



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:40 AM UTC

PDB ID : 7P7R / pdb_00007p7r
EMDB ID : EMD-13242
Title : PoxA-EQ2 antibiotic resistance ABCF bound to E. faecalis 70S ribosome, state I
Authors : Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on : 2021-07-20
Resolution : 2.90 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:

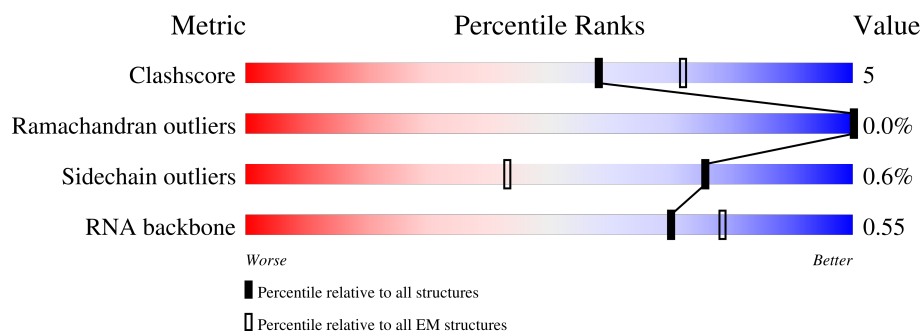
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102
RNA backbone	8273	3508

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	0	586	85% 80% 11% 9%
2	1	62	58% 94% 5%
3	2	59	90% 83% 14%
4	3	89	90% 70% 20% 10%
5	4	59	47% 81% 8% 10%
6	5	48	75% 79% 19%
7	6	44	50% 98%

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Mol	Chain	Length	Quality of chain
8	7	65	
9	8	38	
10	A	2912	
11	B	115	
12	D	77	
13	F	229	
14	G	276	
15	H	209	
16	I	207	
17	J	179	
18	K	178	
19	M	147	
20	N	122	
21	O	146	
22	P	144	
23	Q	127	
24	R	118	
25	S	115	
26	T	119	
27	U	102	
28	V	115	
29	W	96	
30	X	103	
31	Y	95	
32	Z	62	

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Mol	Chain	Length	Quality of chain
33	a	1558	
34	b	19	
35	c	261	
36	d	218	
37	e	203	
38	f	166	
39	g	99	
40	h	156	
41	i	132	
42	j	130	
43	k	102	
44	l	129	
45	m	137	
46	n	121	
47	o	61	
48	p	89	
49	q	91	
50	r	88	
51	s	79	
52	t	92	
53	u	83	

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 147576 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called ARE-ABC-F family resistance factor PoxA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	534	Total	C	N	O	S	0	0
			4347	2789	720	823	15		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			491	307	91	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			428	266	80	81	1		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	80	Total	C	N	O	S	0	0
			647	409	110	126	2		

- Molecule 5 is a protein called 50S ribosomal protein L32-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	53	Total	C	N	O	S	0	0
			406	248	84	69	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	55	UNK	MET	conflict	UNP Q836R0

- Molecule 6 is a protein called 50S ribosomal protein L33 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	48	Total	C	N	O	S	0	0
			411	247	84	76	4		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	64	Total	C	N	O	S	0	0
			523	320	122	79	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	38	Total	C	N	O	S	0	0
			305	188	66	45	6		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2901	Total	C	N	O	P	0	0
			62268	27794	11451	20122	2901		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	114	Total	C	N	O	P	0	0
			2439	1088	439	798	114		

- Molecule 12 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	76	Total	C	N	O	P	0	0
			1624	724	295	529	76		

- Molecule 13 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	226	Total	C	N	O	S	0	0
			1693	1073	287	327	6		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	274	Total	C	N	O	S	0	0
			2106	1305	414	380	7		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	206	Total	C	N	O	S	0	0
			1572	990	291	287	4		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	205	Total	C	N	O	S	0	0
			1572	984	289	297	2		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	177	Total	C	N	O	S	0	0
			1392	887	239	260	6		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	174	Total	C	N	O	S	0	0
			1335	838	242	251	4		

- Molecule 19 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	147	Total	C	N	O	S	0	0
			1146	726	207	209	4		

- Molecule 20 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	122	Total	C	N	O	S	0	0
			923	574	176	171	2		

- Molecule 21 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	146	Total	C	N	O	S	0	0
			1096	677	212	206	1		

- Molecule 22 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	134	Total	C	N	O	S	0	0
			1070	683	209	173	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	136	UNK	GLU	conflict	UNP Q839F7

- Molecule 23 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	125	Total	C	N	O	S	0	0
			997	615	192	187	3		

- Molecule 24 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	118	Total	C	N	O	S	0	0
			908	561	176	169	2		

- Molecule 25 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	S	114	Total	C	N	O	0	0
			925	582	185	158		

- Molecule 26 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	118	Total	C	N	O	S	0	0
			950	602	184	160	4		

- Molecule 27 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	101	Total	C	N	O	S	0	0
			779	497	138	142	2		

- Molecule 28 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	111	Total	C	N	O	S	0	0
			841	527	154	158	2		

- Molecule 29 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	91	Total	C	N	O	S	0	0
			736	469	129	134	4		

- Molecule 30 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	102	UNK	ASP	conflict	UNP Q839F3

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	74	Total	C	N	O		0	0
			559	344	107	108			

- Molecule 32 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	61	Total	C	N	O	S	0	0
			480	299	97	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1521	Total	C	N	O	P	0	0
			32595	14542	5954	10578	1521		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	13	Total	C	N	O	P	0	0
			285	127	57	88	13		

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	222	Total	C	N	O	S	0	0
			1773	1126	312	326	9		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	205	Total	C	N	O	S	0	0
			1618	1018	304	293	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	200	Total	C	N	O	S	0	0
			1611	1010	301	296	4		

- Molecule 38 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	163	Total	C	N	O	S	0	0
			1204	759	222	221	2		

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	96	Total	C	N	O	S	0	0
			787	496	135	153	3		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	153	Total	C	N	O	S	0	0
			1218	759	232	221	6		

- Molecule 41 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	131	Total	C	N	O	S	0	0
			1041	662	184	193	2		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	127	Total	C	N	O	S	0	0
			980	610	195	174	1		

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	96	Total	C	N	O	S	0	0
			773	487	142	142	2		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	116	Total	C	N	O	S	0	0
			854	527	163	160	4		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	134	Total	C	N	O	S	0	0
			1051	652	211	186	2		

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	114	Total	C	N	O	S	0	0
			902	552	183	166	1		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	60	Total	C	N	O	S	0	0
			492	310	100	77	5		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	85	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	87	Total	C	N	O	S	0	0
			692	437	128	125	2		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	80	Total	C	N	O	S	0	0
			660	414	124	119	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	63	Total	C	N	O	S	0	0
			511	328	95	87	1		

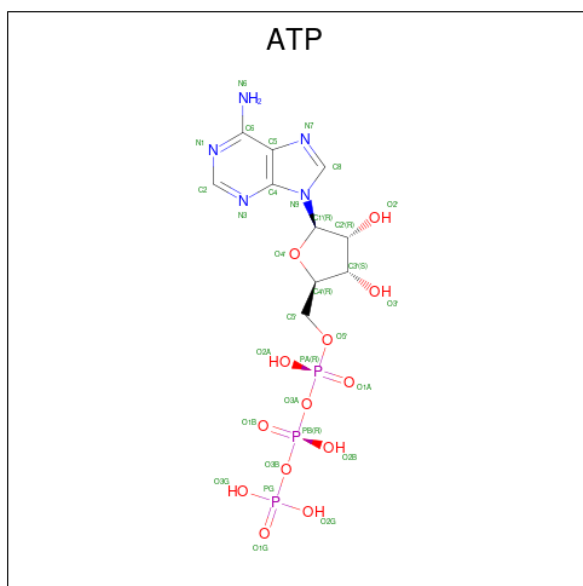
- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	82	Total	C	N	O	S	0	0
			663	426	122	113	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	81	Total	C	N	O	S	0	0
			608	371	118	117	2		

- Molecule 54 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
54	0	1	Total	C	N	O	P	0
			31	10	5	13	3	
54	0	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	0	2	Total	Mg	0
			2	2	
55	A	139	Total	Mg	0
			139	139	
55	B	1	Total	Mg	0
			1	1	
55	G	1	Total	Mg	0
			1	1	
55	Q	1	Total	Mg	0
			1	1	
55	a	44	Total	Mg	0
			44	44	
55	n	1	Total	Mg	0
			1	1	

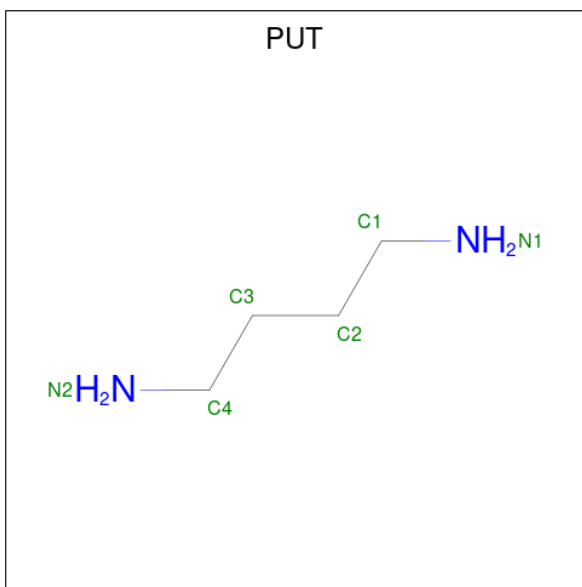
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	4	1	Total 1	Zn 1	0
56	5	1	Total 1	Zn 1	0
56	8	1	Total 1	Zn 1	0
56	o	1	Total 1	Zn 1	0

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

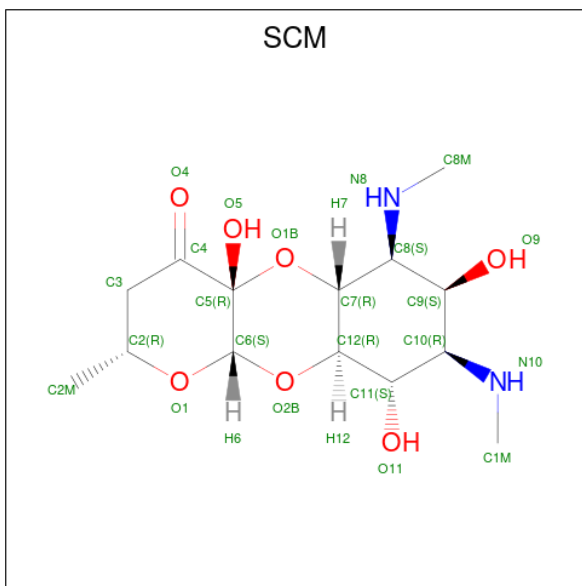
Mol	Chain	Residues	Atoms		AltConf
57	7	2	Total 2	K 2	0
57	A	103	Total 103	K 103	0
57	B	3	Total 3	K 3	0
57	G	3	Total 3	K 3	0
57	P	1	Total 1	K 1	0
57	a	38	Total 38	K 38	0
57	g	1	Total 1	K 1	0
57	o	1	Total 1	K 1	0

- Molecule 58 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
58	a	1	Total	C	N	0
			6	4	2	

- Molecule 59 is SPECTINOMYCIN (CCD ID: SCM) (formula: $C_{14}H_{24}N_2O_7$).

