Full wwPDB EM Validation Report

Mar 5, 2026 – 07:47 PM UTC

PDB ID	:	7QGN / pdb_00007qgn
EMDB ID	:	EMD-13956
Title	:	Structure of the SmrB-bound E. coli disome - stalled 70S ribosome
Authors	:	Kratzat, H.; Buschauer, R.; Berninghausen, O.; Beckmann, R.
Deposited on	:	2021-12-09
Resolution	:	3.37 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:

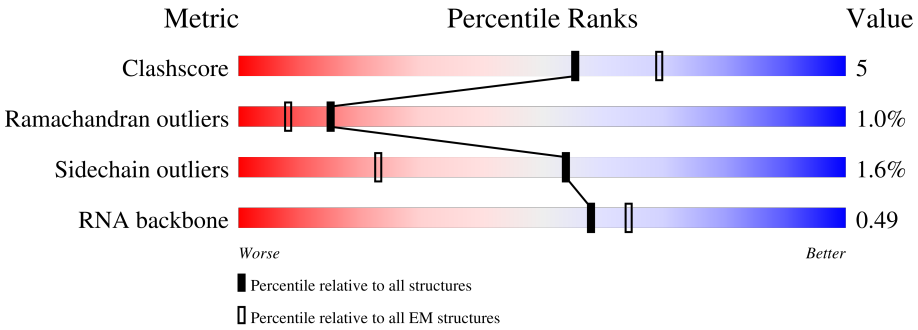
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh &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

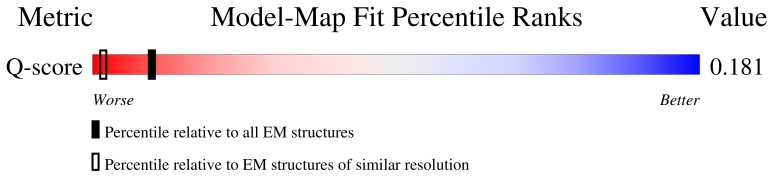
1 Overall quality at a glance

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

The reported resolution of this entry is 3.37 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	14287 (2.87 - 3.87)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	73	8% 67% 27% 5%
2	B	183	14% 19% . 79%
3	s	179	17% . 79%

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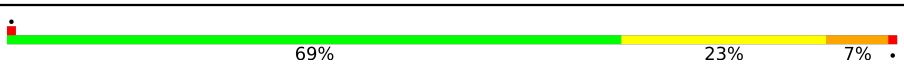
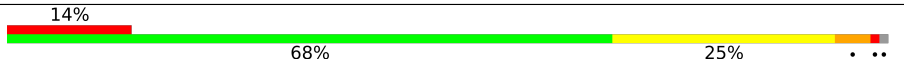
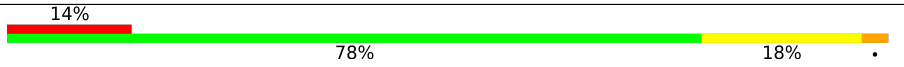
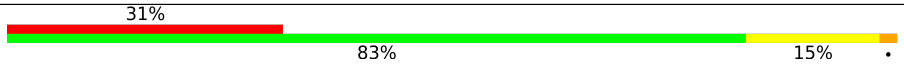
Mol	Chain	Length	Quality of chain
4	M	75	
5	O	120	
6	P	273	
7	Q	209	
8	R	201	
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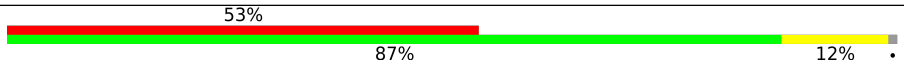
10	T	177	
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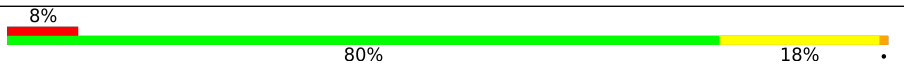
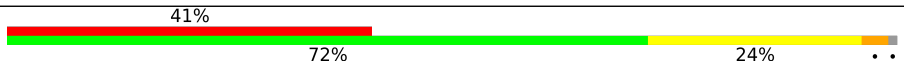
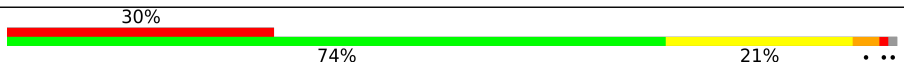
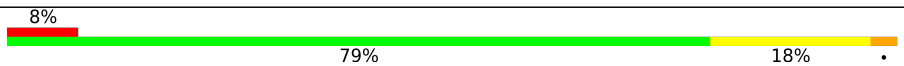
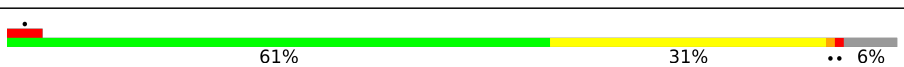
12	V	142	
13	W	142	
14	X	123	
15	Y	144	
16	Z	136	
17	a	127	
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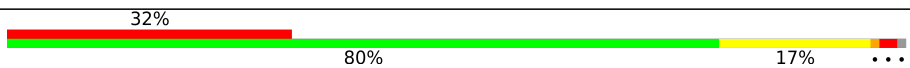
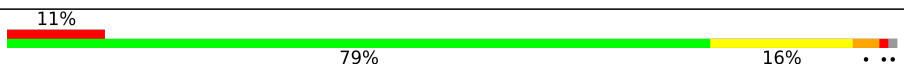
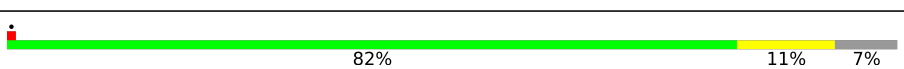
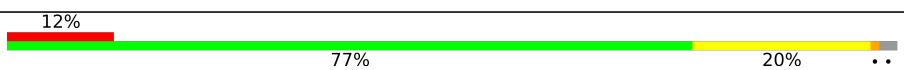
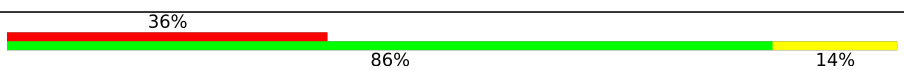
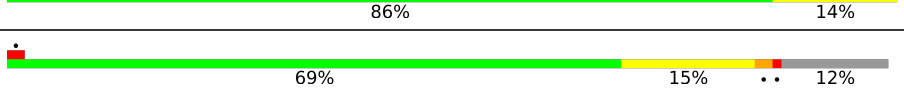
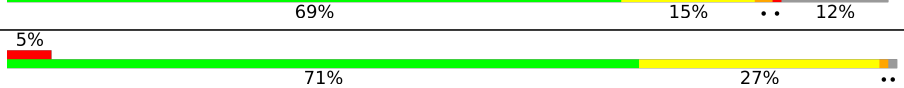
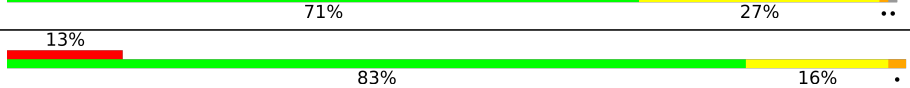
19	c	115	
20	d	118	
21	e	103	
22	f	110	
23	g	100	
24	h	104	
25	i	94	
26	j	85	
27	k	78	
28	l	63	

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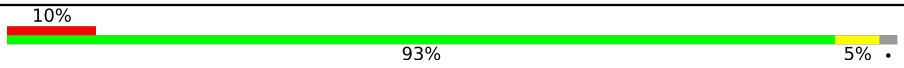
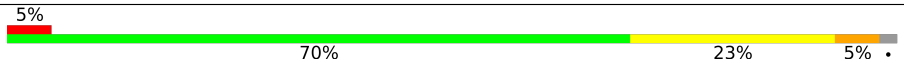
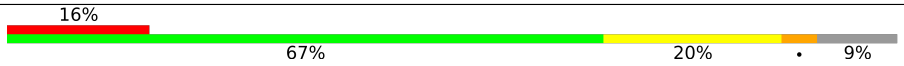
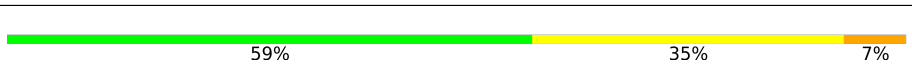
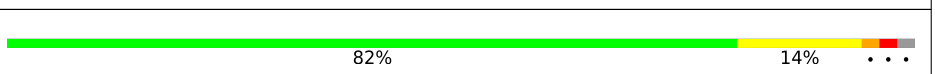
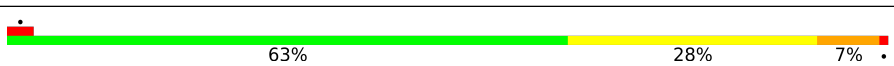
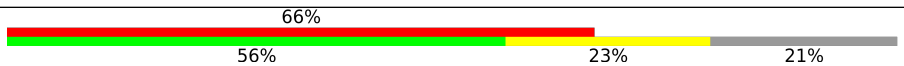
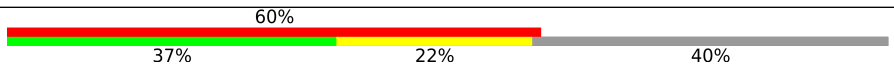
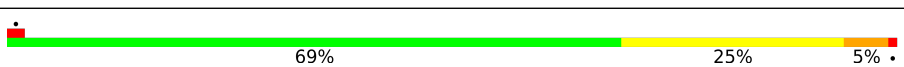
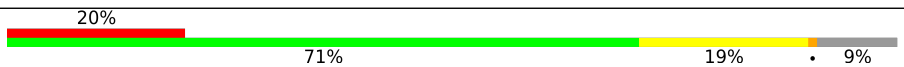
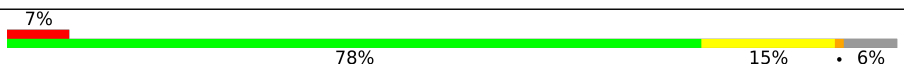
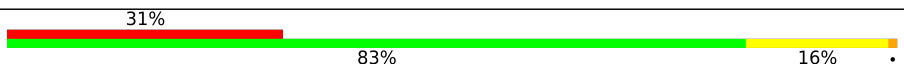
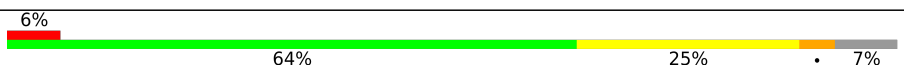
Mol	Chain	Length	Quality of chain
29	m	59	
30	n	57	
31	o	55	
32	p	46	
33	q	65	
34	r	55	
35	N	2903	
36	L	70	
37	C	223	
38	0	1539	
39	1	239	
40	2	218	
41	3	206	
42	4	162	
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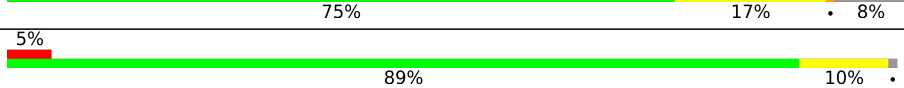
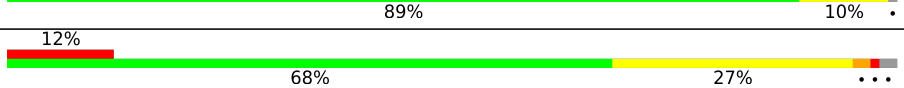
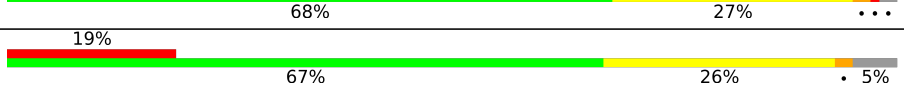
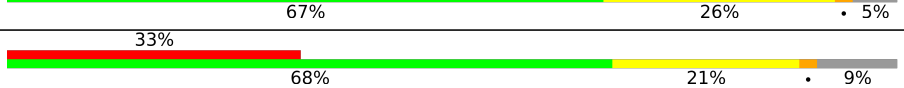
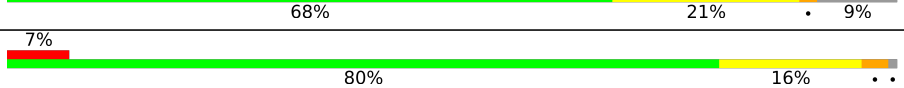
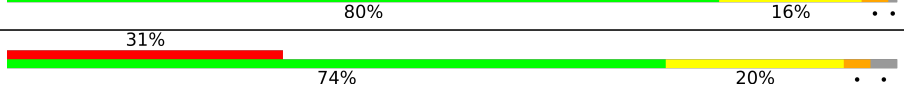
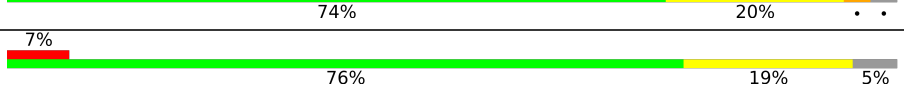
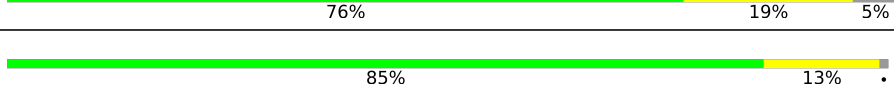
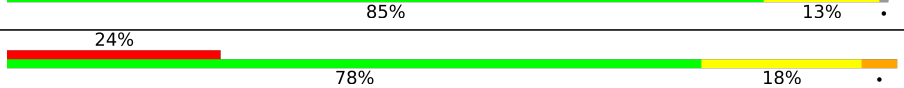
45	7	130	
46	8	130	
47	9	103	
48	D	129	
49	E	124	
50	F	118	
51	G	101	
52	H	89	
53	I	82	

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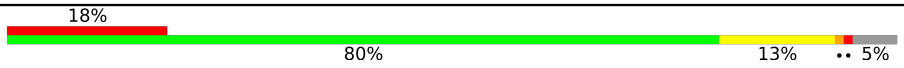
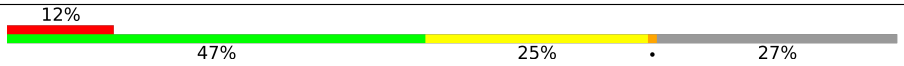
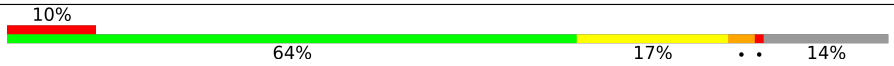
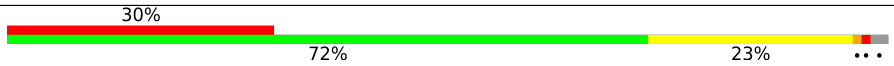
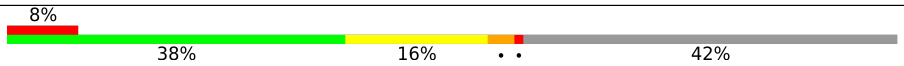
Mol	Chain	Length	Quality of chain
54	J	84	
55	K	75	
56	t	92	
57	u	87	
58	v	88	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 147306 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 A-site tRNA.

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

- Molecule 2 is a protein called UPF0115 protein YfcN.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	B	39	194	116	39	39	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	99	ALA	ASP	variant	UNP Q6KCY1
B	101	ALA	HIS	variant	UNP Q6KCY1

- Molecule 3 is a protein called VemP nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	s	37	316	198	58	58	2	0	0

- Molecule 4 is a RNA chain called P-site tRNA.

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

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

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

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

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

- Molecule 11 is a protein called 50S ribosomal protein L9.

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

- Molecule 12 is a protein called 50S ribosomal protein L11.

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

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called Ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	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	variant	UNP A0A829CNM8

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	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	variant	UNP A0A829CFV1

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

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

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a RNA chain called 23S rRNA.

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

- Molecule 36 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	55	Total	C	N	O	S	0	0
			419	258	76	79	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	68	SER	GLY	variant	UNP J7R8B2

- Molecule 37 is a protein called 50S ribosomal protein L1.

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

- Molecule 38 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	0	1532	Total	C	N	O	P	0	0
			32873	14661	6031	10649	1532		

- Molecule 39 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

- Molecule 40 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	2	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 41 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	205	Total	C	N	O	S	0	0
			1642	1026	315	297	4		

- Molecule 42 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	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	variant	UNP A0A377C6M5

- Molecule 43 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	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	variant	UNP C3SFQ7

- Molecule 44 is a protein called Ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	6	144	Total	C	N	O	S	0	0
			1129	705	213	207	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	78	HIS	ARG	variant	UNP A0A829CQ35

- Molecule 45 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	7	129	Total	C	N	O	S	0	0
			978	616	173	183	6		

- Molecule 46 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	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	variant	UNP A0A1Z3UZ18

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	9	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	D	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
D	5	ALA	PRO	variant	UNP A0A829AF87

- Molecule 49 is a protein called 30S ribosomal protein S12.

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

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	F	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
F	1	VAL	MET	variant	UNP A0A7U9IV78

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	G	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
G	40	ALA	GLU	variant	UNP A0A090BZT4

- Molecule 52 is a protein called 30S ribosomal protein S15.

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

- Molecule 53 is a protein called 30S ribosomal protein S16.

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

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	J	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
J	2	ALA	THR	variant	UNP A0A829A8C6

- Molecule 55 is a protein called 30S ribosomal protein S18.

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

- Molecule 56 is a protein called 30S ribosomal protein S19.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
t	82	TYR	GLY	variant	UNP S1EA57
t	83	TYR	HIS	variant	UNP S1EA57

- Molecule 57 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	u	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
u	1	LEU	MET	variant	UNP C3TRH7

- Molecule 58 is a protein called 30S ribosomal protein S21.

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

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

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

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

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

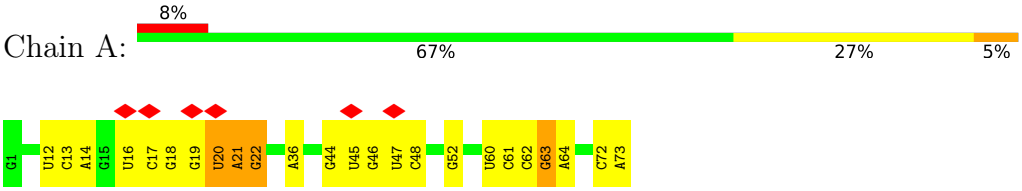
- Molecule 61 is water.

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

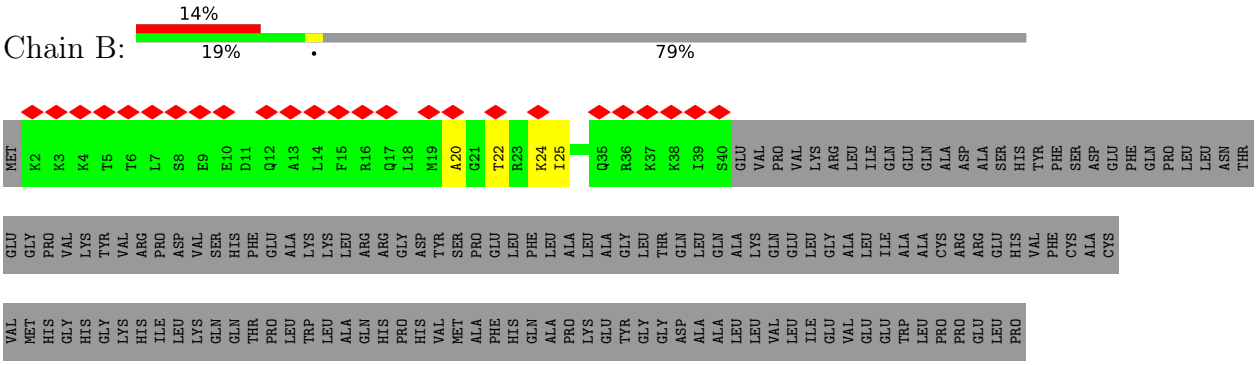
3 Residue-property plots (i)

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.

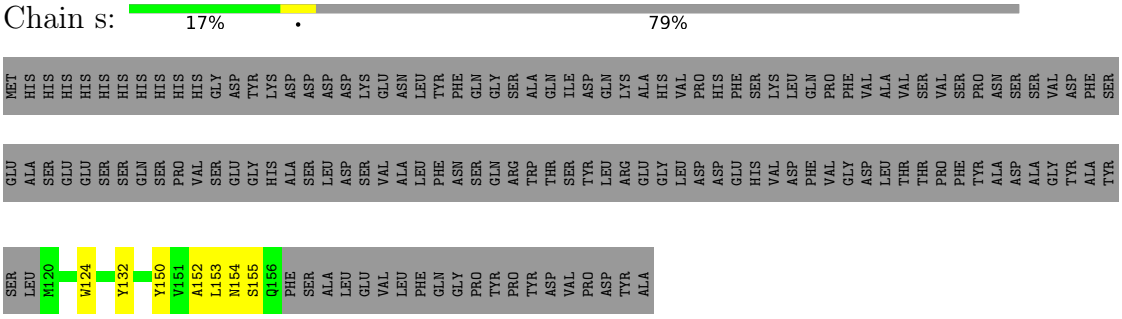
• Molecule 1: A-site tRNA



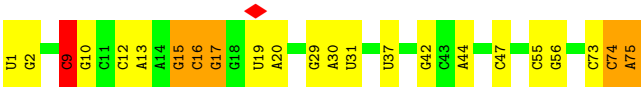
• Molecule 2: UPF0115 protein YfcN



• Molecule 3: VemP nascent chain

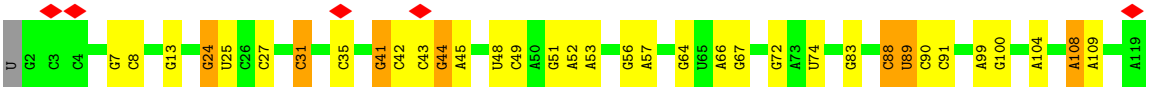


• Molecule 4: P-site tRNA



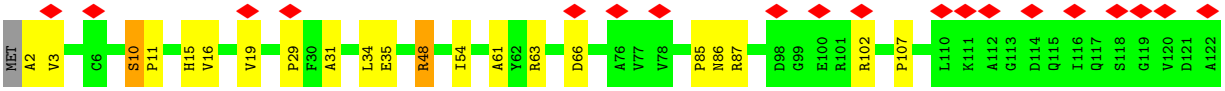
• Molecule 5: 5S rRNA

Chain O:



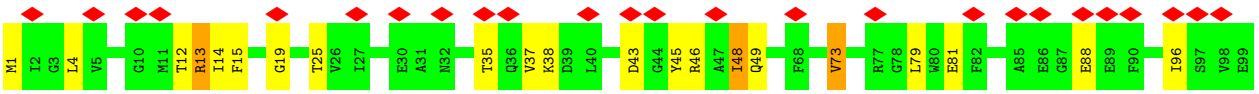
• Molecule 6: 50S ribosomal protein L2

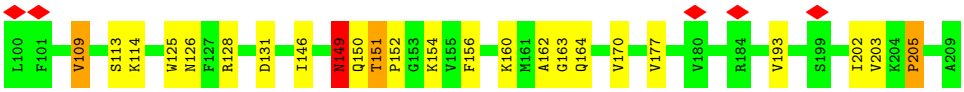
Chain P:



• Molecule 7: 50S ribosomal protein L3

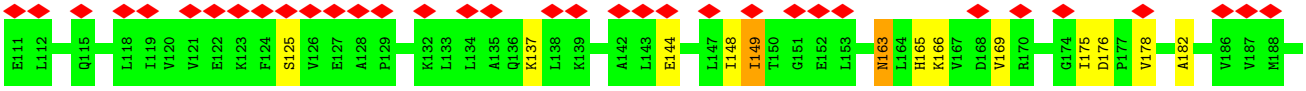
Chain Q:

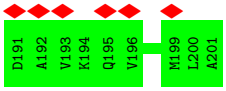




• Molecule 8: 50S ribosomal protein L4

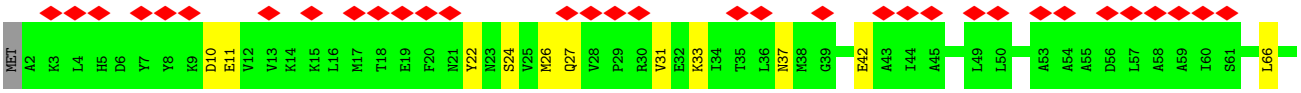
Chain R:

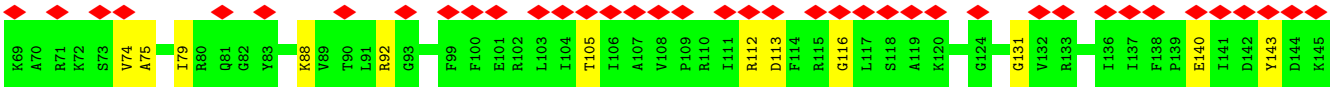


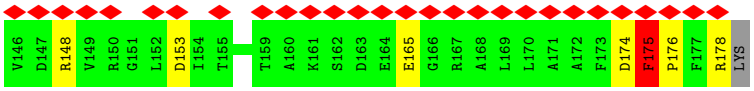


• Molecule 9: 50S ribosomal protein L5

Chain S:

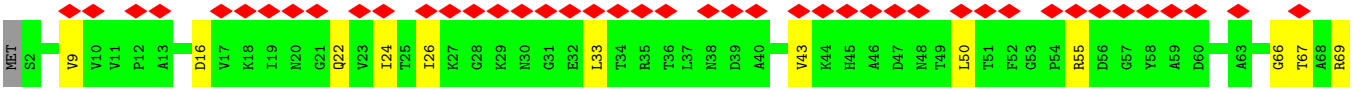


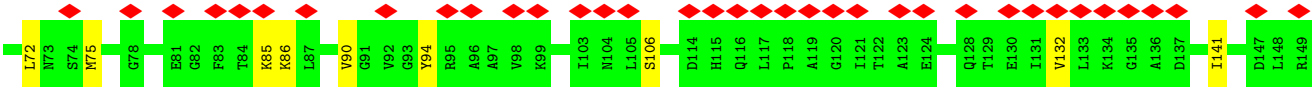


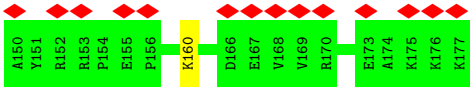


• Molecule 10: 50S ribosomal protein L6

Chain T:

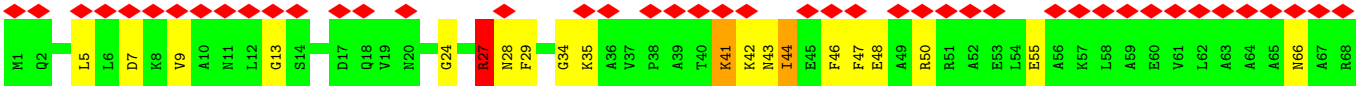


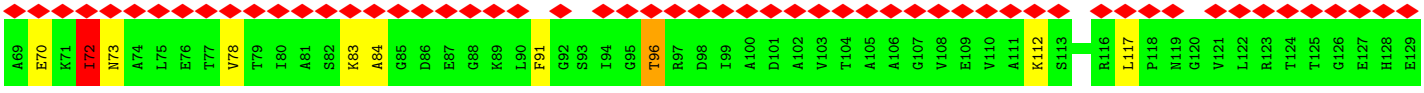


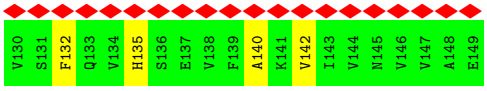


• Molecule 11: 50S ribosomal protein L9

Chain U:

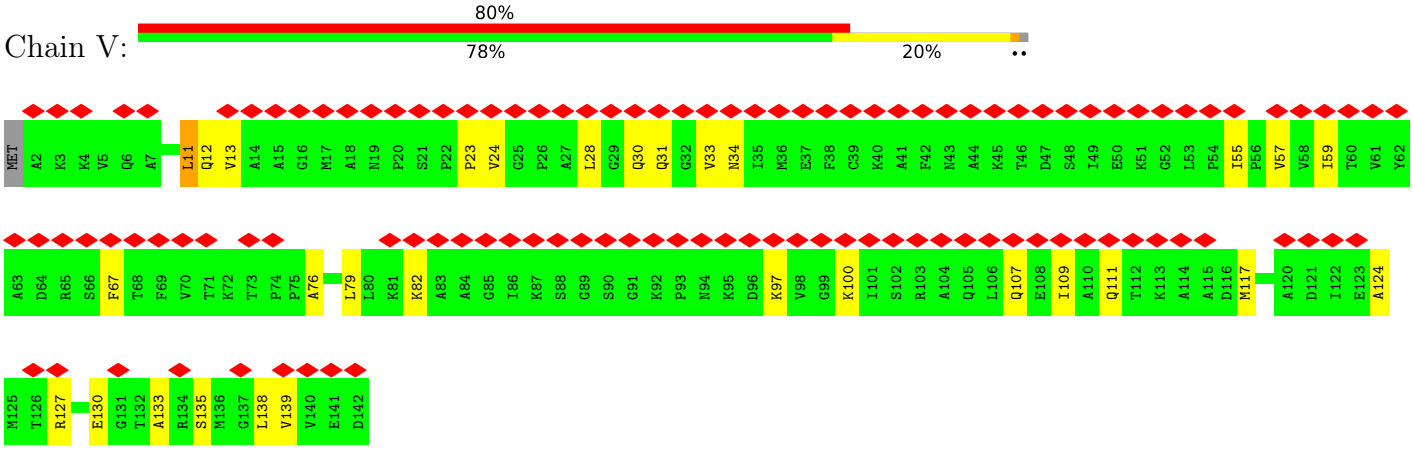






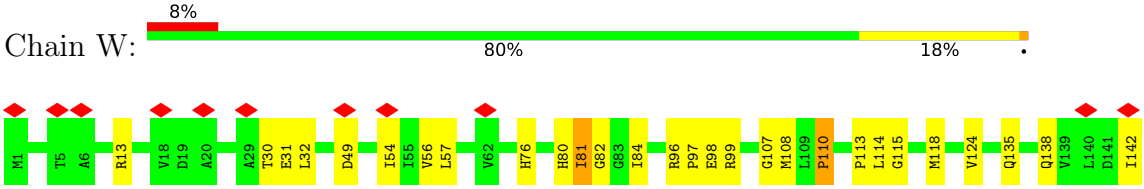
• Molecule 12: 50S ribosomal protein L11

Chain V:



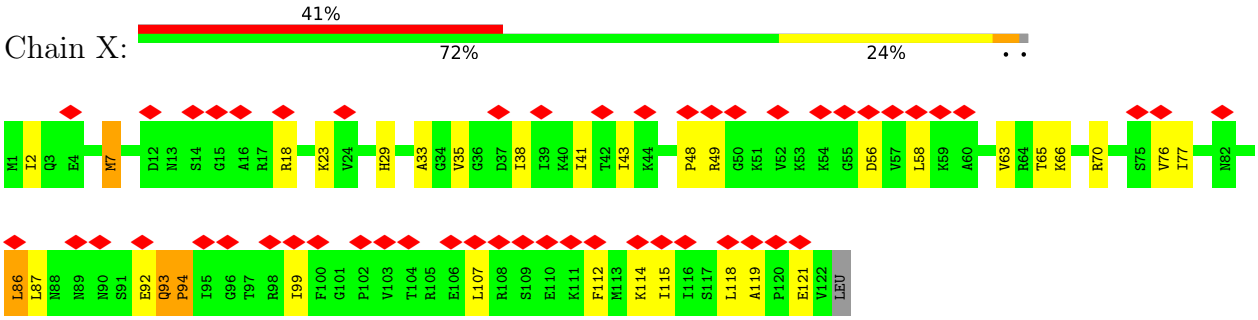
• Molecule 13: 50S ribosomal protein L13

Chain W:



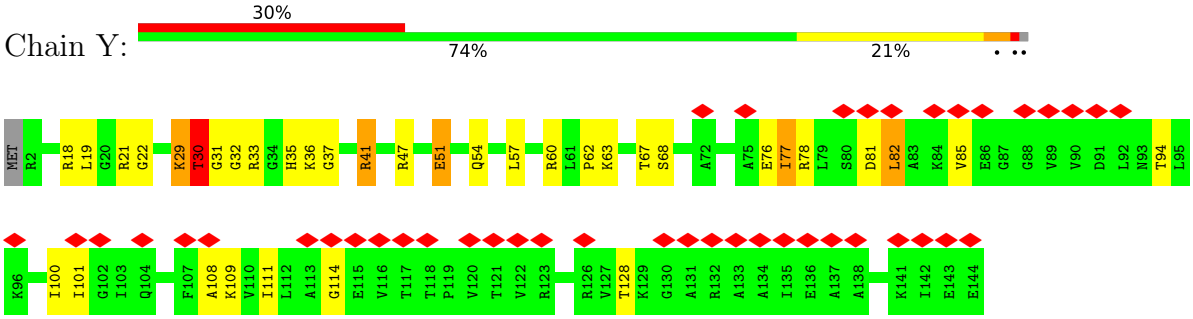
• Molecule 14: 50S ribosomal protein L14

Chain X:



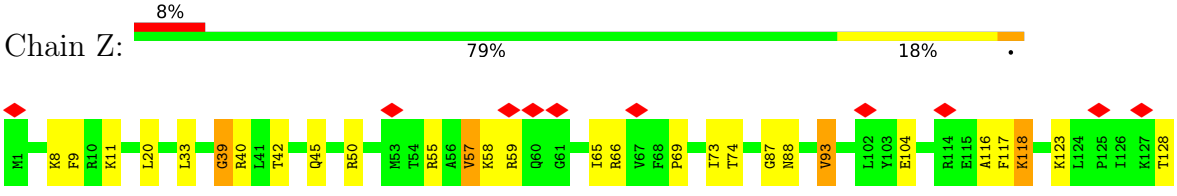
• Molecule 15: 50S ribosomal protein L15

Chain Y:



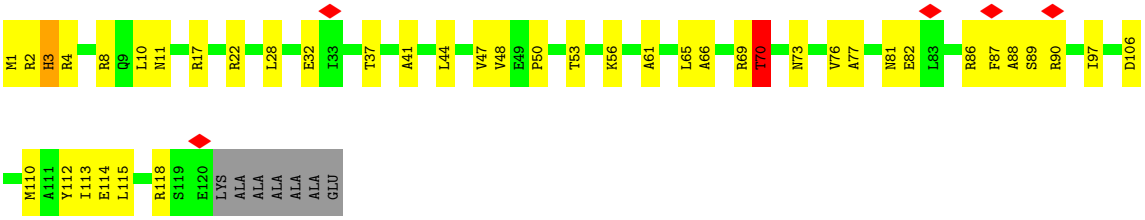
• Molecule 16: 50S ribosomal protein L16

Chain Z:



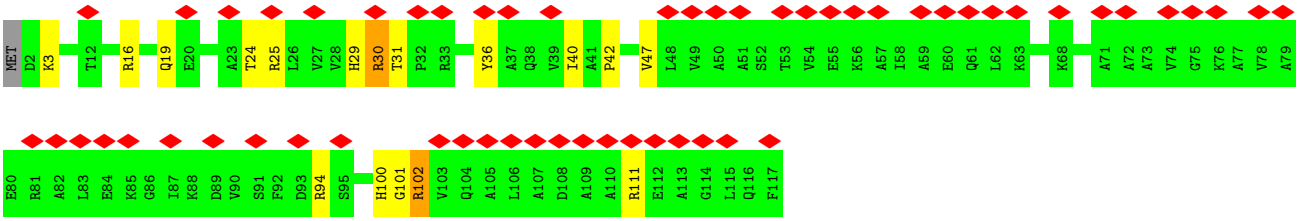
• Molecule 17: Ribosomal protein L17

Chain a:



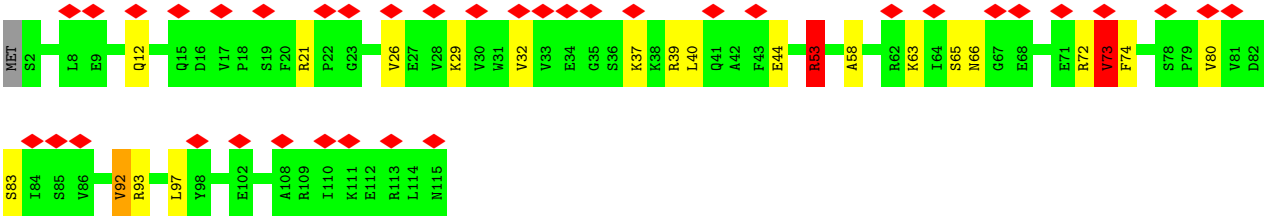
• Molecule 18: 50S ribosomal protein L18

Chain b:



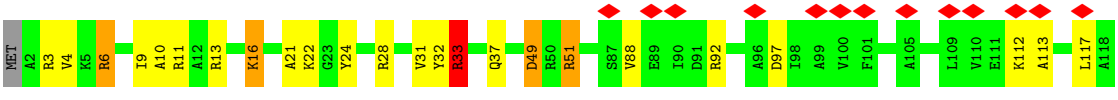
• Molecule 19: 50S ribosomal protein L19

Chain c:



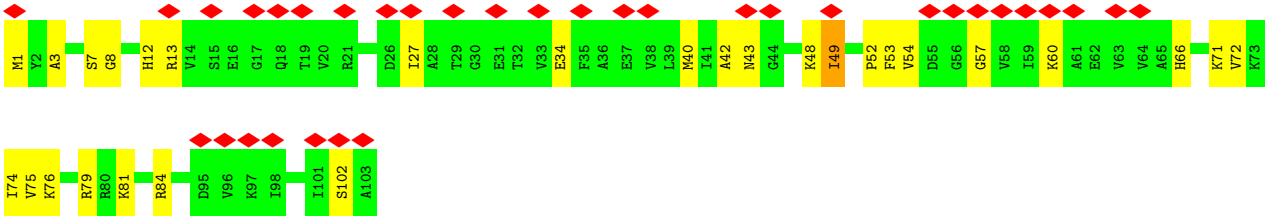
• Molecule 20: 50S ribosomal protein L20

