



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 04:28 AM UTC

PDB ID : 6HA8 / pdb_00006ha8
EMDB ID : EMD-0177
Title : Cryo-EM structure of the ABCF protein VmlR bound to the Bacillus subtilis ribosome
Authors : Crowe-McAuliffe, C.; Graf, M.; Huter, P.; Abdelshahid, M.; Novacek, J.; Wilson, D.N.
Deposited on : 2018-08-07
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

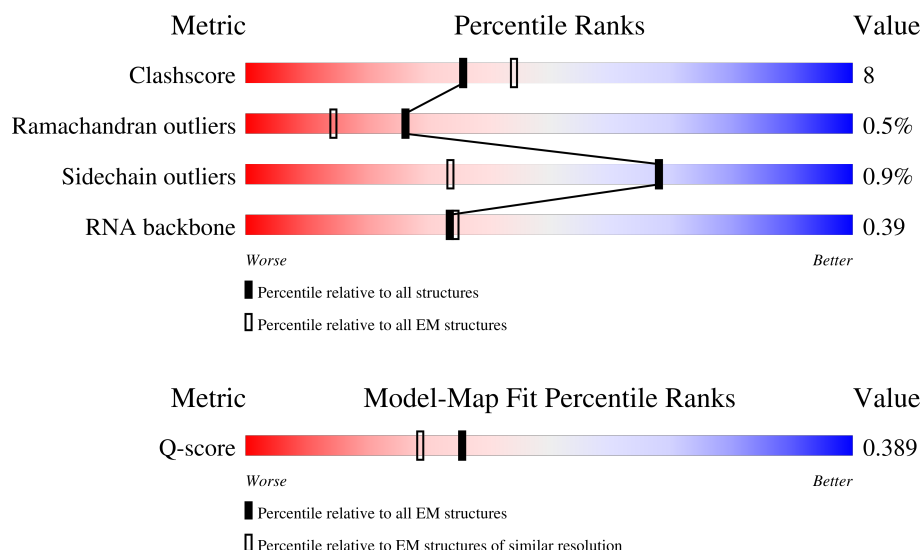
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



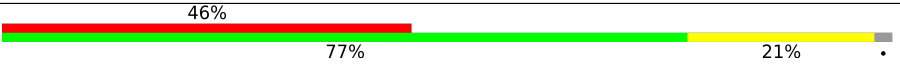
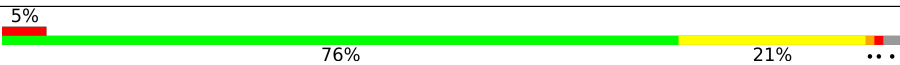
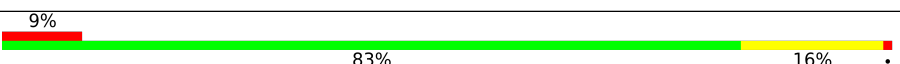
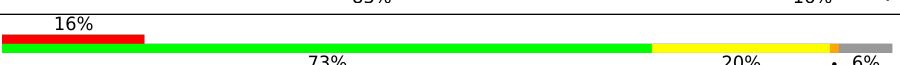
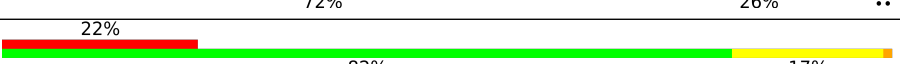
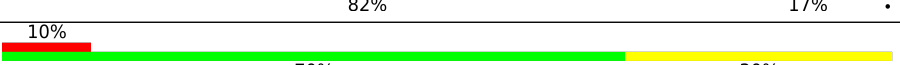
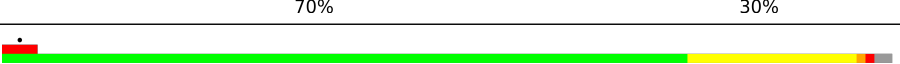
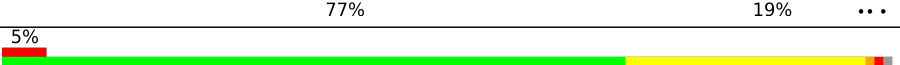
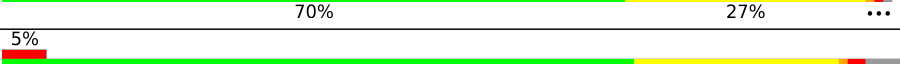
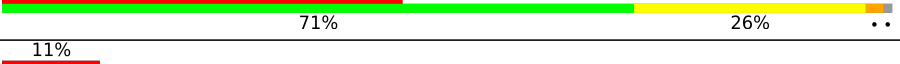
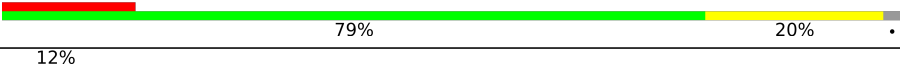
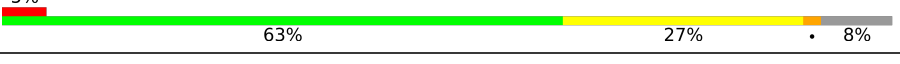
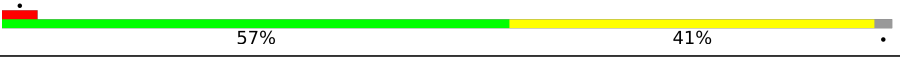
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	A	2928	
2	B	112	
3	C	277	

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Mol	Chain	Length	Quality of chain
4	D	209	
5	E	207	
6	F	179	
7	G	179	
8	J	145	
9	K	122	
10	L	146	
11	M	144	
12	N	120	
13	O	120	
14	P	115	
15	Q	119	
16	R	102	
17	S	113	
18	T	95	
19	U	103	
20	V	548	
21	W	94	
22	X	62	
23	Y	66	
24	Z	59	
25	0	59	
26	1	49	
27	2	44	
28	3	66	

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Mol	Chain	Length	Quality of chain
29	4	37	
30	6	66	
31	7	3	
32	8	232	
33	a	1554	
34	b	246	
35	c	218	
36	d	200	
37	e	166	
38	f	95	
39	g	156	
40	h	132	
41	i	130	
42	j	102	
43	k	131	
44	l	138	
45	m	121	
46	n	61	
47	o	89	
48	p	90	
49	q	87	
50	r	79	
51	s	92	
52	t	88	
53	x	75	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
54	TEL	A	3001	X	-	-	-
55	ATP	V	900	-	-	X	-
55	ATP	V	901	-	-	X	-

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 146404 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2887	Total	C	N	O	P	0	0
			61997	27661	11460	19992	2884		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	272	Total	C	N	O	S	0	0
			2083	1296	408	373	6		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	206	Total	C	N	O	S	0	0
			1569	985	289	290	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	205	Total	C	N	O	S	0	0
			1561	980	289	290	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	176	Total	C	N	O	S	0	0
			1386	882	241	256	7		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	142	Total	C	N	O	S	0	0
			1123	710	206	202	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	122	Total	C	N	O	S	0	0
			920	571	173	172	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	146	Total	C	N	O	S	0	0
			1081	671	207	201	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	119	Total	C	N	O	S	0	0
			953	583	186	180	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	120	Total	C	N	O	S	0	0
			912	564	176	171	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	115	Total	C	N	O	S	0	0
			944	600	185	158	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	117	Total	C	N	O	S	0	0
			940	591	189	156	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	101	Total	C	N	O		0	0
			786	501	139	146			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	109	Total	C	N	O	S	0	0
			842	525	164	150	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	90	Total	C	N	O	S	0	0
			725	452	134	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	101	Total	C	N	O	S	0	0
			762	478	142	138	4		

- Molecule 20 is a protein called Nucleotide-binding protein ExpZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	541	Total	C	N	O	S	0	0
			4177	2637	737	796	7		

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-5	MET	-	initiating methionine	UNP P39115
V	-4	HIS	-	expression tag	UNP P39115
V	-3	HIS	-	expression tag	UNP P39115
V	-2	HIS	-	expression tag	UNP P39115
V	-1	HIS	-	expression tag	UNP P39115
V	0	HIS	-	expression tag	UNP P39115
V	1	HIS	-	expression tag	UNP P39115
V	129	GLN	GLU	engineered mutation	UNP P39115
V	432	GLN	GLU	engineered mutation	UNP P39115
V	486	ALA	-	expression tag	UNP P39115
V	487	ALA	-	expression tag	UNP P39115
V	488	ALA	-	expression tag	UNP P39115
V	489	ALA	-	expression tag	UNP P39115
V	490	ALA	-	expression tag	UNP P39115
V	491	ALA	-	expression tag	UNP P39115
V	492	ALA	-	expression tag	UNP P39115
V	493	ALA	-	expression tag	UNP P39115
V	494	ALA	-	expression tag	UNP P39115
V	495	ALA	-	expression tag	UNP P39115
V	496	ALA	-	expression tag	UNP P39115
V	497	ALA	-	expression tag	UNP P39115
V	498	ALA	-	expression tag	UNP P39115
V	499	ALA	-	expression tag	UNP P39115
V	500	ALA	-	expression tag	UNP P39115
V	501	ALA	-	expression tag	UNP P39115
V	502	ALA	-	expression tag	UNP P39115
V	503	ALA	-	expression tag	UNP P39115
V	504	ALA	-	expression tag	UNP P39115
V	505	ALA	-	expression tag	UNP P39115
V	506	ALA	-	expression tag	UNP P39115
V	507	ALA	-	expression tag	UNP P39115
V	508	ALA	-	expression tag	UNP P39115
V	509	ALA	-	expression tag	UNP P39115
V	510	ALA	-	expression tag	UNP P39115
V	511	ALA	-	expression tag	UNP P39115
V	512	ALA	-	expression tag	UNP P39115
V	513	ALA	-	expression tag	UNP P39115
V	514	ALA	-	expression tag	UNP P39115
V	515	ALA	-	expression tag	UNP P39115
V	516	ALA	-	expression tag	UNP P39115
V	517	ALA	-	expression tag	UNP P39115
V	518	ALA	-	expression tag	UNP P39115
V	519	ALA	-	expression tag	UNP P39115

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Chain	Residue	Modelled	Actual	Comment	Reference
V	520	ALA	-	expression tag	UNP P39115
V	521	ALA	-	expression tag	UNP P39115
V	522	ALA	-	expression tag	UNP P39115
V	523	ALA	-	expression tag	UNP P39115
V	524	ALA	-	expression tag	UNP P39115
V	525	ALA	-	expression tag	UNP P39115
V	526	ALA	-	expression tag	UNP P39115
V	527	ALA	-	expression tag	UNP P39115
V	528	ALA	-	expression tag	UNP P39115
V	529	ALA	-	expression tag	UNP P39115
V	530	ALA	-	expression tag	UNP P39115
V	531	ALA	-	expression tag	UNP P39115
V	532	ALA	-	expression tag	UNP P39115
V	533	ALA	-	expression tag	UNP P39115
V	534	ALA	-	expression tag	UNP P39115
V	535	ALA	-	expression tag	UNP P39115
V	536	ALA	-	expression tag	UNP P39115
V	537	ALA	-	expression tag	UNP P39115
V	538	ALA	-	expression tag	UNP P39115
V	539	ALA	-	expression tag	UNP P39115
V	540	ALA	-	expression tag	UNP P39115
V	541	ALA	-	expression tag	UNP P39115
V	542	ALA	-	expression tag	UNP P39115

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	82	Total	C	N	O	0	0
			630	390	123	117		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	58	Total	C	N	O	S	0	0
			444	275	92	75	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	65	Total	C	N	O	S	0	0
			530	328	102	98	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	58	Total	C	N	O	S	0	0
			455	281	89	84	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	0	54	Total	C	N	O	S	0	0
			426	262	86	71	7		

- Molecule 26 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1	48	Total	C	N	O	S	0	0
			401	244	80	73	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	44	Total	C	N	O	S	0	0
			367	222	89	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	4	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 30 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	63	Total	C	N	O	S	0	0
			499	312	91	91	5		

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	3	Total	C	N	O	P	0	0
			60	27	7	23	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	212	Total	C	N	O	S	0	0
			1599	1015	273	306	5		

- Molecule 33 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1533	Total	C	N	O	P	0	0
			32891	14667	6034	10657	1533		

- Molecule 34 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	218	Total	C	N	O	S	0	0
			1757	1119	309	323	6		

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	206	Total	C	N	O	S	0	0
			1619	1011	304	301	3		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	195	Total	C	N	O	S	0	0
			1568	991	291	284	2		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	164	Total	C	N	O	S	0	0
			1218	767	225	224	2		

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	92	Total	C	N	O	S	0	0
			755	476	132	146	1		

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	149	Total	C	N	O	S	0	0
			1181	740	220	215	6		

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	131	Total	C	N	O	S	0	0
			1036	655	191	187	3		

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	125	Total	C	N	O	S	0	0
			966	599	191	175	1		

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	95	Total	C	N	O	S	0	0
			761	479	139	141	2		

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	114	Total	C	N	O	S	0	0
			838	516	164	156	2		

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	136	Total	C	N	O	S	0	0
			1052	653	211	186	2		

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	m	108	Total	C	N	O		
			868	534	176	158	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	60	Total	C	N	O	S		
			497	317	98	77	5	0	0

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	85	Total	C	N	O	S		
			710	436	144	129	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	88	Total	C	N	O	S		
			695	441	128	124	2	0	0

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	84	Total	C	N	O	S		
			691	435	128	126	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	64	Total	C	N	O	S		
			518	332	96	88	2	0	0

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	78	Total	C	N	O	S		
			633	409	112	110	2	0	0

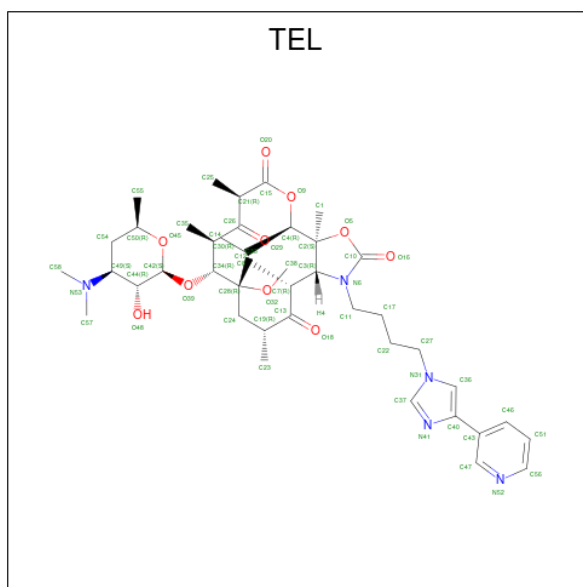
- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	83	Total	C	N	O	S	0	0
			637	390	130	116	1		

- Molecule 53 is a RNA chain called P-tRNA(Leu).

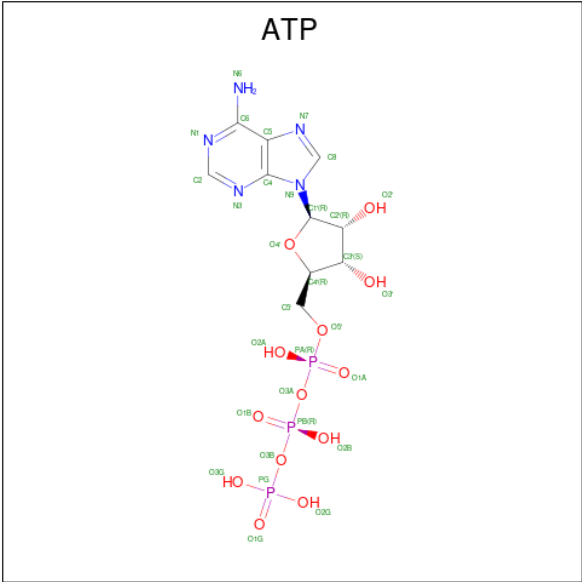
Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	75	Total	C	N	O	P	0	0
			1603	714	284	530	75		

- Molecule 54 is TELITHROMYCIN (CCD ID: TEL) (formula: $C_{43}H_{65}N_5O_{10}$).



Mol	Chain	Residues	Atoms				AltConf
54	A	1	Total	C	N	O	0
			58	43	5	10	

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

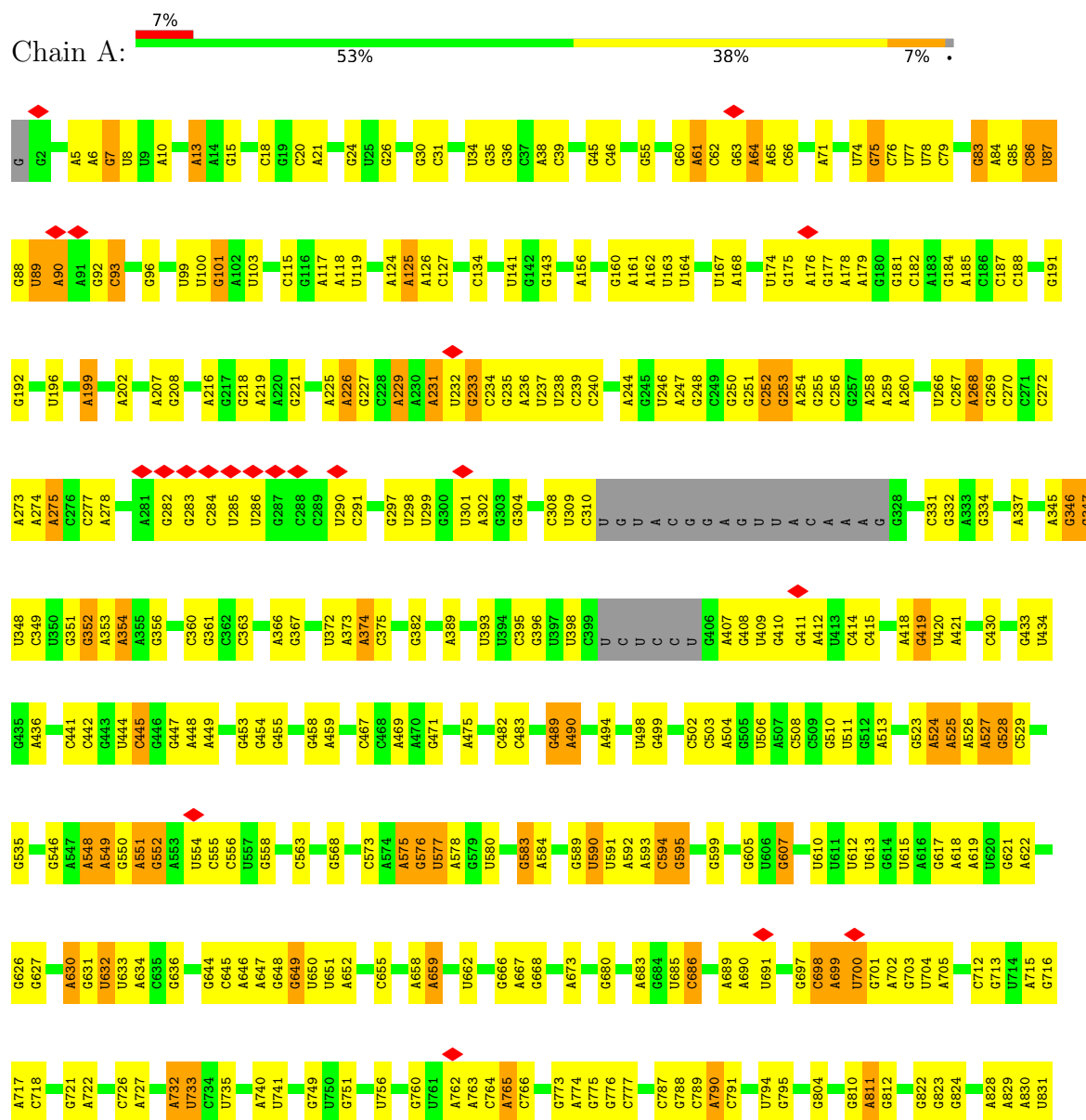


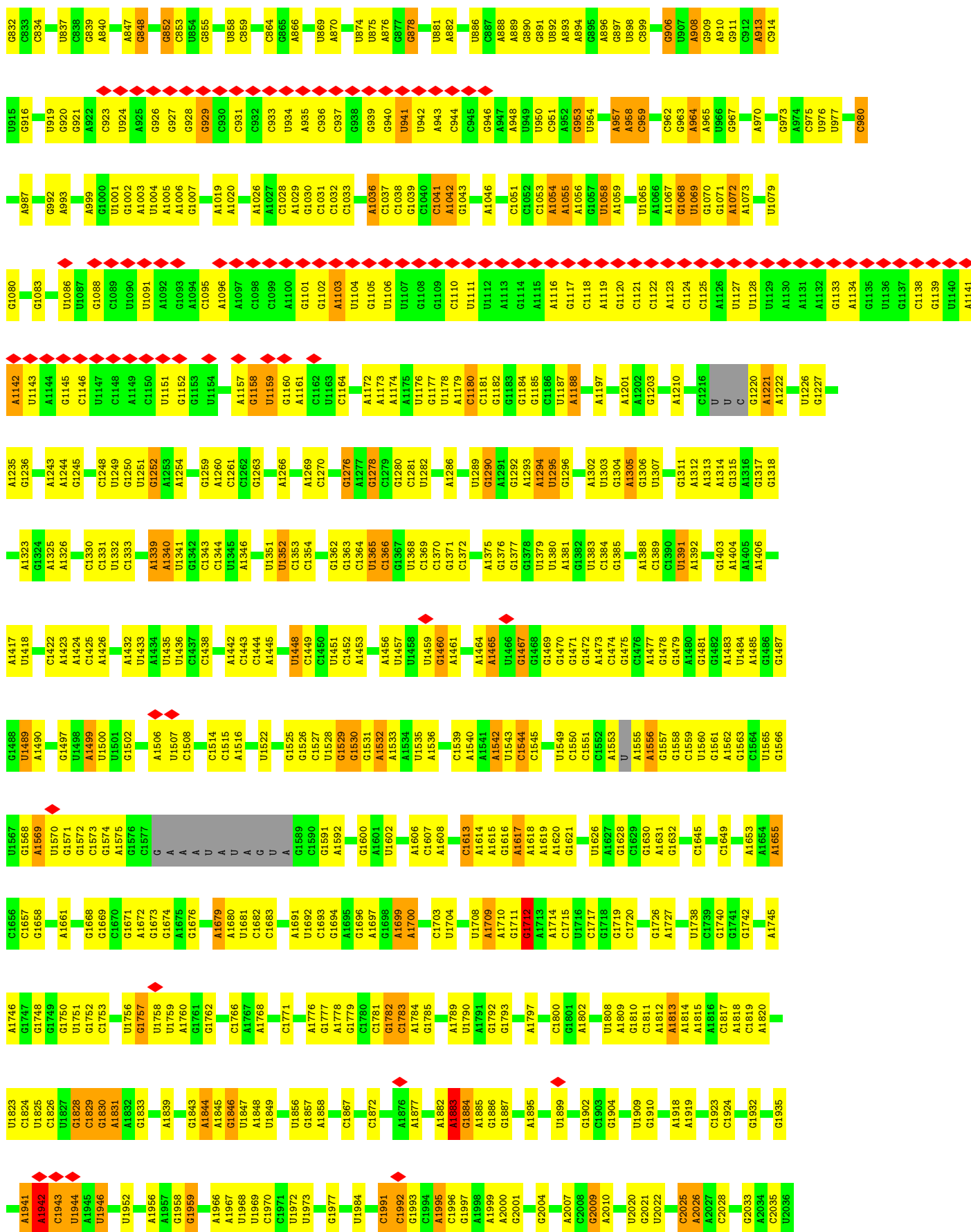
Mol	Chain	Residues	Atoms					AltConf
55	V	1	Total	C	N	O	P	0
			31	10	5	13	3	
55	V	1	Total	C	N	O	P	0
			31	10	5	13	3	

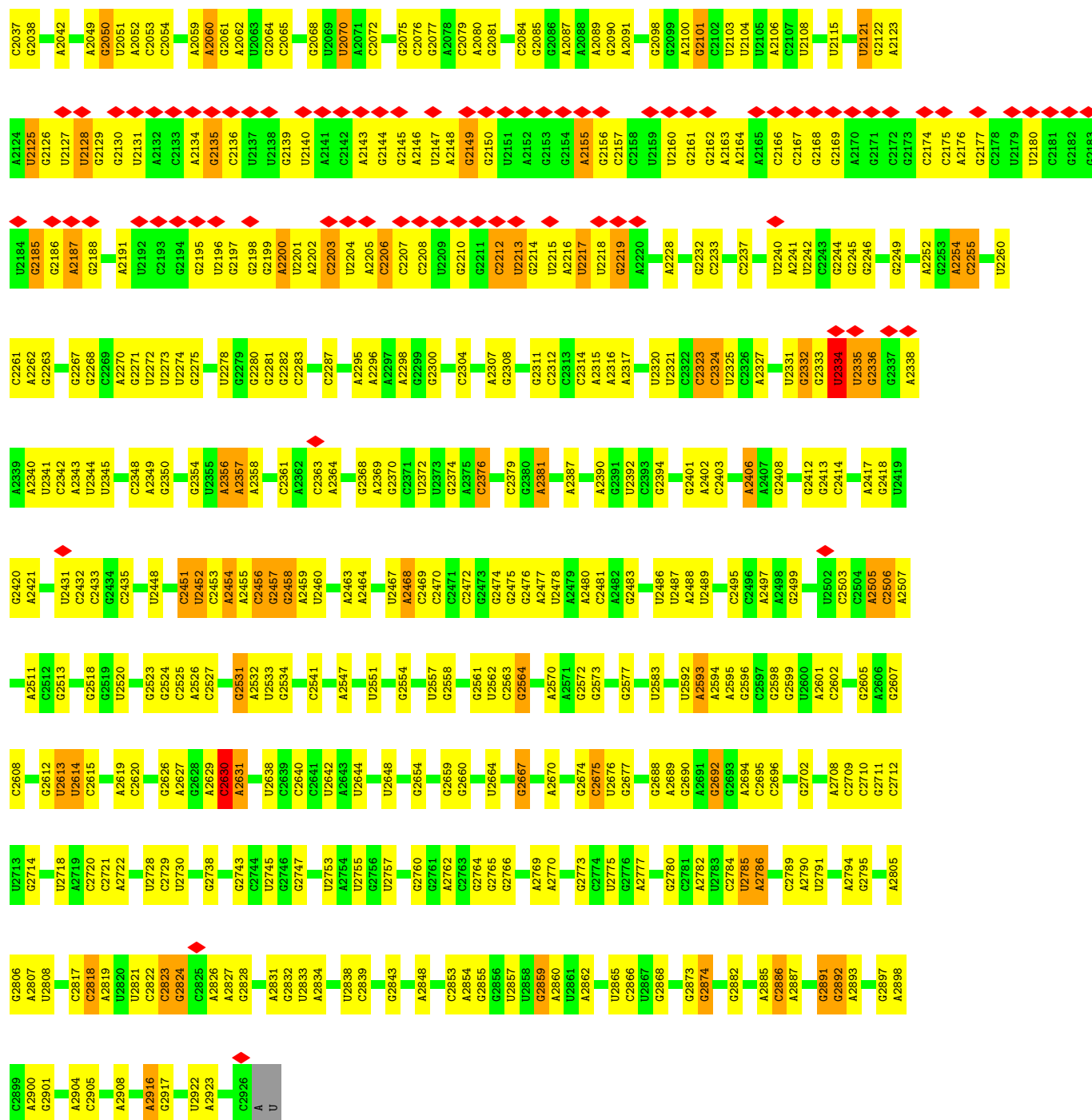
3 Residue-property plots

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

• Molecule 1: 23S rRNA

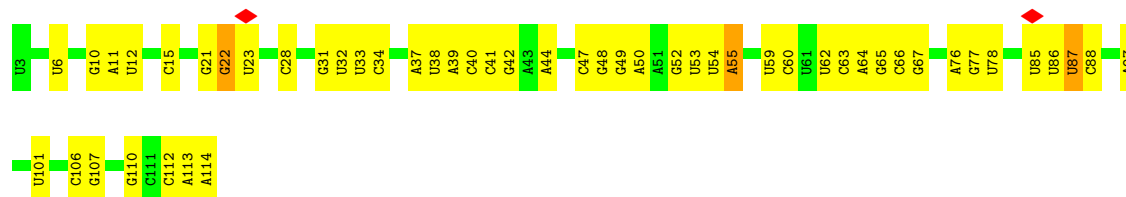




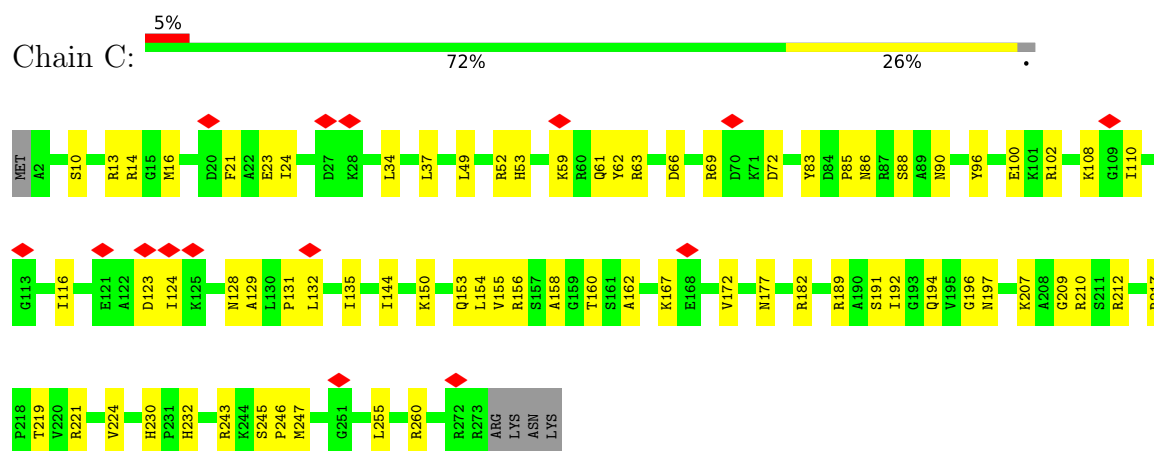


• Molecule 2: 5S rRNA

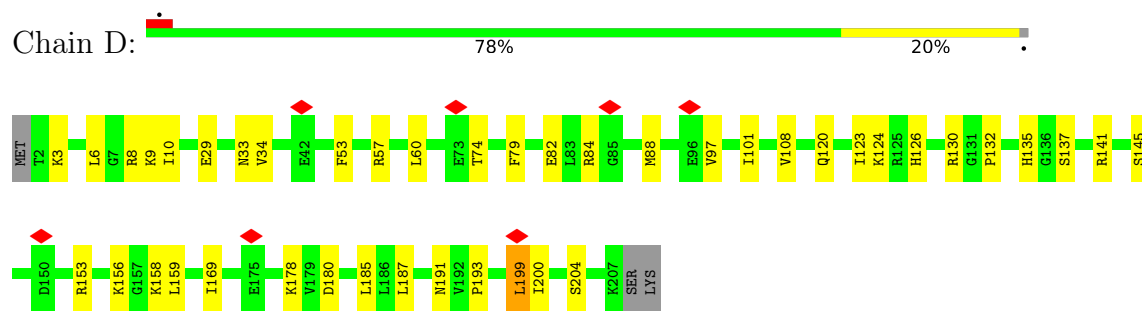
Chain B:



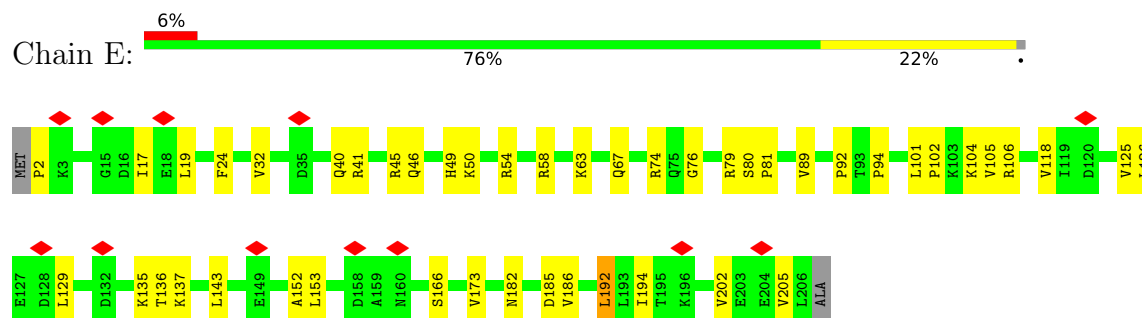
- Molecule 3: 50S ribosomal protein L2



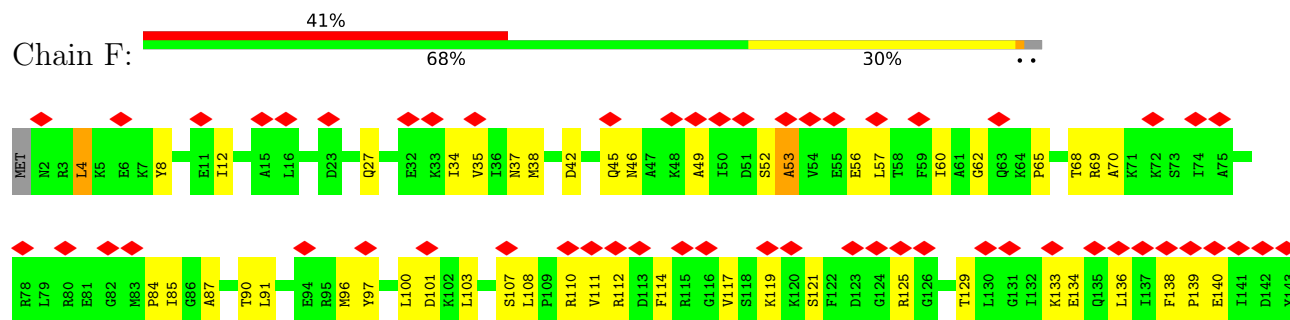
- Molecule 4: 50S ribosomal protein L3

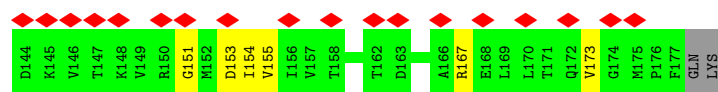


- Molecule 5: 50S ribosomal protein L4

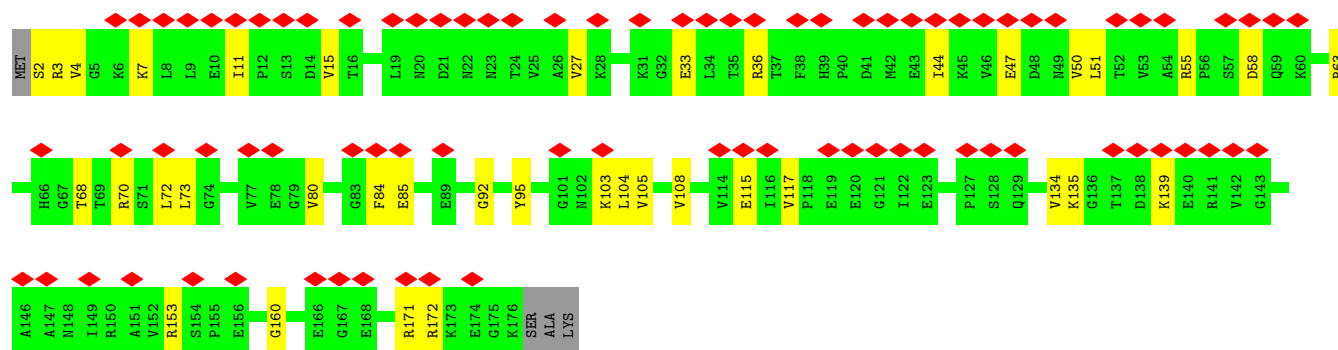
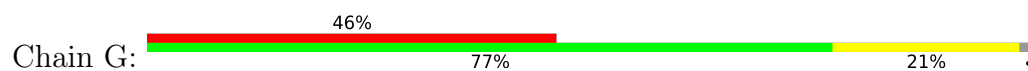


- Molecule 6: 50S ribosomal protein L5

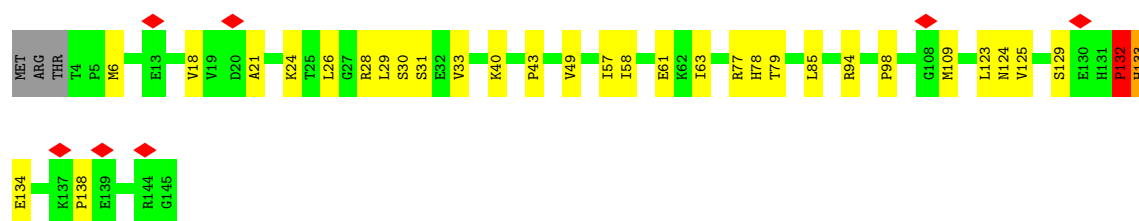
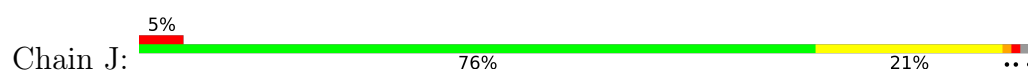




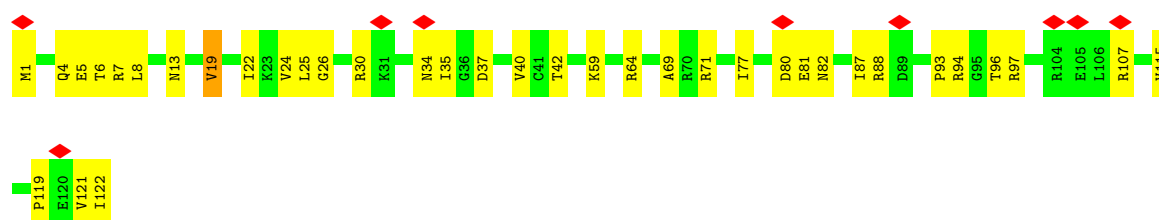
• Molecule 7: 50S ribosomal protein L6



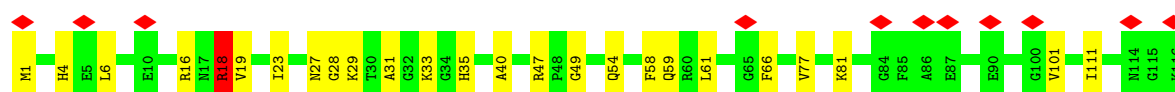
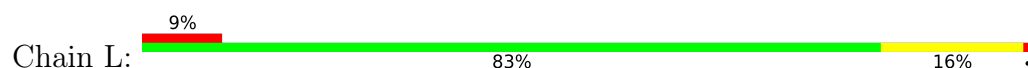
• Molecule 8: 50S ribosomal protein L13

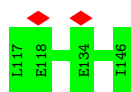


• Molecule 9: 50S ribosomal protein L14

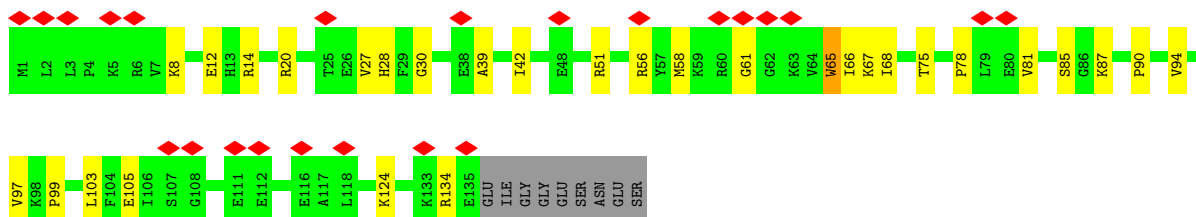
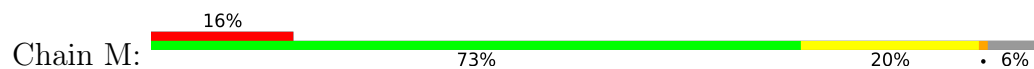


• Molecule 10: 50S ribosomal protein L15

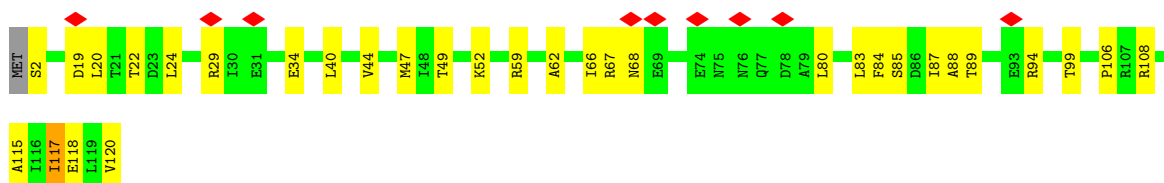




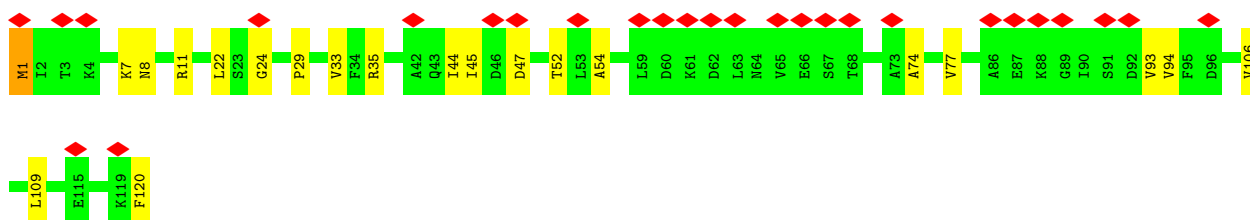
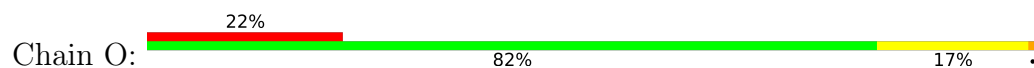
- Molecule 11: 50S ribosomal protein L16