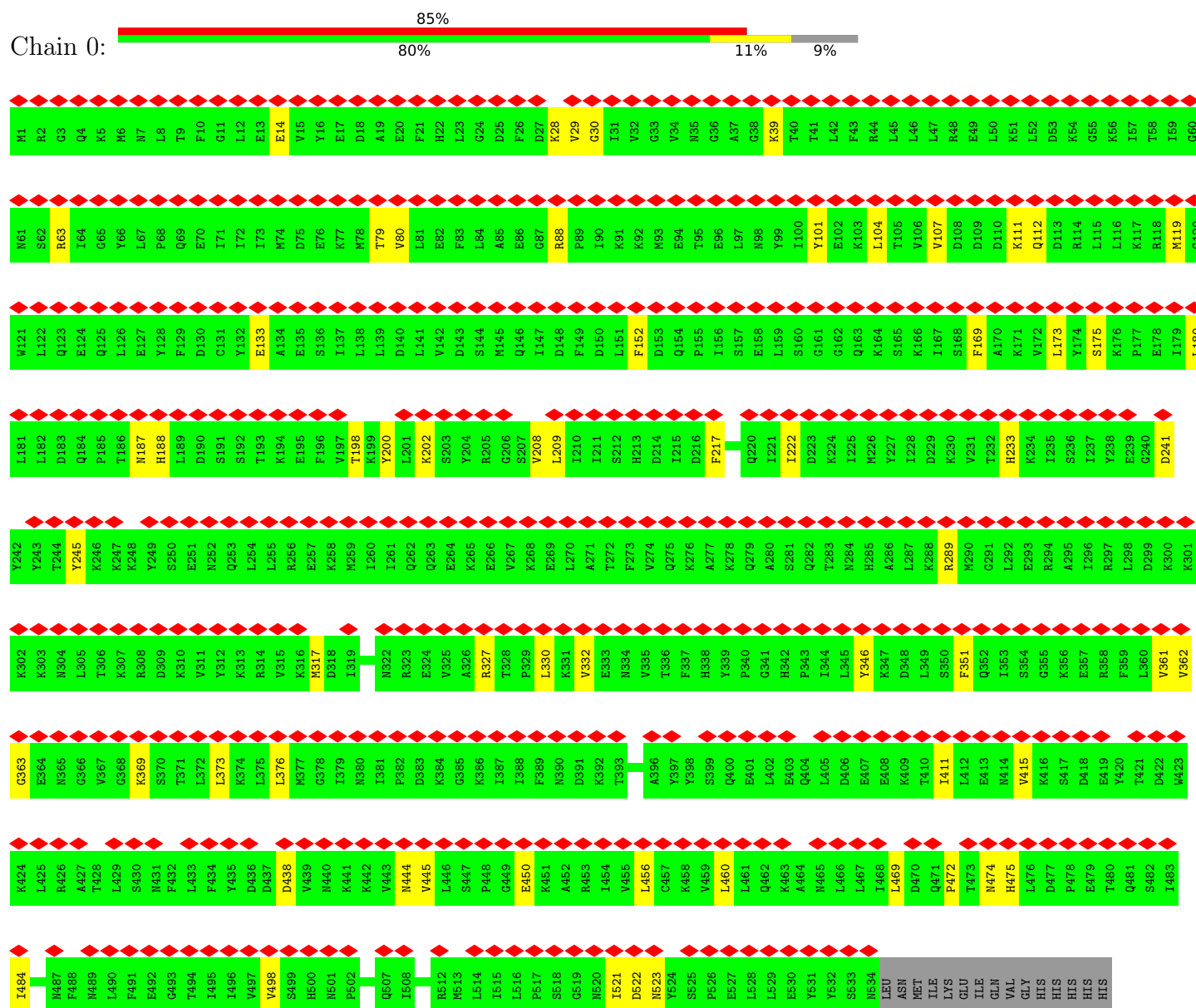


Mol	Chain	Residues	Atoms				AltConf
59	a	1	Total	C	N	O	0
			23	14	2	7	

3 Residue-property plots

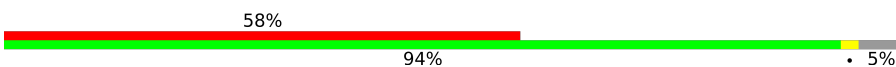
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

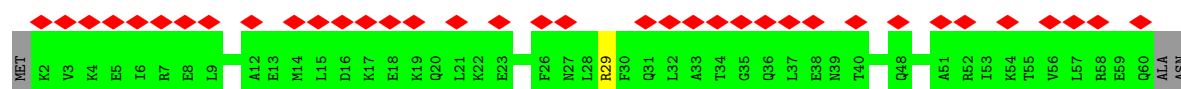
- Molecule 1: ARE-ABC-F family resistance factor PoxA



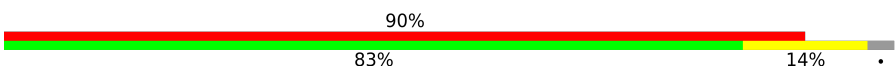
HIS
ALA
LYS
GLY
GLY
GLU
ASN
LEU
TYR
PHE
GLN
GLY
VAL
VAL
ALA
ASP
TYR
LYS
LYS
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GLY
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LYS
GLY

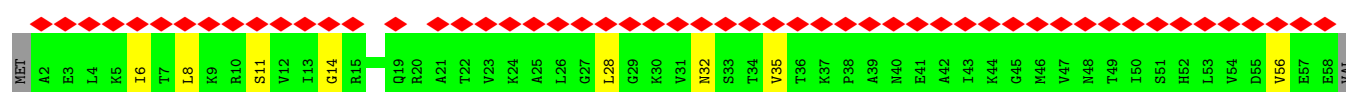
• Molecule 2: 50S ribosomal protein L29

Chain 1: 

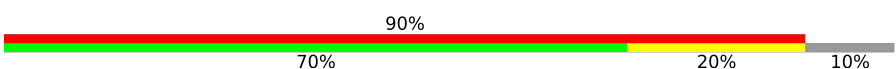


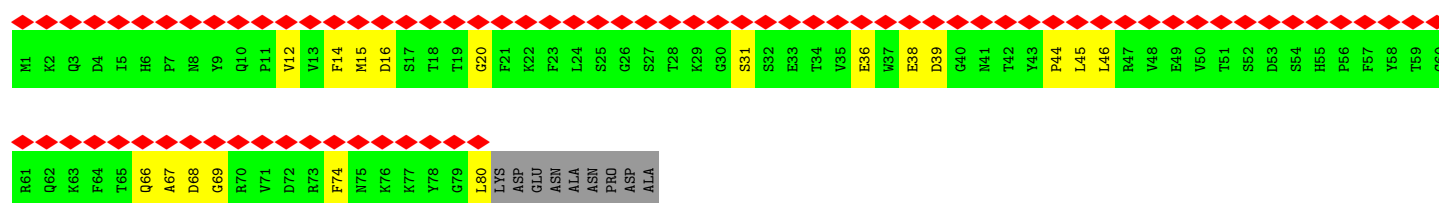
• Molecule 3: 50S ribosomal protein L30

Chain 2: 



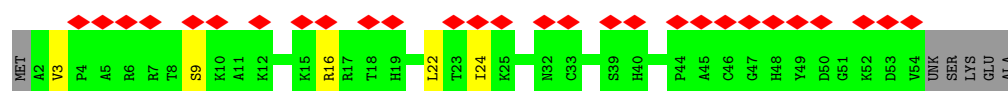
• Molecule 4: 50S ribosomal protein L31 type B

Chain 3: 



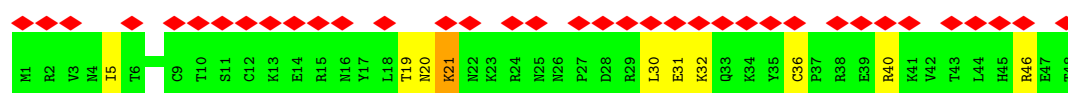
• Molecule 5: 50S ribosomal protein L32-3

Chain 4: 

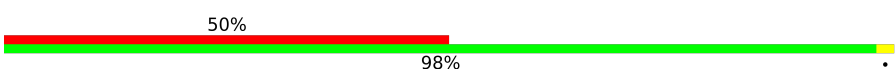


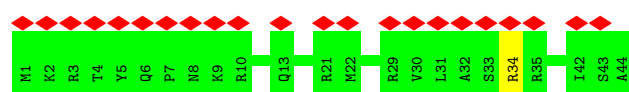
• Molecule 6: 50S ribosomal protein L33 3

Chain 5: 