Chain d:

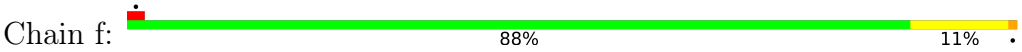


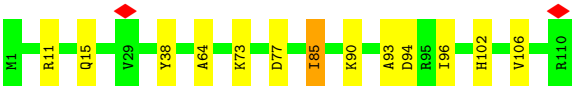
• Molecule 21: 50S ribosomal protein L21

Chain e:

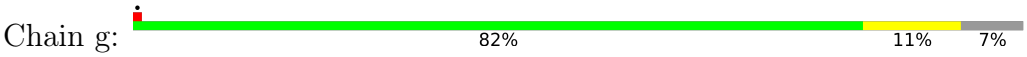


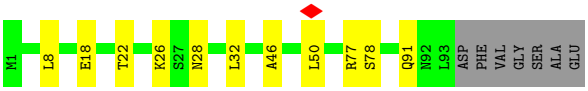
• Molecule 22: 50S ribosomal protein L22



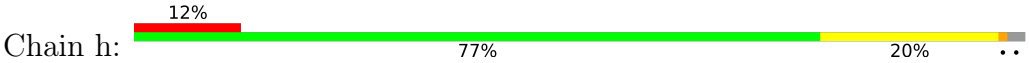


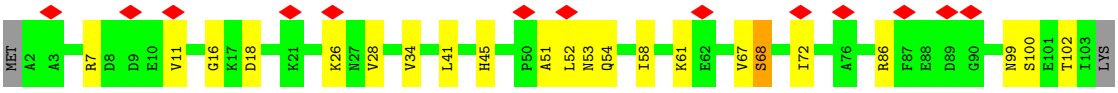
• Molecule 23: 50S ribosomal protein L23



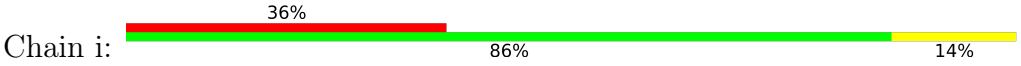


• Molecule 24: 50S ribosomal protein L24

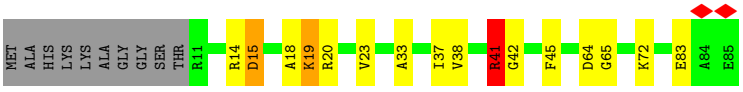




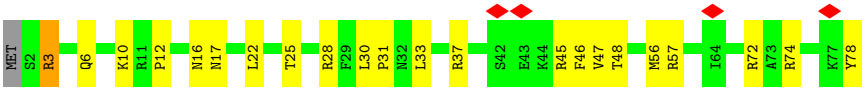
• Molecule 25: 50S ribosomal protein L25



• Molecule 26: 50S ribosomal protein L27

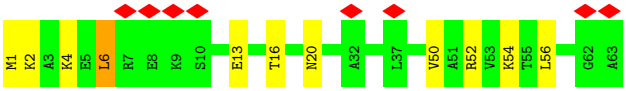


• Molecule 27: 50S ribosomal protein L28



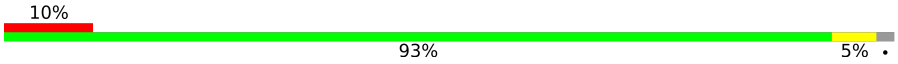
• Molecule 28: 50S ribosomal protein L29

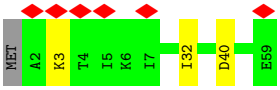
Chain l:



• Molecule 29: 50S ribosomal protein L30

Chain m:



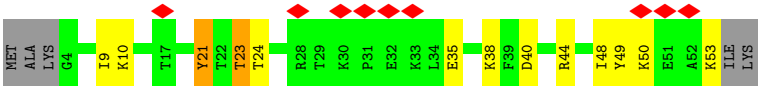


• Molecule 30: 50S ribosomal protein L32

Chain n:

• Molecule 31: 50S ribosomal protein L33

Chain o:

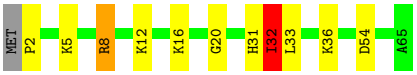


• Molecule 32: 50S ribosomal protein L34

Chain p:

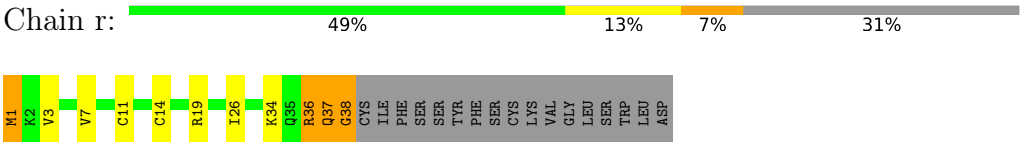
• Molecule 33: 50S ribosomal protein L35

Chain q:



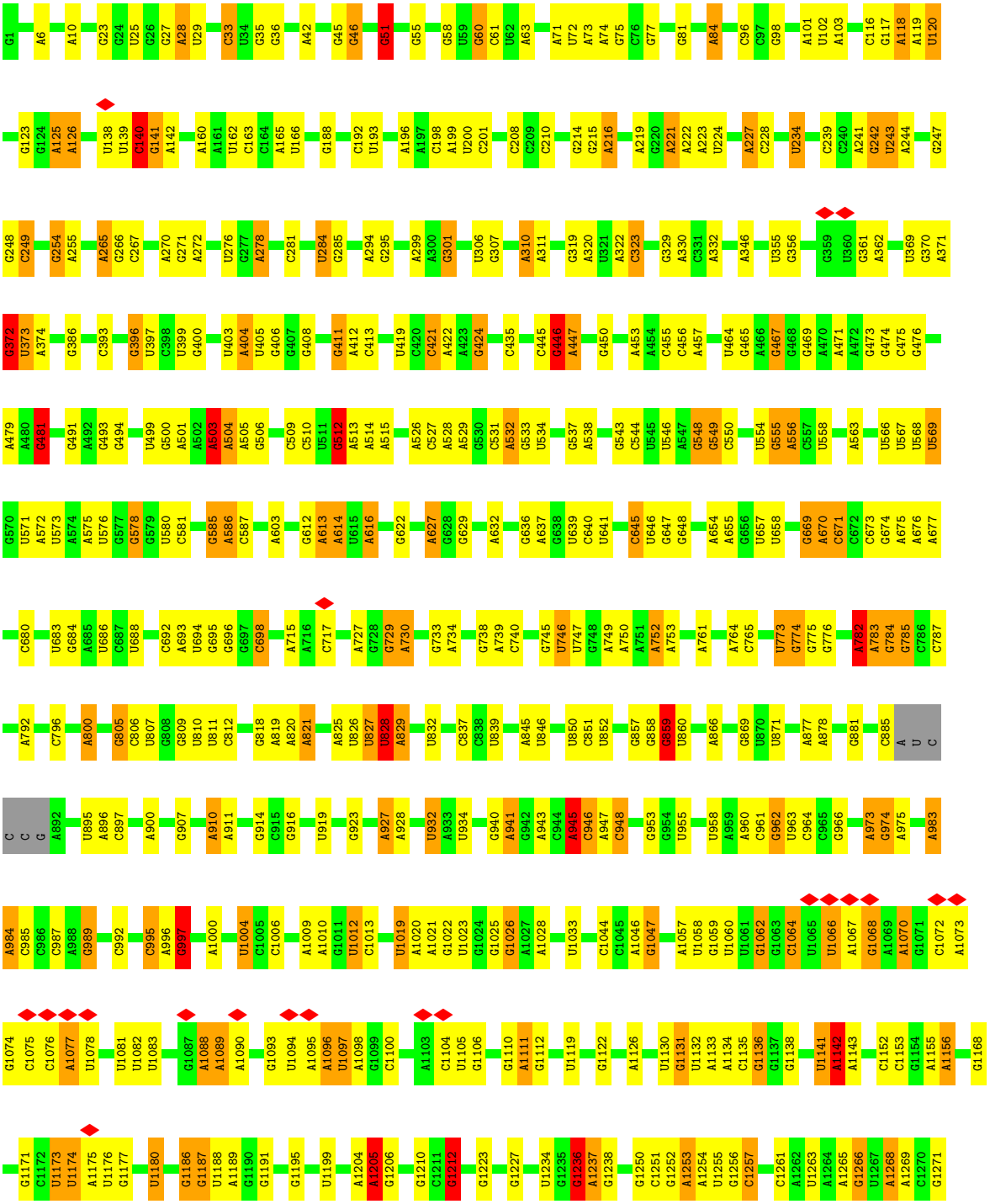
• Molecule 34: 50S ribosomal protein L36

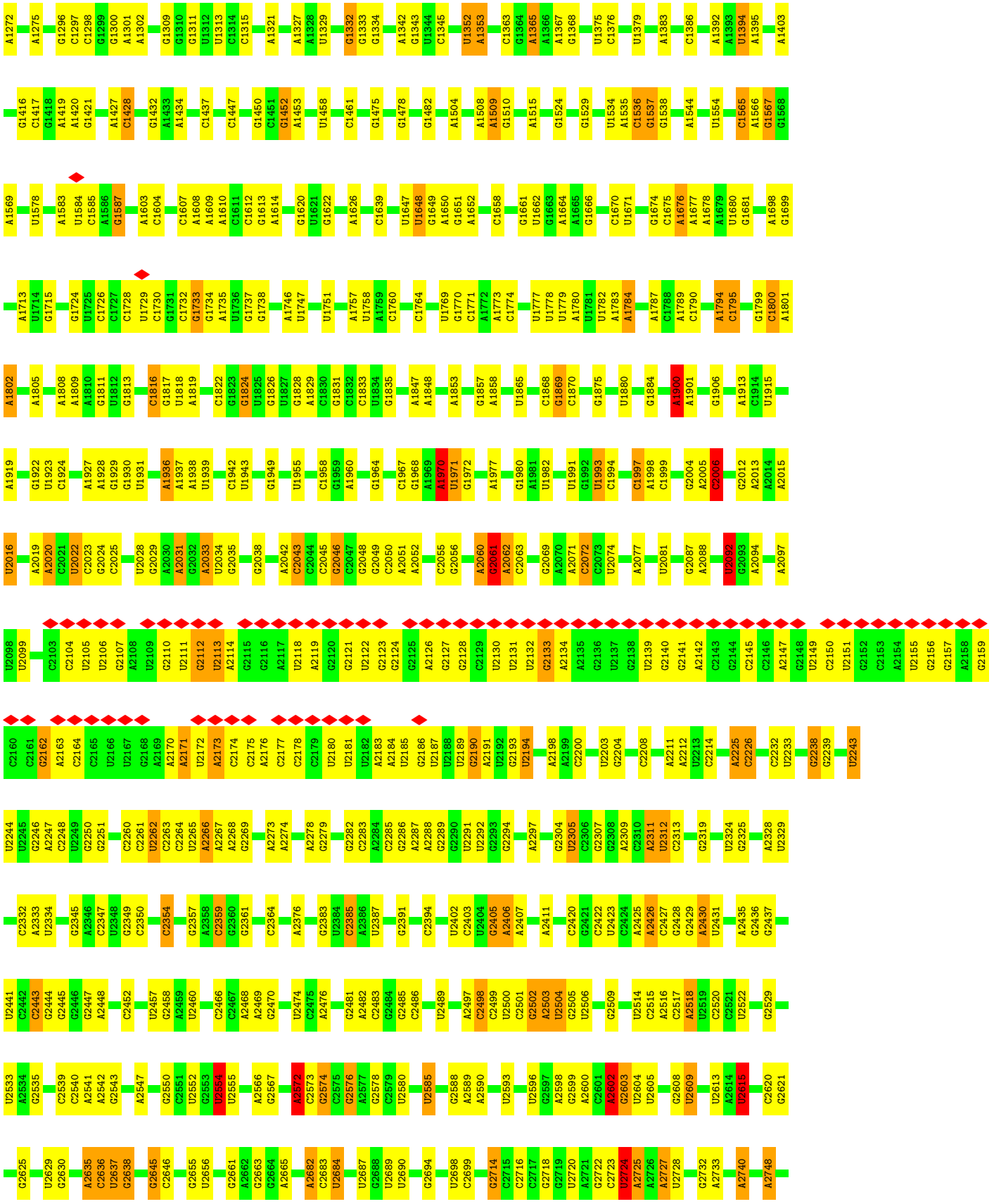
Chain r:

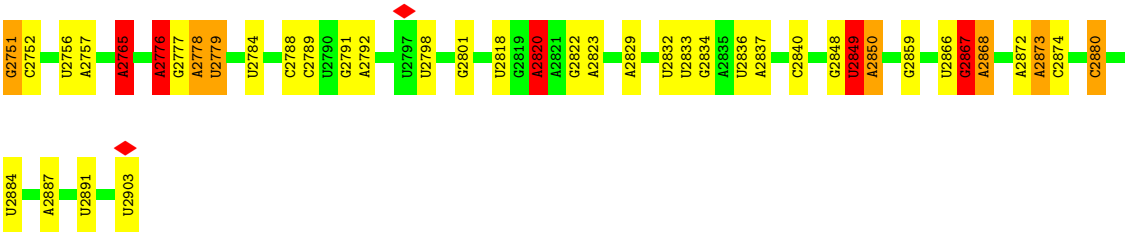


• Molecule 35: 23S rRNA

Chain N:





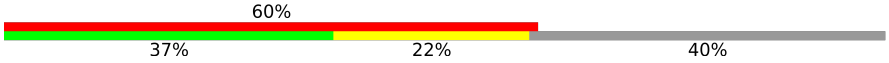


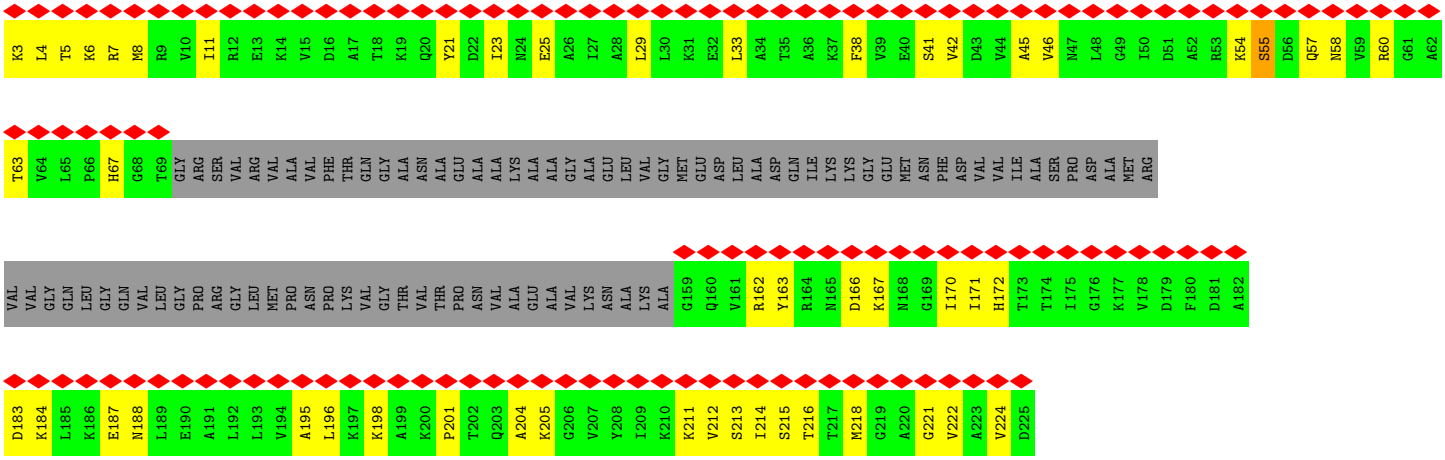
• Molecule 36: 50S ribosomal protein L31

Chain L:

• Molecule 37: 50S ribosomal protein L1

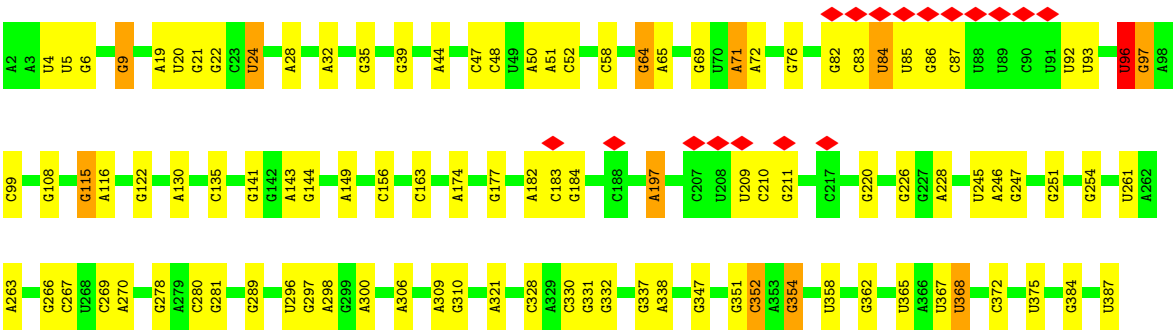
Chain C:

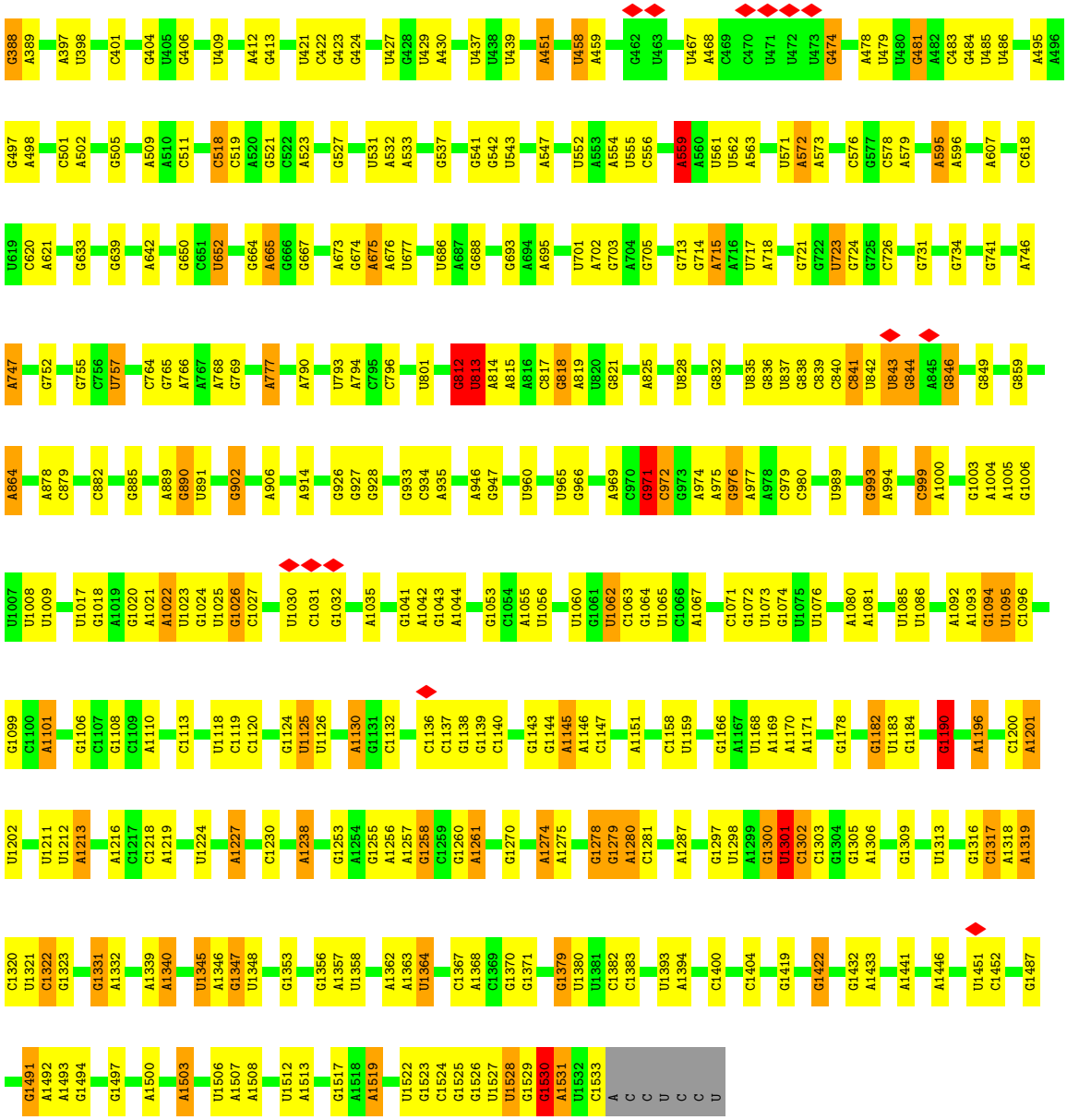




• Molecule 38: 16S rRNA

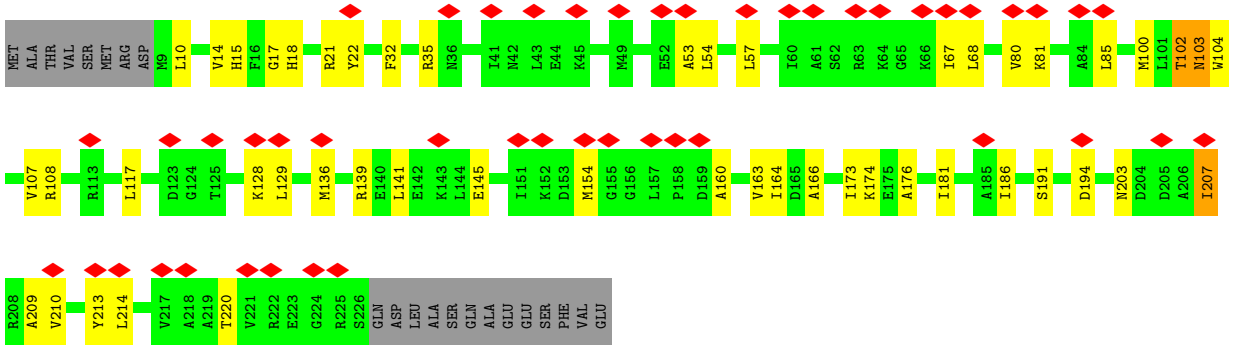
Chain 0:





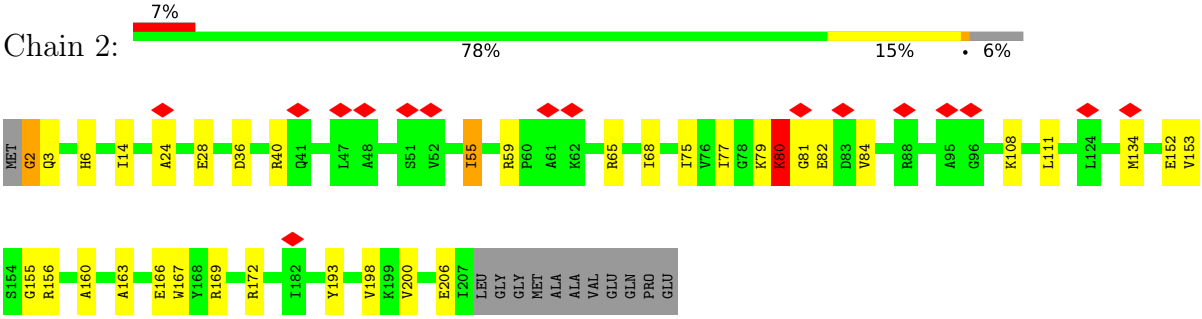
- Molecule 39: 30S ribosomal protein S2

Chain 1:



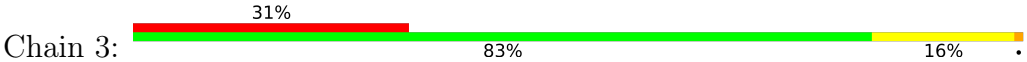
• Molecule 40: 30S ribosomal protein S3

Chain 2:



• Molecule 41: 30S ribosomal protein S4

Chain 3:



• Molecule 42: 30S ribosomal protein S5

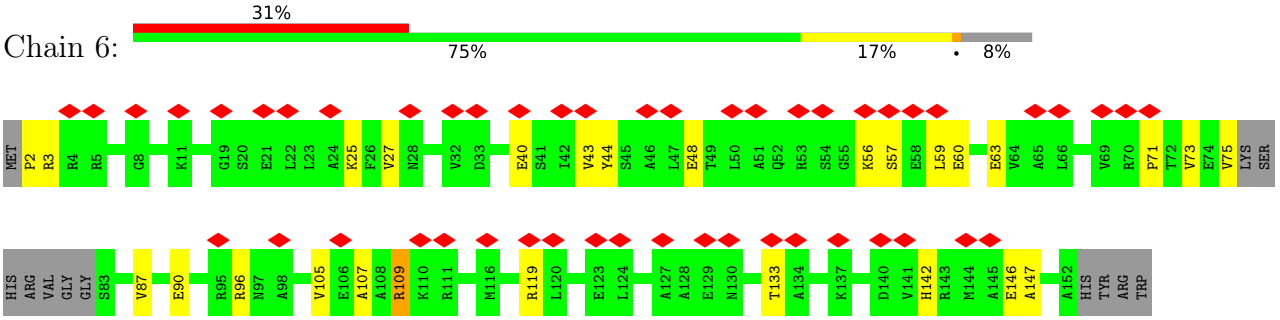
Chain 4:

• Molecule 43: 30S ribosomal protein S6

Chain 5:

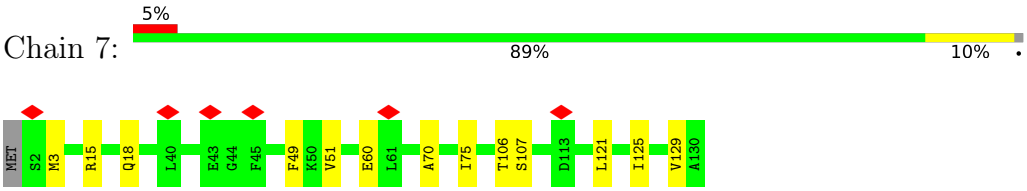
• Molecule 44: Ribosomal protein S7

Chain 6:



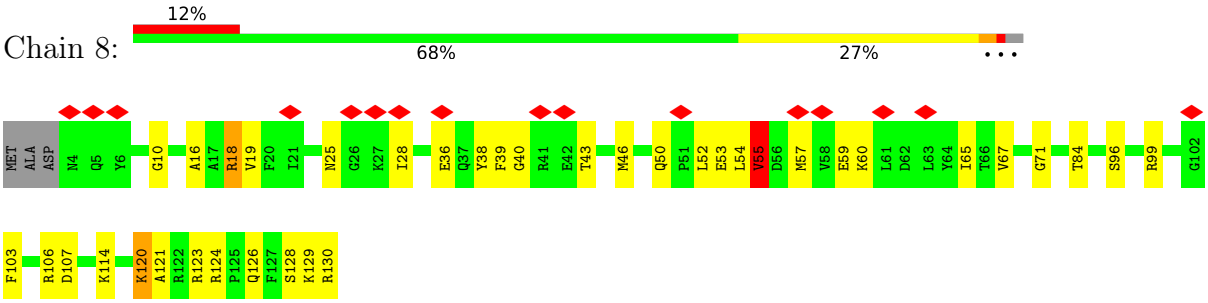
• Molecule 45: 30S ribosomal protein S8

Chain 7:



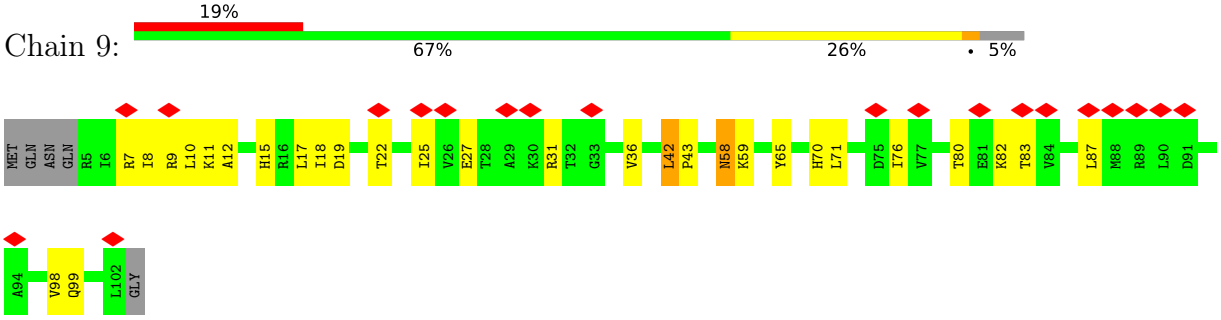
• Molecule 46: 30S ribosomal protein S9

Chain 8:



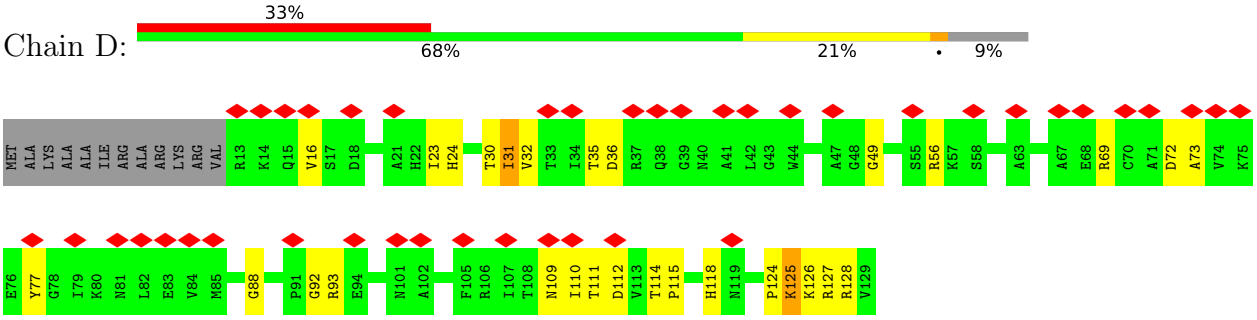
• Molecule 47: 30S ribosomal protein S10

Chain 9:



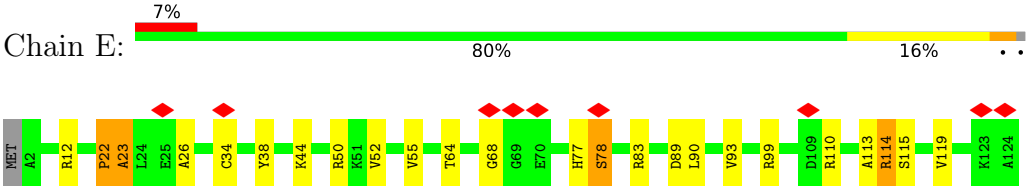
• Molecule 48: 30S ribosomal protein S11

Chain D:



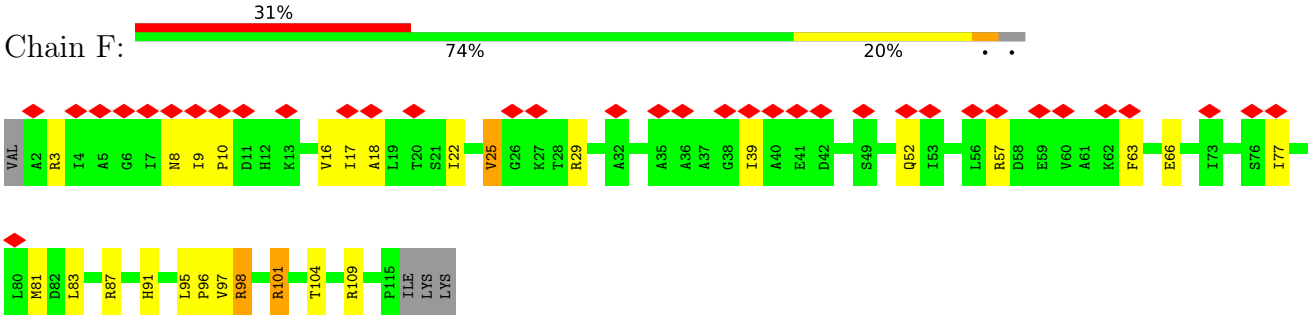
• Molecule 49: 30S ribosomal protein S12

Chain E:



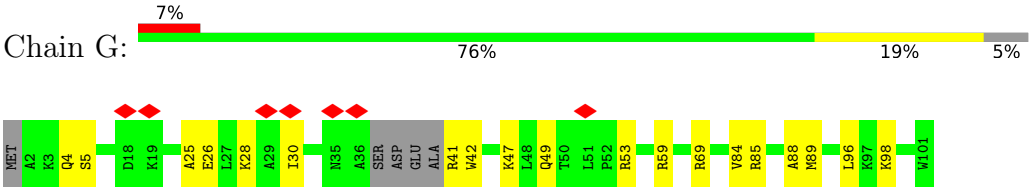
• Molecule 50: 30S ribosomal protein S13

Chain F:



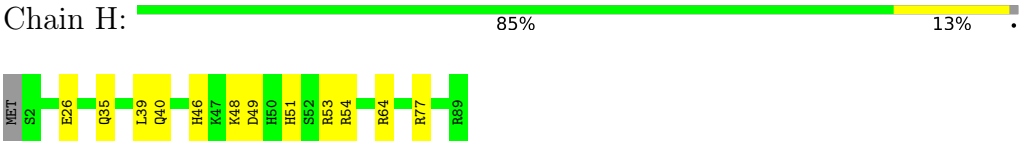
• Molecule 51: 30S ribosomal protein S14

Chain G:



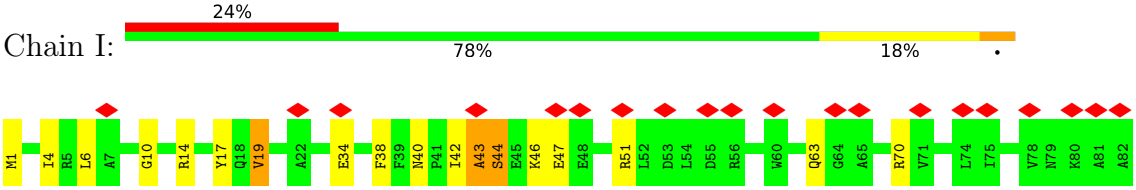
• Molecule 52: 30S ribosomal protein S15

Chain H:



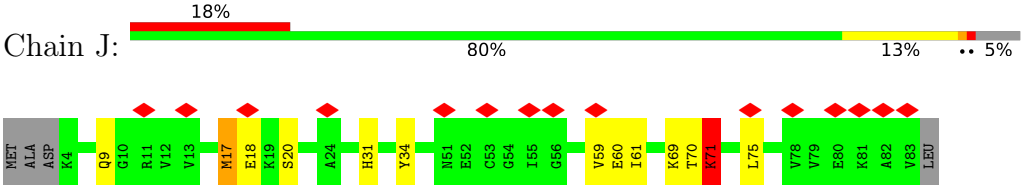
• Molecule 53: 30S ribosomal protein S16

Chain I:



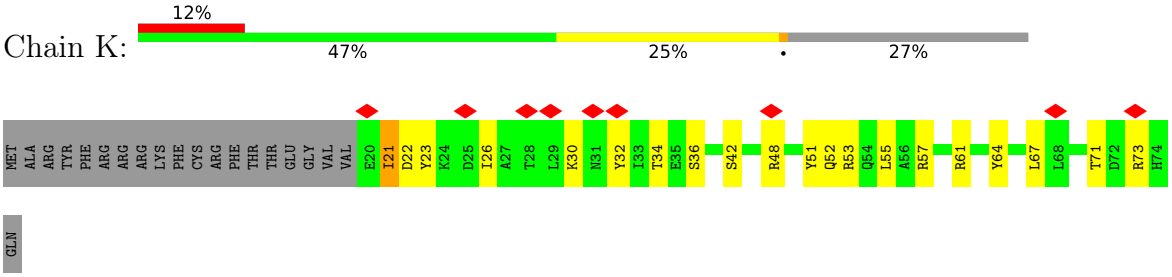
• Molecule 54: 30S ribosomal protein S17

Chain J:



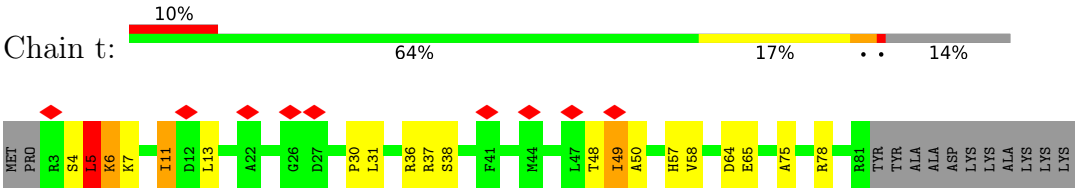
• Molecule 55: 30S ribosomal protein S18

Chain K:



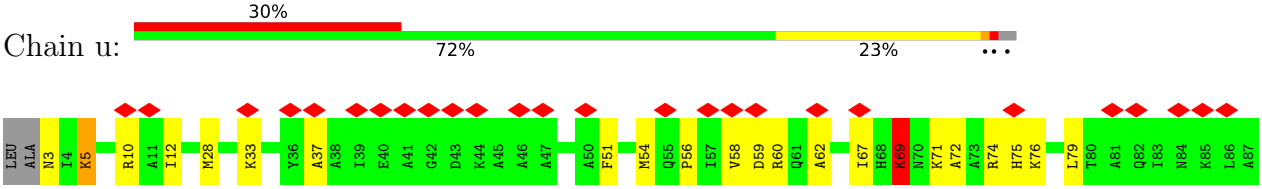
• Molecule 56: 30S ribosomal protein S19

Chain t:



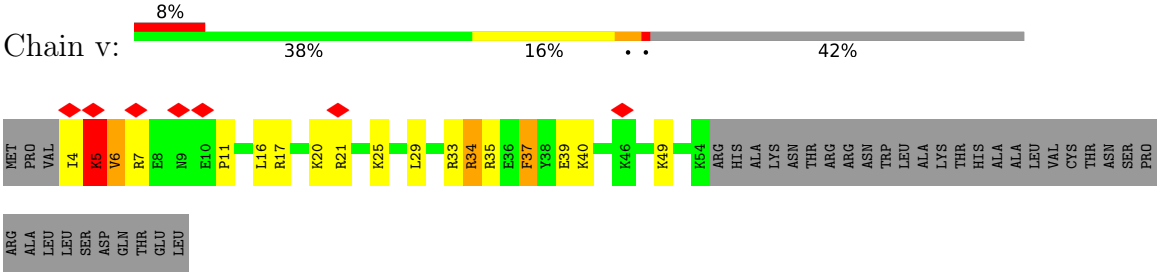
• Molecule 57: 30S ribosomal protein S20

Chain u:



• Molecule 58: 30S ribosomal protein S21

Chain v:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	32412	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 ($e^-/Å^2$)	42.4	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.782	Depositor
Minimum map value	-0.457	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.141	Depositor
Recommended contour level	0.45	Depositor
Map size (Å)	476.55002, 476.55002, 476.55002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.059, 1.059, 1.059	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	A	0.51	0/1744	0.72	0/2716
2	B	0.43	0/193	0.82	0/268
3	s	0.96	1/326 (0.3%)	0.92	0/441
4	M	0.51	0/1779	0.77	3/2768 (0.1%)
5	O	0.65	1/2828 (0.0%)	0.83	7/4410 (0.2%)
6	P	1.72	39/2121 (1.8%)	1.42	17/2852 (0.6%)
7	Q	1.54	14/1585 (0.9%)	1.29	10/2134 (0.5%)
8	R	1.21	8/1571 (0.5%)	1.09	5/2113 (0.2%)
9	S	0.84	0/1434	0.89	0/1926
10	T	0.83	0/1342	0.87	0/1816
11	U	0.68	1/1122 (0.1%)	1.02	3/1515 (0.2%)
12	V	0.76	0/1045	0.74	0/1410
13	W	1.42	10/1151 (0.9%)	1.10	0/1551
14	X	1.53	8/947 (0.8%)	1.28	4/1268 (0.3%)
15	Y	1.65	14/1053 (1.3%)	1.44	7/1403 (0.5%)
16	Z	1.42	4/1092 (0.4%)	1.20	2/1460 (0.1%)
17	a	1.65	11/973 (1.1%)	1.35	5/1301 (0.4%)
18	b	1.05	2/901 (0.2%)	1.04	5/1209 (0.4%)
19	c	1.38	4/927 (0.4%)	1.21	4/1240 (0.3%)
20	d	1.57	7/959 (0.7%)	1.32	8/1278 (0.6%)
21	e	1.39	6/828 (0.7%)	1.21	1/1107 (0.1%)
22	f	1.33	2/864 (0.2%)	1.14	1/1156 (0.1%)
23	g	1.22	0/744	1.10	0/994
24	h	1.00	1/787 (0.1%)	1.06	0/1051
25	i	0.96	0/765	0.90	0/1025
26	j	1.50	5/575 (0.9%)	1.37	6/762 (0.8%)
27	k	1.35	1/634 (0.2%)	1.16	2/848 (0.2%)
28	l	0.89	0/509	1.00	1/677 (0.1%)
29	m	1.18	0/452	1.14	1/605 (0.2%)
30	n	1.48	2/449 (0.4%)	1.40	6/599 (1.0%)
31	o	1.45	5/416 (1.2%)	1.02	0/554
32	p	1.73	5/379 (1.3%)	1.61	5/498 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	q	1.50	0/512	1.35	2/676 (0.3%)
34	r	1.43	3/302 (1.0%)	1.34	3/397 (0.8%)
35	N	0.95	272/69681 (0.4%)	0.95	169/108706 (0.2%)
36	L	0.77	0/426	0.90	1/570 (0.2%)
37	C	0.32	0/1034	0.81	1/1387 (0.1%)
38	0	0.76	27/36809 (0.1%)	0.85	48/57423 (0.1%)
39	1	1.01	1/1735 (0.1%)	1.00	2/2338 (0.1%)
40	2	1.08	4/1651 (0.2%)	0.97	3/2225 (0.1%)
41	3	0.95	2/1664 (0.1%)	1.02	2/2227 (0.1%)
42	4	1.53	6/1118 (0.5%)	1.35	8/1504 (0.5%)
43	5	1.16	5/835 (0.6%)	1.14	3/1128 (0.3%)
44	6	0.83	0/1142	0.86	1/1532 (0.1%)
45	7	1.15	1/988 (0.1%)	1.04	0/1326
46	8	1.09	1/1033 (0.1%)	1.13	2/1375 (0.1%)
47	9	0.94	1/796 (0.1%)	1.02	2/1077 (0.2%)
48	D	1.11	0/892	1.12	3/1205 (0.2%)
49	E	1.37	5/968 (0.5%)	1.25	3/1300 (0.2%)
50	F	1.09	1/892 (0.1%)	1.07	0/1193
51	G	1.09	0/784	1.14	0/1043
52	H	1.20	2/717 (0.3%)	1.03	1/959 (0.1%)
53	I	1.18	3/658 (0.5%)	1.19	5/884 (0.6%)
54	J	1.08	1/657 (0.2%)	1.06	1/881 (0.1%)
55	K	1.20	0/462	1.15	1/621 (0.2%)
56	t	1.02	1/652 (0.2%)	1.00	1/877 (0.1%)
57	u	1.19	2/670 (0.3%)	1.20	2/888 (0.2%)
58	v	1.24	5/430 (1.2%)	1.27	3/570 (0.5%)
All	All	0.99	494/160003 (0.3%)	0.97	370/239267 (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	B	0	1
6	P	0	3
7	Q	0	1
9	S	0	2
11	U	0	1
12	V	0	1
15	Y	0	2
16	Z	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
24	h	0	1
33	q	0	1
35	N	0	6
38	0	0	5
39	1	0	2
40	2	0	2
42	4	0	5
43	5	0	2
46	8	0	4
48	D	0	1
49	E	0	2
54	J	0	2
56	t	0	1
57	u	0	1
58	v	0	1
All	All	0	49

All (494) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	2502	G	P-OP2	14.15	1.77	1.49
35	N	1156	A	P-OP2	12.94	1.74	1.49
35	N	1333	G	P-OP2	10.91	1.70	1.49
35	N	783	A	P-OP2	10.79	1.70	1.49
42	4	127	ALA	C-O	-10.63	1.10	1.23
6	P	221	ARG	CA-C	-10.46	1.38	1.53
35	N	945	A	P-OP2	10.43	1.69	1.49
35	N	1639	C	P-OP1	10.30	1.69	1.49
15	Y	51	GLU	C-O	10.19	1.37	1.23
35	N	1664	A	P-OP2	10.09	1.69	1.49
6	P	219	THR	C-O	10.06	1.35	1.24
35	N	945	A	P-OP1	10.06	1.69	1.49
35	N	1670	C	P-OP1	9.81	1.68	1.49
35	N	2074	U	P-OP1	9.69	1.68	1.49
49	E	23	ALA	N-CA	9.69	1.58	1.46
6	P	213	TRP	CD2-CE2	9.67	1.57	1.41
17	a	2	ARG	C-O	-9.64	1.11	1.24
43	5	63	ASN	C-O	-9.39	1.09	1.23
35	N	2588	G	P-OP1	9.36	1.67	1.49
35	N	2005	A	P-OP1	9.11	1.67	1.49
35	N	450	G	P-OP2	9.03	1.67	1.49
35	N	827	U	P-OP1	9.03	1.67	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	o	50	LYS	C-O	-8.83	1.14	1.24
35	N	943	A	P-OP2	8.77	1.66	1.49
35	N	828	U	O3'-P	-8.74	1.48	1.61
57	u	5	LYS	C-O	-8.70	1.17	1.24
35	N	2349	G	O3'-P	-8.63	1.48	1.61
35	N	2025	C	P-OP2	8.59	1.66	1.49
35	N	2445	G	O3'-P	-8.57	1.48	1.61
35	N	567	U	P-OP1	8.51	1.66	1.49
38	0	578	C	P-OP1	8.47	1.65	1.49
35	N	800	A	P-OP1	8.47	1.65	1.49
6	P	213	TRP	CA-C	-8.45	1.39	1.52
35	N	963	U	O3'-P	-8.32	1.48	1.61
7	Q	162	ALA	CA-C	-8.29	1.41	1.52
6	P	48	ARG	C-O	-8.29	1.13	1.23
34	r	38	GLY	N-CA	8.24	1.58	1.45
35	N	1604	C	P-OP1	8.24	1.65	1.49
38	0	21	G	P-OP1	8.23	1.65	1.49
35	N	2615	U	P-OP1	8.22	1.65	1.49
35	N	2589	A	O3'-P	-8.19	1.48	1.61
35	N	1777	U	O3'-P	-8.19	1.48	1.61
35	N	1774	C	P-OP1	8.18	1.65	1.49
8	R	80	SER	C-O	-8.11	1.11	1.23
35	N	2502	G	O5'-C5'	-8.08	1.30	1.42
35	N	2060	A	O3'-P	-8.08	1.49	1.61
38	0	757	U	O3'-P	-8.03	1.49	1.61
15	Y	22	GLY	C-O	-8.02	1.11	1.23
6	P	238	ARG	C-O	8.00	1.34	1.24
35	N	963	U	P-OP1	7.93	1.64	1.49
35	N	1828	G	P-OP2	7.91	1.64	1.49
6	P	204	VAL	CA-C	-7.90	1.42	1.52
35	N	782	A	O3'-P	-7.89	1.49	1.61
35	N	692	C	O3'-P	-7.85	1.49	1.61
35	N	787	C	O3'-P	-7.85	1.49	1.61
35	N	1968	G	O3'-P	-7.84	1.49	1.61
15	Y	62	PRO	C-O	7.84	1.33	1.23
38	0	20	U	O3'-P	-7.84	1.49	1.61
35	N	576	U	P-OP1	7.83	1.64	1.49
42	4	30	ILE	C-O	-7.80	1.16	1.24
35	N	825	A	O3'-P	-7.80	1.49	1.61
6	P	230	HIS	CA-C	-7.79	1.43	1.52
35	N	2687	U	O3'-P	-7.78	1.49	1.61
35	N	1009	A	O3'-P	-7.78	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	18	ARG	CZ-NH1	7.74	1.43	1.32
35	N	585	G	O3'-P	-7.71	1.49	1.61
35	N	948	C	P-OP1	7.70	1.64	1.49
35	N	1269	A	P-OP2	7.70	1.64	1.49
35	N	1257	C	O3'-P	-7.59	1.49	1.61
6	P	11	PRO	N-CA	7.48	1.56	1.47
35	N	2588	G	P-OP2	7.44	1.63	1.49
35	N	809	G	O3'-P	-7.43	1.50	1.61
35	N	2019	A	O3'-P	-7.42	1.50	1.61
35	N	2025	C	O3'-P	-7.41	1.50	1.61
35	N	554	U	O3'-P	-7.41	1.50	1.61
35	N	2543	G	P-OP1	7.39	1.63	1.49
35	N	2593	U	O3'-P	-7.38	1.50	1.61
35	N	116	C	O3'-P	-7.36	1.50	1.61
35	N	2550	G	O3'-P	-7.34	1.50	1.61
13	W	97	PRO	C-O	7.34	1.33	1.24
35	N	2576	G	P-OP1	7.32	1.63	1.49
32	p	38	GLY	CA-C	-7.32	1.41	1.51
19	c	93	ARG	CD-NE	-7.29	1.36	1.46
35	N	120	U	P-OP1	7.29	1.63	1.49
35	N	445	C	O3'-P	-7.28	1.50	1.61
38	0	667	G	O3'-P	-7.27	1.50	1.61
35	N	984	A	O3'-P	-7.25	1.50	1.61
35	N	1664	A	P-OP1	7.24	1.63	1.49
35	N	2050	C	O3'-P	-7.24	1.50	1.61
38	0	882	C	O3'-P	-7.23	1.50	1.61
35	N	2714	G	P-OP2	7.21	1.63	1.49
15	Y	19	LEU	C-O	7.19	1.32	1.23
6	P	213	TRP	CZ3-CH2	7.18	1.58	1.40
43	5	63	ASN	N-CA	7.18	1.56	1.46
35	N	1375	U	O3'-P	-7.17	1.50	1.61
35	N	1152	C	O3'-P	-7.16	1.50	1.61
18	b	30	ARG	CZ-NH1	7.16	1.42	1.32
35	N	2873	A	C6-N1	-7.14	1.21	1.35
35	N	2588	G	O3'-P	-7.13	1.50	1.61
35	N	673	C	O3'-P	-7.05	1.50	1.61
14	X	86	LEU	C-O	-7.05	1.15	1.24
35	N	397	U	O3'-P	-7.02	1.50	1.61
26	j	14	ARG	C-O	-7.01	1.15	1.23
35	N	2503	A	P-OP2	7.00	1.62	1.49
17	a	47	VAL	C-O	-6.99	1.15	1.23
8	R	77	ILE	CB-CG1	-6.97	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	826	U	P-OP1	6.96	1.62	1.49
7	Q	125	TRP	CA-C	-6.95	1.43	1.52
35	N	2498	C	P-OP2	6.95	1.62	1.49
35	N	859	G	O3'-P	6.94	1.71	1.61
35	N	2022	U	P-OP1	6.92	1.62	1.49
30	n	11	SER	N-CA	-6.91	1.38	1.46
35	N	453	A	P-OP1	6.91	1.62	1.49
35	N	1780	A	P-OP1	6.91	1.62	1.49
35	N	1774	C	O3'-P	-6.91	1.50	1.61
35	N	1019	U	O3'-P	-6.90	1.50	1.61
35	N	2052	A	O3'-P	-6.90	1.50	1.61
49	E	22	PRO	CA-C	6.86	1.62	1.52
54	J	71	LYS	C-O	-6.83	1.15	1.24
6	P	222	GLY	C-O	-6.81	1.14	1.23
35	N	1612	C	O3'-P	-6.80	1.50	1.61
35	N	1658	C	P-OP1	6.80	1.62	1.49
35	N	2635	A	O3'-P	-6.80	1.50	1.61
35	N	2698	U	O3'-P	-6.78	1.50	1.61
35	N	200	U	O3'-P	-6.77	1.50	1.61
6	P	221	ARG	C-O	-6.77	1.15	1.23
17	a	66	ALA	CA-C	-6.75	1.43	1.52
13	W	81	ILE	C-O	6.73	1.32	1.24
6	P	86	ASN	C-O	-6.73	1.15	1.24
35	N	1994	C	O3'-P	-6.71	1.51	1.61
6	P	15	HIS	C-O	-6.71	1.14	1.24
35	N	2006	C	P-OP1	6.68	1.62	1.49
24	h	68	SER	CB-OG	6.68	1.55	1.42
35	N	2466	C	O3'-P	-6.68	1.51	1.61
38	0	812	G	O3'-P	6.67	1.71	1.61
35	N	1658	C	O3'-P	-6.66	1.51	1.61
20	d	49	ASP	CA-C	-6.63	1.43	1.52
35	N	1751	U	O3'-P	-6.63	1.51	1.61
38	0	1500	A	O3'-P	-6.63	1.51	1.61
35	N	2062	A	P-OP2	6.62	1.62	1.49
20	d	49	ASP	C-O	6.62	1.32	1.24
17	a	2	ARG	C-N	-6.61	1.24	1.33
35	N	192	C	P-OP1	6.61	1.62	1.49
35	N	1782	U	P-OP1	6.59	1.62	1.49
35	N	641	U	O3'-P	-6.59	1.51	1.61
35	N	1831	G	O3'-P	-6.59	1.51	1.61
35	N	1900	A	O3'-P	6.59	1.71	1.61
35	N	1993	U	O5'-C5'	-6.58	1.32	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	2740	A	O3'-P	-6.58	1.51	1.61
35	N	955	U	O3'-P	-6.57	1.51	1.61
35	N	2035	G	O5'-C5'	-6.55	1.33	1.42
30	n	10	ARG	CA-C	6.55	1.61	1.52
35	N	2765	A	C6-N1	-6.53	1.22	1.35
19	c	21	ARG	C-O	-6.50	1.18	1.24
35	N	1268	A	P-OP1	6.50	1.61	1.49
6	P	221	ARG	CB-CG	-6.50	1.32	1.52
35	N	1353	A	O3'-P	-6.49	1.51	1.61
35	N	2518	A	P-OP2	6.49	1.61	1.49
14	X	66	LYS	CA-C	-6.46	1.44	1.52
16	Z	39	GLY	C-O	-6.46	1.15	1.23
35	N	810	U	P-OP1	6.44	1.61	1.49
6	P	213	TRP	CB-CG	-6.44	1.30	1.50
35	N	1254	A	O3'-P	-6.43	1.51	1.61
17	a	1	MET	C-O	6.43	1.36	1.23
21	e	79	ARG	C-O	6.41	1.31	1.23
46	8	121	ALA	C-O	-6.41	1.16	1.24
35	N	2605	U	O3'-P	-6.41	1.51	1.61
14	X	7	MET	N-CA	6.40	1.54	1.46
35	N	2489	U	O3'-P	-6.38	1.51	1.61
35	N	2543	G	O5'-C5'	-6.38	1.32	1.42
35	N	2437	G	O3'-P	-6.35	1.51	1.61
6	P	204	VAL	N-CA	-6.35	1.39	1.46
35	N	1970	A	P-OP2	6.34	1.61	1.49
35	N	2264	C	O3'-P	-6.34	1.51	1.61
6	P	234	GLY	C-O	-6.34	1.15	1.23
35	N	2031	A	P-OP1	-6.34	1.36	1.49
35	N	1813	G	O3'-P	-6.34	1.51	1.61
6	P	271	ARG	CZ-NH1	6.33	1.41	1.32
35	N	1678	A	P-OP2	6.32	1.61	1.49
35	N	1828	G	P-OP1	6.32	1.61	1.49
15	Y	62	PRO	CA-CB	-6.30	1.45	1.53
7	Q	126	ASN	CA-C	-6.29	1.45	1.53
35	N	839	U	O3'-P	-6.26	1.51	1.61
35	N	975	A	P-OP2	6.26	1.61	1.49
35	N	2590	A	O3'-P	-6.26	1.51	1.61
49	E	114	ARG	C-O	-6.25	1.16	1.24
35	N	2265	U	O3'-P	-6.23	1.51	1.61
6	P	220	VAL	CA-CB	-6.23	1.46	1.54
19	c	53	ARG	N-CA	-6.23	1.36	1.46
15	Y	41	ARG	CA-C	-6.22	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	p	39	ARG	NE-CZ	6.21	1.39	1.33
35	N	733	G	O3'-P	-6.20	1.51	1.61
38	0	726	C	O3'-P	-6.20	1.51	1.61
35	N	1189	A	O3'-P	-6.20	1.51	1.61
35	N	372	G	O3'-P	6.18	1.70	1.61
35	N	192	C	O3'-P	-6.17	1.51	1.61
20	d	10	ALA	C-O	6.16	1.31	1.24
35	N	1794	A	O3'-P	-6.16	1.51	1.61
7	Q	163	GLY	N-CA	6.16	1.52	1.45
17	a	112	TYR	CA-C	-6.14	1.45	1.52
27	k	22	LEU	C-O	-6.14	1.15	1.23
38	0	24	U	N3-C4	-6.14	1.26	1.38
42	4	24	THR	C-O	-6.14	1.14	1.23
35	N	2447	G	O3'-P	-6.14	1.51	1.61
31	o	10	LYS	C-O	-6.13	1.16	1.24
34	r	37	GLN	CA-C	-6.12	1.44	1.52
35	N	1778	U	O3'-P	-6.12	1.51	1.61
35	N	832	U	O3'-P	-6.11	1.51	1.61
35	N	2572	A	O3'-P	-6.11	1.51	1.61
35	N	572	A	P-OP1	6.10	1.61	1.49
35	N	515	A	O3'-P	-6.10	1.51	1.61
52	H	49	ASP	C-O	6.10	1.31	1.23
35	N	1790	C	O3'-P	-6.09	1.52	1.61
35	N	997	G	O3'-P	-6.09	1.52	1.61
13	W	138	GLN	C-O	-6.07	1.16	1.23
58	v	34	ARG	CZ-NH1	6.06	1.41	1.32
8	R	75	SER	CA-C	-6.04	1.46	1.53
13	W	98	GLU	N-CA	-6.04	1.39	1.46
13	W	107	GLY	C-O	-6.04	1.17	1.24
35	N	569	U	O3'-P	-6.04	1.52	1.61
42	4	24	THR	CA-C	-6.04	1.47	1.53
6	P	10	SER	CA-CB	6.03	1.62	1.53
13	W	84	ILE	CA-C	-6.03	1.46	1.53
58	v	37	PHE	N-CA	6.03	1.53	1.46
35	N	2620	C	O3'-P	-6.02	1.52	1.61
35	N	464	U	O3'-P	-6.02	1.52	1.61
35	N	821	A	O3'-P	-6.02	1.52	1.61
15	Y	37	GLY	C-O	-6.01	1.16	1.23
35	N	1771	C	O3'-P	-6.01	1.52	1.61
35	N	254	G	O3'-P	-6.01	1.52	1.61
35	N	2867	G	O3'-P	6.00	1.70	1.61
35	N	671	C	P-OP2	6.00	1.60	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Y	29	LYS	C-O	5.99	1.31	1.24
35	N	818	G	P-OP2	5.99	1.60	1.49
35	N	2822	G	O3'-P	-5.98	1.52	1.61
6	P	214	ARG	CZ-NH1	5.96	1.41	1.32
38	0	1367	C	O3'-P	-5.95	1.52	1.61
35	N	2406	A	P-OP1	5.95	1.60	1.49
43	5	51	ILE	C-O	-5.95	1.17	1.24
6	P	158	ALA	CA-C	-5.95	1.45	1.52
40	2	3	GLN	N-CA	-5.94	1.39	1.46
35	N	2081	U	O3'-P	-5.94	1.52	1.61
35	N	676	A	O3'-P	-5.94	1.52	1.61
35	N	2025	C	O5'-C5'	-5.94	1.33	1.42
35	N	2385	C	P-OP1	5.93	1.60	1.49
35	N	2499	C	P-OP2	5.93	1.60	1.49
47	9	58	ASN	CA-C	-5.92	1.44	1.52
35	N	2061	G	C2'-O2'	5.92	1.51	1.42
35	N	2625	G	O3'-P	-5.91	1.52	1.61
38	0	1393	U	O3'-P	-5.90	1.52	1.61
15	Y	51	GLU	N-CA	-5.89	1.39	1.46
35	N	2444	G	O3'-P	-5.89	1.52	1.61
35	N	2637	U	O3'-P	-5.89	1.52	1.61
35	N	2072	C	O5'-C5'	-5.88	1.33	1.42
6	P	258	ARG	NE-CZ	-5.86	1.26	1.33
35	N	2359	C	O3'-P	-5.86	1.52	1.61
31	o	48	ILE	C-O	-5.86	1.17	1.24
35	N	566	U	O3'-P	-5.86	1.52	1.61
35	N	538	A	O3'-P	-5.85	1.52	1.61
49	E	23	ALA	C-O	-5.85	1.16	1.24
6	P	235	GLY	C-N	-5.85	1.25	1.33
35	N	2837	A	O3'-P	-5.85	1.52	1.61
34	r	36	ARG	CD-NE	-5.84	1.38	1.46
35	N	2232	C	O3'-P	-5.84	1.52	1.61
35	N	2247	A	O3'-P	-5.83	1.52	1.61
35	N	2072	C	O3'-P	-5.83	1.52	1.61
35	N	730	A	P-OP2	5.83	1.60	1.49
38	0	980	C	P-OP1	5.83	1.60	1.49
35	N	198	C	O3'-P	-5.82	1.52	1.61
35	N	2062	A	O5'-C5'	-5.82	1.34	1.42
42	4	50	TYR	C-O	5.82	1.31	1.24
6	P	235	GLY	CA-C	-5.81	1.43	1.51
35	N	1822	C	O3'-P	-5.81	1.52	1.61
53	I	4	ILE	C-O	-5.81	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	t	6	LYS	N-CA	5.80	1.53	1.46
17	a	106	ASP	N-CA	-5.80	1.40	1.46
35	N	2598	A	O3'-P	-5.79	1.52	1.61
35	N	1824	G	P-OP2	5.79	1.60	1.49
6	P	204	VAL	C-N	-5.77	1.25	1.33
38	0	387	U	O3'-P	-5.76	1.52	1.61
35	N	2457	U	O3'-P	-5.76	1.52	1.61
8	R	62	GLN	N-CA	5.76	1.53	1.46
38	0	22	G	O3'-P	-5.75	1.52	1.61
20	d	51	ARG	CA-CB	-5.74	1.44	1.53
40	2	2	GLY	N-CA	5.74	1.54	1.45
6	P	160	THR	C-O	-5.74	1.16	1.24
35	N	1298	C	O3'-P	-5.73	1.52	1.61
13	W	30	THR	CB-CG2	-5.73	1.33	1.52
35	N	2572	A	P-OP1	-5.73	1.37	1.49
35	N	2268	A	P-OP1	5.72	1.60	1.49
35	N	2684	U	O3'-P	-5.72	1.52	1.61
14	X	65	THR	C-O	-5.72	1.16	1.23
35	N	1805	A	O3'-P	-5.72	1.52	1.61
35	N	2013	A	O3'-P	-5.72	1.52	1.61
35	N	2542	A	O3'-P	-5.71	1.52	1.61
35	N	2602	A	O3'-P	5.71	1.69	1.61
35	N	1261	C	O3'-P	-5.71	1.52	1.61
35	N	783	A	C4'-O4'	5.70	1.54	1.45
14	X	23	LYS	CA-C	-5.70	1.45	1.52
8	R	81	GLY	C-N	-5.70	1.25	1.33
35	N	940	G	O3'-P	-5.70	1.52	1.61
35	N	126	A	O3'-P	-5.69	1.52	1.61
35	N	578	G	P-OP2	5.69	1.60	1.49
7	Q	164	GLN	C-O	5.68	1.30	1.24
35	N	966	G	O3'-P	-5.68	1.52	1.61
35	N	1662	U	P-OP2	5.68	1.60	1.49
35	N	796	C	O3'-P	-5.67	1.52	1.61
32	p	34	ARG	CG-CD	-5.66	1.35	1.52
35	N	1681	G	O3'-P	-5.66	1.52	1.61
31	o	23	THR	C-O	-5.66	1.20	1.24
35	N	29	U	O3'-P	-5.66	1.52	1.61
35	N	2016	U	O3'-P	-5.66	1.52	1.61
38	0	814	A	P-OP2	5.65	1.60	1.49
38	0	505	G	O3'-P	-5.65	1.52	1.61
26	j	42	GLY	N-CA	5.65	1.55	1.45
53	I	10	GLY	N-CA	5.64	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	a	17	ARG	C-O	5.64	1.30	1.24
16	Z	93	VAL	CA-CB	5.63	1.63	1.54
35	N	25	U	O3'-P	-5.63	1.52	1.61
35	N	2499	C	P-OP1	5.62	1.60	1.49
35	N	571	U	O3'-P	-5.62	1.52	1.61
52	H	51	HIS	C-O	5.62	1.30	1.24
14	X	41	ILE	C-O	-5.62	1.17	1.23
5	O	83	G	O3'-P	-5.61	1.52	1.61
35	N	2049	G	O3'-P	-5.60	1.52	1.61
35	N	1795	C	O3'-P	-5.60	1.52	1.61
16	Z	11	LYS	C-O	-5.59	1.17	1.24
35	N	761	A	P-OP1	5.59	1.60	1.49
35	N	773	U	O3'-P	-5.57	1.52	1.61
13	W	110	PRO	CA-C	-5.57	1.45	1.52
35	N	2072	C	P-OP1	5.56	1.60	1.49
13	W	80	HIS	CA-C	-5.56	1.45	1.53
7	Q	162	ALA	C-O	-5.55	1.17	1.23
35	N	1009	A	P-OP2	5.55	1.60	1.49
35	N	2829	A	O3'-P	-5.55	1.52	1.61
6	P	205	LEU	N-CA	5.54	1.53	1.46
35	N	680	C	O3'-P	-5.54	1.52	1.61
35	N	2436	G	O3'-P	-5.54	1.52	1.61
35	N	393	C	P-OP1	5.53	1.60	1.49
49	E	113	ALA	CA-C	-5.53	1.46	1.53
35	N	1949	G	O3'-P	-5.52	1.52	1.61
35	N	2332	C	O3'-P	-5.52	1.52	1.61
38	0	765	G	O3'-P	-5.52	1.52	1.61
35	N	1010	A	P-OP2	5.51	1.59	1.49
7	Q	126	ASN	N-CA	5.51	1.54	1.46
43	5	99	ALA	CA-C	5.51	1.56	1.52
35	N	2051	A	O3'-P	5.49	1.69	1.61
38	0	764	C	O3'-P	-5.49	1.52	1.61
35	N	2248	C	P-OP2	5.49	1.59	1.49
35	N	784	G	O3'-P	5.48	1.69	1.61
7	Q	109	VAL	C-O	-5.48	1.18	1.24
40	2	166	GLU	C-O	-5.47	1.17	1.24
35	N	1186	G	P-OP2	5.47	1.59	1.49
6	P	239	ASN	CA-C	5.47	1.60	1.52
14	X	114	LYS	C-O	-5.45	1.17	1.24
35	N	1255	U	O5'-C5'	-5.45	1.34	1.42
15	Y	35	HIS	CA-C	-5.44	1.45	1.53
20	d	32	TYR	C-N	-5.43	1.25	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	688	U	O3'-P	-5.43	1.53	1.61
6	P	198	ALA	C-O	5.43	1.30	1.24
43	5	62	MET	C-N	-5.42	1.27	1.33
21	e	12	HIS	C-O	5.41	1.30	1.23
6	P	155	ALA	CA-C	-5.39	1.47	1.53
35	N	1671	U	P-OP2	5.39	1.59	1.49
35	N	1394	U	O3'-P	-5.39	1.53	1.61
35	N	2243	U	P-OP1	5.39	1.59	1.49
41	3	123	ILE	C-O	-5.39	1.18	1.24
35	N	2516	A	O3'-P	-5.37	1.53	1.61
21	e	75	VAL	C-O	-5.37	1.18	1.24
35	N	419	U	O3'-P	-5.37	1.53	1.61
7	Q	126	ASN	C-O	-5.36	1.16	1.23
26	j	15	ASP	N-CA	-5.36	1.39	1.45
35	N	923	G	O3'-P	-5.35	1.53	1.61
32	p	34	ARG	C-O	-5.35	1.17	1.24
35	N	239	C	O3'-P	-5.35	1.53	1.61
35	N	2554	U	P-OP2	-5.35	1.38	1.49
21	e	72	VAL	C-O	-5.35	1.18	1.24
58	v	40	LYS	CA-C	5.35	1.59	1.52
35	N	503	A	C6-N1	-5.33	1.24	1.35
35	N	1026	G	P-OP2	-5.33	1.38	1.49
35	N	1327	A	P-OP2	5.33	1.59	1.49
35	N	2048	G	O3'-P	-5.33	1.53	1.61
35	N	2694	G	O3'-P	-5.32	1.53	1.61
35	N	1782	U	O3'-P	-5.32	1.53	1.61
6	P	54	ILE	N-CA	5.31	1.52	1.46
38	0	572	A	P-OP1	5.31	1.59	1.49
13	W	76	HIS	C-O	-5.31	1.17	1.23
8	R	81	GLY	N-CA	-5.30	1.37	1.45
35	N	2045	C	O3'-P	-5.30	1.53	1.61
35	N	2260	C	O3'-P	-5.30	1.53	1.61
15	Y	101	ILE	N-CA	-5.30	1.40	1.46
38	0	1182	G	O3'-P	5.30	1.69	1.61
35	N	411	G	P-OP1	5.29	1.59	1.49
7	Q	170	VAL	CA-C	-5.29	1.46	1.52
26	j	72	LYS	C-O	5.29	1.30	1.23
32	p	42	LEU	N-CA	-5.29	1.41	1.46
14	X	35	VAL	C-O	5.29	1.29	1.24
35	N	117	G	O3'-P	-5.28	1.53	1.61
35	N	120	U	P-OP2	5.28	1.59	1.49
6	P	156	ARG	CD-NE	-5.28	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	698	C	O3'-P	-5.27	1.53	1.61
7	Q	149	ASN	CA-CB	-5.27	1.44	1.53
35	N	1649	G	O3'-P	-5.27	1.53	1.61
35	N	946	C	P-OP2	5.26	1.59	1.49
35	N	1977	A	O3'-P	-5.26	1.53	1.61
35	N	2285	C	O3'-P	-5.26	1.53	1.61
35	N	2452	C	O3'-P	-5.25	1.53	1.61
53	I	34	GLU	CA-C	-5.25	1.46	1.52
8	R	45	ALA	N-CA	-5.25	1.40	1.46
20	d	49	ASP	CB-CG	5.25	1.65	1.52
35	N	1234	U	O3'-P	-5.25	1.53	1.61
35	N	1960	A	O3'-P	-5.25	1.53	1.61
58	v	35	ARG	CA-C	-5.25	1.46	1.52
35	N	2732	G	C3'-O3'	5.25	1.50	1.42
6	P	195	VAL	CB-CG1	-5.25	1.35	1.52
35	N	1342	A	P-OP2	5.25	1.59	1.49
22	f	96	ILE	N-CA	-5.24	1.39	1.46
35	N	2074	U	O3'-P	-5.24	1.53	1.61
35	N	2289	G	O3'-P	-5.24	1.53	1.61
35	N	2723	C	O3'-P	-5.23	1.53	1.61
19	c	92	VAL	CA-C	-5.23	1.46	1.52
41	3	39	GLY	N-CA	5.22	1.52	1.45
6	P	195	VAL	C-O	-5.22	1.17	1.24
21	e	54	VAL	C-O	5.22	1.29	1.24
35	N	2682	A	P-OP2	5.22	1.59	1.49
6	P	239	ASN	N-CA	-5.21	1.39	1.46
17	a	8	ARG	NE-CZ	-5.21	1.27	1.33
35	N	1432	G	O3'-P	-5.21	1.53	1.61
21	e	43	ASN	CA-C	5.21	1.56	1.52
22	f	85	ILE	C-O	-5.20	1.18	1.24
7	Q	12	THR	CA-CB	5.20	1.61	1.54
35	N	1968	G	P-OP1	5.20	1.59	1.49
35	N	2028	U	O3'-P	-5.20	1.53	1.61
35	N	193	U	O3'-P	-5.19	1.53	1.61
35	N	1191	G	O3'-P	-5.19	1.53	1.61
6	P	175	ARG	CA-C	-5.19	1.46	1.52
35	N	1677	A	O3'-P	-5.19	1.53	1.61
31	o	21	TYR	CE2-CZ	-5.18	1.25	1.38
35	N	2426	A	O3'-P	-5.18	1.53	1.61
15	Y	62	PRO	N-CA	-5.18	1.41	1.46
20	d	21	ALA	C-O	-5.18	1.16	1.23
35	N	1680	U	O3'-P	-5.18	1.53	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	1141	U	N3-C4	-5.17	1.28	1.38
58	v	34	ARG	CA-C	5.17	1.59	1.52
35	N	1153	C	P-OP2	5.17	1.59	1.49
7	Q	150	GLN	N-CA	5.16	1.52	1.46
35	N	2727	A	O3'-P	-5.16	1.53	1.61
6	P	213	TRP	CD1-NE1	5.15	1.48	1.37
35	N	960	A	O3'-P	-5.14	1.53	1.61
35	N	1334	G	O3'-P	-5.14	1.53	1.61
35	N	2699	C	O3'-P	-5.14	1.53	1.61
35	N	694	U	O3'-P	-5.14	1.53	1.61
38	0	559	A	N1-C2	5.14	1.44	1.34
35	N	1142	A	O3'-P	5.13	1.68	1.61
35	N	2262	U	O3'-P	-5.13	1.53	1.61
38	0	1062	U	O3'-P	-5.13	1.53	1.61
35	N	1652	A	O3'-P	-5.12	1.53	1.61
38	0	715	A	O3'-P	-5.11	1.53	1.61
35	N	234	U	N3-C4	-5.11	1.28	1.38
35	N	2503	A	P-OP1	5.11	1.59	1.49
17	a	10	LEU	CA-C	-5.11	1.45	1.53
35	N	1648	U	P-OP2	5.11	1.59	1.49
38	0	368	U	N3-C4	-5.11	1.28	1.38
26	j	45	PHE	CA-CB	-5.10	1.45	1.53
35	N	963	U	P-OP2	5.10	1.59	1.49
35	N	1296	G	O3'-P	-5.10	1.53	1.61
11	U	29	PHE	CA-C	-5.10	1.48	1.52
35	N	1367	A	O3'-P	-5.09	1.53	1.61
40	2	152	GLU	CA-C	-5.09	1.47	1.53
16	Z	73	ILE	C-O	-5.09	1.18	1.24
35	N	727	A	P-OP1	5.09	1.59	1.49
38	0	1110	A	P-OP2	5.09	1.59	1.49
57	u	10	ARG	CD-NE	-5.09	1.39	1.46
35	N	745	G	O3'-P	-5.08	1.53	1.61
38	0	19	A	O3'-P	-5.08	1.53	1.61
35	N	208	C	O3'-P	-5.08	1.53	1.61
35	N	632	A	O3'-P	-5.08	1.53	1.61
35	N	2502	G	O3'-P	-5.08	1.53	1.61
8	R	52	VAL	C-O	-5.07	1.18	1.24
3	s	152	ALA	C-O	5.07	1.30	1.24
39	1	18	HIS	C-O	-5.06	1.20	1.24
45	7	106	THR	CA-C	-5.06	1.46	1.53
15	Y	63	LYS	N-CA	-5.06	1.39	1.46
18	b	102	ARG	CZ-NH2	5.04	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	N	1186	G	O3'-P	-5.04	1.53	1.61
50	F	101	ARG	CZ-NH1	5.04	1.39	1.32
35	N	1650	A	O3'-P	-5.03	1.53	1.61
35	N	1004	U	O3'-P	-5.03	1.53	1.61
17	a	11	ASN	CA-C	-5.03	1.46	1.53
42	4	50	TYR	CA-C	-5.02	1.46	1.52
35	N	408	G	O3'-P	-5.02	1.53	1.61
35	N	1006	C	O3'-P	-5.02	1.53	1.61
7	Q	131	ASP	C-O	-5.01	1.17	1.23
35	N	1187	G	P-OP2	5.01	1.58	1.49

