAL
8	W	57	LEU
9	X	58	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	X	86	LEU
10	Y	77	ILE
10	Y	94	THR
11	Z	128	THR
12	a	50	PRO
12	a	70	THR
13	b	3	LYS
14	c	32	VAL
14	c	53	ARG
14	c	73	VAL
15	d	16	LYS
15	d	33	ARG
16	e	49	ILE
18	g	32	LEU
19	h	28	VAL
19	h	68	SER
20	i	65	VAL
21	j	41	ARG
23	l	6	LEU
25	n	28	LEU
28	q	2	PRO
28	q	32	ILE
29	r	26	ILE
32	C	33	LEU
37	1	11	LYS
37	1	207	ILE
38	2	55	ILE
38	2	75	ILE
38	2	200	VAL
39	3	5	LEU
39	3	143	VAL
40	4	15	LEU
40	4	115	LEU
40	4	120	VAL
40	4	123	VAL
40	4	141	ILE
40	4	157	ARG
42	6	25	LYS
43	7	51	VAL
43	7	121	LEU
43	7	125	ILE
44	8	120	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
45	9	17	LEU
46	A	31	ILE
48	D	25	VAL
48	D	98	ARG
51	G	19	VAL
52	H	61	ILE
53	I	21	ILE
54	J	5	LEU
54	J	11	ILE
54	J	49	ILE
54	J	58	VAL
56	s	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
2	P	53	HIS
2	P	86	ASN
2	P	134	ASN
2	P	239	ASN
2	P	260	ASN
3	Q	32	ASN
3	Q	49	GLN
3	Q	149	ASN
3	Q	150	GLN
4	R	136	GLN
4	R	163	ASN
4	R	165	HIS
6	T	22	GLN
6	T	73	ASN
6	T	143	GLN
7	V	12	GLN
8	W	40	HIS
8	W	86	GLN
12	a	3	HIS
12	a	73	ASN
14	c	12	GLN
14	c	52	ASN
15	d	37	GLN
15	d	44	GLN
17	f	15	GLN
20	i	51	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	k	36	HIS
25	n	6	ASN
25	n	38	HIS
26	o	19	HIS
31	L	20	ASN
32	C	57	GLN
32	C	172	HIS
32	C	188	ASN
33	U	2	GLN
33	U	18	GLN
33	U	28	ASN
33	U	43	ASN
37	1	203	ASN
38	2	8	ASN
38	2	123	GLN
38	2	190	HIS
40	4	73	ASN
40	4	89	HIS
40	4	121	HIS
41	5	11	HIS
41	5	14	GLN
41	5	55	HIS
42	6	28	ASN
42	6	148	ASN
44	8	32	GLN
44	8	50	GLN
45	9	58	ASN
46	A	118	HIS
48	D	8	ASN
49	E	49	GLN
49	E	66	GLN
50	F	37	ASN
51	G	63	GLN
52	H	31	HIS
53	I	52	GLN
53	I	54	GLN
54	J	56	GLN
55	K	20	HIS
55	K	48	GLN
55	K	78	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	O	117/120 (97%)	21 (17%)	1 (0%)
30	N	2894/2903 (99%)	521 (18%)	34 (1%)
34	M	74/75 (98%)	11 (14%)	0
35	x	13/692 (1%)	11 (84%)	0
36	0	1538/1539 (99%)	283 (18%)	21 (1%)
58	u	72/73 (98%)	20 (27%)	0
All	All	4708/5402 (87%)	867 (18%)	56 (1%)