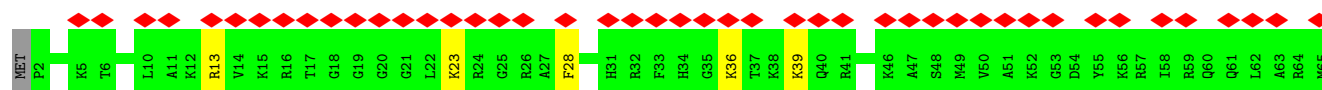


• Molecule 7: 50S ribosomal protein L34

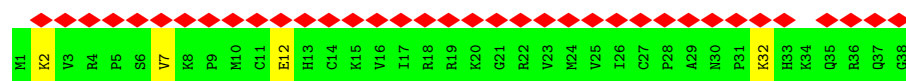
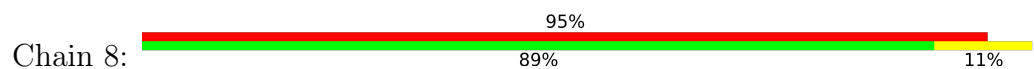
Chain 6: 



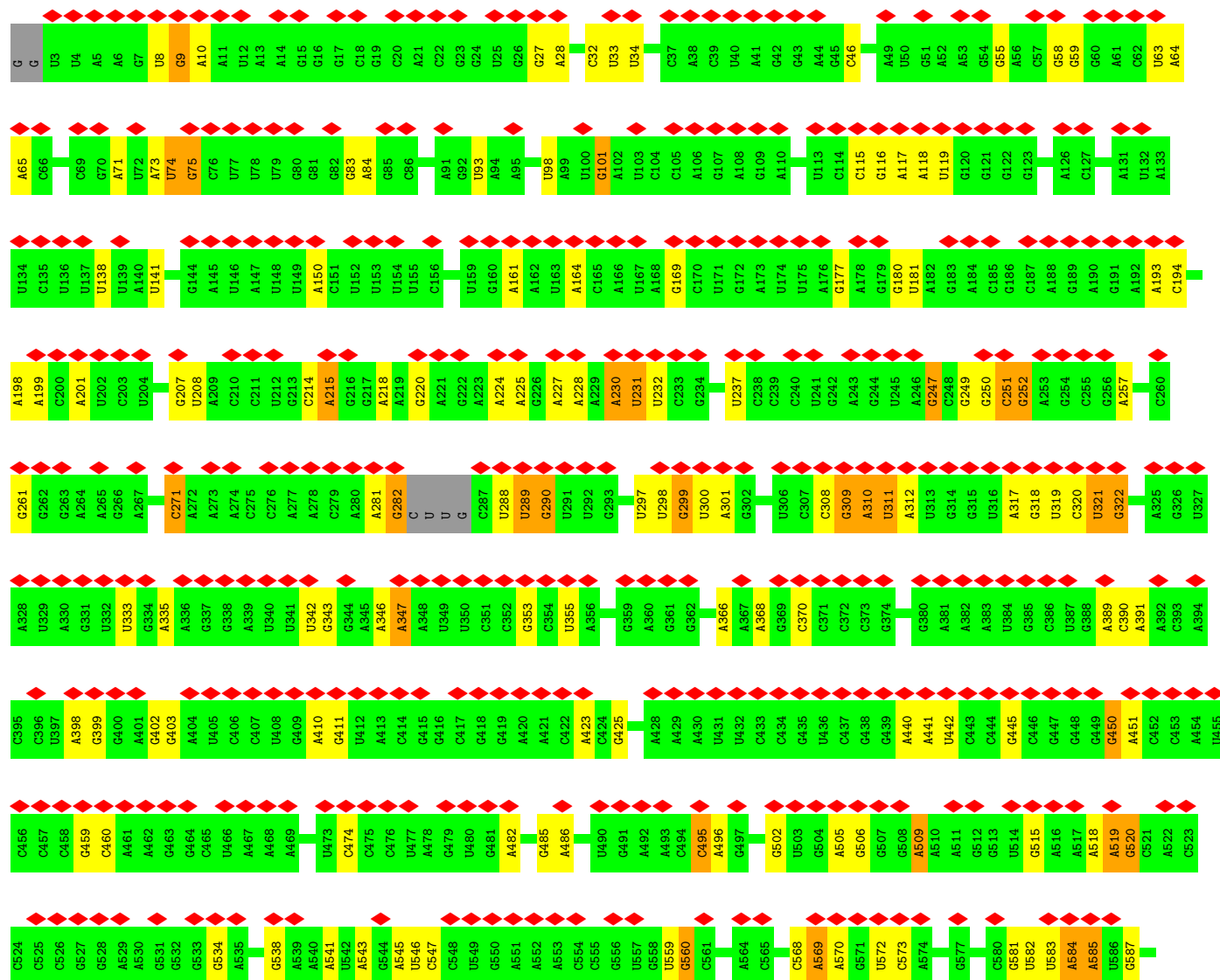
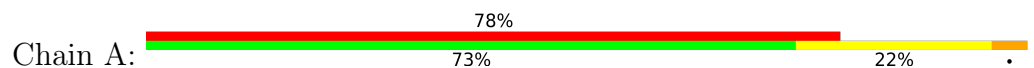
- Molecule 8: 50S ribosomal protein L35

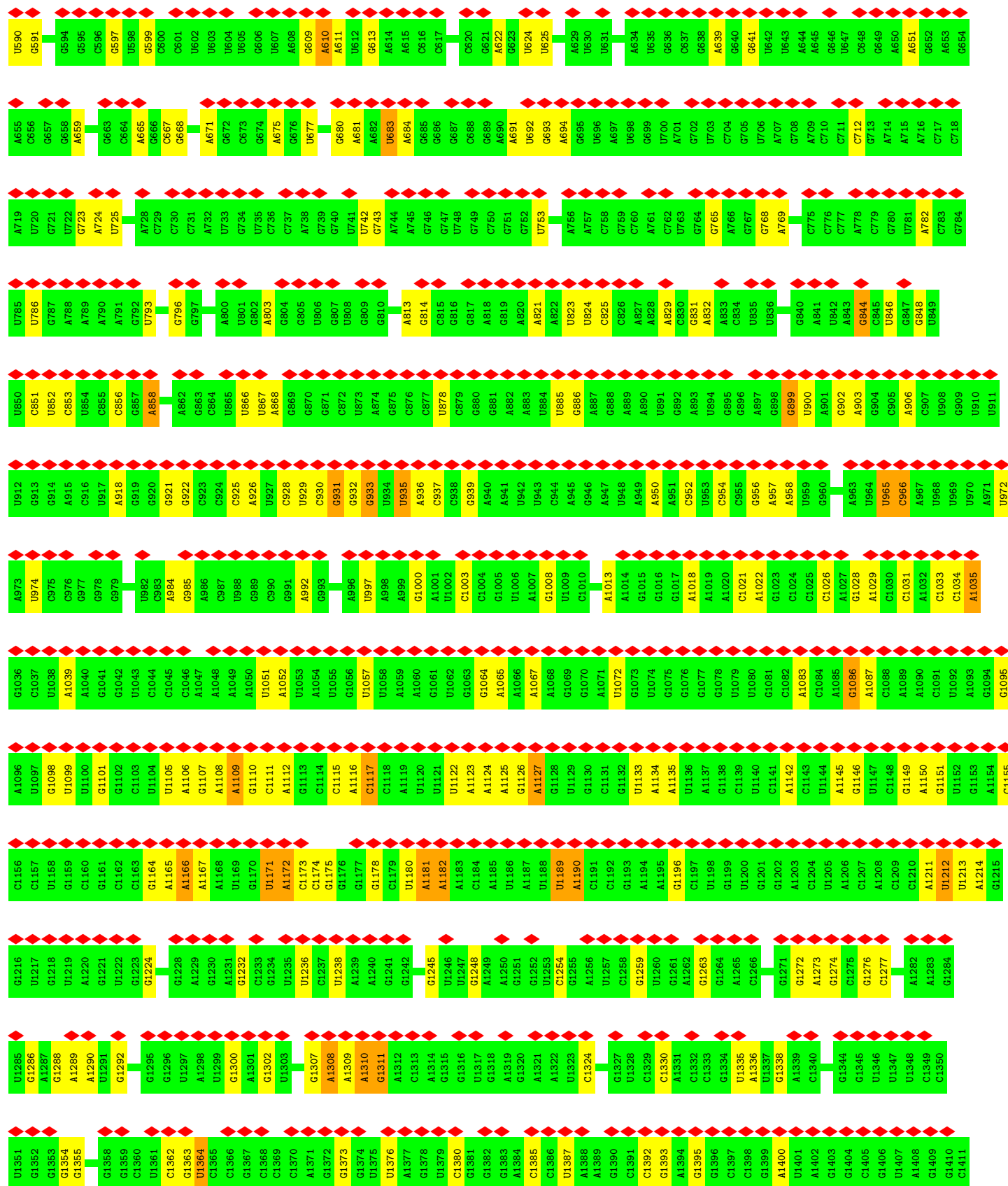


- Molecule 9: 50S ribosomal protein L36



- Molecule 10: 23S rRNA

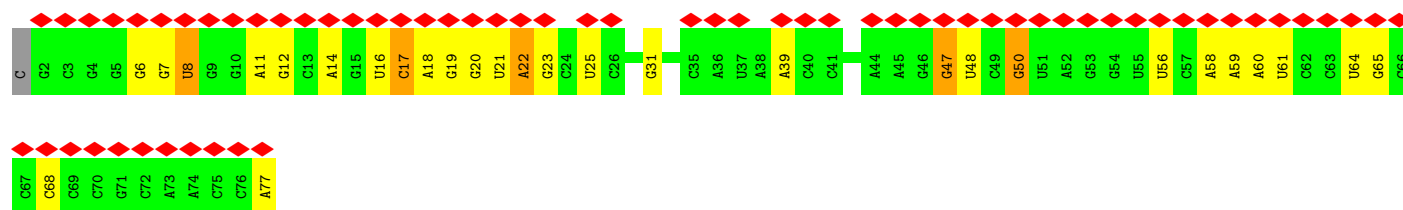
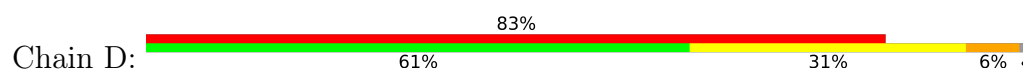