All (370) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	M	73	C	O3'-P-O5'	18.17	131.26	104.00
7	Q	151	THR	CA-C-N	12.75	134.26	119.47
7	Q	151	THR	C-N-CA	12.75	134.26	119.47
35	N	1936	A	C4'-C3'-O3'	-11.06	96.42	113.00
35	N	2725	A	C3'-C2'-O2'	-10.59	94.81	110.70
35	N	242	G	C4'-C3'-O3'	10.00	124.40	109.40
57	u	10	ARG	CB-CG-CD	-9.42	89.63	111.30
35	N	774	G	C1'-C2'-O2'	-9.42	94.27	108.40
58	v	5	LYS	N-CA-C	9.36	124.04	110.10
35	N	2251	G	C3'-C2'-O2'	9.33	124.70	110.70
35	N	774	G	C4'-C3'-O3'	-9.27	99.10	113.00
38	0	561	U	C4'-C3'-O3'	-9.16	99.25	113.00
35	N	995	C	C4'-C3'-O3'	-8.79	96.22	109.40
35	N	2776	A	C2'-C3'-O3'	8.71	122.57	109.50
35	N	670	A	C2'-C3'-O3'	8.68	122.51	109.50
6	P	204	VAL	N-CA-C	8.60	120.34	112.43
35	N	2732	G	C4'-C3'-O3'	-8.47	100.30	113.00
38	0	1528	U	C1'-C2'-O2'	-8.46	99.11	111.80
35	N	1937	A	C4'-C3'-O3'	-8.43	100.36	113.00
35	N	2060	A	O3'-P-O5'	8.30	116.46	104.00
38	0	1347	G	C4'-C3'-O3'	8.28	121.81	109.40
35	N	1136	G	P-O5'-C5'	-8.22	108.57	120.90
35	N	784	G	C2'-C3'-O3'	8.20	126.00	113.70
38	0	717	U	C4'-C3'-O3'	-8.05	100.92	113.00
35	N	1236	G	C4'-C3'-O3'	-8.04	100.94	113.00
35	N	2324	U	C4'-C3'-O3'	-8.01	100.99	113.00
38	0	1345	U	C4'-C3'-O3'	7.98	121.37	109.40
6	P	221	ARG	CG-CD-NE	-7.94	94.54	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	746	U	C4'-C3'-O3'	-7.92	101.13	113.00
6	P	232	HIS	O-C-N	-7.87	113.84	123.04
35	N	1141	U	C2'-C3'-O3'	7.79	121.18	109.50
14	X	94	PRO	N-CA-C	7.76	122.89	110.40
35	N	2266	A	C4'-C3'-O3'	-7.62	97.98	109.40
43	5	90	MET	CA-C-N	7.59	136.04	121.54
43	5	90	MET	C-N-CA	7.59	136.04	121.54
5	O	44	G	C4'-C3'-O3'	-7.53	101.70	113.00
35	N	2406	A	C2'-C3'-O3'	-7.53	102.40	113.70
14	X	35	VAL	O-C-N	7.45	129.91	121.94
38	0	115	G	C2'-C3'-O3'	7.45	120.67	109.50
38	0	518	C	C4'-C3'-O3'	7.41	120.51	109.40
35	N	1142	A	C2'-C3'-O3'	7.39	120.59	109.50
33	q	8	ARG	CD-NE-CZ	-7.38	114.06	124.40
8	R	81	GLY	O-C-N	-7.33	113.17	122.70
18	b	101	GLY	O-C-N	7.30	125.94	121.85
38	0	1278	G	C4'-C3'-O3'	-7.28	102.08	113.00
56	t	5	LEU	CB-CG-CD2	7.25	132.46	110.70
35	N	2543	G	P-O5'-C5'	-7.22	110.07	120.90
8	R	81	GLY	CA-C-N	-7.21	107.28	121.41
8	R	81	GLY	C-N-CA	-7.21	107.28	121.41
35	N	2497	A	C5'-C4'-C3'	-7.20	104.40	115.20
38	0	752	G	C4'-C3'-O3'	-7.14	102.30	113.00
35	N	33	C	C4'-C3'-O3'	-7.08	102.38	113.00
35	N	2225	A	C2'-C3'-O3'	7.07	120.10	109.50
6	P	239	ASN	N-CA-C	7.06	125.83	110.80
32	p	39	ARG	NE-CZ-NH2	-7.02	112.89	119.20
48	D	126	LYS	N-CA-C	7.02	120.73	109.79
35	N	227	A	C4'-C3'-O3'	-7.01	102.48	113.00
38	0	1362	A	C4'-C3'-O3'	-7.00	102.50	113.00
38	0	878	A	C3'-C2'-O2'	7.00	121.20	110.70
35	N	1648	U	P-O5'-C5'	-6.97	110.44	120.90
42	4	111	MET	CG-SD-CE	-6.97	85.56	100.90
35	N	2732	G	C1'-C2'-O2'	-6.96	97.96	108.40
26	j	14	ARG	CG-CD-NE	-6.96	96.69	112.00
7	Q	13	ARG	NE-CZ-NH2	6.91	125.42	119.20
35	N	1993	U	C3'-C2'-O2'	-6.90	100.35	110.70
6	P	157	SER	N-CA-C	-6.89	100.60	110.59
32	p	39	ARG	NE-CZ-NH1	6.87	128.37	121.50
35	N	1666	G	C3'-C2'-O2'	6.86	120.99	110.70
35	N	1865	U	C4'-C3'-O3'	-6.85	102.72	113.00
4	M	73	C	OP1-P-O3'	-6.85	87.46	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	0	1279	G	N9-C1'-C2'	6.85	122.27	112.00
20	d	22	LYS	N-CA-C	-6.84	100.36	110.48
20	d	6	ARG	NE-CZ-NH2	6.80	125.32	119.20
35	N	989	G	C4'-C3'-O3'	-6.78	102.83	113.00
35	N	995	C	C2'-C3'-O3'	6.76	119.64	109.50
58	v	21	ARG	N-CA-C	6.75	118.72	111.36
38	0	1190	G	C1'-C2'-O2'	-6.74	101.69	111.80
6	P	241	GLY	N-CA-C	6.74	124.65	114.61
44	6	109	ARG	CG-CD-NE	-6.74	97.18	112.00
8	R	65	THR	O-C-N	-6.72	114.54	122.81
35	N	2061	G	C4'-C3'-O3'	-6.71	102.93	113.00
35	N	1313	U	N1-C1'-C2'	6.71	122.06	112.00
35	N	974	G	N9-C1'-C2'	6.71	124.06	114.00
35	N	2832	U	C4'-C3'-O3'	-6.68	102.98	113.00
35	N	2238	G	C2'-C3'-O3'	6.65	119.47	109.50
32	p	34	ARG	NE-CZ-NH1	-6.64	114.86	121.50
19	c	93	ARG	CG-CD-NE	-6.63	97.42	112.00
38	0	1190	G	C4'-C3'-O3'	-6.63	99.46	109.40
5	O	108	A	C2'-C3'-O3'	-6.59	103.81	113.70
35	N	1666	G	O4'-C4'-C3'	-6.59	97.41	104.00
35	N	421	C	C2'-C3'-O3'	6.57	119.35	109.50
38	0	388	G	C2'-C3'-O3'	6.55	119.33	109.50
35	N	2509	G	C3'-C2'-O2'	6.55	120.52	110.70
46	8	18	ARG	CB-CG-CD	-6.54	96.25	111.30
18	b	102	ARG	NE-CZ-NH2	6.53	125.08	119.20
36	L	54	GLY	N-CA-C	6.53	120.99	112.25
35	N	2071	A	C3'-C2'-O2'	6.52	120.48	110.70
38	0	1145	A	C4'-C3'-O3'	-6.47	103.30	113.00
38	0	1301	U	N1-C1'-C2'	6.46	121.69	112.00
15	Y	30	THR	N-CA-CB	6.45	121.39	110.49
38	0	665	A	C2'-C3'-O3'	-6.45	104.02	113.70
57	u	69	LYS	N-CA-C	6.45	124.53	110.80
38	0	1151	A	C4'-C3'-O3'	-6.44	103.34	113.00
15	Y	68	SER	N-CA-C	6.44	118.38	111.36
35	N	1452	G	C4'-C3'-O3'	-6.40	103.40	113.00
15	Y	47	ARG	NE-CZ-NH2	6.39	124.95	119.20
35	N	1212	G	C4'-C3'-O3'	-6.38	103.44	113.00
38	0	818	G	C4'-C3'-O3'	-6.36	103.45	113.00
19	c	73	VAL	N-CA-CB	6.34	117.64	110.72
35	N	2443	C	O4'-C4'-C3'	-6.34	97.66	104.00
30	n	25	VAL	CA-C-N	6.31	133.05	121.70
30	n	25	VAL	C-N-CA	6.31	133.05	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	k	57	ARG	NE-CZ-NH2	6.30	124.87	119.20
55	K	57	ARG	CA-CB-CG	6.30	126.70	114.10
35	N	404	A	C4'-C3'-O3'	6.29	118.83	109.40
6	P	11	PRO	CB-CA-C	-6.28	103.35	111.39
38	0	1213	A	C4'-C3'-O3'	-6.27	103.59	113.00
53	I	43	ALA	CA-C-N	6.27	133.52	121.54
53	I	43	ALA	C-N-CA	6.27	133.52	121.54
42	4	127	ALA	N-CA-C	6.26	119.44	110.24
5	O	44	G	N9-C1'-C2'	6.25	121.38	112.00
35	N	2364	C	O4'-C4'-C3'	-6.24	97.76	104.00
40	2	167	TRP	N-CA-C	6.24	119.72	110.48
26	j	41	ARG	CD-NE-CZ	6.24	133.13	124.40
35	N	859	G	C1'-C2'-O2'	-6.22	102.46	111.80
35	N	2728	U	C2'-C3'-O3'	-6.21	104.39	113.70
35	N	446	G	C2'-C3'-O3'	6.16	118.74	109.50
35	N	2501	C	C4'-C3'-O3'	-6.15	103.78	113.00
11	U	72	ILE	N-CA-C	6.14	122.11	109.34
49	E	22	PRO	O-C-N	-6.14	114.35	122.64
26	j	41	ARG	CB-CG-CD	6.12	125.38	111.30
38	0	818	G	N9-C1'-C2'	6.11	121.16	112.00
38	0	1201	A	C2'-C3'-O3'	6.10	118.65	109.50
49	E	44	LYS	N-CA-C	6.10	120.52	112.35
15	Y	78	ARG	NE-CZ-NH2	6.08	124.67	119.20
35	N	2728	U	C4'-C3'-O3'	-6.07	103.89	113.00
32	p	12	ARG	CA-CB-CG	6.06	126.22	114.10
11	U	27	ARG	NE-CZ-NH1	-6.06	115.44	121.50
35	N	1352	U	O4'-C1'-C2'	-6.04	101.56	107.60
35	N	2725	A	C1'-C2'-O2'	-6.04	99.34	108.40
42	4	138	ARG	N-CA-CB	6.04	120.69	110.49
48	D	124	PRO	CA-C-N	6.02	128.95	120.28
48	D	124	PRO	C-N-CA	6.02	128.95	120.28
35	N	2319	G	C4'-C3'-O3'	-6.01	103.98	113.00
6	P	221	ARG	N-CA-CB	6.01	120.07	110.46
53	I	44	SER	N-CA-C	-6.00	98.02	110.80
17	a	69	ARG	NE-CZ-NH2	5.99	124.59	119.20
17	a	70	THR	N-CA-C	5.98	123.54	110.80
35	N	2034	U	C4'-C3'-O3'	-5.97	104.04	113.00
35	N	827	U	C2'-C3'-O3'	-5.96	104.76	113.70
35	N	1567	G	C1'-C2'-O2'	-5.94	102.89	111.80
29	m	32	ILE	N-CA-CB	5.94	117.00	110.53
35	N	2246	G	O4'-C4'-C3'	-5.93	98.07	104.00
35	N	974	G	C4'-C3'-O3'	-5.92	100.52	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	2518	A	C1'-C2'-O2'	-5.92	102.92	111.80
26	j	19	LYS	N-CA-C	5.92	120.50	113.16
38	0	64	G	C2'-C3'-O3'	-5.90	104.84	113.70
35	N	782	A	C4'-C3'-O3'	-5.90	100.55	109.40
35	N	2468	A	C4'-C3'-O3'	-5.90	104.15	113.00
35	N	1254	A	C4'-C3'-O3'	-5.88	104.18	113.00
35	N	2543	G	C5'-C4'-C3'	-5.88	107.18	116.00
34	r	36	ARG	NE-CZ-NH1	-5.88	115.62	121.50
35	N	1626	A	C2'-C3'-O3'	-5.88	104.89	113.70
35	N	2035	G	C4'-C3'-O3'	-5.87	100.59	109.40
26	j	41	ARG	N-CA-C	5.86	120.73	112.93
35	N	871	U	P-O5'-C5'	-5.86	112.11	120.90
35	N	820	A	O4'-C4'-C3'	-5.84	98.16	104.00
30	n	25	VAL	N-CA-C	5.83	116.48	110.82
38	0	330	C	P-O5'-C5'	-5.82	112.17	120.90
35	N	301	G	C4'-C3'-O3'	-5.82	104.28	113.00
7	Q	113	SER	N-CA-C	5.81	117.56	110.41
35	N	974	G	C2'-C3'-O3'	5.80	118.21	109.50
6	P	258	ARG	NE-CZ-NH1	-5.79	115.71	121.50
35	N	2873	A	P-O5'-C5'	-5.79	112.22	120.90
6	P	31	ALA	CA-C-N	-5.78	114.94	120.83
6	P	31	ALA	C-N-CA	-5.78	114.94	120.83
7	Q	151	THR	O-C-N	-5.77	114.97	121.43
35	N	1970	A	C2'-C3'-O3'	5.76	118.15	109.50
42	4	38	VAL	CG1-CB-CG2	-5.76	98.13	110.80
6	P	177	ARG	CG-CD-NE	-5.75	99.34	112.00
6	P	238	ARG	N-CA-C	5.75	123.06	110.80
35	N	782	A	C2'-C3'-O3'	5.74	118.11	109.50
35	N	140	C	N1-C1'-C2'	5.73	120.60	112.00
20	d	33	ARG	CB-CG-CD	-5.73	98.13	111.30
35	N	2267	A	N9-C1'-C2'	5.73	120.59	112.00
35	N	2447	G	P-O3'-C3'	5.72	128.79	120.20
21	e	79	ARG	CD-NE-CZ	-5.71	116.40	124.40
35	N	512	G	P-O3'-C3'	5.71	128.77	120.20
35	N	2543	G	O5'-C5'-C4'	5.70	120.05	111.50
35	N	2035	G	C1'-C2'-O2'	-5.69	103.27	111.80
35	N	2049	G	C3'-C2'-O2'	5.69	119.23	110.70
6	P	156	ARG	CB-CG-CD	-5.68	98.23	111.30
20	d	13	ARG	NE-CZ-NH2	5.68	124.31	119.20
30	n	7	LYS	CD-CE-NZ	5.67	130.05	111.90
42	4	24	THR	N-CA-C	5.66	117.53	110.91
38	0	971	G	C2'-C3'-O3'	-5.65	105.22	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	O	88	C	C4'-C3'-O3'	-5.65	104.53	113.00
35	N	555	G	C4'-C3'-O3'	-5.65	104.53	113.00
38	0	96	U	C2'-C3'-O3'	5.64	122.17	113.70
40	2	3	GLN	N-CA-C	5.63	122.09	113.19
35	N	301	G	N9-C1'-C2'	5.63	120.45	112.00
35	N	2776	A	C8-N9-C1'	-5.63	110.80	127.70
35	N	1900	A	P-O3'-C3'	5.63	128.65	120.20
38	0	1280	A	C4'-C3'-O3'	-5.63	104.55	113.00
40	2	6	HIS	N-CA-C	-5.63	102.56	109.65
35	N	1661	G	C3'-C2'-O2'	5.62	119.13	110.70
35	N	2776	A	C4-N9-C1'	5.62	143.16	126.30
18	b	100	HIS	CA-C-N	-5.62	115.52	123.95
18	b	100	HIS	C-N-CA	-5.62	115.52	123.95
38	0	1196	A	C4'-C3'-O3'	-5.62	104.58	113.00
18	b	102	ARG	NE-CZ-NH1	-5.61	115.89	121.50
19	c	53	ARG	CB-CG-CD	-5.61	98.40	111.30
5	O	24	G	C2'-C3'-O3'	-5.61	105.29	113.70
38	0	1432	G	C4'-C3'-O3'	-5.60	104.60	113.00
17	a	69	ARG	CG-CD-NE	5.59	124.31	112.00
35	N	2019	A	C3'-C2'-O2'	5.59	119.08	110.70
35	N	1261	C	O4'-C4'-C3'	-5.58	98.42	104.00
35	N	1565	C	C2'-C3'-O3'	5.56	117.84	109.50
35	N	2517	C	O3'-P-O5'	-5.55	95.67	104.00
30	n	55	ILE	N-CA-C	5.55	120.89	109.34
33	q	8	ARG	CG-CD-NE	5.55	124.21	112.00
35	N	752	A	N9-C1'-C2'	5.55	122.33	114.00
35	N	2034	U	O3'-P-O5'	-5.55	95.67	104.00
35	N	784	G	P-O3'-C3'	5.54	128.52	120.20
35	N	1205	A	C4'-C3'-O3'	5.53	117.70	109.40
35	N	2645	G	C5'-C4'-C3'	-5.53	106.91	115.20
38	0	686	U	C4'-C3'-O3'	-5.53	104.70	113.00
43	5	63	ASN	N-CA-C	5.53	117.38	110.91
35	N	1565	C	C5'-C4'-C3'	-5.53	106.91	115.20
35	N	727	A	N9-C1'-C2'	5.52	120.28	112.00
46	8	126	GLN	CA-C-O	-5.51	114.99	121.16
35	N	2645	G	P-O5'-C5'	-5.50	112.65	120.90
38	0	665	A	C3'-C2'-O2'	5.49	118.93	110.70
35	N	2751	G	C2'-C3'-O3'	-5.48	105.47	113.70
35	N	1428	C	C2'-C3'-O3'	-5.48	105.48	113.70
7	Q	160	LYS	CG-CD-CE	5.48	123.90	111.30
35	N	645	C	N1-C1'-C2'	5.48	120.22	112.00
35	N	372	G	C1'-C2'-O2'	-5.47	103.59	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	c	21	ARG	NE-CZ-NH1	-5.47	116.03	121.50
42	4	157	ARG	NE-CZ-NH1	-5.47	116.03	121.50
35	N	2724	U	C2'-C3'-O3'	-5.47	105.50	113.70
35	N	1012	U	C2'-C3'-O3'	-5.46	105.50	113.70
39	1	17	GLY	CA-C-O	-5.46	117.87	122.29
35	N	947	A	C3'-C2'-O2'	-5.44	102.54	110.70
38	0	1125	U	N1-C1'-C2'	5.44	120.16	112.00
38	0	1491	G	C4'-C3'-O3'	5.44	121.16	113.00
35	N	962	G	C3'-C2'-O2'	5.43	118.85	110.70
35	N	923	G	C3'-C2'-O2'	5.43	118.84	110.70
38	0	813	U	C4'-C3'-O3'	-5.43	104.86	113.00
38	0	1211	U	C2'-C3'-O3'	-5.41	105.58	113.70
54	J	71	LYS	N-CA-C	5.41	122.33	110.80
30	n	7	LYS	CG-CD-CE	-5.40	98.87	111.30
34	r	1	MET	CB-CG-SD	-5.40	96.50	112.70
35	N	51	G	C4'-C3'-O3'	-5.38	104.92	113.00
35	N	2820	A	C4'-C3'-O3'	-5.38	104.92	113.00
35	N	983	A	C5'-C4'-O4'	-5.38	101.73	109.80
35	N	2038	G	C3'-C2'-O2'	5.37	118.76	110.70
26	j	41	ARG	NH1-CZ-NH2	-5.37	112.32	119.30
38	0	563	A	N9-C1'-C2'	5.37	120.05	112.00
35	N	1819	A	C1'-C2'-O2'	-5.36	103.76	111.80
35	N	2497	A	C2'-C3'-O3'	5.36	117.53	109.50
35	N	1937	A	N9-C1'-C2'	5.35	120.03	112.00
38	0	5	U	C2'-C3'-O3'	-5.34	105.69	113.70
35	N	2552	U	C3'-C2'-O2'	5.33	118.69	110.70
35	N	2354	C	C5'-C4'-C3'	-5.33	108.01	116.00
15	Y	29	LYS	CD-CE-NZ	-5.32	94.87	111.90
35	N	783	A	O4'-C1'-C2'	-5.32	102.28	107.60
35	N	2645	G	C2'-C3'-O3'	5.32	117.48	109.50
47	9	42	LEU	CA-C-N	5.32	126.48	119.84
47	9	42	LEU	C-N-CA	5.32	126.48	119.84
35	N	1236	G	P-O3'-C3'	5.31	128.17	120.20
35	N	1620	G	C3'-C2'-O2'	5.31	118.67	110.70
38	0	388	G	O3'-P-O5'	-5.31	96.04	104.00
32	p	12	ARG	CB-CG-CD	-5.29	99.13	111.30
35	N	1770	G	C3'-C2'-O2'	5.29	118.63	110.70
35	N	310	A	C1'-C2'-O2'	-5.29	100.47	108.40
35	N	2092	U	P-O5'-C5'	-5.29	112.97	120.90
35	N	1977	A	C2'-C3'-O3'	-5.27	105.79	113.70
35	N	2394	C	O4'-C4'-C3'	-5.27	98.73	104.00
16	Z	118	LYS	CB-CG-CD	-5.27	99.19	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	2497	A	C4'-C3'-O3'	-5.26	101.50	109.40
35	N	2430	A	C3'-C2'-O2'	5.26	118.59	110.70
35	N	2498	C	C3'-C2'-O2'	5.26	118.59	110.70
38	0	1094	G	C4'-C3'-O3'	-5.26	105.11	113.00
37	C	55	SER	N-CA-C	5.25	117.01	111.28
52	H	64	ARG	CG-CD-NE	-5.25	100.44	112.00
35	N	785	G	P-O5'-C5'	-5.25	113.02	120.90
35	N	669	G	N9-C1'-C2'	5.25	119.87	112.00
35	N	1650	A	C3'-C2'-O2'	5.24	118.56	110.70
7	Q	114	LYS	CA-CB-CG	5.24	124.57	114.10
35	N	2849	U	P-O5'-C5'	5.23	128.74	120.90
27	k	28	ARG	NE-CZ-NH2	-5.22	114.50	119.20
6	P	226	ASN	CA-C-N	-5.22	114.29	119.56
6	P	226	ASN	C-N-CA	-5.22	114.29	119.56
15	Y	18	ARG	NE-CZ-NH2	-5.22	114.51	119.20
38	0	652	U	C2'-C3'-O3'	-5.22	105.88	113.70
38	0	1530	G	C4'-C3'-O3'	-5.21	105.18	113.00
35	N	372	G	C2'-C3'-O3'	5.21	117.32	109.50
8	R	49	ARG	NE-CZ-NH1	-5.21	116.29	121.50
14	X	29	HIS	CB-CA-C	-5.21	103.49	111.66
35	N	421	C	C4'-C3'-O3'	5.21	117.21	109.40
35	N	2474	U	N1-C1'-C2'	5.21	119.81	112.00
35	N	2311	A	P-O3'-C3'	5.20	128.00	120.20
38	0	812	G	C1'-C2'-O2'	-5.20	100.60	108.40
35	N	2502	G	C3'-C2'-O2'	-5.20	102.91	110.70
49	E	12	ARG	NE-CZ-NH1	-5.19	116.31	121.50
35	N	278	A	N9-C1'-C2'	5.19	119.78	112.00
35	N	2596	U	C2'-C3'-O3'	-5.19	105.92	113.70
6	P	156	ARG	CG-CD-NE	5.19	123.41	112.00
35	N	1343	G	N9-C1'-C2'	5.19	119.78	112.00
7	Q	12	THR	N-CA-C	-5.18	101.50	108.19
38	0	1303	C	N1-C1'-C2'	5.18	119.78	112.00
35	N	2638	G	C4'-C3'-O3'	-5.18	105.23	113.00
41	3	5	LEU	CB-CA-C	-5.18	104.55	112.11
35	N	27	G	C5'-C4'-O4'	-5.17	102.04	109.80
20	d	3	ARG	NE-CZ-NH1	-5.17	116.33	121.50
35	N	2867	G	C4'-C3'-O3'	5.17	117.16	109.40
5	O	41	G	C4'-C3'-O3'	-5.17	105.25	113.00
22	f	11	ARG	N-CA-CB	5.16	118.01	110.58
35	N	2621	G	C3'-C2'-O2'	5.16	118.44	110.70
17	a	69	ARG	N-CA-C	-5.15	103.23	110.50
35	N	2580	U	N1-C1'-C2'	5.15	119.72	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	1676	A	C3'-C2'-O2'	5.15	118.42	110.70
7	Q	128	ARG	CA-C-N	5.14	128.02	120.71
7	Q	128	ARG	C-N-CA	5.14	128.02	120.71
14	X	35	VAL	CA-C-O	-5.14	115.21	121.18
58	v	33	ARG	CA-CB-CG	5.14	124.39	114.10
11	U	96	THR	N-CA-C	-5.14	106.86	113.23
15	Y	41	ARG	CA-CB-CG	-5.12	103.85	114.10
35	N	2035	G	C2'-C3'-O3'	5.12	117.18	109.50
35	N	123	G	C3'-C2'-O2'	5.12	118.38	110.70
35	N	481	G	C2'-C3'-O3'	-5.12	106.02	113.70
35	N	1998	A	O4'-C4'-C3'	-5.12	98.89	104.00
5	O	100	G	C3'-C2'-O2'	5.11	118.37	110.70
35	N	1180	U	N1-C1'-C2'	5.11	119.67	112.00
35	N	2049	G	O4'-C4'-C3'	-5.11	98.89	104.00
35	N	2019	A	C2'-C3'-O3'	-5.10	106.04	113.70
38	0	971	G	P-O5'-C5'	-5.10	113.25	120.90
35	N	566	U	C2'-C3'-O3'	-5.10	106.06	113.70
35	N	2062	A	O4'-C4'-C3'	-5.09	101.01	106.10
35	N	2238	G	C4'-C3'-O3'	-5.09	101.77	109.40
35	N	2732	G	C3'-C2'-O2'	-5.08	103.08	110.70
34	r	36	ARG	CG-CD-NE	-5.08	100.83	112.00
38	0	812	G	P-O3'-C3'	5.08	127.82	120.20
53	I	42	ILE	CA-C-N	5.07	131.23	121.54
53	I	42	ILE	C-N-CA	5.07	131.23	121.54
38	0	595	A	C4'-C3'-O3'	5.07	117.01	109.40
35	N	1253	A	C2'-C3'-O3'	5.07	117.10	109.50
20	d	32	TYR	CA-C-O	5.07	125.83	120.10
41	3	23	SER	O-C-N	5.07	127.99	122.11
4	M	9	C	C2'-C3'-O3'	-5.06	106.11	113.70
35	N	1131	G	O3'-P-O5'	-5.06	96.41	104.00
35	N	1928	A	C3'-C2'-O2'	5.05	118.28	110.70
42	4	30	ILE	CB-CA-C	5.05	117.70	110.33
35	N	2049	G	C2'-C3'-O3'	-5.04	106.13	113.70
35	N	2502	G	P-O5'-C5'	5.04	128.45	120.90
16	Z	8	LYS	CB-CG-CD	-5.03	99.72	111.30
35	N	820	A	O4'-C1'-C2'	-5.03	102.57	107.60
35	N	1997	C	O4'-C4'-C3'	-5.03	98.97	104.00
39	1	103	ASN	N-CA-CB	5.03	119.92	110.56
20	d	9	ILE	N-CA-C	5.03	117.38	111.09
17	a	1	MET	CB-CG-SD	-5.03	97.61	112.70
38	0	801	U	C2'-C3'-O3'	-5.03	106.16	113.70
35	N	60	G	C1'-C2'-O2'	-5.03	104.26	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	N	750	A	C2'-C3'-O3'	-5.03	106.16	113.70
35	N	995	C	C1'-C2'-O2'	-5.02	104.27	111.80
42	4	140	THR	N-CA-C	-5.02	106.01	112.68
28	l	52	ARG	NE-CZ-NH1	-5.02	116.48	121.50
35	N	683	U	N1-C1'-C2'	5.01	119.51	112.00
20	d	32	TYR	N-CA-C	5.01	117.47	111.71

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
38	0	24	U	Sidechain
38	0	368	U	Sidechain
38	0	559	A	Sidechain
38	0	571	U	Sidechain
38	0	864	A	Sidechain
39	1	102	THR	Peptide
39	1	14	VAL	Peptide
40	2	79	LYS	Peptide
40	2	80	LYS	Peptide
42	4	102	GLY	Peptide
42	4	136	VAL	Peptide
42	4	137	VAL	Peptide
42	4	142	ASP	Peptide
42	4	89	HIS	Peptide
43	5	52	ASN	Peptide
43	5	93	LYS	Peptide
46	8	128	SER	Peptide
46	8	53	GLU	Peptide
46	8	54	LEU	Peptide
46	8	55	VAL	Peptide
2	B	22	THR	Peptide
48	D	125	LYS	Peptide
49	E	22	PRO	Peptide
49	E	77	HIS	Peptide
54	J	17	MET	Peptide
54	J	69	LYS	Peptide
35	N	1802	A	Sidechain
35	N	2522	U	Sidechain
35	N	2765	A	Sidechain
35	N	586	A	Sidechain
35	N	850	U	Sidechain

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Mol	Chain	Res	Type	Group
35	N	927	A	Sidechain
6	P	195	VAL	Peptide
6	P	234	GLY	Peptide
6	P	238	ARG	Peptide
7	Q	151	THR	Peptide
9	S	174	ASP	Peptide
9	S	175	PHE	Peptide
11	U	34	GLY	Peptide
12	V	11	LEU	Peptide
15	Y	114	GLY	Peptide
15	Y	82	LEU	Peptide
16	Z	57	VAL	Mainchain,Peptide
24	h	52	LEU	Peptide
33	q	31	HIS	Peptide
56	t	37	ARG	Peptide
57	u	3	ASN	Peptide
58	v	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	A	1561	0	788	13	0
2	B	194	0	83	11	0
3	s	316	0	283	8	0
4	M	1594	0	809	65	0
5	O	2529	0	1281	15	0
6	P	2082	0	2154	40	0
7	Q	1564	0	1616	24	0
8	R	1552	0	1619	18	0
9	S	1410	0	1444	31	0
10	T	1322	0	1371	13	0
11	U	1111	0	1148	28	0
12	V	1031	0	1085	21	0
13	W	1128	0	1162	15	0
14	X	938	0	1012	19	0
15	Y	1044	0	1117	17	0
16	Z	1073	0	1157	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	a	960	0	1000	17	0
18	b	891	0	923	11	0
19	c	915	0	958	14	0
20	d	946	0	1019	22	0
21	e	815	0	839	16	0
22	f	857	0	922	10	0
23	g	738	0	807	5	0
24	h	779	0	831	9	0
25	i	752	0	780	9	0
26	j	568	0	581	10	0
27	k	624	0	652	12	0
28	l	508	0	543	6	0
29	m	448	0	488	1	0
30	n	443	0	458	12	0
31	o	409	0	440	5	0
32	p	376	0	418	20	0
33	q	503	0	572	12	0
34	r	301	0	341	8	0
35	N	62215	0	31275	414	0
36	L	419	0	418	11	0
37	C	1027	0	1091	43	0
38	0	32873	0	16532	182	0
39	1	1704	0	1732	39	0
40	2	1624	0	1696	18	0
41	3	1642	0	1707	21	0
42	4	1105	0	1148	20	0
43	5	817	0	808	16	0
44	6	1129	0	1178	17	0
45	7	978	0	1031	6	0
46	8	1021	0	1070	21	0
47	9	786	0	828	19	0
48	D	876	0	886	24	0
49	E	954	0	1016	16	0
50	F	883	0	941	19	0
51	G	773	0	824	14	0
52	H	709	0	728	13	0
53	I	648	0	666	10	0
54	J	648	0	691	6	0
55	K	455	0	478	12	0
56	t	637	0	665	11	0
57	u	664	0	714	18	0
58	v	425	0	449	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	A	2	0	0	0	0
60	A	1	0	0	0	0
61	A	9	0	0	0	0
All	All	147306	0	99273	1180	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 5.