- Molecule 12: 50S ribosomal protein L17



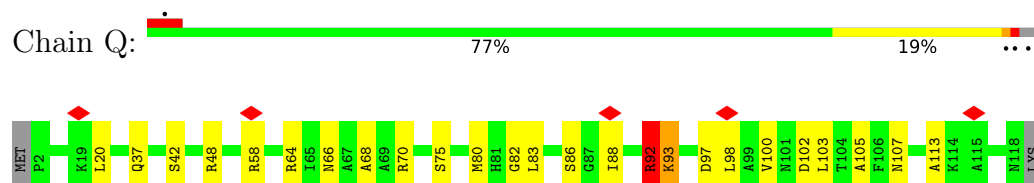
- Molecule 13: 50S ribosomal protein L18



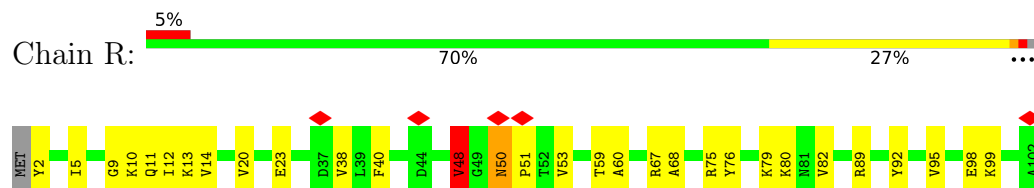
- Molecule 14: 50S ribosomal protein L19



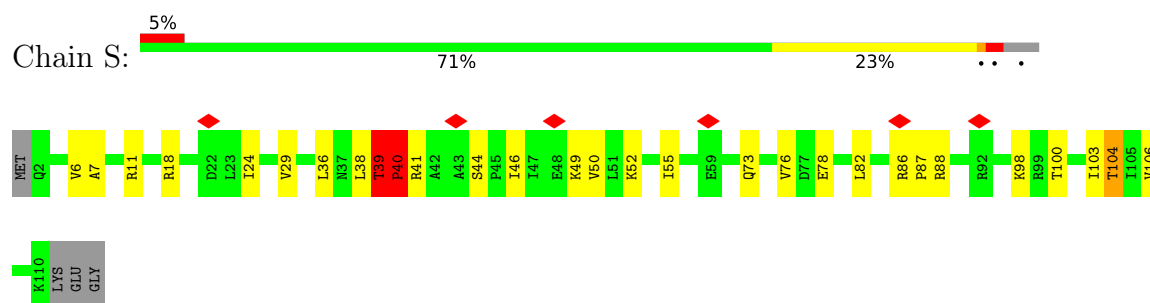
- Molecule 15: 50S ribosomal protein L20



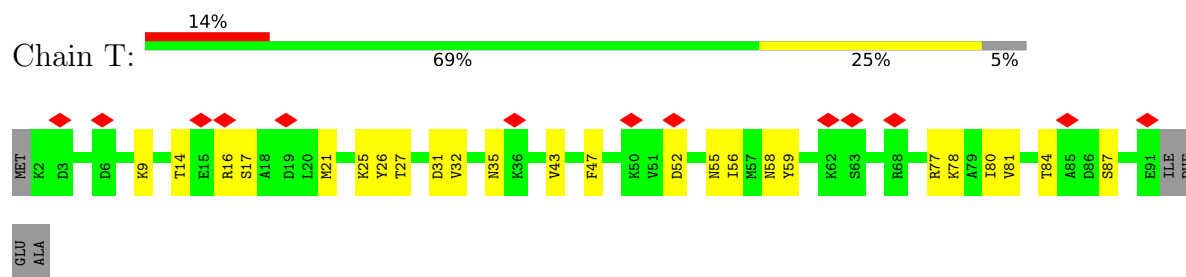
- Molecule 16: 50S ribosomal protein L21



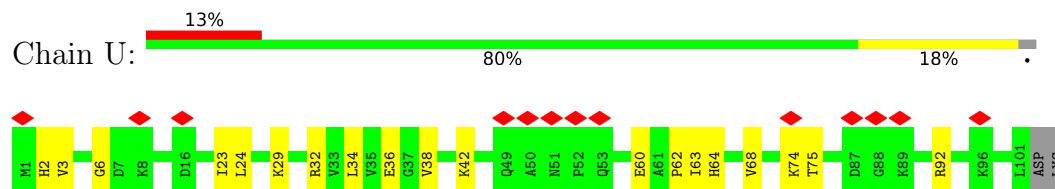
- Molecule 17: 50S ribosomal protein L22



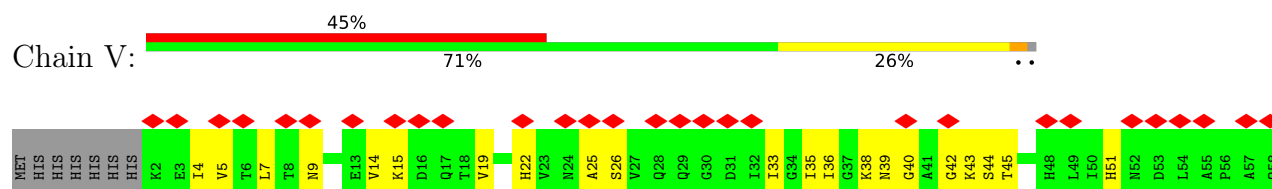
- Molecule 18: 50S ribosomal protein L23

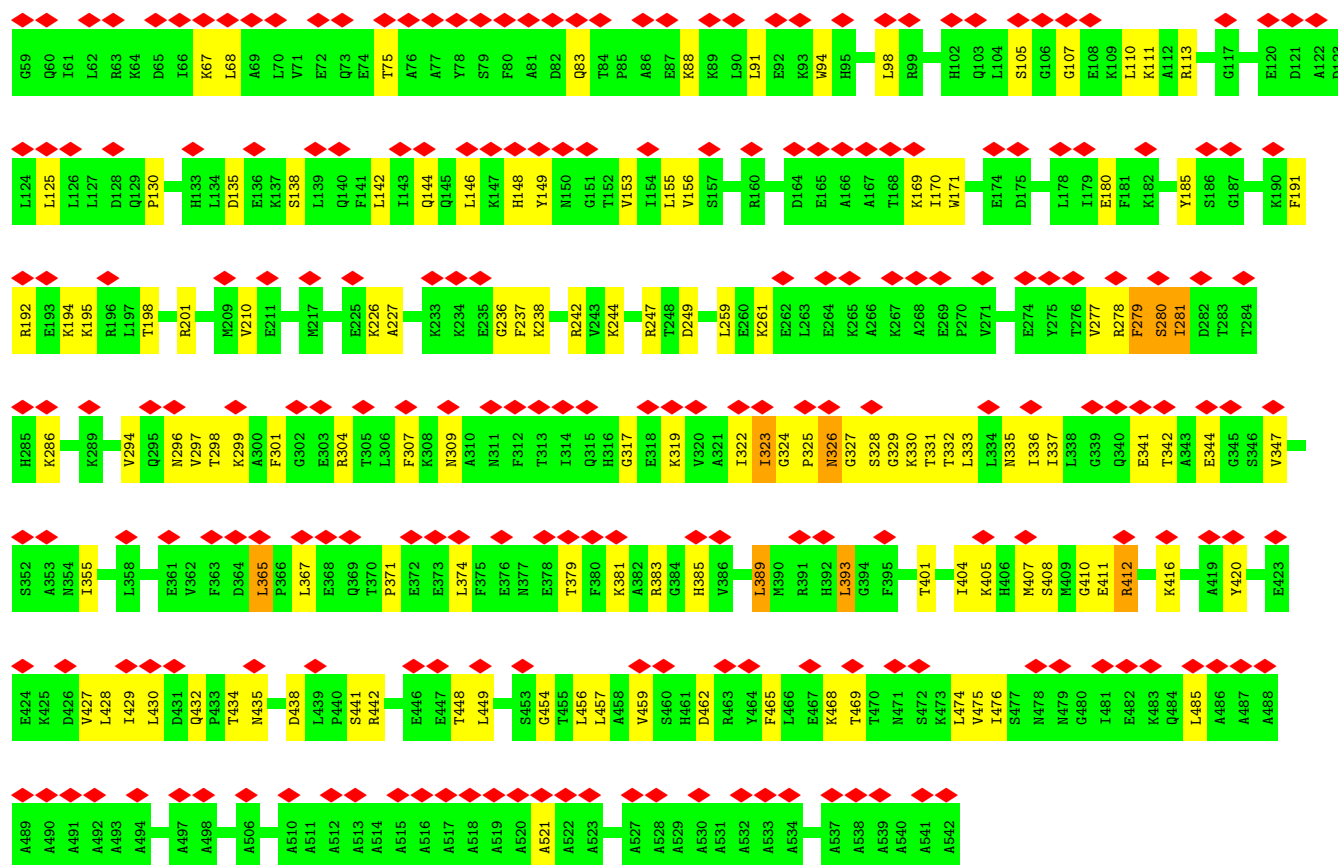


- Molecule 19: 50S ribosomal protein L24

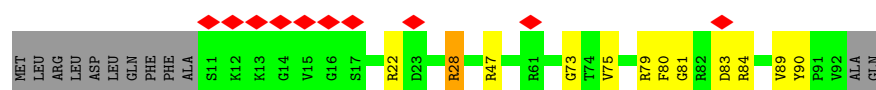
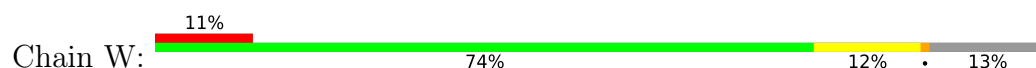


- Molecule 20: Nucleotide-binding protein ExpZ

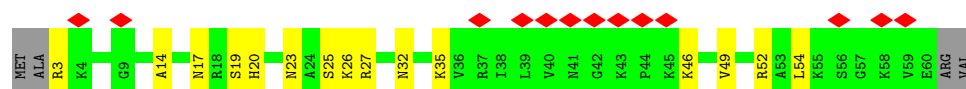




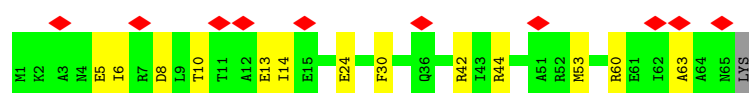
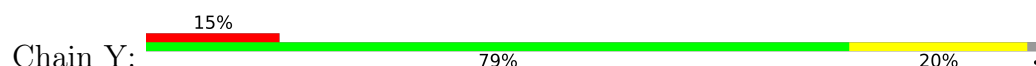
• Molecule 21: 50S ribosomal protein L27



• Molecule 22: 50S ribosomal protein L28



• Molecule 23: 50S ribosomal protein L29



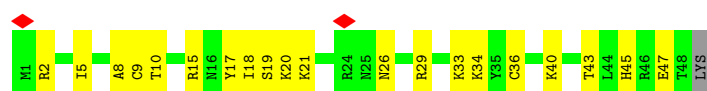
• Molecule 24: 50S ribosomal protein L30



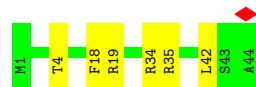
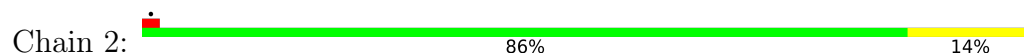
- Molecule 25: 50S ribosomal protein L32



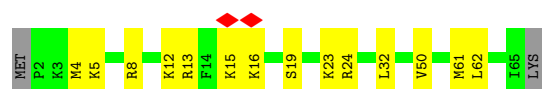
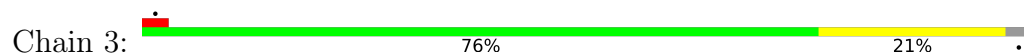
- Molecule 26: 50S ribosomal protein L33 1



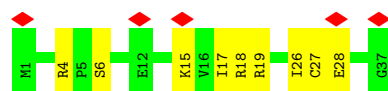
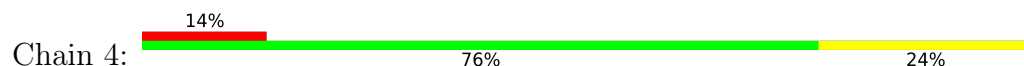
- Molecule 27: 50S ribosomal protein L34



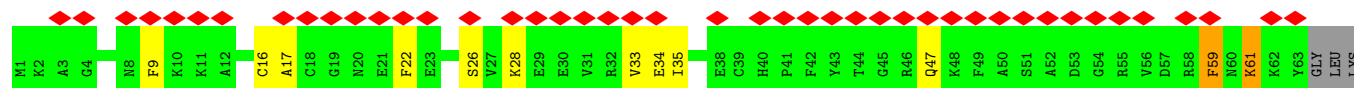
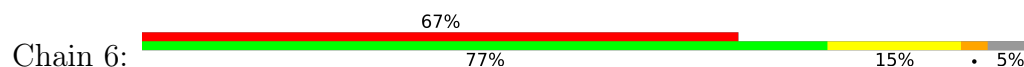
- Molecule 28: 50S ribosomal protein L35



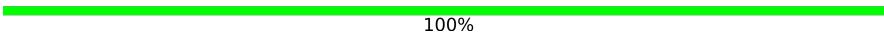
- Molecule 29: 50S ribosomal protein L36



- Molecule 30: 50S ribosomal protein L31

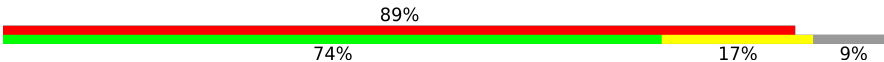


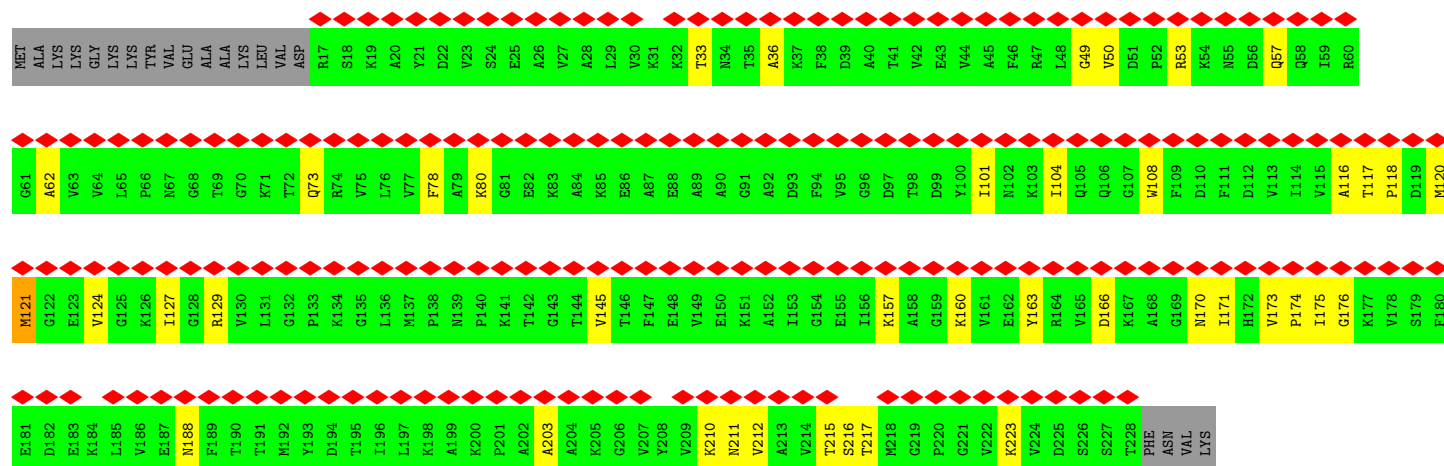
- Molecule 31: mRNA

Chain 7:  100%

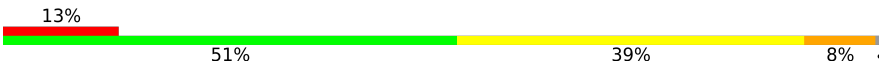
There are no outlier residues recorded for this chain.

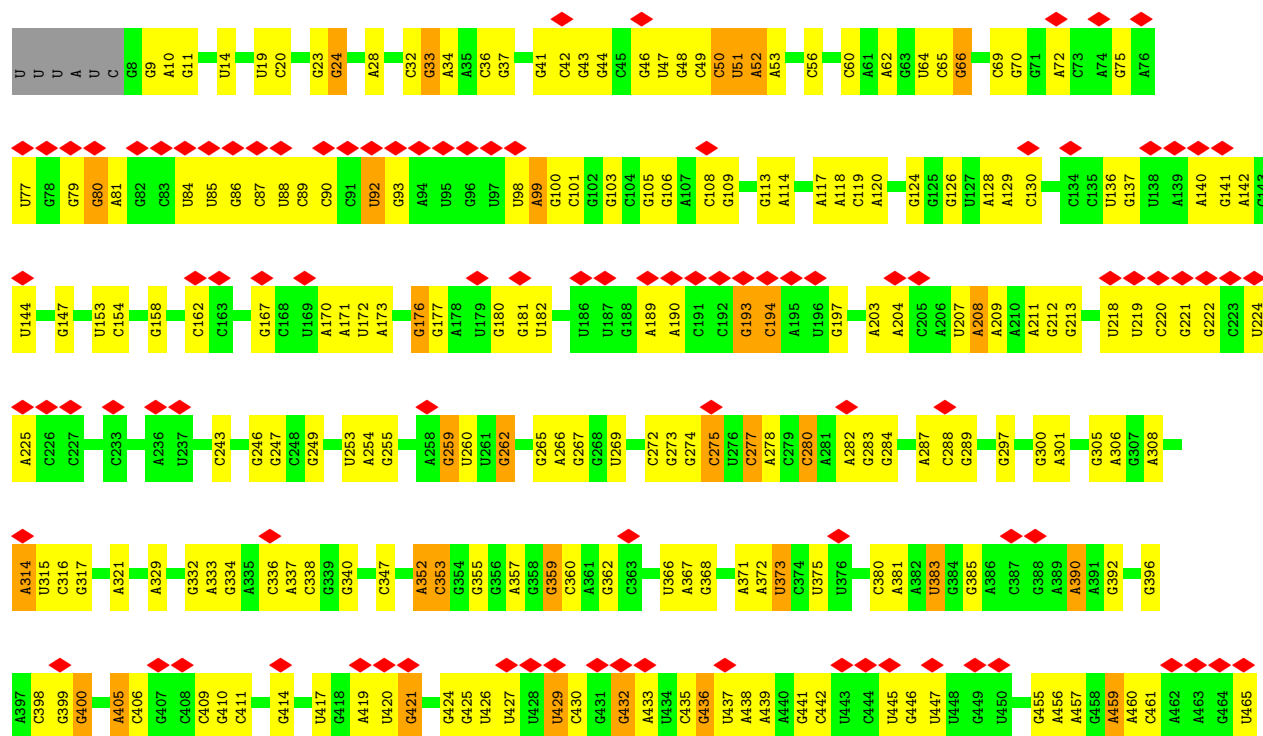
- Molecule 32: 50S ribosomal protein L1

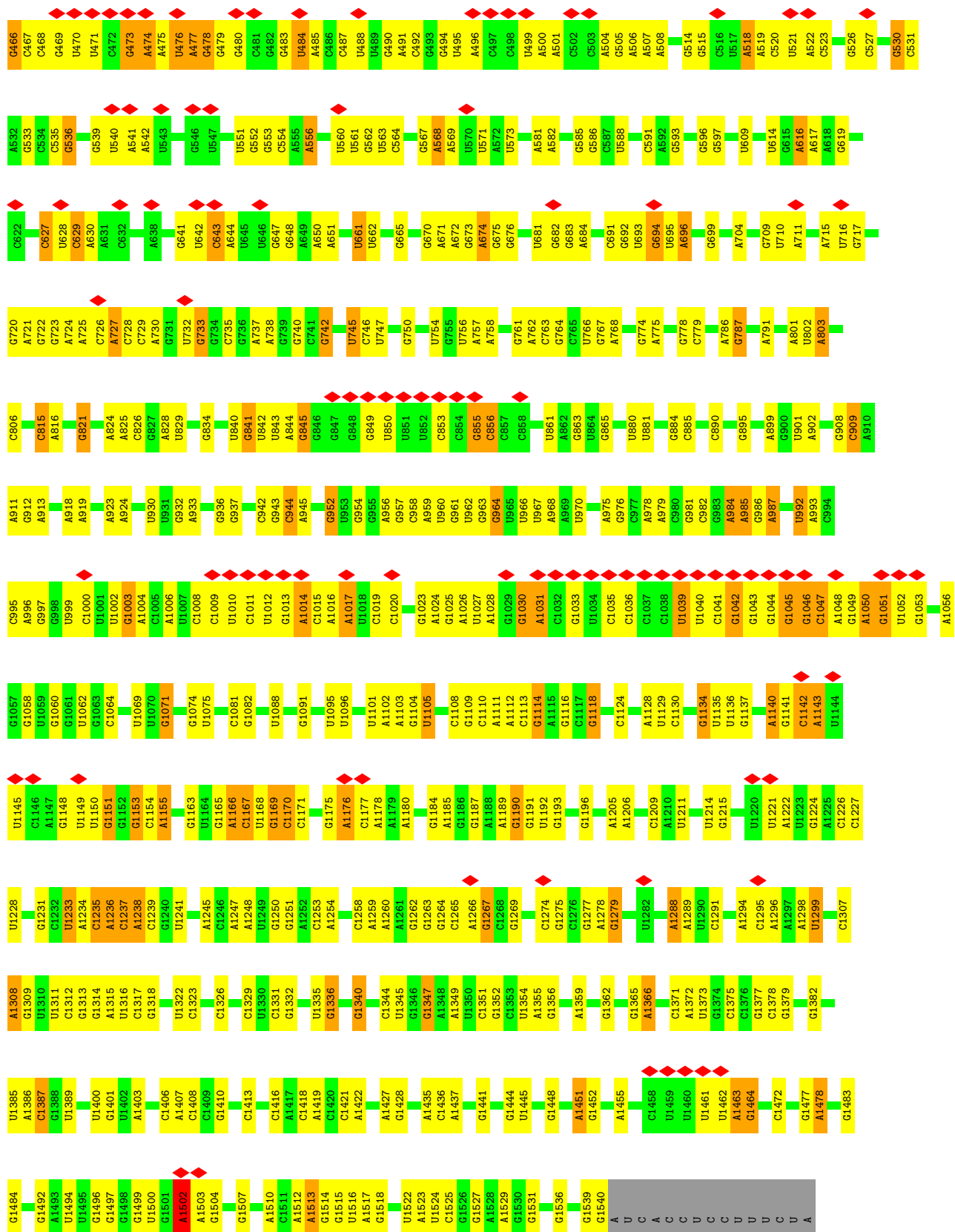
Chain 8:  89%



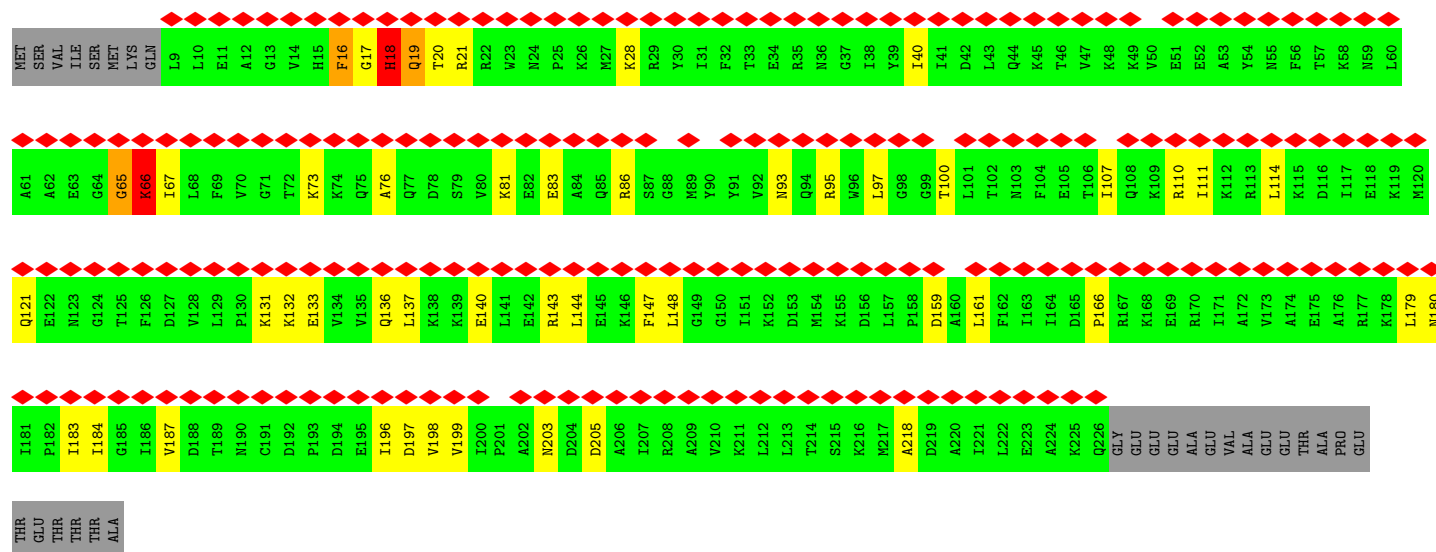
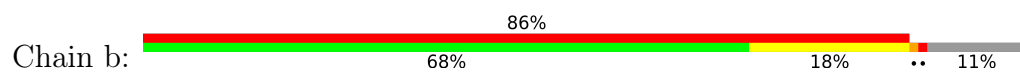
- Molecule 33: 16S rRNA

Chain a:  13%

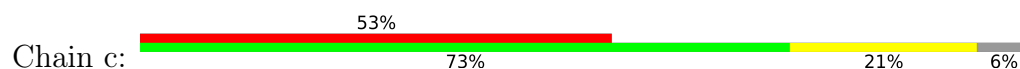




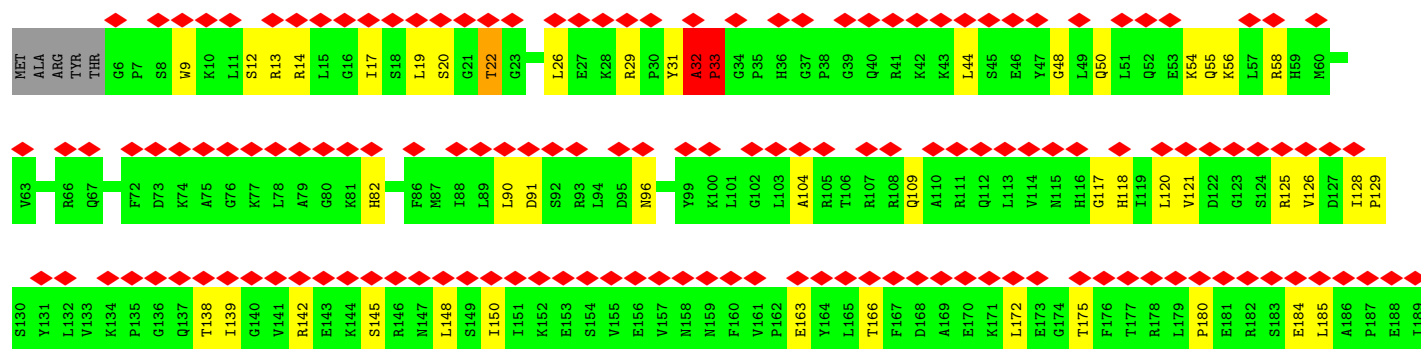
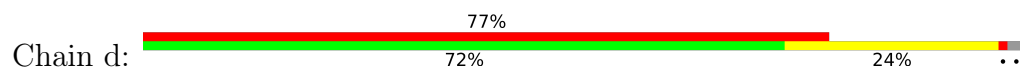
• Molecule 34: 30S ribosomal protein S2



• Molecule 35: 30S ribosomal protein S3

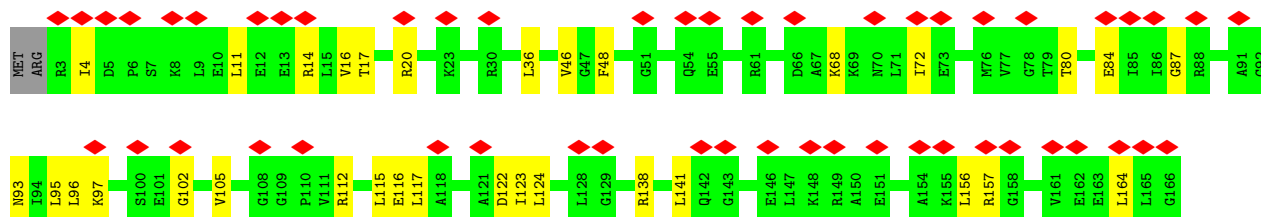
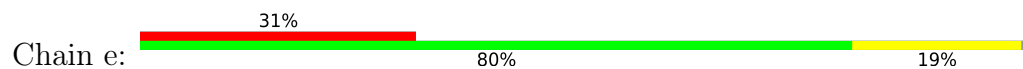


• Molecule 36: 30S ribosomal protein S4

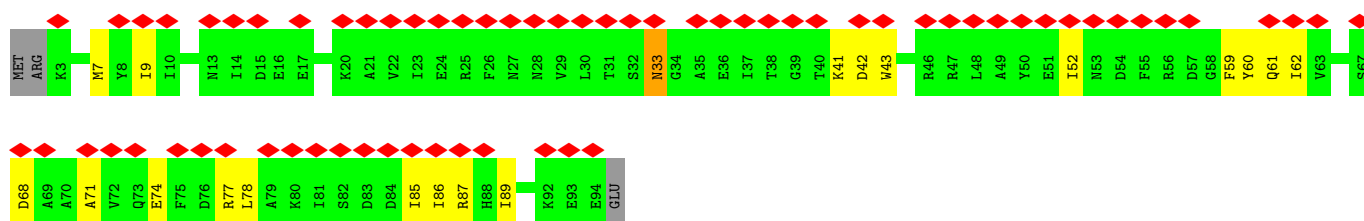
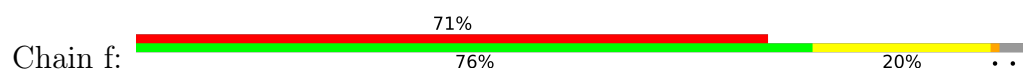




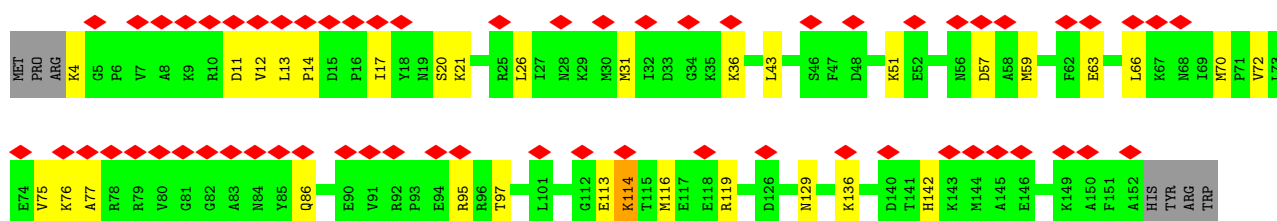
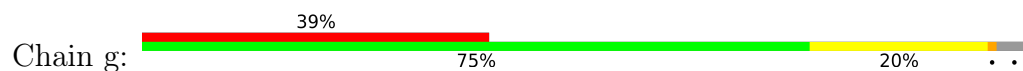
- Molecule 37: 30S ribosomal protein S5



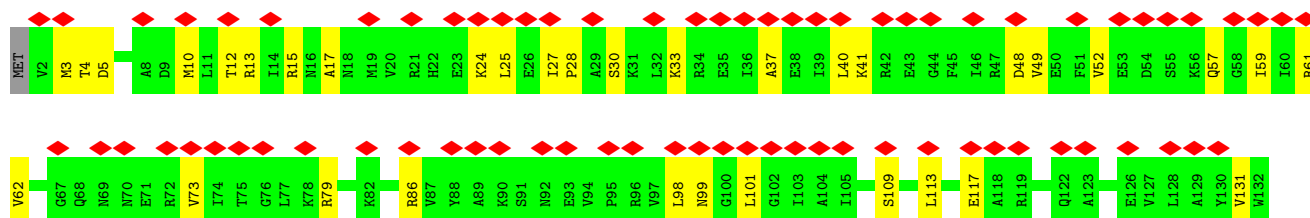
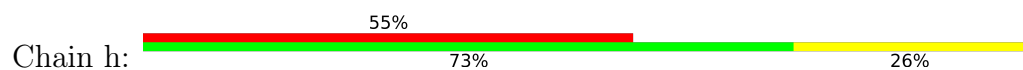
- Molecule 38: 30S ribosomal protein S6



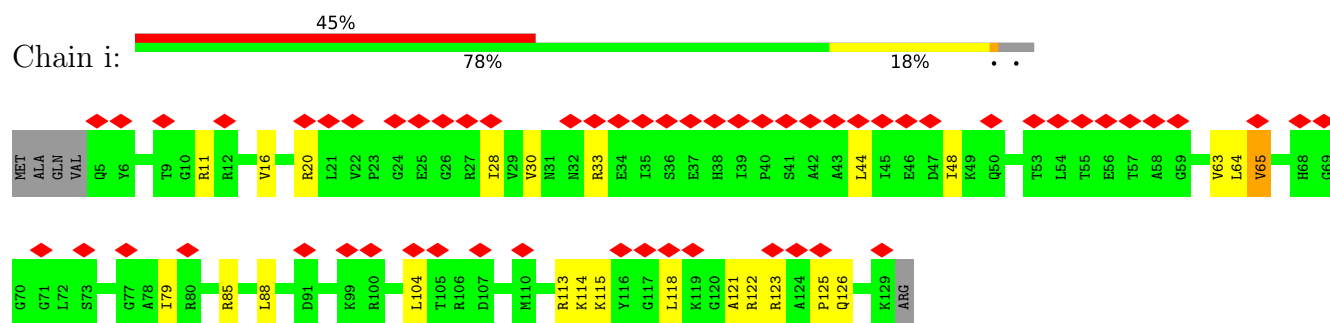
- Molecule 39: 30S ribosomal protein S7



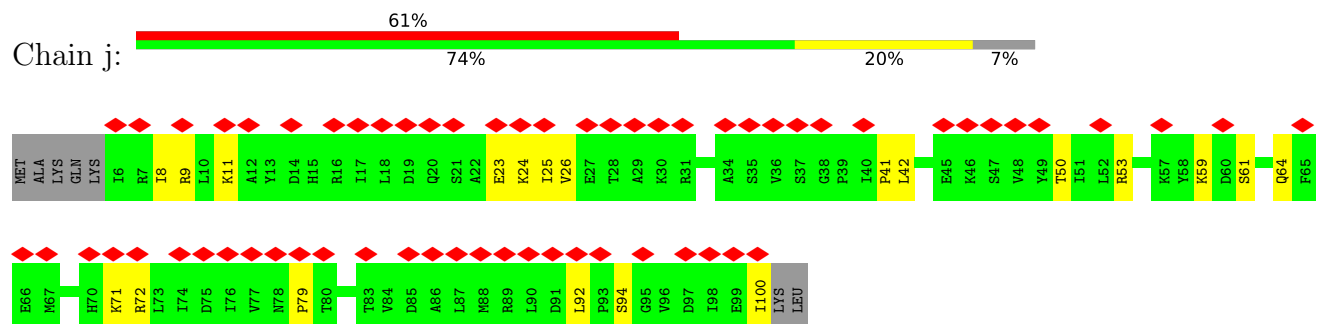
- Molecule 40: 30S ribosomal protein S8



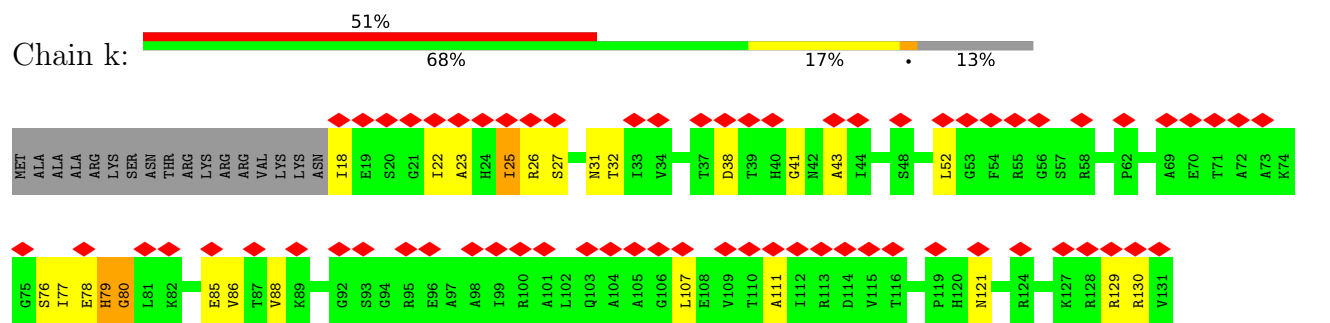
- Molecule 41: 30S ribosomal protein S9



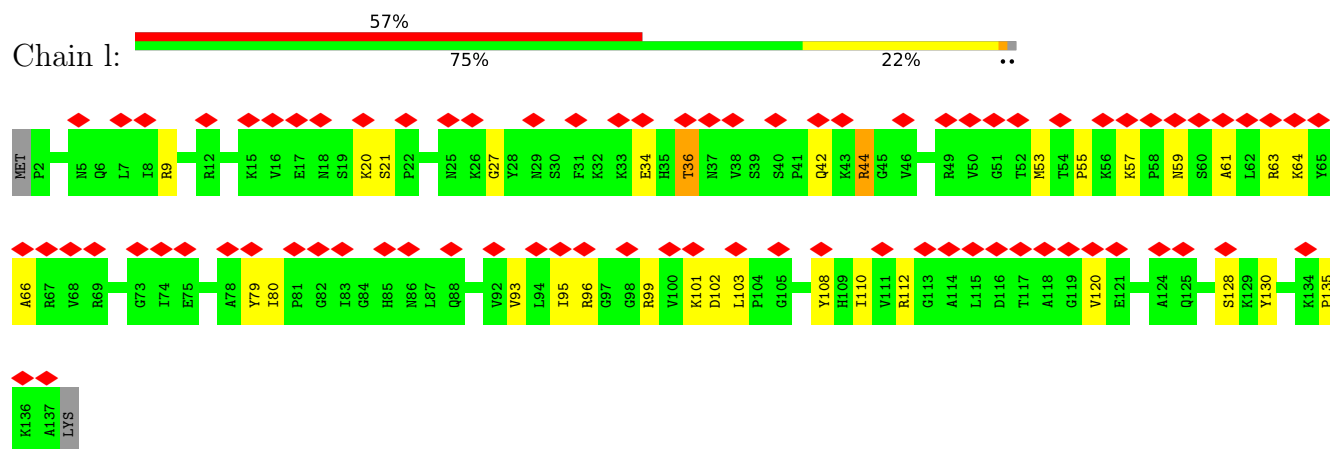
- Molecule 42: 30S ribosomal protein S10



- Molecule 43: 30S ribosomal protein S11

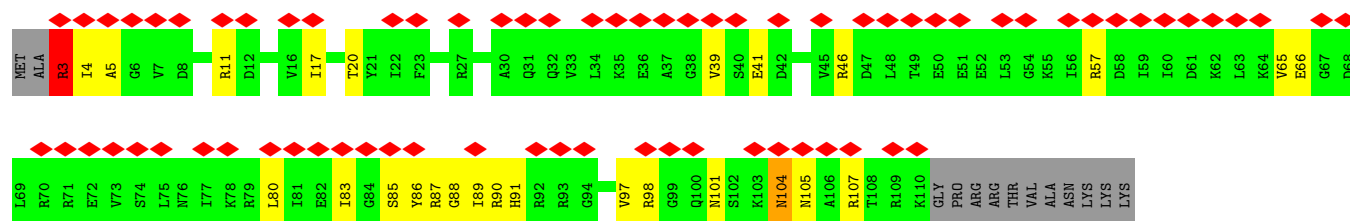


- Molecule 44: 30S ribosomal protein S12

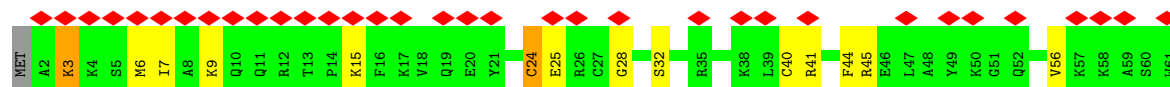
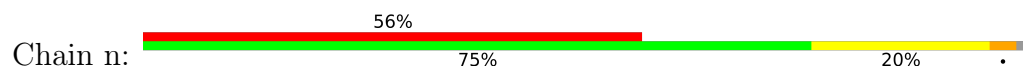