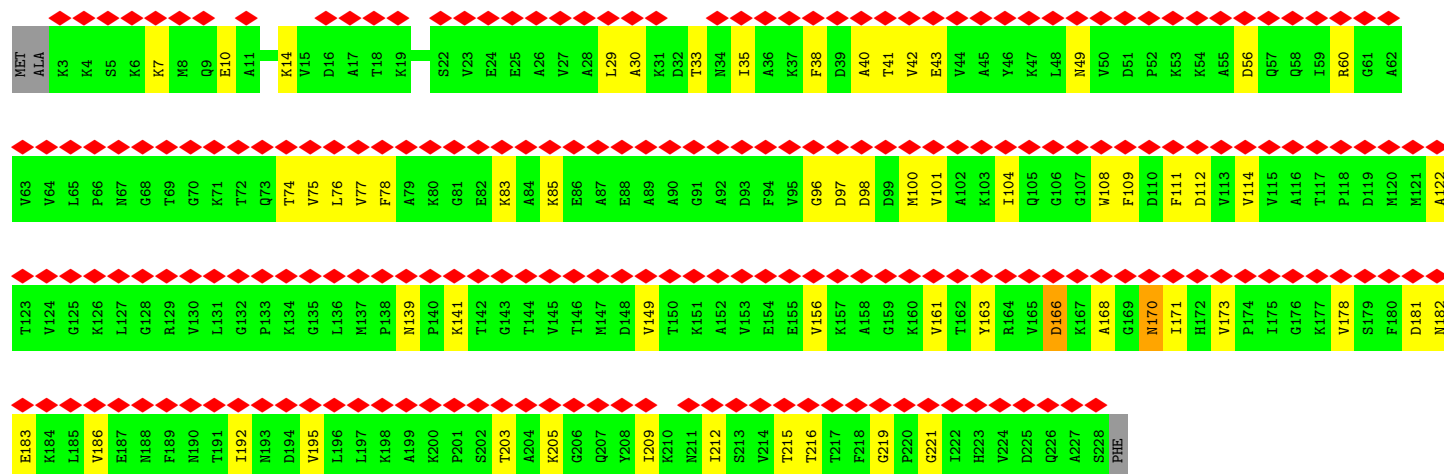
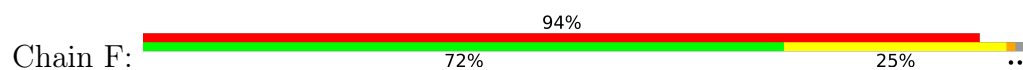
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G2173	U1414		C1610	G1671	U1735	C1795	A1866	U1928	G1988	G2052	U2113	G2173
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G2228	C1478		U1541	C1606	G1667	A1731	U1791	A1984	G2048			G2228
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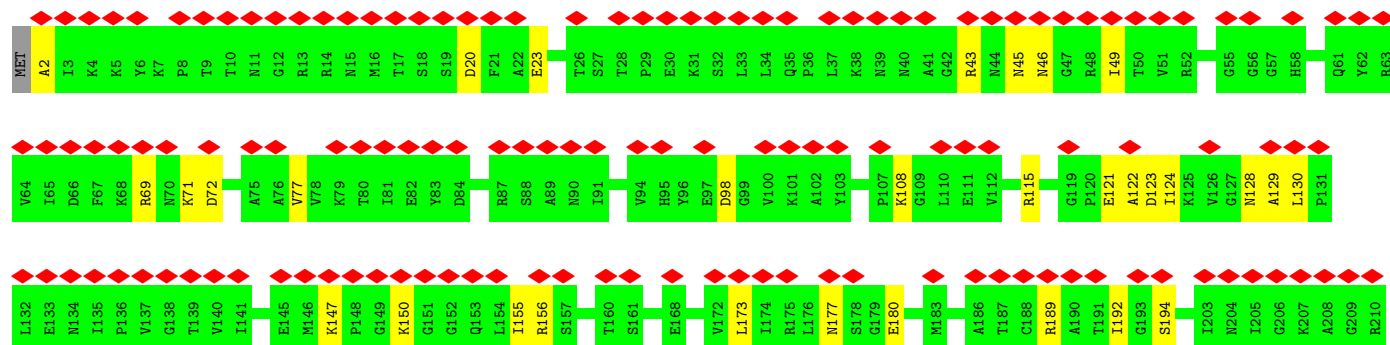
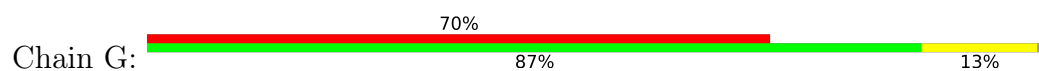
• Molecule 12: tRNA-fMet

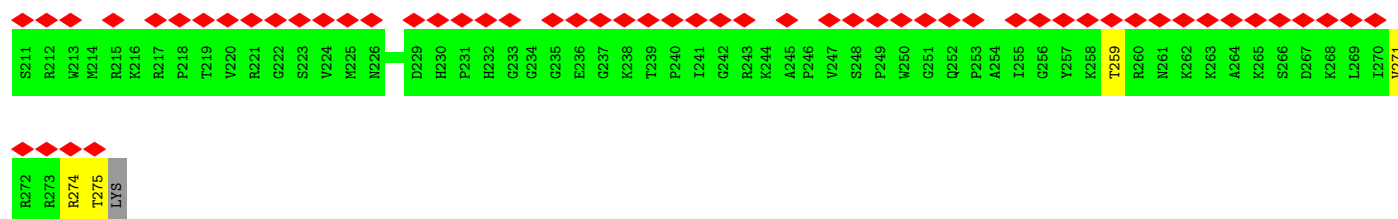


• Molecule 13: 50S ribosomal protein L1

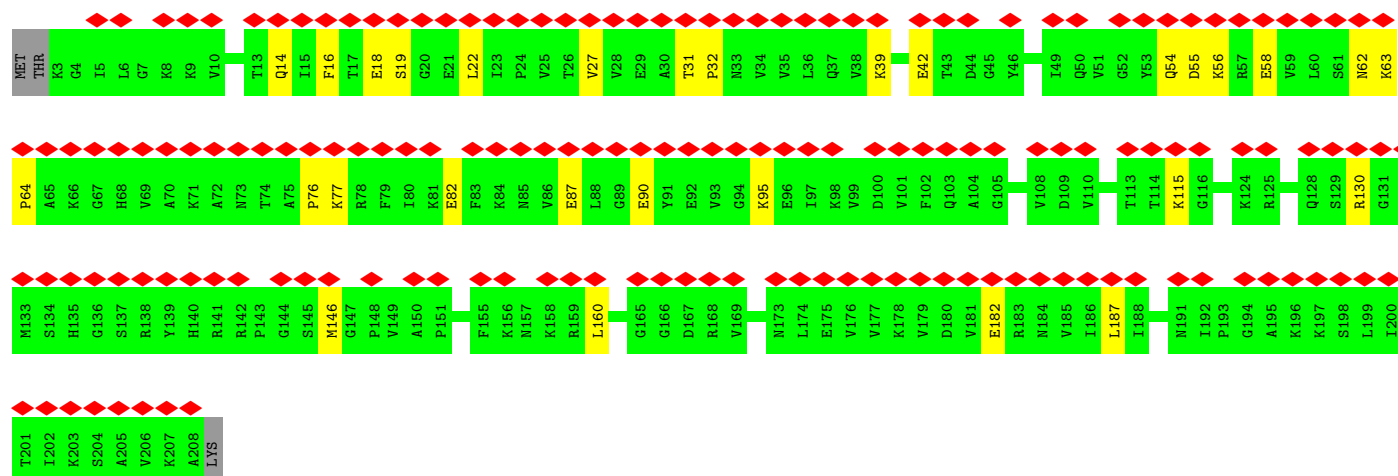
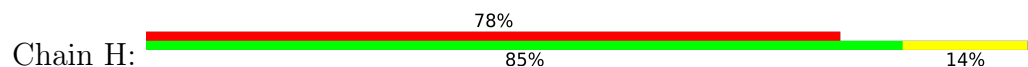


• Molecule 14: 50S ribosomal protein L2

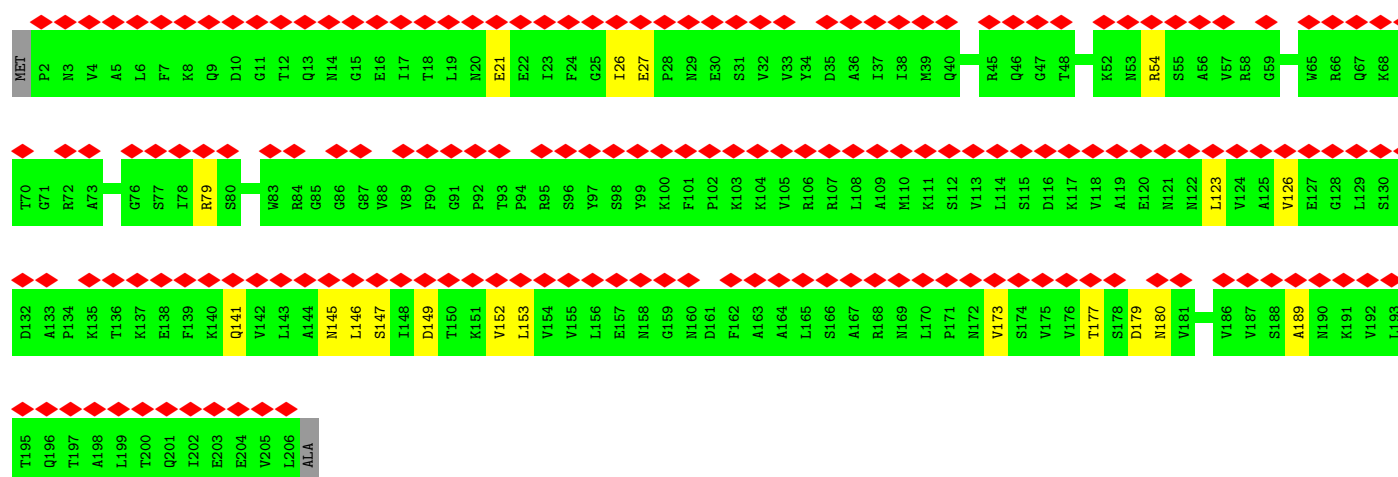
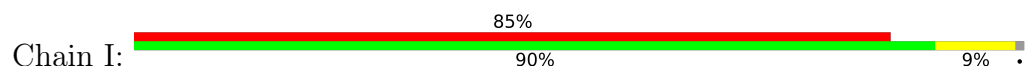