All (1180) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:75:A:H5”	35:N:2602:A:C5	1.40	1.53
35:N:306:U:H3	35:N:310:A:N6	1.15	1.43
38:0:1238:A:N6	38:0:1301:U:H3	1.22	1.37
4:M:75:A:H3’	35:N:2602:A:N6	1.36	1.35
11:U:43:ASN:HB3	11:U:47:PHE:CE2	1.62	1.33
4:M:12:C:O2’	35:N:1923:U:C1’	1.84	1.24
4:M:75:A:H5”	35:N:2602:A:N7	1.53	1.24
35:N:715:A:H1’	52:H:40:GLN:NE2	1.53	1.23
35:N:715:A:C1’	52:H:40:GLN:HE22	1.52	1.23
35:N:499:U:H3	35:N:503:A:N6	1.39	1.21
4:M:12:C:O2’	35:N:1923:U:H1’	1.34	1.17
4:M:56:G:H5’	9:S:75:ALA:HB3	1.27	1.11
4:M:75:A:C5’	35:N:2602:A:N7	2.13	1.10
35:N:715:A:H1’	52:H:40:GLN:HE22	1.01	1.09
4:M:75:A:C5’	35:N:2602:A:C5	2.36	1.08
35:N:306:U:N3	35:N:310:A:N6	1.86	1.06
11:U:43:ASN:CB	11:U:47:PHE:HE2	1.71	1.03
4:M:12:C:O2’	35:N:1923:U:O2’	1.74	1.02
2:B:25:ILE:CB	39:1:32:PHE:HA	1.90	1.02
4:M:12:C:HO2’	35:N:1923:U:C2’	1.74	1.00
4:M:75:A:H3’	35:N:2602:A:C6	1.96	1.00
4:M:15:G:H5”	4:M:15:G:H8	1.31	0.95
4:M:75:A:C3’	35:N:2602:A:N6	2.31	0.94
4:M:15:G:H5”	4:M:15:G:C8	2.02	0.93
11:U:42:LYS:O	11:U:46:PHE:HD2	1.51	0.93
2:B:25:ILE:CB	39:1:32:PHE:O	2.17	0.92
4:M:56:G:H5’	9:S:75:ALA:CB	2.00	0.91
11:U:42:LYS:O	11:U:46:PHE:CD2	2.23	0.90
35:N:715:A:C1’	52:H:40:GLN:NE2	2.22	0.90
38:0:1060:U:C5	40:2:2:GLY:HA3	2.07	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:12:C:O2'	35:N:1923:U:C2'	2.19	0.87
35:N:2304:G:H22	35:N:2312:U:H3	1.23	0.87
4:M:31:U:H5'	38:0:1340:A:O2'	1.74	0.87
35:N:2177:C:O3'	37:C:211:LYS:HE2	1.76	0.86
35:N:715:A:H1'	52:H:40:GLN:CD	1.89	0.86
11:U:43:ASN:O	11:U:47:PHE:CD2	2.29	0.86
2:B:24:LYS:HA	39:1:32:PHE:CZ	2.11	0.85
11:U:43:ASN:O	11:U:47:PHE:HD2	1.57	0.85
1:A:12:U:H4'	35:N:1915:U:H4'	1.58	0.84
4:M:75:A:H5"	35:N:2602:A:C6	2.10	0.84
47:9:83:THR:O	47:9:87:LEU:HB2	1.79	0.83
6:P:35:GLU:OE2	35:N:1816:C:N4	2.10	0.82
4:M:15:G:H5'	4:M:16:C:OP2	1.81	0.81
4:M:30:A:O4'	38:0:1339:A:C2	2.34	0.81
35:N:284:U:H3	35:N:356:G:H1	1.30	0.79
4:M:56:G:C5'	9:S:75:ALA:HB3	2.10	0.78
2:B:20:ALA:H	39:1:35:ARG:HH21	1.31	0.77
50:F:101:ARG:NH1	50:F:104:THR:OG1	2.16	0.77
38:0:1238:A:N7	38:0:1301:U:O4	2.18	0.77
35:N:306:U:C2	35:N:310:A:N6	2.54	0.76
14:X:49:ARG:NH2	38:0:1422:G:O3'	2.18	0.75
37:C:3:LYS:HG3	37:C:4:LEU:H	1.50	0.75
4:M:16:C:H3'	4:M:17:G:H5'	1.68	0.75
38:0:1279:G:OP1	47:9:9:ARG:NH2	2.18	0.75
34:r:3:VAL:HG21	35:N:2539:C:H5'	1.67	0.75
35:N:2177:C:H4'	37:C:211:LYS:HZ1	1.51	0.75
17:a:53:THR:HG21	35:N:2840:C:H5"	1.66	0.75
35:N:499:U:N3	35:N:503:A:N6	2.11	0.75
11:U:42:LYS:HB3	11:U:46:PHE:HE2	1.52	0.75
47:9:65:TYR:HB3	51:G:96:LEU:HD11	1.69	0.75
11:U:43:ASN:CB	11:U:47:PHE:CE2	2.57	0.75
35:N:2112:G:H2'	35:N:2113:U:H5'	1.69	0.75
35:N:1093:G:N2	35:N:1098:A:H62	1.85	0.74
38:0:673:A:O3'	43:5:86:ARG:NH2	2.20	0.74
6:P:221:ARG:NH1	35:N:1789:A:OP2	2.20	0.74
56:t:30:PRO:HA	56:t:48:THR:O	1.88	0.73
50:F:87:ARG:O	50:F:91:HIS:HB2	1.87	0.73
1:A:64:A:H5'	35:N:2482:A:O2'	1.88	0.73
42:4:101:GLU:OE2	42:4:103:THR:OG1	2.05	0.73
4:M:75:A:H5'	35:N:2602:A:N7	2.04	0.73
7:Q:14:ILE:HA	19:c:12:GLN:HE22	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:C:OP1	35:N:1942:C:O3'	2.08	0.72
38:0:1527:U:OP2	58:v:39:GLU:OE1	2.07	0.72
2:B:25:ILE:CB	39:1:32:PHE:CA	2.65	0.72
35:N:1093:G:H21	35:N:1098:A:N6	1.87	0.72
56:t:6:LYS:HG3	56:t:7:LYS:HG2	1.70	0.72
4:M:16:C:C3'	4:M:17:G:H5'	2.20	0.71
17:a:77:ALA:O	17:a:81:ASN:HB2	1.90	0.71
4:M:12:C:C2'	35:N:1923:U:O2'	2.38	0.71
6:P:258:ARG:NH1	6:P:264:ASP:OD1	2.23	0.71
4:M:56:G:C5'	9:S:75:ALA:CB	2.66	0.71
38:0:1081:A:OP2	42:4:52:LYS:NZ	2.23	0.71
38:0:1147:C:O2	46:8:18:ARG:NH2	2.22	0.71
42:4:81:LEU:HD13	42:4:123:VAL:HG11	1.72	0.71
9:S:37:ASN:ND2	35:N:2312:U:O2	2.24	0.71
51:G:47:LYS:HB3	56:t:13:LEU:HD12	1.72	0.70
33:q:8:ARG:NH2	35:N:243:U:OP1	2.24	0.70
38:0:404:G:O2'	38:0:498:A:N1	2.23	0.70
38:0:664:G:H22	38:0:741:G:H1	1.38	0.70
35:N:2637:U:N3	35:N:2776:A:N6	2.40	0.70
8:R:163:ASN:ND2	35:N:323:C:H2'	2.07	0.70
35:N:715:A:C6	52:H:53:ARG:NH1	2.60	0.70
35:N:2128:G:H21	35:N:2173:A:H1'	1.57	0.70
7:Q:45:TYR:HH	35:N:2636:C:HO2'	1.40	0.69
38:0:1309:G:OP2	50:F:98:ARG:NH1	2.25	0.69
38:0:1238:A:N6	38:0:1301:U:N3	2.01	0.69
46:8:84:THR:HG21	46:8:103:PHE:HB3	1.75	0.69
14:X:48:PRO:HB3	38:0:1422:G:OP1	1.92	0.69
22:f:15:GLN:HE22	35:N:1266:G:H5"	1.56	0.69
1:A:72:C:OP2	35:N:1943:U:OP2	2.11	0.69
4:M:12:C:HO2'	35:N:1923:U:C1'	1.88	0.69
38:0:501:C:OP1	49:E:114:ARG:NH2	2.26	0.69
35:N:2134:A:N6	35:N:2157:G:H4'	2.08	0.69
4:M:75:A:C5'	35:N:2602:A:C8	2.76	0.68
5:O:48:U:OP1	18:b:30:ARG:NH2	2.26	0.68
6:P:87:ARG:NH2	35:N:1817:G:OP1	2.26	0.68
35:N:613:A:N7	35:N:616:A:N1	2.41	0.68
4:M:75:A:H5"	35:N:2602:A:C8	2.29	0.68
35:N:962:G:H21	35:N:2250:G:H1	1.41	0.68
11:U:43:ASN:C	11:U:47:PHE:HD2	2.03	0.67
13:W:113:PRO:HD2	35:N:558:U:OP1	1.94	0.67
23:g:46:ALA:O	23:g:50:LEU:HB2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:56:G:O4'	9:S:75:ALA:HB1	1.95	0.67
39:1:209:ALA:O	39:1:213:TYR:HB2	1.94	0.67
4:M:12:C:H4'	35:N:1922:G:H21	1.57	0.67
38:0:1064:G:N2	38:0:1190:G:O2'	2.28	0.67
38:0:427:U:OP1	41:3:13:ARG:NH2	2.28	0.66
50:F:29:ARG:HH21	50:F:63:PHE:HB2	1.59	0.66
35:N:2107:G:OP1	37:C:3:LYS:HE3	1.94	0.66
35:N:2156:G:H2'	35:N:2157:G:H5'	1.78	0.66
51:G:26:GLU:HG2	51:G:30:ILE:HD12	1.77	0.66
10:T:67:THR:HG21	35:N:2757:A:N1	2.11	0.66
38:0:458:U:H3	38:0:474:G:H1	1.44	0.66
2:B:20:ALA:H	39:1:35:ARG:NH2	1.93	0.66
6:P:29:PRO:HG2	6:P:34:LEU:HD11	1.78	0.65
35:N:499:U:C2	35:N:503:A:N6	2.63	0.65
45:7:75:ILE:HD13	45:7:129:VAL:HG22	1.79	0.65
35:N:1019:U:H3	35:N:1142:A:N6	1.95	0.65
33:q:8:ARG:NH2	35:N:243:U:P	2.70	0.65
4:M:74:C:H2'	4:M:75:A:H1'	1.78	0.65
48:D:24:HIS:HB3	48:D:31:ILE:HG23	1.78	0.65
38:0:437:U:OP1	41:3:152:GLN:NE2	2.30	0.65
35:N:2405:G:O2'	35:N:2411:A:N6	2.30	0.65
7:Q:38:LYS:O	7:Q:46:ARG:HA	1.97	0.64
38:0:974:A:OP1	51:G:69:ARG:NH2	2.30	0.64
45:7:15:ARG:NH1	45:7:75:ILE:O	2.30	0.64
1:A:12:U:C4'	35:N:1915:U:H4'	2.28	0.64
35:N:2637:U:H3	35:N:2776:A:N6	1.96	0.64
1:A:21:A:H4'	1:A:22:G:OP1	1.96	0.64
38:0:554:A:H5'	49:E:26:ALA:HB1	1.78	0.64
9:S:88:LYS:HD3	35:N:2313:C:H5"	1.80	0.64
32:p:37:LYS:HE2	35:N:469:G:O6	1.97	0.64
35:N:1311:G:H21	35:N:1603:A:H62	1.45	0.64
35:N:2141:G:H2'	35:N:2142:A:H8	1.63	0.64
11:U:84:ALA:HA	11:U:91:PHE:H	1.62	0.64
35:N:2121:G:H4'	37:C:167:LYS:HD3	1.79	0.64
14:X:2:ILE:HB	14:X:33:ALA:HB3	1.80	0.63
38:0:1060:U:OP1	51:G:85:ARG:NH2	2.30	0.63
5:O:31:C:H4'	9:S:26:MET:HE1	1.79	0.63
35:N:2178:C:P	37:C:211:LYS:HE2	2.37	0.63
38:0:1086:U:H3	38:0:1099:G:H22	1.46	0.63
46:8:46:MET:HE2	46:8:50:GLN:HE21	1.63	0.63
32:p:44:VAL:HG13	32:p:44:VAL:O	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:140:C:OP1	35:N:141:G:N2	2.30	0.63
54:J:9:GLN:HG2	54:J:60:GLU:HG2	1.81	0.63
35:N:1066:U:O2'	35:N:1074:G:N2	2.32	0.63
10:T:86:LYS:HG3	10:T:132:VAL:HG22	1.81	0.63
38:0:1527:U:OP2	58:v:39:GLU:CD	2.42	0.63
56:t:11:ILE:HG22	56:t:38:SER:HB3	1.81	0.63
16:Z:55:ARG:NH2	35:N:2469:A:O2'	2.32	0.62
2:B:25:ILE:CB	39:1:32:PHE:C	2.72	0.62
7:Q:49:GLN:HE21	7:Q:79:LEU:HB3	1.64	0.62
20:d:6:ARG:NH1	35:N:585:G:N7	2.47	0.62
38:0:972:C:OP2	47:9:59:LYS:HD3	1.98	0.62
46:8:123:ARG:NH1	46:8:124:ARG:O	2.31	0.62
35:N:693:A:O2'	35:N:1353:A:N3	2.33	0.62
3:s:132:TYR:OH	8:R:67:ARG:NH1	2.33	0.62
44:6:147:ALA:O	48:D:56:ARG:NH2	2.32	0.62
11:U:5:LEU:HD13	11:U:13:GLY:HA2	1.82	0.62
16:Z:20:LEU:HD13	25:i:81:PRO:HG2	1.82	0.62
18:b:16:ARG:NH2	18:b:19:GLN:OE1	2.33	0.62
25:i:51:GLN:HE22	25:i:86:LEU:HD21	1.65	0.62
4:M:31:U:C5'	38:0:1340:A:O2'	2.48	0.62
14:X:92:GLU:O	14:X:93:GLN:HB2	1.98	0.62
27:k:12:PRO:HB3	27:k:30:LEU:HD23	1.82	0.62
38:0:1238:A:N6	38:0:1301:U:C2	2.68	0.61
35:N:475:C:O2	35:N:479:A:N6	2.33	0.61
46:8:52:LEU:HB3	46:8:57:MET:HB3	1.81	0.61
35:N:1779:U:H5	35:N:1784:A:N7	1.99	0.61
36:L:20:ASN:ND2	36:L:37:CYS:SG	2.73	0.61
46:8:25:ASN:HA	46:8:59:GLU:HG3	1.81	0.61
35:N:1105:U:H2'	35:N:1106:G:H8	1.64	0.61
35:N:1093:G:N2	35:N:1098:A:N6	2.48	0.61
27:k:16:ASN:HA	27:k:25:THR:O	2.00	0.61
33:q:12:LYS:NZ	35:N:249:C:O2	2.33	0.61
11:U:42:LYS:HB3	11:U:46:PHE:CE2	2.36	0.60
22:f:15:GLN:NE2	35:N:1266:G:H5"	2.16	0.60
5:O:24:G:O2'	5:O:27:C:N4	2.34	0.60
35:N:613:A:H62	35:N:616:A:H61	1.50	0.60
35:N:2127:G:H4'	37:C:38:PHE:CD1	2.36	0.60
1:A:72:C:P	35:N:1942:C:O3'	2.59	0.60
12:V:135:SER:OG	35:N:1062:G:N3	2.34	0.60
4:M:75:A:C3'	35:N:2602:A:C6	2.80	0.60
23:g:28:ASN:OD1	23:g:91:GLN:NE2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:1093:G:H21	35:N:1098:A:H62	1.46	0.59
38:0:933:G:N7	44:6:3:ARG:NH1	2.49	0.59
7:Q:156:PHE:CE1	13:W:81:ILE:HD12	2.37	0.59
11:U:96:THR:HG23	11:U:112:LYS:HE2	1.84	0.59
32:p:9:VAL:HG23	35:N:1309:G:OP1	2.01	0.59
56:t:31:LEU:HB2	56:t:49:ILE:HG22	1.84	0.59
6:P:236:GLU:HG2	35:N:2600:A:N7	2.18	0.59
35:N:2849:U:O2'	35:N:2866:U:O2	2.15	0.59
39:1:141:LEU:O	39:1:145:GLU:HB2	2.02	0.59
41:3:60:LYS:HE3	41:3:195:ILE:HG22	1.84	0.59
55:K:26:ILE:O	55:K:30:LYS:HB2	2.02	0.59
38:0:946:A:H2'	38:0:947:G:C8	2.38	0.59
38:0:693:G:OP1	48:D:127:ARG:NH2	2.36	0.59
4:M:30:A:C1'	38:0:1339:A:C2	2.86	0.59
47:9:19:ASP:HA	47:9:22:THR:HG22	1.83	0.59
49:E:68:GLY:O	49:E:99:ARG:NH1	2.36	0.59
38:0:769:G:H4'	38:0:1513:A:H4'	1.84	0.59
48:D:93:ARG:HH12	58:v:25:LYS:HD3	1.68	0.59
3:s:124:TRP:HB2	22:f:85:ILE:HD11	1.84	0.59
20:d:88:VAL:HA	21:e:49:ILE:HD12	1.85	0.59
33:q:16:LYS:HE2	33:q:20:GLY:HA2	1.84	0.59
38:0:246:A:N1	38:0:278:G:O2'	2.35	0.59
38:0:1526:G:H3'	58:v:39:GLU:OE1	2.03	0.59
35:N:2128:G:H4'	37:C:218:MET:HE1	1.85	0.59
5:O:43:C:O2	9:S:92:ARG:NH2	2.36	0.59
26:j:15:ASP:OD1	35:N:2263:C:N4	2.35	0.59
35:N:1068:G:N1	35:N:1073:A:N6	2.50	0.59
40:2:40:ARG:NH1	40:2:55:ILE:O	2.36	0.59
38:0:890:G:O2'	38:0:906:A:N6	2.36	0.58
20:d:92:ARG:HG2	35:N:997:G:OP1	2.03	0.58
49:E:50:ARG:NH1	49:E:89:ASP:OD2	2.35	0.58
16:Z:66:ARG:NH1	16:Z:104:GLU:OE2	2.36	0.58
35:N:481:G:O2'	35:N:506:G:N2	2.37	0.58
38:0:1055:A:H1'	40:2:156:ARG:HH21	1.66	0.58
50:F:83:LEU:HD21	56:t:65:GLU:HG2	1.85	0.58
35:N:1019:U:N3	35:N:1142:A:N6	2.50	0.58
26:j:18:ALA:O	26:j:20:ARG:NH1	2.35	0.58
35:N:1019:U:C4	35:N:1142:A:N6	2.71	0.58
38:0:1302:C:C5	50:F:17:ILE:HD13	2.38	0.58
40:2:36:ASP:OD1	40:2:59:ARG:NH2	2.34	0.58
4:M:13:A:H4'	35:N:1924:C:H5'	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:75:A:H5”	35:N:2602:A:C4	2.24	0.58
40:2:156:ARG:HD3	40:2:193:TYR:HB3	1.86	0.58
4:M:12:C:HO2’	35:N:1923:U:H1’	1.48	0.58
35:N:1212:G:O2’	35:N:1237:A:N6	2.36	0.58
35:N:1726:C:N4	35:N:1735:A:N6	2.51	0.58
27:k:6:GLN:O	27:k:74:ARG:NH1	2.37	0.58
27:k:10:LYS:NZ	35:N:396:G:OP2	2.37	0.58
33:q:5:LYS:HE2	35:N:254:G:N7	2.19	0.58
14:X:70:ARG:NH1	35:N:2684:U:O4’	2.37	0.58
35:N:2848:G:O2’	35:N:2867:G:N2	2.36	0.58
38:0:812:G:OP1	38:0:902:G:N2	2.34	0.58
38:0:579:A:O2’	52:H:54:ARG:NH1	2.36	0.57
38:0:1224:U:O2’	38:0:1322:C:OP1	2.21	0.57
35:N:2850:A:N7	35:N:2868:A:O2’	2.35	0.57
38:0:675:A:H1’	48:D:118:HIS:CD2	2.38	0.57
41:3:91:LEU:HD13	41:3:191:LEU:HD11	1.86	0.57
4:M:12:C:H2’	35:N:1923:U:O2’	2.04	0.57
12:V:34:ASN:H	12:V:67:PHE:HE2	1.52	0.57
13:W:32:LEU:HD22	13:W:54:ILE:HG21	1.85	0.57
38:0:1316:G:H22	38:0:1319:A:H5”	1.69	0.57
11:U:43:ASN:C	11:U:47:PHE:CD2	2.81	0.57
35:N:1980:G:O2’	35:N:1982:U:OP2	2.22	0.57
37:C:201:PRO:HB2	37:C:204:ALA:HB2	1.86	0.57
6:P:144:VAL:HB	6:P:154:LEU:HB2	1.86	0.57
35:N:413:C:HO2’	35:N:1880:U:HO2’	1.52	0.57
38:0:796:C:O3’	48:D:127:ARG:NH1	2.38	0.57
3:s:150:TYR:O	3:s:154:ASN:ND2	2.35	0.57
26:j:23:VAL:HG22	26:j:38:VAL:HG22	1.87	0.57
15:Y:76:GLU:OE2	35:N:627:A:O2’	2.23	0.57
10:T:24:ILE:HD11	10:T:43:VAL:HG11	1.86	0.57
39:1:81:LYS:O	39:1:85:LEU:HB2	2.04	0.57
47:9:27:GLU:O	47:9:31:ARG:HB2	2.04	0.57
37:C:54:LYS:HD2	37:C:57:GLN:HE21	1.70	0.57
33:q:32:ILE:O	33:q:36:LYS:NZ	2.36	0.57
4:M:75:A:H3’	35:N:2602:A:H61	1.55	0.56
7:Q:46:ARG:NH2	7:Q:88:GLU:O	2.36	0.56
12:V:97:LYS:HD2	12:V:139:VAL:HG21	1.87	0.56
37:C:54:LYS:HD2	37:C:57:GLN:HG3	1.85	0.56
38:0:451:A:H61	38:0:481:G:H5’	1.70	0.56
5:O:42:C:C5	9:S:66:LEU:HD22	2.40	0.56
35:N:805:G:N2	35:N:829:A:OP1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:C:63:THR:HG22	37:C:163:TYR:HE1	1.69	0.56
11:U:132:PHE:HB2	11:U:140:ALA:HB3	1.87	0.56
27:k:72:ARG:NH2	27:k:78:TYR:OH	2.33	0.56
35:N:2506[A]:U:OP2	35:N:2576:G:N1	2.33	0.56
43:5:38:ARG:HG2	43:5:63:ASN:HB2	1.85	0.56
46:8:36:GLU:HA	46:8:40:GLY:HA3	1.87	0.56
8:R:149:ILE:HD12	8:R:175:ILE:HG21	1.88	0.56
27:k:45:ARG:HH21	27:k:47:VAL:HG22	1.71	0.56
2:B:24:LYS:HA	39:1:32:PHE:CE1	2.40	0.56
4:M:30:A:O4'	38:0:1339:A:H2	1.86	0.56
8:R:69:ARG:HG3	35:N:674:G:O2'	2.05	0.56
35:N:1332:G:N7	35:N:1609:A:O2'	2.37	0.56
37:C:213:SER:C	37:C:214:ILE:HD12	2.30	0.56
13:W:135:GLN:NE2	35:N:6:A:N3	2.53	0.56
25:i:62:THR:HG22	25:i:71:LYS:HG2	1.86	0.56
35:N:370:G:O2'	35:N:424:G:OP1	2.22	0.56
35:N:2177:C:O3'	37:C:211:LYS:CE	2.53	0.56
35:N:1726:C:H42	35:N:1735:A:N6	2.04	0.56
38:0:409:U:OP1	41:3:24:GLY:HA3	2.06	0.56
13:W:13:ARG:NH1	13:W:49:ASP:O	2.39	0.56
15:Y:111:ILE:HD12	15:Y:111:ILE:H	1.70	0.56
35:N:1315:C:O2'	35:N:1392:A:N3	2.30	0.56
32:p:31:LEU:HD22	32:p:42:LEU:HD23	1.88	0.56
32:p:34:ARG:HD3	35:N:467:G:OP2	2.05	0.56
35:N:2176:A:H5"	37:C:221:GLY:N	2.20	0.56
38:0:979:C:O2	51:G:59:ARG:NH1	2.36	0.56
6:P:2:ALA:N	6:P:199:GLU:OE1	2.39	0.55
35:N:2163:A:H2'	35:N:2164:C:H5'	1.88	0.55
48:D:93:ARG:NH2	48:D:112:ASP:OD1	2.39	0.55
9:S:140:GLU:OE2	36:L:27:THR:HG23	2.07	0.55
35:N:1724:G:O6	35:N:1737:G:C2	2.59	0.55
44:6:40:GLU:OE2	46:8:43:THR:HG23	2.06	0.55
35:N:837:C:N3	35:N:941:A:N6	2.54	0.55
38:0:673:A:H2'	38:0:674:G:C8	2.42	0.55
38:0:993:G:O2'	38:0:994:A:N7	2.40	0.55
42:4:13:GLU:OE1	42:4:68:ARG:NH2	2.39	0.55
47:9:10:LEU:HG	47:9:98:VAL:HG12	1.88	0.55
8:R:176:ASP:OD1	8:R:176:ASP:N	2.40	0.55
38:0:1368:A:OP2	46:8:114:LYS:HD3	2.05	0.55
50:F:3:ARG:O	50:F:57:ARG:NH1	2.38	0.55
37:C:67:HIS:HB2	37:C:188:ASN:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:74:THR:HA	16:Z:88:ASN:O	2.07	0.55
17:a:53:THR:HA	17:a:56:LYS:HD3	1.88	0.55
30:n:43:ILE:HG22	30:n:49:TYR:HB2	1.88	0.55
35:N:987:C:O2'	35:N:1000:A:N3	2.36	0.55
4:M:15:G:C8	4:M:15:G:C5'	2.86	0.55
16:Z:50:ARG:HD3	16:Z:65:ILE:HD11	1.87	0.54
21:e:1:MET:HA	21:e:42:ALA:O	2.07	0.54
35:N:1450:G:N2	35:N:1452:G:O6	2.40	0.54
43:5:11:HIS:HD2	43:5:12:PRO:HD2	1.72	0.54
4:M:16:C:O2	4:M:16:C:H5"	2.07	0.54
8:R:178:VAL:O	8:R:182:ALA:HB2	2.08	0.54
4:M:13:A:H4'	35:N:1924:C:C4'	2.37	0.54
38:0:1261:A:N6	38:0:1274:A:O2'	2.35	0.54
21:e:49:ILE:HB	21:e:52:PRO:HA	1.89	0.54
35:N:2156:G:C2'	35:N:2157:G:H5'	2.36	0.54
43:5:41:ASP:OD1	43:5:58:HIS:NE2	2.41	0.54
57:u:59:ASP:OD1	57:u:76:LYS:NZ	2.33	0.54
52:H:46:HIS:O	52:H:48:LYS:N	2.36	0.54
6:P:235:GLY:O	6:P:239:ASN:ND2	2.39	0.54
7:Q:13:ARG:NH1	35:N:2683:C:H4'	2.22	0.54
10:T:33:LEU:HD22	10:T:75:MET:HG2	1.89	0.54
20:d:37:GLN:HE21	35:N:1252:G:H1	1.55	0.54
35:N:299:A:N3	35:N:319:G:O2'	2.37	0.54
35:N:1536:C:O2	35:N:1537:G:N2	2.41	0.54
51:G:41:ARG:NH1	51:G:42:TRP:O	2.41	0.54
11:U:42:LYS:C	11:U:46:PHE:HD2	2.15	0.54
22:f:73:LYS:HB2	22:f:106:VAL:HB	1.90	0.54
34:r:36:ARG:HD2	34:r:37:GLN:HB2	1.89	0.54
39:1:117:LEU:HB3	39:1:141:LEU:HD11	1.89	0.54
12:V:100:LYS:HA	12:V:139:VAL:O	2.08	0.54
38:0:768:A:N3	38:0:1512:U:O2'	2.40	0.54
50:F:39:ILE:HD12	50:F:52:GLN:HE21	1.73	0.54
1:A:72:C:OP2	35:N:1943:U:P	2.66	0.53
5:O:72:G:H21	5:O:104:A:H62	1.55	0.53
35:N:2162:G:H2'	35:N:2163:A:H8	1.73	0.53
38:0:676:A:H5"	48:D:115:PRO:HB3	1.90	0.53
38:0:1166:G:N1	38:0:1169:A:OP2	2.40	0.53
9:S:143:TYR:CE2	50:F:9:ILE:HD12	2.44	0.53
30:n:53:LYS:HE2	30:n:56:ALA:HB2	1.89	0.53
35:N:306:U:O4	35:N:310:A:N7	2.41	0.53
38:0:1003:G:H21	38:0:1005:A:H5'	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:204:VAL:O	6:P:206:GLY:N	2.40	0.53
48:D:30:THR:HG21	48:D:92:GLY:HA3	1.89	0.53
50:F:77:ILE:HG22	50:F:81:MET:HE2	1.89	0.53
4:M:74:C:H2'	4:M:75:A:C1'	2.38	0.53
15:Y:21:ARG:HA	35:N:811:U:H2'	1.90	0.53
17:a:22:ARG:HG3	17:a:70:THR:HA	1.91	0.53
47:9:8:ILE:HA	47:9:99:GLN:O	2.08	0.53
6:P:160:THR:HG23	6:P:177:ARG:HG2	1.91	0.53
35:N:28:A:N6	35:N:512:G:H1'	2.23	0.53
39:1:67:ILE:HD12	39:1:160:ALA:HB3	1.91	0.53
56:t:36:ARG:NH2	56:t:75:ALA:O	2.42	0.53
38:0:927:G:O2'	38:0:1503:A:N7	2.35	0.53
38:0:1006:G:O6	38:0:1023:U:O2	2.27	0.53
35:N:1726:C:N4	35:N:1735:A:H61	2.06	0.53
13:W:56:VAL:HB	13:W:124:VAL:HG12	1.88	0.53
35:N:1936:A:H2	35:N:1943:U:H3	1.56	0.53
12:V:12:GLN:HE21	12:V:55:ILE:H	1.57	0.53
12:V:76:ALA:HA	12:V:79:LEU:HB3	1.91	0.52
14:X:43:ILE:HD12	14:X:56:ASP:HB2	1.89	0.52
26:j:41:ARG:HH11	35:N:2387:U:H1'	1.74	0.52
34:r:3:VAL:HG12	34:r:36:ARG:HE	1.73	0.52
35:N:1070:A:N7	35:N:1096:A:O2'	2.36	0.52
5:O:89:U:H6	35:N:958:U:H2'	1.74	0.52
14:X:77:ILE:HG12	19:c:72:ARG:HD2	1.90	0.52
35:N:51:G:O2'	35:N:118:A:N6	2.42	0.52
39:1:68:LEU:HD12	39:1:154:MET:HE1	1.92	0.52
48:D:111:THR:HG22	58:v:5:LYS:CA	2.39	0.52
1:A:20:U:O2'	1:A:21:A:P	2.67	0.52
9:S:116:GLY:HA3	9:S:178:ARG:HB3	1.91	0.52
17:a:114:GLU:OE1	17:a:118:ARG:NH2	2.42	0.52
39:1:80:VAL:HG12	39:1:214:LEU:HD21	1.91	0.52
48:D:109:ASN:HA	58:v:6:VAL:O	2.09	0.52
57:u:28:MET:HE1	57:u:67:ILE:HG12	1.91	0.52
6:P:3:VAL:HG12	6:P:19:VAL:HG22	1.92	0.52
15:Y:76:GLU:HG3	15:Y:111:ILE:HD13	1.91	0.52
21:e:74:ILE:HD13	35:N:992:C:H4'	1.90	0.52
38:0:263:A:OP2	57:u:74:ARG:NH1	2.42	0.52
52:H:46:HIS:C	52:H:48:LYS:H	2.17	0.52
20:d:88:VAL:HG22	21:e:49:ILE:O	2.09	0.52
24:h:86:ARG:NH1	24:h:100:SER:OG	2.42	0.52
35:N:2114:A:N3	35:N:2114:A:H2'	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1:54:LEU:HG	39:1:220:THR:HG21	1.92	0.52
42:4:99:ALA:O	42:4:102:GLY:N	2.39	0.52
30:n:4:GLN:HA	35:N:2615:U:C2	2.45	0.52
12:V:31:GLN:NE2	35:N:1097:U:O4	2.34	0.52
2:B:24:LYS:CA	39:1:32:PHE:CZ	2.91	0.52
11:U:83:LYS:HG3	11:U:91:PHE:HB3	1.92	0.52
23:g:8:LEU:HD23	23:g:50:LEU:HD21	1.91	0.52
32:p:12:ARG:NH1	35:N:465:G:OP1	2.42	0.52
38:0:76:G:H1	38:0:93:U:H3	1.56	0.52
47:9:80:THR:HG22	47:9:82:LYS:H	1.74	0.52
4:M:16:C:H4'	4:M:17:G:OP2	2.10	0.52
6:P:48:ARG:HD3	35:N:773:U:O2'	2.09	0.52
16:Z:45:GLN:NE2	35:N:2485:G:OP1	2.34	0.52
33:q:8:ARG:HH21	35:N:243:U:P	2.33	0.52
40:2:77:ILE:HA	40:2:84:VAL:HG23	1.92	0.52
55:K:42:SER:HB3	55:K:52:GLN:HE21	1.75	0.52
4:M:30:A:C4'	38:0:1339:A:C2	2.93	0.51
10:T:24:ILE:HG21	10:T:72:LEU:HD21	1.91	0.51
35:N:1070:A:H2'	35:N:1097:U:H4'	1.92	0.51
35:N:1939:U:OP1	35:N:2604:U:O2'	2.27	0.51
44:6:109:ARG:O	44:6:119:ARG:NH2	2.44	0.51
24:h:86:ARG:NH2	24:h:102:THR:OG1	2.42	0.51
35:N:877:A:O2'	35:N:900:A:N6	2.43	0.51
38:0:502:A:OP1	49:E:115:SER:HB3	2.09	0.51
46:8:19:VAL:HA	46:8:65:ILE:HG22	1.92	0.51
8:R:19:PHE:HE1	8:R:109:LEU:HD13	1.75	0.51
35:N:639:U:H2'	35:N:640:C:C6	2.45	0.51
54:J:17:MET:HG3	54:J:20:SER:HB3	1.92	0.51
8:R:2:GLU:HB3	8:R:11:ALA:HB1	1.92	0.51
32:p:29:GLN:NE2	35:N:210:C:OP1	2.40	0.51
40:2:55:ILE:HG22	40:2:68:ILE:HG12	1.92	0.51
8:R:144:GLU:HG2	8:R:166:LYS:HD2	1.92	0.51
21:e:57:GLY:HA2	21:e:102:SER:O	2.10	0.51
28:l:6:LEU:HD13	28:l:56:LEU:HD22	1.93	0.51
40:2:156:ARG:NH1	40:2:160:ALA:O	2.43	0.51
41:3:58:LYS:NZ	41:3:69:GLU:OE1	2.44	0.51
14:X:99:ILE:HD12	14:X:118:LEU:HB2	1.93	0.51
35:N:612:G:N2	35:N:614:A:O2'	2.44	0.51
54:J:59:VAL:HG21	54:J:75:LEU:HD22	1.92	0.51
4:M:13:A:H4'	35:N:1924:C:C5'	2.41	0.51
4:M:30:A:H4'	38:0:1339:A:N1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:V:117:MET:HA	35:N:1058:U:O2'	2.11	0.51
14:X:76:VAL:HG12	19:c:73:VAL:HG22	1.92	0.51
33:q:8:ARG:NH2	35:N:243:U:OP2	2.44	0.51
35:N:2638:G:O2'	35:N:2778:A:N6	2.44	0.51
38:0:401:C:O2'	38:0:621:A:N3	2.40	0.51
38:0:812:G:HO2'	38:0:813:U:H6	1.58	0.51
38:0:1527:U:OP2	58:v:39:GLU:OE2	2.28	0.51
48:D:35:THR:OG1	48:D:36:ASP:N	2.44	0.51
4:M:29:G:H4'	38:0:1230:C:OP1	2.10	0.51
6:P:220:VAL:HG21	35:N:782:A:N7	2.26	0.51
19:c:37:LYS:HD2	19:c:39:ARG:HH11	1.75	0.51
24:h:34:VAL:HG13	24:h:67:VAL:HG22	1.93	0.51
38:0:1076:U:OP1	39:1:174:LYS:NZ	2.43	0.51
4:M:56:G:C4'	9:S:75:ALA:HB1	2.41	0.51
28:l:54:LYS:HE3	35:N:72:U:OP2	2.11	0.51
30:n:17:ARG:NE	35:N:1266:G:OP2	2.40	0.51
43:5:90:MET:SD	55:K:61:ARG:NH1	2.83	0.51
54:J:31:HIS:HD2	54:J:34:TYR:H	1.59	0.51
8:R:21:ARG:HD3	8:R:106:LYS:HB3	1.93	0.50
35:N:948:C:O2	35:N:984:A:O2'	2.28	0.50
40:2:172:ARG:NH2	40:2:206:GLU:OE2	2.44	0.50
14:X:77:ILE:HG12	19:c:72:ARG:CD	2.41	0.50
6:P:165:VAL:HG21	6:P:181:MET:HE1	1.93	0.50
8:R:163:ASN:HD21	35:N:323:C:H2'	1.74	0.50
17:a:41:ALA:HB1	17:a:97:ILE:HD12	1.92	0.50
38:0:552:U:H5'	49:E:83:ARG:HH11	1.76	0.50
35:N:1297:C:O2'	35:N:1302:A:N1	2.39	0.50
35:N:2105:U:H2'	35:N:2106:U:O4'	2.12	0.50
35:N:2533:U:OP1	35:N:2665:A:O2'	2.29	0.50
37:C:183:ASP:O	37:C:187:GLU:HG2	2.12	0.50
38:0:976:G:OP2	38:0:1358:U:O2'	2.29	0.50
20:d:49:ASP:OD2	35:N:534:U:O2'	2.20	0.50
38:0:1522:U:OP1	48:D:128:ARG:NH1	2.40	0.50
49:E:34:CYS:SG	49:E:78:SER:OG	2.67	0.50
11:U:72:ILE:HG22	11:U:73:ASN:N	2.27	0.50
41:3:141:ASP:O	41:3:181:THR:HA	2.12	0.50
46:8:55:VAL:O	46:8:60:LYS:NZ	2.43	0.50
12:V:55:ILE:HG22	12:V:57:VAL:HB	1.94	0.50
21:e:27:ILE:O	21:e:66:HIS:NE2	2.42	0.50
24:h:7:ARG:NH2	24:h:26:LYS:O	2.45	0.50
36:L:37:CYS:SG	36:L:38:SER:N	2.85	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
57:u:54:MET:HE3	57:u:58:VAL:HG21	1.94	0.50
21:e:76:LYS:O	21:e:84:ARG:HA	2.11	0.50
35:N:698:C:O2'	35:N:734:A:N6	2.44	0.50
35:N:1417:C:HO2'	35:N:1587:G:HO2'	1.55	0.50
35:N:2185:U:H2'	35:N:2186:G:C8	2.47	0.50
44:6:57:SER:HB3	44:6:60:GLU:HG2	1.93	0.50
47:9:11:LYS:HA	47:9:70:HIS:O	2.12	0.50
47:9:15:HIS:HA	47:9:18:ILE:HG22	1.93	0.50
35:N:503:A:O2'	35:N:506:G:OP2	2.28	0.50
42:4:122:ASN:N	42:4:122:ASN:OD1	2.43	0.50
12:V:127:ARG:HA	12:V:130:GLU:HB2	1.94	0.49
35:N:160:A:N3	35:N:2208:C:O2'	2.44	0.49
55:K:32:TYR:HB3	55:K:55:LEU:HD21	1.93	0.49
2:B:20:ALA:N	39:1:35:ARG:NH2	2.60	0.49
17:a:32:GLU:HG2	17:a:115:LEU:HD12	1.93	0.49
29:m:3:LYS:HE2	29:m:40:ASP:HB3	1.94	0.49
30:n:3:VAL:HG23	35:N:2015:A:C6	2.47	0.49
48:D:72:ASP:O	48:D:73:ALA:HB3	2.12	0.49
4:M:16:C:O2	4:M:16:C:H2'	2.11	0.49
35:N:2113:U:H2'	35:N:2114:A:H8	1.77	0.49
24:h:51:ALA:O	24:h:54:GLN:NE2	2.44	0.49
37:C:23:ILE:HG12	37:C:224:VAL:HB	1.93	0.49
38:0:197:A:N1	38:0:220:G:O2'	2.45	0.49
39:1:176:ALA:HB1	39:1:181:ILE:HB	1.94	0.49
48:D:109:ASN:OD1	58:v:7:ARG:HA	2.12	0.49
6:P:207:LYS:HB2	35:N:729:G:C6	2.48	0.49
12:V:124:ALA:HB1	35:N:1081:U:H4'	1.93	0.49
4:M:37:U:O2'	38:0:790:A:OP1	2.30	0.49
5:O:74:U:O2	25:i:29:ILE:HD13	2.13	0.49
8:R:83:VAL:HB	8:R:86:ALA:HB2	1.95	0.49
11:U:7:ASP:HB3	11:U:9:VAL:HG23	1.94	0.49
24:h:11:VAL:HG12	24:h:72:ILE:HG22	1.93	0.49
35:N:527:C:N4	35:N:2779:U:OP2	2.44	0.49
35:N:1447:C:O2'	35:N:1544:A:N3	2.39	0.49
35:N:2540:C:O2'	35:N:2740:A:N3	2.42	0.49
21:e:7:SER:OG	21:e:8:GLY:N	2.45	0.49
35:N:1724:G:C6	35:N:1737:G:N2	2.81	0.49
35:N:2128:G:N2	35:N:2173:A:H1'	2.27	0.49
35:N:2149:U:H2'	35:N:2150:C:O4'	2.13	0.49
42:4:99:ALA:HB2	42:4:124:LEU:HG	1.94	0.49
53:I:6:LEU:HG	53:I:17:TYR:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Z:33:LEU:HD13	16:Z:117:PHE:HB3	1.95	0.49
20:d:4:VAL:HG22	35:N:1199:U:H1'	1.95	0.49
32:p:18:PHE:HA	32:p:43:THR:HG21	1.95	0.49
37:C:212:VAL:HG23	37:C:224:VAL:HG23	1.95	0.49
38:0:972:C:P	47:9:59:LYS:HD3	2.53	0.49
4:M:1:U:H2'	4:M:2:G:H8	1.78	0.49
25:i:6:ALA:HB1	25:i:40:ILE:HG23	1.95	0.49
31:o:35:GLU:HA	31:o:49:TYR:O	2.13	0.49
35:N:2106:U:H2'	35:N:2107:G:C8	2.48	0.49
35:N:2150:C:H2'	35:N:2151:U:O4'	2.13	0.49
8:R:58:LYS:HG3	8:R:71:GLY:HA2	1.95	0.48
10:T:67:THR:HG22	35:N:2748:A:H1'	1.95	0.48
18:b:40:ILE:HG12	18:b:47:VAL:HG12	1.94	0.48
21:e:71:LYS:NZ	35:N:1223:G:N7	2.61	0.48
23:g:18:GLU:OE2	35:N:1392:A:N6	2.43	0.48
32:p:33:ARG:NH2	35:N:467:G:OP1	2.46	0.48
46:8:120:LYS:HG2	46:8:123:ARG:HB3	1.94	0.48
47:9:27:GLU:O	47:9:31:ARG:CB	2.61	0.48
48:D:110:ILE:HD12	58:v:17:ARG:HD2	1.94	0.48
50:F:10:PRO:HB2	50:F:18:ALA:HB1	1.94	0.48
57:u:69:LYS:O	57:u:72:ALA:HB3	2.12	0.48
38:0:542:G:H5'	41:3:39:GLY:HA3	1.94	0.48
11:U:27:ARG:NH2	27:k:56:MET:HE2	2.29	0.48
46:8:38:TYR:HD2	46:8:39:PHE:HD1	1.61	0.48
11:U:43:ASN:HB3	11:U:47:PHE:HE2	0.74	0.48
28:l:2:LYS:HD3	35:N:77:G:OP1	2.13	0.48
35:N:1868:C:N4	35:N:1869:G:O6	2.46	0.48
49:E:64:THR:HG23	49:E:93:VAL:HG12	1.95	0.48
13:W:108:MET:HE2	35:N:1138:G:N3	2.27	0.48
15:Y:51:GLU:OE1	15:Y:60:ARG:NH1	2.46	0.48
38:0:1270:G:O2'	38:0:1313:U:O2'	2.31	0.48
39:1:141:LEU:O	39:1:145:GLU:CB	2.61	0.48
44:6:142:HIS:O	44:6:146:GLU:HB2	2.13	0.48
48:D:16:VAL:HG12	48:D:77:TYR:HB3	1.96	0.48
4:M:55:C:H4'	9:S:74:VAL:HA	1.96	0.48
15:Y:67:THR:HG21	35:N:244:A:H5"	1.95	0.48
32:p:1:MET:SD	35:N:752:A:H3'	2.53	0.48
35:N:355:U:H2'	35:N:356:G:H8	1.78	0.48
38:0:705:G:H21	48:D:31:ILE:HD11	1.78	0.48
39:1:104:TRP:O	39:1:108:ARG:N	2.47	0.48
50:F:8:ASN:HD22	50:F:22:ILE:HG13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:P:66:ASP:OD2	6:P:102:ARG:NH1	2.46	0.48
35:N:33:C:O2	35:N:447:A:N6	2.47	0.48
48:D:23:ILE:HG22	48:D:32:VAL:HG13	1.96	0.48
58:v:37:PHE:HB3	58:v:39:GLU:H	1.79	0.48
13:W:81:ILE:O	35:N:1131:G:OP1	2.32	0.48
35:N:372:G:HO2'	35:N:400:G:H1	1.60	0.48
35:N:1047:G:O2'	35:N:1111:A:N6	2.46	0.48
35:N:2139:U:H2'	35:N:2140:G:C8	2.48	0.48
35:N:2189:U:H2'	35:N:2190:G:C8	2.49	0.48
1:A:63:G:HO2'	35:N:2482:A:HO2'	1.62	0.48
6:P:167:ARG:HG2	6:P:172:VAL:HG12	1.96	0.48
20:d:51:ARG:HG2	35:N:1156:A:C8	2.49	0.48
35:N:476:G:N1	35:N:479:A:OP2	2.46	0.48
38:0:362:G:N1	38:0:365:U:OP2	2.43	0.48
38:0:1130:A:H61	38:0:1144:G:H1'	1.79	0.48
55:K:34:THR:HG23	55:K:36:SER:H	1.79	0.48
6:P:235:GLY:O	35:N:2599:G:N7	2.47	0.48
37:C:25:GLU:O	37:C:29:LEU:HG	2.13	0.48
48:D:111:THR:HG22	58:v:5:LYS:HA	1.95	0.48
4:M:16:C:H3'	4:M:17:G:C5'	2.40	0.47
6:P:132:MET:HG2	6:P:135:ILE:HD12	1.96	0.47
17:a:61:ALA:O	17:a:65:LEU:HB2	2.13	0.47
32:p:19:ARG:HG2	35:N:126:A:O5'	2.14	0.47
35:N:58:G:O2'	35:N:73:A:N1	2.46	0.47
35:N:270:A:N1	35:N:369:U:O2'	2.38	0.47
36:L:55:GLY:C	56:t:64:ASP:OD2	2.57	0.47
38:0:757:U:O2'	38:0:879:C:O2	2.31	0.47
38:0:1006:G:O6	38:0:1023:U:C2	2.67	0.47
53:I:46:LYS:HG3	53:I:47:GLU:H	1.79	0.47
1:A:72:C:OP1	35:N:1942:C:H4'	2.14	0.47
13:W:114:LEU:HG	13:W:118:MET:HE3	1.97	0.47
15:Y:57:LEU:HD22	33:q:54:ASP:HB3	1.96	0.47
23:g:22:THR:O	23:g:26:LYS:HB3	2.14	0.47
35:N:1187:G:N2	35:N:1188:U:O4	2.47	0.47
35:N:1724:G:O6	35:N:1737:G:N2	2.47	0.47
35:N:2176:A:H2'	35:N:2177:C:C6	2.49	0.47
6:P:153:GLN:O	35:N:1818:U:O2'	2.31	0.47
17:a:82:GLU:OE2	17:a:86:ARG:NH2	2.47	0.47
26:j:65:GLY:HA3	26:j:83:GLU:O	2.15	0.47
35:N:1534:U:O2'	35:N:1537:G:O6	2.29	0.47
38:0:642:A:C5	45:7:107:SER:HA	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1:136:MET:SD	39:1:139:ARG:NH2	2.87	0.47
42:4:105:ILE:HD11	42:4:115:LEU:HD23	1.96	0.47
1:A:20:U:HO2'	1:A:21:A:P	2.38	0.47
15:Y:81:ASP:HB2	15:Y:100:ILE:HD11	1.96	0.47
35:N:219:A:N3	35:N:234:U:O2'	2.41	0.47
9:S:42:GLU:OE1	9:S:148:ARG:NH1	2.48	0.47
35:N:1028:A:N3	35:N:2486:C:O2'	2.42	0.47
35:N:1847:A:O2'	35:N:1848:A:H8	1.98	0.47
37:C:171:ILE:HD13	37:C:196:LEU:HD11	1.96	0.47
38:0:812:G:O2'	38:0:813:U:H6	1.96	0.47
41:3:95:GLU:HA	41:3:100:ASN:ND2	2.29	0.47
24:h:45:HIS:HB3	24:h:58:ILE:HG12	1.95	0.47
26:j:19:LYS:NZ	35:N:2261:C:OP1	2.33	0.47
30:n:6:ASN:ND2	35:N:2020:A:H62	2.12	0.47
35:N:84:A:N1	35:N:98:G:O2'	2.46	0.47
35:N:1783:A:H5'	35:N:2608:G:H4'	1.95	0.47
38:0:1073:U:O2	39:1:103:ASN:ND2	2.48	0.47
38:0:1302:C:C6	50:F:17:ILE:HD13	2.50	0.47
39:1:81:LYS:O	39:1:85:LEU:CB	2.62	0.47
22:f:90:LYS:NZ	35:N:746:U:O2'	2.47	0.47
35:N:1475:G:H1'	35:N:1732:C:H41	1.79	0.47