All (867) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	O	13	G
1	O	25	U
1	O	31	C
1	O	35	C
1	O	41	G
1	O	44	G
1	O	45	A
1	O	51	G
1	O	53	A
1	O	56	G
1	O	57	A
1	O	64	G
1	O	66	A
1	O	67	G
1	O	88	C
1	O	89	U
1	O	90	C
1	O	91	C
1	O	99	A
1	O	108	A
1	O	109	A
30	N	10	A
30	N	23	G
30	N	28	A
30	N	35	G
30	N	36	G
30	N	42	A
30	N	46	G
30	N	51	G
30	N	55	G
30	N	60	G
30	N	61	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	63	A
30	N	71	A
30	N	74	A
30	N	75	G
30	N	84	A
30	N	96	C
30	N	101	A
30	N	102	U
30	N	103	A
30	N	118	A
30	N	119	A
30	N	120	U
30	N	125	A
30	N	138	U
30	N	139	U
30	N	140	C
30	N	141	G
30	N	142	A
30	N	162	U
30	N	163	C
30	N	165	A
30	N	166	U
30	N	188	G
30	N	196	A
30	N	199	A
30	N	201	C
30	N	215	G
30	N	216	A
30	N	221	A
30	N	222	A
30	N	223	A
30	N	224	U
30	N	228	C
30	N	241	A
30	N	242	G
30	N	243	U
30	N	248	G
30	N	255	A
30	N	265	A
30	N	266	G
30	N	267	C
30	N	272	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	276	U
30	N	278	A
30	N	281	C
30	N	284	U
30	N	294	A
30	N	301	G
30	N	311	A
30	N	323	C
30	N	329	G
30	N	330	A
30	N	332	A
30	N	346	A
30	N	361	G
30	N	362	A
30	N	371	A
30	N	372	G
30	N	373	U
30	N	386	G
30	N	396	G
30	N	399	U
30	N	403	U
30	N	404	A
30	N	405	U
30	N	406	G
30	N	411	G
30	N	412	A
30	N	421	C
30	N	422	A
30	N	424	G
30	N	435	C
30	N	447	A
30	N	455	C
30	N	456	C
30	N	457	A
30	N	467	G
30	N	471	A
30	N	473	G
30	N	481	G
30	N	491	G
30	N	501	A
30	N	504	A
30	N	505	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	509	C
30	N	513	A
30	N	529	A
30	N	531	C
30	N	532	A
30	N	543	G
30	N	544	C
30	N	546	U
30	N	548	G
30	N	549	G
30	N	550	C
30	N	556	A
30	N	563	A
30	N	573	U
30	N	575	A
30	N	578	G
30	N	586	A
30	N	603	A
30	N	613	A
30	N	614	A
30	N	616	A
30	N	622	G
30	N	627	A
30	N	637	A
30	N	645	C
30	N	646	U
30	N	647	G
30	N	648	G
30	N	654	A
30	N	655	A
30	N	669	G
30	N	670	A
30	N	671	C
30	N	677	A
30	N	686	U
30	N	695	G
30	N	696	G
30	N	717	C
30	N	729	G
30	N	730	A
30	N	738	G
30	N	747	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	764	A
30	N	765	C
30	N	775	G
30	N	776	G
30	N	782	A
30	N	783	A
30	N	784	G
30	N	785	G
30	N	792	A
30	N	800	A
30	N	805	G
30	N	806	C
30	N	812	C
30	N	819	A
30	N	827	U
30	N	828	U
30	N	829	A
30	N	845	A
30	N	846	U
30	N	858	G
30	N	860	U
30	N	866	A
30	N	869	G
30	N	878	A
30	N	885	C
30	N	896	A
30	N	897	C
30	N	907	G
30	N	910	A
30	N	914	G
30	N	919	U
30	N	932	U
30	N	941	A
30	N	945	A
30	N	946	C
30	N	953	G
30	N	961	C
30	N	973	A
30	N	974	G
30	N	983	A
30	N	985	C
30	N	989	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	995	C
30	N	996	A
30	N	997	G
30	N	1004	U
30	N	1012	U
30	N	1013	C
30	N	1020	A
30	N	1021	A
30	N	1022	G
30	N	1023	U
30	N	1025	G
30	N	1026	G
30	N	1033	U
30	N	1046	A
30	N	1047	G
30	N	1057	A
30	N	1060	U
30	N	1062	G
30	N	1064	C
30	N	1066	U
30	N	1067	A
30	N	1068	G
30	N	1070	A
30	N	1077	A
30	N	1082	U
30	N	1083	U
30	N	1088	A
30	N	1089	A
30	N	1090	A
30	N	1094	U
30	N	1096	A
30	N	1097	U
30	N	1100	C
30	N	1104	C
30	N	1110	G
30	N	1111	A
30	N	1112	G
30	N	1119	U
30	N	1122	G
30	N	1130	U
30	N	1132	U
30	N	1133	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	1135	C
30	N	1136	G
30	N	1141	U
30	N	1142	A
30	N	1143	A
30	N	1155	A
30	N	1168	G
30	N	1171	G
30	N	1173	U
30	N	1174	U
30	N	1175	A
30	N	1180	U
30	N	1186	G
30	N	1195	G
30	N	1204	A
30	N	1205	A
30	N	1206	G
30	N	1210	G
30	N	1212	G
30	N	1237	A
30	N	1238	G
30	N	1250	G
30	N	1251	C
30	N	1253	A
30	N	1256	G
30	N	1257	C
30	N	1265	A
30	N	1266	G
30	N	1268	A
30	N	1271	G
30	N	1272	A
30	N	1275	A
30	N	1300	G
30	N	1301	A
30	N	1321	A
30	N	1329	U
30	N	1332	G
30	N	1345	C
30	N	1352	U
30	N	1365	A
30	N	1368	G
30	N	1376	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	1379	U
30	N	1383	A
30	N	1386	C
30	N	1395	A
30	N	1403	A
30	N	1416	G
30	N	1419	A
30	N	1420	A
30	N	1421	G
30	N	1427	A
30	N	1428	C
30	N	1434	A
30	N	1437	C
30	N	1453	A
30	N	1458	U
30	N	1461	C
30	N	1478	G
30	N	1482	G
30	N	1504	A
30	N	1508	A
30	N	1509	A
30	N	1515	A
30	N	1524	G
30	N	1529	G
30	N	1535	A
30	N	1536	C
30	N	1537	G
30	N	1538	G
30	N	1554	U
30	N	1565	C
30	N	1566	A
30	N	1569	A
30	N	1578	U
30	N	1583	A
30	N	1584	U
30	N	1585	C
30	N	1587	G
30	N	1607	C
30	N	1608	A
30	N	1610	A
30	N	1613	G
30	N	1622	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	1647	U
30	N	1648	U
30	N	1651	G
30	N	1674	G
30	N	1675	C
30	N	1676	A
30	N	1698	A
30	N	1699	G
30	N	1713	A
30	N	1715	G
30	N	1728	C
30	N	1729	U
30	N	1730	C
30	N	1733	G
30	N	1738	G
30	N	1757	A
30	N	1758	U
30	N	1760	C
30	N	1764	C
30	N	1773	A
30	N	1784	A
30	N	1787	A
30	N	1800	C
30	N	1801	A
30	N	1802	A
30	N	1808	A
30	N	1811	G
30	N	1816	C
30	N	1829	A
30	N	1833	C
30	N	1835	G
30	N	1857	G
30	N	1869	G
30	N	1870	C
30	N	1900	A
30	N	1901	A
30	N	1905	C
30	N	1906	G
30	N	1913	A
30	N	1919	A
30	N	1927	A
30	N	1929	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	1930	G
30	N	1931	U
30	N	1938	A
30	N	1955	U
30	N	1964	G
30	N	1967	C
30	N	1970	A
30	N	1971	U
30	N	1972	G
30	N	1991	U
30	N	1993	U
30	N	1997	C
30	N	2004	G
30	N	2006	C
30	N	2020	A
30	N	2022	U
30	N	2023	C
30	N	2031	A
30	N	2033	A
30	N	2043	C
30	N	2046	G
30	N	2055	C
30	N	2056	G
30	N	2060	A
30	N	2061	G
30	N	2062	A
30	N	2063	C
30	N	2069	G
30	N	2072	C
30	N	2077	A
30	N	2092	U
30	N	2094	A
30	N	2097	A
30	N	2099	U
30	N	2110	G
30	N	2111	U
30	N	2112	G
30	N	2113	U
30	N	2118	U
30	N	2119	A
30	N	2132	U
30	N	2133	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	2145	C
30	N	2147	A
30	N	2162	G
30	N	2171	A
30	N	2172	U
30	N	2173	A
30	N	2190	G
30	N	2191	A
30	N	2194	U
30	N	2198	A
30	N	2200	C
30	N	2203	U
30	N	2204	G
30	N	2211	A
30	N	2212	A
30	N	2214	C
30	N	2225	A
30	N	2226	C
30	N	2238	G
30	N	2239	G
30	N	2266	A