- Molecule 45: 30S ribosomal protein S13

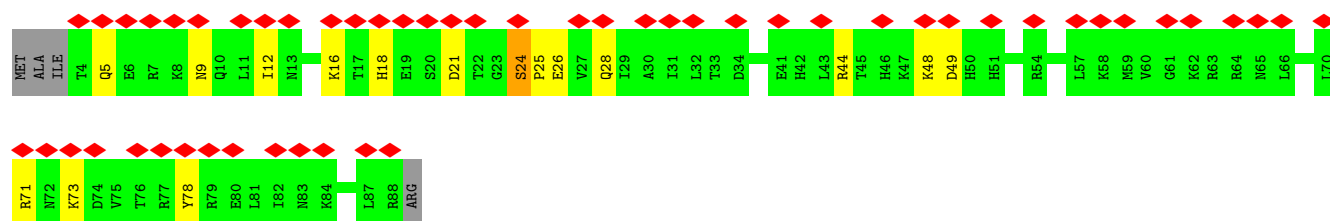
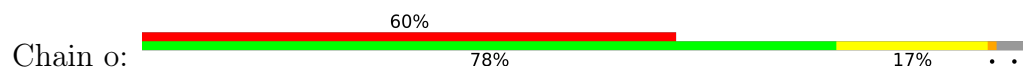




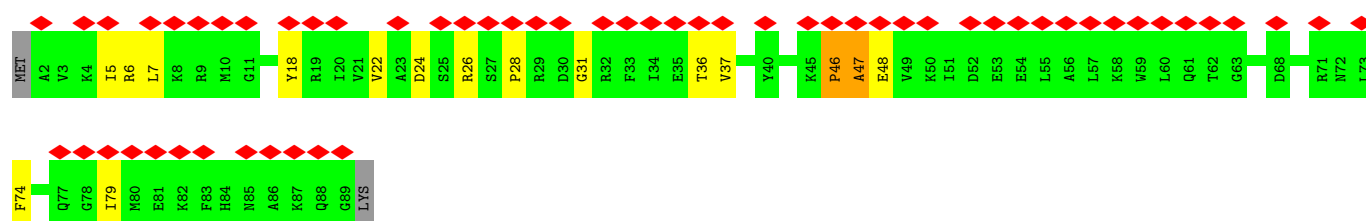
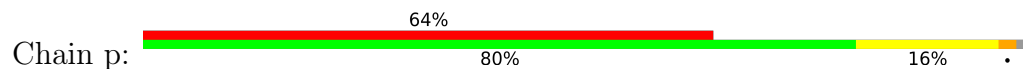
- Molecule 46: 30S ribosomal protein S14



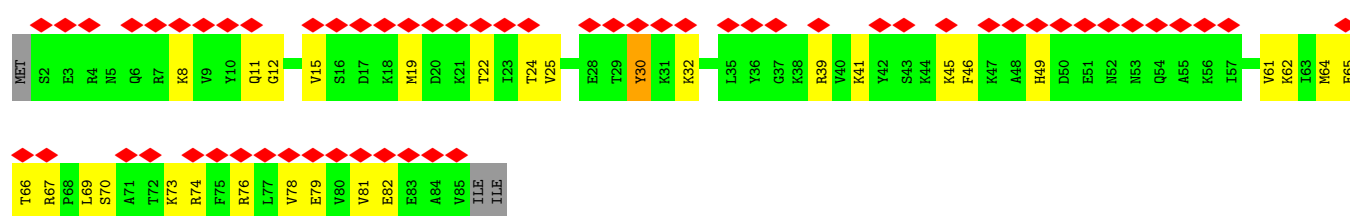
- Molecule 47: 30S ribosomal protein S15



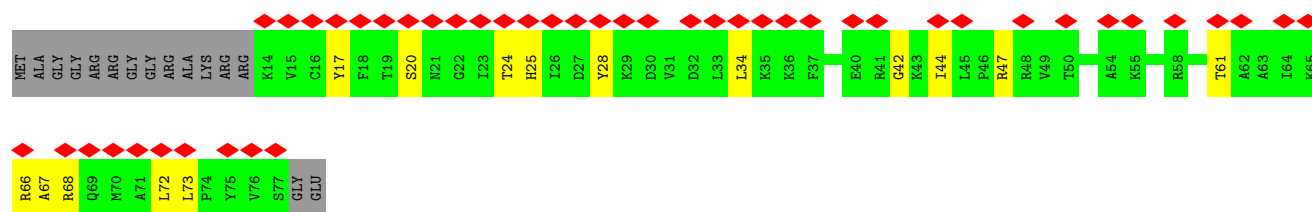
- Molecule 48: 30S ribosomal protein S16



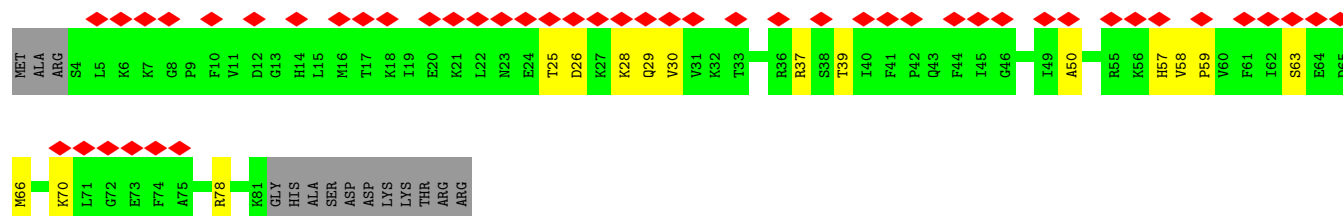
- Molecule 49: 30S ribosomal protein S17



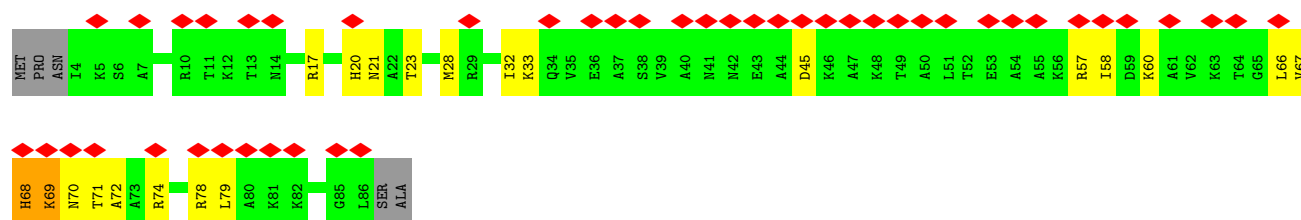
- Molecule 50: 30S ribosomal protein S18



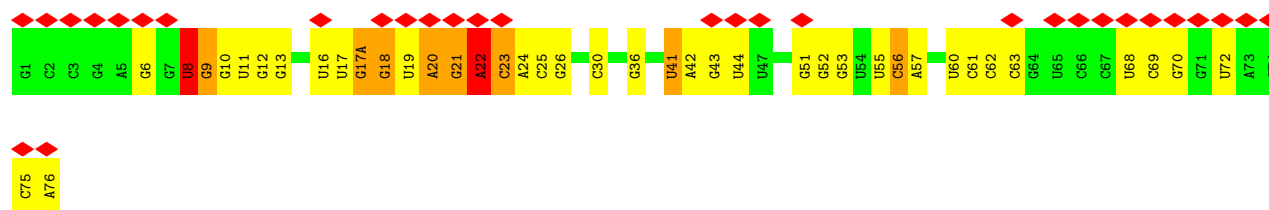
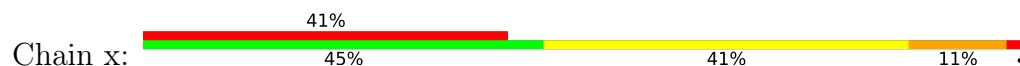
- Molecule 51: 30S ribosomal protein S19



- Molecule 52: 30S ribosomal protein S20



- Molecule 53: P-tRNA(Leu)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	28972	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.425	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.634	Depositor
Minimum map value	-0.379	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.11	Depositor
Map size ($\text{\AA}$)	381.96, 381.96, 381.96	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.061, 1.061, 1.061	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.52	2/69438 (0.0%)	0.61	7/108311 (0.0%)
2	B	0.40	0/2675	0.60	0/4170
3	C	0.60	0/2120	0.94	1/2845 (0.0%)
4	D	0.59	0/1591	0.89	0/2132
5	E	0.53	0/1580	0.81	0/2132
6	F	0.44	0/1405	0.93	1/1887 (0.1%)
7	G	0.37	0/1360	0.82	0/1832
8	J	0.57	0/1146	0.90	0/1542
9	K	0.57	0/927	0.92	0/1245
10	L	0.54	0/1093	0.94	1/1457 (0.1%)
11	M	0.52	0/1099	0.93	1/1468 (0.1%)
12	N	0.55	0/960	0.81	0/1284
13	O	0.43	0/921	0.87	0/1236
14	P	0.51	0/957	0.90	1/1279 (0.1%)
15	Q	0.63	1/952 (0.1%)	0.89	3/1266 (0.2%)
16	R	0.56	0/797	0.95	1/1070 (0.1%)
17	S	0.57	0/851	0.95	4/1146 (0.3%)
18	T	0.46	0/731	0.83	0/974
19	U	0.47	0/772	0.94	0/1032
20	V	0.39	0/4247	0.85	5/5736 (0.1%)
21	W	0.60	0/638	1.08	2/847 (0.2%)
22	X	0.44	0/448	0.91	0/596
23	Y	0.42	0/531	0.85	0/707
24	Z	0.46	0/457	0.92	0/613
25	0	0.56	0/433	0.93	0/574
26	1	0.50	0/406	0.93	0/540
27	2	0.60	0/370	0.84	0/483
28	3	0.56	0/519	0.82	0/680
29	4	0.46	0/299	0.79	0/393
30	6	0.38	0/509	0.98	2/678 (0.3%)
31	7	0.33	0/65	0.51	0/98
32	8	0.29	0/1624	0.78	1/2192 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.33	0/36826	0.57	7/57450 (0.0%)
34	b	0.32	0/1782	0.89	6/2392 (0.3%)
35	c	0.33	0/1641	0.82	0/2208
36	d	0.35	0/1598	0.93	4/2147 (0.2%)
37	e	0.38	0/1230	0.86	0/1655
38	f	0.28	0/766	0.75	0/1031
39	g	0.40	0/1196	0.89	3/1604 (0.2%)
40	h	0.36	0/1048	0.89	2/1407 (0.1%)
41	i	0.36	0/979	0.88	1/1315 (0.1%)
42	j	0.37	0/773	0.84	0/1044
43	k	0.37	0/852	1.02	5/1153 (0.4%)
44	l	0.36	0/1069	0.95	4/1435 (0.3%)
45	m	0.34	0/873	0.94	2/1166 (0.2%)
46	n	0.38	0/507	1.00	3/672 (0.4%)
47	o	0.31	0/718	0.72	0/960
48	p	0.37	0/708	0.93	4/950 (0.4%)
49	q	0.35	0/699	0.83	0/933
50	r	0.31	0/526	0.81	0/705
51	s	0.33	0/649	0.87	0/872
52	t	0.36	0/639	0.81	2/852 (0.2%)
53	x	0.36	0/1790	0.83	6/2787 (0.2%)
All	All	0.46	3/158790 (0.0%)	0.69	79/237183 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
4	D	0	1
6	F	0	3
8	J	0	1
10	L	0	2
13	O	0	1
15	Q	0	1
16	R	0	2
17	S	0	1
20	V	0	11
25	0	0	2
30	6	0	1
34	b	0	5

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Mol	Chain	#Chirality outliers	#Planarity outliers
36	d	0	5
37	e	0	1
38	f	0	1
39	g	0	2
40	h	0	1
44	l	0	2
45	m	0	3
47	o	0	1
49	q	0	1
50	r	0	2
All	All	0	51

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	20	LEU	CA-C	-5.98	1.44	1.52
1	A	700	U	C1'-N1	5.90	1.57	1.48
1	A	1489	U	C1'-N1	5.67	1.55	1.47

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	k	80	GLY	N-CA-C	16.91	131.24	112.29
43	k	79	HIS	N-CA-C	-11.19	97.79	111.33
11	M	65	TRP	N-CA-C	8.59	121.76	111.02
33	a	1176	A	O5'-C5'-C4'	8.35	124.22	111.70
21	W	28	ARG	CB-CG-CD	7.66	128.93	111.30
33	a	1502	A	C5'-C4'-O4'	-7.43	98.65	109.80
34	b	18	HIS	CA-C-N	7.28	135.44	121.54
34	b	18	HIS	C-N-CA	7.28	135.44	121.54
44	l	44	ARG	CA-CB-CG	7.05	128.20	114.10
1	A	1712	G	N9-C1'-C2'	6.74	122.11	112.00
20	V	323	ILE	N-CA-C	6.63	117.45	108.17
44	l	44	ARG	N-CA-CB	6.61	120.93	110.23
17	S	39	THR	N-CA-C	6.59	124.36	109.81
34	b	66	LYS	CA-C-N	6.51	133.70	121.97
34	b	66	LYS	C-N-CA	6.51	133.70	121.97
41	i	122	ARG	CB-CG-CD	6.45	126.13	111.30
20	V	341	GLU	CA-C-N	6.37	131.17	122.19
20	V	341	GLU	C-N-CA	6.37	131.17	122.19
17	S	38	LEU	CA-C-N	6.26	137.07	121.80
17	S	38	LEU	C-N-CA	6.26	137.07	121.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	28	LYS	N-CA-C	-6.25	105.97	113.97
1	A	2630	C	C4'-C3'-O3'	6.23	122.35	113.00
53	x	42	A	P-O3'-C3'	6.20	129.49	120.20
33	a	1175	G	OP1-P-O3'	-6.19	89.42	108.00
17	S	40	PRO	N-CA-C	6.16	125.16	112.47
43	k	80	GLY	CA-C-O	6.15	126.47	122.23
1	A	2334	U	O4'-C1'-N1	6.03	117.24	108.20
10	L	18	ARG	CA-CB-CG	6.01	126.12	114.10
53	x	20	A	P-O3'-C3'	6.00	129.19	120.20
30	6	61	LYS	CA-C-N	5.97	129.77	120.82
30	6	61	LYS	C-N-CA	5.97	129.77	120.82
21	W	28	ARG	NE-CZ-NH2	5.91	124.52	119.20
32	8	176	GLY	N-CA-C	5.77	117.95	110.45
48	p	47	ALA	CA-C-N	5.73	132.49	121.54
48	p	47	ALA	C-N-CA	5.73	132.49	121.54
15	Q	92	ARG	CA-CB-CG	5.61	125.33	114.10
34	b	17	GLY	N-CA-C	5.55	126.33	113.18
33	a	92	U	P-O3'-C3'	5.48	128.42	120.20
1	A	185	A	P-O5'-C5'	5.44	129.06	120.90
44	l	36	THR	N-CA-C	5.41	117.28	110.24
53	x	62	C	P-O3'-C3'	5.37	128.25	120.20
40	h	3	MET	CA-C-N	5.36	131.78	121.54
40	h	3	MET	C-N-CA	5.36	131.78	121.54
36	d	145	SER	CA-C-N	5.35	127.72	120.65
36	d	145	SER	C-N-CA	5.35	127.72	120.65
53	x	22	A	P-O3'-C3'	5.35	128.22	120.20
36	d	148	LEU	CA-C-N	5.30	127.39	120.28
36	d	148	LEU	C-N-CA	5.30	127.39	120.28
44	l	44	ARG	CB-CG-CD	5.30	123.48	111.30
1	A	1883	A	C2'-C3'-O3'	5.29	121.64	113.70
39	g	114	LYS	CA-C-N	5.28	131.62	121.54
39	g	114	LYS	C-N-CA	5.28	131.62	121.54
43	k	121	ASN	CA-C-N	5.26	130.49	120.07
43	k	121	ASN	C-N-CA	5.26	130.49	120.07
45	m	3	ARG	CA-C-N	5.25	127.64	120.77
45	m	3	ARG	C-N-CA	5.25	127.64	120.77
53	x	8	U	O5'-P-OP1	5.24	123.73	108.00
1	A	1448	U	C4'-C3'-O3'	5.22	117.23	109.40
46	n	24	CYS	CA-C-N	5.20	131.47	121.54
46	n	24	CYS	C-N-CA	5.20	131.47	121.54
6	F	112	ARG	CA-CB-CG	5.19	124.49	114.10
48	p	46	PRO	CA-C-N	5.17	131.42	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	p	46	PRO	C-N-CA	5.17	131.42	121.54
39	g	17	ILE	N-CA-C	-5.16	101.05	108.89
33	a	944	C	O5'-C5'-C4'	5.13	119.40	111.70
1	A	1942	A	O3'-P-O5'	-5.11	96.33	104.00
33	a	1499	G	C2'-C3'-O3'	5.11	121.37	113.70
15	Q	92	ARG	CA-C-N	5.10	131.28	121.54
15	Q	92	ARG	C-N-CA	5.10	131.28	121.54
20	V	149	TYR	CA-C-N	5.10	128.06	120.31
20	V	149	TYR	C-N-CA	5.10	128.06	120.31
52	t	66	LEU	CA-C-N	-5.09	115.79	121.85
52	t	66	LEU	C-N-CA	-5.09	115.79	121.85
16	R	48	VAL	CG1-CB-CG2	5.08	121.98	110.80
46	n	3	LYS	CD-CE-NZ	-5.08	95.65	111.90
53	x	22	A	O3'-P-O5'	5.06	111.60	104.00
14	P	44	GLU	CA-CB-CG	5.06	124.22	114.10
33	a	1045	G	C4'-C3'-O3'	5.02	120.53	113.00
3	C	196	GLY	N-CA-C	5.01	125.05	113.18

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
25	0	50	ASN	Peptide
25	0	51	GLY	Peptide
30	6	59	PHE	Peptide
3	C	153	GLN	Peptide
4	D	53	PHE	Peptide
6	F	117	VAL	Peptide
6	F	138	PHE	Peptide
6	F	53	ALA	Peptide
8	J	132	PRO	Peptide
10	L	18	ARG	Peptide
10	L	35	HIS	Peptide
13	O	1	MET	Peptide
15	Q	102	ASP	Peptide
16	R	50	ASN	Peptide
16	R	51	PRO	Peptide
17	S	39	THR	Peptide
20	V	15	LYS	Peptide
20	V	19	VAL	Peptide
20	V	278	ARG	Peptide
20	V	279	PHE	Peptide

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Mol	Chain	Res	Type	Group
20	V	281	ILE	Peptide
20	V	342	THR	Peptide
20	V	405	LYS	Peptide
20	V	412	ARG	Peptide
20	V	521	ALA	Peptide
20	V	75	THR	Peptide
20	V	98	LEU	Peptide
34	b	148	LEU	Peptide
34	b	16	PHE	Peptide
34	b	18	HIS	Peptide
34	b	65	GLY	Peptide
34	b	66	LYS	Peptide
36	d	117	GLY	Peptide
36	d	192	ALA	Peptide
36	d	31	TYR	Peptide
36	d	32	ALA	Peptide
36	d	33	PRO	Peptide
37	e	20	ARG	Peptide
38	f	33	ASN	Peptide
39	g	114	LYS	Peptide
39	g	129	ASN	Peptide
40	h	98	LEU	Peptide
44	l	34	GLU	Peptide
44	l	57	LYS	Peptide
45	m	104	ASN	Peptide
45	m	3	ARG	Peptide
45	m	65	VAL	Peptide
47	o	24	SER	Peptide
49	q	30	TYR	Peptide
50	r	24	THR	Peptide
50	r	25	HIS	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	61997	0	31214	501	0
2	B	2392	0	1213	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2083	0	2168	56	0
4	D	1569	0	1637	32	0
5	E	1561	0	1647	37	0
6	F	1386	0	1446	39	0
7	G	1342	0	1388	22	0
8	J	1123	0	1162	25	0
9	K	920	0	977	24	0
10	L	1081	0	1132	19	0
11	M	1076	0	1145	19	0
12	N	953	0	983	21	0
13	O	912	0	947	16	0
14	P	944	0	1020	26	0
15	Q	940	0	1005	21	0
16	R	786	0	826	19	0
17	S	842	0	899	18	0
18	T	725	0	770	18	0
19	U	762	0	821	11	0
20	V	4177	0	4221	202	0
21	W	630	0	644	9	0
22	X	444	0	487	11	0
23	Y	530	0	568	10	0
24	Z	455	0	491	14	0
25	0	426	0	441	12	0
26	1	401	0	413	16	0
27	2	367	0	410	5	0
28	3	512	0	564	13	0
29	4	296	0	342	8	0
30	6	499	0	491	10	0
31	7	60	0	32	0	0
32	8	1599	0	1640	48	0
33	a	32891	0	16559	347	0
34	b	1757	0	1830	29	0
35	c	1619	0	1658	31	0
36	d	1568	0	1604	33	0
37	e	1218	0	1300	22	0
38	f	755	0	746	14	0
39	g	1181	0	1235	23	0
40	h	1036	0	1095	20	0
41	i	966	0	1005	17	0
42	j	761	0	795	15	0
43	k	838	0	854	20	0
44	l	1052	0	1112	24	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	m	868	0	925	18	0
46	n	497	0	531	11	0
47	o	710	0	735	10	0
48	p	695	0	721	9	0
49	q	691	0	728	21	0
50	r	518	0	555	9	0
51	s	633	0	649	9	0
52	t	637	0	696	14	0
53	x	1603	0	808	17	0
54	A	58	0	65	16	0
55	V	62	0	24	59	0
All	All	146404	0	99374	1700	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 8.