35:N:1853:A:N3	35:N:2233:U:O2'	2.43	0.47
35:N:2506[A]:U:OP2	35:N:2576:G:N2	2.47	0.47
37:C:163:TYR:CD2	37:C:171:ILE:HD11	2.50	0.47
38:0:35:G:O2'	49:E:115:SER:O	2.31	0.47
38:0:674:G:P	43:5:86:ARG:HH22	2.38	0.47
42:4:153:VAL:HG12	42:4:156:LYS:HZ1	1.79	0.47
43:5:88:MET:HE3	55:K:64:TYR:CD2	2.49	0.47
15:Y:111:ILE:HD11	35:N:636:G:C6	2.49	0.47
35:N:528:A:C2	35:N:2042:A:H2'	2.50	0.47
35:N:2243:U:H2'	35:N:2244:U:C6	2.50	0.47
51:G:89:MET:HE1	51:G:98:LYS:HD3	1.96	0.47
19:c:26:VAL:O	19:c:44:GLU:HA	2.14	0.47
26:j:41:ARG:NH1	35:N:2262:U:OP1	2.47	0.47
30:n:25:VAL:HG21	30:n:28:LEU:HD23	1.97	0.47
32:p:12:ARG:CZ	32:p:44:VAL:HG21	2.45	0.47
35:N:2006:C:O2'	35:N:2823:A:N3	2.48	0.47
37:C:3:LYS:HG3	37:C:4:LEU:N	2.25	0.47
38:0:677:U:H3	38:0:713:G:H22	1.62	0.47
38:0:1227:A:OP2	50:F:95:LEU:HD21	2.15	0.47
20:d:16:LYS:NZ	35:N:1227:G:OP2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:h:41:LEU:HA	24:h:61:LYS:O	2.15	0.47
35:N:910:A:H2'	35:N:911:A:C8	2.49	0.47
46:8:28:ILE:HD11	46:8:57:MET:HE1	1.96	0.47
55:K:51:TYR:O	55:K:55:LEU:HB2	2.15	0.47
16:Z:57:VAL:HG13	16:Z:116:ALA:HB2	1.96	0.46
16:Z:136:MET:HE3	25:i:57:TYR:HB3	1.96	0.46
49:E:38:TYR:HB2	49:E:52:VAL:O	2.15	0.46
7:Q:35:THR:HG22	7:Q:73:VAL:HG11	1.96	0.46
19:c:29:LYS:HD3	19:c:40:LEU:HD21	1.97	0.46
34:r:11:CYS:SG	34:r:14:CYS:N	2.88	0.46
35:N:2029:G:N1	35:N:2033:A:OP2	2.34	0.46
38:0:928:G:O2'	38:0:1533:C:OP1	2.34	0.46
41:3:58:LYS:HD3	41:3:203:LEU:HD23	1.98	0.46
7:Q:81:GLU:OE1	35:N:2635:A:O2'	2.30	0.46
7:Q:146:ILE:HG21	7:Q:146:ILE:HD13	1.62	0.46
12:V:30:GLN:OE1	35:N:1095:A:N6	2.48	0.46
18:b:31:THR:O	18:b:102:ARG:NH1	2.41	0.46
22:f:38:TYR:CD2	30:n:28:LEU:HD22	2.50	0.46
33:q:5:LYS:CE	35:N:254:G:N7	2.79	0.46
35:N:1999:C:O3'	35:N:2722:G:N2	2.48	0.46
35:N:2126:A:H2'	35:N:2162:G:C2	2.50	0.46
35:N:2177:C:O2'	37:C:170:ILE:HG12	2.15	0.46
37:C:55:SER:O	37:C:58:ASN:ND2	2.48	0.46
40:2:108:LYS:HD3	40:2:111:LEU:HD12	1.96	0.46
15:Y:41:ARG:NH1	35:N:807:U:OP2	2.48	0.46
16:Z:9:PHE:HZ	35:N:911:A:H2'	1.80	0.46
16:Z:42:THR:HG22	16:Z:93:VAL:HG12	1.97	0.46
35:N:675:A:N3	35:N:2443:C:O2'	2.47	0.46
35:N:2273:A:H2'	35:N:2274:A:C8	2.50	0.46
35:N:2776:A:O5'	35:N:2776:A:H8	1.97	0.46
38:0:618:C:O2'	53:I:14:ARG:NH2	2.47	0.46
40:2:65:ARG:O	40:2:65:ARG:HG3	2.16	0.46
56:t:50:ALA:HB1	56:t:57:HIS:HB3	1.97	0.46
8:R:77:ILE:HD13	8:R:77:ILE:HG21	1.24	0.46
11:U:24:GLY:O	11:U:28:ASN:HB2	2.15	0.46
17:a:44:LEU:HD23	17:a:113:ILE:HD13	1.97	0.46
35:N:715:A:C1'	52:H:40:GLN:CD	2.65	0.46
41:3:140:ASN:N	41:3:182:PHE:O	2.49	0.46
13:W:31:GLU:HG2	13:W:142:ILE:HG12	1.97	0.46
20:d:37:GLN:NE2	35:N:1252:G:H22	2.14	0.46
35:N:548:G:H5"	35:N:549:G:H5'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:N:1266:G:O2'	35:N:2012:G:O6	2.22	0.46
38:0:254:G:O3'	54:J:71:LYS:NZ	2.47	0.46
38:0:1006:G:C6	38:0:1023:U:O2	2.68	0.46
38:0:1218:C:H2'	38:0:1219:A:C8	2.51	0.46
39:1:207:ILE:HA	39:1:210:VAL:HG22	1.96	0.46
40:2:155:GLY:HA2	40:2:163:ALA:HB1	1.98	0.46
6:P:260:ASN:ND2	6:P:263:THR:OG1	2.48	0.46
12:V:107:GLN:O	12:V:111:GLN:HB2	2.15	0.46
25:i:48:MET:SD	25:i:51:GLN:NE2	2.89	0.46
35:N:2104:C:H2'	35:N:2105:U:C6	2.51	0.46
37:C:163:TYR:HB2	37:C:171:ILE:HD11	1.97	0.46
6:P:251:GLN:NE2	6:P:252:THR:O	2.48	0.46
20:d:11:ARG:HA	20:d:11:ARG:HD2	1.81	0.46
20:d:97:ASP:OD2	21:e:13:ARG:NE	2.47	0.46
35:N:503:A:H4'	35:N:504:A:H5'	1.97	0.46
35:N:715:A:N6	52:H:53:ARG:NH1	2.64	0.46
35:N:857:G:N2	35:N:2269:G:O4'	2.49	0.46
35:N:1064:C:N4	35:N:1070:A:OP2	2.49	0.46
37:C:163:TYR:HD2	37:C:171:ILE:HD11	1.79	0.46
38:0:71:A:N1	38:0:99:C:O2'	2.47	0.46
38:0:261:U:OP2	57:u:74:ARG:NH2	2.47	0.46
43:5:62:MET:HG2	43:5:64:VAL:HG23	1.97	0.46
47:9:10:LEU:O	47:9:71:LEU:HA	2.15	0.46
9:S:140:GLU:CD	36:L:27:THR:HG23	2.41	0.46
35:N:1078:U:O2'	35:N:1088:A:OP1	2.34	0.46
38:0:999:C:N3	38:0:1042:A:N6	2.63	0.46
38:0:1126:U:OP1	47:9:7:ARG:NH2	2.49	0.46
42:4:18:VAL:HA	42:4:34:THR:O	2.16	0.46
20:d:37:GLN:HE21	35:N:1252:G:H22	1.62	0.46
35:N:2141:G:H2'	35:N:2142:A:C8	2.48	0.46
36:L:13:THR:HA	36:L:23:LYS:HA	1.97	0.46
39:1:53:ALA:O	39:1:57:LEU:HB2	2.16	0.46
47:9:12:ALA:HB3	47:9:18:ILE:HB	1.98	0.46
9:S:24:SER:HB3	9:S:27:GLN:HB2	1.97	0.45
19:c:92:VAL:HG21	19:c:97:LEU:HD21	1.98	0.45
21:e:34:GLU:HG2	21:e:60:LYS:HG2	1.98	0.45
30:n:4:GLN:NE2	35:N:2016:U:O2	2.49	0.45
35:N:1509:A:H2'	35:N:1510:G:C8	2.50	0.45
35:N:2183:A:H2'	35:N:2184:A:C8	2.51	0.45
38:0:309:A:H2'	38:0:310:G:H8	1.81	0.45
6:P:155:ALA:HB2	6:P:162:VAL:HG23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:131:GLY:HA3	35:N:2305:U:H5”	1.98	0.45
35:N:1176:U:H2’	35:N:1177:G:C8	2.51	0.45
38:0:1106:G:O2’	40:2:169:ARG:NH1	2.50	0.45
42:4:89:HIS:CD2	42:4:90:THR:H	2.33	0.45
9:S:74:VAL:HG22	9:S:79:ILE:HD11	1.97	0.45
35:N:2186:G:H2’	35:N:2187:U:O4’	2.16	0.45
38:0:523:A:N1	49:E:89:ASP:HB2	2.31	0.45
38:0:1067:A:N1	38:0:1108:G:O2’	2.34	0.45
38:0:1255:G:O2’	38:0:1258:G:N3	2.46	0.45
39:1:100:MET:HA	39:1:107:VAL:HG21	1.99	0.45
42:4:133:PRO:HA	42:4:136:VAL:HG12	1.98	0.45
49:E:114:ARG:HG2	49:E:119:VAL:HB	1.99	0.45
16:Z:55:ARG:NH2	35:N:2469:A:O3’	2.49	0.45
19:c:29:LYS:HB2	19:c:83:SER:HB2	1.98	0.45
32:p:1:MET:HE2	32:p:1:MET:HB3	1.83	0.45
34:r:1:MET:HE2	34:r:34:LYS:HD3	1.98	0.45
34:r:7:VAL:HG22	34:r:38:GLY:HA3	1.99	0.45
35:N:284:U:O4	35:N:356:G:O6	2.33	0.45
35:N:1900:A:H1’	35:N:1970:A:H2’	1.97	0.45
35:N:2180:U:H2’	35:N:2181:U:O4’	2.16	0.45
35:N:2514:U:H2’	35:N:2515:C:C6	2.51	0.45
38:0:297:G:N2	38:0:300:A:OP2	2.47	0.45
38:0:1356:G:H2’	38:0:1357:A:C8	2.51	0.45
39:1:53:ALA:O	39:1:57:LEU:CB	2.65	0.45
42:4:107:ALA:HA	42:4:125:ALA:HB3	1.99	0.45
48:D:49:GLY:O	48:D:69:ARG:NH1	2.50	0.45
1:A:12:U:C5’	35:N:1915:U:H4’	2.47	0.45
12:V:79:LEU:HD21	12:V:109:ILE:HG21	1.99	0.45
15:Y:54:GLN:HE21	35:N:2428:G:N2	2.14	0.45
35:N:1733:G:H2’	35:N:1734:G:C8	2.51	0.45
6:P:182:ARG:NH1	35:N:1800:C:OP2	2.49	0.45
13:W:82:GLY:HA2	35:N:1131:G:OP1	2.17	0.45
35:N:306:U:H3	35:N:310:A:H62	0.61	0.45
35:N:499:U:O4	35:N:503:A:N7	2.49	0.45
38:0:1101:A:H61	39:1:102:THR:HG21	1.81	0.45
42:4:80:THR:OG1	42:4:81:LEU:N	2.50	0.45
43:5:51:ILE:HG21	43:5:51:ILE:HD13	1.64	0.45
8:R:148:ILE:HB	8:R:169:VAL:HG22	1.98	0.45
15:Y:82:LEU:HA	15:Y:85:VAL:HG13	1.99	0.45
21:e:3:ALA:HA	21:e:40:MET:O	2.17	0.45
35:N:1363:C:O2’	35:N:1809:A:N3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:L:8:LYS:HA	36:L:8:LYS:HD3	1.82	0.45
37:C:45:ALA:HA	37:C:172:HIS:CD2	2.52	0.45
38:0:1096:C:O2	38:0:1170:A:O2'	2.34	0.45
38:0:1113:C:H4'	40:2:14:ILE:HD12	1.97	0.45
5:O:7:G:H5'	18:b:29:HIS:CE1	2.51	0.45
11:U:72:ILE:HG22	11:U:73:ASN:H	1.81	0.45
12:V:33:VAL:HG13	12:V:59:ILE:HG21	1.97	0.45
35:N:1794:A:H2'	35:N:1795:C:C6	2.52	0.45
37:C:5:THR:OG1	37:C:6:LYS:N	2.49	0.45
53:I:70:ARG:HA	53:I:70:ARG:HD2	1.62	0.45
44:6:56:LYS:HE3	44:6:60:GLU:HG3	1.99	0.45
16:Z:123:LYS:HE3	35:N:2483:C:N3	2.32	0.45
20:d:88:VAL:HA	21:e:49:ILE:CD1	2.47	0.45
35:N:881:G:N2	35:N:895:U:O2	2.49	0.45
38:0:1178:G:C5	46:8:99:ARG:NH2	2.86	0.45
53:I:38:PHE:CE1	53:I:51:ARG:HG2	2.52	0.45
15:Y:33:ARG:NH1	35:N:587:C:O2	2.46	0.44
16:Z:118:LYS:HE3	16:Z:118:LYS:HB3	1.84	0.44
19:c:63:LYS:HE3	19:c:65:SER:HB2	1.99	0.44
35:N:1311:G:N2	35:N:1603:A:H62	2.14	0.44
37:C:184:LYS:O	37:C:188:ASN:ND2	2.50	0.44
38:0:1062:U:H2'	38:0:1063:C:C6	2.52	0.44
38:0:1093:A:O2'	38:0:1095:U:OP1	2.29	0.44
3:s:155:SER:HB3	35:N:2061:G:H22	1.81	0.44
4:M:30:A:C4'	38:0:1339:A:N1	2.80	0.44
16:Z:9:PHE:CZ	35:N:911:A:H2'	2.52	0.44
28:l:20:ASN:HB3	28:l:50:VAL:HG22	2.00	0.44
32:p:35:ARG:HG3	32:p:42:LEU:HD21	1.98	0.44
35:N:2123:G:H2'	35:N:2124:G:C8	2.52	0.44
38:0:825:A:H4'	45:7:3:MET:HE2	1.99	0.44
41:3:100:ASN:OD1	41:3:111:ARG:NH1	2.51	0.44
46:8:106:ARG:NH1	46:8:107:ASP:O	2.50	0.44
58:v:17:ARG:H	58:v:17:ARG:HD3	1.82	0.44
3:s:153:LEU:C	3:s:153:LEU:HD23	2.43	0.44
7:Q:43:ASP:OD1	35:N:2784:U:H4'	2.17	0.44
18:b:29:HIS:HB3	18:b:36:TYR:HB2	2.00	0.44
28:l:13:GLU:HA	28:l:16:THR:HG22	1.99	0.44
35:N:569:U:H5"	35:N:821:A:C2	2.52	0.44
35:N:613:A:N7	35:N:616:A:C6	2.85	0.44
38:0:9:G:OP2	42:4:126:LYS:HD2	2.18	0.44
38:0:352:C:O2'	38:0:354:G:OP1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:3:95:GLU:HG3	41:3:191:LEU:HD22	2.00	0.44
55:K:71:THR:HG23	55:K:73:ARG:H	1.82	0.44
3:s:153:LEU:HD21	35:N:2585:U:O2'	2.17	0.44
12:V:11:LEU:HD11	12:V:28:LEU:HB3	1.99	0.44
14:X:99:ILE:HD13	14:X:115:ILE:HG23	1.99	0.44
16:Z:40:ARG:HD3	16:Z:93:VAL:HG21	2.00	0.44
30:n:16:ARG:HA	35:N:2046:G:H5'	1.99	0.44
31:o:40:ASP:O	31:o:44:ARG:N	2.50	0.44
35:N:45:G:H5"	35:N:46:G:H5'	1.97	0.44
37:C:166:ASP:OD1	37:C:170:ILE:N	2.47	0.44
38:0:1074:G:O2'	38:0:1101:A:N1	2.44	0.44
39:1:163:VAL:HG21	39:1:173:ILE:HD11	1.98	0.44
46:8:16:ALA:O	46:8:67:VAL:HA	2.17	0.44
20:d:31:VAL:HG13	35:N:580:U:O3'	2.17	0.44
28:l:1:MET:HG2	28:l:4:LYS:HD3	2.00	0.44
35:N:500:G:N1	35:N:503:A:OP2	2.42	0.44
35:N:2130:U:H5'	35:N:2159:G:N2	2.33	0.44
4:M:13:A:H4'	35:N:1924:C:H4'	2.00	0.44
12:V:11:LEU:HD23	35:N:1097:U:O2	2.16	0.44
13:W:113:PRO:HD2	35:N:558:U:P	2.58	0.44
38:0:841:C:H2'	38:0:843:U:H5"	2.00	0.44
38:0:971:G:O6	38:0:1364:U:O2'	2.35	0.44
6:P:19:VAL:HG23	6:P:203:ARG:HB3	1.99	0.44
6:P:145:GLU:HB2	6:P:188:CYS:HB3	1.98	0.44
8:R:165:HIS:CD2	35:N:1205:A:C5	3.06	0.44
10:T:66:GLY:O	10:T:69:ARG:HB3	2.17	0.44
10:T:85:LYS:HG2	10:T:141:ILE:HD12	1.99	0.44
53:I:6:LEU:HD12	53:I:19:VAL:HB	1.99	0.44
4:M:30:A:H1'	38:0:1339:A:C2	2.53	0.44
6:P:141:VAL:HG13	6:P:190:ALA:HB1	1.99	0.44
7:Q:37:VAL:HG22	7:Q:48:ILE:HG22	2.00	0.44
8:R:165:HIS:CD2	35:N:1205:A:C6	3.05	0.44
10:T:9:VAL:HB	10:T:50:LEU:HB2	2.00	0.44
31:o:21:TYR:HE2	31:o:38:LYS:HB3	1.83	0.44
38:0:620:C:C2	41:3:132:ILE:HD13	2.53	0.44
38:0:714:G:H2'	38:0:715:A:C8	2.53	0.44
38:0:1321:U:O2'	56:t:78:ARG:NH1	2.51	0.44
41:3:62:ARG:HH21	41:3:68:LEU:HA	1.82	0.44
12:V:133:ALA:O	12:V:138:LEU:N	2.51	0.44
19:c:53:ARG:NH2	35:N:2720:U:OP1	2.51	0.44
20:d:113:ALA:O	20:d:117:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:k:37:ARG:HG2	27:k:46:PHE:HB3	1.99	0.44
35:N:1769:U:O2'	35:N:1958:C:OP1	2.36	0.44
38:0:296:U:O2'	38:0:556:C:O2	2.33	0.44
38:0:481:G:O2'	38:0:483:C:N4	2.50	0.44
38:0:552:U:H5'	49:E:83:ARG:NH1	2.32	0.44
38:0:1317:C:H4'	51:G:49:GLN:HE21	1.83	0.44
43:5:70:VAL:HA	43:5:73:GLU:HG2	1.99	0.44
7:Q:4:LEU:HD21	7:Q:96:ILE:HG22	1.99	0.43
35:N:514:A:N3	35:N:581:C:O2'	2.44	0.43
35:N:1072:C:H42	35:N:1098:A:N6	2.16	0.43
38:0:1060:U:P	51:G:85:ARG:HH22	2.41	0.43
38:0:1064:G:O2'	38:0:1190:G:N2	2.51	0.43
38:0:1379:G:O6	44:6:2:PRO:HB2	2.17	0.43
7:Q:149:ASN:HD22	35:N:2572:A:H2'	1.81	0.43
35:N:299:A:N1	35:N:322:A:O2'	2.46	0.43
35:N:1077:A:N6	35:N:1089:A:OP1	2.46	0.43
42:4:114:VAL:O	42:4:118:ALA:HB2	2.18	0.43
44:6:59:LEU:O	44:6:63:GLU:HB2	2.18	0.43
44:6:71:PRO:O	44:6:96:ARG:NH1	2.51	0.43
44:6:107:ALA:HB1	44:6:133:THR:HB	2.00	0.43
6:P:61:ALA:O	6:P:63:ARG:NH2	2.52	0.43
6:P:85:PRO:HG3	35:N:1567:G:H2'	2.00	0.43
6:P:201:MET:HG3	6:P:202:LEU:HD12	2.00	0.43
7:Q:109:VAL:HG22	7:Q:203:VAL:HG22	2.00	0.43
26:j:33:ALA:N	26:j:64:ASP:OD1	2.51	0.43
35:N:2092:U:N3	35:N:2226:C:OP2	2.44	0.43
38:0:723:U:C5'	58:v:49:LYS:HE2	2.48	0.43
38:0:1026:G:C6	38:0:1035:A:C6	3.06	0.43
34:r:19:ARG:NE	35:N:2756:U:OP2	2.43	0.43
38:0:766:A:OP2	38:0:812:G:N2	2.50	0.43
38:0:1143:G:H2'	38:0:1144:G:H8	1.83	0.43
38:0:1507:A:H2'	38:0:1508:A:C8	2.53	0.43
39:1:186:ILE:HB	39:1:213:TYR:CZ	2.54	0.43
27:k:17:ASN:HB2	27:k:25:THR:HB	1.99	0.43
33:q:33:LEU:HB2	35:N:2420:C:OP2	2.19	0.43
35:N:221:A:N1	35:N:265:A:O2'	2.51	0.43
35:N:372:G:O2'	35:N:400:G:N1	2.50	0.43
35:N:2177:C:H4'	37:C:211:LYS:NZ	2.26	0.43
44:6:73:VAL:HG12	44:6:90:GLU:HA	2.00	0.43
45:7:49:PHE:HA	45:7:60:GLU:O	2.19	0.43
51:G:53:ARG:HH11	51:G:53:ARG:HD3	1.62	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:t:4:SER:HB3	56:t:5:LEU:HD12	2.00	0.43
10:T:94:TYR:HA	10:T:106:SER:O	2.19	0.43
11:U:44:ILE:O	11:U:48:GLU:HG3	2.17	0.43
35:N:2291:U:H2'	35:N:2292:U:C6	2.54	0.43
36:L:11:GLU:HA	36:L:25:ARG:HA	2.01	0.43
38:0:1080:A:OP1	42:4:52:LYS:HD2	2.18	0.43
38:0:1081:A:H5'	42:4:23:LYS:HG3	2.01	0.43
57:u:51:PHE:HA	57:u:54:MET:HG2	2.01	0.43
57:u:67:ILE:HG13	57:u:71:LYS:HD3	2.00	0.43
7:Q:45:TYR:OH	35:N:2636:C:O2'	2.07	0.43
15:Y:100:ILE:HG21	15:Y:100:ILE:HD13	1.75	0.43
22:f:77:ASP:HB2	22:f:102:HIS:HB2	2.00	0.43
35:N:629:G:N3	35:N:639:U:O2'	2.52	0.43
50:F:16:VAL:HG23	50:F:17:ILE:HG13	2.00	0.43
9:S:37:ASN:ND2	35:N:2313:C:O4'	2.52	0.43
9:S:105:THR:HG21	36:L:22:MET:SD	2.59	0.43
25:i:75:GLN:HB2	25:i:92:VAL:HG23	2.01	0.43
35:N:2170:A:H2'	35:N:2171:A:O4'	2.19	0.43
35:N:2602:A:H4'	35:N:2603:G:H5'	2.00	0.43
36:L:30:HIS:ND1	36:L:31:ASP:O	2.52	0.43
38:0:723:U:H5"	58:v:49:LYS:HE2	2.01	0.43
38:0:838:G:H2'	38:0:839:C:C6	2.54	0.43
39:1:166:ALA:HB3	39:1:191:SER:HB3	2.00	0.43
40:2:153:VAL:HG12	40:2:198:VAL:HG22	2.01	0.43
52:H:35:GLN:HE21	52:H:39:LEU:HD13	1.84	0.43
7:Q:13:ARG:HD2	7:Q:15:PHE:CZ	2.53	0.43
14:X:63:VAL:HG12	14:X:107:LEU:HD21	2.00	0.43
35:N:2174:C:O2'	35:N:2175:C:H5'	2.19	0.43
35:N:2458:G:O2'	35:N:2460:U:O4	2.34	0.43
38:0:1380:U:O2	38:0:1382:C:N4	2.49	0.43
47:9:83:THR:O	47:9:87:LEU:CB	2.58	0.43
6:P:161:TYR:HB3	6:P:194:GLU:HB3	2.01	0.43
30:n:8:PRO:HD2	35:N:1263:U:O2'	2.19	0.43
35:N:33:C:N4	35:N:446:G:O2'	2.46	0.43
35:N:537:G:O2'	35:N:556:A:N6	2.50	0.43
38:0:71:A:H61	38:0:99:C:H1'	1.83	0.43
38:0:537:G:H5"	49:E:110:ARG:HH12	1.84	0.43
39:1:15:HIS:HB2	39:1:203:ASN:HD22	1.84	0.43
5:O:72:G:N2	5:O:104:A:H62	2.17	0.42
7:Q:19:GLY:HA3	19:c:80:VAL:HG23	2.00	0.42
9:S:175:PHE:HA	9:S:176:PRO:HD3	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:a:3:HIS:O	17:a:4:ARG:HB2	2.17	0.42
17:a:37:THR:HG22	17:a:110:MET:HE1	2.00	0.42
26:j:37:ILE:HG22	26:j:38:VAL:HG23	2.01	0.42
35:N:828:U:H2'	35:N:829:A:C8	2.53	0.42
35:N:2541:A:HO2'	35:N:2765:A:H2	1.67	0.42
37:C:42:VAL:HG12	37:C:216:THR:HG22	2.00	0.42
38:0:228:A:C4'	53:I:63:GLN:HE21	2.32	0.42
41:3:95:GLU:HA	41:3:100:ASN:HD22	1.84	0.42
44:6:105:VAL:O	44:6:109:ARG:HG2	2.19	0.42
57:u:33:LYS:O	57:u:37:ALA:HB3	2.19	0.42
4:M:1:U:H2'	4:M:2:G:C8	2.54	0.42
7:Q:152:PRO:HG2	7:Q:156:PHE:CZ	2.55	0.42
14:X:77:ILE:HG21	14:X:77:ILE:HD13	1.75	0.42
17:a:90:ARG:HD2	35:N:2880:C:O2'	2.18	0.42
31:o:23:THR:OG1	31:o:24:THR:N	2.52	0.42
35:N:320:A:H4'	35:N:322:A:C8	2.54	0.42
35:N:932:U:O2'	35:N:934:U:O4	2.36	0.42
38:0:135:C:O2	53:I:1:MET:HB2	2.20	0.42
38:0:555:U:H2'	38:0:556:C:C6	2.54	0.42
38:0:1119:C:H2'	38:0:1120:C:H6	1.84	0.42
38:0:1404:C:O2	38:0:1519:A:O2'	2.36	0.42
38:0:1530:G:H2'	38:0:1531:A:C8	2.54	0.42
41:3:109:ALA:HA	41:3:161:LEU:HD11	2.00	0.42
7:Q:149:ASN:ND2	35:N:2572:A:H2'	2.35	0.42
12:V:24:VAL:HG12	35:N:1070:A:H61	1.83	0.42
15:Y:77:ILE:CD1	15:Y:108:ALA:HB1	2.48	0.42
17:a:3:HIS:CD2	35:N:2820:A:H4'	2.54	0.42
38:0:228:A:H5'	53:I:63:GLN:NE2	2.34	0.42
38:0:1380:U:C5	44:6:3:ARG:HA	2.54	0.42
10:T:16:ASP:O	10:T:26:ILE:HA	2.19	0.42
11:U:66:ASN:CG	11:U:135:HIS:HD2	2.26	0.42
35:N:749:A:N1	35:N:753:A:O2'	2.43	0.42
38:0:844:G:C5	38:0:846:G:H4'	2.55	0.42
41:3:157:ALA:O	41:3:160:GLU:HB3	2.19	0.42
43:5:90:MET:HE3	43:5:90:MET:HB2	1.92	0.42
4:M:55:C:O3'	9:S:75:ALA:CB	2.67	0.42
27:k:31:PRO:HG2	27:k:33:LEU:HD13	2.01	0.42
35:N:247:G:OP2	35:N:249:C:N4	2.47	0.42
35:N:373:U:H2'	35:N:374:A:H8	1.84	0.42
35:N:1075:C:H2'	35:N:1076:C:C6	2.54	0.42
37:C:7:ARG:O	37:C:11:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:1118:U:H2'	38:0:1119:C:H6	1.85	0.42
39:1:21:ARG:HG3	39:1:22:TYR:CD2	2.55	0.42
57:u:33:LYS:O	57:u:37:ALA:CB	2.68	0.42
7:Q:1:MET:HG2	7:Q:205:PRO:HG2	2.00	0.42
14:X:121:GLU:HG3	19:c:66:ASN:HD21	1.85	0.42
20:d:37:GLN:NE2	35:N:1252:G:H1	2.17	0.42
37:C:60:ARG:HE	37:C:162:ARG:HH11	1.68	0.42
38:0:269:C:H2'	38:0:270:A:C8	2.54	0.42
38:0:509:A:N3	38:0:543:U:O2'	2.49	0.42
38:0:1101:A:H61	39:1:102:THR:CG2	2.32	0.42
42:4:112:ARG:O	42:4:116:GLU:HB2	2.19	0.42
2:B:20:ALA:N	39:1:35:ARG:HH21	2.07	0.42
4:M:9:C:O2'	4:M:44:A:O2'	2.33	0.42
6:P:146:MET:HE1	35:N:1800:C:C5'	2.50	0.42
7:Q:25:THR:HG21	7:Q:193:VAL:HG22	2.00	0.42
14:X:70:ARG:NH2	35:N:2683:C:O2	2.52	0.42
20:d:112:LYS:HG3	21:e:48:LYS:HE2	2.01	0.42
21:e:81:LYS:HD2	35:N:973:A:OP2	2.20	0.42
31:o:9:ILE:HG22	31:o:53:LYS:HB2	2.00	0.42
35:N:81:G:HO2'	35:N:295:G:HO2'	1.61	0.42
35:N:1058:U:H2'	35:N:1059:G:C8	2.55	0.42
38:0:713:G:H2'	38:0:714:G:C8	2.54	0.42
45:7:18:GLN:NE2	45:7:70:ALA:HB1	2.35	0.42
55:K:21:ILE:HD12	55:K:22:ASP:HB2	2.01	0.42
57:u:56:PRO:O	57:u:60:ARG:HB2	2.20	0.42
4:M:12:C:H4'	35:N:1922:G:N2	2.31	0.42
9:S:140:GLU:HA	36:L:28:VAL:HG22	2.01	0.42
14:X:7:MET:HB3	14:X:18:ARG:HD2	2.02	0.42
14:X:49:ARG:HH21	38:0:1422:G:H4'	1.85	0.42
22:f:85:ILE:HA	22:f:94:ASP:O	2.19	0.42
32:p:16:HIS:ND1	35:N:684:G:OP1	2.48	0.42
35:N:285:G:O6	35:N:355:U:O2	2.36	0.42
35:N:2175:C:OP1	37:C:8:MET:HG2	2.20	0.42
49:E:34:CYS:HA	49:E:55:VAL:HA	2.01	0.42
15:Y:30:THR:O	15:Y:32:GLY:N	2.52	0.42
17:a:28:LEU:HD23	17:a:48:VAL:HG21	2.01	0.42
32:p:19:ARG:NH2	35:N:125:A:OP2	2.53	0.42
33:q:54:ASP:OD2	35:N:2359:C:O2'	2.30	0.42
35:N:1875:G:O3'	37:C:205:LYS:HE3	2.13	0.42
37:C:46:VAL:HG13	37:C:212:VAL:HG12	2.01	0.42
38:0:839:C:H2'	38:0:840:C:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:1306:A:N6	38:0:1331:G:H1’	2.35	0.42
49:E:50:ARG:HG3	49:E:90:LEU:HD11	2.01	0.42
57:u:79:LEU:HD23	57:u:79:LEU:HA	1.83	0.42
7:Q:154:LYS:HE2	35:N:2024:G:O3’	2.20	0.42
9:S:112:ARG:NH2	9:S:113:ASP:OD2	2.53	0.42
11:U:78:VAL:HG23	11:U:142:VAL:HG11	2.01	0.42
22:f:93:ALA:HB2	35:N:1614:A:C2	2.55	0.42
32:p:44:VAL:O	32:p:44:VAL:CG1	2.67	0.42
35:N:1173:U:H3’	35:N:1174:U:H4’	2.02	0.42
35:N:1394:U:H4’	35:N:1603:A:H4’	2.02	0.42
38:0:96:U:H2’	38:0:97:G:C8	2.54	0.42
38:0:1216:A:H5”	51:G:5:SER:HB2	2.02	0.42
38:0:1300:G:O2’	38:0:1301:U:O5’	2.38	0.42
55:K:26:ILE:HG21	55:K:67:LEU:HB3	2.01	0.42
57:u:28:MET:HE3	57:u:58:VAL:HG22	2.02	0.42
6:P:16:VAL:HG22	6:P:206:GLY:HA3	2.02	0.41
7:Q:156:PHE:CD1	13:W:81:ILE:HD12	2.55	0.41
13:W:96:ARG:HH21	13:W:99:ARG:HG2	1.84	0.41
16:Z:136:MET:SD	25:i:75:GLN:O	2.78	0.41
32:p:34:ARG:HD3	32:p:34:ARG:HH11	1.53	0.41
35:N:2554:U:H2’	35:N:2555:U:C6	2.55	0.41
37:C:63:THR:HG22	37:C:163:TYR:CE1	2.53	0.41
39:1:128:LYS:HG3	39:1:129:LEU:HG	2.01	0.41
43:5:3:HIS:CE1	43:5:95:ALA:HB2	2.55	0.41
3:s:153:LEU:O	35:N:2585:U:O2	2.37	0.41
9:S:153:ASP:OD1	9:S:153:ASP:N	2.53	0.41
17:a:87:PHE:O	17:a:89:SER:N	2.49	0.41
30:n:16:ARG:NE	35:N:1266:G:OP1	2.37	0.41
38:0:835:U:OP1	55:K:53:ARG:NH2	2.32	0.41
38:0:837:U:H2’	38:0:838:G:C8	2.54	0.41
38:0:1041:G:H2’	38:0:1042:A:C8	2.55	0.41
38:0:1071:C:H2’	38:0:1072:G:H8	1.86	0.41
40:2:134:MET:HE2	40:2:134:MET:HB3	1.91	0.41
44:6:27:VAL:HG12	44:6:43:VAL:HG21	2.02	0.41
9:S:22:TYR:OH	9:S:165:GLU:OE2	2.34	0.41
10:T:22:GLN:HE22	10:T:55:ARG:HH21	1.66	0.41
19:c:58:ALA:HA	19:c:74:PHE:O	2.20	0.41
35:N:307:G:N1	35:N:310:A:OP2	2.50	0.41
35:N:1028:A:OP2	35:N:1126:A:N6	2.46	0.41
35:N:2124:G:O2’	37:C:41:SER:HB3	2.20	0.41
38:0:28:A:O2’	38:0:296:U:OP1	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:0:331:G:H2'	57:u:5:LYS:NZ	2.35	0.41
41:3:72:PHE:HE1	41:3:94:LEU:HD11	1.85	0.41
47:9:36:VAL:HG22	47:9:76:ILE:HG12	2.03	0.41
6:P:236:GLU:HB3	35:N:2599:G:N7	2.35	0.41
14:X:38:ILE:HD11	14:X:112:PHE:HZ	1.84	0.41
35:N:859:G:HO2'	35:N:916:G:H1	1.68	0.41
35:N:964:C:O2'	35:N:2273:A:N3	2.49	0.41
35:N:1509:A:H2'	35:N:1510:G:H8	1.84	0.41
35:N:2176:A:H4'	37:C:215:SER:CB	2.50	0.41
38:0:746:A:H2'	38:0:747:A:C8	2.54	0.41
38:0:1118:U:H2'	38:0:1119:C:C6	2.54	0.41
50:F:96:PRO:HA	50:F:109:ARG:HG2	2.01	0.41
57:u:12:ILE:HD13	57:u:12:ILE:HG21	1.72	0.41
20:d:33:ARG:HG2	35:N:1252:G:N3	2.35	0.41
35:N:2866:U:H4'	35:N:2867:G:H5'	2.02	0.41
38:0:1371:G:O3'	46:8:71:GLY:HA3	2.20	0.41
41:3:159:LEU:HD13	41:3:175:ALA:HB1	2.01	0.41
43:5:51:ILE:N	43:5:53:LYS:O	2.52	0.41
48:D:31:ILE:HD13	48:D:31:ILE:HG21	1.70	0.41
5:O:42:C:C6	9:S:66:LEU:HB2	2.56	0.41
10:T:90:VAL:O	10:T:160:LYS:HA	2.21	0.41
18:b:94:ARG:HH12	35:N:2294:G:P	2.43	0.41
26:j:41:ARG:HH12	35:N:2262:U:H5"	1.84	0.41
35:N:526:A:O2'	35:N:2043:C:O2	2.34	0.41
35:N:2328:A:H2'	35:N:2329:U:C6	2.55	0.41
35:N:2788:C:H2'	35:N:2789:C:C6	2.56	0.41
43:5:42:TRP:HB2	43:5:59:TYR:HB2	2.01	0.41
46:8:96:SER:O	46:8:99:ARG:HB3	2.21	0.41
5:O:8:C:O3'	18:b:25:ARG:NH1	2.54	0.41
5:O:89:U:O2'	35:N:958:U:O2	2.38	0.41
12:V:79:LEU:O	12:V:82:LYS:NZ	2.52	0.41
35:N:1212:G:H2'	35:N:1236:G:H22	1.85	0.41
35:N:2193:G:H2'	35:N:2194:U:C6	2.56	0.41
35:N:2469:A:N6	35:N:2481:G:O2'	2.50	0.41
35:N:2500:U:O2'	35:N:2504:U:OP1	2.39	0.41
41:3:151:LYS:HA	41:3:156:LYS:HE3	2.03	0.41
32:p:24:THR:HG23	32:p:27:GLY:H	1.86	0.41
35:N:372:G:H1'	35:N:373:U:H5	1.85	0.41
35:N:2155:U:H2'	35:N:2156:G:H5'	2.01	0.41
38:0:501:C:H2'	38:0:502:A:C8	2.56	0.41
38:0:677:U:O2	38:0:777:A:O2'	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1:164:ILE:HD11	39:1:210:VAL:HB	2.02	0.41
57:u:5:LYS:HE3	57:u:5:LYS:HB2	1.90	0.41
57:u:62:ALA:HA	57:u:67:ILE:HG22	2.02	0.41
6:P:107:PRO:HA	6:P:195:VAL:HA	2.03	0.41
6:P:178:SER:HB2	35:N:1799:G:N7	2.36	0.41
9:S:33:LYS:HD3	9:S:92:ARG:NH1	2.35	0.41
11:U:96:THR:HB	11:U:117:LEU:HD21	2.03	0.41
12:V:13:VAL:HG21	12:V:23:PRO:HG2	2.02	0.41
15:Y:109:LYS:HE2	15:Y:128:THR:HG22	2.02	0.41
22:f:85:ILE:HG23	22:f:93:ALA:HB1	2.03	0.41
24:h:16:GLY:C	24:h:18:ASP:H	2.28	0.41
32:p:34:ARG:CD	35:N:467:G:OP2	2.69	0.41
35:N:1236:G:O2'	35:N:1237:A:O5'	2.37	0.41
35:N:1826:G:O2'	35:N:1971:U:OP2	2.35	0.41
35:N:2087:G:H2'	35:N:2088:A:H8	1.86	0.41
35:N:2572:A:OP1	35:N:2574:G:H4'	2.20	0.41
38:0:337:G:H2'	38:0:338:A:C8	2.56	0.41
38:0:837:U:H2'	38:0:838:G:H8	1.85	0.41
40:2:24:ALA:HB1	40:2:28:GLU:HG2	2.02	0.41
44:6:75:VAL:HA	44:6:87:VAL:O	2.21	0.41
46:8:129:LYS:HG3	46:8:130:ARG:H	1.86	0.41
50:F:25:VAL:HG23	50:F:29:ARG:HB3	2.03	0.41
50:F:29:ARG:NH2	50:F:63:PHE:HB2	2.32	0.41
51:G:25:ALA:O	51:G:28:LYS:HG2	2.21	0.41
58:v:17:ARG:HD3	58:v:17:ARG:N	2.36	0.41
3:s:150:TYR:OH	35:N:2609:U:H5'	2.21	0.41
4:M:12:C:O2'	35:N:1923:U:O4'	2.32	0.41
5:O:49:C:OP1	18:b:102:ARG:HG2	2.21	0.41
6:P:247:PRO:HD3	35:N:1824:G:O3'	2.20	0.41
14:X:87:LEU:HD23	14:X:94:PRO:HB3	2.03	0.41
20:d:24:TYR:CD1	35:N:533:G:H5'	2.55	0.41
20:d:24:TYR:CE1	35:N:533:G:H5'	2.56	0.41
34:r:3:VAL:HG12	34:r:36:ARG:HB3	2.02	0.41
35:N:927:A:H2'	35:N:928:A:C8	2.56	0.41
35:N:2122:U:H2'	35:N:2123:G:O4'	2.21	0.41
37:C:21:TYR:CD2	37:C:222:VAL:HG23	2.56	0.41
37:C:195:ALA:O	37:C:198:LYS:HB2	2.20	0.41
38:0:254:G:H5"	54:J:71:LYS:HE3	2.02	0.41
38:0:1524:C:H2'	38:0:1525:G:C8	2.56	0.41
43:5:6:ILE:HB	43:5:62:MET:HB3	2.02	0.41
53:I:40:ASN:HB3	53:I:43:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:75:A:C5'	35:N:2602:A:C6	2.92	0.40
35:N:1044:C:O2'	35:N:1111:A:N1	2.48	0.40
35:N:1746:A:H2'	35:N:1747:U:C6	2.56	0.40
40:2:80:LYS:O	40:2:82:GLU:N	2.54	0.40
43:5:90:MET:HE1	55:K:23:TYR:CE1	2.56	0.40
11:U:41:LYS:HD3	11:U:41:LYS:HA	1.90	0.40
18:b:24:THR:HG22	18:b:42:PRO:HD3	2.03	0.40
18:b:111:ARG:NH1	35:N:2376:A:N3	2.69	0.40
35:N:568:U:O5'	35:N:945:A:N6	2.54	0.40
35:N:657:U:H2'	35:N:658:U:C6	2.56	0.40
35:N:851:C:H2'	35:N:852:U:C6	2.57	0.40
38:0:1526:G:OP2	58:v:39:GLU:HB2	2.22	0.40
8:R:125:SER:O	8:R:137:LYS:NZ	2.54	0.40
35:N:214:G:N2	35:N:216:A:N3	2.68	0.40
35:N:962:G:N2	35:N:2250:G:H1	2.15	0.40
35:N:1858:A:H61	35:N:1884:G:H1'	1.86	0.40
35:N:2131:U:O5'	35:N:2133:G:H4'	2.21	0.40
35:N:2724:U:H2'	35:N:2725:A:C8	2.56	0.40
38:0:82:G:N2	38:0:84:U:O4	2.55	0.40
38:0:427:U:O2'	38:0:541:G:OP1	2.39	0.40
42:4:12:GLN:HG3	42:4:117:VAL:HG12	2.04	0.40
47:9:22:THR:HA	47:9:25:ILE:HG22	2.02	0.40
52:H:26:GLU:OE2	52:H:77:ARG:NE	2.53	0.40
5:O:89:U:H1'	35:N:958:U:H2'	2.02	0.40
13:W:110:PRO:O	13:W:115:GLY:HA3	2.20	0.40
20:d:28:ARG:NH1	35:N:532:A:H3'	2.36	0.40
27:k:3:ARG:HD3	35:N:1365:A:OP1	2.21	0.40
35:N:475:C:H4'	35:N:510:C:H5'	2.04	0.40
35:N:493:G:H2'	35:N:494:G:O4'	2.21	0.40
35:N:739:A:H1'	35:N:740:C:H5	1.87	0.40
38:0:1021:A:H2'	38:0:1022:A:C8	2.57	0.40
38:0:1523:G:OP1	48:D:125:LYS:CE	2.70	0.40
48:D:88:GLY:N	48:D:114:THR:HG22	2.37	0.40
50:F:87:ARG:HG3	50:F:97:VAL:HG13	2.03	0.40
51:G:84:VAL:O	51:G:88:ALA:HB2	2.22	0.40
57:u:71:LYS:HE2	57:u:75:HIS:HE1	1.86	0.40
6:P:154:LEU:HD13	6:P:176:LEU:HD21	2.03	0.40
6:P:243:HIS:HA	6:P:244:PRO:HD3	1.94	0.40
9:S:10:ASP:OD1	9:S:11:GLU:N	2.54	0.40
17:a:73:ASN:HA	17:a:76:VAL:HG12	2.03	0.40
27:k:37:ARG:HG3	27:k:48:THR:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:6:44:TYR:O	44:6:48:GLU:HB2	2.21	0.40
46:8:129:LYS:HB2	46:8:129:LYS:HE3	1.71	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	B	37/183 (20%)	36 (97%)	1 (3%)	0	100 100
3	s	35/179 (20%)	32 (91%)	3 (9%)	0	100 100
6	P	269/273 (98%)	247 (92%)	18 (7%)	4 (2%)	8 29
7	Q	207/209 (99%)	195 (94%)	11 (5%)	1 (0%)	24 53
8	R	199/201 (99%)	191 (96%)	8 (4%)	0	100 100
9	S	175/179 (98%)	163 (93%)	11 (6%)	1 (1%)	21 49
10	T	174/177 (98%)	165 (95%)	9 (5%)	0	100 100
11	U	147/149 (99%)	125 (85%)	19 (13%)	3 (2%)	6 24
12	V	139/142 (98%)	112 (81%)	27 (19%)	0	100 100
13	W	140/142 (99%)	136 (97%)	4 (3%)	0	100 100
14	X	120/123 (98%)	109 (91%)	9 (8%)	2 (2%)	7 27
15	Y	141/144 (98%)	121 (86%)	16 (11%)	4 (3%)	4 19
16	Z	134/136 (98%)	118 (88%)	11 (8%)	5 (4%)	2 15
17	a	118/127 (93%)	102 (86%)	14 (12%)	2 (2%)	7 27
18	b	114/117 (97%)	108 (95%)	6 (5%)	0	100 100
19	c	112/115 (97%)	104 (93%)	8 (7%)	0	100 100
20	d	115/118 (98%)	115 (100%)	0	0	100 100
21	e	101/103 (98%)	92 (91%)	8 (8%)	1 (1%)	12 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
22	f	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	14 41
23	g	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	5 23
24	h	100/104 (96%)	84 (84%)	14 (14%)	2 (2%)	6 24
25	i	92/94 (98%)	89 (97%)	3 (3%)	0	100 100
26	j	73/85 (86%)	71 (97%)	2 (3%)	0	100 100
27	k	75/78 (96%)	71 (95%)	3 (4%)	1 (1%)	9 32
28	l	61/63 (97%)	56 (92%)	5 (8%)	0	100 100
29	m	56/59 (95%)	52 (93%)	4 (7%)	0	100 100
30	n	54/57 (95%)	48 (89%)	5 (9%)	1 (2%)	6 25
31	o	48/55 (87%)	45 (94%)	3 (6%)	0	100 100
32	p	44/46 (96%)	40 (91%)	4 (9%)	0	100 100
33	q	62/65 (95%)	56 (90%)	5 (8%)	1 (2%)	7 29
34	r	36/55 (66%)	35 (97%)	1 (3%)	0	100 100
36	L	53/70 (76%)	45 (85%)	7 (13%)	1 (2%)	6 25
37	C	130/223 (58%)	123 (95%)	7 (5%)	0	100 100
39	1	216/239 (90%)	188 (87%)	27 (12%)	1 (0%)	24 53
40	2	204/218 (94%)	186 (91%)	16 (8%)	2 (1%)	12 39
41	3	203/206 (98%)	182 (90%)	21 (10%)	0	100 100
42	4	148/162 (91%)	116 (78%)	30 (20%)	2 (1%)	9 30
43	5	98/131 (75%)	81 (83%)	11 (11%)	6 (6%)	1 7
44	6	140/156 (90%)	130 (93%)	10 (7%)	0	100 100
45	7	127/130 (98%)	121 (95%)	6 (5%)	0	100 100
46	8	125/130 (96%)	103 (82%)	20 (16%)	2 (2%)	7 29
47	9	96/103 (93%)	84 (88%)	9 (9%)	3 (3%)	3 18
48	D	115/129 (89%)	102 (89%)	13 (11%)	0	100 100
49	E	121/124 (98%)	104 (86%)	15 (12%)	2 (2%)	7 27
50	F	112/118 (95%)	103 (92%)	8 (7%)	1 (1%)	14 41
51	G	92/101 (91%)	77 (84%)	14 (15%)	1 (1%)	11 37
52	H	86/89 (97%)	81 (94%)	5 (6%)	0	100 100
53	I	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	9 32
54	J	78/84 (93%)	66 (85%)	9 (12%)	3 (4%)	2 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
55	K	53/75 (71%)	49 (92%)	3 (6%)	1 (2%)	6 25
56	t	77/92 (84%)	73 (95%)	4 (5%)	0	100 100
57	u	83/87 (95%)	78 (94%)	4 (5%)	1 (1%)	10 34
58	v	49/88 (56%)	41 (84%)	7 (14%)	1 (2%)	6 24
All	All	5863/6625 (88%)	5300 (90%)	504 (9%)	59 (1%)	15 39