30	N	2278	A
30	N	2279	G
30	N	2283	C
30	N	2286	G
30	N	2287	A
30	N	2288	A
30	N	2297	A
30	N	2305	U
30	N	2307	G
30	N	2309	A
30	N	2312	U
30	N	2325	G
30	N	2333	A
30	N	2334	U
30	N	2345	G
30	N	2347	C
30	N	2350	C
30	N	2354	C
30	N	2357	G
30	N	2361	G
30	N	2383	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	2385	C
30	N	2391	G
30	N	2402	U
30	N	2403	C
30	N	2406	A
30	N	2407	A
30	N	2422	C
30	N	2423	U
30	N	2425	A
30	N	2426	A
30	N	2427	C
30	N	2429	G
30	N	2430	A
30	N	2431	U
30	N	2435	A
30	N	2441	U
30	N	2448	A
30	N	2470	G
30	N	2476	A
30	N	2498	C
30	N	2502	G
30	N	2503	A
30	N	2504	U
30	N	2505	G
30	N	2518	A
30	N	2520	C
30	N	2529	G
30	N	2535	G
30	N	2547	A
30	N	2554	U
30	N	2566	A
30	N	2567	G
30	N	2572	A
30	N	2573	C
30	N	2574	G
30	N	2578	G
30	N	2585	U
30	N	2602	A
30	N	2603	G
30	N	2609	U
30	N	2613	U
30	N	2615	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	2629	U
30	N	2630	G
30	N	2636	C
30	N	2645	G
30	N	2646	C
30	N	2655	G
30	N	2656	U
30	N	2661	G
30	N	2663	G
30	N	2682	A
30	N	2689	U
30	N	2690	U
30	N	2714	G
30	N	2716	C
30	N	2718	G
30	N	2724	U
30	N	2727	A
30	N	2733	A
30	N	2748	A
30	N	2751	G
30	N	2752	C
30	N	2765	A
30	N	2776	A
30	N	2777	G
30	N	2778	A
30	N	2779	U
30	N	2791	G
30	N	2792	A
30	N	2798	U
30	N	2801	G
30	N	2818	U
30	N	2820	A
30	N	2833	U
30	N	2834	G
30	N	2836	U
30	N	2849	U
30	N	2850	A
30	N	2859	G
30	N	2867	G
30	N	2868	A
30	N	2872	A
30	N	2873	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	2874	C
30	N	2880	C
30	N	2884	U
30	N	2887	A
30	N	2891	U
30	N	2903	U
34	M	9	C
34	M	10	G
34	M	15	G
34	M	16	C
34	M	17	G
34	M	19	U
34	M	20	A
34	M	42	G
34	M	47	C
34	M	74	C
34	M	75	A
35	x	449	A
35	x	450	C
35	x	451	G
35	x	452	U
35	x	453	C
35	x	455	C
35	x	457	C
35	x	458	U
35	x	459	C
35	x	460	A
35	x	461	A
36	0	4	U
36	0	6	G
36	0	9	G
36	0	32	A
36	0	39	G
36	0	44	A
36	0	47	C
36	0	48	C
36	0	50	A
36	0	51	A
36	0	52	C
36	0	58	C
36	0	65	A
36	0	69	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	0	71	A
36	0	72	A
36	0	83	C
36	0	84	U
36	0	85	U
36	0	86	G
36	0	87	C
36	0	92	U
36	0	97	G
36	0	108	G
36	0	115	G
36	0	116	A
36	0	122	G
36	0	130	A
36	0	141	G
36	0	143	A
36	0	144	G
36	0	149	A
36	0	156	C
36	0	163	C
36	0	174	A
36	0	177	G
36	0	182	A
36	0	183	C
36	0	184	G
36	0	197	A
36	0	209	U
36	0	210	C
36	0	211	G
36	0	226	G
36	0	245	U
36	0	247	G
36	0	251	G
36	0	266	G
36	0	267	C
36	0	280	C
36	0	281	G
36	0	289	G
36	0	298	A
36	0	306	A
36	0	321	A
36	0	328	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	0	332	G
36	0	347	G
36	0	351	G
36	0	352	C
36	0	354	G
36	0	358	U
36	0	367	U
36	0	372	C
36	0	375	U
36	0	384	G
36	0	388	G
36	0	389	A
36	0	397	A
36	0	398	U
36	0	406	G
36	0	412	A
36	0	413	G
36	0	421	U
36	0	422	C
36	0	423	G
36	0	424	G
36	0	429	U
36	0	430	A
36	0	439	U
36	0	451	A
36	0	458	U
36	0	459	A
36	0	467	U
36	0	468	A
36	0	474	G
36	0	478	A
36	0	479	U
36	0	481	G
36	0	484	G
36	0	485	U
36	0	486	U
36	0	495	A
36	0	497	G
36	0	511	C
36	0	518	C
36	0	519	C
36	0	521	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	0	527	G
36	0	531	U
36	0	532	A
36	0	533	A
36	0	547	A
36	0	559	A
36	0	562	U
36	0	572	A
36	0	573	A
36	0	576	C
36	0	595	A
36	0	596	A
36	0	607	A
36	0	633	G
36	0	639	G
36	0	650	G
36	0	652	U
36	0	665	A
36	0	675	A
36	0	688	G
36	0	695	A
36	0	701	U
36	0	702	A
36	0	703	G
36	0	718	A
36	0	721	G
36	0	723	U
36	0	724	G
36	0	731	G
36	0	734	G
36	0	747	A
36	0	755	G
36	0	760	G
36	0	777	A
36	0	793	U
36	0	794	A
36	0	813	U
36	0	815	A
36	0	817	C
36	0	818	G
36	0	819	A
36	0	821	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	0	828	U
36	0	832	G
36	0	836	G
36	0	841	C
36	0	843	U
36	0	844	G
36	0	846	G
36	0	849	G
36	0	859	G
36	0	864	A
36	0	885	G
36	0	889	A
36	0	890	G
36	0	891	U
36	0	902	G
36	0	914	A
36	0	922	G
36	0	926	G
36	0	934	C
36	0	935	A
36	0	960	U
36	0	965	U
36	0	966	G
36	0	969	A
36	0	971	G
36	0	972	C
36	0	975	A
36	0	976	G
36	0	977	A
36	0	989	U
36	0	993	G
36	0	996	A
36	0	999	C
36	0	1000	A
36	0	1004	A
36	0	1008	U
36	0	1009	U
36	0	1017	U
36	0	1018	G
36	0	1020	G
36	0	1022	A
36	0	1024	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	0	1025	U
36	0	1026	G
36	0	1027	C
36	0	1030	U
36	0	1031	C
36	0	1032	G
36	0	1043	G
36	0	1044	A
36	0	1053	G
36	0	1056	U
36	0	1065	U
36	0	1085	U
36	0	1092	A
36	0	1094	G
36	0	1095	U
36	0	1101	A
36	0	1125	U
36	0	1130	A
36	0	1132	C
36	0	1136	C
36	0	1137	C
36	0	1138	G
36	0	1139	G
36	0	1140	C
36	0	1146	A
36	0	1158	C
36	0	1159	U
36	0	1168	U
36	0	1171	A
36	0	1182	G
36	0	1183	U
36	0	1184	G
36	0	1190	G
36	0	1196	A
36	0	1200	C
36	0	1201	A
36	0	1202	U
36	0	1212	U
36	0	1213	A
36	0	1227	A
36	0	1238	A
36	0	1253	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	0	1256	A
36	0	1257	A
36	0	1258	G
36	0	1260	G
36	0	1261	A
36	0	1274	A
36	0	1275	A
36	0	1278	G
36	0	1280	A
36	0	1281	C
36	0	1287	A
36	0	1297	G
36	0	1298	U
36	0	1300	G
36	0	1301	U
36	0	1302	C
36	0	1305	G
36	0	1317	C
36	0	1318	A
36	0	1319	A
36	0	1320	C
36	0	1322	C
36	0	1323	G
36	0	1331	G
36	0	1332	A
36	0	1340	A
36	0	1346	A
36	0	1347	G
36	0	1348	U
36	0	1353	G
36	0	1363	A
36	0	1364	U
36	0	1370	G
36	0	1379	G
36	0	1383	C
36	0	1394	A
36	0	1400	C
36	0	1419	G
36	0	1422	G
36	0	1433	A
36	0	1441	A
36	0	1446	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	0	1451	U
36	0	1452	C
36	0	1487	G
36	0	1491	G
36	0	1492	A
36	0	1493	A
36	0	1497	G
36	0	1503	A
36	0	1506	U
36	0	1517	G
36	0	1519	A
36	0	1529	G
36	0	1530	G
36	0	1531	A
36	0	1534	A
36	0	1535	C
36	0	1537	U
58	u	13	C
58	u	14	A
58	u	16	U
58	u	17	C
58	u	18	G
58	u	19	G
58	u	20	U
58	u	21	A
58	u	22	G
58	u	36	A
58	u	45	U
58	u	46	G
58	u	47	U
58	u	48	C
58	u	52	G
58	u	60	U
58	u	61	C
58	u	62	C
58	u	63	G
58	u	73	A