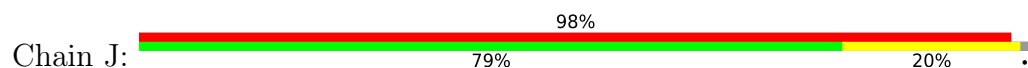
• Molecule 15: 50S ribosomal protein L3



• Molecule 16: 50S ribosomal protein L4

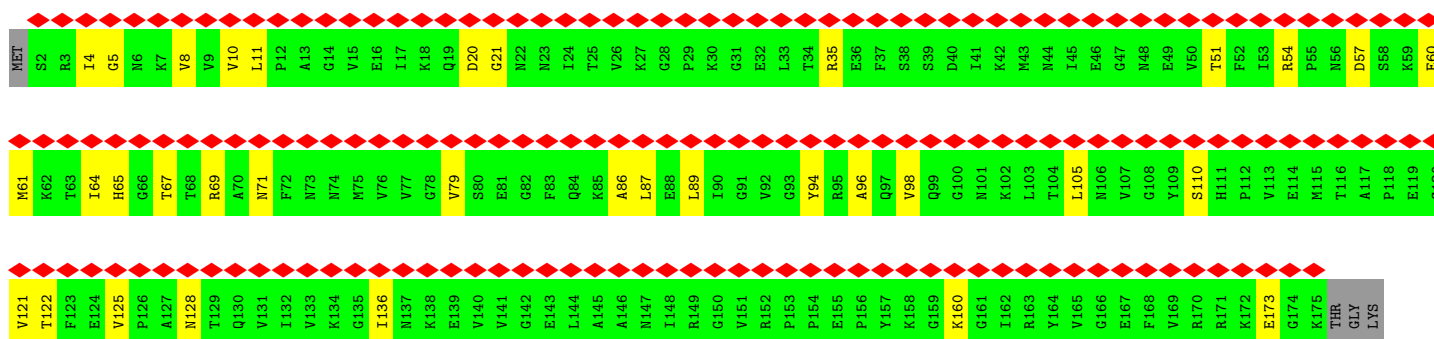
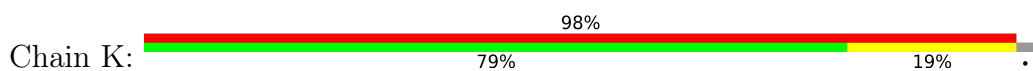


• Molecule 17: 50S ribosomal protein L5

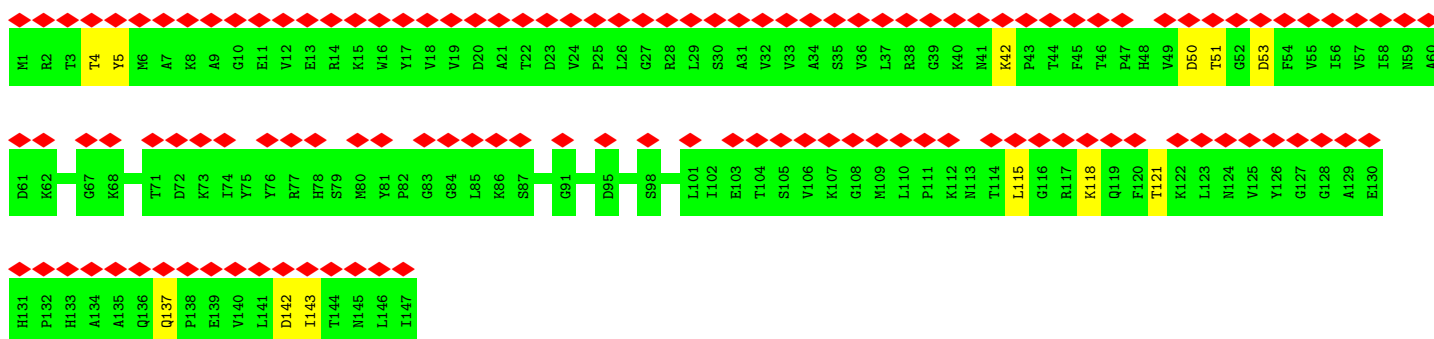
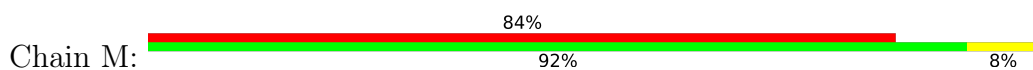




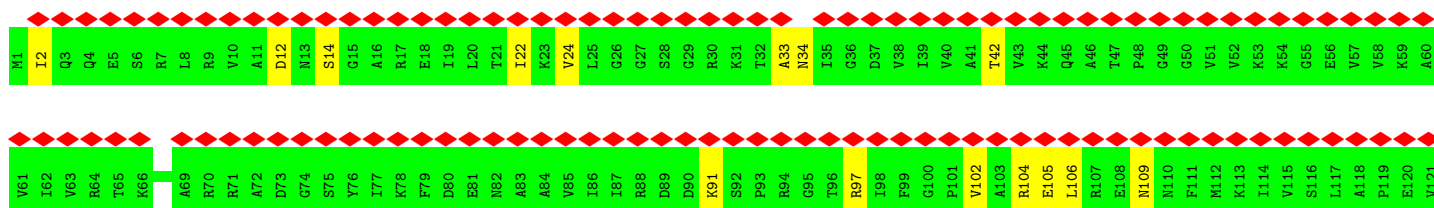
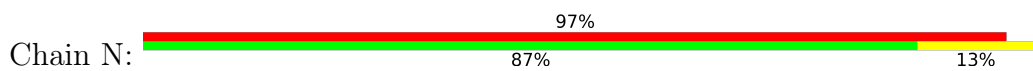
• Molecule 18: 50S ribosomal protein L6



• Molecule 19: 50S ribosomal protein L13

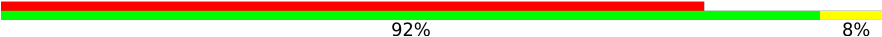


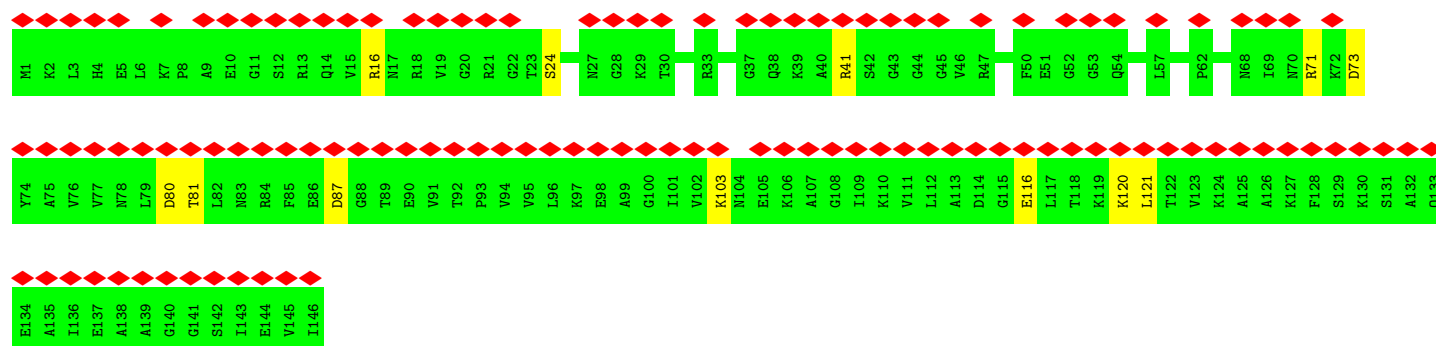
• Molecule 20: 50S ribosomal protein L14



◆
L122

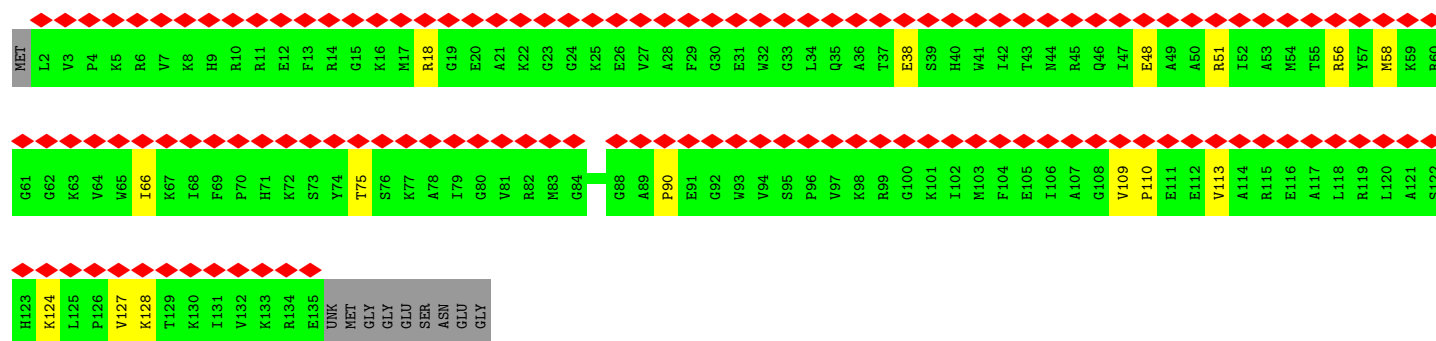
• Molecule 21: 50S ribosomal protein L15

Chain O: 