All (59) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	P	239	ASN
11	U	72	ILE
15	Y	36	LYS
16	Z	58	LYS
21	e	53	PHE
30	n	55	ILE
33	q	32	ILE
43	5	53	LYS
47	9	58	ASN
53	I	44	SER
54	J	70	THR
58	v	11	PRO
11	U	41	LYS
16	Z	59	ARG
17	a	3	HIS
40	2	81	GLY
43	5	56	LYS
43	5	91	ARG
46	8	55	VAL
49	E	23	ALA
54	J	18	GLU
57	u	69	LYS
6	P	235	GLY
16	Z	39	GLY
23	g	78	SER
24	h	99	ASN
27	k	3	ARG
40	2	80	LYS
43	5	54	LEU
43	5	94	HIS
47	9	43	PRO
49	E	78	SER

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Mol	Chain	Res	Type
54	J	71	LYS
55	K	48	ARG
6	P	10	SER
6	P	238	ARG
7	Q	149	ASN
9	S	175	PHE
11	U	35	LYS
14	X	93	GLN
15	Y	29	LYS
15	Y	30	THR
15	Y	31	GLY
16	Z	69	PRO
23	g	77	ARG
36	L	3	LYS
42	4	51	GLY
43	5	86	ARG
50	F	66	GLU
17	a	88	ALA
22	f	64	ALA
24	h	53	ASN
39	1	194	ASP
42	4	90	THR
51	G	4	GLN
16	Z	87	GLY
47	9	42	LEU
46	8	10	GLY
14	X	119	ALA

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	s	34/158 (22%)	34 (100%)	0	100	100
6	P	216/218 (99%)	213 (99%)	3 (1%)	59	70
7	Q	164/164 (100%)	159 (97%)	5 (3%)	36	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	R	165/165 (100%)	162 (98%)	3 (2%)	51 67
9	S	148/150 (99%)	147 (99%)	1 (1%)	76 78
10	T	137/138 (99%)	137 (100%)	0	100 100
11	U	114/114 (100%)	109 (96%)	5 (4%)	25 51
12	V	109/110 (99%)	109 (100%)	0	100 100
13	W	116/116 (100%)	115 (99%)	1 (1%)	70 76
14	X	103/104 (99%)	101 (98%)	2 (2%)	50 66
15	Y	102/103 (99%)	100 (98%)	2 (2%)	48 66
16	Z	109/109 (100%)	108 (99%)	1 (1%)	70 76
17	a	100/102 (98%)	98 (98%)	2 (2%)	48 66
18	b	86/87 (99%)	85 (99%)	1 (1%)	63 72
19	c	98/100 (98%)	95 (97%)	3 (3%)	35 59
20	d	89/90 (99%)	87 (98%)	2 (2%)	45 63
21	e	84/84 (100%)	83 (99%)	1 (1%)	63 72
22	f	93/93 (100%)	93 (100%)	0	100 100
23	g	80/85 (94%)	79 (99%)	1 (1%)	61 71
24	h	83/85 (98%)	81 (98%)	2 (2%)	43 62
25	i	78/78 (100%)	77 (99%)	1 (1%)	61 71
26	j	56/63 (89%)	55 (98%)	1 (2%)	51 67
27	k	67/68 (98%)	67 (100%)	0	100 100
28	l	55/55 (100%)	54 (98%)	1 (2%)	51 67
29	m	48/49 (98%)	48 (100%)	0	100 100
30	n	47/48 (98%)	46 (98%)	1 (2%)	47 64
31	o	45/49 (92%)	45 (100%)	0	100 100
32	p	38/38 (100%)	38 (100%)	0	100 100
33	q	51/52 (98%)	49 (96%)	2 (4%)	28 53
34	r	34/50 (68%)	33 (97%)	1 (3%)	37 60
36	L	48/63 (76%)	48 (100%)	0	100 100
37	C	110/174 (63%)	109 (99%)	1 (1%)	70 76
39	1	180/198 (91%)	178 (99%)	2 (1%)	65 74
40	2	170/178 (96%)	167 (98%)	3 (2%)	51 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
41	3	172/173 (99%)	170 (99%)	2 (1%)	63 72
42	4	113/123 (92%)	107 (95%)	6 (5%)	20 47
43	5	87/112 (78%)	87 (100%)	0	100 100
44	6	119/129 (92%)	118 (99%)	1 (1%)	73 77
45	7	104/105 (99%)	101 (97%)	3 (3%)	37 60
46	8	105/107 (98%)	104 (99%)	1 (1%)	68 75
47	9	86/90 (96%)	85 (99%)	1 (1%)	63 72
48	D	90/98 (92%)	89 (99%)	1 (1%)	65 74
49	E	103/104 (99%)	103 (100%)	0	100 100
50	F	92/96 (96%)	90 (98%)	2 (2%)	45 63
51	G	79/83 (95%)	79 (100%)	0	100 100
52	H	75/77 (97%)	75 (100%)	0	100 100
53	I	65/65 (100%)	64 (98%)	1 (2%)	57 69
54	J	74/77 (96%)	73 (99%)	1 (1%)	59 70
55	K	48/66 (73%)	47 (98%)	1 (2%)	47 64
56	t	70/80 (88%)	66 (94%)	4 (6%)	18 45
57	u	65/66 (98%)	65 (100%)	0	100 100
58	v	44/76 (58%)	38 (86%)	6 (14%)	3 15
All	All	4848/5265 (92%)	4770 (98%)	78 (2%)	54 68

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	P	141	VAL
6	P	165	VAL
6	P	218	PRO
7	Q	48	ILE
7	Q	73	VAL
7	Q	177	VAL
7	Q	202	ILE
7	Q	205	PRO
8	R	69	ARG
8	R	149	ILE
8	R	163	ASN
9	S	31	VAL
11	U	27	ARG

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Mol	Chain	Res	Type
11	U	44	ILE
11	U	50	ARG
11	U	55	GLU
11	U	70	GLU
13	W	57	LEU
14	X	58	LEU
14	X	86	LEU
15	Y	77	ILE
15	Y	94	THR
16	Z	128	THR
17	a	50	PRO
17	a	70	THR
18	b	3	LYS
19	c	32	VAL
19	c	53	ARG
19	c	73	VAL
20	d	16	LYS
20	d	33	ARG
21	e	49	ILE
23	g	32	LEU
24	h	28	VAL
24	h	68	SER
25	i	65	VAL
26	j	41	ARG
28	l	6	LEU
30	n	28	LEU
33	q	2	PRO
33	q	32	ILE
34	r	26	ILE
37	C	33	LEU
39	1	10	LEU
39	1	207	ILE
40	2	55	ILE
40	2	75	ILE
40	2	200	VAL
41	3	5	LEU
41	3	143	VAL
42	4	15	LEU
42	4	115	LEU
42	4	120	VAL
42	4	123	VAL
42	4	141	ILE

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Mol	Chain	Res	Type
42	4	157	ARG
44	6	25	LYS
45	7	51	VAL
45	7	121	LEU
45	7	125	ILE
46	8	120	LYS
47	9	17	LEU
48	D	31	ILE
50	F	25	VAL
50	F	98	ARG
53	I	19	VAL
54	J	61	ILE
55	K	21	ILE
56	t	5	LEU
56	t	11	ILE
56	t	49	ILE
56	t	58	VAL
58	v	4	ILE
58	v	5	LYS
58	v	6	VAL
58	v	16	LEU
58	v	20	LYS
58	v	29	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
3	s	126	HIS
6	P	53	HIS
6	P	86	ASN
6	P	239	ASN
6	P	260	ASN
7	Q	32	ASN
7	Q	49	GLN
7	Q	149	ASN
7	Q	150	GLN
8	R	136	GLN
8	R	163	ASN
8	R	165	HIS
10	T	22	GLN
10	T	73	ASN
10	T	143	GLN

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Mol	Chain	Res	Type
11	U	2	GLN
11	U	11	ASN
11	U	135	HIS
12	V	12	GLN
13	W	40	HIS
13	W	86	GLN
17	a	3	HIS
17	a	73	ASN
19	c	12	GLN
19	c	15	GLN
19	c	52	ASN
20	d	37	GLN
20	d	44	GLN
22	f	15	GLN
25	i	51	GLN
27	k	36	HIS
30	n	6	ASN
30	n	38	HIS
30	n	42	HIS
31	o	19	HIS
36	L	20	ASN
37	C	57	GLN
37	C	67	HIS
37	C	172	HIS
37	C	188	ASN
39	1	203	ASN
40	2	8	ASN
40	2	123	GLN
40	2	190	HIS
42	4	73	ASN
42	4	89	HIS
42	4	121	HIS
43	5	11	HIS
43	5	55	HIS
44	6	28	ASN
44	6	148	ASN
46	8	25	ASN
46	8	32	GLN
46	8	50	GLN
47	9	15	HIS
47	9	56	HIS
47	9	58	ASN

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Mol	Chain	Res	Type
48	D	118	HIS
50	F	8	ASN
51	G	49	GLN
51	G	66	GLN
52	H	35	GLN
52	H	37	ASN
53	I	63	GLN
54	J	31	HIS
55	K	52	GLN
55	K	54	GLN
56	t	56	GLN
57	u	20	HIS
57	u	48	GLN
57	u	78	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	72/73 (98%)	20 (27%)	8 (11%)
35	N	2894/2903 (99%)	521 (18%)	34 (1%)
38	0	1531/1539 (99%)	277 (18%)	22 (1%)
4	M	74/75 (98%)	11 (14%)	0
5	O	117/120 (97%)	21 (17%)	1 (0%)
All	All	4688/4710 (99%)	850 (18%)	65 (1%)

All (850) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	13	C
1	A	14	A
1	A	16	U
1	A	17	C
1	A	18	G
1	A	19	G
1	A	20	U
1	A	21	A
1	A	22	G
1	A	36	A
1	A	45	U
1	A	46	G
1	A	47	U

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Mol	Chain	Res	Type
1	A	48	C
1	A	52	G
1	A	60	U
1	A	61	C
1	A	62	C
1	A	63	G
1	A	73	A
4	M	9	C
4	M	10	G
4	M	15	G
4	M	16	C
4	M	17	G
4	M	19	U
4	M	20	A
4	M	42	G
4	M	47	C
4	M	74	C
4	M	75	A
5	O	13	G
5	O	25	U
5	O	31	C
5	O	35	C
5	O	41	G
5	O	44	G
5	O	45	A
5	O	51	G
5	O	53	A
5	O	56	G
5	O	57	A
5	O	64	G
5	O	66	A
5	O	67	G
5	O	88	C
5	O	89	U
5	O	90	C
5	O	91	C
5	O	99	A
5	O	108	A
5	O	109	A
35	N	10	A
35	N	23	G
35	N	28	A

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Mol	Chain	Res	Type
35	N	35	G
35	N	36	G
35	N	42	A
35	N	46	G
35	N	51	G
35	N	55	G
35	N	60	G
35	N	61	C
35	N	63	A
35	N	71	A
35	N	74	A
35	N	75	G
35	N	84	A
35	N	96	C
35	N	101	A
35	N	102	U
35	N	103	A
35	N	118	A
35	N	119	A
35	N	120	U
35	N	125	A
35	N	138	U
35	N	139	U
35	N	140	C
35	N	141	G
35	N	142	A
35	N	162	U
35	N	163	C
35	N	165	A
35	N	166	U
35	N	188	G
35	N	196	A
35	N	199	A
35	N	201	C
35	N	215	G
35	N	216	A
35	N	221	A
35	N	222	A
35	N	223	A
35	N	224	U
35	N	228	C
35	N	241	A

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Mol	Chain	Res	Type
35	N	242	G
35	N	243	U
35	N	248	G
35	N	255	A
35	N	265	A
35	N	266	G
35	N	267	C
35	N	271	G
35	N	272	A
35	N	276	U
35	N	278	A
35	N	281	C
35	N	284	U
35	N	294	A
35	N	301	G
35	N	311	A
35	N	323	C
35	N	329	G
35	N	330	A
35	N	332	A
35	N	346	A
35	N	361	G
35	N	362	A
35	N	371	A
35	N	372	G
35	N	373	U
35	N	386	G
35	N	396	G
35	N	399	U
35	N	403	U
35	N	404	A
35	N	405	U
35	N	406	G
35	N	411	G
35	N	412	A
35	N	421	C
35	N	422	A
35	N	424	G
35	N	435	C
35	N	447	A
35	N	455	C
35	N	456	C

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Mol	Chain	Res	Type
35	N	457	A
35	N	467	G
35	N	471	A
35	N	473	G
35	N	481	G
35	N	491	G
35	N	501	A
35	N	504	A
35	N	505	A
35	N	509	C
35	N	513	A
35	N	529	A
35	N	531	C
35	N	532	A
35	N	543	G
35	N	544	C
35	N	546	U
35	N	548	G
35	N	549	G
35	N	550	C
35	N	556	A
35	N	563	A
35	N	573	U
35	N	575	A
35	N	578	G
35	N	586	A
35	N	603	A
35	N	613	A
35	N	614	A
35	N	616	A
35	N	622	G
35	N	627	A
35	N	637	A
35	N	645	C
35	N	646	U
35	N	647	G
35	N	648	G
35	N	654	A
35	N	655	A
35	N	669	G
35	N	670	A
35	N	671	C

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Mol	Chain	Res	Type
35	N	677	A
35	N	686	U
35	N	695	G
35	N	696	G
35	N	717	C
35	N	729	G
35	N	730	A
35	N	738	G
35	N	747	U
35	N	764	A
35	N	765	C
35	N	775	G
35	N	776	G
35	N	782	A
35	N	783	A
35	N	784	G
35	N	785	G
35	N	792	A
35	N	800	A
35	N	805	G
35	N	806	C
35	N	812	C
35	N	819	A
35	N	827	U
35	N	828	U
35	N	829	A
35	N	845	A
35	N	846	U
35	N	858	G
35	N	860	U
35	N	866	A
35	N	869	G
35	N	878	A
35	N	885	C
35	N	896	A
35	N	897	C
35	N	907	G
35	N	910	A
35	N	914	G
35	N	919	U
35	N	932	U
35	N	941	A

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Mol	Chain	Res	Type
35	N	945	A
35	N	946	C
35	N	953	G
35	N	961	C
35	N	973	A
35	N	974	G
35	N	983	A
35	N	985	C
35	N	989	G
35	N	995	C
35	N	996	A
35	N	997	G
35	N	1004	U
35	N	1012	U
35	N	1013	C
35	N	1020	A
35	N	1021	A
35	N	1022	G
35	N	1023	U
35	N	1025	G
35	N	1026	G
35	N	1033	U
35	N	1046	A
35	N	1047	G
35	N	1057	A
35	N	1060	U
35	N	1062	G
35	N	1064	C
35	N	1066	U
35	N	1067	A
35	N	1068	G
35	N	1070	A
35	N	1077	A
35	N	1082	U
35	N	1083	U
35	N	1088	A
35	N	1089	A
35	N	1090	A
35	N	1094	U
35	N	1096	A
35	N	1097	U
35	N	1100	C

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Mol	Chain	Res	Type
35	N	1104	C
35	N	1110	G
35	N	1111	A
35	N	1112	G
35	N	1119	U
35	N	1122	G
35	N	1130	U
35	N	1132	U
35	N	1133	A
35	N	1135	C
35	N	1136	G
35	N	1141	U
35	N	1142	A
35	N	1143	A
35	N	1155	A
35	N	1168	G
35	N	1171	G
35	N	1173	U
35	N	1174	U
35	N	1175	A
35	N	1180	U
35	N	1186	G
35	N	1195	G
35	N	1204	A
35	N	1205	A
35	N	1206	G
35	N	1210	G
35	N	1212	G
35	N	1237	A
35	N	1238	G
35	N	1250	G
35	N	1251	C
35	N	1253	A
35	N	1256	G
35	N	1257	C
35	N	1265	A
35	N	1266	G
35	N	1268	A
35	N	1271	G
35	N	1272	A
35	N	1275	A
35	N	1300	G

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Mol	Chain	Res	Type
35	N	1301	A
35	N	1321	A
35	N	1329	U
35	N	1332	G
35	N	1345	C
35	N	1352	U
35	N	1365	A
35	N	1368	G
35	N	1376	C
35	N	1379	U
35	N	1383	A
35	N	1386	C
35	N	1395	A
35	N	1403	A
35	N	1416	G
35	N	1419	A
35	N	1420	A
35	N	1421	G
35	N	1427	A
35	N	1428	C
35	N	1434	A
35	N	1437	C
35	N	1453	A
35	N	1458	U
35	N	1461	C
35	N	1478	G
35	N	1482	G
35	N	1504	A
35	N	1508	A
35	N	1509	A
35	N	1515	A
35	N	1524	G
35	N	1529	G
35	N	1535	A
35	N	1536	C
35	N	1537	G
35	N	1538	G
35	N	1554	U
35	N	1565	C
35	N	1566	A
35	N	1569	A
35	N	1578	U

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Mol	Chain	Res	Type
35	N	1583	A
35	N	1584	U
35	N	1585	C
35	N	1587	G
35	N	1607	C
35	N	1608	A
35	N	1610	A
35	N	1613	G
35	N	1622	G
35	N	1647	U
35	N	1648	U
35	N	1651	G
35	N	1674	G
35	N	1675	C
35	N	1676	A
35	N	1698	A
35	N	1699	G
35	N	1713	A
35	N	1715	G
35	N	1728	C
35	N	1729	U
35	N	1730	C
35	N	1733	G
35	N	1738	G
35	N	1757	A
35	N	1758	U
35	N	1760	C
35	N	1764	C
35	N	1773	A
35	N	1784	A
35	N	1787	A
35	N	1800	C
35	N	1801	A
35	N	1802	A
35	N	1808	A
35	N	1811	G
35	N	1816	C
35	N	1829	A
35	N	1833	C
35	N	1835	G
35	N	1857	G
35	N	1869	G

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Mol	Chain	Res	Type
35	N	1870	C
35	N	1900	A
35	N	1901	A
35	N	1906	G
35	N	1913	A
35	N	1919	A
35	N	1927	A
35	N	1929	G
35	N	1930	G
35	N	1931	U
35	N	1938	A
35	N	1955	U
35	N	1964	G
35	N	1967	C
35	N	1970	A
35	N	1971	U
35	N	1972	G
35	N	1991	U
35	N	1993	U
35	N	1997	C
35	N	2004	G
35	N	2006	C
35	N	2020	A
35	N	2022	U
35	N	2023	C
35	N	2031	A
35	N	2033	A
35	N	2043	C
35	N	2046	G
35	N	2055	C
35	N	2056	G
35	N	2060	A
35	N	2061	G
35	N	2062	A
35	N	2063	C
35	N	2069	G
35	N	2072	C
35	N	2077	A
35	N	2092	U
35	N	2094	A
35	N	2097	A
35	N	2099	U

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Mol	Chain	Res	Type
35	N	2110	G
35	N	2111	U
35	N	2112	G
35	N	2113	U
35	N	2118	U
35	N	2119	A
35	N	2132	U
35	N	2133	G
35	N	2145	C
35	N	2147	A
35	N	2162	G
35	N	2171	A
35	N	2172	U
35	N	2173	A
35	N	2190	G
35	N	2191	A
35	N	2194	U
35	N	2198	A
35	N	2200	C
35	N	2203	U
35	N	2204	G
35	N	2211	A
35	N	2212	A
35	N	2214	C
35	N	2225	A
35	N	2226	C
35	N	2238	G
35	N	2239	G
35	N	2266	A
35	N	2278	A
35	N	2279	G
35	N	2283	C
35	N	2286	G
35	N	2287	A
35	N	2288	A
35	N	2297	A
35	N	2305	U
35	N	2307	G
35	N	2309	A
35	N	2312	U
35	N	2325	G
35	N	2333	A