All (56) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	O	52	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	N	60	G
30	N	227	A
30	N	242	G
30	N	249	C
30	N	372	G
30	N	404	A
30	N	421	C
30	N	446	G
30	N	456	C
30	N	474	G
30	N	503	A
30	N	512	G
30	N	555	G
30	N	670	A
30	N	774	G
30	N	784	G
30	N	859	G
30	N	995	C
30	N	1020	A
30	N	1134	A
30	N	1141	U
30	N	1142	A
30	N	1236	G
30	N	1900	A
30	N	2062	A
30	N	2225	A
30	N	2282	G
30	N	2286	G
30	N	2311	A
30	N	2405	G
30	N	2655	G
30	N	2776	A
30	N	2867	G
30	N	2873	A
36	0	64	G
36	0	85	U
36	0	96	U
36	0	115	G
36	0	388	G
36	0	429	U
36	0	518	C
36	0	595	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	0	812	G
36	0	890	G
36	0	965	U
36	0	1124	G
36	0	1145	A
36	0	1182	G
36	0	1190	G
36	0	1201	A
36	0	1300	G
36	0	1345	U
36	0	1347	G
36	0	1491	G
36	0	1528	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

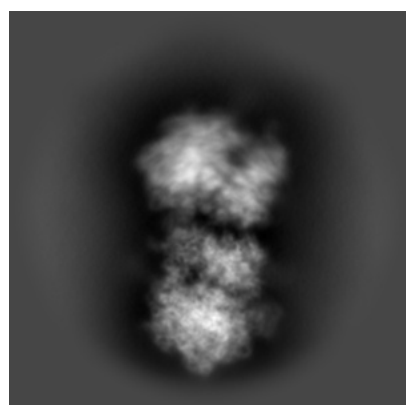
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13955. These allow visual inspection of the internal detail of the map and identification of artifacts.

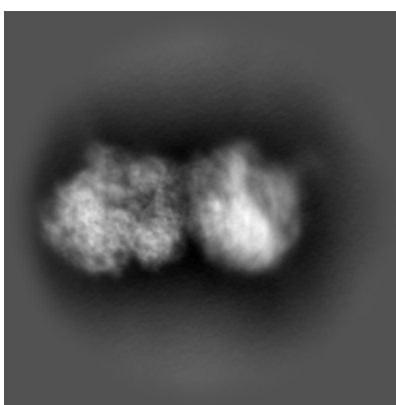
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

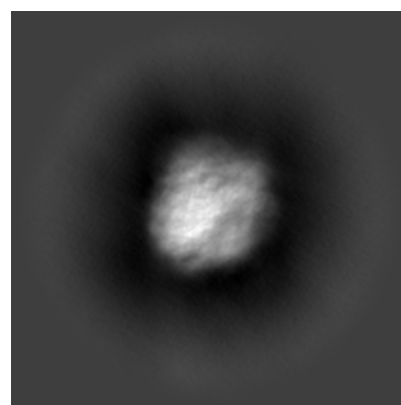
6.1.1 Primary map



X



Y

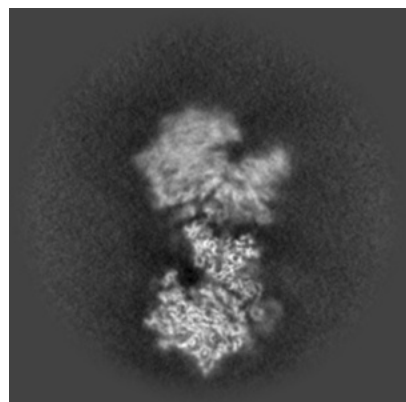


Z

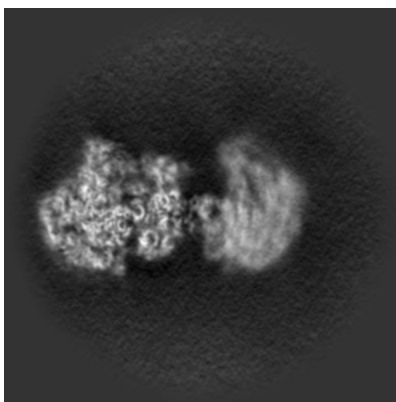
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

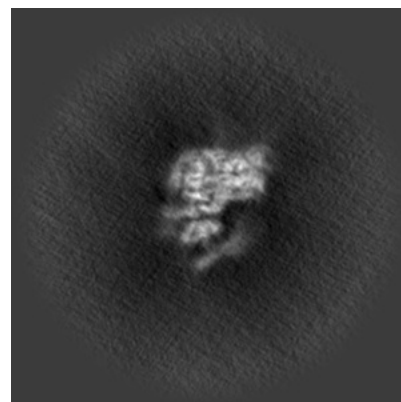
6.2.1 Primary map



X Index: 300



Y Index: 300

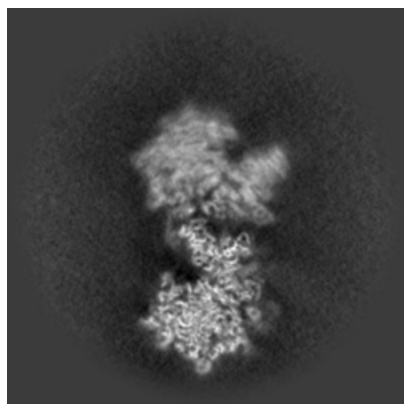


Z Index: 300

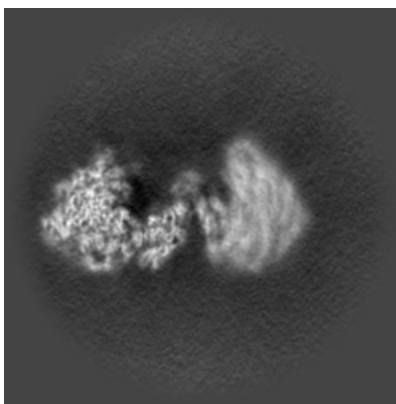
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