All (1700) 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)
20:V:328:SER:HB3	20:V:476:ILE:CG2	1.25	1.64
20:V:43:LYS:CD	20:V:156:VAL:CG1	1.78	1.59
20:V:43:LYS:CE	20:V:156:VAL:HG11	1.39	1.49
20:V:328:SER:CB	20:V:476:ILE:CG2	1.92	1.44
20:V:43:LYS:NZ	20:V:156:VAL:HG11	1.28	1.42
20:V:43:LYS:NZ	20:V:156:VAL:CG1	1.83	1.39
20:V:328:SER:CB	20:V:476:ILE:HG23	1.52	1.34
20:V:327:GLY:HA2	55:V:900:ATP:O1B	1.22	1.34
20:V:43:LYS:NZ	20:V:156:VAL:CB	1.96	1.28
20:V:43:LYS:HD2	20:V:156:VAL:CG1	1.42	1.27
20:V:43:LYS:CD	20:V:156:VAL:HG11	1.45	1.26
20:V:408:SER:HB3	55:V:901:ATP:O3'	1.38	1.19
20:V:45:THR:OG1	55:V:901:ATP:O2A	1.59	1.18
20:V:43:LYS:CE	20:V:156:VAL:CG1	2.07	1.18
32:8:116:ALA:HB1	32:8:121:MET:CE	1.73	1.18
20:V:324:GLY:HA3	20:V:330:LYS:HD2	1.27	1.16
20:V:43:LYS:HZ3	20:V:156:VAL:CB	1.55	1.15
20:V:43:LYS:CG	20:V:156:VAL:CG1	2.23	1.14
20:V:43:LYS:CG	20:V:156:VAL:HG11	1.78	1.12
20:V:328:SER:CB	20:V:476:ILE:HG21	1.63	1.12
20:V:43:LYS:HZ2	20:V:156:VAL:CG1	1.48	1.10
20:V:329:GLY:N	55:V:900:ATP:O1A	1.85	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:8:116:ALA:HB1	32:8:121:MET:HE1	1.09	1.07
20:V:40:GLY:HA2	55:V:901:ATP:H5'2	1.36	1.06
20:V:43:LYS:HZ3	20:V:156:VAL:HB	0.95	1.05
20:V:40:GLY:CA	55:V:901:ATP:H5'2	1.87	1.04
1:A:1995:A:N6	1:A:2631:A:C2	2.26	1.04
20:V:40:GLY:C	55:V:901:ATP:H5'2	1.82	1.03
1:A:1995:A:N6	1:A:2631:A:H2	1.56	1.02
20:V:328:SER:HB3	20:V:476:ILE:HG21	1.18	1.00
1:A:2631:A:H5'	20:V:227:ALA:HB2	1.43	0.99
20:V:43:LYS:CD	20:V:156:VAL:HG12	1.67	0.99
20:V:407:MET:O	55:V:901:ATP:H2'	1.64	0.98
20:V:328:SER:HB2	20:V:476:ILE:HG21	1.46	0.98
32:8:116:ALA:CB	32:8:121:MET:SD	2.52	0.97
20:V:328:SER:HB3	20:V:476:ILE:HG23	1.04	0.97
20:V:43:LYS:HG2	20:V:156:VAL:CG1	1.93	0.97
1:A:334:G:H1	1:A:393:U:H3	1.01	0.96
33:a:774:G:H1	33:a:821:G:HO2'	1.01	0.95
32:8:121:MET:HE2	32:8:121:MET:HA	1.48	0.95
20:V:328:SER:HB2	20:V:476:ILE:CG2	1.96	0.95
20:V:328:SER:O	20:V:476:ILE:HG12	1.66	0.94
20:V:329:GLY:CA	55:V:900:ATP:O1A	2.15	0.94
43:k:18:ILE:O	43:k:80:GLY:O	1.85	0.94
20:V:43:LYS:HD2	20:V:156:VAL:HG12	0.95	0.93
32:8:116:ALA:CB	32:8:121:MET:HE1	1.98	0.93
20:V:43:LYS:NZ	20:V:156:VAL:HB	1.72	0.91
20:V:40:GLY:N	55:V:901:ATP:O2B	2.04	0.91
32:8:117:THR:O	32:8:121:MET:SD	2.29	0.91
33:a:300:G:H21	33:a:617:A:H61	0.93	0.90
20:V:408:SER:HB3	55:V:901:ATP:C3'	2.02	0.90
33:a:300:G:N2	33:a:617:A:H61	1.68	0.90
20:V:330:LYS:HE2	55:V:900:ATP:O2B	1.71	0.90
20:V:301:PHE:CE1	55:V:900:ATP:N6	2.40	0.90
20:V:43:LYS:HZ2	20:V:156:VAL:CG2	1.84	0.89
33:a:427:U:H3	33:a:432:G:H1	1.20	0.89
20:V:43:LYS:CG	20:V:156:VAL:HG13	1.99	0.89
20:V:301:PHE:CD1	55:V:900:ATP:C6	2.60	0.89
33:a:964:G:H21	33:a:1236:A:H62	1.18	0.88
20:V:332:THR:OG1	55:V:900:ATP:O2A	1.91	0.88
32:8:116:ALA:HB3	32:8:121:MET:SD	2.12	0.88
32:8:101:ILE:CD1	32:8:124:VAL:HG23	2.04	0.88
20:V:43:LYS:HG2	20:V:156:VAL:HG11	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:327:GLY:CA	55:V:900:ATP:O1B	2.16	0.88
20:V:40:GLY:O	55:V:901:ATP:C5'	2.21	0.88
20:V:43:LYS:NZ	20:V:156:VAL:CG2	2.37	0.88
20:V:324:GLY:CA	20:V:330:LYS:HD2	2.03	0.87
20:V:301:PHE:CE1	55:V:900:ATP:C6	2.62	0.87
20:V:42:GLY:N	55:V:901:ATP:O1A	2.08	0.87
32:8:117:THR:O	32:8:121:MET:HG2	1.75	0.87
32:8:116:ALA:HB1	32:8:121:MET:SD	2.13	0.87
33:a:300:G:H21	33:a:617:A:N6	1.71	0.87
20:V:135:ASP:HB3	20:V:325:PRO:O	1.73	0.86
1:A:2481:C:O2	1:A:2481:C:H2'	1.75	0.85
32:8:101:ILE:HD13	32:8:124:VAL:HG23	1.55	0.85
1:A:2480:A:H5'	20:V:238:LYS:HE3	1.59	0.85
1:A:2629:A:O2'	1:A:2630:C:H5'	1.77	0.85
34:b:133:GLU:O	34:b:137:LEU:HB3	1.76	0.85
1:A:2087:A:H2	54:A:3001:TEL:H351	1.42	0.84
20:V:43:LYS:HZ2	20:V:156:VAL:CB	1.69	0.84
32:8:124:VAL:O	32:8:127:ILE:HG22	1.78	0.83
20:V:328:SER:OG	20:V:476:ILE:HG23	1.79	0.82
32:8:117:THR:O	32:8:121:MET:CG	2.27	0.82
1:A:2480:A:C5'	20:V:238:LYS:HE3	2.08	0.82
26:1:5:ILE:HB	26:1:19:SER:O	1.79	0.82
1:A:2631:A:OP1	20:V:244:LYS:HB3	1.80	0.82
20:V:226:LYS:NZ	53:x:72:U:OP1	2.13	0.82
20:V:408:SER:CB	55:V:901:ATP:O3'	2.23	0.82
44:l:42:GLN:HA	44:l:95:ILE:O	1.80	0.81
33:a:455:G:H21	33:a:496:A:H62	1.25	0.81
20:V:324:GLY:HA3	20:V:330:LYS:CD	2.10	0.81
44:l:44:ARG:HA	44:l:93:VAL:O	1.79	0.81
32:8:116:ALA:CB	32:8:121:MET:CE	2.57	0.81
20:V:43:LYS:NZ	20:V:156:VAL:HG21	1.97	0.80
20:V:329:GLY:O	20:V:332:THR:N	2.15	0.80
40:h:25:LEU:O	40:h:61:ARG:HA	1.81	0.80
1:A:1088:G:H1	1:A:1159:U:H3	0.82	0.79
20:V:42:GLY:CA	55:V:901:ATP:O1A	2.30	0.79
1:A:1995:A:C6	1:A:2631:A:H2	2.00	0.79
20:V:43:LYS:HZ2	20:V:156:VAL:HG21	1.48	0.79
1:A:2148:A:H61	1:A:2197:G:H21	1.31	0.79
20:V:329:GLY:HA2	55:V:900:ATP:O1A	1.83	0.78
33:a:445:U:H3	33:a:504:A:H62	1.29	0.78
1:A:2631:A:H5'	20:V:227:ALA:CB	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:43:LYS:HG2	20:V:156:VAL:HG13	1.63	0.77
33:a:1142:C:O2	33:a:1151:G:N2	2.18	0.76
6:F:96:MET:N	6:F:96:MET:SD	2.58	0.76
1:A:2640:C:C5	54:A:3001:TEL:H352	2.20	0.76
20:V:408:SER:HB3	55:V:901:ATP:HO3'	1.50	0.75
20:V:328:SER:HB3	20:V:476:ILE:CB	2.14	0.75
54:A:3001:TEL:H112	54:A:3001:TEL:O18	1.87	0.75
20:V:43:LYS:HZ2	20:V:156:VAL:HG11	1.02	0.74
33:a:964:G:N2	33:a:1236:A:H62	1.84	0.74
20:V:135:ASP:CB	20:V:325:PRO:O	2.36	0.74
46:n:3:LYS:NZ	46:n:28:GLY:O	2.20	0.74
49:q:25:VAL:O	49:q:45:LYS:HA	1.87	0.74
1:A:2557:U:H3	1:A:2564:G:H1	1.35	0.74
1:A:2640:C:C6	54:A:3001:TEL:H352	2.22	0.74
20:V:40:GLY:C	55:V:901:ATP:C5'	2.59	0.74
46:n:24:CYS:SG	46:n:25:GLU:N	2.61	0.74
1:A:607:G:H21	15:Q:37:GLN:HE22	1.33	0.73
1:A:2157:C:H5'	32:8:36:ALA:HB1	1.70	0.73
12:N:84:PHE:O	12:N:88:ALA:HB3	1.88	0.73
9:K:7:ARG:HA	9:K:19:VAL:O	1.88	0.73
20:V:226:LYS:CE	53:x:72:U:OP1	2.37	0.73
33:a:890:C:H5''	44:l:9:ARG:HH12	1.54	0.73
20:V:43:LYS:N	55:V:901:ATP:O1B	2.22	0.72
35:c:66:THR:HA	35:c:101:ASN:O	1.89	0.72
32:8:121:MET:HE2	32:8:121:MET:CA	2.20	0.72
49:q:22:THR:HG22	49:q:49:HIS:HA	1.72	0.72
37:e:84:GLU:HA	37:e:96:LEU:O	1.91	0.71
1:A:2613:U:H5'	1:A:2614:U:OP2	1.91	0.71
39:g:66:LEU:HB3	39:g:70:MET:HE3	1.72	0.71
33:a:964:G:H21	33:a:1236:A:N6	1.87	0.71
1:A:1847:U:H2'	3:C:156:ARG:HG2	1.71	0.70
1:A:894:A:N6	1:A:980:C:C4	2.60	0.70
7:G:85:GLU:HA	7:G:134:VAL:O	1.92	0.70
1:A:246:U:OP2	28:3:8:ARG:NH2	2.25	0.70
35:c:182:ASP:O	35:c:200:TRP:HA	1.92	0.70
20:V:40:GLY:HA2	55:V:901:ATP:C5'	2.19	0.70
33:a:551:U:H5''	36:d:33:PRO:HG2	1.72	0.70
20:V:40:GLY:O	55:V:901:ATP:H5'2	1.89	0.69
49:q:64:MET:HB3	49:q:76:ARG:HE	1.57	0.69
33:a:674:A:H62	33:a:733:G:H1	1.41	0.69
49:q:30:TYR:HB2	49:q:41:LYS:HA	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:A:HO2'	1:A:414:C:HO2'	1.33	0.69
1:A:1756:U:H5'	1:A:1757:G:H5''	1.73	0.69
1:A:1995:A:C6	1:A:2631:A:C2	2.79	0.69
33:a:665:G:O2'	47:o:28:GLN:NE2	2.26	0.68
33:a:1441:G:HO2'	33:a:1477:G:H1	1.41	0.68
33:a:1116:G:H5''	35:c:171:THR:HG22	1.75	0.68
1:A:160:G:O2'	1:A:168:A:N6	2.26	0.68
24:Z:37:HIS:HB3	24:Z:43:ILE:HD13	1.76	0.68
26:1:9:CYS:SG	26:1:10:THR:N	2.66	0.68
48:p:6:ARG:NH1	48:p:24:ASP:O	2.26	0.68
1:A:64:A:H61	1:A:90:A:H61	1.42	0.68
20:V:226:LYS:HE2	53:x:72:U:OP1	1.94	0.68
20:V:301:PHE:CE1	55:V:900:ATP:C5	2.81	0.68
43:k:77:ILE:HD11	43:k:107:LEU:HD21	1.75	0.68
41:i:65:VAL:HG11	41:i:79:ILE:HG12	1.75	0.68
33:a:1502:A:N6	33:a:1504:G:N7	2.43	0.67
20:V:389:LEU:HD23	53:x:17(A):G:H1'	1.76	0.67
1:A:2087:A:C2	54:A:3001:TEL:H351	2.26	0.67
20:V:135:ASP:CG	20:V:325:PRO:O	2.37	0.67
7:G:104:LEU:O	7:G:115:GLU:HA	1.95	0.67
36:d:82:HIS:H	37:e:102:GLY:HA3	1.60	0.67
1:A:2631:A:OP1	20:V:244:LYS:CB	2.42	0.67
9:K:26:GLY:HA3	9:K:30:ARG:HE	1.58	0.67
1:A:1820:A:N6	1:A:1857:G:O2'	2.28	0.67
1:A:2108:U:O2'	22:X:23:ASN:ND2	2.28	0.66
1:A:221:G:H22	1:A:238:U:H4'	1.60	0.66
33:a:692:G:N2	43:k:41:GLY:O	2.28	0.66
1:A:1542:A:O2'	1:A:1544:C:N4	2.29	0.66
1:A:1856:U:OP2	3:C:221:ARG:NH2	2.27	0.66
2:B:44:A:OP1	13:O:7:LYS:NZ	2.27	0.66
20:V:329:GLY:HA2	55:V:900:ATP:PA	2.35	0.66
20:V:43:LYS:HD2	20:V:156:VAL:HG13	1.65	0.66
33:a:269:U:OP2	52:t:74:ARG:NH2	2.29	0.66
1:A:2640:C:C4	54:A:3001:TEL:C35	2.79	0.66
1:A:1304:G:OP1	25:0:16:ARG:NH2	2.28	0.66
33:a:1088:U:H4'	37:e:138:ARG:HH12	1.60	0.66
4:D:9:LYS:HB2	4:D:200:ILE:HD12	1.77	0.66
14:P:62:ARG:NH1	14:P:100:LEU:O	2.28	0.66
44:l:20:LYS:HE3	44:l:99:ARG:HE	1.61	0.66
44:l:80:ILE:HG12	44:l:110:ILE:HD12	1.77	0.66
51:s:50:ALA:HB1	51:s:57:HIS:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2135:G:N2	1:A:2212:C:C2	2.64	0.65
6:F:110:ARG:HH22	30:6:34:GLU:H	1.43	0.65
32:8:212:VAL:O	32:8:223:LYS:HA	1.96	0.65
1:A:2204:U:H4'	32:8:215:THR:HG21	1.77	0.65
5:E:182:ASN:ND2	5:E:185:ASP:OD2	2.29	0.65
33:a:982:C:OP2	42:j:59:LYS:NZ	2.30	0.65
33:a:1109:G:H3'	34:b:95:ARG:HH22	1.61	0.65
3:C:88:SER:O	3:C:197:ASN:ND2	2.30	0.65
13:O:7:LYS:O	13:O:11:ARG:HB2	1.97	0.65
1:A:760:G:H21	1:A:765:A:H2	1.42	0.65
33:a:260:U:O2	33:a:283:G:N2	2.29	0.65
1:A:721:G:H5''	5:E:76:GLY:H	1.61	0.65
12:N:20:LEU:HB3	12:N:40:LEU:HD11	1.78	0.65
8:J:78:HIS:ND1	8:J:79:THR:O	2.29	0.65
40:h:12:THR:HG22	40:h:15:ARG:HH12	1.61	0.65
1:A:1042:A:H4'	15:Q:92:ARG:HD3	1.78	0.65
20:V:407:MET:O	55:V:901:ATP:C2'	2.44	0.64
33:a:1365:G:H2'	33:a:1366:A:H8	1.62	0.64
1:A:1847:U:O2'	3:C:154:LEU:O	2.15	0.64
20:V:42:GLY:HA2	55:V:901:ATP:O1A	1.97	0.64
1:A:1830:G:OP2	3:C:150:LYS:NZ	2.30	0.64
1:A:2824:G:H21	1:A:2827:A:H62	1.43	0.64
1:A:1263:G:OP2	16:R:89:ARG:NH2	2.31	0.64
49:q:11:GLN:HA	49:q:62:LYS:HA	1.80	0.64
1:A:184:G:O6	5:E:58:ARG:NH1	2.30	0.64
33:a:317:G:O2'	33:a:616:A:N1	2.31	0.64
33:a:1187:G:N2	33:a:1190:G:OP2	2.30	0.64
1:A:254:A:H4'	10:L:47:ARG:HH12	1.63	0.64
40:h:28:PRO:O	40:h:57:GLN:NE2	2.30	0.64
8:J:63:ILE:O	8:J:94:ARG:NH1	2.30	0.64
11:M:39:ALA:HB2	11:M:99:PRO:HD3	1.78	0.64
35:c:47:SER:O	35:c:121:ARG:NH2	2.31	0.64
33:a:834:G:O2'	40:h:13:ARG:NH2	2.31	0.64
20:V:331:THR:HG21	55:V:900:ATP:O2G	1.98	0.63
1:A:2695:C:H41	7:G:153:ARG:HH22	1.47	0.63
6:F:125:ARG:HB3	13:O:1:MET:HG2	1.81	0.63
34:b:161:LEU:HB3	34:b:183:ILE:HG22	1.80	0.63
13:O:29:PRO:HG2	13:O:93:VAL:HG23	1.79	0.63
32:8:101:ILE:HD11	32:8:124:VAL:HG23	1.81	0.63
3:C:167:LYS:HG2	3:C:172:VAL:HG22	1.81	0.63
48:p:28:PRO:HG2	48:p:31:GLY:HA3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:ILE:HD11	7:G:51:LEU:HG	1.80	0.63
20:V:39:ASN:HB2	55:V:901:ATP:O2G	1.99	0.63
33:a:277:C:H2'	33:a:278:A:H8	1.63	0.63
36:d:104:ALA:HB1	36:d:109:GLN:HB3	1.80	0.63
1:A:1286:A:H4'	5:E:45:ARG:HH12	1.63	0.63
1:A:1942:A:N6	33:a:1502:A:N3	2.47	0.63
33:a:421:G:N2	33:a:436:G:O2'	2.30	0.63
1:A:2640:C:C4	54:A:3001:TEL:H352	2.34	0.62
5:E:101:LEU:O	5:E:106:ARG:NH2	2.32	0.62
32:8:80:LYS:NZ	32:8:120:MET:HB2	2.14	0.62
1:A:2196:U:H3	1:A:2200:A:H62	1.47	0.62
4:D:178:LYS:HB3	4:D:187:LEU:HD12	1.81	0.62
1:A:510:G:N2	1:A:513:A:OP2	2.33	0.62
4:D:8:ARG:HH21	4:D:79:PHE:HE2	1.45	0.62
1:A:1846:G:OP2	3:C:156:ARG:NH2	2.32	0.62
1:A:2314:C:OP2	26:1:2:ARG:NH2	2.32	0.62
6:F:37:ASN:HB3	6:F:153:ASP:HB2	1.80	0.62
33:a:180:G:H1	33:a:208:A:H2'	1.64	0.62
20:V:438:ASP:H	20:V:441:SER:HB2	1.63	0.62
30:6:9:PHE:HA	30:6:26:SER:O	1.99	0.62
5:E:153:LEU:HD12	5:E:192:LEU:HD12	1.82	0.62
33:a:1026:A:HO2'	33:a:1226:C:HO2'	1.47	0.62
1:A:1497:G:N2	1:A:1499:A:N1	2.47	0.62
20:V:135:ASP:OD2	20:V:325:PRO:O	2.17	0.62
33:a:682:G:H4'	38:f:87:ARG:HH12	1.65	0.62
9:K:80:ASP:OD2	14:P:62:ARG:NH2	2.32	0.62
13:O:45:ILE:HG12	13:O:52:THR:HG22	1.81	0.62
1:A:253:G:OP1	28:3:13:ARG:NH2	2.33	0.61
18:T:56:ILE:HG21	18:T:77:ARG:HH21	1.64	0.61
32:8:78:PHE:HB3	32:8:120:MET:HE3	1.81	0.61
34:b:180:ASN:HB2	37:e:4:ILE:HD12	1.80	0.61
1:A:2480:A:OP1	1:A:2526:A:N6	2.33	0.61
20:V:328:SER:HB3	20:V:476:ILE:CG1	2.30	0.61
33:a:64:U:H3	33:a:103:G:H1	1.47	0.61
33:a:536:G:O6	44:l:59:ASN:ND2	2.33	0.61
33:a:1315:A:N6	33:a:1340:G:O2'	2.34	0.61
1:A:1941:A:N6	33:a:1416:C:O2'	2.34	0.61
20:V:301:PHE:HE1	55:V:900:ATP:N6	1.92	0.61
15:Q:82:GLY:O	15:Q:86:SER:HB2	2.01	0.61
33:a:124:G:OP1	33:a:614:U:O2'	2.17	0.61
33:a:499:U:OP1	36:d:142:ARG:NH1	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:b:86:ARG:HH21	34:b:218:ALA:HB3	1.65	0.61
40:h:30:SER:H	40:h:33:LYS:HD2	1.65	0.61
41:i:44:LEU:O	41:i:48:ILE:HB	2.00	0.61
38:f:42:ASP:OD1	38:f:61:GLN:NE2	2.33	0.61
36:d:91:ASP:HA	36:d:96:ASN:HD22	1.66	0.61
1:A:1649:C:O2'	1:A:1655:A:N6	2.34	0.61
1:A:2708:A:H5'	4:D:169:ILE:HD13	1.83	0.61
1:A:2541:C:O2'	4:D:158:LYS:NZ	2.34	0.60
37:e:14:ARG:HG2	37:e:117:LEU:HD11	1.83	0.60
11:M:65:TRP:HB3	11:M:67:LYS:HZ3	1.66	0.60
1:A:965:A:N3	2:B:78:U:O2'	2.35	0.60
34:b:121:GLN:HB3	34:b:137:LEU:HD11	1.82	0.60
1:A:523:G:H4'	1:A:548:A:H61	1.65	0.60
1:A:2640:C:C5	54:A:3001:TEL:C35	2.84	0.60
14:P:6:GLU:O	14:P:10:LYS:HB2	2.01	0.60
33:a:177:G:OP2	52:t:60:LYS:NZ	2.34	0.60
33:a:1359:A:OP1	41:i:123:ARG:NH1	2.35	0.60
1:A:894:A:C6	1:A:980:C:N3	2.69	0.60
1:A:1485:A:H2	1:A:1600:G:H21	1.47	0.60
3:C:230:HIS:HD2	3:C:232:HIS:H	1.48	0.60
20:V:44:SER:N	55:V:901:ATP:O1B	2.34	0.60
36:d:180:PRO:HB2	36:d:185:LEU:HD21	1.83	0.60
1:A:1056:A:OP1	15:Q:66:ASN:ND2	2.34	0.60
1:A:2315:A:H2'	26:1:26:ASN:HD21	1.66	0.60
36:d:12:SER:HB3	36:d:19:LEU:HD22	1.82	0.60
53:x:9:G:O2'	53:x:10:G:N7	2.35	0.60
12:N:24:LEU:HD13	12:N:44:VAL:HG21	1.82	0.60
37:e:97:LYS:HB2	37:e:124:LEU:HB2	1.84	0.60
1:A:2480:A:O2'	20:V:237:PHE:HB3	2.01	0.60
49:q:81:VAL:HG12	49:q:82:GLU:HG3	1.83	0.60
1:A:535:G:H4'	17:S:49:LYS:HD2	1.84	0.60
1:A:589:G:N2	1:A:590:U:O4	2.35	0.60
13:O:33:VAL:HG11	13:O:106:VAL:HG22	1.83	0.60
33:a:1387:C:O2	39:g:76:LYS:NZ	2.34	0.60
38:f:86:ILE:HG22	38:f:87:ARG:HG2	1.83	0.60
39:g:116:MET:HA	39:g:119:ARG:HB2	1.83	0.60
43:k:38:ASP:O	43:k:41:GLY:N	2.35	0.60
1:A:1290:G:N7	10:L:18:ARG:NH2	2.50	0.59
2:B:55:A:O2'	6:F:27:GLN:NE2	2.25	0.59
7:G:3:ARG:HH22	7:G:55:ARG:HH22	1.50	0.59
49:q:24:THR:HA	49:q:46:PHE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:C:OP2	28:3:5:LYS:NZ	2.35	0.59
1:A:2712:C:OP1	14:P:51:ARG:NH1	2.34	0.59
7:G:105:VAL:HG22	7:G:115:GLU:HG2	1.82	0.59
1:A:1055:A:OP2	8:J:40:LYS:NZ	2.31	0.59
19:U:74:LYS:HD3	19:U:75:THR:HG23	1.84	0.59
36:d:91:ASP:OD1	36:d:96:ASN:ND2	2.34	0.59
7:G:4:VAL:O	7:G:70:ARG:NH1	2.36	0.59
20:V:408:SER:HB3	55:V:901:ATP:H3'	1.83	0.59
33:a:673:G:H22	33:a:750:G:H1	1.51	0.59
2:B:11:A:N6	2:B:67:G:O2'	2.32	0.59
51:s:50:ALA:HA	51:s:58:VAL:O	2.03	0.59
1:A:1184:G:H21	8:J:109:MET:HE3	1.68	0.59
11:M:78:PRO:HG2	11:M:81:VAL:HG21	1.83	0.59
20:V:412:ARG:HH12	20:V:416:LYS:HE3	1.67	0.59
12:N:94:ARG:NH1	12:N:120:VAL:O	2.36	0.59
24:Z:10:ARG:HB3	24:Z:53:LEU:HA	1.85	0.59
1:A:2376:C:O2'	26:1:17:TYR:OH	2.21	0.59
1:A:2605:G:O2'	1:A:2608:C:OP2	2.18	0.59
33:a:455:G:N2	33:a:496:A:H62	1.99	0.59
48:p:5:ILE:HG12	48:p:22:VAL:HG22	1.85	0.59
52:t:32:ILE:HG23	52:t:79:LEU:HD21	1.84	0.59
10:L:58:PHE:O	28:3:13:ARG:NH1	2.36	0.58
25:0:32:SER:OG	25:0:46:CYS:SG	2.61	0.58
35:c:16:ARG:NH2	35:c:182:ASP:OD1	2.35	0.58
20:V:130:PRO:HB2	20:V:142:LEU:HD21	1.85	0.58
33:a:992:U:H5''	46:n:6:MET:HE2	1.85	0.58
3:C:72:ASP:OD2	3:C:189:ARG:NH2	2.36	0.58
1:A:2474:G:OP1	5:E:74:ARG:NH2	2.29	0.58
15:Q:105:ALA:HB1	16:R:40:PHE:HZ	1.68	0.58
33:a:815:C:H2'	33:a:816:A:H8	1.68	0.58
33:a:908:G:N2	33:a:911:A:OP2	2.37	0.58
34:b:114:LEU:HB2	34:b:144:LEU:HD23	1.84	0.58
50:r:44:ILE:HG21	50:r:61:THR:HG22	1.83	0.58
1:A:959:C:OP1	11:M:8:LYS:NZ	2.30	0.58
1:A:75:G:O5'	23:Y:44:ARG:NH2	2.37	0.58
37:e:157:ARG:NH2	40:h:101:LEU:O	2.37	0.58
49:q:78:VAL:HG12	49:q:79:GLU:HG2	1.85	0.58
20:V:40:GLY:O	55:V:901:ATP:H5'1	2.03	0.58
41:i:20:ARG:HG3	41:i:64:LEU:HB2	1.84	0.58
1:A:1036:A:O2'	1:A:1038:C:OP2	2.22	0.58
1:A:2513:G:H1'	11:M:124:LYS:HG3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2782:A:O2'	29:4:15:LYS:NZ	2.36	0.58
33:a:436:G:O2'	36:d:29:ARG:NH1	2.37	0.58
33:a:937:G:O2'	33:a:1513:A:N7	2.37	0.58
1:A:1403:G:OP1	22:X:3:ARG:NH1	2.36	0.58
1:A:1943:C:H2'	1:A:1944:U:H2'	1.86	0.58
20:V:408:SER:CB	55:V:901:ATP:H3'	2.34	0.58
42:j:41:PRO:HA	42:j:72:ARG:HG2	1.85	0.58
6:F:110:ARG:HH12	30:6:35:ILE:H	1.50	0.57
7:G:47:GLU:HB2	7:G:50:VAL:HB	1.86	0.57
20:V:4:ILE:HG23	20:V:5:VAL:HG23	1.86	0.57
20:V:301:PHE:HB2	20:V:304:ARG:HB2	1.85	0.57
23:Y:10:THR:HG22	23:Y:60:ARG:HH11	1.69	0.57
52:t:67:VAL:O	52:t:71:THR:OG1	2.22	0.57
1:A:621:G:O2'	1:A:1294:A:OP1	2.21	0.57
24:Z:11:SER:OG	24:Z:12:VAL:N	2.35	0.57
37:e:80:THR:HG22	37:e:122:ASP:HB2	1.84	0.57
1:A:125:A:H5'	27:2:18:PHE:HB3	1.86	0.57
1:A:2561:G:N2	1:A:2692:G:O2'	2.37	0.57
9:K:71:ARG:NH2	9:K:122:ILE:O	2.38	0.57
13:O:44:ILE:HD12	13:O:54:ALA:HB3	1.86	0.57
55:V:900:ATP:O1B	55:V:900:ATP:H5'2	2.04	0.57
33:a:530:G:N7	44:l:63:ARG:NH1	2.52	0.57
44:l:55:PRO:HD3	44:l:63:ARG:HG2	1.85	0.57
1:A:83:G:O2'	1:A:101:G:N2	2.37	0.57
1:A:252:C:O2	28:3:12:LYS:NZ	2.37	0.57
3:C:66:ASP:OD2	3:C:102:ARG:NH1	2.37	0.57
20:V:236:GLY:O	20:V:237:PHE:C	2.45	0.57
20:V:301:PHE:CZ	55:V:900:ATP:N7	2.72	0.57
33:a:609:U:H3	33:a:647:G:H1	1.52	0.57
33:a:1427:A:N6	33:a:1492:G:O2'	2.38	0.57
37:e:48:PHE:HZ	37:e:138:ARG:HE	1.52	0.57
49:q:64:MET:HG2	49:q:76:ARG:HH21	1.69	0.57
9:K:115:VAL:HG13	9:K:121:VAL:HG21	1.85	0.57
33:a:42:C:H2'	33:a:43:G:H8	1.70	0.57
33:a:1382:G:H5''	39:g:36:LYS:HD3	1.87	0.57
39:g:113:GLU:O	39:g:119:ARG:NH2	2.37	0.57
53:x:18:G:O6	53:x:57:A:O2'	2.20	0.57
40:h:5:ASP:OD2	40:h:79:ARG:NH1	2.38	0.57
9:K:107:ARG:HE	9:K:115:VAL:HG11	1.69	0.57
12:N:59:ARG:HD2	12:N:80:LEU:HD21	1.86	0.57
33:a:1081:C:H2'	33:a:1082:G:H8	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1352:U:OP2	1:A:1353:C:N4	2.38	0.57
1:A:1699:A:N1	1:A:2077:G:O2'	2.37	0.57
1:A:2060:A:O2'	1:A:2483:G:N2	2.37	0.57
12:N:52:LYS:NZ	12:N:94:ARG:O	2.38	0.57
20:V:326:ASN:OD1	20:V:326:ASN:N	2.36	0.57
20:V:408:SER:CB	55:V:901:ATP:C3'	2.79	0.57
36:d:120:LEU:HD11	36:d:142:ARG:HE	1.69	0.57
2:B:6:U:OP1	13:O:11:ARG:NH1	2.35	0.57
33:a:1387:C:O4'	39:g:95:ARG:NH2	2.37	0.57
43:k:25:ILE:HG23	43:k:88:VAL:HA	1.86	0.57
1:A:447:G:O6	22:X:52:ARG:NH1	2.37	0.57
33:a:1025:G:N3	33:a:1227:C:O2'	2.37	0.57
33:a:1167:C:O2'	34:b:131:LYS:NZ	2.35	0.57
4:D:132:PRO:O	4:D:137:SER:OG	2.23	0.56
6:F:119:LYS:HA	6:F:167:ARG:HH12	1.69	0.56
38:f:43:TRP:HB2	38:f:60:TYR:HB2	1.86	0.56
1:A:1188:A:H4'	8:J:28:ARG:HH22	1.69	0.56
1:A:2280:G:O6	20:V:242:ARG:NH1	2.38	0.56
3:C:63:ARG:NH1	3:C:83:TYR:O	2.37	0.56
12:N:19:ASP:OD1	12:N:67:ARG:NH1	2.39	0.56
20:V:144:GLN:O	20:V:148:HIS:ND1	2.34	0.56
32:8:49:GLY:HA2	32:8:210:LYS:HE3	1.87	0.56
53:x:21:G:O2'	53:x:22:A:N7	2.34	0.56
1:A:2381:A:N6	1:A:2394:G:O2'	2.39	0.56
11:M:30:GLY:N	11:M:105:GLU:OE1	2.38	0.56
11:M:75:THR:HA	11:M:90:PRO:HA	1.87	0.56
19:U:2:HIS:O	19:U:92:ARG:NH1	2.37	0.56
20:V:365:LEU:HD12	20:V:367:LEU:HD23	1.87	0.56
35:c:43:SER:O	35:c:47:SER:HB2	2.05	0.56
35:c:75:VAL:HG12	35:c:102:ILE:HD13	1.87	0.56
1:A:722:A:O2'	5:E:67:GLN:OE1	2.20	0.56
1:A:791:C:H4'	1:A:1703:C:H4'	1.86	0.56
28:3:24:ARG:HD3	28:3:50:VAL:HG22	1.87	0.56
36:d:196:GLU:OE2	37:e:105:VAL:N	2.38	0.56
1:A:2357:A:H2'	1:A:2358:A:C8	2.41	0.56
15:Q:92:ARG:NH1	16:R:9:GLY:O	2.39	0.56
33:a:259:G:O6	33:a:280:C:N4	2.39	0.56
33:a:429:U:O2	35:c:126:ARG:NH2	2.38	0.56
49:q:8:LYS:HB3	49:q:65:GLU:HG2	1.86	0.56
54:A:3001:TEL:H122	54:A:3001:TEL:C11	2.36	0.56
20:V:40:GLY:O	55:V:901:ATP:H4'	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:66:G:OP1	33:a:390:A:N6	2.38	0.56
33:a:961:G:O6	45:m:104:ASN:ND2	2.38	0.56
20:V:43:LYS:CE	20:V:156:VAL:HG12	2.08	0.56
33:a:987:A:N6	33:a:1233:U:O4'	2.39	0.56
46:n:40:CYS:SG	46:n:41:ARG:N	2.79	0.56
1:A:2551:U:O2'	1:A:2676:U:OP1	2.22	0.56
1:A:2648:U:H5'	4:D:156:LYS:HG2	1.88	0.56
6:F:129:THR:HA	6:F:154:ILE:O	2.05	0.56
11:M:51:ARG:HG3	11:M:66:ILE:HD11	1.88	0.56
12:N:29:ARG:HA	12:N:117:ILE:O	2.06	0.56
33:a:398:C:H2'	33:a:399:G:H8	1.71	0.56
33:a:455:G:H21	33:a:496:A:N6	2.01	0.56
1:A:351:G:H21	1:A:374:A:H62	1.54	0.56
1:A:2332:G:H4'	6:F:121:SER:HA	1.88	0.56
33:a:284:G:H5''	49:q:19:MET:HE3	1.87	0.56
1:A:1709:A:H61	1:A:2025:C:H5	1.54	0.55
9:K:24:VAL:HG11	9:K:30:ARG:HD2	1.88	0.55
17:S:24:ILE:HD11	17:S:36:LEU:HD21	1.88	0.55
18:T:59:TYR:HE2	18:T:78:LYS:HD3	1.71	0.55
33:a:560:U:O2'	44:l:96:ARG:NH2	2.39	0.55
33:a:733:G:OP1	33:a:841:G:N2	2.39	0.55
33:a:1318:G:N7	45:m:98:ARG:NH2	2.54	0.55
1:A:926:G:H2'	1:A:927:G:H8	1.71	0.55
1:A:2314:C:H5	26:l:2:ARG:HH12	1.54	0.55
3:C:158:ALA:HB1	3:C:197:ASN:HB2	1.88	0.55
1:A:1068:G:N2	1:A:1069:U:O4	2.38	0.55
1:A:1292:G:H1	15:Q:37:GLN:HE21	1.54	0.55
10:L:77:VAL:HB	10:L:111:ILE:HG12	1.89	0.55
33:a:445:U:O4	33:a:504:A:N7	2.39	0.55
33:a:468:C:H2'	33:a:469:G:H8	1.71	0.55
33:a:1316:U:O4	33:a:1340:G:N2	2.38	0.55
1:A:1005:A:N3	1:A:2486:U:O2'	2.40	0.55
1:A:1103:A:N6	1:A:1133:G:OP2	2.39	0.55
6:F:70:ALA:HB2	6:F:85:ILE:HD12	1.88	0.55
38:f:33:ASN:HD21	38:f:68:ASP:H	1.54	0.55
49:q:66:THR:OG1	49:q:67:ARG:N	2.38	0.55
50:r:42:GLY:O	50:r:68:ARG:NH2	2.39	0.55
1:A:2520:U:H5'	1:A:2599:G:H5''	1.88	0.55
54:A:3001:TEL:H122	54:A:3001:TEL:H111	1.89	0.55
10:L:61:LEU:O	28:3:13:ARG:NH1	2.39	0.55
14:P:113:ILE:HD12	14:P:115:ARG:HE	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1016:A:H3'	33:a:1017:A:H8	1.72	0.55
42:j:8:ILE:HG12	42:j:100:ILE:HG12	1.87	0.55
43:k:23:ALA:HB3	43:k:86:VAL:HG22	1.89	0.55
6:F:65:PRO:HB2	6:F:87:ALA:HB1	1.89	0.55
16:R:5:ILE:O	16:R:11:GLN:HA	2.07	0.55
32:8:73:GLN:O	32:8:157:LYS:NZ	2.40	0.55
33:a:1096:U:H3	33:a:1109:G:H22	1.53	0.55
44:l:112:ARG:HB3	44:l:130:TYR:HA	1.89	0.55
3:C:100:GLU:OE1	3:C:102:ARG:NH2	2.40	0.55
11:M:30:GLY:O	11:M:134:ARG:NH2	2.38	0.55
33:a:1226:C:OP1	46:n:9:LYS:NZ	2.40	0.55
34:b:16:PHE:HB2	34:b:40:ILE:HG12	1.89	0.55
36:d:13:ARG:NE	36:d:32:ALA:O	2.39	0.55
43:k:78:GLU:O	43:k:79:HIS:C	2.46	0.55
1:A:612:U:N3	1:A:615:U:OP2	2.32	0.55
3:C:144:ILE:HB	3:C:154:LEU:HB2	1.87	0.55
14:P:114:ARG:NH2	33:a:1451:A:O2'	2.37	0.55
20:V:389:LEU:O	20:V:393:LEU:HB3	2.07	0.55
1:A:911:G:N2	1:A:913:A:H61	2.04	0.55
1:A:1043:G:OP2	15:Q:58:ARG:NE	2.39	0.55
33:a:352:A:H5''	33:a:353:C:H5	1.72	0.55
39:g:63:GLU:HA	39:g:66:LEU:HD12	1.88	0.55
1:A:2823:C:H2'	1:A:2824:G:C8	2.42	0.54
7:G:103:LYS:HG2	7:G:117:VAL:HG22	1.89	0.54
33:a:1277:G:N3	33:a:1335:U:O2'	2.39	0.54
43:k:77:ILE:HD11	43:k:107:LEU:CD2	2.35	0.54
1:A:1088:G:N2	1:A:1159:U:O2	2.33	0.54
1:A:2481:C:O2	1:A:2481:C:C2'	2.45	0.54
33:a:424:G:H2'	33:a:425:G:H8	1.73	0.54
1:A:549:A:N3	1:A:551:A:O2'	2.36	0.54
1:A:1574:G:N1	1:A:1592:A:OP2	2.34	0.54
33:a:596:G:OP1	40:h:86:ARG:NH2	2.40	0.54
33:a:791:A:OP1	33:a:1531:G:N2	2.35	0.54
20:V:40:GLY:CA	55:V:901:ATP:O2B	2.54	0.54
32:8:175:ILE:HB	32:8:188:ASN:HB3	1.89	0.54
33:a:1237:C:OP2	45:m:107:ARG:NH2	2.40	0.54
1:A:1381:A:O2'	1:A:1383:U:OP2	2.26	0.54
1:A:2169:G:H1	1:A:2180:U:H3	1.54	0.54
32:8:80:LYS:HZ2	32:8:120:MET:HB2	1.72	0.54
37:e:16:VAL:HG12	37:e:17:THR:HG23	1.88	0.54
38:f:52:ILE:HG21	38:f:86:ILE:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:911:G:H21	1:A:913:A:N6	2.05	0.54
1:A:2332:G:H21	6:F:129:THR:HG21	1.72	0.54
6:F:8:TYR:O	6:F:12:ILE:HB	2.08	0.54
24:Z:6:ILE:HG23	24:Z:54:VAL:HG13	1.89	0.54
34:b:65:GLY:HA3	34:b:159:ASP:HB2	1.89	0.54
36:d:166:THR:OG1	36:d:175:THR:OG1	2.26	0.54
1:A:2356:A:N7	1:A:2417:A:N6	2.56	0.54
23:Y:8:ASP:HB3	23:Y:13:GLU:HB2	1.90	0.54
6:F:68:THR:O	6:F:85:ILE:N	2.39	0.54
32:8:104:ILE:HA	32:8:108:TRP:HB2	1.90	0.54
33:a:56:C:OP1	33:a:359:G:N2	2.40	0.54
33:a:411:C:H5''	36:d:129:PRO:HD2	1.90	0.54
33:a:1196:G:H4'	41:i:113:ARG:HH11	1.72	0.54
36:d:196:GLU:OE1	37:e:112:ARG:NH1	2.33	0.54
3:C:69:ARG:O	3:C:189:ARG:NH1	2.41	0.54
35:c:70:ALA:HB2	35:c:105:ILE:HB	1.90	0.54
1:A:2421:A:OP2	1:A:2451:C:N4	2.39	0.53
3:C:37:LEU:HG	3:C:62:TYR:HB2	1.89	0.53
12:N:22:THR:HG22	12:N:66:ILE:HG23	1.91	0.53
33:a:468:C:H2'	33:a:469:G:C8	2.43	0.53
35:c:14:VAL:HG12	35:c:15:ILE:HG13	1.90	0.53
35:c:66:THR:HG22	35:c:101:ASN:HB2	1.91	0.53
36:d:55:GLN:HA	36:d:58:ARG:HG2	1.91	0.53
39:g:13:LEU:HA	39:g:21:LYS:HD2	1.90	0.53
26:1:8:ALA:HA	26:1:15:ARG:HA	1.90	0.53
33:a:495:U:H2'	33:a:496:A:H8	1.72	0.53
6:F:91:LEU:HB3	6:F:96:MET:HG3	1.89	0.53
21:W:79:ARG:HD2	21:W:81:GLY:H	1.74	0.53
1:A:2104:U:OP1	3:C:243:ARG:NH2	2.41	0.53
1:A:2315:A:N6	26:1:19:SER:OG	2.40	0.53
1:A:2757:U:O2	4:D:191:ASN:ND2	2.40	0.53
13:O:45:ILE:HA	13:O:52:THR:HA	1.91	0.53
32:8:121:MET:CE	32:8:121:MET:CA	2.86	0.53
33:a:1264:G:O2'	33:a:1267:G:N3	2.36	0.53
35:c:15:ILE:HD11	35:c:178:ARG:HG2	1.89	0.53
40:h:52:VAL:HB	40:h:59:ILE:HB	1.90	0.53
1:A:563:C:OP1	25:0:13:LYS:NZ	2.38	0.53
1:A:993:A:O2'	1:A:1030:G:N2	2.35	0.53
1:A:1295:U:OP2	1:A:2531:G:N2	2.36	0.53
1:A:2898:A:HO2'	12:N:2:SER:N	2.06	0.53
16:R:5:ILE:HG22	16:R:38:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:333:LEU:O	20:V:337:ILE:N	2.38	0.53
32:8:117:THR:N	32:8:121:MET:SD	2.82	0.53
33:a:1262:G:H2'	33:a:1263:G:H8	1.73	0.53
1:A:650:U:H5''	5:E:102:PRO:HB3	1.91	0.53
1:A:911:G:H21	1:A:913:A:H61	1.55	0.53
1:A:1712:G:O2'	1:A:1714:A:N6	2.41	0.53
1:A:2149:G:O6	1:A:2206:C:N4	2.41	0.53
3:C:129:ALA:HA	3:C:191:SER:HA	1.89	0.53
3:C:132:LEU:HD23	3:C:135:ILE:HD12	1.90	0.53
7:G:27:VAL:O	7:G:33:GLU:HA	2.09	0.53
20:V:327:GLY:CA	55:V:900:ATP:H5'2	2.39	0.53
33:a:105:G:OP1	33:a:333:A:N6	2.39	0.53
1:A:1065:U:H3	1:A:1188:A:H62	1.57	0.53
1:A:2054:C:OP1	4:D:153:ARG:NE	2.33	0.53
1:A:2278:U:N3	1:A:2282:G:OP2	2.37	0.53
16:R:67:ARG:HB3	16:R:89:ARG:HB3	1.90	0.53
20:V:33:ILE:HG12	20:V:169:LYS:HB2	1.90	0.53
20:V:407:MET:HE2	20:V:411:GLU:HG2	1.91	0.53
33:a:381:A:O2'	33:a:459:A:N7	2.42	0.53
33:a:596:G:N1	33:a:763:C:OP2	2.41	0.53
33:a:890:C:OP1	44:l:9:ARG:NH2	2.27	0.53
1:A:2334:U:O2'	1:A:2335:U:O4'	2.27	0.52
33:a:48:G:O2'	33:a:373:U:O2	2.24	0.52
33:a:243:C:H5'	49:q:74:ARG:HG3	1.90	0.52
33:a:779:C:O2'	33:a:909:C:N3	2.37	0.52
35:c:18:TRP:HB2	35:c:21:LYS:HG2	1.91	0.52
39:g:31:MET:HE2	39:g:36:LYS:HG3	1.91	0.52
4:D:57:ARG:HH11	4:D:60:LEU:HD11	1.75	0.52
28:3:15:LYS:HB3	28:3:23:LYS:HB3	1.90	0.52
33:a:366:U:H2'	33:a:367:A:H8	1.75	0.52
33:a:1071:G:OP1	42:j:53:ARG:NH1	2.42	0.52
6:F:107:SER:OG	6:F:108:LEU:N	2.42	0.52
7:G:7:LYS:HB2	7:G:70:ARG:HH22	1.73	0.52
33:a:643:C:H2'	33:a:644:A:H8	1.74	0.52
33:a:1235:C:OP1	45:m:90:ARG:NH1	2.39	0.52
1:A:1080:G:O4'	29:4:18:ARG:NH1	2.42	0.52
1:A:1302:A:N3	25:0:7:ARG:NH2	2.57	0.52
12:N:84:PHE:O	12:N:88:ALA:CB	2.56	0.52
32:8:124:VAL:O	32:8:127:ILE:CG2	2.54	0.52
1:A:331:C:H2'	1:A:332:G:H8	1.75	0.52
1:A:924:U:H2'	1:A:946:G:H22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:N:83:LEU:HA	12:N:87:ILE:HD12	1.90	0.52
20:V:7:LEU:HD12	20:V:25:ALA:HB3	1.90	0.52
20:V:26:SER:OG	20:V:169:LYS:NZ	2.43	0.52
33:a:761:G:OP1	47:o:73:LYS:NZ	2.38	0.52
33:a:1288:A:H5''	42:j:9:ARG:HH22	1.73	0.52
6:F:139:PRO:HG2	30:6:33:VAL:HG22	1.91	0.52
22:X:49:VAL:HG11	22:X:54:LEU:HD13	1.91	0.52
33:a:821:G:OP1	33:a:912:G:N2	2.38	0.52
1:A:929:G:H1	1:A:941:U:H3	1.58	0.52
1:A:1831:A:OP2	1:A:1844:A:N6	2.33	0.52
14:P:21:ARG:HD3	14:P:22:PRO:HD2	1.89	0.52
19:U:36:GLU:HA	19:U:60:GLU:HG2	1.91	0.52
42:j:23:GLU:HA	42:j:26:VAL:HB	1.91	0.52
48:p:74:PHE:HD1	48:p:79:ILE:HD13	1.75	0.52
1:A:740:A:O2'	1:A:1392:A:N3	2.39	0.52
1:A:2356:A:H2'	1:A:2357:A:C8	2.45	0.52
33:a:691:C:H2'	33:a:692:G:H8	1.73	0.52
36:d:163:GLU:N	36:d:184:GLU:OE2	2.38	0.52
49:q:67:ARG:HE	49:q:69:LEU:HD23	1.75	0.52
1:A:445:C:OP1	22:X:32:ASN:ND2	2.34	0.52
20:V:329:GLY:O	20:V:330:LYS:C	2.52	0.52
33:a:1129:U:OP1	41:i:85:ARG:NH1	2.43	0.52
38:f:9:ILE:HA	38:f:59:PHE:O	2.10	0.52
38:f:43:TRP:HE1	38:f:62:ILE:HD11	1.75	0.52
1:A:1033:C:O2'	1:A:1046:A:N3	2.35	0.52
1:A:1618:A:OP1	3:C:61:GLN:NE2	2.43	0.52
1:A:2287:C:O2'	1:A:2456:C:OP2	2.22	0.52
16:R:79:LYS:HB2	16:R:80:LYS:HD2	1.92	0.52
20:V:40:GLY:O	55:V:901:ATP:C4'	2.58	0.52
20:V:442:ARG:NH1	20:V:462:ASP:OD2	2.43	0.52
29:4:27:CYS:SG	29:4:28:GLU:N	2.83	0.52
33:a:1441:G:N2	33:a:1478:A:OP2	2.40	0.52
37:e:105:VAL:O	37:e:112:ARG:NH2	2.43	0.52
43:k:18:ILE:C	43:k:80:GLY:O	2.53	0.52
44:l:63:ARG:HB3	44:l:79:TYR:HE1	1.75	0.52
46:n:44:PHE:HZ	46:n:56:VAL:HG11	1.75	0.52
14:P:88:ARG:NH2	33:a:1472:C:OP1	2.42	0.51
32:8:211:ASN:HD21	32:8:223:LYS:HE3	1.74	0.51
6:F:69:ARG:HA	6:F:84:PRO:HA	1.92	0.51
20:V:294:VAL:HG13	20:V:347:VAL:HG22	1.92	0.51
20:V:328:SER:HB2	20:V:330:LYS:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:17:ASN:HB3	22:X:25:SER:HB2	1.92	0.51
36:d:121:VAL:HG22	36:d:139:ILE:HG12	1.92	0.51
39:g:113:GLU:H	39:g:119:ARG:HH21	1.57	0.51
46:n:24:CYS:SG	46:n:28:GLY:HA2	2.51	0.51
1:A:1529:G:H2'	1:A:1530:G:H8	1.76	0.51
15:Q:80:MET:HE2	15:Q:93:LYS:HE3	1.92	0.51
1:A:253:G:H4'	10:L:59:GLN:HE21	1.74	0.51
1:A:721:G:H5''	5:E:76:GLY:N	2.25	0.51
1:A:1252:G:O2'	1:A:1276:G:N2	2.41	0.51
20:V:135:ASP:OD1	20:V:135:ASP:N	2.41	0.51
33:a:273:G:H4'	49:q:70:SER:HA	1.91	0.51
33:a:1279:G:HO2'	33:a:1322:U:HO2'	1.56	0.51
50:r:28:TYR:OH	50:r:66:ARG:NH1	2.43	0.51
1:A:407:A:H2'	1:A:408:G:H8	1.76	0.51
1:A:610:U:OP1	10:L:29:LYS:NZ	2.42	0.51
1:A:651:U:H2'	1:A:652:A:H8	1.75	0.51
1:A:1095:C:H2'	1:A:1096:A:H8	1.75	0.51
1:A:2372:U:HO2'	1:A:2402:A:HO2'	1.53	0.51
33:a:1410:G:O6	33:a:1514:G:N2	2.44	0.51
36:d:138:THR:HG22	36:d:175:THR:HG22	1.92	0.51
1:A:2106:A:O2'	20:V:261:LYS:NZ	2.44	0.51
1:A:2818:C:H1'	1:A:2916:A:H2	1.75	0.51
17:S:76:VAL:HG22	17:S:103:ILE:HG13	1.92	0.51
20:V:43:LYS:HB3	55:V:901:ATP:O1B	2.11	0.51
33:a:400:G:HO2'	33:a:492:C:HO2'	1.57	0.51
33:a:593:G:H1	33:a:766:U:H3	1.58	0.51
35:c:8:VAL:HG23	35:c:183:TYR:HB3	1.92	0.51
53:x:68:U:H2'	53:x:69:C:H6	1.75	0.51
1:A:15:G:H4'	25:0:18:THR:HG22	1.93	0.51
1:A:775:G:H5'	3:C:13:ARG:HH21	1.75	0.51
1:A:1088:G:O6	1:A:1159:U:O4	2.29	0.51
1:A:2577:G:O2'	9:K:4:GLN:OE1	2.28	0.51
8:J:18:VAL:HG13	8:J:58:ILE:HD12	1.92	0.51
33:a:446:G:N2	33:a:505:G:N7	2.41	0.51
33:a:1047:C:H2'	33:a:1048:A:H8	1.75	0.51
33:a:1288:A:H5''	42:j:9:ARG:HH12	1.76	0.51
39:g:76:LYS:HG2	39:g:77:ALA:H	1.76	0.51
1:A:7:G:H5'	8:J:133:HIS:HE1	1.76	0.51
12:N:106:PRO:HG3	17:S:40:PRO:HG3	1.92	0.51
33:a:552:G:OP1	36:d:14:ARG:NE	2.44	0.51
1:A:594:C:OP1	16:R:92:TYR:OH	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:G:H2'	1:A:1479:G:C8	2.46	0.51
7:G:58:ASP:HB3	7:G:63:ARG:HH21	1.76	0.51
8:J:21:ALA:HB1	8:J:63:ILE:HD12	1.92	0.51
17:S:18:ARG:HD2	17:S:76:VAL:HB	1.92	0.51
20:V:298:THR:HB	20:V:344:GLU:HB3	1.93	0.51
34:b:81:LYS:HD2	34:b:93:ASN:HD22	1.76	0.51
44:l:64:LYS:HG2	44:l:80:ILE:HB	1.93	0.51
1:A:304:G:N2	1:A:414:C:O2	2.33	0.51
1:A:1083:G:H1	1:A:1164:C:H42	1.58	0.51
24:Z:10:ARG:HE	24:Z:15:ARG:HH21	1.57	0.51
33:a:62:A:OP1	33:a:109:G:N2	2.44	0.51
33:a:66:G:C6	33:a:98:U:C4	2.99	0.51
33:a:775:A:OP2	33:a:821:G:N2	2.44	0.51
33:a:960:U:OP2	45:m:101:ASN:ND2	2.39	0.51
39:g:72:VAL:HB	39:g:142:HIS:HE1	1.75	0.51
51:s:30:VAL:HG11	51:s:59:PRO:HB3	1.92	0.51
1:A:2629:A:C2'	1:A:2630:C:H5'	2.41	0.50
14:P:23:GLY:HA3	14:P:92:VAL:HG21	1.91	0.50
23:Y:14:ILE:HG23	23:Y:53:MET:HE2	1.93	0.50
11:M:42:ILE:HD12	11:M:97:VAL:HG21	1.93	0.50
17:S:6:VAL:HG13	17:S:104:THR:HG22	1.92	0.50
33:a:170:A:H2'	33:a:171:A:C8	2.46	0.50
36:d:17:ILE:HG21	36:d:56:LYS:HG2	1.92	0.50
39:g:51:LYS:NZ	39:g:57:ASP:OD1	2.44	0.50
1:A:226:A:N1	1:A:454:G:O2'	2.44	0.50
1:A:633:U:H2'	1:A:634:A:H8	1.75	0.50
1:A:881:U:H2'	1:A:882:A:H8	1.75	0.50
20:V:429:ILE:HG12	20:V:457:LEU:HB2	1.93	0.50
32:8:120:MET:HG2	32:8:120:MET:O	2.10	0.50
45:m:85:SER:O	45:m:88:GLY:N	2.43	0.50
1:A:576:G:OP1	1:A:2050:G:O2'	2.25	0.50
3:C:124:ILE:HG13	3:C:192:ILE:HD13	1.93	0.50
5:E:50:LYS:HB2	5:E:94:PRO:HG3	1.94	0.50
9:K:71:ARG:HE	9:K:77:ILE:HD11	1.77	0.50
41:i:11:ARG:HG2	41:i:16:VAL:HG22	1.93	0.50
43:k:22:ILE:HG22	43:k:85:GLU:HB3	1.93	0.50
1:A:1058:U:O4	8:J:31:SER:OG	2.28	0.50
1:A:1177:G:H5'	8:J:85:LEU:HD22	1.93	0.50
3:C:123:ASP:O	3:C:128:ASN:ND2	2.44	0.50
11:M:20:ARG:HD3	11:M:99:PRO:HG2	1.93	0.50
33:a:1169:G:O6	33:a:1191:G:O6	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1260:A:N3	33:a:1378:C:O2'	2.38	0.50
34:b:184:ILE:HA	34:b:198:VAL:HB	1.93	0.50
1:A:2049:A:H5'	25:0:9:SER:HB3	1.92	0.50
33:a:23:G:H2'	33:a:24:G:C8	2.47	0.50
33:a:651:A:C5	40:h:109:SER:HA	2.47	0.50
33:a:842:U:H3	33:a:863:G:H1	1.58	0.50
33:a:1317:C:OP1	45:m:97:VAL:N	2.43	0.50
1:A:419:G:N2	1:A:448:A:OP2	2.28	0.50
1:A:645:C:O2'	5:E:104:LYS:NZ	2.44	0.50
1:A:713:G:H1'	28:3:4:MET:HE2	1.93	0.50
1:A:1036:A:N3	16:R:75:ARG:NH1	2.58	0.50
16:R:68:ALA:O	16:R:89:ARG:NE	2.43	0.50
1:A:594:C:H4'	1:A:595:G:OP1	2.10	0.50
1:A:1305:A:H61	1:A:2042:A:H5''	1.77	0.50
1:A:1783:C:N3	1:A:2745:U:O2'	2.41	0.50
1:A:2128:U:H3	1:A:2219:G:H1	1.59	0.50
9:K:4:GLN:HG2	9:K:5:GLU:HG2	1.93	0.50
9:K:64:ARG:NH1	9:K:81:GLU:OE2	2.36	0.50
16:R:76:TYR:HA	16:R:82:VAL:O	2.11	0.50
18:T:14:THR:H	18:T:17:SER:HG	1.60	0.50
22:X:19:SER:OG	22:X:20:HIS:N	2.45	0.50
30:6:16:CYS:SG	30:6:17:ALA:N	2.85	0.50
33:a:716:U:H2'	33:a:717:G:H8	1.77	0.50
33:a:1365:G:H2'	33:a:1366:A:C8	2.46	0.50
1:A:89:U:H3'	1:A:90:A:H2'	1.93	0.50
1:A:1141:A:N1	1:A:1142:A:N6	2.59	0.50
1:A:2857:U:H5'	1:A:2859:G:H5'	1.94	0.50
19:U:32:ARG:HB3	19:U:62:PRO:HB2	1.94	0.50
33:a:47:U:H5''	33:a:315:U:H1'	1.92	0.50
33:a:962:U:H2'	33:a:963:G:H8	1.77	0.50
35:c:56:ILE:HG12	35:c:65:ILE:HG12	1.94	0.50
35:c:57:GLU:OE1	42:j:94:SER:OG	2.25	0.50
1:A:751:G:H2'	1:A:773:G:H22	1.77	0.49
3:C:155:VAL:HG21	3:C:162:ALA:HB2	1.94	0.49
15:Q:83:LEU:HD23	15:Q:113:ALA:HB2	1.93	0.49
20:V:331:THR:CG2	55:V:900:ATP:O2G	2.60	0.49
24:Z:47:ILE:HD13	24:Z:56:VAL:HG11	1.94	0.49
42:j:50:THR:HG22	42:j:64:GLN:HG2	1.94	0.49
43:k:85:GLU:HG3	43:k:111:ALA:HB3	1.94	0.49
52:t:20:HIS:O	52:t:23:THR:OG1	2.27	0.49
8:J:124:ASN:N	8:J:124:ASN:OD1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:8:121:MET:SD	32:8:145:VAL:HG13	2.52	0.49
33:a:277:C:H2'	33:a:278:A:C8	2.45	0.49
33:a:1047:C:H2'	33:a:1048:A:C8	2.47	0.49
1:A:2709:C:H5'	4:D:193:PRO:HA	1.95	0.49
1:A:2730:U:O2'	12:N:68:ASN:ND2	2.45	0.49
6:F:57:LEU:HB2	6:F:65:PRO:HG3	1.94	0.49
17:S:86:ARG:HD3	17:S:87:PRO:HD2	1.93	0.49
20:V:355:ILE:HA	20:V:427:VAL:HB	1.93	0.49
20:V:381:LYS:O	20:V:385:HIS:N	2.45	0.49
33:a:693:U:O2'	43:k:43:ALA:O	2.29	0.49
33:a:754:U:O3'	33:a:845:G:N2	2.41	0.49
33:a:778:G:H4'	33:a:1523:A:H4'	1.93	0.49
33:a:1318:G:OP1	45:m:87:ARG:NH1	2.45	0.49
34:b:73:LYS:H	34:b:76:ALA:HB3	1.76	0.49
1:A:87:U:OP2	19:U:29:LYS:NZ	2.40	0.49
1:A:229:A:O2'	1:A:231:A:N1	2.45	0.49
8:J:132:PRO:O	8:J:134:GLU:N	2.45	0.49
33:a:33:G:N2	33:a:50:C:OP1	2.44	0.49
35:c:123:LEU:HD13	35:c:195:LEU:HD13	1.93	0.49
40:h:10:MET:HE3	40:h:27:ILE:HD13	1.94	0.49
1:A:115:C:O2'	1:A:125:A:N3	2.42	0.49
1:A:331:C:H2'	1:A:332:G:C8	2.47	0.49
1:A:1710:A:O2'	9:K:1:MET:O	2.30	0.49
55:V:901:ATP:H3'	55:V:901:ATP:C8	2.48	0.49
23:Y:24:GLU:OE2	23:Y:42:ARG:NH2	2.45	0.49
33:a:1264:G:H3'	33:a:1288:A:H61	1.76	0.49
33:a:1335:U:H2'	33:a:1336:G:H8	1.78	0.49
41:i:115:LYS:HB2	41:i:118:LEU:HD12	1.95	0.49
44:l:66:ALA:HB2	44:l:80:ILE:HD11	1.94	0.49
1:A:774:A:OP1	1:A:1477:A:O2'	2.23	0.49
1:A:1514:C:O2	1:A:1572:G:N2	2.40	0.49
17:S:73:GLN:HB2	17:S:106:VAL:HB	1.95	0.49
37:e:156:LEU:HD22	40:h:73:VAL:HG22	1.94	0.49
1:A:352:G:N2	1:A:524:A:N7	2.61	0.49
1:A:852:G:N2	1:A:876:A:OP1	2.45	0.49
1:A:1808:U:OP2	1:A:1813:A:N6	2.35	0.49
6:F:4:LEU:HD12	6:F:97:TYR:HD1	1.78	0.49
32:8:57:GLN:NE2	32:8:203:ALA:O	2.45	0.49
1:A:896:A:H2'	1:A:897:G:H8	1.77	0.49
20:V:371:PRO:HA	20:V:374:LEU:HB3	1.94	0.49
32:8:163:TYR:HB3	32:8:171:ILE:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:531:C:H41	44:l:63:ARG:HH22	1.61	0.49
34:b:83:GLU:OE1	34:b:86:ARG:NH2	2.46	0.49
1:A:631:G:H22	10:L:33:LYS:HE2	1.76	0.49
33:a:51:U:N3	33:a:372:A:C6	2.81	0.49
33:a:840:U:H5'	34:b:21:ARG:HD2	1.95	0.49
33:a:1448:G:OP1	52:t:33:LYS:NZ	2.42	0.49
1:A:2475:G:N2	1:A:2478:U:O2	2.43	0.49
33:a:24:G:O2'	33:a:923:A:N1	2.44	0.49
33:a:301:A:H5'	33:a:619:G:C2	2.48	0.49
33:a:715:A:H5''	43:k:26:ARG:HH21	1.78	0.49
33:a:956:A:H2'	33:a:957:G:H8	1.77	0.49
33:a:1039:U:O4	33:a:1042:G:N1	2.45	0.49
33:a:1234:A:O2'	33:a:1235:C:H5'	2.13	0.49
1:A:2150:G:OP1	1:A:2199:G:N2	2.45	0.48
7:G:44:ILE:HD13	7:G:73:LEU:HD11	1.95	0.48
20:V:322:ILE:HG12	20:V:474:LEU:HD12	1.94	0.48
33:a:265:G:H2'	33:a:266:A:H8	1.78	0.48
33:a:381:A:H61	33:a:399:G:H1'	1.77	0.48
36:d:9:TRP:O	36:d:12:SER:OG	2.28	0.48
40:h:37:ALA:HB1	40:h:49:VAL:HG21	1.93	0.48
1:A:31:C:O2'	1:A:1278:G:OP1	2.30	0.48
1:A:250:G:OP2	1:A:252:C:N4	2.43	0.48
1:A:580:U:H5'	15:Q:42:SER:HB2	1.95	0.48
1:A:2076:C:H2'	1:A:2077:G:H8	1.78	0.48
15:Q:70:ARG:HE	15:Q:75:SER:HA	1.78	0.48
17:S:52:LYS:HA	17:S:55:ILE:HD12	1.94	0.48
20:V:319:LYS:HG2	20:V:456:LEU:HD21	1.95	0.48
33:a:147:G:H1	33:a:173:A:H61	1.60	0.48
33:a:466:G:H1	33:a:484:U:H3	1.61	0.48
1:A:733:U:O2'	27:2:4:THR:O	2.30	0.48
1:A:2026:A:O5'	4:D:130:ARG:NH1	2.45	0.48
1:A:2304:C:H1'	11:M:85:SER:HA	1.96	0.48
3:C:23:GLU:OE1	3:C:90:ASN:ND2	2.46	0.48
5:E:49:HIS:ND1	5:E:92:PRO:HB2	2.28	0.48
10:L:23:ILE:HA	10:L:28:GLY:HA3	1.95	0.48
33:a:80:G:H2'	33:a:81:A:H8	1.79	0.48
33:a:267:G:H5''	52:t:78:ARG:HH22	1.78	0.48
33:a:1231:G:H5''	51:s:78:ARG:HH11	1.78	0.48
33:a:1347:G:N3	53:x:41:U:O2'	2.46	0.48
5:E:136:THR:HG22	5:E:166:SER:HA	1.96	0.48
6:F:62:GLY:H	30:6:9:PHE:HZ	1.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:33:LYS:HE3	10:L:40:ALA:HA	1.96	0.48
33:a:801:A:O2'	33:a:803:A:N7	2.40	0.48
45:m:11:ARG:HB3	45:m:46:ARG:HB3	1.95	0.48
1:A:789:C:H2'	1:A:790:A:C8	2.48	0.48
1:A:2150:G:N2	32:8:166:ASP:OD2	2.47	0.48
1:A:2541:C:O2	4:D:145:SER:OG	2.31	0.48
6:F:100:LEU:HD23	6:F:103:LEU:HD12	1.96	0.48
8:J:43:PRO:HB3	15:Q:68:ALA:HB2	1.96	0.48
20:V:39:ASN:ND2	20:V:410:GLY:O	2.45	0.48
20:V:371:PRO:HD2	20:V:401:THR:HA	1.95	0.48
26:1:29:ARG:HG3	26:1:47:GLU:HB3	1.96	0.48
42:j:42:LEU:HB3	42:j:71:LYS:HG3	1.95	0.48
53:x:11:U:H2'	53:x:12:G:C8	2.48	0.48
1:A:235:G:N2	1:A:467:C:OP1	2.39	0.48
1:A:848:G:O4'	5:E:54:ARG:NH1	2.46	0.48
1:A:1456:A:HO2'	1:A:1460:G:HO2'	1.57	0.48
1:A:1817:C:H4'	3:C:224:VAL:HG11	1.96	0.48
1:A:2121:U:H4'	1:A:2122:G:H5'	1.95	0.48
14:P:60:THR:HA	14:P:73:THR:HA	1.96	0.48
16:R:2:TYR:HA	16:R:14:VAL:O	2.13	0.48
33:a:52:A:O2'	33:a:368:G:N2	2.47	0.48
33:a:699:G:OP2	43:k:31:ASN:ND2	2.36	0.48
33:a:865:G:OP2	33:a:881:U:N3	2.29	0.48
48:p:6:ARG:NH2	48:p:28:PRO:O	2.47	0.48
3:C:16:MET:HE1	3:C:207:LYS:HG3	1.96	0.48
4:D:3:LYS:HD3	4:D:101:ILE:HG22	1.96	0.48
5:E:54:ARG:HD2	5:E:81:PRO:HD3	1.94	0.48
8:J:78:HIS:HD2	8:J:85:LEU:HB3	1.78	0.48
10:L:49:GLY:H	28:3:61:MET:HE3	1.78	0.48
50:r:67:ALA:HB1	50:r:72:LEU:HB2	1.96	0.48
3:C:62:TYR:HA	3:C:86:ASN:HD21	1.79	0.48
6:F:4:LEU:HD11	6:F:173:VAL:HG13	1.96	0.48