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Mol	Chain	Res	Type
35	N	2334	U
35	N	2345	G
35	N	2347	C
35	N	2350	C
35	N	2354	C
35	N	2357	G
35	N	2361	G
35	N	2383	G
35	N	2385	C
35	N	2391	G
35	N	2402	U
35	N	2403	C
35	N	2406	A
35	N	2407	A
35	N	2422	C
35	N	2423	U
35	N	2425	A
35	N	2426	A
35	N	2427	C
35	N	2429	G
35	N	2430	A
35	N	2431	U
35	N	2435	A
35	N	2441	U
35	N	2448	A
35	N	2470	G
35	N	2476	A
35	N	2498	C
35	N	2502	G
35	N	2503	A
35	N	2504	U
35	N	2505	G
35	N	2518	A
35	N	2520	C
35	N	2529	G
35	N	2535	G
35	N	2547	A
35	N	2554	U
35	N	2566	A
35	N	2567	G
35	N	2572	A
35	N	2573	C

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Mol	Chain	Res	Type
35	N	2574	G
35	N	2578	G
35	N	2585	U
35	N	2602	A
35	N	2603	G
35	N	2609	U
35	N	2613	U
35	N	2615	U
35	N	2629	U
35	N	2630	G
35	N	2636	C
35	N	2645	G
35	N	2646	C
35	N	2655	G
35	N	2656	U
35	N	2661	G
35	N	2663	G
35	N	2682	A
35	N	2689	U
35	N	2690	U
35	N	2714	G
35	N	2716	C
35	N	2718	G
35	N	2724	U
35	N	2727	A
35	N	2733	A
35	N	2748	A
35	N	2751	G
35	N	2752	C
35	N	2765	A
35	N	2776	A
35	N	2777	G
35	N	2778	A
35	N	2779	U
35	N	2791	G
35	N	2792	A
35	N	2798	U
35	N	2801	G
35	N	2818	U
35	N	2820	A
35	N	2833	U
35	N	2834	G

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Mol	Chain	Res	Type
35	N	2836	U
35	N	2849	U
35	N	2850	A
35	N	2859	G
35	N	2867	G
35	N	2868	A
35	N	2872	A
35	N	2873	A
35	N	2874	C
35	N	2880	C
35	N	2884	U
35	N	2887	A
35	N	2891	U
35	N	2903	U
38	0	4	U
38	0	6	G
38	0	9	G
38	0	32	A
38	0	39	G
38	0	44	A
38	0	47	C
38	0	48	C
38	0	50	A
38	0	51	A
38	0	52	C
38	0	58	C
38	0	65	A
38	0	69	G
38	0	71	A
38	0	72	A
38	0	83	C
38	0	84	U
38	0	85	U
38	0	86	G
38	0	87	C
38	0	92	U
38	0	97	G
38	0	108	G
38	0	115	G
38	0	116	A
38	0	122	G
38	0	130	A

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Mol	Chain	Res	Type
38	0	141	G
38	0	143	A
38	0	144	G
38	0	149	A
38	0	156	C
38	0	163	C
38	0	174	A
38	0	177	G
38	0	182	A
38	0	183	C
38	0	184	G
38	0	197	A
38	0	209	U
38	0	210	C
38	0	211	G
38	0	226	G
38	0	245	U
38	0	247	G
38	0	251	G
38	0	266	G
38	0	267	C
38	0	280	C
38	0	281	G
38	0	289	G
38	0	298	A
38	0	306	A
38	0	321	A
38	0	328	C
38	0	332	G
38	0	347	G
38	0	351	G
38	0	352	C
38	0	354	G
38	0	358	U
38	0	367	U
38	0	372	C
38	0	375	U
38	0	384	G
38	0	388	G
38	0	389	A
38	0	397	A
38	0	398	U

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Mol	Chain	Res	Type
38	0	406	G
38	0	412	A
38	0	413	G
38	0	421	U
38	0	422	C
38	0	423	G
38	0	424	G
38	0	429	U
38	0	430	A
38	0	439	U
38	0	451	A
38	0	458	U
38	0	459	A
38	0	467	U
38	0	468	A
38	0	474	G
38	0	478	A
38	0	479	U
38	0	481	G
38	0	484	G
38	0	485	U
38	0	486	U
38	0	495	A
38	0	497	G
38	0	511	C
38	0	518	C
38	0	519	C
38	0	521	G
38	0	527	G
38	0	531	U
38	0	532	A
38	0	533	A
38	0	547	A
38	0	559	A
38	0	562	U
38	0	572	A
38	0	573	A
38	0	576	C
38	0	595	A
38	0	596	A
38	0	607	A
38	0	633	G

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Mol	Chain	Res	Type
38	0	639	G
38	0	650	G
38	0	652	U
38	0	665	A
38	0	675	A
38	0	688	G
38	0	695	A
38	0	701	U
38	0	702	A
38	0	703	G
38	0	718	A
38	0	721	G
38	0	723	U
38	0	724	G
38	0	731	G
38	0	734	G
38	0	747	A
38	0	755	G
38	0	777	A
38	0	793	U
38	0	794	A
38	0	813	U
38	0	815	A
38	0	817	C
38	0	818	G
38	0	819	A
38	0	821	G
38	0	828	U
38	0	832	G
38	0	836	G
38	0	841	C
38	0	842	U
38	0	843	U
38	0	844	G
38	0	846	G
38	0	849	G
38	0	859	G
38	0	864	A
38	0	885	G
38	0	889	A
38	0	890	G
38	0	891	U

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Mol	Chain	Res	Type
38	0	902	G
38	0	914	A
38	0	926	G
38	0	934	C
38	0	935	A
38	0	960	U
38	0	965	U
38	0	966	G
38	0	969	A
38	0	971	G
38	0	972	C
38	0	975	A
38	0	976	G
38	0	977	A
38	0	989	U
38	0	993	G
38	0	999	C
38	0	1000	A
38	0	1004	A
38	0	1008	U
38	0	1009	U
38	0	1017	U
38	0	1018	G
38	0	1020	G
38	0	1022	A
38	0	1024	G
38	0	1025	U
38	0	1026	G
38	0	1027	C
38	0	1030	U
38	0	1031	C
38	0	1032	G
38	0	1043	G
38	0	1044	A
38	0	1053	G
38	0	1056	U
38	0	1065	U
38	0	1085	U
38	0	1092	A
38	0	1094	G
38	0	1095	U
38	0	1101	A

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Mol	Chain	Res	Type
38	0	1125	U
38	0	1130	A
38	0	1132	C
38	0	1136	C
38	0	1137	C
38	0	1138	G
38	0	1139	G
38	0	1140	C
38	0	1146	A
38	0	1158	C
38	0	1159	U
38	0	1168	U
38	0	1171	A
38	0	1182	G
38	0	1183	U
38	0	1184	G
38	0	1190	G
38	0	1196	A
38	0	1200	C
38	0	1201	A
38	0	1202	U
38	0	1212	U
38	0	1213	A
38	0	1227	A
38	0	1238	A
38	0	1253	G
38	0	1256	A
38	0	1257	A
38	0	1258	G
38	0	1260	G
38	0	1261	A
38	0	1274	A
38	0	1275	A
38	0	1278	G
38	0	1280	A
38	0	1281	C
38	0	1287	A
38	0	1297	G
38	0	1298	U
38	0	1300	G
38	0	1301	U
38	0	1302	C

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Mol	Chain	Res	Type
38	0	1305	G
38	0	1317	C
38	0	1318	A
38	0	1319	A
38	0	1320	C
38	0	1322	C
38	0	1323	G
38	0	1331	G
38	0	1332	A
38	0	1340	A
38	0	1346	A
38	0	1347	G
38	0	1348	U
38	0	1353	G
38	0	1363	A
38	0	1364	U
38	0	1370	G
38	0	1379	G
38	0	1383	C
38	0	1394	A
38	0	1400	C
38	0	1419	G
38	0	1422	G
38	0	1433	A
38	0	1441	A
38	0	1446	A
38	0	1451	U
38	0	1452	C
38	0	1487	G
38	0	1492	A
38	0	1494	G
38	0	1497	G
38	0	1503	A
38	0	1506	U
38	0	1517	G
38	0	1519	A
38	0	1529	G
38	0	1530	G
38	0	1531	A

All (65) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	16	U
1	A	19	G
1	A	20	U
1	A	21	A
1	A	44	G
1	A	45	U
1	A	46	G
1	A	60	U
5	O	52	A
35	N	60	G
35	N	227	A
35	N	242	G
35	N	249	C
35	N	372	G
35	N	404	A
35	N	421	C
35	N	446	G
35	N	456	C
35	N	474	G
35	N	503	A
35	N	512	G
35	N	555	G
35	N	670	A
35	N	774	G
35	N	784	G
35	N	859	G
35	N	995	C
35	N	1020	A
35	N	1134	A
35	N	1141	U
35	N	1142	A
35	N	1236	G
35	N	1900	A
35	N	2062	A
35	N	2225	A
35	N	2282	G
35	N	2286	G
35	N	2311	A
35	N	2405	G
35	N	2655	G
35	N	2776	A
35	N	2867	G
35	N	2873	A

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Mol	Chain	Res	Type
38	0	64	G
38	0	85	U
38	0	96	U
38	0	115	G
38	0	388	G
38	0	429	U
38	0	518	C
38	0	595	A
38	0	812	G
38	0	890	G
38	0	965	U
38	0	1124	G
38	0	1145	A
38	0	1182	G
38	0	1190	G
38	0	1201	A
38	0	1300	G
38	0	1345	U
38	0	1347	G
38	0	1491	G
38	0	1493	A
38	0	1528	U

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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 (i)

There are no chain breaks in this entry.

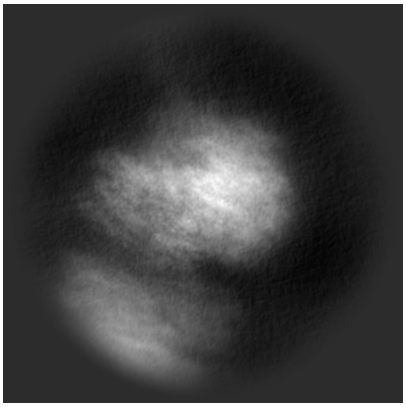
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13956. These allow visual inspection of the internal detail of the map and identification of artifacts.

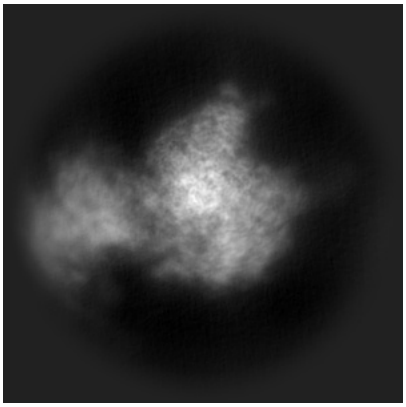
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

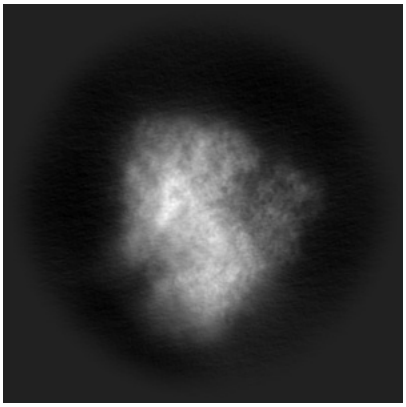
6.1.1 Primary map



X



Y

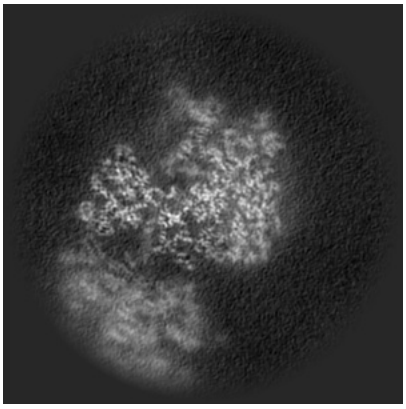


Z

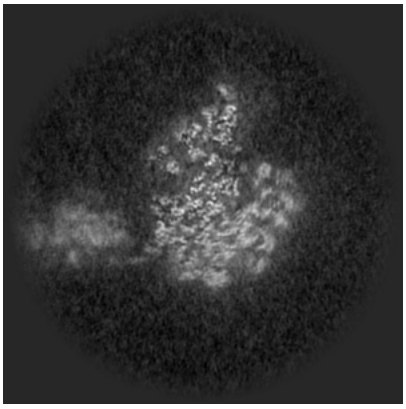
The images above show the map projected in three orthogonal directions.

6.2 Central slices

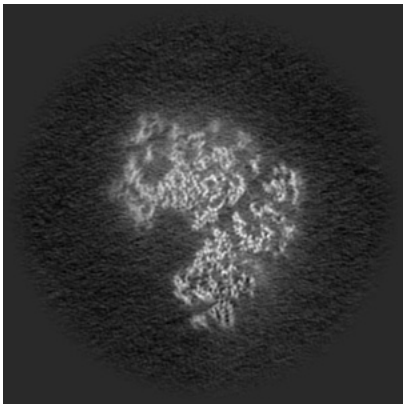
6.2.1 Primary map



X Index: 225



Y Index: 225

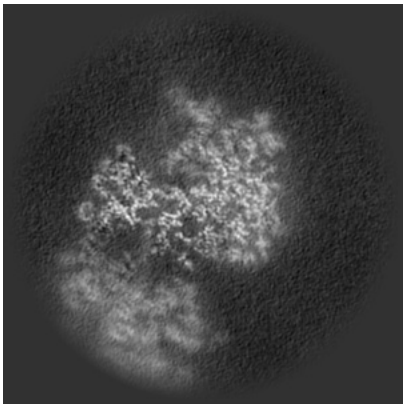


Z Index: 225

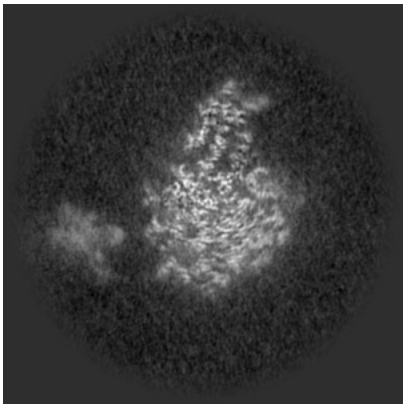
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

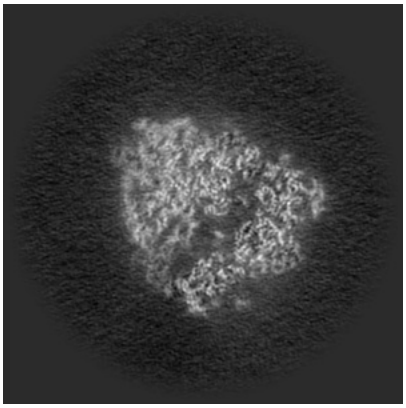
6.3.1 Primary map



X Index: 223



Y Index: 245

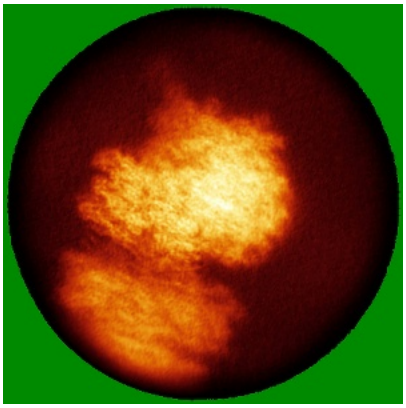


Z Index: 250

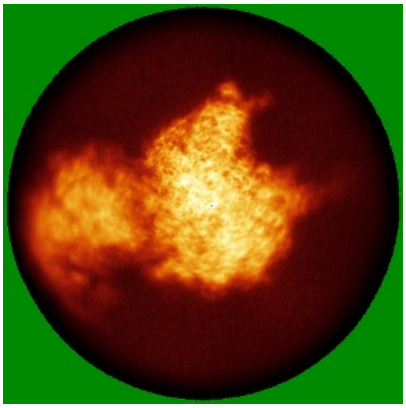
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

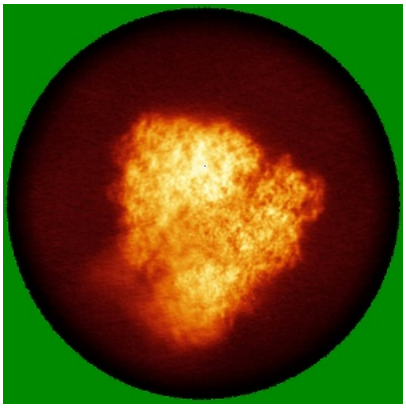
6.4.1 Primary map



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.

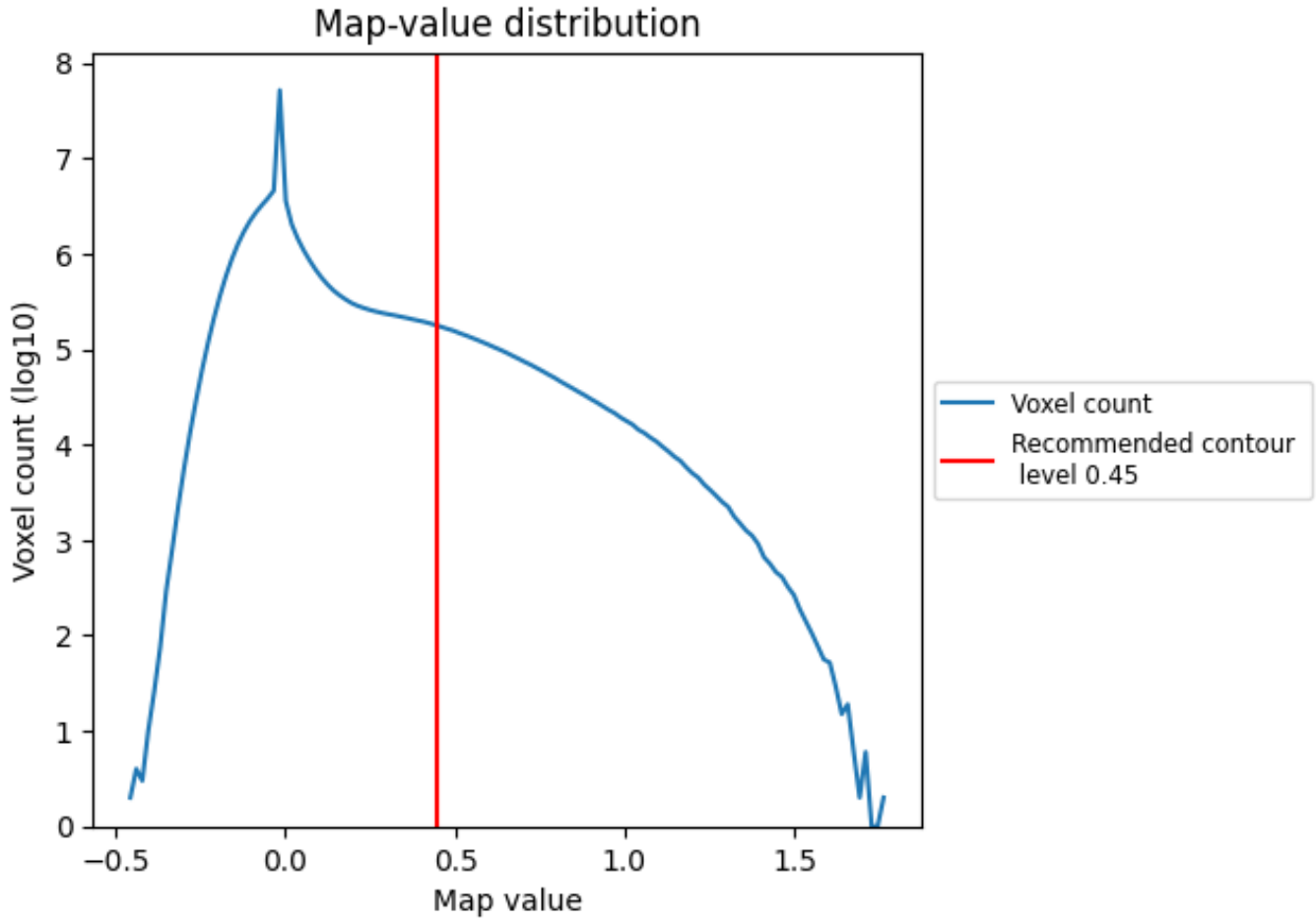
6.6 Mask visualisation (i)

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

7 Map analysis

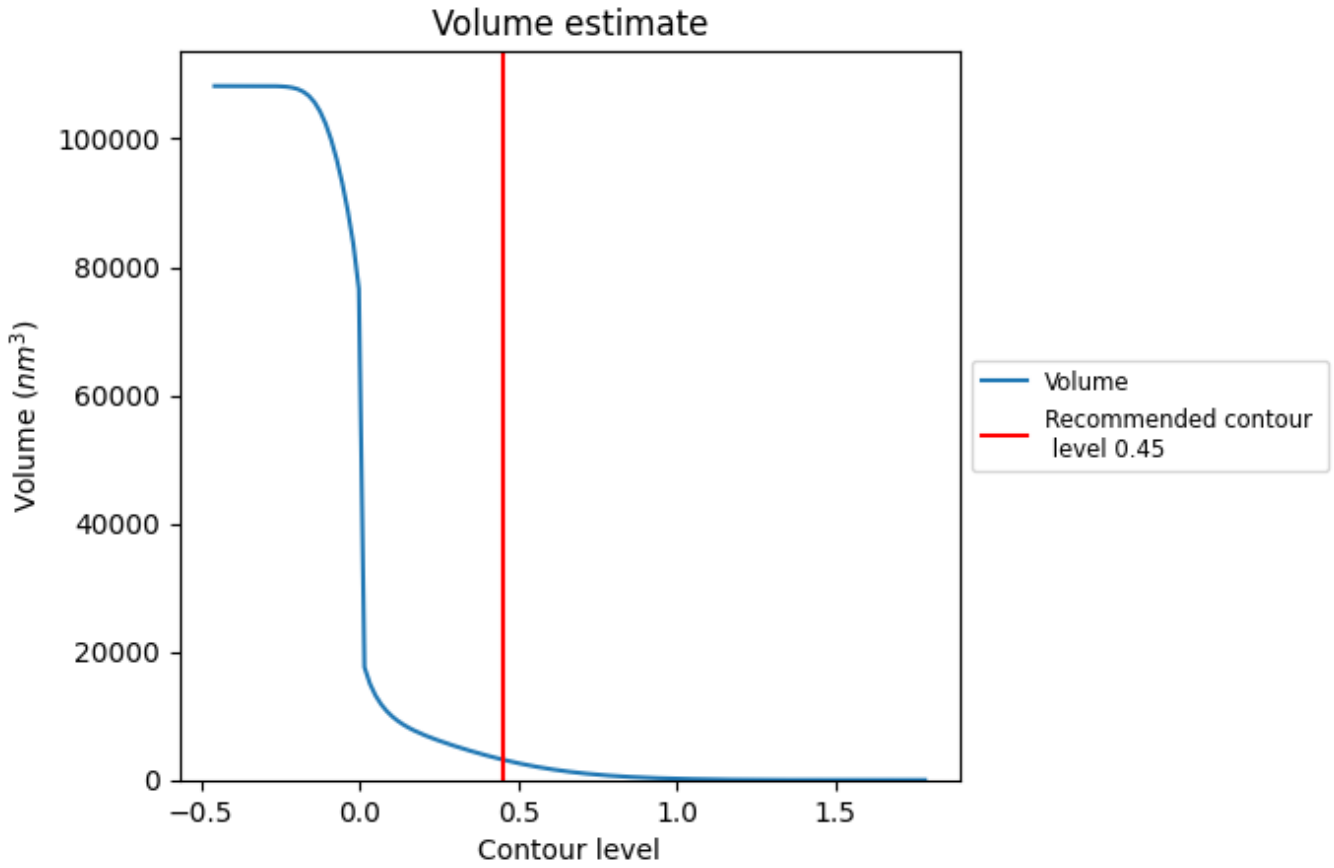
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

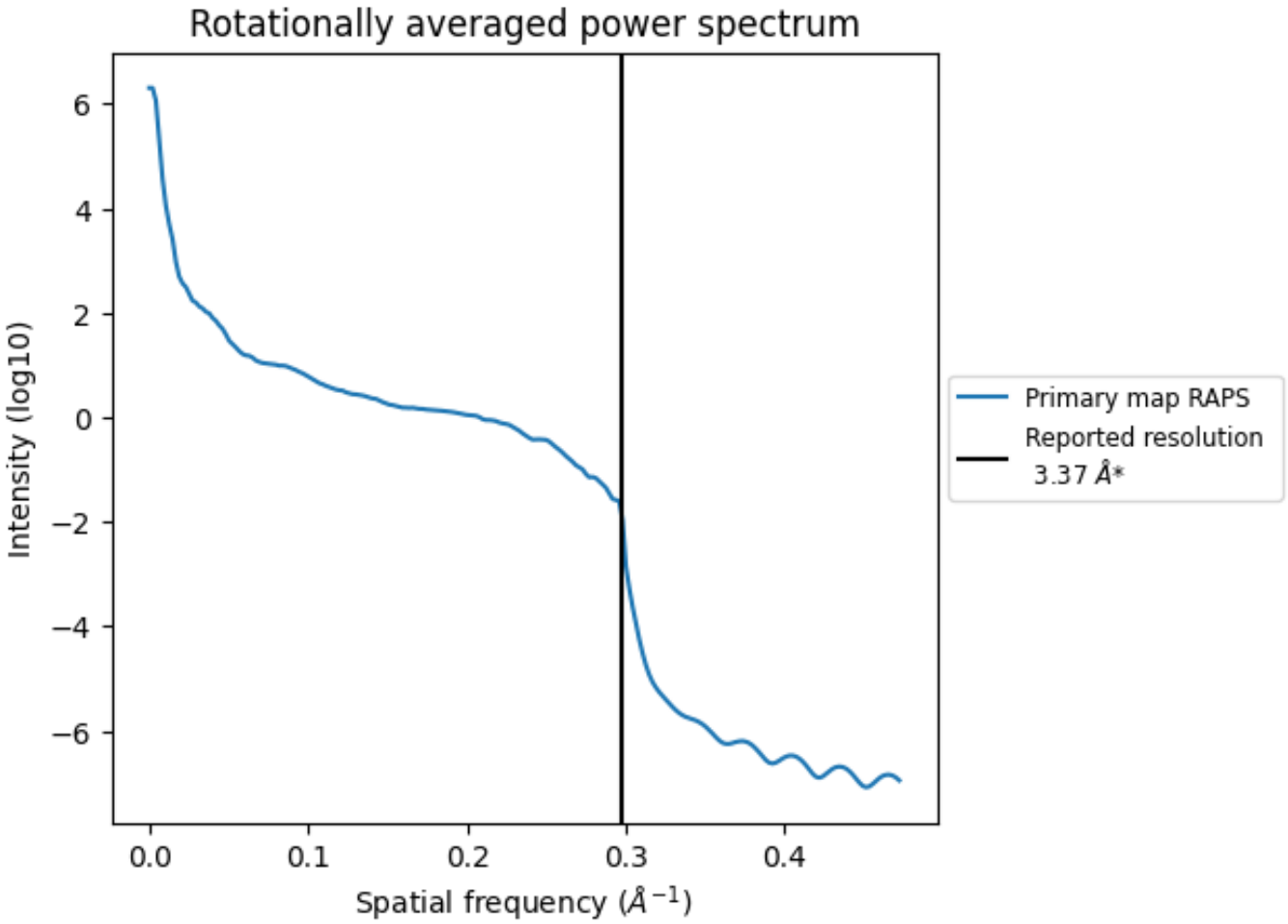
7.2 Volume estimate



The volume at the recommended contour level is 3188 nm^3; this corresponds to an approximate mass of 2880 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 (i)



*Reported resolution corresponds to spatial frequency of 0.297 Å^{-1}

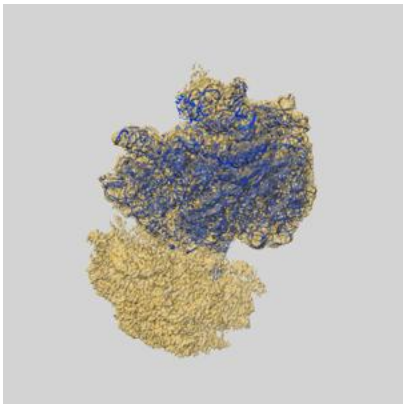
8 Fourier-Shell correlation

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

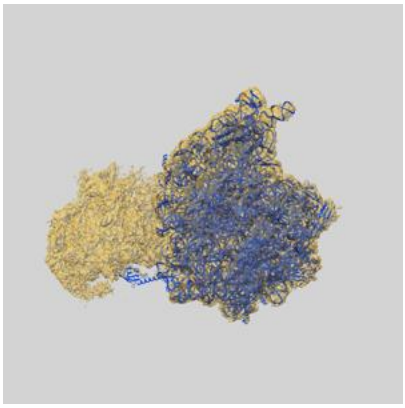
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13956 and PDB model 7QGN. Per-residue inclusion information can be found in section 3 on page 17.

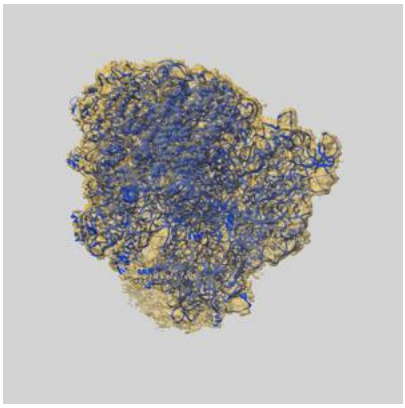
9.1 Map-model overlay



X



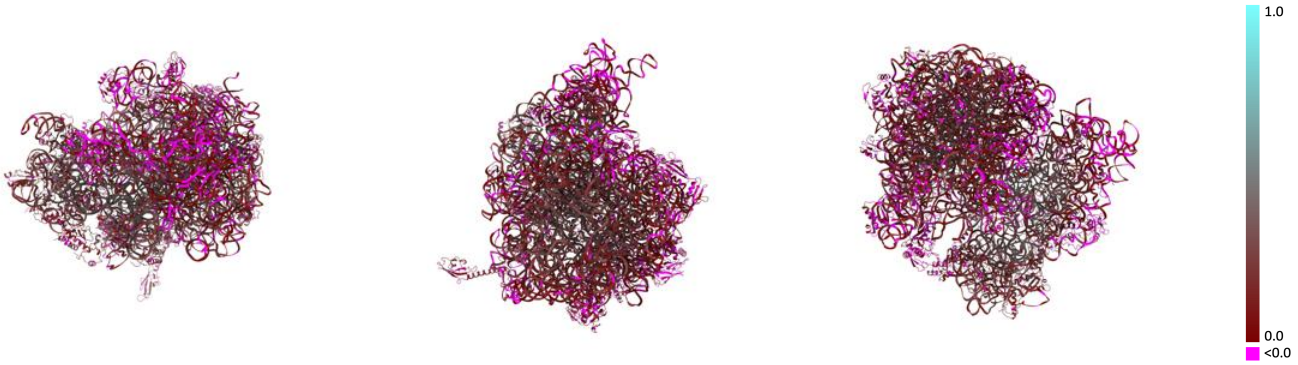
Y



Z

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.

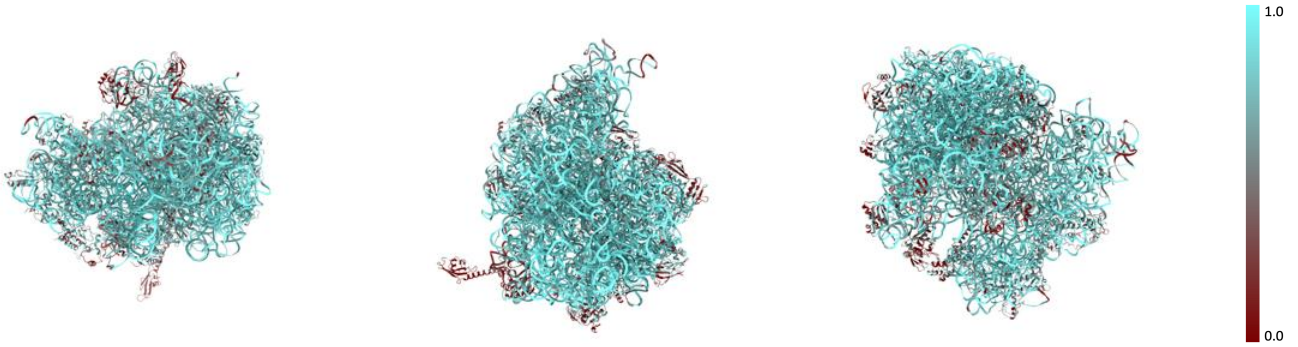
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

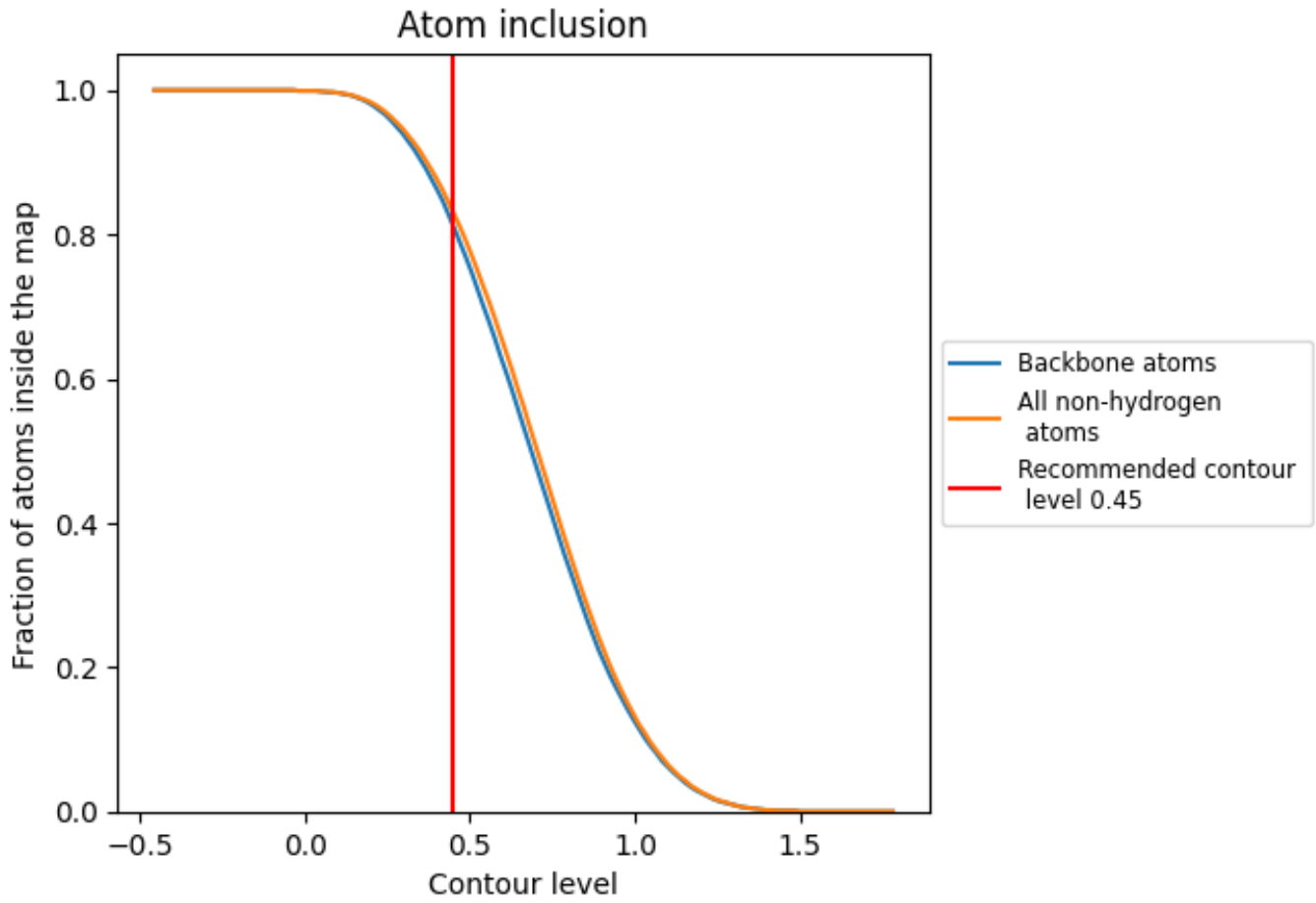
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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, 81% of all backbone atoms, 83% 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	0.8300	0.1810
0	0.9180	0.2440
1	0.6360	0.1660
2	0.7410	0.2820
3	0.5910	0.0580
4	0.8140	0.2370
5	0.5280	0.1490
6	0.5480	0.1290
7	0.7670	0.2440
8	0.6910	0.1920
9	0.6620	0.2430
A	0.7370	0.1610
B	0.3250	0.1890
C	0.0120	0.0460
D	0.5350	0.1080
E	0.7850	0.2330
F	0.5780	0.1350
G	0.7600	0.2470
H	0.7960	0.2870
I	0.6450	0.0550
J	0.6660	0.0690
K	0.5960	0.2170
L	0.1810	0.0110
M	0.9210	0.2460
N	0.9270	0.1880
O	0.8580	0.1050
P	0.7560	0.1160
Q	0.7290	0.0760
R	0.6250	0.1170
S	0.3800	0.0260
T	0.4020	0.0260
U	0.2000	0.1020
V	0.1920	0.0210
W	0.8570	0.0920
X	0.4880	0.0270

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Chain	Atom inclusion	Q-score
Y	0.6730	0.1330
Z	0.7720	0.1600
a	0.8290	0.1080
b	0.4300	0.0360
c	0.5450	-0.0020
d	0.8450	0.1180
e	0.6220	0.0650
f	0.8740	0.2120
g	0.8240	0.2060
h	0.6980	0.1080
i	0.5650	0.0630
j	0.9060	0.0930
k	0.8200	0.1870
l	0.7040	0.1660
m	0.7890	0.1120
n	0.8270	0.2010
o	0.7060	0.0740
p	0.9690	0.2970
q	0.9180	0.1700
r	0.8280	0.1380
s	0.9450	0.2580
t	0.7070	0.1800
u	0.5950	0.0730
v	0.6480	0.2470