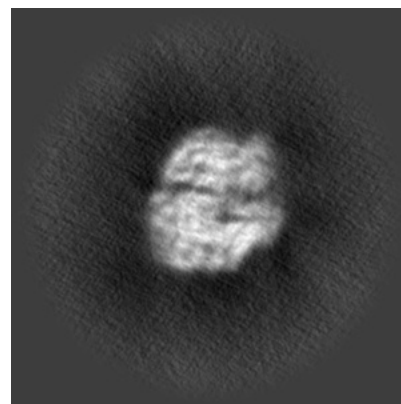
6.3.1 Primary map



X Index: 294



Y Index: 273

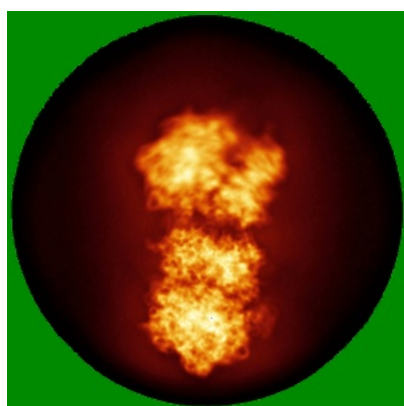


Z Index: 348

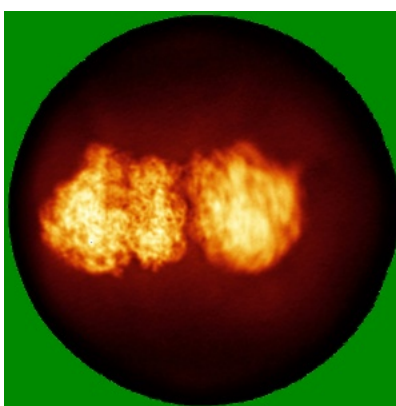
The images above show the largest variance slices of the map in three orthogonal directions.

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

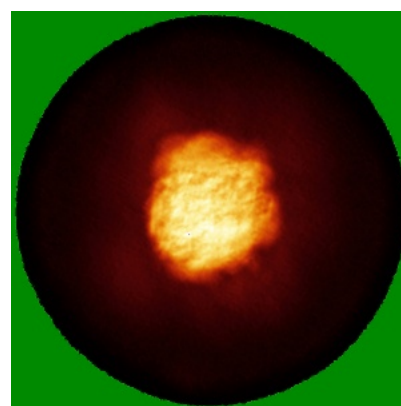
6.4.1 Primary map



X



Y



Z

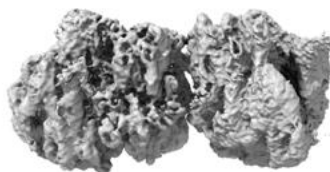
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

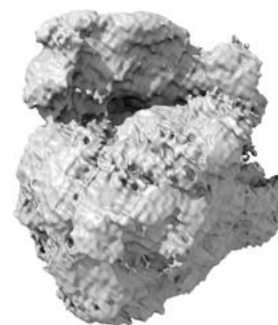
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.45. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

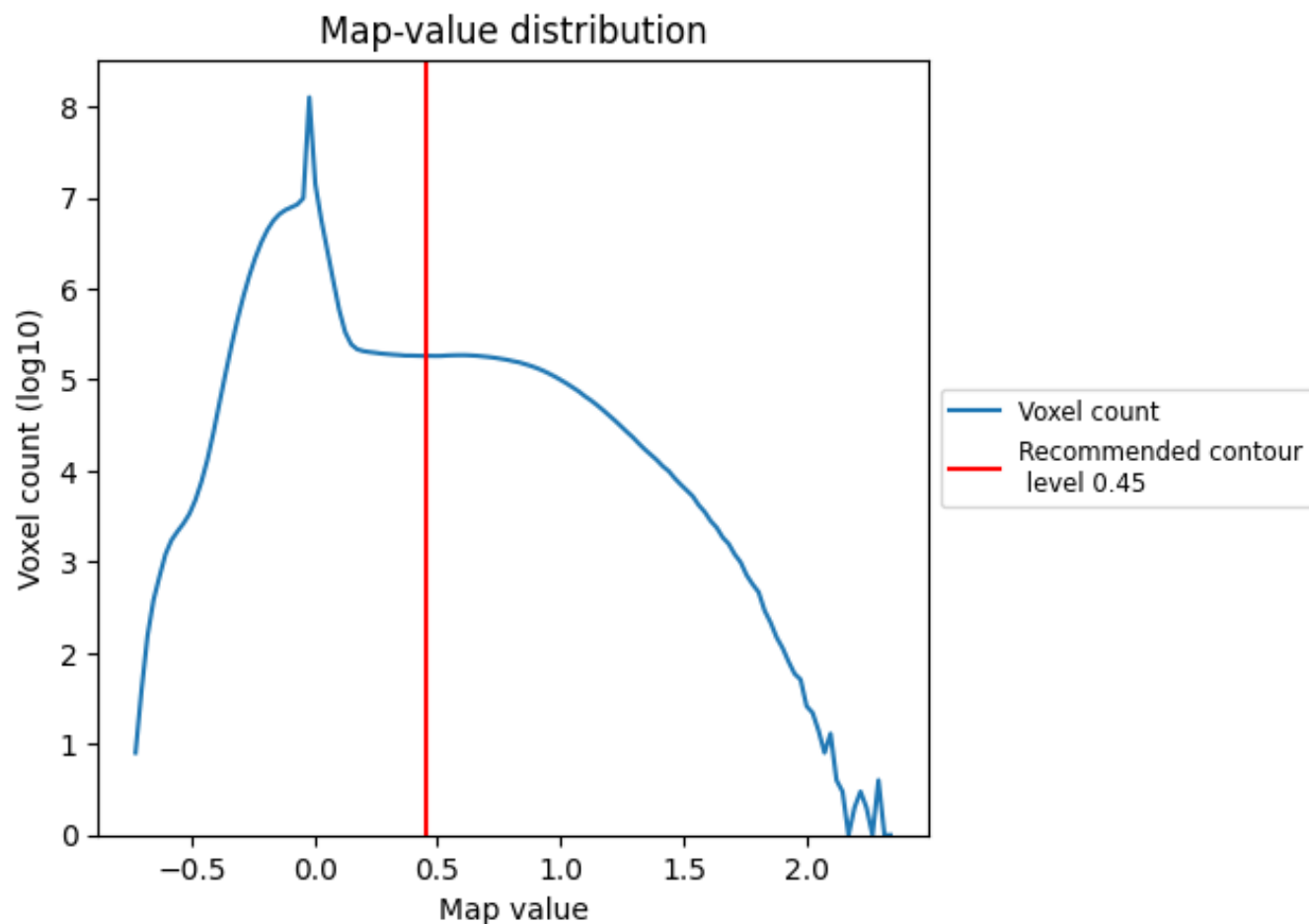
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