6:F:69:ARG:HG2	6:F:84:PRO:HB3	1.95	0.48
20:V:43:LYS:CA	55:V:901:ATP:O1B	2.61	0.48
20:V:420:TYR:CZ	20:V:428:LEU:HB3	2.48	0.48
23:Y:6:ILE:O	23:Y:60:ARG:NH2	2.46	0.48
24:Z:7:THR:HG22	24:Z:34:THR:HG22	1.96	0.48
33:a:912:G:H2'	33:a:913:A:H8	1.78	0.48
1:A:1613:C:H5''	3:C:21:PHE:HE2	1.79	0.48
1:A:2129:G:N2	1:A:2218:U:O2	2.47	0.48
1:A:2300:G:H5'	21:W:28:ARG:HE	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2480:A:C5	1:A:2481:C:H5	2.32	0.48
8:J:24:LYS:HD2	8:J:29:LEU:HD12	1.95	0.48
20:V:296:ASN:OD1	20:V:309:ASN:ND2	2.46	0.48
20:V:301:PHE:CD1	55:V:900:ATP:N6	2.75	0.48
21:W:22:ARG:H	21:W:22:ARG:HD3	1.78	0.48
22:X:35:LYS:HE2	22:X:46:LYS:HG2	1.94	0.48
1:A:828:A:OP1	3:C:217:ARG:NH1	2.47	0.48
20:V:331:THR:O	20:V:335:ASN:ND2	2.47	0.48
26:1:2:ARG:HD2	26:1:20:LYS:HB3	1.96	0.48
33:a:661:U:O4	33:a:761:G:O2'	2.27	0.48
51:s:63:SER:H	51:s:66:MET:HE3	1.78	0.48
1:A:490:A:H62	5:E:41:ARG:HG2	1.78	0.47
1:A:1072:A:OP2	1:A:1180:C:O2'	2.31	0.47
1:A:1365:U:O2'	1:A:1366:C:O4'	2.32	0.47
1:A:2562:U:OP1	1:A:2694:A:O2'	2.31	0.47
4:D:185:LEU:HD13	14:P:8:ILE:HD11	1.96	0.47
18:T:9:LYS:HE3	18:T:31:ASP:HB3	1.96	0.47
55:V:901:ATP:C3'	55:V:901:ATP:C8	2.97	0.47
40:h:17:ALA:HB2	40:h:25:LEU:HD21	1.95	0.47
52:t:32:ILE:HG12	52:t:79:LEU:HD11	1.96	0.47
1:A:1177:G:H4'	8:J:85:LEU:HD13	1.95	0.47
1:A:1471:G:N2	1:A:1621:G:N7	2.62	0.47
1:A:1817:C:H3'	1:A:1818:A:H8	1.79	0.47
1:A:2261:C:OP2	22:X:27:ARG:NH2	2.43	0.47
54:A:3001:TEL:H333	54:A:3001:TEL:O45	2.15	0.47
33:a:473:G:N1	33:a:476:U:OP2	2.47	0.47
20:V:327:GLY:HA3	55:V:900:ATP:H5'2	1.96	0.47
33:a:477:A:H3'	33:a:478:G:H8	1.79	0.47
33:a:933:A:O2'	33:a:1408:C:OP2	2.30	0.47
1:A:575:A:H62	1:A:2070:U:H3	1.63	0.47
1:A:834:C:OP1	1:A:1809:A:N6	2.45	0.47
1:A:1668:G:H2'	1:A:1669:G:H8	1.78	0.47
1:A:2670:A:P	8:J:77:ARG:HH12	2.37	0.47
9:K:97:ARG:NE	33:a:347:C:OP2	2.48	0.47
47:o:24:SER:O	47:o:26:GLU:N	2.48	0.47
1:A:920:G:H2'	1:A:921:G:H8	1.78	0.47
1:A:1317:G:H2'	1:A:1318:G:H8	1.79	0.47
1:A:1452:C:H2'	1:A:1453:A:C8	2.50	0.47
1:A:2164:A:O4'	1:A:2188:G:O2'	2.32	0.47
1:A:2334:U:O4	6:F:151:GLY:N	2.48	0.47
4:D:10:ILE:HD11	4:D:29:GLU:HB2	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:69:C:H2'	33:a:70:G:C8	2.49	0.47
33:a:176:G:OP1	52:t:57:ARG:NH2	2.39	0.47
33:a:224:U:H2'	33:a:225:A:C8	2.50	0.47
33:a:500:A:H2'	33:a:501:A:H8	1.80	0.47
33:a:984:A:OP2	46:n:41:ARG:NH2	2.48	0.47
51:s:39:THR:HA	51:s:70:LYS:HG2	1.96	0.47
1:A:273:A:OP2	1:A:297:G:N2	2.38	0.47
1:A:448:A:H2'	1:A:449:A:C8	2.49	0.47
1:A:1614:A:OP1	3:C:210:ARG:NH1	2.48	0.47
1:A:1829:C:O2	1:A:1846:G:N2	2.47	0.47
1:A:2103:U:HO2'	1:A:2626:G:HO2'	1.61	0.47
32:8:118:PRO:HG3	32:8:145:VAL:HG12	1.97	0.47
33:a:728:C:O2'	50:r:44:ILE:O	2.32	0.47
33:a:1050:A:H2'	33:a:1051:G:C8	2.49	0.47
36:d:50:GLN:HB3	36:d:197:PHE:HB2	1.97	0.47
1:A:528:G:O2'	1:A:552:G:N2	2.48	0.47
1:A:763:A:O2'	47:o:44:ARG:NH2	2.46	0.47
1:A:976:U:O2'	24:Z:25:THR:O	2.23	0.47
1:A:1474:C:O2'	1:A:1617:A:OP2	2.28	0.47
1:A:2125:U:H2'	1:A:2126:G:C8	2.49	0.47
1:A:2320:U:H2'	1:A:2321:U:C6	2.50	0.47
1:A:2320:U:O2'	1:A:2403:C:O2	2.33	0.47
4:D:126:HIS:CD2	4:D:159:LEU:HB3	2.49	0.47
9:K:13:ASN:ND2	9:K:96:THR:OG1	2.47	0.47
16:R:48:VAL:HG21	16:R:53:VAL:N	2.30	0.47
20:V:322:ILE:HB	20:V:459:VAL:HG22	1.96	0.47
24:Z:5:GLU:OE2	24:Z:59:GLN:NE2	2.48	0.47
27:2:35:ARG:HG3	27:2:42:LEU:HD11	1.96	0.47
32:8:62:ALA:HB3	32:8:160:LYS:HE3	1.95	0.47
33:a:203:A:H2'	33:a:204:A:C8	2.50	0.47
33:a:514:G:H2'	33:a:515:G:C8	2.50	0.47
33:a:724:A:H2'	33:a:725:A:C8	2.49	0.47
33:a:1013:G:N2	33:a:1014:A:O2'	2.46	0.47
33:a:1049:G:H2'	33:a:1050:A:H8	1.80	0.47
33:a:1137:G:H1	33:a:1154:C:H42	1.61	0.47
35:c:20:SER:HB2	35:c:22:TRP:CZ3	2.50	0.47
36:d:126:VAL:HG12	36:d:128:ILE:H	1.80	0.47
1:A:869:U:H2'	1:A:870:A:H8	1.80	0.47
1:A:2480:A:H5''	20:V:238:LYS:HE3	1.95	0.47
1:A:2499:G:O6	1:A:2505:A:O2'	2.29	0.47
5:E:2:PRO:HG2	5:E:19:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:83:GLN:OE1	32:8:129:ARG:NH1	2.47	0.47
24:Z:23:VAL:HG21	24:Z:53:LEU:HD22	1.97	0.47
33:a:535:C:OP1	44:l:101:LYS:NZ	2.47	0.47
33:a:1318:G:OP1	45:m:91:HIS:NE2	2.37	0.47
47:o:18:HIS:N	47:o:21:ASP:OD2	2.39	0.47
1:A:957:A:H2'	1:A:958:A:C8	2.50	0.47
1:A:2786:A:N1	7:G:68:THR:HG21	2.30	0.47
16:R:60:ALA:HB1	16:R:95:VAL:HG13	1.96	0.47
33:a:919:A:N3	33:a:1422:A:O2'	2.42	0.47
41:i:28:ILE:HG12	41:i:63:VAL:HB	1.96	0.47
45:m:3:ARG:HG3	45:m:4:ILE:H	1.79	0.47
1:A:626:G:H2'	1:A:627:G:C8	2.49	0.47
5:E:40:GLN:HE22	5:E:182:ASN:HB3	1.79	0.47
6:F:45:GLN:HE21	20:V:379:THR:HB	1.80	0.47
33:a:262:G:H5'	49:q:73:LYS:HE3	1.97	0.47
33:a:381:A:N1	33:a:399:G:O2'	2.46	0.47
33:a:985:A:N6	42:j:50:THR:OG1	2.47	0.47
33:a:1385:U:H2'	33:a:1386:A:H8	1.80	0.47
1:A:795:G:O6	54:A:3001:TEL:H56	2.15	0.46
1:A:864:C:O2'	1:A:886:U:OP1	2.30	0.46
1:A:1941:A:H2	1:A:1946:U:H3	1.60	0.46
1:A:2406:A:O2'	13:O:120:PHE:O	2.33	0.46
7:G:171:ARG:NH2	29:4:28:GLU:O	2.48	0.46
10:L:19:VAL:HG13	10:L:27:ASN:HB3	1.96	0.46
14:P:35:GLY:C	14:P:37:ARG:H	2.21	0.46
21:W:73:GLY:HA3	21:W:90:TYR:O	2.15	0.46
21:W:80:PHE:N	21:W:84:ARG:O	2.39	0.46
44:l:61:ALA:HB3	44:l:63:ARG:HH11	1.80	0.46
50:r:34:LEU:HB3	50:r:73:LEU:HD11	1.97	0.46
1:A:909:G:O2'	2:B:76:A:N3	2.48	0.46
3:C:21:PHE:HB3	3:C:24:ILE:HD12	1.96	0.46
3:C:53:HIS:HA	3:C:217:ARG:HB2	1.96	0.46
9:K:19:VAL:HA	9:K:42:THR:O	2.15	0.46
10:L:19:VAL:HG12	10:L:31:ALA:HB1	1.98	0.46
16:R:10:LYS:NZ	16:R:23:GLU:OE2	2.45	0.46
20:V:35:ILE:HD13	20:V:171:TRP:HB2	1.97	0.46
20:V:88:LYS:HA	20:V:91:LEU:HB2	1.97	0.46
20:V:428:LEU:HD13	20:V:430:LEU:HG	1.96	0.46
33:a:36:C:H1'	44:l:42:GLN:HE22	1.80	0.46
33:a:954:G:N1	33:a:1347:G:OP2	2.40	0.46
38:f:41:LYS:HB3	38:f:62:ILE:HB	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:644:G:N2	1:A:649:G:O3'	2.48	0.46
1:A:1782:G:OP1	14:P:93:ARG:NH2	2.48	0.46
3:C:131:PRO:HA	3:C:189:ARG:HA	1.97	0.46
6:F:4:LEU:HB3	6:F:97:TYR:HB3	1.98	0.46
14:P:49:LYS:HB3	14:P:60:THR:HG22	1.96	0.46
33:a:70:G:H1	33:a:99:A:N6	2.13	0.46
33:a:930:U:O2'	33:a:1091:G:O2'	2.23	0.46
44:l:53:MET:HE3	44:l:103:LEU:HD21	1.98	0.46
1:A:897:G:H21	24:Z:46:MET:HE3	1.79	0.46
20:V:365:LEU:HD11	20:V:404:ILE:HB	1.96	0.46
33:a:69:C:O2'	33:a:170:A:N3	2.45	0.46
33:a:737:A:H2'	33:a:738:A:C8	2.50	0.46
33:a:815:C:H2'	33:a:816:A:C8	2.48	0.46
33:a:1113:C:H5''	34:b:97:LEU:HD22	1.98	0.46
51:s:28:LYS:HG2	51:s:29:GLN:H	1.79	0.46
1:A:86:C:H4'	1:A:103:U:H1'	1.98	0.46
1:A:1001:U:OP1	11:M:87:LYS:NZ	2.32	0.46
1:A:1184:G:N2	8:J:109:MET:HE3	2.30	0.46
1:A:1221:A:H2'	1:A:1222:A:C8	2.51	0.46
1:A:1432:A:H62	18:T:16:ARG:HE	1.64	0.46
1:A:1959:G:O2'	1:A:1997:G:O6	2.30	0.46
6:F:49:ALA:O	6:F:52:SER:HB3	2.15	0.46
17:S:82:LEU:HB2	17:S:98:LYS:HB2	1.98	0.46
20:V:277:VAL:HG12	20:V:279:PHE:HB2	1.98	0.46
27:2:34:ARG:HG3	27:2:42:LEU:HD12	1.97	0.46
32:8:104:ILE:HG12	32:8:108:TRP:CD1	2.50	0.46
33:a:106:G:OP1	33:a:334:G:N2	2.47	0.46
33:a:843:U:OP1	50:r:47:ARG:NH1	2.44	0.46
1:A:1339:A:H4'	1:A:1340:A:H5'	1.95	0.46
14:P:29:HIS:HD2	14:P:83:LYS:HB3	1.80	0.46
16:R:12:ILE:HG21	16:R:20:VAL:HG11	1.97	0.46
16:R:59:THR:OG1	16:R:98:GLU:O	2.30	0.46
20:V:333:LEU:HA	20:V:336:ILE:HG12	1.97	0.46
26:1:5:ILE:HG13	26:1:21:LYS:HG2	1.97	0.46
33:a:254:A:H62	33:a:289:G:N2	2.13	0.46
33:a:643:C:H2'	33:a:644:A:C8	2.50	0.46
43:k:78:GLU:C	43:k:80:GLY:N	2.72	0.46
1:A:5:A:H2'	1:A:6:A:C8	2.51	0.46
1:A:259:A:H2'	1:A:260:A:C8	2.51	0.46
8:J:61:GLU:HB3	8:J:98:PRO:HG3	1.97	0.46
9:K:34:ASN:N	9:K:37:ASP:OD2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:51:ARG:O	14:P:57:GLU:HA	2.16	0.46
15:Q:98:LEU:HB3	16:R:13:LYS:HD2	1.97	0.46
20:V:43:LYS:CB	55:V:901:ATP:O1B	2.63	0.46
20:V:125:LEU:HD12	20:V:153:VAL:HG22	1.96	0.46
20:V:294:VAL:HG22	20:V:347:VAL:HG13	1.98	0.46
33:a:282:A:H1'	33:a:283:G:C8	2.51	0.46
33:a:956:A:H2'	33:a:957:G:C8	2.49	0.46
33:a:1046:G:O2'	33:a:1047:C:O4'	2.27	0.46
1:A:1465:A:H2'	1:A:1467:G:N7	2.31	0.46
1:A:1469:G:H2'	1:A:1470:G:H8	1.80	0.46
4:D:180:ASP:HB2	4:D:185:LEU:HB2	1.98	0.46
5:E:32:VAL:HG13	5:E:105:VAL:HG13	1.97	0.46
33:a:126:G:O2'	49:q:65:GLU:OE2	2.25	0.46
33:a:960:U:H2'	33:a:961:G:C8	2.50	0.46
40:h:40:LEU:HD21	40:h:131:VAL:HG21	1.98	0.46
52:t:28:MET:HE3	52:t:58:ILE:HG12	1.98	0.46
1:A:1575:A:N6	1:A:1591:G:O2'	2.49	0.46
54:A:3001:TEL:H541	54:A:3001:TEL:H572	1.68	0.46
6:F:111:VAL:HB	6:F:114:PHE:HB2	1.97	0.46
10:L:81:LYS:HD3	10:L:101:VAL:HG13	1.97	0.46
26:1:5:ILE:O	26:1:18:ILE:HA	2.15	0.46
33:a:1238:A:O2'	53:x:30:C:OP1	2.34	0.46
35:c:68:HIS:CD2	35:c:103:LEU:HB2	2.51	0.46
42:j:24:LYS:HG2	42:j:92:LEU:HD21	1.98	0.46
43:k:129:ARG:HH21	43:k:130:ARG:HH22	1.64	0.46
1:A:231:A:H1'	1:A:233:G:H5'	1.98	0.46
1:A:704:U:H2'	1:A:705:A:C8	2.51	0.46
1:A:776:G:OP1	3:C:10:SER:OG	2.32	0.46
1:A:2125:U:H2'	1:A:2126:G:H8	1.81	0.46
20:V:432:GLN:NE2	20:V:435:ASN:HD22	2.14	0.46
33:a:477:A:H3'	33:a:478:G:C8	2.50	0.46
1:A:1918:A:N3	1:A:2115:U:O2'	2.44	0.45
1:A:2721:C:H2'	1:A:2722:A:H8	1.81	0.45
33:a:1436:C:H2'	33:a:1437:A:H8	1.81	0.45
1:A:1303:U:O3'	25:0:8:THR:OG1	2.34	0.45
26:1:34:LYS:HB2	26:1:45:HIS:CE1	2.50	0.45
33:a:850:U:H3	33:a:855:G:H22	1.65	0.45
33:a:985:A:N1	33:a:1375:C:O2'	2.43	0.45
33:a:1522:U:H2'	33:a:1523:A:C8	2.52	0.45
34:b:136:GLN:O	34:b:140:GLU:HB3	2.16	0.45
33:a:746:C:H2'	33:a:747:U:H6	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:f:77:ARG:HD3	38:f:78:LEU:HG	1.97	0.45
1:A:910:A:H2'	1:A:911:G:C8	2.51	0.45
1:A:2452:U:H1'	1:A:2454:A:C5	2.51	0.45
14:P:29:HIS:CD2	14:P:83:LYS:HB3	2.52	0.45
33:a:710:U:OP1	33:a:711:A:O2'	2.29	0.45
1:A:2144:G:O2'	1:A:2195:G:N2	2.49	0.45
1:A:2281:G:N2	20:V:242:ARG:O	2.48	0.45
7:G:36:ARG:HG2	7:G:72:LEU:HD22	1.99	0.45
9:K:88:ARG:HB3	9:K:94:ARG:HB3	1.97	0.45
20:V:51:HIS:HA	20:V:68:LEU:HD13	1.98	0.45
20:V:238:LYS:O	20:V:242:ARG:CG	2.64	0.45
55:V:901:ATP:H3'	55:V:901:ATP:H8	1.80	0.45
21:W:83:ASP:N	21:W:83:ASP:OD1	2.47	0.45
33:a:108:C:O2'	48:p:26:ARG:O	2.31	0.45
39:g:70:MET:HE2	39:g:97:THR:HA	1.97	0.45
1:A:577:U:OP1	1:A:605:G:N1	2.50	0.45
1:A:685:U:H2'	1:A:686:C:C6	2.51	0.45
1:A:2186:G:O2'	1:A:2187:A:O4'	2.34	0.45
1:A:2592:U:O2'	1:A:2594:A:N7	2.38	0.45
4:D:3:LYS:HG2	4:D:204:SER:HB3	1.99	0.45
8:J:58:ILE:HG23	8:J:129:SER:HA	1.99	0.45
17:S:24:ILE:HD11	17:S:36:LEU:HD11	1.99	0.45
20:V:105:SER:CB	55:V:900:ATP:O3A	2.65	0.45
33:a:43:G:H2'	33:a:44:G:H8	1.82	0.45
33:a:514:G:H2'	33:a:515:G:H8	1.81	0.45
33:a:737:A:H2'	33:a:738:A:H8	1.80	0.45
34:b:100:THR:HA	34:b:107:ILE:HG13	1.99	0.45
37:e:11:LEU:HD12	37:e:68:LYS:HE2	1.97	0.45
53:x:23:C:H2'	53:x:24:A:C8	2.51	0.45
1:A:636:G:H1	1:A:712:C:H42	1.63	0.45
1:A:2215:U:H2'	1:A:2216:A:H8	1.82	0.45
14:P:27:ARG:HE	14:P:87:VAL:HG11	1.82	0.45
20:V:301:PHE:CZ	55:V:900:ATP:C5	3.05	0.45
33:a:1165:G:O2'	33:a:1189:A:N1	2.42	0.45
39:g:11:ASP:N	39:g:11:ASP:OD1	2.48	0.45
1:A:1002:G:OP2	11:M:14:ARG:NH2	2.46	0.45
1:A:2272:U:H2'	1:A:2273:U:C6	2.52	0.45
12:N:47:MET:HE1	12:N:62:ALA:HA	1.98	0.45
17:S:18:ARG:NE	17:S:76:VAL:O	2.43	0.45
33:a:1044:G:H2'	33:a:1045:G:C8	2.52	0.45
33:a:1483:G:H2'	33:a:1484:G:C8	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:23:TYR:CE2	42:j:11:LYS:HG3	2.52	0.45
1:A:811:A:N3	3:C:212:ARG:NH2	2.65	0.45
1:A:1825:U:H2'	1:A:1826:C:H6	1.82	0.45
1:A:2075:G:H5'	25:0:16:ARG:HG2	1.99	0.45
1:A:2203:C:O2'	32:8:217:THR:O	2.28	0.45
1:A:2572:G:H21	1:A:2675:C:H5''	1.82	0.45
4:D:123:ILE:HD12	4:D:141:ARG:HA	1.98	0.45
5:E:24:PHE:HB3	5:E:118:VAL:HG21	1.99	0.45
9:K:87:ILE:HA	9:K:93:PRO:HA	1.99	0.45
33:a:500:A:H2'	33:a:501:A:C8	2.52	0.45
33:a:671:A:H2'	33:a:672:A:C8	2.52	0.45
37:e:72:ILE:HG21	37:e:141:LEU:HD22	1.99	0.45
42:j:11:LYS:HB3	42:j:71:LYS:HB3	1.99	0.45
1:A:61:A:H61	1:A:93:C:H42	1.65	0.45
1:A:1461:A:H62	1:A:1630:G:H21	1.65	0.45
1:A:2640:C:O4'	54:A:3001:TEL:H81	2.17	0.45
1:A:2817:C:O2'	1:A:2834:A:N3	2.44	0.45
20:V:238:LYS:O	20:V:242:ARG:HG2	2.17	0.45
20:V:389:LEU:O	20:V:393:LEU:CB	2.64	0.45
33:a:37:G:O2'	44:l:128:SER:O	2.25	0.45
33:a:417:U:O2	33:a:441:G:N2	2.44	0.45
38:f:78:LEU:HD23	38:f:78:LEU:HA	1.89	0.45
1:A:1616:G:H4'	3:C:59:LYS:HG3	1.98	0.44
1:A:1883:A:H3'	1:A:1884:G:H8	1.82	0.44
1:A:2487:U:O2'	1:A:2489:U:O4	2.34	0.44
3:C:108:LYS:HB3	3:C:194:GLN:HB3	1.99	0.44
3:C:243:ARG:NE	3:C:247:MET:SD	2.90	0.44
5:E:143:LEU:HD13	5:E:173:VAL:HG21	1.99	0.44
9:K:22:ILE:HD12	9:K:40:VAL:HG12	1.98	0.44
9:K:25:LEU:HD11	9:K:59:LYS:HE3	1.99	0.44
12:N:29:ARG:HE	12:N:118:GLU:HG2	1.82	0.44
20:V:110:LEU:HD13	20:V:113:ARG:HH11	1.81	0.44
33:a:1140:A:O3'	41:i:20:ARG:NH2	2.50	0.44
33:a:1444:G:H2'	33:a:1445:U:C6	2.52	0.44
34:b:20:THR:OG1	34:b:21:ARG:N	2.44	0.44
1:A:354:A:O2'	1:A:356:G:N7	2.45	0.44
1:A:957:A:H62	11:M:12:GLU:HA	1.82	0.44
33:a:383:U:H5'	48:p:7:LEU:HD12	1.99	0.44
33:a:1044:G:H2'	33:a:1045:G:H8	1.82	0.44
1:A:125:A:H5''	27:2:19:ARG:HG2	1.99	0.44
1:A:967:G:H21	1:A:2298:A:H8	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1444:C:H2'	1:A:1445:A:C8	2.53	0.44
1:A:1800:C:H42	1:A:2009:G:H1	1.65	0.44
1:A:1923:C:H5'	20:V:198:THR:HG22	2.00	0.44
1:A:2518:G:N2	1:A:2520:U:O4	2.42	0.44
1:A:2769:A:H2'	1:A:2770:A:C8	2.52	0.44
6:F:38:MET:HB3	6:F:87:ALA:H	1.82	0.44
23:Y:14:ILE:HG23	23:Y:53:MET:HB3	1.99	0.44
32:8:50:VAL:HB	32:8:57:GLN:HB3	2.00	0.44
33:a:568:A:H4'	33:a:569:A:H3'	1.99	0.44
33:a:627:C:N4	33:a:630:A:N7	2.66	0.44
33:a:696:A:N1	33:a:709:G:O2'	2.48	0.44
34:b:166:PRO:HG3	34:b:187:VAL:HG12	1.99	0.44
35:c:174:LEU:HD21	35:c:200:TRP:CD1	2.53	0.44
36:d:120:LEU:HD22	36:d:125:ARG:HA	1.98	0.44
48:p:36:THR:OG1	48:p:37:VAL:O	2.35	0.44
49:q:15:VAL:HB	49:q:24:THR:HG23	1.99	0.44
1:A:30:G:O2'	1:A:1254:A:N3	2.42	0.44
1:A:1004:U:H2'	2:B:87:U:H1'	1.99	0.44
1:A:2506:C:O2	29:4:4:ARG:NH1	2.50	0.44
54:A:3001:TEL:H13	54:A:3001:TEL:H7	1.49	0.44
3:C:230:HIS:CD2	3:C:232:HIS:H	2.33	0.44
7:G:15:VAL:HG22	7:G:80:VAL:HG12	1.99	0.44
14:P:14:ARG:NH1	14:P:78:THR:O	2.50	0.44
15:Q:93:LYS:H	15:Q:93:LYS:HD2	1.83	0.44
33:a:855:G:H2'	33:a:856:C:C6	2.53	0.44
33:a:952:G:H21	41:i:126:GLN:NE2	2.15	0.44
35:c:39:ARG:HA	35:c:42:ILE:HG22	1.98	0.44
5:E:152:ALA:HB3	5:E:173:VAL:HG22	1.99	0.44
20:V:301:PHE:HE1	55:V:900:ATP:HN61	1.60	0.44
33:a:42:C:H2'	33:a:43:G:C8	2.52	0.44
33:a:265:G:H2'	33:a:266:A:C8	2.53	0.44
51:s:37:ARG:H	51:s:37:ARG:HG2	1.55	0.44
1:A:898:U:H2'	1:A:899:C:H6	1.81	0.44
1:A:1909:U:H2'	1:A:1910:G:C8	2.52	0.44
1:A:2270:A:H2'	1:A:2271:G:C8	2.52	0.44
20:V:432:GLN:HE21	20:V:435:ASN:HD22	1.66	0.44
21:W:75:VAL:HG22	21:W:89:VAL:HG22	1.99	0.44
34:b:166:PRO:HB3	34:b:196:ILE:HD11	1.99	0.44
40:h:5:ASP:HB2	40:h:79:ARG:HH12	1.83	0.44
1:A:363:C:OP2	5:E:137:LYS:NZ	2.34	0.44
6:F:34:ILE:O	6:F:91:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:27:THR:HG22	18:T:80:ILE:HG13	2.00	0.44
24:Z:44:ARG:NH2	24:Z:58:GLU:OE2	2.51	0.44
33:a:722:G:H2'	33:a:723:G:C8	2.53	0.44
35:c:71:LYS:HE3	35:c:71:LYS:HB3	1.90	0.44
1:A:143:G:O3'	18:T:35:ASN:ND2	2.50	0.44
1:A:184:G:OP1	1:A:184:G:N2	2.37	0.44
1:A:274:A:N3	1:A:415:C:O2'	2.50	0.44
1:A:632:U:H2'	1:A:633:U:C6	2.53	0.44
1:A:2091:A:C6	54:A:3001:TEL:H551	2.53	0.44
1:A:2149:G:N1	1:A:2207:C:O2	2.49	0.44
4:D:34:VAL:HG11	4:D:74:THR:HG21	1.99	0.44
8:J:18:VAL:HG23	8:J:138:PRO:HB2	1.98	0.44
14:P:37:ARG:HH22	33:a:352:A:H4'	1.83	0.44
33:a:43:G:H2'	33:a:44:G:C8	2.53	0.44
33:a:1134:G:N2	33:a:1135:U:O4	2.51	0.44
33:a:1400:U:H2'	33:a:1401:G:C8	2.52	0.44
39:g:13:LEU:HD22	39:g:21:LYS:HE3	2.00	0.44
40:h:113:LEU:HD22	40:h:117:GLU:HB3	2.00	0.44
42:j:61:SER:O	42:j:61:SER:OG	2.35	0.44
46:n:7:ILE:HD11	46:n:28:GLY:HA3	2.00	0.44
1:A:20:C:H2'	1:A:21:A:H8	1.83	0.44
1:A:334:G:O6	1:A:393:U:O4	2.36	0.44
1:A:633:U:P	10:L:16:ARG:HH22	2.41	0.44
1:A:1909:U:H2'	1:A:1910:G:H8	1.83	0.44
1:A:2376:C:HO2'	26:l:17:TYR:HH	1.60	0.44
1:A:2572:G:H2'	1:A:2573:G:C8	2.53	0.44
6:F:53:ALA:HA	6:F:56:GLU:HB3	1.99	0.44
23:Y:5:GLU:HG2	23:Y:53:MET:HE3	2.00	0.44
33:a:19:U:H2'	33:a:20:C:C6	2.53	0.44
33:a:551:U:H2'	33:a:552:G:C8	2.53	0.44
33:a:1227:C:H2'	33:a:1228:U:C6	2.53	0.44
40:h:24:LYS:HA	40:h:62:VAL:O	2.18	0.44
1:A:199:A:H61	1:A:878:G:H21	1.66	0.43
1:A:1053:C:H5''	1:A:1054:A:H2'	1.98	0.43
3:C:14:ARG:HD3	3:C:14:ARG:HA	1.79	0.43
8:J:78:HIS:HA	8:J:85:LEU:HA	1.99	0.43
33:a:1142:C:H2'	33:a:1143:A:C8	2.52	0.43
38:f:7:MET:HE2	38:f:89:ILE:HD11	2.00	0.43
43:k:76:SER:O	43:k:80:GLY:HA2	2.18	0.43
1:A:546:G:N1	1:A:549:A:OP2	2.51	0.43
1:A:2853:C:H2'	1:A:2854:A:H8	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:34:LEU:HD23	3:C:63:ARG:HG3	2.00	0.43
17:S:11:ARG:HA	17:S:100:THR:HG23	2.00	0.43
19:U:3:VAL:HG21	19:U:68:VAL:HG12	1.99	0.43
33:a:505:G:N2	33:a:507:A:OP2	2.40	0.43
33:a:551:U:O3'	36:d:14:ARG:NH2	2.50	0.43
33:a:1129:U:H2'	33:a:1130:C:H6	1.83	0.43
45:m:86:TYR:HA	45:m:89:ILE:HD12	2.00	0.43
1:A:1289:U:O2'	10:L:18:ARG:NH2	2.52	0.43
1:A:1403:G:N2	1:A:1406:A:OP2	2.48	0.43
1:A:1991:C:O2'	1:A:1992:C:O5'	2.37	0.43
1:A:2922:U:H2'	1:A:2923:A:C8	2.53	0.43
3:C:49:LEU:HD21	3:C:52:ARG:HA	1.99	0.43
8:J:6:MET:O	15:Q:64:ARG:NH2	2.43	0.43
18:T:58:ASN:OD1	18:T:58:ASN:N	2.51	0.43
24:Z:5:GLU:HG3	24:Z:36:VAL:HG22	1.99	0.43
33:a:681:U:H2'	33:a:682:G:H8	1.83	0.43
33:a:1088:U:H4'	37:e:138:ARG:NH1	2.29	0.43
33:a:1389:U:C5	39:g:4:LYS:HE3	2.52	0.43
35:c:154:GLY:HA3	35:c:195:LEU:HD23	1.99	0.43
37:e:87:GLY:O	37:e:93:ASN:HA	2.18	0.43
39:g:75:VAL:HG12	39:g:86:GLN:HB3	1.99	0.43
43:k:77:ILE:HG22	43:k:77:ILE:O	2.18	0.43
1:A:698:C:HO2'	1:A:699:A:H8	1.65	0.43
1:A:2155:A:N1	1:A:2191:A:O2'	2.35	0.43
1:A:2619:A:H2'	1:A:2620:C:H6	1.82	0.43
1:A:2785:U:OP2	29:4:19:ARG:NE	2.44	0.43
5:E:186:VAL:HG13	5:E:192:LEU:HD13	2.00	0.43
7:G:160:GLY:H	7:G:172:ARG:HH22	1.66	0.43
14:P:35:GLY:C	14:P:37:ARG:N	2.77	0.43
20:V:105:SER:OG	55:V:900:ATP:O3B	2.36	0.43
33:a:1025:G:H2'	33:a:1026:A:C8	2.53	0.43
33:a:1418:C:H2'	33:a:1419:A:C8	2.54	0.43
1:A:1380:U:H1'	18:T:55:ASN:HB3	1.99	0.43
1:A:2130:G:H1	1:A:2217:U:H3	1.67	0.43
1:A:2357:A:H2'	1:A:2358:A:H8	1.80	0.43
29:4:17:ILE:HD12	29:4:26:ILE:HD12	2.00	0.43
33:a:1153:G:N2	33:a:1155:A:H62	2.16	0.43
41:i:30:VAL:N	41:i:33:ARG:O	2.49	0.43
1:A:1783:C:H5'	14:P:99:TYR:CZ	2.53	0.43
4:D:6:LEU:HD12	4:D:199:LEU:HD11	2.00	0.43
18:T:32:VAL:O	18:T:77:ARG:NH1	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:170:ILE:O	20:V:180:GLU:HA	2.19	0.43
33:a:267:G:H1	33:a:275:C:H42	1.65	0.43
33:a:727:A:OP2	33:a:729:C:N4	2.40	0.43
33:a:729:C:H2'	33:a:730:A:C8	2.54	0.43
33:a:942:C:H2'	33:a:943:G:C8	2.54	0.43
33:a:995:C:H2'	33:a:996:A:C8	2.54	0.43
33:a:1003:G:O2'	33:a:1004:A:N7	2.50	0.43
1:A:1681:U:H2'	1:A:1682:C:C6	2.54	0.43
1:A:2874:G:O6	1:A:2892:G:C2	2.72	0.43
6:F:35:VAL:HG22	6:F:90:THR:HG22	2.00	0.43
19:U:6:GLY:H	19:U:23:ILE:HB	1.82	0.43
20:V:107:GLY:O	20:V:111:LYS:NZ	2.42	0.43
25:0:33:CYS:N	25:0:46:CYS:SG	2.91	0.43
32:8:117:THR:C	32:8:121:MET:SD	2.98	0.43
33:a:332:G:O2'	33:a:334:G:O6	2.34	0.43
33:a:366:U:H2'	33:a:367:A:C8	2.52	0.43
33:a:694:G:O2'	33:a:695:U:O4'	2.33	0.43
33:a:1385:U:H2'	33:a:1386:A:C8	2.54	0.43
33:a:1524:U:H2'	33:a:1525:C:C6	2.52	0.43
36:d:44:LEU:HB3	36:d:48:GLY:HA3	1.99	0.43
40:h:24:LYS:HD2	40:h:61:ARG:HH11	1.83	0.43
44:l:21:SER:HB2	44:l:108:TYR:CE1	2.53	0.43
52:t:45:ASP:N	52:t:45:ASP:OD1	2.52	0.43
1:A:2838:U:H2'	1:A:2839:C:H6	1.83	0.43
4:D:6:LEU:H	4:D:33:ASN:HD21	1.67	0.43
12:N:34:GLU:HG2	12:N:115:ALA:HB2	2.00	0.43
20:V:319:LYS:NZ	20:V:468:LYS:O	2.45	0.43
33:a:1250:G:H2'	33:a:1251:G:H8	1.84	0.43
34:b:111:ILE:HD12	34:b:111:ILE:HA	1.79	0.43
36:d:20:SER:OG	36:d:22:THR:OG1	2.27	0.43
3:C:160:THR:HB	3:C:177:ASN:ND2	2.34	0.43
7:G:84:PHE:O	7:G:135:LYS:HA	2.19	0.43
9:K:8:LEU:HD22	9:K:82:ASN:HB3	2.00	0.43
17:S:7:ALA:HB3	17:S:103:ILE:H	1.84	0.43
20:V:324:GLY:N	20:V:330:LYS:HD2	2.33	0.43
33:a:246:G:H2'	33:a:247:G:C8	2.54	0.43
35:c:57:GLU:HB2	35:c:64:ASN:HB2	2.00	0.43
52:t:17:ARG:O	52:t:21:ASN:HB2	2.19	0.43
1:A:896:A:H2'	1:A:897:G:C8	2.54	0.43
1:A:1038:C:H2'	1:A:1039:G:H8	1.84	0.43
1:A:2021:G:N2	1:A:2025:C:O2'	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2035:C:O2'	1:A:2848:A:N3	2.52	0.43
4:D:33:ASN:O	4:D:97:VAL:N	2.48	0.43
18:T:52:ASP:HB2	18:T:84:THR:HG22	2.01	0.43
33:a:47:U:H4'	33:a:314:A:H2	1.83	0.43
33:a:683:G:H2'	33:a:684:A:H8	1.83	0.43
33:a:745:U:H2'	33:a:746:C:C6	2.54	0.43
36:d:54:LYS:HE3	36:d:54:LYS:HB3	1.92	0.43
1:A:633:U:H2'	1:A:634:A:C8	2.53	0.42
1:A:953:G:H4'	11:M:28:HIS:CE1	2.54	0.42
1:A:1432:A:N7	18:T:16:ARG:NH2	2.46	0.42
1:A:2463:A:O3'	20:V:261:LYS:NZ	2.41	0.42
14:P:67:GLY:O	14:P:104:ARG:NH1	2.52	0.42
18:T:47:PHE:HZ	23:Y:30:PHE:HE2	1.66	0.42
33:a:561:U:H2'	33:a:562:G:H8	1.84	0.42
36:d:90:LEU:HA	36:d:90:LEU:HD23	1.81	0.42
41:i:88:LEU:HD11	41:i:104:LEU:HD11	2.00	0.42
41:i:114:LYS:HA	41:i:121:ALA:HB2	2.00	0.42
45:m:39:VAL:HG23	45:m:41:GLU:H	1.84	0.42
47:o:71:ARG:NH2	47:o:78:TYR:OH	2.52	0.42
1:A:239:C:H2'	1:A:240:C:H6	1.84	0.42
1:A:697:G:OP1	28:3:19:SER:OG	2.37	0.42
1:A:1823:U:H2'	1:A:1824:C:C6	2.53	0.42
1:A:1828:G:O2'	3:C:182:ARG:NH1	2.52	0.42
1:A:2212:C:H2'	1:A:2213:U:C6	2.53	0.42
13:O:24:GLY:N	13:O:47:ASP:OD2	2.52	0.42
20:V:146:LEU:HD22	20:V:153:VAL:HG21	2.01	0.42
20:V:323:ILE:HD11	20:V:475:VAL:HG22	2.01	0.42
33:a:28:A:N6	33:a:567:G:O2'	2.49	0.42
33:a:1421:C:H2'	33:a:1422:A:C8	2.54	0.42
35:c:198:LYS:HB3	35:c:200:TRP:HZ3	1.84	0.42
36:d:118:HIS:HE1	36:d:142:ARG:HB3	1.83	0.42
37:e:115:LEU:HB3	37:e:123:ILE:HD13	2.02	0.42
1:A:762:A:H2'	1:A:763:A:C8	2.54	0.42
1:A:1532:A:H2'	1:A:1533:A:C8	2.54	0.42
1:A:2728:U:H2'	1:A:2729:C:C6	2.54	0.42
1:A:2818:C:H2'	1:A:2819:A:C8	2.54	0.42
2:B:112:C:H2'	2:B:113:A:C8	2.54	0.42
3:C:246:PRO:HG2	3:C:255:LEU:HD12	2.00	0.42
17:S:41:ARG:O	17:S:44:SER:OG	2.28	0.42
18:T:84:THR:OG1	18:T:87:SER:OG	2.33	0.42
33:a:1025:G:O2'	46:n:15:LYS:NZ	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:m:3:ARG:HH12	45:m:57:ARG:HH21	1.66	0.42
49:q:12:GLY:N	49:q:61:VAL:O	2.42	0.42
1:A:524:A:H2'	1:A:525:A:C8	2.54	0.42
1:A:1995:A:N6	1:A:2631:A:N3	2.63	0.42
1:A:2100:A:H2'	1:A:2101:G:H8	1.83	0.42
1:A:2121:U:N3	1:A:2255:C:OP2	2.38	0.42
1:A:2163:A:H61	1:A:2185:G:H2'	1.84	0.42
1:A:2283:C:H5'	20:V:249:ASP:HB3	2.01	0.42
20:V:210:VAL:HG22	20:V:259:LEU:HD21	2.00	0.42
20:V:389:LEU:HG	53:x:18:G:C8	2.54	0.42
33:a:305:G:N2	33:a:308:A:OP2	2.42	0.42
33:a:495:U:H2'	33:a:496:A:C8	2.52	0.42
33:a:716:U:H2'	33:a:717:G:C8	2.55	0.42
33:a:726:C:H5'	33:a:742:G:H3'	2.02	0.42
33:a:1140:A:H4'	41:i:20:ARG:HH21	1.85	0.42
39:g:20:SER:HB2	39:g:59:MET:HE1	2.01	0.42
41:i:88:LEU:HD11	41:i:104:LEU:HD21	2.02	0.42
1:A:499:G:C8	5:E:58:ARG:HG2	2.55	0.42
1:A:630:A:H5'	5:E:89:VAL:HG21	2.02	0.42
1:A:2392:U:O2	21:W:47:ARG:NH2	2.49	0.42
1:A:2790:A:H2'	1:A:2791:U:C6	2.55	0.42
1:A:2882:G:N2	1:A:2885:A:OP2	2.39	0.42
6:F:129:THR:HG22	6:F:155:VAL:HG22	2.02	0.42
10:L:1:MET:HE3	10:L:6:LEU:HD23	2.02	0.42
12:N:85:SER:O	12:N:89:THR:OG1	2.30	0.42
19:U:24:LEU:HB2	19:U:34:LEU:HD12	2.01	0.42
20:V:485:LEU:HB3	39:g:136:LYS:HE2	2.02	0.42
33:a:272:C:H2'	33:a:273:G:O4'	2.19	0.42
33:a:720:G:H2'	33:a:721:A:C8	2.55	0.42
33:a:786:A:H2'	33:a:787:G:C8	2.54	0.42
39:g:13:LEU:HD13	39:g:21:LYS:HD3	2.02	0.42
45:m:17:ILE:O	45:m:20:THR:OG1	2.26	0.42
53:x:68:U:H2'	53:x:69:C:C6	2.54	0.42
1:A:268:A:O2'	1:A:475:A:N6	2.53	0.42
1:A:353:A:N7	1:A:374:A:N6	2.68	0.42
1:A:840:A:OP2	1:A:2100:A:O2'	2.38	0.42
1:A:1377:G:O2'	1:A:1432:A:N1	2.48	0.42
1:A:1379:U:OP2	18:T:59:TYR:OH	2.37	0.42
1:A:2121:U:O2	1:A:2254:A:O2'	2.37	0.42
1:A:2667:G:OP2	4:D:84:ARG:NH1	2.41	0.42
6:F:140:GLU:HG2	30:6:28:LYS:HE3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:92:GLY:HA3	7:G:95:TYR:CG	2.55	0.42
11:M:58:MET:HE2	11:M:61:GLY:HA2	2.02	0.42
13:O:22:LEU:HD12	13:O:94:VAL:HG12	2.01	0.42
13:O:74:ALA:HA	13:O:77:VAL:HG12	2.02	0.42
20:V:192:ARG:HA	20:V:192:ARG:HD3	1.83	0.42
20:V:299:LYS:HB3	20:V:307:PHE:HD2	1.83	0.42
20:V:449:LEU:HD23	20:V:469:THR:HG21	2.02	0.42
26:1:33:LYS:HA	26:1:43:THR:O	2.19	0.42
33:a:36:C:H2'	33:a:37:G:H8	1.85	0.42
33:a:470:U:H2'	33:a:471:U:C6	2.55	0.42
33:a:767:G:H4'	33:a:890:C:H4'	2.00	0.42
33:a:1069:U:O2'	46:n:45:ARG:NH2	2.52	0.42
33:a:1274:C:H2'	33:a:1275:G:H8	1.84	0.42
34:b:203:ASN:ND2	34:b:205:ASP:OD1	2.52	0.42
1:A:2149:G:H2'	1:A:2150:G:C8	2.54	0.42
1:A:2433:C:H1'	10:L:66:PHE:CZ	2.54	0.42
1:A:2456:C:H5''	1:A:2458:G:H5'	2.02	0.42
1:A:2874:G:O2'	1:A:2891:G:N2	2.53	0.42
1:A:2886:C:H2'	1:A:2887:A:H8	1.84	0.42
8:J:30:SER:HA	8:J:33:VAL:HB	2.02	0.42
15:Q:97:ASP:HA	15:Q:100:VAL:HB	2.00	0.42
33:a:212:G:H2'	33:a:213:G:H8	1.85	0.42
1:A:39:C:O2'	1:A:659:A:N1	2.48	0.42
1:A:161:A:N3	1:A:2237:C:O2'	2.46	0.42
1:A:906:G:N2	1:A:964:A:OP2	2.34	0.42
1:A:950:U:H2'	1:A:951:C:C6	2.55	0.42
1:A:1676:G:N2	1:A:1679:A:OP2	2.45	0.42
5:E:202:VAL:HA	5:E:205:VAL:HG12	2.01	0.42
25:O:30:CYS:SG	25:O:37:LYS:HB2	2.60	0.42
33:a:521:U:H2'	33:a:522:A:C8	2.55	0.42
35:c:53:LYS:NZ	35:c:55:GLU:OE2	2.52	0.42
36:d:17:ILE:HD12	36:d:17:ILE:HA	1.87	0.42
38:f:7:MET:HA	38:f:61:GLN:O	2.19	0.42
1:A:1438:C:OP1	18:T:25:LYS:NZ	2.52	0.42
20:V:36:ILE:HD13	20:V:185:TYR:HE1	1.84	0.42
20:V:286:LYS:HE2	20:V:286:LYS:HB3	1.90	0.42
20:V:286:LYS:HE2	33:a:1344:C:H5	1.85	0.42
26:1:36:CYS:O	26:1:40:LYS:N	2.51	0.42
33:a:14:U:H4'	33:a:535:C:H4'	2.02	0.42
33:a:843:U:H2'	33:a:844:A:C8	2.55	0.42
33:a:1418:C:H2'	33:a:1419:A:H8	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:t:69:LYS:HA	52:t:72:ALA:HB3	2.02	0.42
53:x:55:U:O2'	53:x:57:A:N7	2.46	0.42
1:A:192:G:O6	1:A:208:G:O2'	2.34	0.42
1:A:583:G:OP1	1:A:1041:C:N4	2.53	0.42
1:A:2144:G:N2	1:A:2148:A:OP1	2.53	0.42
1:A:2467:U:O3'	1:A:2468:A:H3'	2.20	0.42
13:O:8:ASN:OD1	13:O:11:ARG:NH2	2.53	0.42
24:Z:6:ILE:HD12	24:Z:37:HIS:HD2	1.84	0.42
28:3:15:LYS:HD2	28:3:23:LYS:HD3	2.01	0.42
33:a:180:G:N1	33:a:208:A:H2'	2.32	0.42
39:g:26:LEU:HD22	39:g:43:LEU:HD12	2.02	0.42
1:A:277:C:H2'	1:A:278:A:H8	1.84	0.41
1:A:499:G:H5'	5:E:79:ARG:HH12	1.85	0.41
1:A:1331:C:H2'	1:A:1332:U:C6	2.55	0.41
1:A:1700:A:H4'	4:D:120:GLN:HA	2.01	0.41
1:A:1977:G:O2'	33:a:1427:A:N1	2.43	0.41
1:A:2664:U:O2'	4:D:82:GLU:OE1	2.36	0.41
4:D:178:LYS:NZ	14:P:11:GLU:OE2	2.39	0.41
32:8:78:PHE:O	32:8:120:MET:CE	2.68	0.41
33:a:193:G:H2'	33:a:194:C:H2'	2.02	0.41
33:a:225:A:O2'	33:a:479:G:N3	2.52	0.41
33:a:409:C:H2'	33:a:410:G:C8	2.55	0.41
33:a:1062:U:O2	33:a:1215:G:O6	2.38	0.41
33:a:1241:U:H5''	41:i:126:GLN:HB2	2.02	0.41
37:e:164:LEU:HD23	37:e:164:LEU:HA	1.85	0.41
1:A:489:G:O4'	5:E:46:GLN:NE2	2.53	0.41
1:A:908:A:N3	2:B:77:G:O2'	2.53	0.41
1:A:1042:A:O2'	15:Q:92:ARG:NH1	2.53	0.41
1:A:1220:G:O6	1:A:1221:A:N6	2.53	0.41
1:A:1673:G:H2'	1:A:1674:G:H8	1.85	0.41
1:A:2129:G:H1	1:A:2218:U:H3	1.66	0.41
1:A:2167:C:H2'	1:A:2168:G:C8	2.54	0.41
1:A:2323:C:H2'	1:A:2324:C:H5'	2.02	0.41
2:B:21:G:H2'	2:B:22:G:C8	2.56	0.41
9:K:35:ILE:HD12	9:K:69:ALA:HB2	2.02	0.41
9:K:119:PRO:HB2	14:P:66:TYR:CZ	2.55	0.41
13:O:35:ARG:NH1	13:O:106:VAL:HG23	2.35	0.41
20:V:297:VAL:O	20:V:309:ASN:N	2.51	0.41
20:V:434:THR:HG21	20:V:465:PHE:CG	2.55	0.41
32:8:33:THR:O	32:8:216:SER:OG	2.30	0.41
32:8:166:ASP:OD1	32:8:170:ASN:N	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:474:A:H2'	33:a:475:A:C8	2.55	0.41
33:a:629:C:C2	36:d:128:ILE:HD13	2.54	0.41
33:a:901:U:H2'	33:a:902:A:H8	1.85	0.41
33:a:1408:C:O2	33:a:1512:A:N6	2.53	0.41
52:t:68:HIS:O	52:t:70:ASN:N	2.54	0.41
1:A:24:G:O2'	17:S:78:GLU:O	2.33	0.41
1:A:191:G:H5'	22:X:14:ALA:HB3	2.02	0.41
1:A:722:A:N3	1:A:2472:C:O2'	2.50	0.41
1:A:1555:A:H2'	1:A:1556:A:C8	2.55	0.41
1:A:2593:A:OP1	1:A:2677:G:O2'	2.35	0.41
1:A:2775:U:H5''	7:G:139:LYS:HB3	2.01	0.41
15:Q:103:LEU:HD13	15:Q:107:ASN:HD21	1.84	0.41
20:V:9:ASN:HA	20:V:22:HIS:HA	2.01	0.41
20:V:328:SER:HB2	20:V:330:LYS:CD	2.49	0.41
20:V:410:GLY:HA3	55:V:901:ATP:O2G	2.20	0.41
33:a:432:G:H2'	33:a:433:A:H8	1.84	0.41
33:a:478:G:H2'	33:a:479:G:C8	2.55	0.41
33:a:1169:G:H22	33:a:1185:A:H2	1.69	0.41
33:a:1184:G:H2'	33:a:1185:A:H8	1.84	0.41
33:a:1277:G:H2'	33:a:1278:A:C8	2.55	0.41
47:o:5:GLN:O	47:o:9:ASN:ND2	2.53	0.41
1:A:1452:C:H2'	1:A:1453:A:H8	1.85	0.41
1:A:1613:C:O2'	1:A:1614:A:H8	2.04	0.41
1:A:1683:C:O3'	1:A:2738:G:N2	2.54	0.41
1:A:2215:U:H2'	1:A:2216:A:C8	2.55	0.41
1:A:2557:U:O4	1:A:2564:G:O6	2.38	0.41
3:C:62:TYR:HA	3:C:86:ASN:ND2	2.35	0.41
5:E:63:LYS:HD2	5:E:76:GLY:HA2	2.03	0.41
23:Y:60:ARG:O	23:Y:63:ALA:HB3	2.20	0.41
33:a:100:G:H2'	33:a:101:C:H6	1.84	0.41
33:a:405:A:N7	33:a:556:A:O2'	2.53	0.41
33:a:518:A:N3	33:a:552:G:O2'	2.52	0.41
33:a:918:A:H2'	33:a:919:A:C8	2.56	0.41
33:a:958:C:H2'	33:a:959:A:H8	1.85	0.41
33:a:1101:U:O2'	33:a:1103:A:N7	2.46	0.41
1:A:1619:A:H2'	1:A:1620:A:C8	2.55	0.41
1:A:2613:U:O2	1:A:2613:U:H2'	2.19	0.41
1:A:2865:U:H5''	12:N:49:THR:HG21	2.02	0.41
5:E:17:ILE:HD12	5:E:125:VAL:HG11	2.02	0.41
14:P:75:PRO:HG2	14:P:78:THR:HG23	2.01	0.41
20:V:383:ARG:NH2	53:x:56:C:O4'	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:26:LYS:HA	22:X:26:LYS:HD3	1.91	0.41
44:l:27:GLY:N	44:l:36:THR:O	2.54	0.41
44:l:112:ARG:HH12	44:l:120:VAL:HG23	1.85	0.41
45:m:80:LEU:HA	45:m:83:ILE:HG12	2.02	0.41
49:q:32:LYS:HA	49:q:39:ARG:HA	2.02	0.41
50:r:17:TYR:O	50:r:20:SER:OG	2.34	0.41
53:x:8:U:H4'	53:x:8:U:OP1	2.20	0.41
1:A:732:A:O2'	1:A:735:U:O4	2.29	0.41
1:A:1483:A:H2'	1:A:1484:U:H6	1.85	0.41
1:A:1532:A:H2'	1:A:1533:A:H8	1.85	0.41
1:A:2361:C:OP1	21:W:84:ARG:NH1	2.53	0.41
1:A:2495:C:H5''	29:4:6:SER:HB3	2.01	0.41
1:A:2630:C:OP1	20:V:247:ARG:NH1	2.53	0.41
3:C:232:HIS:CE1	3:C:247:MET:H	2.39	0.41
16:R:99:LYS:HA	16:R:99:LYS:HD3	1.91	0.41
20:V:67:LYS:NZ	32:8:53:ARG:O	2.43	0.41
33:a:435:C:H2'	33:a:436:G:N2	2.35	0.41
33:a:1351:C:H2'	33:a:1352:G:H8	1.86	0.41
33:a:1463:A:H2'	33:a:1464:G:C8	2.56	0.41
1:A:346:G:H2'	1:A:347:G:C8	2.55	0.41
1:A:490:A:H2'	5:E:45:ARG:HD3	2.02	0.41
1:A:790:A:O2'	1:A:1704:U:OP1	2.31	0.41
1:A:1366:C:O2'	12:N:108:ARG:NH2	2.54	0.41
1:A:1819:C:H2'	1:A:1820:A:C5	2.56	0.41
1:A:2369:A:H2'	1:A:2370:G:C8	2.55	0.41
4:D:29:GLU:HA	4:D:185:LEU:HD23	2.02	0.41
5:E:54:ARG:HE	5:E:80:SER:HA	1.85	0.41
5:E:135:LYS:HG2	5:E:137:LYS:H	1.85	0.41
20:V:94:TRP:NE1	20:V:138:SER:OG	2.53	0.41
32:8:173:VAL:HA	32:8:174:PRO:HD2	1.93	0.41
33:a:1049:G:H2'	33:a:1050:A:C8	2.56	0.41
33:a:1248:A:H62	33:a:1308:A:H61	1.67	0.41
34:b:183:ILE:HG13	34:b:197:ASP:H	1.85	0.41
35:c:148:VAL:HG22	35:c:201:ILE:HG23	2.01	0.41
45:m:5:ALA:HB1	45:m:66:GLU:HB2	2.03	0.41
1:A:1104:U:H2'	1:A:1105:G:C8	2.56	0.41
1:A:2143:A:N3	1:A:2196:U:O2'	2.50	0.41
1:A:2369:A:H2'	1:A:2370:G:H8	1.86	0.41
1:A:2480:A:O2'	20:V:237:PHE:HD1	2.03	0.41
1:A:2619:A:H2'	1:A:2620:C:C6	2.56	0.41
3:C:207:LYS:HB3	3:C:209:GLY:H	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:245:SER:O	3:C:247:MET:HG3	2.21	0.41
12:N:99:THR:HA	12:N:118:GLU:O	2.21	0.41
20:V:280:SER:HA	20:V:448:THR:HG21	2.02	0.41
28:3:16:LYS:HB2	28:3:16:LYS:HE3	1.91	0.41
33:a:720:G:H2'	33:a:721:A:H8	1.85	0.41
33:a:1298:A:H5''	33:a:1299:U:H5	1.86	0.41
33:a:1351:C:H2'	33:a:1352:G:C8	2.56	0.41
1:A:527:A:O2'	19:U:42:LYS:O	2.39	0.41
1:A:1151:U:H2'	1:A:1152:G:H8	1.84	0.41
1:A:1711:G:O2'	9:K:6:THR:HG22	2.21	0.41
1:A:1712:G:N2	1:A:2021:G:OP2	2.38	0.41
1:A:1828:G:OP1	3:C:260:ARG:NE	2.47	0.41
1:A:2688:G:O2'	1:A:2690:G:N7	2.45	0.41
3:C:53:HIS:CE1	3:C:219:THR:HA	2.55	0.41
4:D:88:MET:HE2	4:D:88:MET:HB3	1.99	0.41
6:F:101:ASP:HB3	30:6:22:PHE:HE2	1.86	0.41
18:T:43:VAL:HG11	18:T:81:VAL:HG11	2.03	0.41
20:V:317:GLY:HA2	20:V:454:GLY:HA3	2.03	0.41
30:6:47:GLN:H	30:6:47:GLN:HG2	1.68	0.41
33:a:551:U:H2'	33:a:552:G:H8	1.86	0.41
33:a:675:G:H5'	33:a:735:C:H1'	2.03	0.41
33:a:676:G:O2'	47:o:49:ASP:OD1	2.28	0.41
33:a:825:A:OP1	33:a:1536:G:O2'	2.29	0.41
33:a:996:A:H2'	33:a:997:G:C8	2.56	0.41
33:a:1030:G:H2'	33:a:1031:A:C8	2.56	0.41
33:a:1114:G:O3'	34:b:110:ARG:NH1	2.54	0.41
33:a:1510:A:H5''	33:a:1518:G:H5''	2.03	0.41
35:c:63:VAL:HG23	35:c:96:LYS:HE3	2.03	0.41
35:c:68:HIS:HB3	35:c:105:ILE:HD11	2.03	0.41
38:f:71:ALA:HA	38:f:74:GLU:HB2	2.03	0.41
43:k:18:ILE:HG13	43:k:80:GLY:O	2.20	0.41
47:o:12:ILE:HG22	47:o:16:LYS:HE3	2.02	0.41
51:s:25:THR:OG1	51:s:26:ASP:N	2.54	0.41
1:A:1380:U:OP2	1:A:1433:U:O2'	2.25	0.41
1:A:2042:A:H2	17:S:88:ARG:HH22	1.69	0.41
20:V:38:LYS:NZ	20:V:441:SER:OG	2.54	0.41
33:a:1356:G:O2'	33:a:1382:G:O6	2.32	0.41
34:b:95:ARG:HG2	34:b:147:PHE:CD1	2.55	0.41
39:g:12:VAL:HG12	39:g:14:PRO:HD2	2.02	0.41
1:A:13:A:O2'	1:A:15:G:N7	2.47	0.40
1:A:38:A:H2'	1:A:39:C:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:894:A:N6	1:A:980:C:N3	2.69	0.40
1:A:1158:G:H1'	1:A:1159:U:H5'	2.03	0.40
1:A:1515:C:H2'	1:A:1569:A:N6	2.36	0.40
1:A:1918:A:H2'	1:A:1919:A:C8	2.56	0.40
1:A:2028:C:OP1	4:D:124:LYS:NZ	2.36	0.40
1:A:2213:U:H2'	1:A:2214:G:C8	2.56	0.40
6:F:42:ASP:O	6:F:46:ASN:N	2.45	0.40
17:S:50:VAL:HG11	17:S:103:ILE:HG22	2.02	0.40
18:T:21:MET:HG2	18:T:26:TYR:CD1	2.56	0.40
20:V:191:PHE:CZ	20:V:195:LYS:HD2	2.56	0.40
25:O:43:CYS:HB3	25:O:46:CYS:HB2	2.03	0.40
33:a:745:U:OP1	50:r:66:ARG:NH2	2.38	0.40
33:a:960:U:H2'	33:a:961:G:H8	1.86	0.40
33:a:1105:U:P	33:a:1118:G:H1	2.44	0.40
34:b:18:HIS:HB3	34:b:19:GLN:H	1.66	0.40
35:c:6:ASN:HA	35:c:7:PRO:HD3	1.96	0.40
48:p:7:LEU:HB3	48:p:18:TYR:HB3	2.03	0.40
49:q:64:MET:HB3	49:q:76:ARG:NE	2.30	0.40
1:A:881:U:H2'	1:A:882:A:C8	2.56	0.40
1:A:1615:A:H3'	3:C:85:PRO:HG3	2.02	0.40
1:A:1715:C:O2	4:D:135:HIS:NE2	2.47	0.40
1:A:2626:G:H2'	1:A:2627:A:C8	2.56	0.40
1:A:2873:G:O2'	1:A:2893:A:N6	2.54	0.40
13:O:77:VAL:HG13	13:O:109:LEU:HD21	2.04	0.40
15:Q:88:ILE:HD12	15:Q:88:ILE:HG23	1.87	0.40
20:V:35:ILE:N	20:V:155:LEU:O	2.42	0.40
25:O:27:MET:HA	25:O:37:LYS:O	2.21	0.40
33:a:522:A:H2'	33:a:523:C:C6	2.56	0.40
33:a:746:C:H2'	33:a:747:U:C6	2.57	0.40
33:a:1436:C:H2'	33:a:1437:A:C8	2.56	0.40
40:h:41:LYS:HD3	40:h:48:ASP:HA	2.02	0.40
43:k:27:SER:HA	43:k:32:THR:HA	2.02	0.40
45:m:17:ILE:HA	45:m:20:THR:HG23	2.03	0.40
1:A:372:U:H4'	19:U:64:HIS:CG	2.56	0.40
1:A:1515:C:H2'	1:A:1569:A:H61	1.86	0.40
1:A:1742:G:H4'	1:A:2007:A:H5''	2.02	0.40
1:A:1848:A:H5''	3:C:160:THR:HG21	2.03	0.40
1:A:2037:C:H2'	1:A:2038:G:H8	1.85	0.40
1:A:2262:A:H2'	1:A:2263:G:C8	2.57	0.40
1:A:2335:U:H5''	1:A:2336:G:H5''	2.04	0.40
1:A:2457:G:N2	10:L:54:GLN:HE21	2.19	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:57:LEU:HA	6:F:60:ILE:HB	2.03	0.40
30:6:59:PHE:O	30:6:61:LYS:N	2.54	0.40
32:8:121:MET:HG3	32:8:145:VAL:HG11	2.02	0.40
33:a:561:U:H2'	33:a:562:G:C8	2.56	0.40
33:a:1166:A:N6	33:a:1187:G:H1'	2.36	0.40
33:a:1170:C:H2'	33:a:1171:C:H6	1.86	0.40
33:a:1253:C:H2'	33:a:1254:A:C8	2.57	0.40
33:a:1253:C:H2'	33:a:1254:A:H8	1.86	0.40
1:A:888:A:H2'	1:A:889:A:C8	2.57	0.40
1:A:906:G:O2'	1:A:963:G:O6	2.37	0.40
1:A:2780:G:C4	7:G:2:SER:HA	2.57	0.40
3:C:96:TYR:HE2	3:C:102:ARG:HD2	1.87	0.40
3:C:110:ILE:HD11	3:C:116:ILE:HD11	2.04	0.40
5:E:126:LEU:HD13	5:E:129:LEU:HD21	2.03	0.40
5:E:129:LEU:HD23	5:E:129:LEU:HA	1.91	0.40
6:F:133:LYS:HG2	6:F:134:GLU:HG3	2.04	0.40
8:J:57:ILE:HD12	8:J:125:VAL:HG22	2.03	0.40
11:M:68:ILE:HD13	11:M:103:LEU:HD22	2.03	0.40
33:a:79:G:H2'	33:a:80:G:C8	2.57	0.40
33:a:98:U:H1'	33:a:99:A:H2	1.87	0.40
33:a:409:C:H2'	33:a:410:G:H8	1.85	0.40
34:b:132:LYS:O	34:b:136:GLN:HB3	2.20	0.40
44:l:59:ASN:ND2	44:l:102:ASP:OD2	2.54	0.40
1:A:605:G:H1'	15:Q:48:ARG:HH22	1.86	0.40
1:A:726:C:H2'	1:A:727:A:C8	2.56	0.40
1:A:1138:C:H2'	1:A:1139:G:C8	2.56	0.40
1:A:1391:U:H1'	1:A:1618:A:H2	1.86	0.40
1:A:1923:C:H4'	20:V:194:LYS:HD2	2.03	0.40
1:A:1924:C:OP2	20:V:201:ARG:NH1	2.44	0.40
1:A:2076:C:H2'	1:A:2077:G:C8	2.55	0.40
1:A:2274:U:H5''	1:A:2275:G:H5'	2.03	0.40
1:A:2874:G:O6	1:A:2892:G:N3	2.55	0.40
11:M:56:ARG:HH11	11:M:56:ARG:HD2	1.70	0.40
19:U:38:VAL:HG12	19:U:63:ILE:HD12	2.04	0.40
33:a:1108:C:OP2	34:b:143:ARG:NH1	2.53	0.40
37:e:14:ARG:NH2	37:e:116:GLU:OE1	2.42	0.40
37:e:157:ARG:HD2	37:e:164:LEU:HD11	2.03	0.40
47:o:48:LYS:HA	47:o:48:LYS:HD3	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	270/277 (98%)	253 (94%)	17 (6%)	0	100	100
4	D	204/209 (98%)	195 (96%)	9 (4%)	0	100	100
5	E	203/207 (98%)	187 (92%)	16 (8%)	0	100	100
6	F	174/179 (97%)	159 (91%)	15 (9%)	0	100	100
7	G	173/179 (97%)	153 (88%)	20 (12%)	0	100	100
8	J	140/145 (97%)	129 (92%)	9 (6%)	2 (1%)	9	38
9	K	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
10	L	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
11	M	133/144 (92%)	125 (94%)	8 (6%)	0	100	100
12	N	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
13	O	118/120 (98%)	107 (91%)	11 (9%)	0	100	100
14	P	113/115 (98%)	105 (93%)	8 (7%)	0	100	100
15	Q	115/119 (97%)	107 (93%)	6 (5%)	2 (2%)	7	35
16	R	99/102 (97%)	83 (84%)	15 (15%)	1 (1%)	12	44
17	S	107/113 (95%)	92 (86%)	13 (12%)	2 (2%)	6	33
18	T	88/95 (93%)	84 (96%)	4 (4%)	0	100	100
19	U	99/103 (96%)	86 (87%)	13 (13%)	0	100	100
20	V	539/548 (98%)	464 (86%)	73 (14%)	2 (0%)	30	62
21	W	80/94 (85%)	71 (89%)	9 (11%)	0	100	100
22	X	56/62 (90%)	46 (82%)	10 (18%)	0	100	100
23	Y	63/66 (96%)	60 (95%)	3 (5%)	0	100	100
24	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
25	0	52/59 (88%)	49 (94%)	2 (4%)	1 (2%)	6	33
26	1	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
27	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	3	62/66 (94%)	60 (97%)	2 (3%)	0	100	100
29	4	35/37 (95%)	32 (91%)	3 (9%)	0	100	100
30	6	61/66 (92%)	53 (87%)	8 (13%)	0	100	100
32	8	210/232 (90%)	192 (91%)	18 (9%)	0	100	100
34	b	216/246 (88%)	188 (87%)	24 (11%)	4 (2%)	6	33
35	c	204/218 (94%)	185 (91%)	19 (9%)	0	100	100
36	d	193/200 (96%)	173 (90%)	18 (9%)	2 (1%)	12	44
37	e	162/166 (98%)	150 (93%)	12 (7%)	0	100	100
38	f	90/95 (95%)	83 (92%)	7 (8%)	0	100	100
39	g	147/156 (94%)	136 (92%)	11 (8%)	0	100	100
40	h	129/132 (98%)	107 (83%)	20 (16%)	2 (2%)	7	36
41	i	123/130 (95%)	104 (85%)	18 (15%)	1 (1%)	16	49
42	j	93/102 (91%)	83 (89%)	9 (10%)	1 (1%)	11	43
43	k	112/131 (86%)	100 (89%)	12 (11%)	0	100	100
44	l	134/138 (97%)	117 (87%)	16 (12%)	1 (1%)	18	51
45	m	106/121 (88%)	94 (89%)	11 (10%)	1 (1%)	14	47
46	n	58/61 (95%)	46 (79%)	11 (19%)	1 (2%)	7	35
47	o	83/89 (93%)	79 (95%)	3 (4%)	1 (1%)	10	41
48	p	86/90 (96%)	76 (88%)	7 (8%)	3 (4%)	3	23
49	q	82/87 (94%)	77 (94%)	5 (6%)	0	100	100
50	r	62/79 (78%)	57 (92%)	5 (8%)	0	100	100
51	s	76/92 (83%)	66 (87%)	10 (13%)	0	100	100
52	t	81/88 (92%)	76 (94%)	3 (4%)	2 (2%)	4	28
All	All	5956/6298 (95%)	5382 (90%)	545 (9%)	29 (0%)	26	57