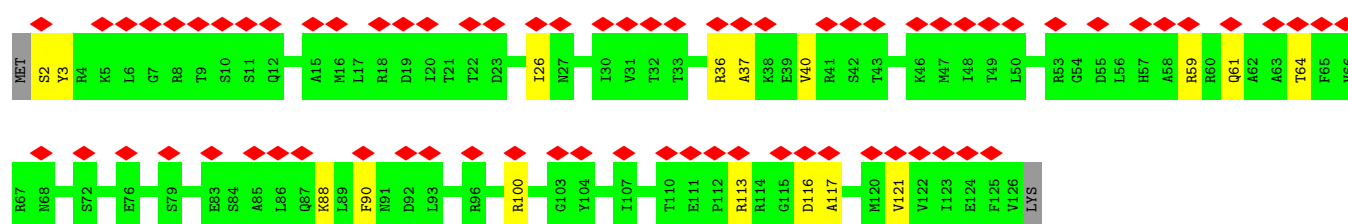
• Molecule 22: 50S ribosomal protein L16

Chain P: 



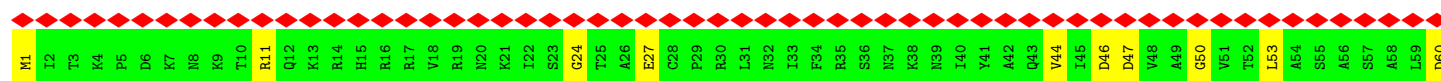
• Molecule 23: 50S ribosomal protein L17

Chain Q: 

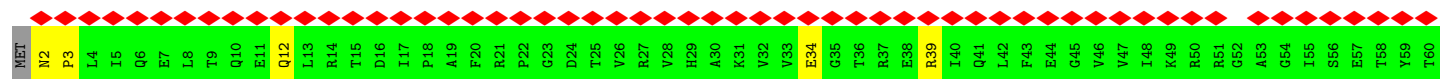
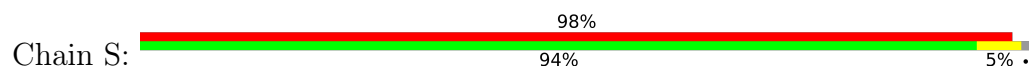


• Molecule 24: 50S ribosomal protein L18

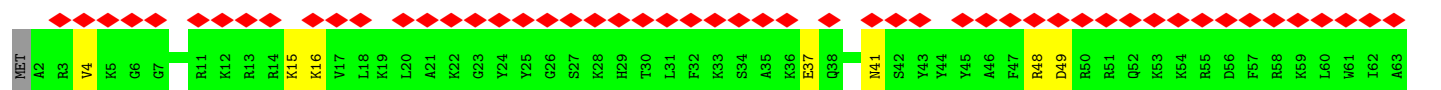
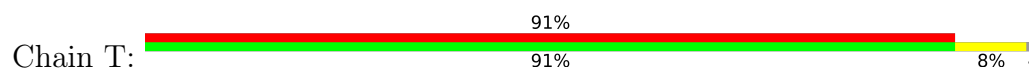
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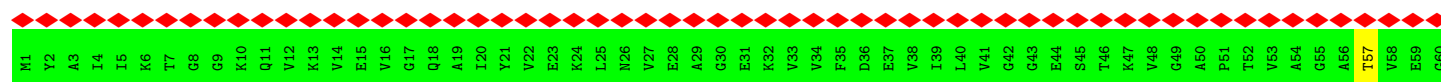
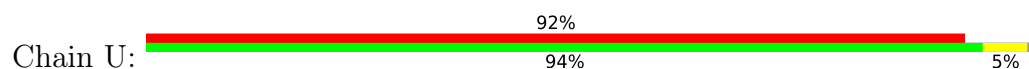
• Molecule 25: 50S ribosomal protein L19



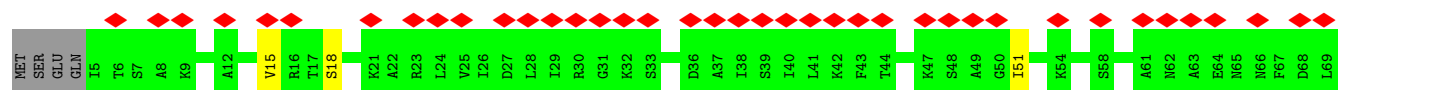
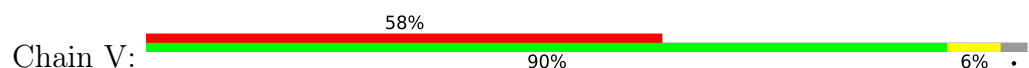
• Molecule 26: 50S ribosomal protein L20

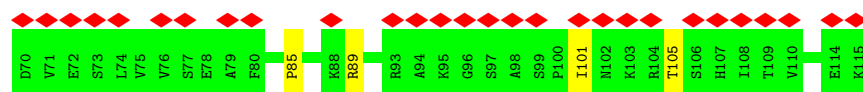


• Molecule 27: 50S ribosomal protein L21

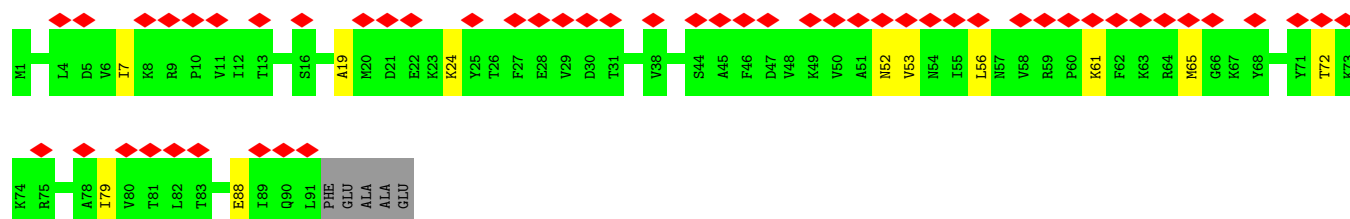
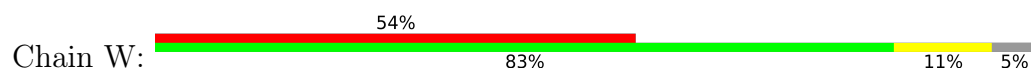


• Molecule 28: 50S ribosomal protein L22

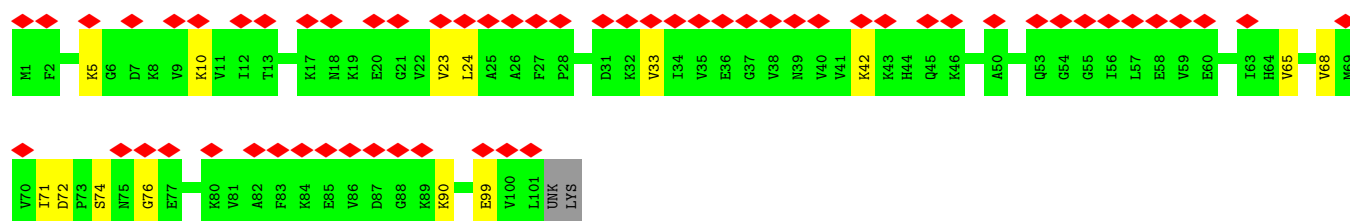
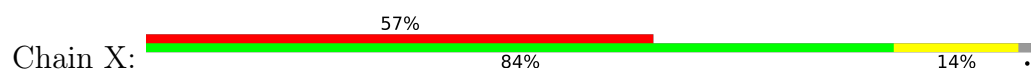




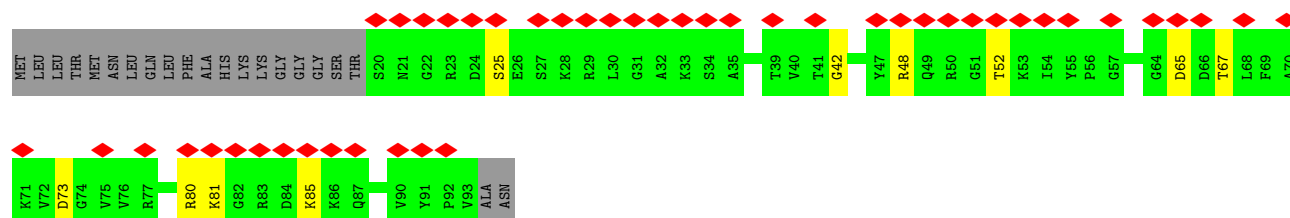
• Molecule 29: 50S ribosomal protein L23



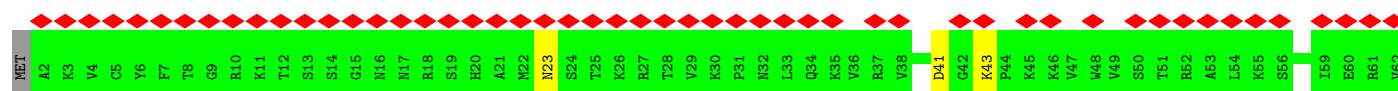
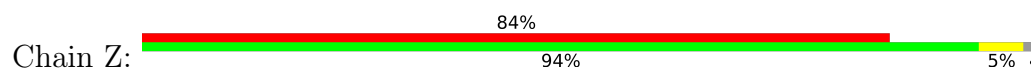
• Molecule 30: 50S ribosomal protein L24



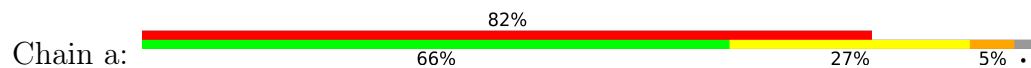
• Molecule 31: 50S ribosomal protein L27