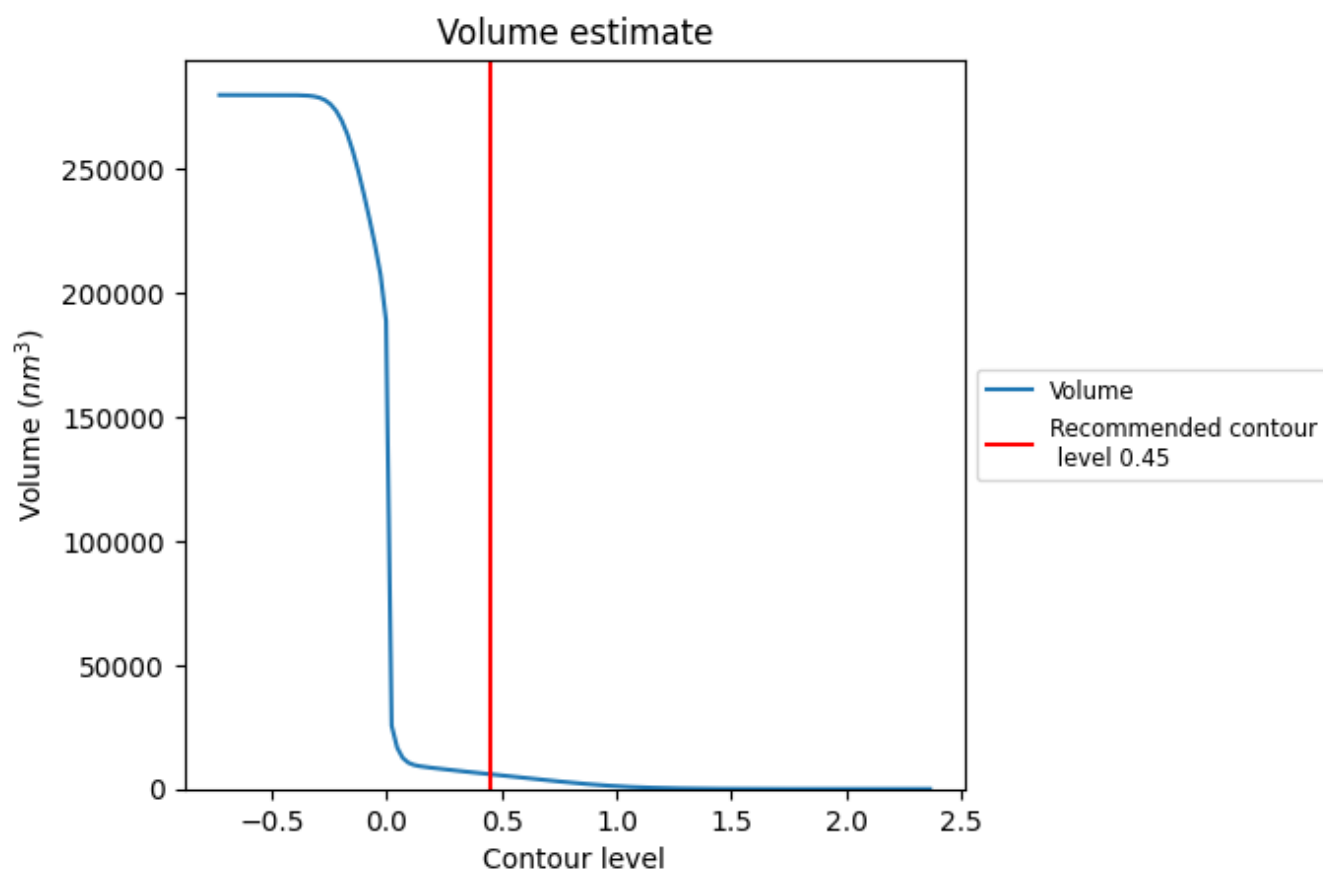
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