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	133	HIS
15	Q	93	LYS
17	S	40	PRO
20	V	280	SER
34	b	18	HIS
34	b	19	GLN

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Mol	Chain	Res	Type
36	d	32	ALA
40	h	99	ASN
48	p	47	ALA
52	t	69	LYS
8	J	132	PRO
15	Q	92	ARG
34	b	67	ILE
36	d	33	PRO
40	h	4	THR
46	n	32	SER
34	b	66	LYS
45	m	105	ASN
17	S	39	THR
25	0	51	GLY
44	l	135	PRO
48	p	48	GLU
52	t	68	HIS
16	R	50	ASN
41	i	125	PRO
48	p	46	PRO
20	V	281	ILE
42	j	79	PRO
47	o	25	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	220/225 (98%)	220 (100%)	0	100	100
4	D	167/170 (98%)	165 (99%)	2 (1%)	63	73
5	E	169/170 (99%)	167 (99%)	2 (1%)	63	73
6	F	151/154 (98%)	149 (99%)	2 (1%)	61	72
7	G	148/151 (98%)	147 (99%)	1 (1%)	76	78
8	J	120/123 (98%)	117 (98%)	3 (2%)	42	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	K	101/101 (100%)	100 (99%)	1 (1%)	68	75
10	L	110/110 (100%)	109 (99%)	1 (1%)	70	76
11	M	109/116 (94%)	107 (98%)	2 (2%)	51	69
12	N	99/100 (99%)	98 (99%)	1 (1%)	68	75
13	O	93/93 (100%)	93 (100%)	0	100	100
14	P	100/100 (100%)	100 (100%)	0	100	100
15	Q	96/98 (98%)	96 (100%)	0	100	100
16	R	83/84 (99%)	82 (99%)	1 (1%)	63	73
17	S	90/93 (97%)	87 (97%)	3 (3%)	33	58
18	T	81/85 (95%)	81 (100%)	0	100	100
19	U	85/87 (98%)	85 (100%)	0	100	100
20	V	424/431 (98%)	419 (99%)	5 (1%)	63	73
21	W	64/74 (86%)	64 (100%)	0	100	100
22	X	47/50 (94%)	47 (100%)	0	100	100
23	Y	56/57 (98%)	56 (100%)	0	100	100
24	Z	52/53 (98%)	52 (100%)	0	100	100
25	0	48/53 (91%)	46 (96%)	2 (4%)	26	52
26	1	46/47 (98%)	46 (100%)	0	100	100
27	2	39/39 (100%)	39 (100%)	0	100	100
28	3	54/56 (96%)	52 (96%)	2 (4%)	30	56
29	4	35/35 (100%)	35 (100%)	0	100	100
30	6	53/55 (96%)	53 (100%)	0	100	100
32	8	169/185 (91%)	168 (99%)	1 (1%)	78	79
34	b	189/212 (89%)	187 (99%)	2 (1%)	65	74
35	c	168/178 (94%)	167 (99%)	1 (1%)	78	79
36	d	169/173 (98%)	165 (98%)	4 (2%)	43	64
37	e	128/130 (98%)	125 (98%)	3 (2%)	44	64
38	f	81/84 (96%)	80 (99%)	1 (1%)	63	73
39	g	125/132 (95%)	125 (100%)	0	100	100
40	h	111/112 (99%)	111 (100%)	0	100	100
41	i	98/102 (96%)	97 (99%)	1 (1%)	68	75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	j	86/92 (94%)	85 (99%)	1 (1%)	63	73
43	k	86/100 (86%)	84 (98%)	2 (2%)	44	64
44	l	114/116 (98%)	114 (100%)	0	100	100
45	m	94/104 (90%)	94 (100%)	0	100	100
46	n	53/54 (98%)	53 (100%)	0	100	100
47	o	80/83 (96%)	80 (100%)	0	100	100
48	p	74/76 (97%)	74 (100%)	0	100	100
49	q	77/80 (96%)	77 (100%)	0	100	100
50	r	56/64 (88%)	56 (100%)	0	100	100
51	s	70/81 (86%)	70 (100%)	0	100	100
52	t	66/70 (94%)	66 (100%)	0	100	100
All	All	5034/5238 (96%)	4990 (99%)	44 (1%)	68	76