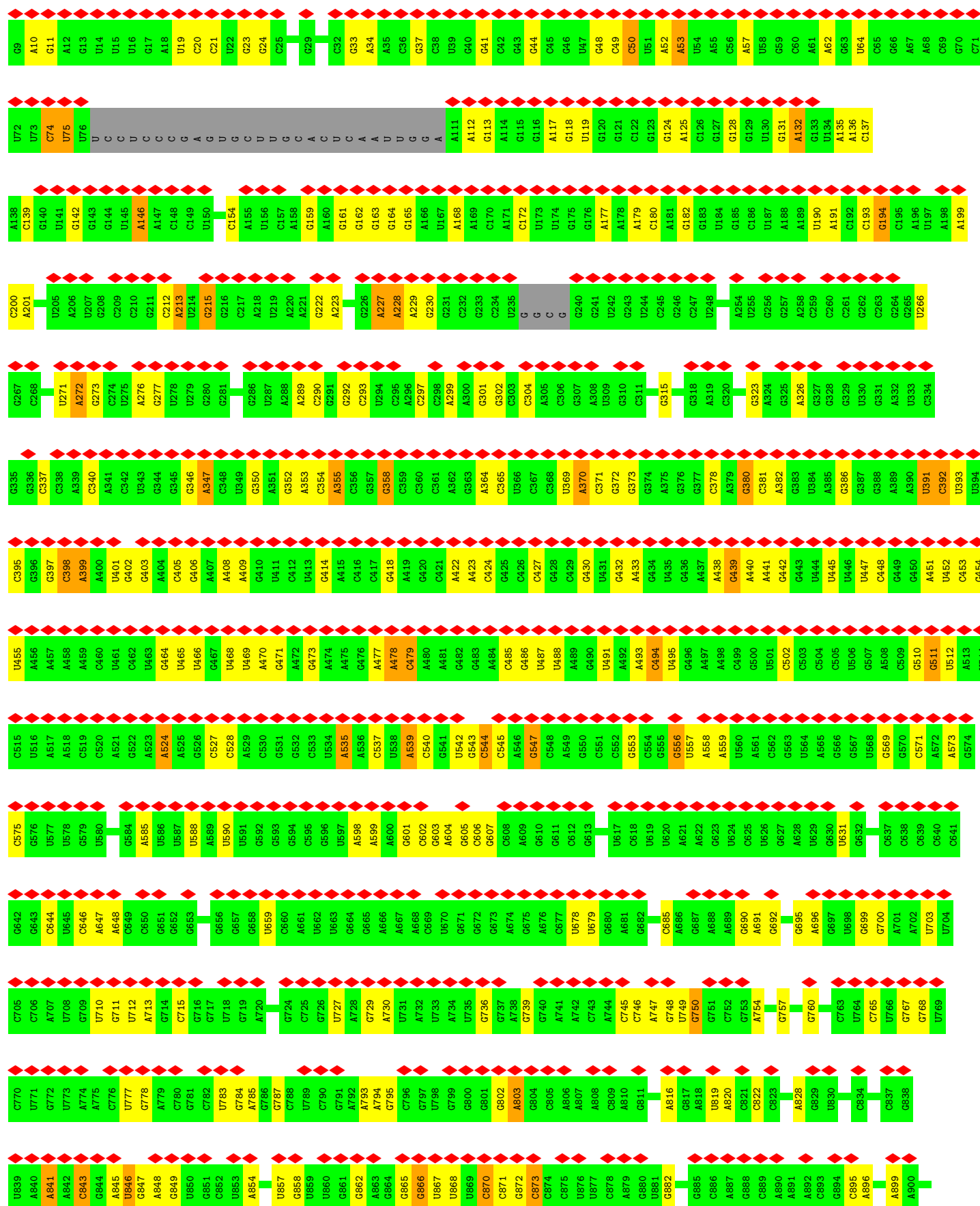


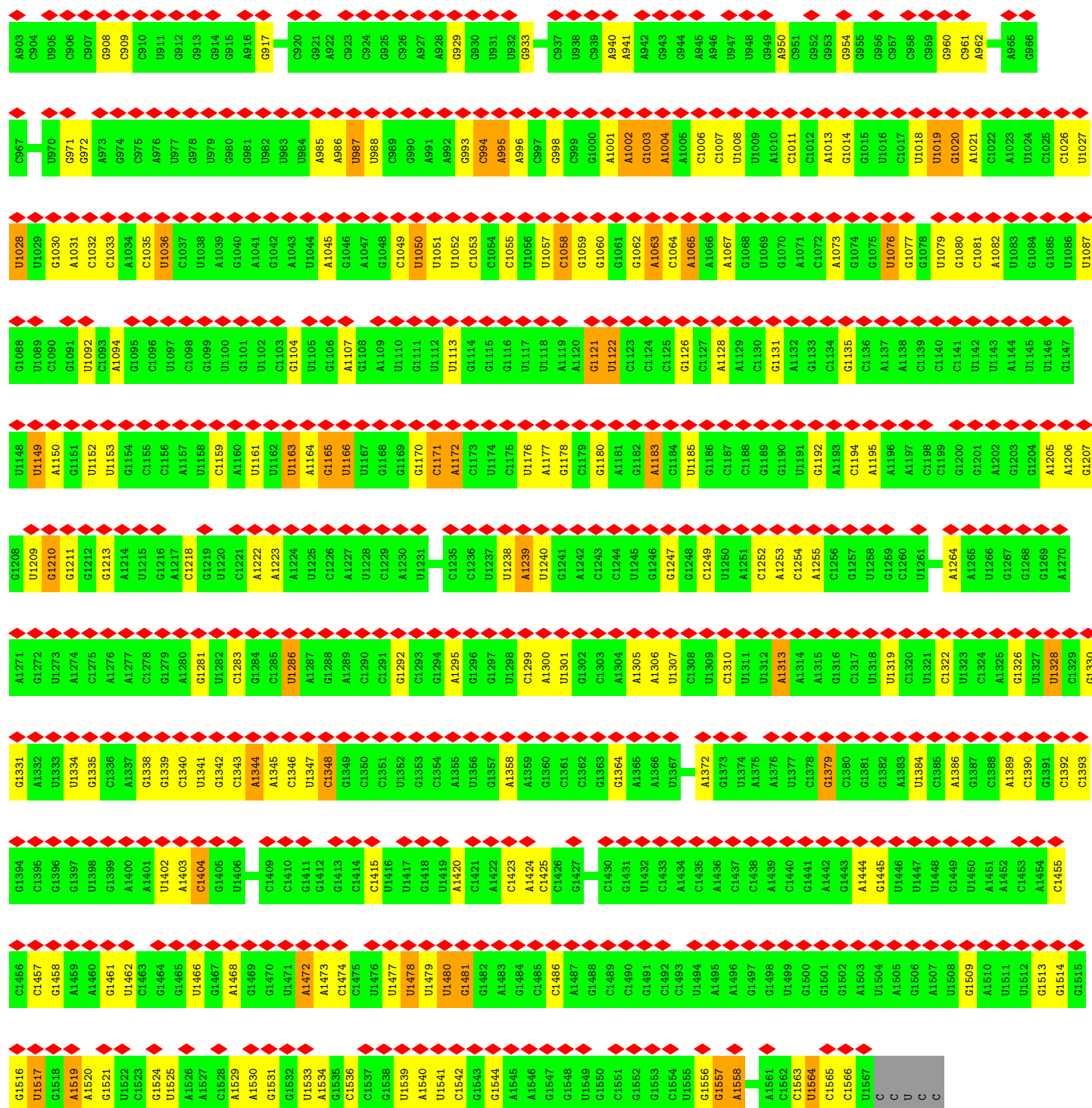
• Molecule 32: 50S ribosomal protein L28

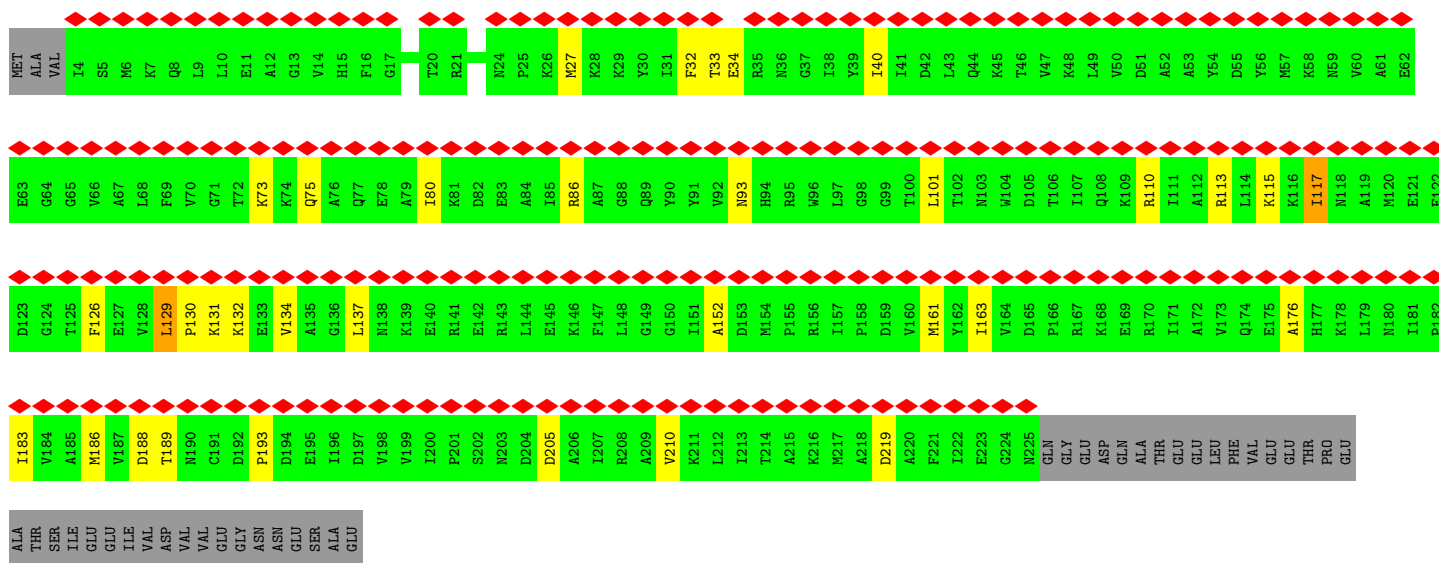
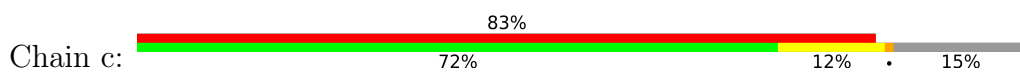