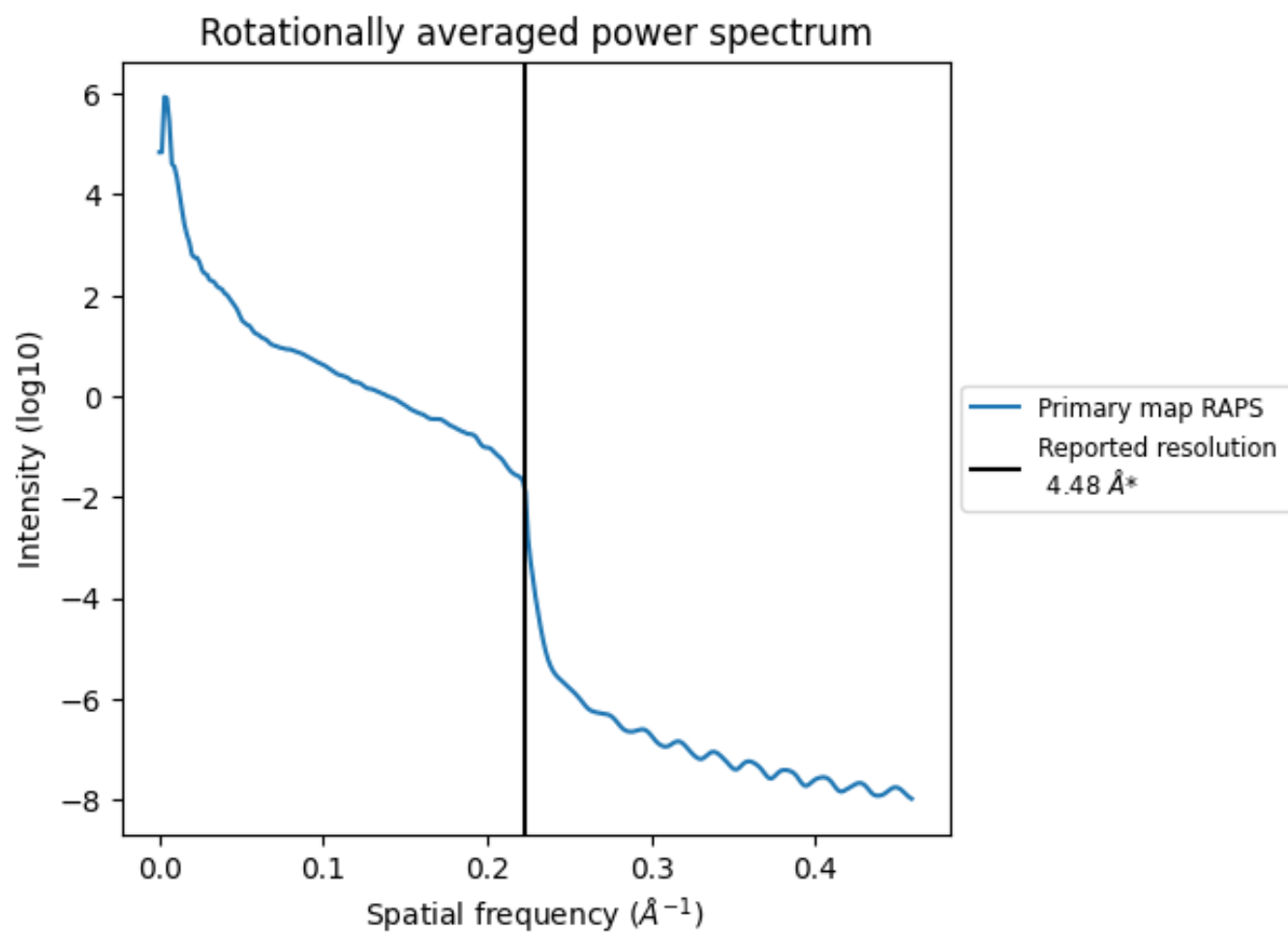
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5945 nm^3 ; this corresponds to an approximate mass of 5371 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 0.223 Å⁻¹

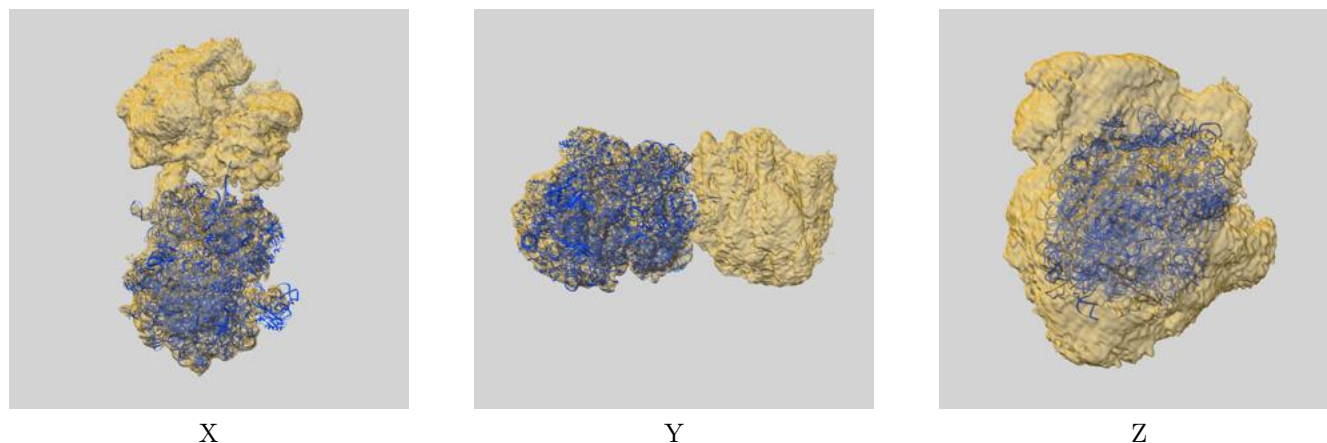
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

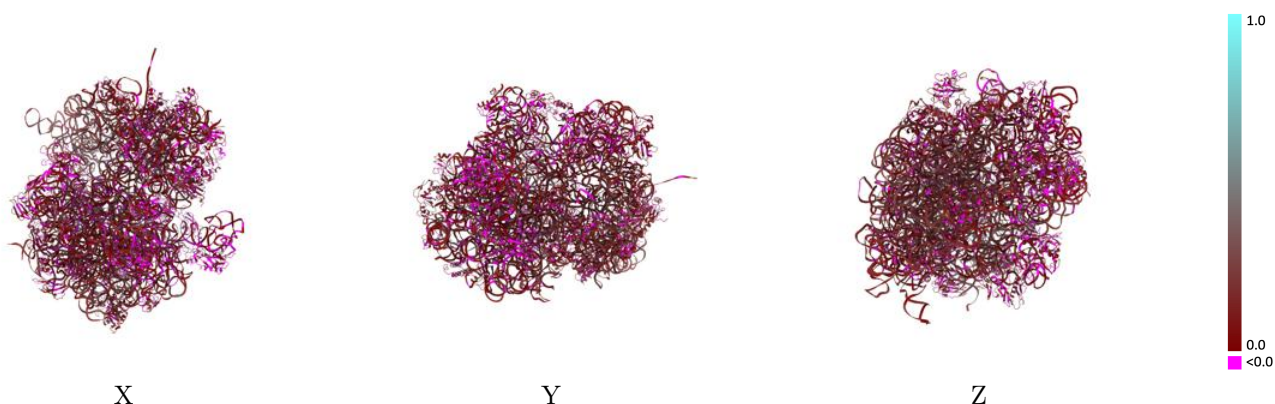
This section contains information regarding the fit between EMDB map EMD-13955 and PDB model 7QGH. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



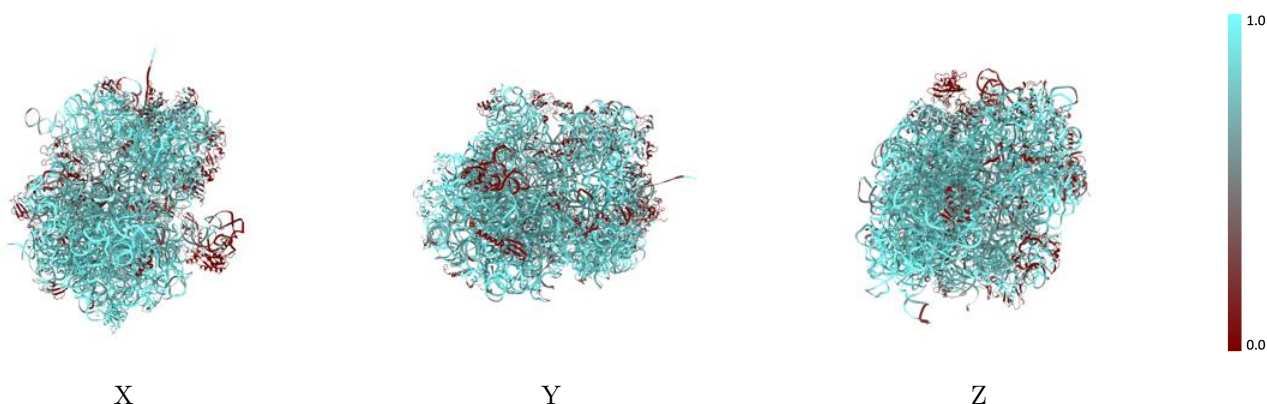
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