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	108	VAL
4	D	199	LEU
5	E	192	LEU
5	E	194	ILE
6	F	4	LEU
6	F	136	LEU
7	G	108	VAL
8	J	26	LEU
8	J	49	VAL
8	J	123	LEU
9	K	19	VAL
10	L	4	HIS
11	M	27	VAL
11	M	94	VAL
12	N	117	ILE
16	R	48	VAL
17	S	29	VAL
17	S	46	ILE
17	S	104	THR
20	V	14	VAL
20	V	326	ASN
20	V	365	LEU

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Mol	Chain	Res	Type
20	V	389	LEU
20	V	393	LEU
25	0	22	LEU
25	0	38	LEU
28	3	32	LEU
28	3	62	LEU
32	8	121	MET
34	b	179	LEU
34	b	199	VAL
35	c	71	LYS
36	d	22	THR
36	d	26	LEU
36	d	150	ILE
36	d	172	LEU
37	e	36	LEU
37	e	46	VAL
37	e	95	LEU
38	f	85	ILE
41	i	65	VAL
42	j	25	ILE
43	k	25	ILE
43	k	52	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (101) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	86	ASN
3	C	177	ASN
3	C	232	HIS
4	D	33	ASN
4	D	126	HIS
5	E	10	ASN
5	E	29	ASN
5	E	46	GLN
5	E	188	ASN
6	F	45	GLN
6	F	127	ASN
6	F	135	GLN
6	F	172	GLN
8	J	54	HIS
8	J	81	HIS
8	J	118	GLN

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Mol	Chain	Res	Type
9	K	4	GLN
10	L	54	GLN
10	L	78	ASN
10	L	126	ASN
11	M	13	HIS
12	N	27	ASN
12	N	61	GLN
12	N	68	ASN
13	O	15	HIS
13	O	37	ASN
14	P	36	ASN
15	Q	29	HIS
15	Q	37	GLN
15	Q	66	ASN
16	R	83	HIS
19	U	2	HIS
19	U	59	GLN
19	U	64	HIS
20	V	73	GLN
20	V	102	HIS
20	V	140	GLN
20	V	158	HIS
20	V	230	GLN
20	V	296	ASN
20	V	309	ASN
20	V	360	GLN
20	V	388	ASN
20	V	406	HIS
20	V	435	ASN
20	V	436	HIS
20	V	461	HIS
21	W	37	GLN
22	X	17	ASN
22	X	23	ASN
23	Y	31	GLN
24	Z	52	HIS
24	Z	59	GLN
25	0	40	HIS
25	0	50	ASN
26	1	22	ASN
26	1	26	ASN
29	4	36	GLN

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Mol	Chain	Res	Type
30	6	60	ASN
32	8	67	ASN
32	8	106	GLN
32	8	188	ASN
34	b	18	HIS
34	b	24	ASN
34	b	36	ASN
34	b	93	ASN
34	b	123	ASN
34	b	136	GLN
34	b	203	ASN
35	c	113	GLN
35	c	136	GLN
36	d	85	ASN
36	d	96	ASN
36	d	112	GLN
36	d	116	HIS
36	d	118	HIS
37	e	83	HIS
38	f	33	ASN
38	f	88	HIS
39	g	19	ASN
39	g	84	ASN
39	g	142	HIS
40	h	22	HIS
40	h	57	GLN
41	i	38	HIS
41	i	81	HIS
41	i	126	GLN
44	l	42	GLN
44	l	59	ASN
44	l	85	HIS
44	l	90	HIS
44	l	109	HIS
45	m	105	ASN
46	n	10	GLN
47	o	5	GLN
47	o	28	GLN
47	o	46	HIS
47	o	51	HIS
47	o	83	ASN
50	r	25	HIS

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Mol	Chain	Res	Type
52	t	84	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2928 (98%)	864 (30%)	90 (3%)
2	B	111/112 (99%)	40 (36%)	3 (2%)
31	7	2/3 (66%)	0	0
33	a	1532/1554 (98%)	412 (26%)	0
53	x	73/75 (97%)	29 (39%)	0
All	All	4597/4672 (98%)	1345 (29%)	93 (2%)

All (1345) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	U
1	A	10	A
1	A	13	A
1	A	18	C
1	A	26	G
1	A	34	U
1	A	35	G
1	A	36	G
1	A	45	G
1	A	46	C
1	A	55	G
1	A	60	G
1	A	61	A
1	A	62	C
1	A	63	G
1	A	64	A
1	A	65	A
1	A	66	C
1	A	71	A
1	A	74	U
1	A	75	G
1	A	76	C
1	A	77	U
1	A	78	U
1	A	79	C

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Mol	Chain	Res	Type
1	A	83	G
1	A	84	A
1	A	85	G
1	A	86	C
1	A	87	U
1	A	89	U
1	A	90	A
1	A	92	G
1	A	93	C
1	A	96	G
1	A	99	U
1	A	100	U
1	A	101	G
1	A	117	A
1	A	118	A
1	A	119	U
1	A	124	A
1	A	125	A
1	A	126	A
1	A	127	C
1	A	134	C
1	A	141	U
1	A	156	A
1	A	162	A
1	A	163	U
1	A	164	U
1	A	167	U
1	A	174	U
1	A	175	G
1	A	176	A
1	A	177	G
1	A	178	A
1	A	179	A
1	A	182	C
1	A	187	C
1	A	188	C
1	A	196	U
1	A	199	A
1	A	202	A
1	A	207	A
1	A	216	A
1	A	218	G

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Mol	Chain	Res	Type
1	A	219	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	229	A
1	A	231	A
1	A	232	U
1	A	233	G
1	A	234	C
1	A	236	A
1	A	237	U
1	A	244	A
1	A	247	A
1	A	248	G
1	A	251	G
1	A	252	C
1	A	253	G
1	A	255	G
1	A	258	A
1	A	266	U
1	A	267	C
1	A	268	A
1	A	269	G
1	A	270	C
1	A	272	C
1	A	275	A
1	A	282	G
1	A	283	G
1	A	284	C
1	A	285	U
1	A	286	U
1	A	290	U
1	A	291	C
1	A	298	U
1	A	299	U
1	A	301	U
1	A	302	A
1	A	308	C
1	A	309	U
1	A	310	C
1	A	337	A
1	A	345	A

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Mol	Chain	Res	Type
1	A	346	G
1	A	348	U
1	A	349	C
1	A	352	G
1	A	354	A
1	A	360	C
1	A	361	G
1	A	366	A
1	A	367	G
1	A	373	A
1	A	374	A
1	A	375	C
1	A	382	G
1	A	389	A
1	A	395	C
1	A	396	G
1	A	398	U
1	A	409	U
1	A	411	G
1	A	412	A
1	A	418	A
1	A	419	G
1	A	420	U
1	A	421	A
1	A	430	C
1	A	433	G
1	A	434	U
1	A	436	A
1	A	442	C
1	A	444	U
1	A	445	C
1	A	453	G
1	A	458	G
1	A	459	A
1	A	469	A
1	A	471	G
1	A	482	C
1	A	483	C
1	A	489	G
1	A	490	A
1	A	494	A
1	A	498	U

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Mol	Chain	Res	Type
1	A	502	C
1	A	503	C
1	A	504	A
1	A	506	U
1	A	508	C
1	A	511	U
1	A	524	A
1	A	526	A
1	A	527	A
1	A	528	G
1	A	529	C
1	A	548	A
1	A	550	G
1	A	551	A
1	A	552	G
1	A	554	U
1	A	555	C
1	A	556	C
1	A	558	G
1	A	568	G
1	A	573	C
1	A	575	A
1	A	577	U
1	A	578	A
1	A	583	G
1	A	584	A
1	A	590	U
1	A	591	U
1	A	592	A
1	A	593	A
1	A	594	C
1	A	595	G
1	A	599	G
1	A	607	G
1	A	613	U
1	A	617	G
1	A	618	A
1	A	619	A
1	A	622	A
1	A	630	A
1	A	632	U
1	A	646	A

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Mol	Chain	Res	Type
1	A	647	A
1	A	648	G
1	A	649	G
1	A	655	C
1	A	658	A
1	A	659	A
1	A	662	U
1	A	667	A
1	A	668	G
1	A	673	A
1	A	680	G
1	A	683	A
1	A	686	C
1	A	689	A
1	A	690	A
1	A	691	U
1	A	698	C
1	A	699	A
1	A	700	U
1	A	701	G
1	A	702	A
1	A	703	G
1	A	715	A
1	A	716	G
1	A	717	A
1	A	718	C
1	A	733	U
1	A	741	U
1	A	749	G
1	A	764	C
1	A	765	A
1	A	766	C
1	A	777	C
1	A	787	C
1	A	788	G
1	A	790	A
1	A	794	U
1	A	804	G
1	A	810	G
1	A	811	A
1	A	812	G
1	A	822	G

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Mol	Chain	Res	Type
1	A	823	G
1	A	824	G
1	A	829	A
1	A	830	A
1	A	831	U
1	A	832	G
1	A	837	U
1	A	839	G
1	A	847	A
1	A	852	G
1	A	853	C
1	A	858	U
1	A	859	C
1	A	866	A
1	A	874	U
1	A	875	U
1	A	878	G
1	A	890	G
1	A	891	G
1	A	892	U
1	A	893	A
1	A	906	G
1	A	908	A
1	A	913	A
1	A	914	C
1	A	916	G
1	A	919	U
1	A	923	C
1	A	928	G
1	A	929	G
1	A	931	C
1	A	933	C
1	A	934	U
1	A	935	A
1	A	936	C
1	A	937	C
1	A	939	G
1	A	940	G
1	A	941	U
1	A	942	U
1	A	943	A
1	A	944	C

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Mol	Chain	Res	Type
1	A	948	A
1	A	953	G
1	A	954	U
1	A	957	A
1	A	958	A
1	A	959	C
1	A	962	C
1	A	964	A
1	A	970	A
1	A	973	G
1	A	975	C
1	A	977	U
1	A	980	C
1	A	987	A
1	A	992	G
1	A	999	A
1	A	1003	A
1	A	1006	A
1	A	1007	G
1	A	1019	A
1	A	1020	A
1	A	1026	A
1	A	1029	A
1	A	1031	C
1	A	1036	A
1	A	1037	C
1	A	1042	A
1	A	1051	C
1	A	1054	A
1	A	1055	A
1	A	1058	U
1	A	1059	A
1	A	1067	A
1	A	1068	G
1	A	1069	U
1	A	1070	G
1	A	1071	G
1	A	1072	A
1	A	1073	A
1	A	1079	U
1	A	1086	U
1	A	1091	U

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Mol	Chain	Res	Type
1	A	1101	G
1	A	1102	G
1	A	1103	A
1	A	1106	U
1	A	1110	C
1	A	1111	U
1	A	1116	A
1	A	1117	G
1	A	1118	C
1	A	1119	A
1	A	1120	G
1	A	1121	C
1	A	1122	C
1	A	1123	A
1	A	1124	C
1	A	1125	C
1	A	1127	U
1	A	1128	U
1	A	1134	A
1	A	1142	A
1	A	1143	U
1	A	1145	G
1	A	1146	C
1	A	1157	A
1	A	1158	G
1	A	1159	U
1	A	1160	G
1	A	1161	A
1	A	1173	A
1	A	1174	A
1	A	1176	U
1	A	1178	U
1	A	1179	A
1	A	1180	C
1	A	1181	C
1	A	1182	G
1	A	1185	G
1	A	1188	A
1	A	1197	A
1	A	1201	A
1	A	1203	G
1	A	1210	A

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Mol	Chain	Res	Type
1	A	1221	A
1	A	1226	U
1	A	1227	G
1	A	1235	A
1	A	1236	G
1	A	1244	A
1	A	1245	G
1	A	1248	C
1	A	1249	U
1	A	1250	G
1	A	1251	U
1	A	1252	G
1	A	1259	G
1	A	1260	A
1	A	1261	C
1	A	1270	C
1	A	1276	G
1	A	1278	G
1	A	1280	G
1	A	1281	C
1	A	1282	U
1	A	1290	G
1	A	1293	A
1	A	1294	A
1	A	1295	U
1	A	1296	G
1	A	1306	G
1	A	1307	U
1	A	1311	G
1	A	1312	A
1	A	1313	A
1	A	1314	A
1	A	1315	G
1	A	1323	A
1	A	1325	A
1	A	1326	A
1	A	1330	C
1	A	1333	C
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1343	C

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Mol	Chain	Res	Type
1	A	1344	C
1	A	1346	A
1	A	1351	U
1	A	1352	U
1	A	1354	C
1	A	1362	G
1	A	1363	G
1	A	1364	C
1	A	1365	U
1	A	1366	C
1	A	1368	U
1	A	1369	C
1	A	1370	C
1	A	1371	G
1	A	1372	C
1	A	1375	A
1	A	1376	G
1	A	1384	C
1	A	1385	G
1	A	1388	A
1	A	1389	C
1	A	1391	U
1	A	1404	A
1	A	1417	A
1	A	1418	U
1	A	1422	C
1	A	1423	A
1	A	1424	A
1	A	1425	C
1	A	1426	A
1	A	1435	U
1	A	1436	U
1	A	1442	A
1	A	1443	C
1	A	1448	U
1	A	1449	C
1	A	1451	U
1	A	1457	U
1	A	1459	U
1	A	1460	G
1	A	1464	A
1	A	1465	A

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Mol	Chain	Res	Type
1	A	1467	G
1	A	1472	G
1	A	1473	A
1	A	1475	G
1	A	1481	G
1	A	1487	G
1	A	1489	U
1	A	1490	A
1	A	1499	A
1	A	1500	U
1	A	1502	G
1	A	1506	A
1	A	1507	U
1	A	1508	C
1	A	1516	A
1	A	1522	U
1	A	1525	G
1	A	1526	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1530	G
1	A	1531	G
1	A	1532	A
1	A	1536	A
1	A	1539	C
1	A	1540	A
1	A	1542	A
1	A	1543	U
1	A	1544	C
1	A	1545	C
1	A	1549	U
1	A	1550	C
1	A	1551	C
1	A	1553	A
1	A	1556	A
1	A	1557	G
1	A	1558	G
1	A	1559	C
1	A	1560	U
1	A	1561	G
1	A	1562	A

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Mol	Chain	Res	Type
1	A	1563	G
1	A	1566	G
1	A	1568	G
1	A	1569	A
1	A	1570	U
1	A	1571	G
1	A	1573	C
1	A	1602	U
1	A	1606	A
1	A	1607	C
1	A	1608	A
1	A	1613	C
1	A	1617	A
1	A	1626	U
1	A	1628	G
1	A	1631	A
1	A	1632	G
1	A	1645	C
1	A	1653	A
1	A	1655	A
1	A	1657	C
1	A	1658	G
1	A	1661	A
1	A	1672	A
1	A	1679	A
1	A	1680	A
1	A	1691	A
1	A	1692	U
1	A	1693	C
1	A	1694	G
1	A	1696	G
1	A	1697	A
1	A	1699	A
1	A	1700	A
1	A	1708	U
1	A	1709	A
1	A	1712	G
1	A	1717	C
1	A	1719	G
1	A	1720	C
1	A	1727	A
1	A	1738	U

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Mol	Chain	Res	Type
1	A	1740	G
1	A	1745	A
1	A	1746	A
1	A	1748	G
1	A	1750	G
1	A	1752	G
1	A	1753	C
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1762	G
1	A	1766	C
1	A	1768	A
1	A	1771	C
1	A	1776	A
1	A	1777	G
1	A	1778	A
1	A	1779	G
1	A	1781	C
1	A	1782	G
1	A	1783	C
1	A	1785	G
1	A	1789	A
1	A	1790	U
1	A	1792	G
1	A	1793	G
1	A	1797	A
1	A	1802	A
1	A	1810	G
1	A	1811	C
1	A	1812	A
1	A	1813	A
1	A	1814	A
1	A	1815	A
1	A	1829	C
1	A	1830	G
1	A	1831	A
1	A	1833	G
1	A	1839	A
1	A	1843	G
1	A	1845	A

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Mol	Chain	Res	Type
1	A	1846	G
1	A	1849	U
1	A	1858	A
1	A	1867	C
1	A	1872	C
1	A	1877	A
1	A	1882	A
1	A	1883	A
1	A	1884	G
1	A	1885	A
1	A	1887	G
1	A	1895	A
1	A	1899	U
1	A	1902	G
1	A	1904	G
1	A	1932	G
1	A	1935	G
1	A	1941	A
1	A	1942	A
1	A	1943	C
1	A	1944	U
1	A	1946	U
1	A	1952	U
1	A	1956	A
1	A	1958	G
1	A	1959	G
1	A	1966	A
1	A	1967	A
1	A	1968	U
1	A	1969	U
1	A	1970	C
1	A	1972	U
1	A	1973	U
1	A	1984	U
1	A	1992	C
1	A	1993	G
1	A	1995	A
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2004	G

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Mol	Chain	Res	Type
1	A	2010	A
1	A	2020	U
1	A	2022	U
1	A	2025	C
1	A	2026	A
1	A	2033	G
1	A	2050	G
1	A	2051	U
1	A	2052	A
1	A	2053	C
1	A	2059	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2064	G
1	A	2065	C
1	A	2068	G
1	A	2070	U
1	A	2072	C
1	A	2079	C
1	A	2080	A
1	A	2081	G
1	A	2084	C
1	A	2085	G
1	A	2089	A
1	A	2090	G
1	A	2098	G
1	A	2101	G
1	A	2121	U
1	A	2123	A
1	A	2125	U
1	A	2128	U
1	A	2131	U
1	A	2134	A
1	A	2135	G
1	A	2136	C
1	A	2139	G
1	A	2140	U
1	A	2145	G
1	A	2146	A
1	A	2147	U
1	A	2149	G

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Mol	Chain	Res	Type
1	A	2156	G
1	A	2160	U
1	A	2161	G
1	A	2162	G
1	A	2166	C
1	A	2174	C
1	A	2175	C
1	A	2176	A
1	A	2177	G
1	A	2185	G
1	A	2187	A
1	A	2198	G
1	A	2200	A
1	A	2201	U
1	A	2202	A
1	A	2203	C
1	A	2205	A
1	A	2206	C
1	A	2208	C
1	A	2210	G
1	A	2212	C
1	A	2213	U
1	A	2217	U
1	A	2219	G
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2240	U
1	A	2241	A
1	A	2242	U
1	A	2244	G
1	A	2245	G
1	A	2246	G
1	A	2249	G
1	A	2252	A
1	A	2254	A
1	A	2255	C
1	A	2260	U
1	A	2267	G
1	A	2268	G
1	A	2295	A
1	A	2296	A

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Mol	Chain	Res	Type
1	A	2307	A
1	A	2308	G
1	A	2311	G
1	A	2312	C
1	A	2316	A
1	A	2317	A
1	A	2323	C
1	A	2324	C
1	A	2325	U
1	A	2327	A
1	A	2331	U
1	A	2332	G
1	A	2333	G
1	A	2334	U
1	A	2335	U
1	A	2336	G
1	A	2338	A
1	A	2340	A
1	A	2341	U
1	A	2342	C
1	A	2343	A
1	A	2344	U
1	A	2345	U
1	A	2348	C
1	A	2349	A
1	A	2350	G
1	A	2354	G
1	A	2356	A
1	A	2357	A
1	A	2363	C
1	A	2364	A
1	A	2368	G
1	A	2374	G
1	A	2376	C
1	A	2379	C
1	A	2381	A
1	A	2387	A
1	A	2390	A
1	A	2401	G
1	A	2406	A
1	A	2408	G
1	A	2412	G

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Mol	Chain	Res	Type
1	A	2413	G
1	A	2414	C
1	A	2418	G
1	A	2420	G
1	A	2431	U
1	A	2432	C
1	A	2435	C
1	A	2448	U
1	A	2451	C
1	A	2452	U
1	A	2453	C
1	A	2454	A
1	A	2455	A
1	A	2456	C
1	A	2457	G
1	A	2458	G
1	A	2459	A
1	A	2460	U
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2476	G
1	A	2477	A
1	A	2488	A
1	A	2497	A
1	A	2503	C
1	A	2505	A
1	A	2506	C
1	A	2507	A
1	A	2511	A
1	A	2523	G
1	A	2524	G
1	A	2525	C
1	A	2527	C
1	A	2531	G
1	A	2532	A
1	A	2533	U
1	A	2534	G
1	A	2547	A
1	A	2554	G
1	A	2558	G

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Mol	Chain	Res	Type
1	A	2563	C
1	A	2564	G
1	A	2570	A
1	A	2583	U
1	A	2593	A
1	A	2595	A
1	A	2596	G
1	A	2598	G
1	A	2601	A
1	A	2602	C
1	A	2607	G
1	A	2612	G
1	A	2613	U
1	A	2614	U
1	A	2615	C
1	A	2630	C
1	A	2631	A
1	A	2638	U
1	A	2642	U
1	A	2644	U
1	A	2654	G
1	A	2659	G
1	A	2660	G
1	A	2667	G
1	A	2674	G
1	A	2675	C
1	A	2689	A
1	A	2692	G
1	A	2696	C
1	A	2702	G
1	A	2711	G
1	A	2714	G
1	A	2718	U
1	A	2720	C
1	A	2743	G
1	A	2747	G
1	A	2753	U
1	A	2755	U
1	A	2760	G
1	A	2762	A
1	A	2764	G
1	A	2765	G

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Mol	Chain	Res	Type
1	A	2766	G
1	A	2773	G
1	A	2777	A
1	A	2784	C
1	A	2785	U
1	A	2786	A
1	A	2789	C
1	A	2794	A
1	A	2795	G
1	A	2806	G
1	A	2807	A
1	A	2808	U
1	A	2818	C
1	A	2821	U
1	A	2822	C
1	A	2823	C
1	A	2824	G
1	A	2826	A
1	A	2828	G
1	A	2831	A
1	A	2832	G
1	A	2833	U
1	A	2843	G
1	A	2855	G
1	A	2859	G
1	A	2860	A
1	A	2862	A
1	A	2866	C
1	A	2868	G
1	A	2874	G
1	A	2886	C
1	A	2891	G
1	A	2892	G
1	A	2897	G
1	A	2900	A
1	A	2901	G
1	A	2905	C
1	A	2908	A
1	A	2916	A
1	A	2917	G
2	B	10	G
2	B	12	U

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Mol	Chain	Res	Type
2	B	15	C
2	B	22	G
2	B	23	U
2	B	28	C
2	B	31	G
2	B	32	U
2	B	33	U
2	B	34	C
2	B	38	U
2	B	39	A
2	B	40	C
2	B	41	C
2	B	42	G
2	B	47	C
2	B	48	G
2	B	49	G
2	B	50	A
2	B	52	G
2	B	53	U
2	B	54	U
2	B	55	A
2	B	59	U
2	B	60	C
2	B	62	U
2	B	63	C
2	B	64	A
2	B	65	G
2	B	66	C
2	B	85	U
2	B	86	U
2	B	87	U
2	B	88	C
2	B	97	A
2	B	101	U
2	B	106	C
2	B	107	G
2	B	110	G
2	B	114	A
33	a	9	G
33	a	10	A
33	a	11	G
33	a	24	G

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Mol	Chain	Res	Type
33	a	32	C
33	a	33	G
33	a	34	A
33	a	41	G
33	a	46	G
33	a	49	C
33	a	50	C
33	a	51	U
33	a	52	A
33	a	53	A
33	a	60	C
33	a	65	C
33	a	66	G
33	a	72	A
33	a	75	G
33	a	77	U
33	a	80	G
33	a	84	U
33	a	85	U
33	a	86	G
33	a	87	C
33	a	88	U
33	a	89	C
33	a	90	C
33	a	92	U
33	a	93	G
33	a	99	A
33	a	113	G
33	a	114	A
33	a	117	A
33	a	118	A
33	a	119	C
33	a	120	A
33	a	128	A
33	a	129	A
33	a	130	C
33	a	136	U
33	a	137	G
33	a	140	A
33	a	141	G
33	a	142	A
33	a	144	U

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Mol	Chain	Res	Type
33	a	153	U
33	a	154	C
33	a	158	G
33	a	162	C
33	a	167	G
33	a	172	U
33	a	176	G
33	a	181	G
33	a	182	U
33	a	189	A
33	a	190	A
33	a	193	G
33	a	194	C
33	a	197	G
33	a	207	U
33	a	208	A
33	a	209	A
33	a	211	A
33	a	218	U
33	a	219	U
33	a	220	C
33	a	221	G
33	a	222	G
33	a	249	G
33	a	253	U
33	a	255	G
33	a	259	G
33	a	262	G
33	a	274	G
33	a	275	C
33	a	277	C
33	a	280	C
33	a	287	A
33	a	288	C
33	a	297	G
33	a	306	A
33	a	314	A
33	a	316	C
33	a	321	A
33	a	329	A
33	a	336	C
33	a	337	A

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Mol	Chain	Res	Type
33	a	338	C
33	a	340	G
33	a	352	A
33	a	353	C
33	a	355	G
33	a	357	A
33	a	359	G
33	a	360	C
33	a	362	G
33	a	371	A
33	a	373	U
33	a	375	U
33	a	380	C
33	a	383	U
33	a	385	G
33	a	390	A
33	a	392	G
33	a	396	G
33	a	400	G
33	a	405	A
33	a	406	C
33	a	414	G
33	a	419	A
33	a	420	U
33	a	421	G
33	a	426	U
33	a	429	U
33	a	430	C
33	a	432	G
33	a	436	G
33	a	437	U
33	a	438	A
33	a	439	A
33	a	442	C
33	a	447	U
33	a	456	A
33	a	457	A
33	a	459	A
33	a	460	A
33	a	461	C
33	a	465	U
33	a	466	G

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Mol	Chain	Res	Type
33	a	467	C
33	a	473	G
33	a	474	A
33	a	476	U
33	a	477	A
33	a	478	G
33	a	480	G
33	a	483	G
33	a	484	U
33	a	485	A
33	a	487	C
33	a	488	U
33	a	490	G
33	a	491	A
33	a	494	G
33	a	506	A
33	a	508	A
33	a	518	A
33	a	519	A
33	a	520	C
33	a	526	G
33	a	527	C
33	a	530	G
33	a	533	G
33	a	536	G
33	a	539	G
33	a	540	U
33	a	541	A
33	a	542	A
33	a	553	G
33	a	554	C
33	a	556	A
33	a	563	U
33	a	564	C
33	a	568	A
33	a	571	U
33	a	573	U
33	a	581	A
33	a	582	A
33	a	585	G
33	a	586	G
33	a	588	U

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Mol	Chain	Res	Type
33	a	591	C
33	a	597	G
33	a	616	A
33	a	627	C
33	a	628	U
33	a	629	C
33	a	641	G
33	a	642	U
33	a	643	C
33	a	648	G
33	a	650	A
33	a	661	U
33	a	662	U
33	a	670	G
33	a	674	A
33	a	694	G
33	a	696	A
33	a	704	A
33	a	727	A
33	a	732	U
33	a	733	G
33	a	740	G
33	a	742	G
33	a	745	U
33	a	756	U
33	a	757	A
33	a	758	A
33	a	762	A
33	a	764	G
33	a	768	A
33	a	787	G
33	a	802	U
33	a	803	A
33	a	806	C
33	a	815	C
33	a	821	G
33	a	824	A
33	a	826	C
33	a	828	A
33	a	829	U
33	a	841	G
33	a	845	G

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Mol	Chain	Res	Type
33	a	849	G
33	a	853	C
33	a	855	G
33	a	856	C
33	a	861	U
33	a	880	U
33	a	884	G
33	a	885	C
33	a	895	G
33	a	899	A
33	a	909	C
33	a	924	A
33	a	932	G
33	a	936	G
33	a	944	C
33	a	945	A
33	a	952	G
33	a	964	G
33	a	966	U
33	a	967	U
33	a	968	A
33	a	970	U
33	a	975	A
33	a	976	G
33	a	978	A
33	a	979	A
33	a	981	G
33	a	984	A
33	a	985	A
33	a	986	G
33	a	987	A
33	a	992	U
33	a	993	A
33	a	999	U
33	a	1000	C
33	a	1002	U
33	a	1003	G
33	a	1006	A
33	a	1008	C
33	a	1009	C
33	a	1010	U
33	a	1011	C

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Mol	Chain	Res	Type
33	a	1012	U
33	a	1014	A
33	a	1015	C
33	a	1017	A
33	a	1019	C
33	a	1020	C
33	a	1023	G
33	a	1024	A
33	a	1027	U
33	a	1028	A
33	a	1030	G
33	a	1031	A
33	a	1033	G
33	a	1035	C
33	a	1036	C
33	a	1039	U
33	a	1040	U
33	a	1041	C
33	a	1042	G
33	a	1043	G
33	a	1046	G
33	a	1047	C
33	a	1050	A
33	a	1051	G
33	a	1052	U
33	a	1053	G
33	a	1056	A
33	a	1058	G
33	a	1060	G
33	a	1064	C
33	a	1071	G
33	a	1074	G
33	a	1075	U
33	a	1095	U
33	a	1102	A
33	a	1104	G
33	a	1105	U
33	a	1110	C
33	a	1111	A
33	a	1112	A
33	a	1114	G
33	a	1118	G

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Mol	Chain	Res	Type
33	a	1124	C
33	a	1128	A
33	a	1134	G
33	a	1136	U
33	a	1140	A
33	a	1141	G
33	a	1142	C
33	a	1143	A
33	a	1145	U
33	a	1148	G
33	a	1149	U
33	a	1150	U
33	a	1151	G
33	a	1153	G
33	a	1155	A
33	a	1163	G
33	a	1166	A
33	a	1167	C
33	a	1168	U
33	a	1169	G
33	a	1170	C
33	a	1176	A
33	a	1177	C
33	a	1178	A
33	a	1180	A
33	a	1190	G
33	a	1192	U
33	a	1193	G
33	a	1205	A
33	a	1206	A
33	a	1209	C
33	a	1211	U
33	a	1214	U
33	a	1221	U
33	a	1222	A
33	a	1224	G
33	a	1233	U
33	a	1235	C
33	a	1236	A
33	a	1237	C
33	a	1238	A
33	a	1239	C

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Mol	Chain	Res	Type
33	a	1245	A
33	a	1247	A
33	a	1258	C
33	a	1259	A
33	a	1265	C
33	a	1266	A
33	a	1267	G
33	a	1269	G
33	a	1279	G
33	a	1288	A
33	a	1289	A
33	a	1291	C
33	a	1294	A
33	a	1295	C
33	a	1296	A
33	a	1299	U
33	a	1307	C
33	a	1308	A
33	a	1309	G
33	a	1311	U
33	a	1312	C
33	a	1313	G
33	a	1314	G
33	a	1323	C
33	a	1326	C
33	a	1329	C
33	a	1331	C
33	a	1332	G
33	a	1336	G
33	a	1340	G
33	a	1345	U
33	a	1347	G
33	a	1349	A
33	a	1354	U
33	a	1355	A
33	a	1362	G
33	a	1366	A
33	a	1371	C
33	a	1372	A
33	a	1373	U
33	a	1377	G
33	a	1379	G

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Mol	Chain	Res	Type
33	a	1387	C
33	a	1403	A
33	a	1406	C
33	a	1407	A
33	a	1413	C
33	a	1428	G
33	a	1435	A
33	a	1451	A
33	a	1452	G
33	a	1455	A
33	a	1461	U
33	a	1462	U
33	a	1463	A
33	a	1464	G
33	a	1478	A
33	a	1494	U
33	a	1496	G
33	a	1497	G
33	a	1500	U
33	a	1502	A
33	a	1503	A
33	a	1507	G
33	a	1513	A
33	a	1515	G
33	a	1516	U
33	a	1517	A
33	a	1527	G
33	a	1529	A
33	a	1539	G
33	a	1540	G
53	x	6	G
53	x	8	U
53	x	9	G
53	x	13	G
53	x	16	U
53	x	17	U
53	x	17(A)	G
53	x	18	G
53	x	19	U
53	x	20	A
53	x	21	G
53	x	22	A

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Mol	Chain	Res	Type
53	x	23	C
53	x	25	C
53	x	26	G
53	x	36	G
53	x	41	U
53	x	43	G
53	x	44	U
53	x	51	G
53	x	52	G
53	x	53	G
53	x	56	C
53	x	60	U
53	x	61	C
53	x	63	C
53	x	70	G
53	x	75	C
53	x	76	A

All (93) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	C
1	A	88	G
1	A	92	G
1	A	118	A
1	A	163	U
1	A	181	G
1	A	199	A
1	A	236	A
1	A	252	C
1	A	347	G
1	A	410	G
1	A	411	G
1	A	441	C
1	A	455	G
1	A	458	G
1	A	459	A
1	A	482	C
1	A	525	A
1	A	549	A
1	A	554	U
1	A	576	G

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Mol	Chain	Res	Type
1	A	594	C
1	A	666	G
1	A	689	A
1	A	702	A
1	A	732	A
1	A	756	U
1	A	810	G
1	A	831	U
1	A	848	G
1	A	855	G
1	A	933	C
1	A	1028	C
1	A	1032	C
1	A	1036	A
1	A	1041	C
1	A	1172	A
1	A	1176	U
1	A	1187	U
1	A	1210	A
1	A	1226	U
1	A	1243	A
1	A	1250	G
1	A	1260	A
1	A	1266	A
1	A	1269	A
1	A	1294	A
1	A	1305	A
1	A	1325	A
1	A	1339	A
1	A	1351	U
1	A	1365	U
1	A	1448	U
1	A	1464	A
1	A	1507	U
1	A	1525	G
1	A	1529	G
1	A	1530	G
1	A	1535	U
1	A	1543	U
1	A	1565	U
1	A	1570	U
1	A	1631	A

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Mol	Chain	Res	Type
1	A	1671	G
1	A	1726	G
1	A	1751	U
1	A	1784	A
1	A	1813	A
1	A	1828	G
1	A	1844	A
1	A	1882	A
1	A	1883	A
1	A	1886	G
1	A	1991	C
1	A	2009	G
1	A	2127	U
1	A	2139	G
1	A	2155	A
1	A	2254	A
1	A	2295	A
1	A	2316	A
1	A	2356	A
1	A	2454	A
1	A	2456	C
1	A	2468	A
1	A	2531	G
1	A	2630	C
1	A	2710	C
1	A	2805	A
1	A	2904	A
2	B	37	A
2	B	48	G
2	B	49	G

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

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
54	TEL	A	3001	-	60,62,62	1.34	5 (8%)	78,92,92	1.98	17 (21%)
55	ATP	V	900	-	32,33,33	1.29	5 (15%)	48,52,52	1.89	11 (22%)
55	ATP	V	901	-	32,33,33	1.38	6 (18%)	48,52,52	1.80	10 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	TEL	A	3001	-	1/1/19/19	16/73/108/108	0/4/5/5
55	ATP	V	900	-	-	3/22/38/38	0/3/3/3
55	ATP	V	901	-	-	5/22/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A	3001	TEL	O5-C10	5.76	1.45	1.35
54	A	3001	TEL	O9-C15	5.01	1.45	1.34
55	V	901	ATP	C5-C4	4.57	1.47	1.39
55	V	900	ATP	C5-C4	4.19	1.46	1.39
54	A	3001	TEL	C40-N41	-3.21	1.35	1.38
54	A	3001	TEL	O5-C2	-2.78	1.43	1.47
55	V	901	ATP	C5-N7	-2.64	1.34	1.39
55	V	901	ATP	C5-C6	2.59	1.48	1.41
55	V	901	ATP	C8-N9	-2.52	1.33	1.37
55	V	900	ATP	C5-C6	2.48	1.47	1.41
55	V	900	ATP	C5-N7	-2.35	1.34	1.39
55	V	900	ATP	C8-N7	2.33	1.36	1.31
54	A	3001	TEL	C36-N31	-2.29	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	V	901	ATP	C4-N9	-2.21	1.33	1.37
55	V	901	ATP	C8-N7	2.08	1.35	1.31
55	V	900	ATP	C4-N9	-2.07	1.33	1.37

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A	3001	TEL	O9-C15-C21	9.49	120.30	110.93
55	V	900	ATP	C5-C4-N3	-5.98	118.48	126.72
54	A	3001	TEL	C17-C11-N6	-5.49	104.94	113.25
55	V	901	ATP	C5-C4-N3	-5.30	119.42	126.72
55	V	900	ATP	N3-C4-N9	4.80	135.34	127.17
55	V	901	ATP	N3-C4-N9	4.72	135.19	127.17
54	A	3001	TEL	N31-C37-N41	-4.50	108.76	112.35
54	A	3001	TEL	C36-N31-C37	4.05	108.70	106.71
55	V	900	ATP	C2-N3-C4	3.93	121.42	111.83
54	A	3001	TEL	C4-O9-C15	-3.73	111.69	118.20
55	V	900	ATP	C4-C5-N7	-3.54	106.54	110.58
55	V	901	ATP	C2-N3-C4	3.52	120.42	111.83
55	V	901	ATP	C4-N9-C8	3.46	109.37	105.74
55	V	900	ATP	N3-C2-N1	-3.46	123.35	128.58
55	V	900	ATP	C4-N9-C8	3.25	109.15	105.74
55	V	901	ATP	N3-C2-N1	-3.23	123.69	128.58
54	A	3001	TEL	O20-C15-C21	-3.16	120.55	124.65
54	A	3001	TEL	C8-C4-C2	-3.10	110.96	115.23
55	V	901	ATP	C4-C5-N7	-3.09	107.05	110.58
54	A	3001	TEL	C28-C24-C19	-3.08	111.07	116.10
55	V	901	ATP	C2'-C1'-N9	-3.08	105.65	113.30
54	A	3001	TEL	C43-C40-N41	2.84	126.39	122.45
54	A	3001	TEL	C1-C2-C3	-2.80	111.15	116.36
55	V	900	ATP	C5-N7-C8	2.68	107.67	103.45
54	A	3001	TEL	O9-C15-O20	-2.66	119.15	123.95
54	A	3001	TEL	C56-N52-C47	2.47	121.17	116.85
55	V	900	ATP	N9-C8-N7	-2.46	110.44	113.94
54	A	3001	TEL	C42-O39-C34	-2.45	112.10	116.26
54	A	3001	TEL	C24-C19-C13	-2.35	109.38	113.32
54	A	3001	TEL	C37-N41-C40	2.31	107.79	105.94
55	V	901	ATP	O3A-PA-O1A	-2.29	103.82	110.70
55	V	900	ATP	C6-C5-N7	2.25	136.43	132.09
55	V	901	ATP	C5-N7-C8	2.25	106.98	103.45
54	A	3001	TEL	C43-C40-C36	-2.22	126.26	129.65
54	A	3001	TEL	C54-C49-N53	-2.17	109.48	115.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	V	900	ATP	O2A-PA-O1A	2.16	122.50	112.44
55	V	901	ATP	C6-C5-N7	2.07	136.08	132.09
55	V	900	ATP	O3G-PG-O2G	2.06	115.51	107.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
54	A	3001	TEL	C21

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	A	3001	TEL	C15-C21-C26-O29
54	A	3001	TEL	C15-C21-C26-C30
55	V	900	ATP	C5'-O5'-PA-O1A
55	V	900	ATP	C5'-O5'-PA-O3A
55	V	901	ATP	C5'-O5'-PA-O1A
55	V	901	ATP	C5'-O5'-PA-O3A
54	A	3001	TEL	C21-C15-O9-C4
54	A	3001	TEL	O20-C15-O9-C4
54	A	3001	TEL	O9-C4-C8-C14
54	A	3001	TEL	N6-C3-C7-C12
54	A	3001	TEL	O20-C15-C21-C25
54	A	3001	TEL	O9-C15-C21-C25
54	A	3001	TEL	C17-C22-C27-N31
54	A	3001	TEL	O9-C15-C21-C26
55	V	900	ATP	C5'-O5'-PA-O2A
55	V	901	ATP	C5'-O5'-PA-O2A
54	A	3001	TEL	C2-C4-C8-C14
54	A	3001	TEL	C35-C30-C34-C28
55	V	901	ATP	PB-O3A-PA-O1A
54	A	3001	TEL	C17-C11-N6-C10
54	A	3001	TEL	O20-C15-C21-C26
54	A	3001	TEL	C2-C3-C7-C12
55	V	901	ATP	PB-O3A-PA-O2A
54	A	3001	TEL	N6-C11-C17-C22

There are no ring outliers.