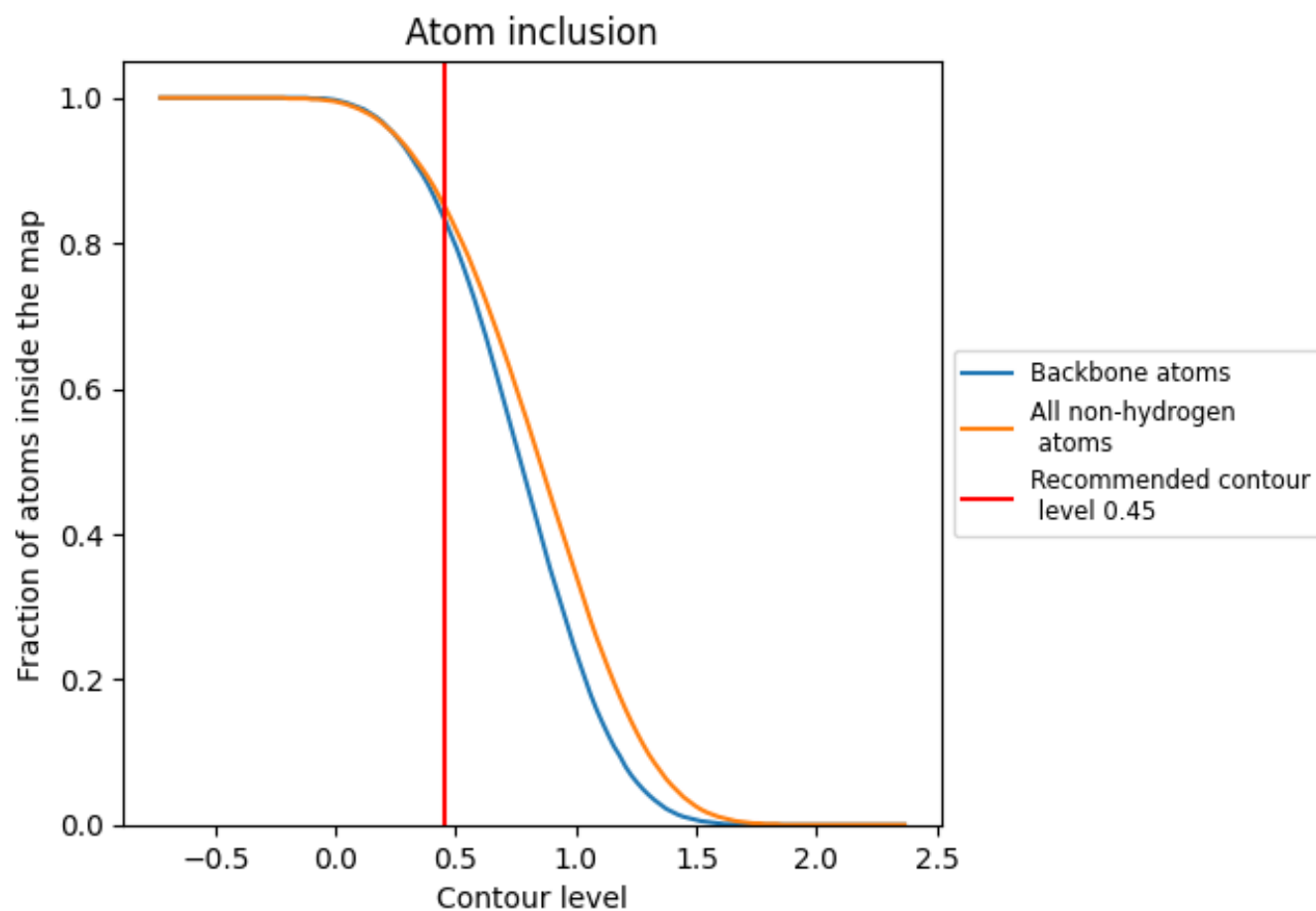
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 85% 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 (0.45) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8530	 0.1260
0	 0.9470	 0.1750
1	 0.5300	 0.1370
2	 0.5970	 0.1260
3	 0.4370	 0.1170
4	 0.7880	 0.1780
5	 0.6680	 0.1140
6	 0.6370	 0.1040
7	 0.8380	 0.1220
8	 0.6570	 0.0640
9	 0.6870	 0.0780
A	 0.6270	 0.1110
B	 0.8960	 0.1470
C	 0.0020	 0.0400
D	 0.6710	 0.0590
E	 0.7250	 0.0510
F	 0.8700	 0.1310
G	 0.8510	 0.1410
H	 0.8840	 0.1200
I	 0.8530	 0.1100
J	 0.6140	 0.0190
K	 0.8520	 0.1010
L	 0.3380	 0.0890
M	 0.8590	 0.1080
N	 0.9270	 0.1290
O	 0.9350	 0.1110
P	 0.7520	 0.0440
Q	 0.7160	 0.0520
R	 0.9240	 0.1200
S	 0.7110	 0.0620
T	 0.4970	 0.0780
U	 0.1410	 0.0450
V	 0.3040	 0.0550
W	 0.9390	 0.0820
X	 0.6060	 0.0450



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Y	 0.9340	 0.0880
Z	 0.7980	 0.0800
a	 0.9430	 0.0940
b	 0.6200	 0.0510
c	 0.7010	 0.0640
d	 0.8750	 0.0840
e	 0.6420	 0.0980
f	 0.8530	 0.1010
g	 0.9090	 0.1010
h	 0.8460	 0.1170
i	 0.7480	 0.0790
j	 0.9530	 0.0720
k	 0.9550	 0.0540
l	 0.6830	 0.1010
m	 0.8900	 0.1020
n	 0.9130	 0.1070
o	 0.5640	 0.0540
p	 0.8360	 0.0530
q	 0.9760	 0.0870
r	 0.7220	 0.0730
s	 0.6380	 0.1440
t	 0.0670	 0.0660
u	 0.6700	 0.0970
x	 0.3500	 0.0950