3 monomers are involved in 75 short contacts:

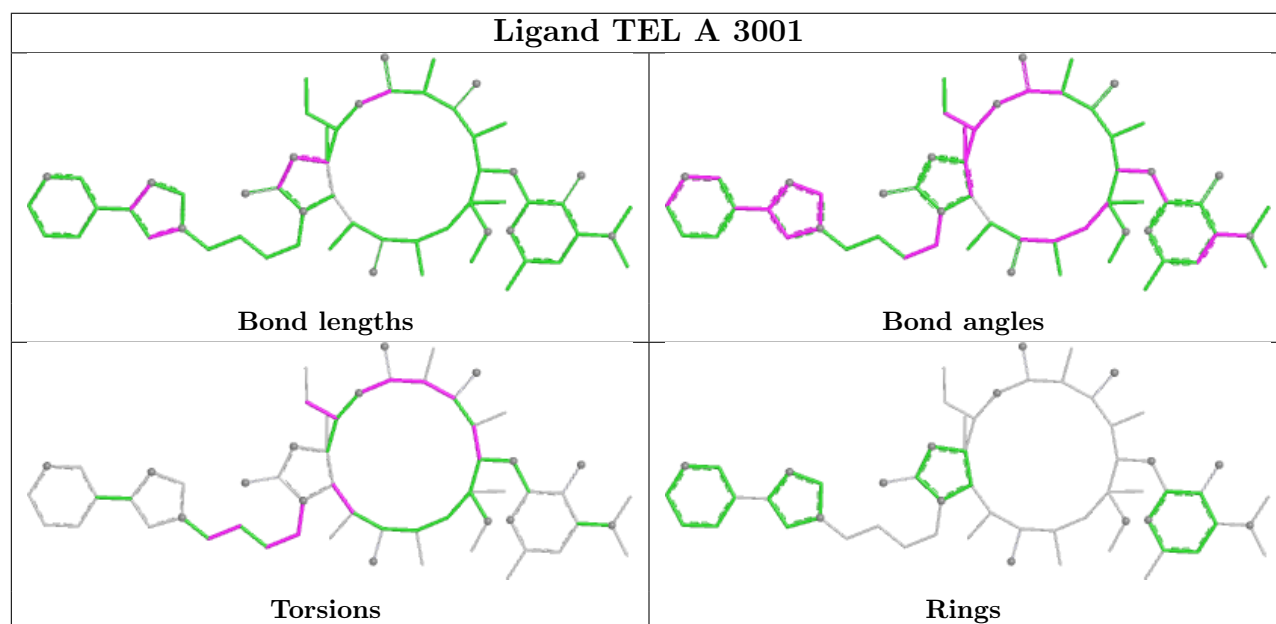
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	A	3001	TEL	16	0

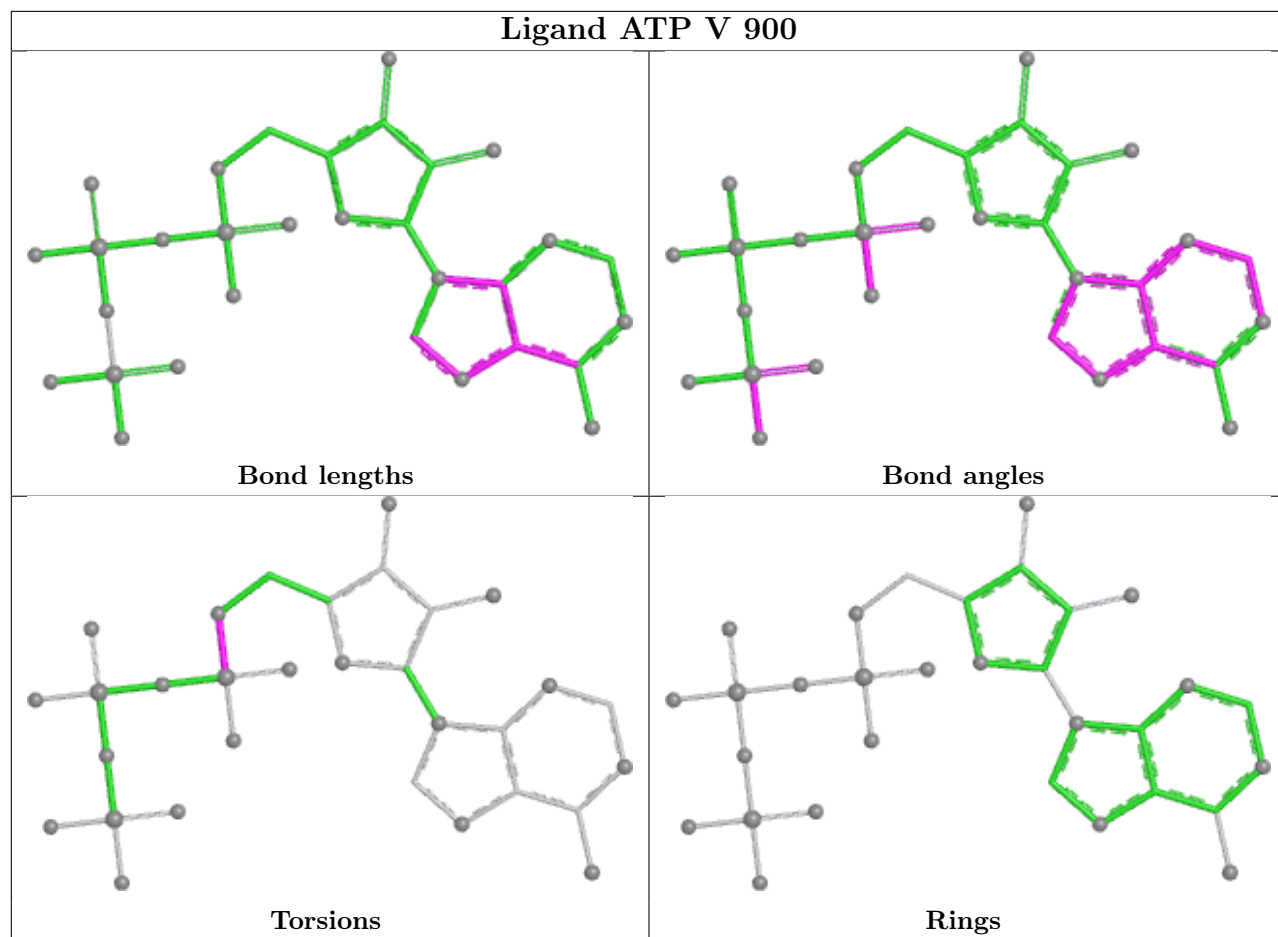
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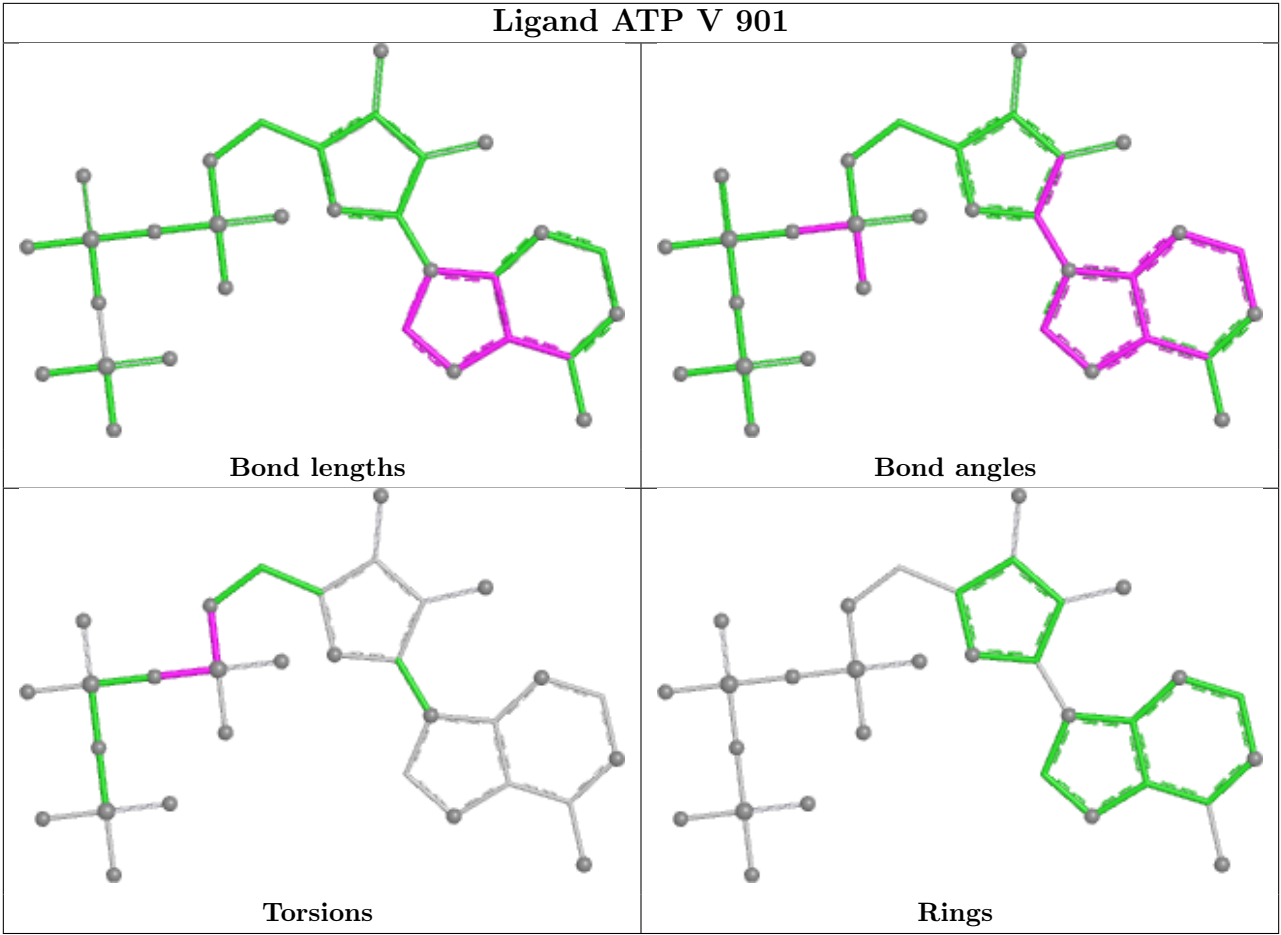
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	V	900	ATP	24	0
55	V	901	ATP	35	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
53	x	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	44:U	O3'	47:U	P	14.81
1	A	182:C	O3'	183:A	P	6.43
1	A	1449:C	O3'	1450:C	P	4.34
1	A	1451:U	O3'	1452:C	P	3.29

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1452:C	O3'	1453:A	P	3.25
1	A	183:A	O3'	184:G	P	3.12

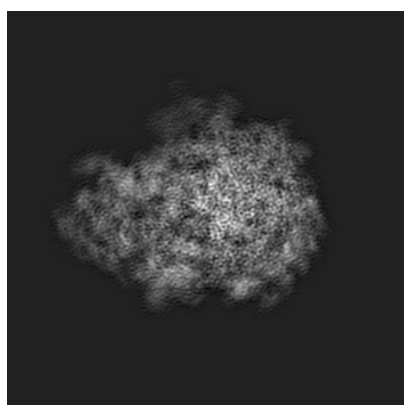
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0177. These allow visual inspection of the internal detail of the map and identification of artifacts.

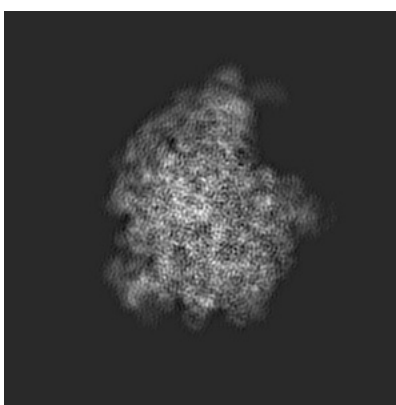
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

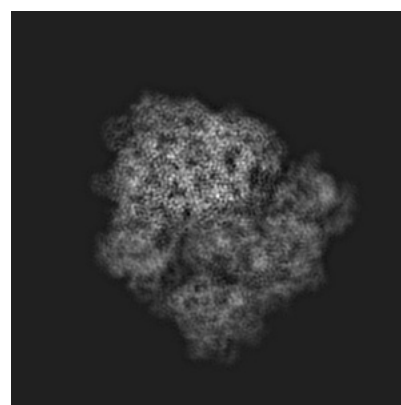
6.1.1 Primary map



X



Y

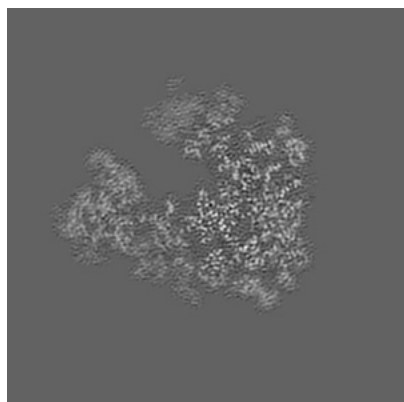


Z

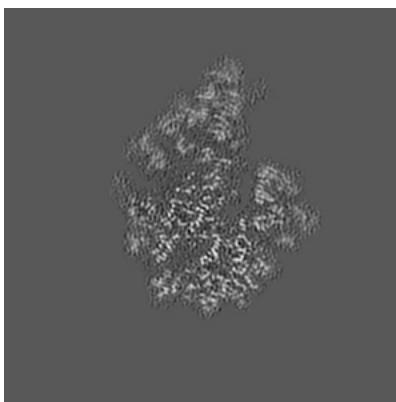
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

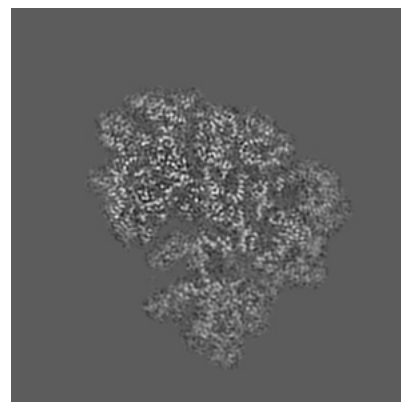
6.2.1 Primary map



X Index: 180



Y Index: 180

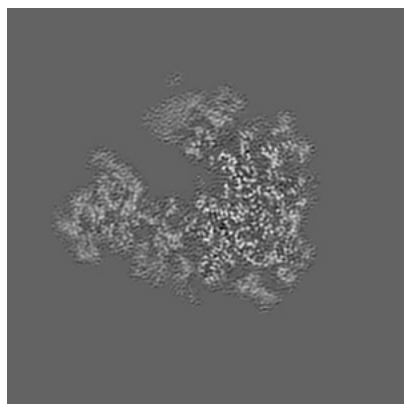


Z Index: 180

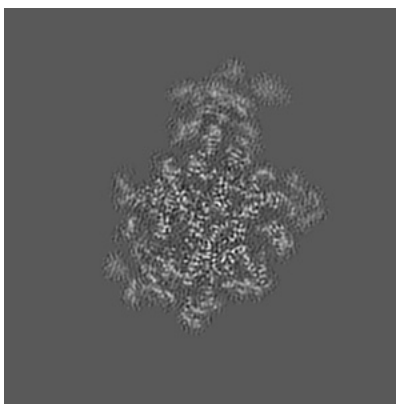
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

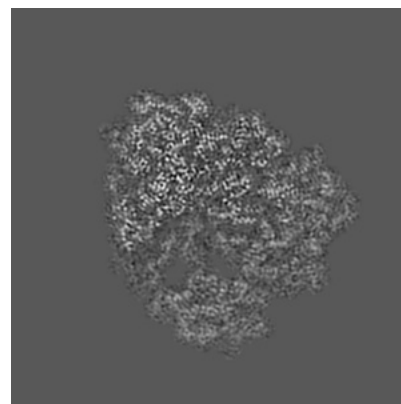
6.3.1 Primary map



X Index: 177



Y Index: 199

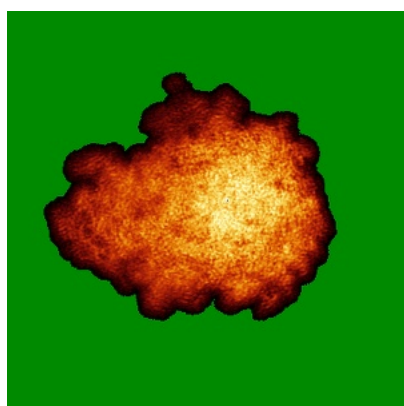


Z Index: 189

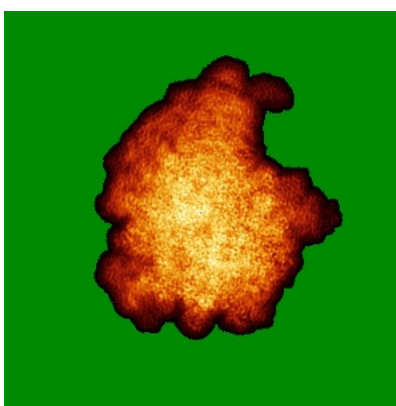
The images above show the largest variance slices of the map in three orthogonal directions.

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

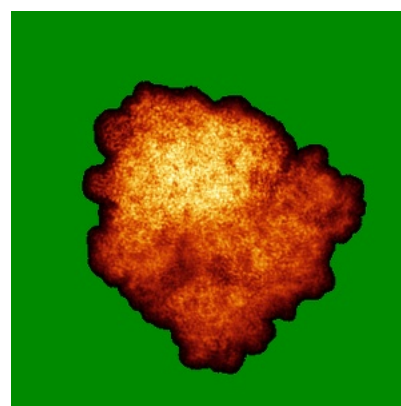
6.4.1 Primary map



X



Y

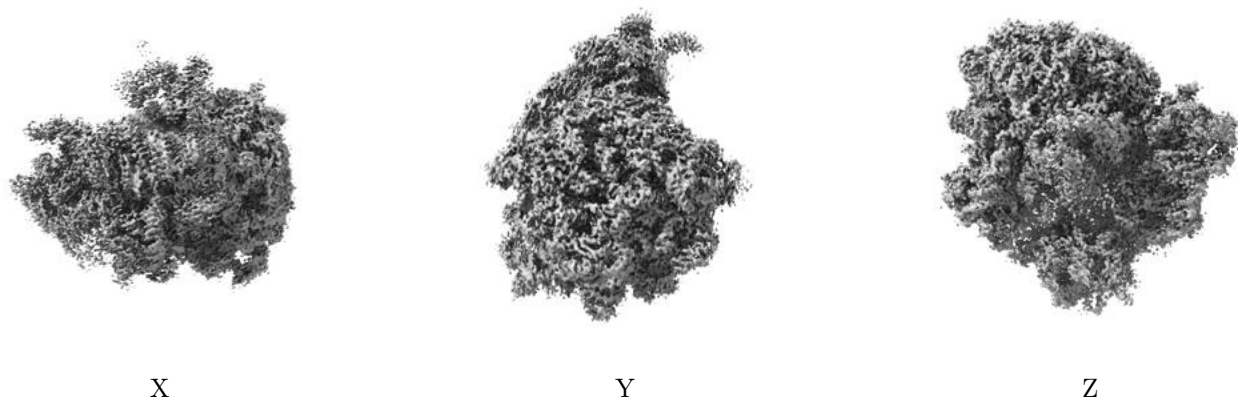


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.11. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

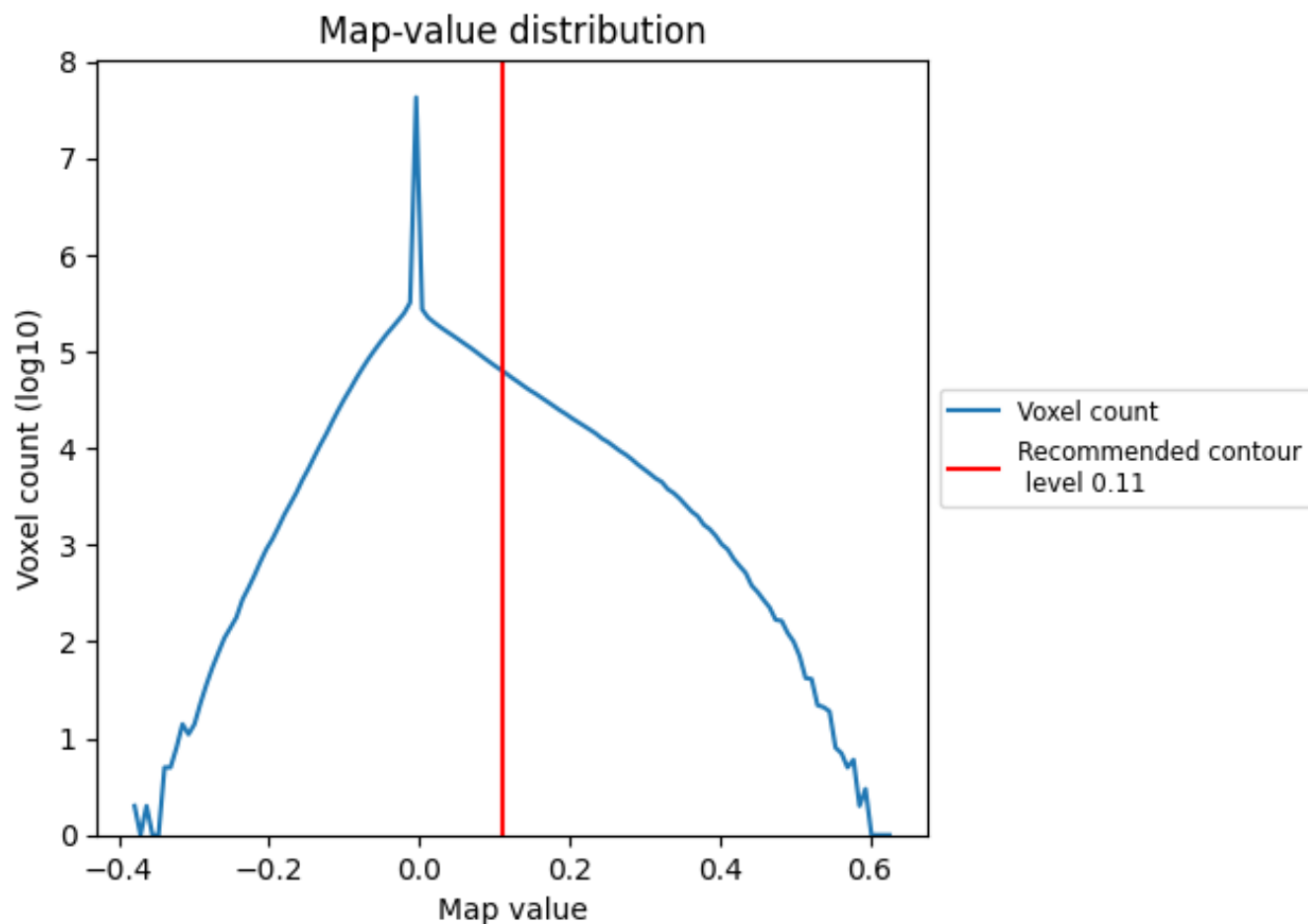
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

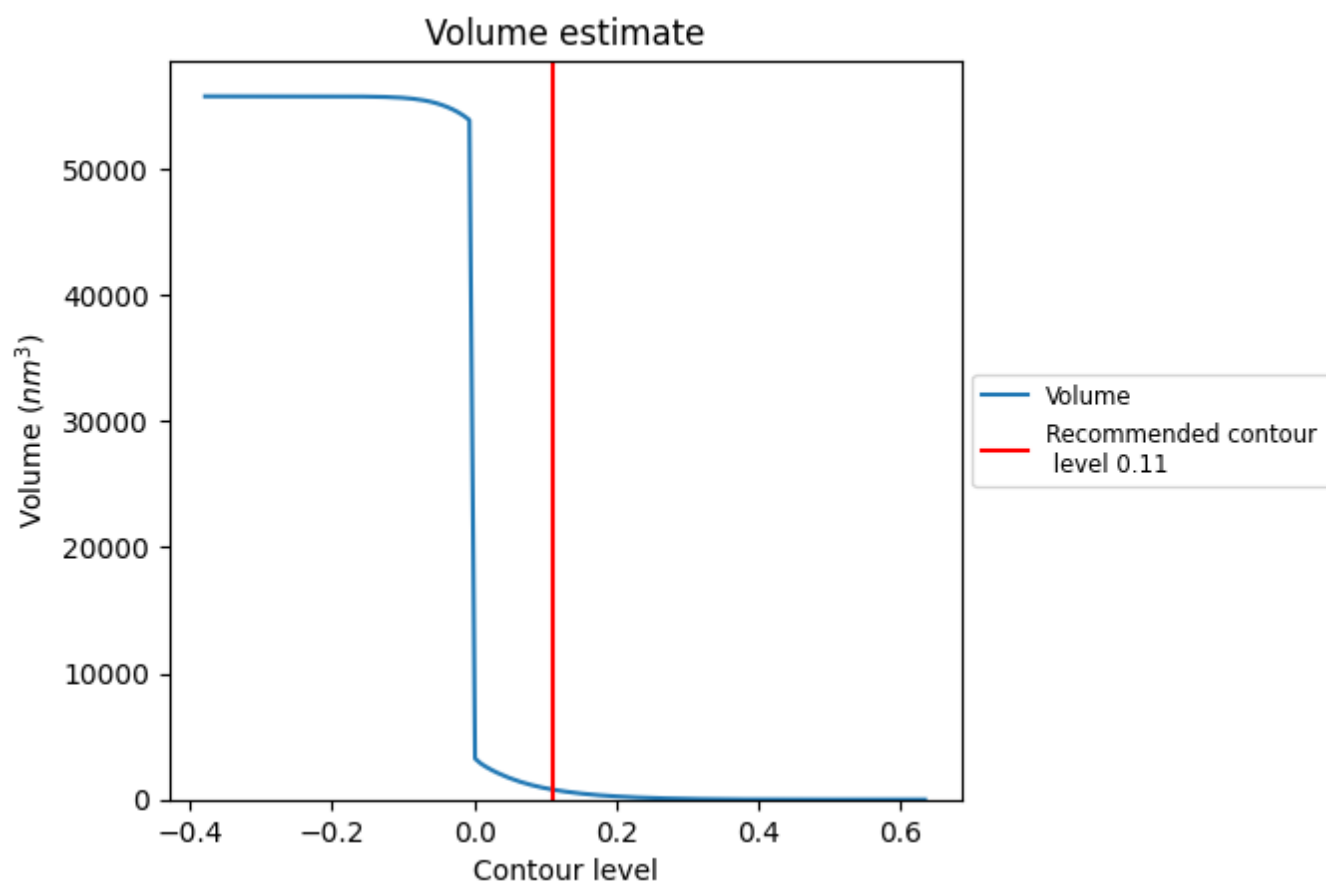
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

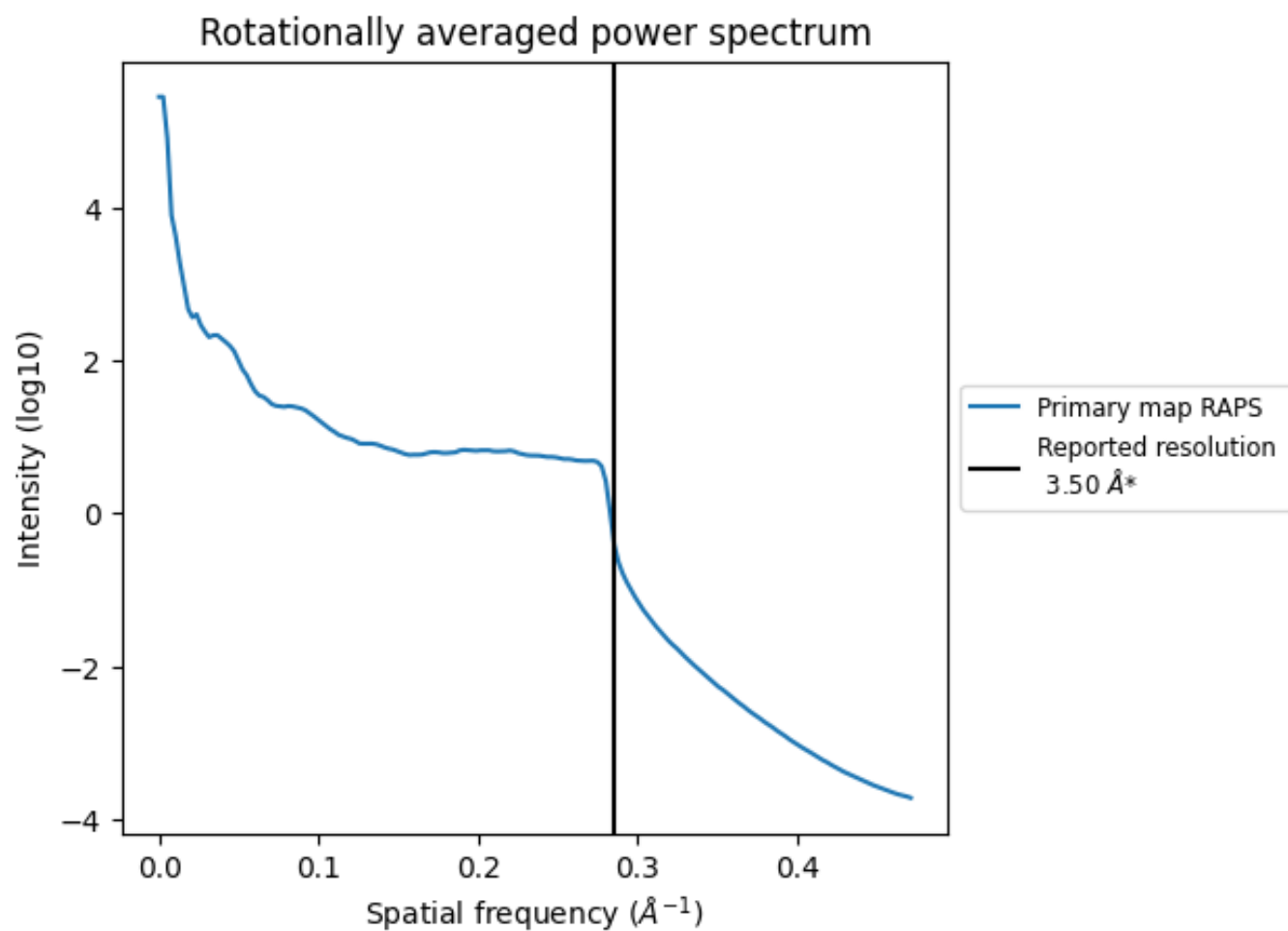
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 793 nm³; this corresponds to an approximate mass of 716 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

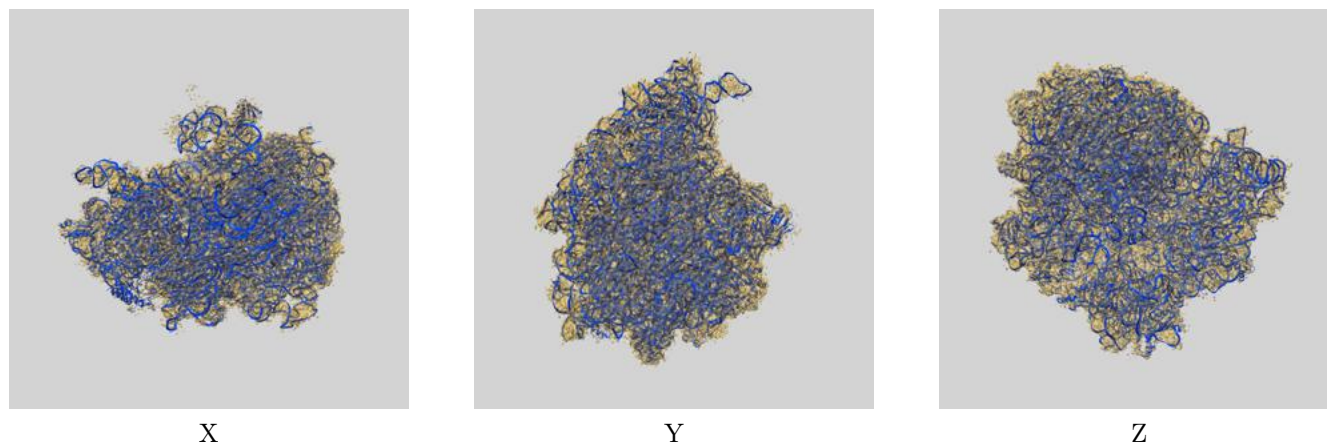
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

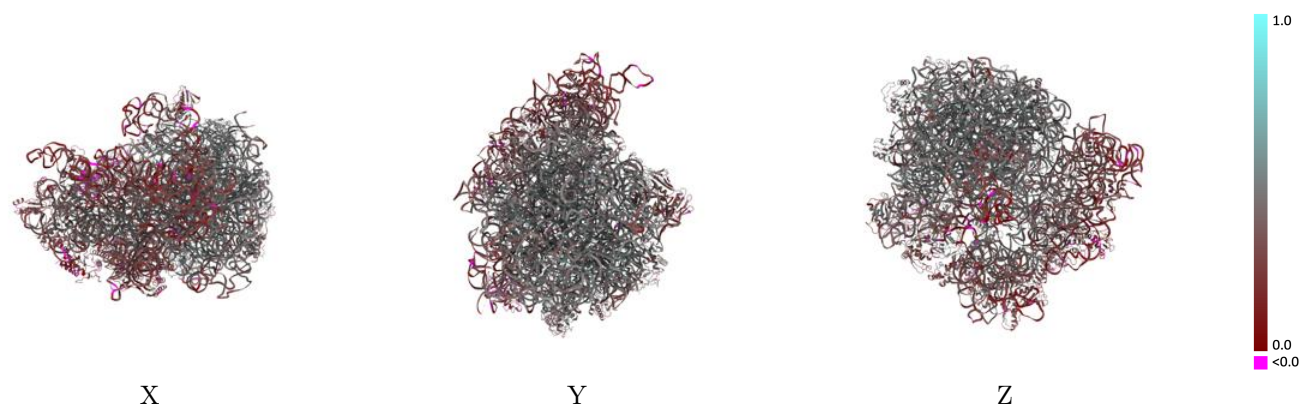
This section contains information regarding the fit between EMDB map EMD-0177 and PDB model 6HA8. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



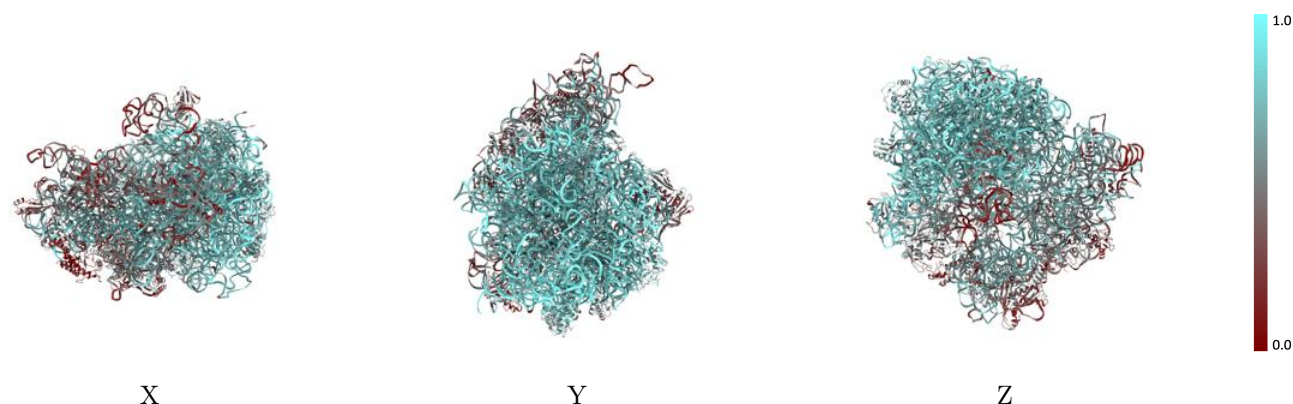
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



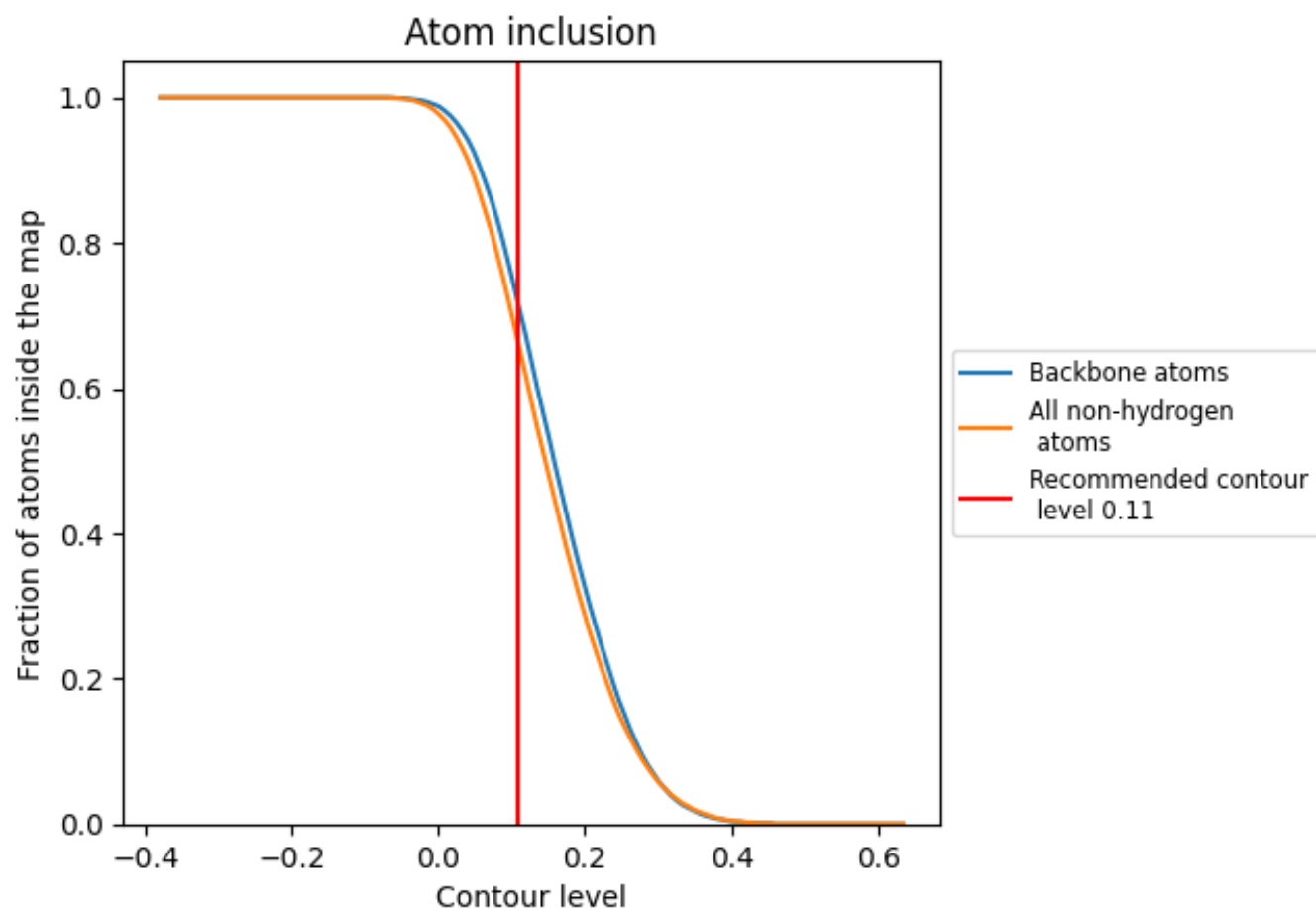
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 66% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.3890
0	 0.7190	 0.4870
1	 0.6740	 0.4410
2	 0.7360	 0.5030
3	 0.7260	 0.5080
4	 0.6140	 0.4620
6	 0.2940	 0.2640
7	 0.6670	 0.4050
8	 0.0760	 0.1430
A	 0.7960	 0.4370
B	 0.7850	 0.4020
C	 0.6760	 0.4800
D	 0.6960	 0.4810
E	 0.6820	 0.4500
F	 0.4590	 0.3260
G	 0.4150	 0.3170
J	 0.7100	 0.4720
K	 0.6450	 0.4620
L	 0.6630	 0.4490
M	 0.6350	 0.4500
N	 0.6840	 0.4640
O	 0.5470	 0.3630
P	 0.6320	 0.4500
Q	 0.7070	 0.4500
R	 0.6890	 0.4530
S	 0.7030	 0.4810
T	 0.6140	 0.4430
U	 0.6150	 0.4040
V	 0.4240	 0.3890
W	 0.6490	 0.4500
X	 0.5230	 0.4500
Y	 0.5880	 0.3610
Z	 0.6360	 0.4400
a	 0.6450	 0.3360
b	 0.1210	 0.1970



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Chain	Atom inclusion	Q-score
c	 0.3990	 0.3340
d	 0.2450	 0.2270
e	 0.4970	 0.3750
f	 0.2840	 0.2490
g	 0.4500	 0.3240
h	 0.3960	 0.2870
i	 0.4340	 0.3220
j	 0.3410	 0.3210
k	 0.3790	 0.2970
l	 0.3720	 0.3080
m	 0.3810	 0.2880
n	 0.3810	 0.3480
o	 0.3850	 0.2490
p	 0.3260	 0.2690
q	 0.2850	 0.2390
r	 0.3410	 0.2730
s	 0.3460	 0.2600
t	 0.3710	 0.2630
x	 0.4340	 0.3210