• Molecule 33: 16S rRNA

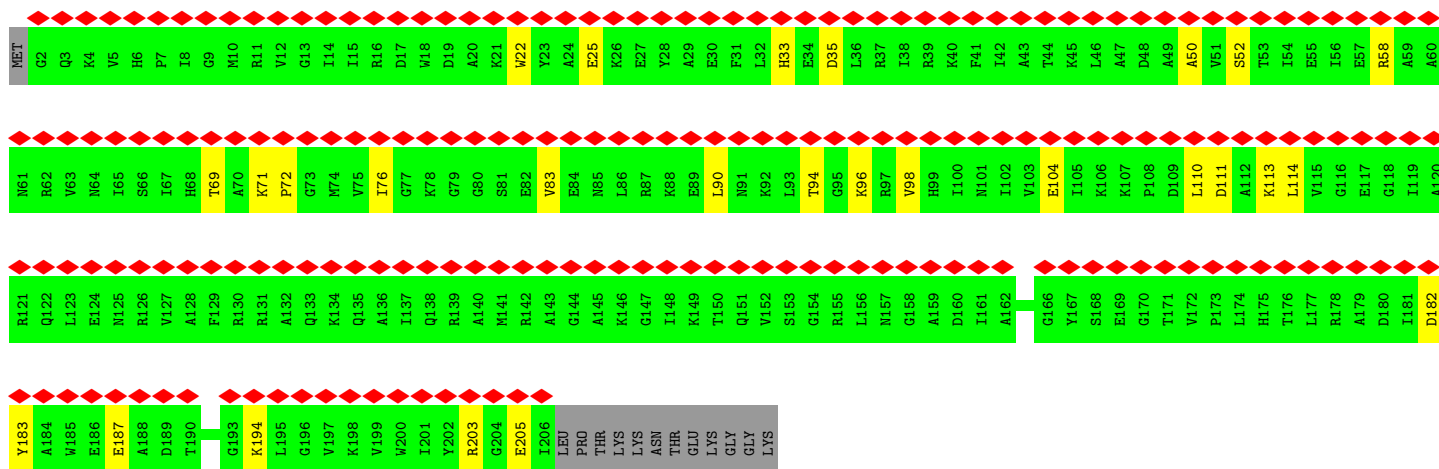
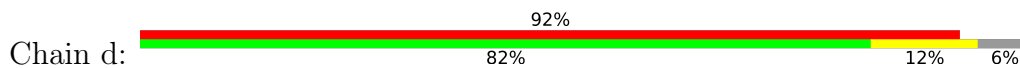




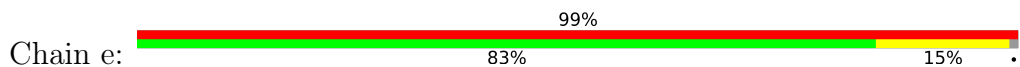


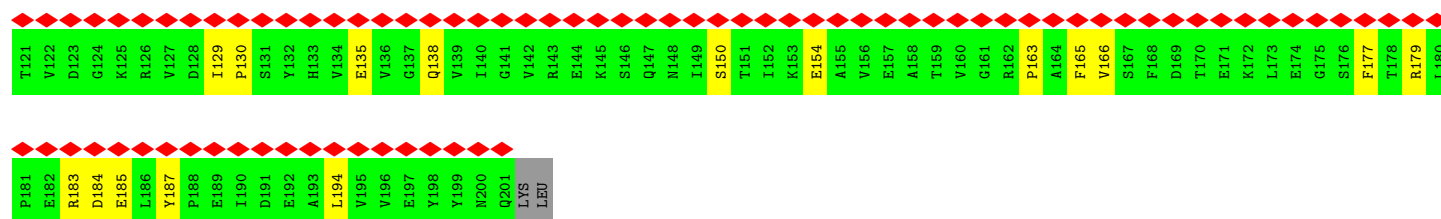


- Molecule 36: 30S ribosomal protein S3

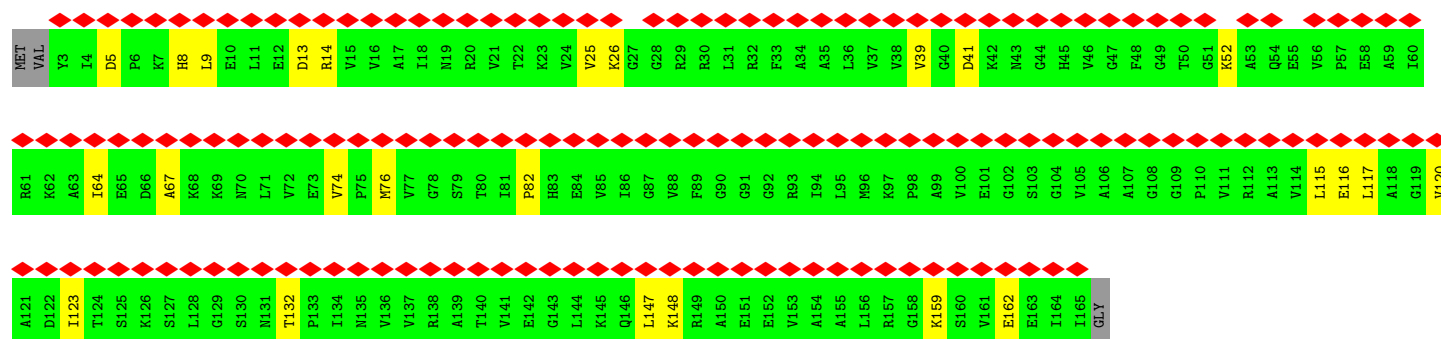
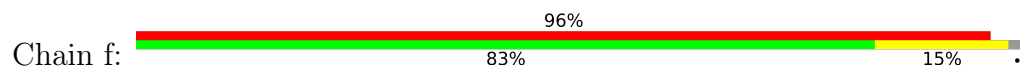


- Molecule 37: 30S ribosomal protein S4

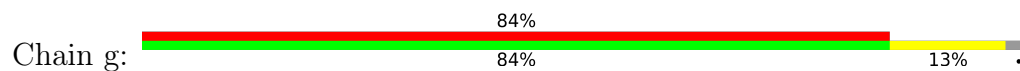




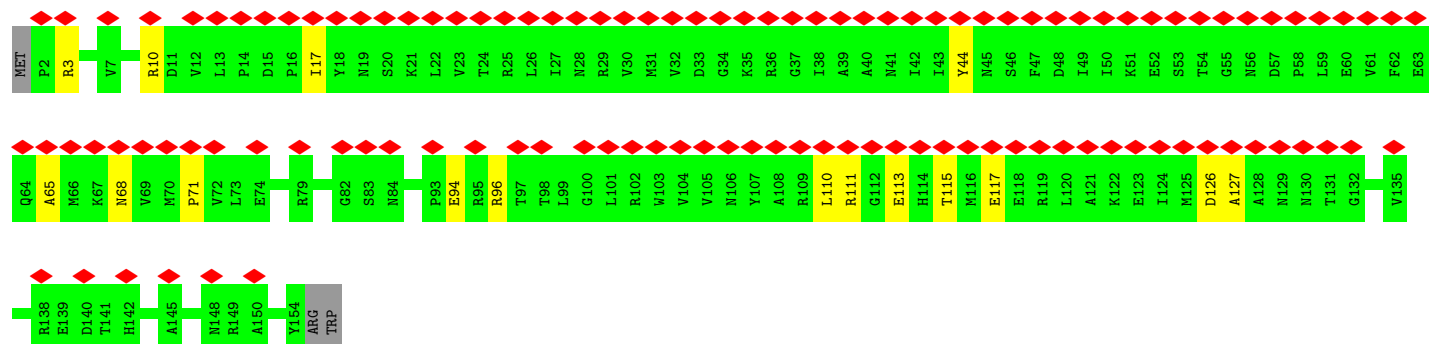
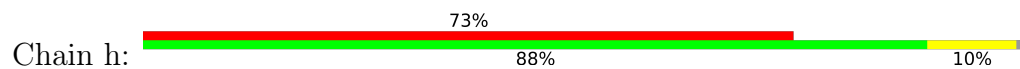
• Molecule 38: 30S ribosomal protein S5



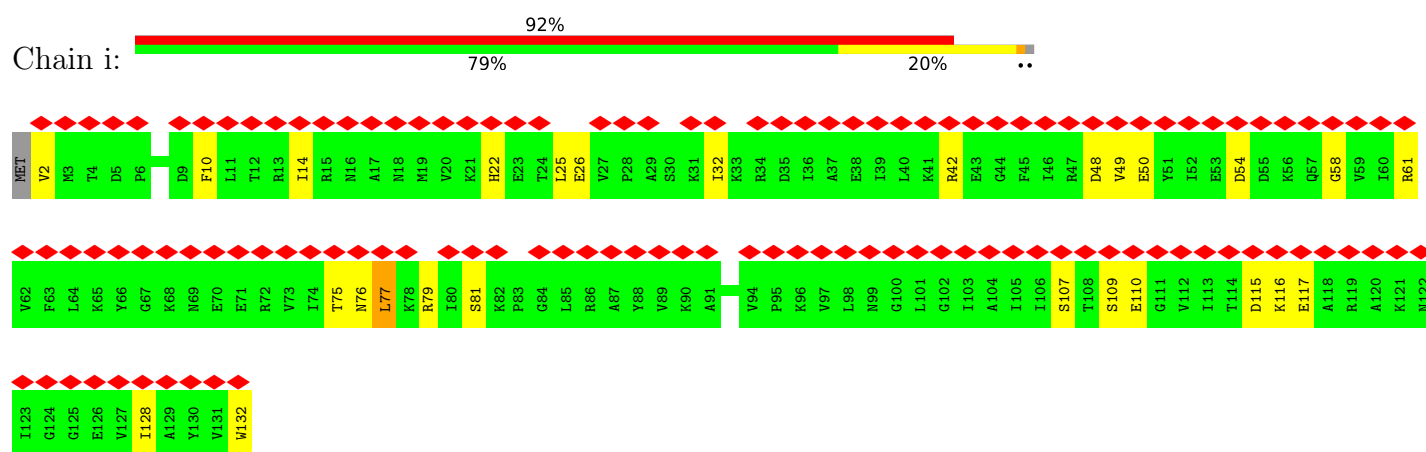
• Molecule 39: 30S ribosomal protein S6



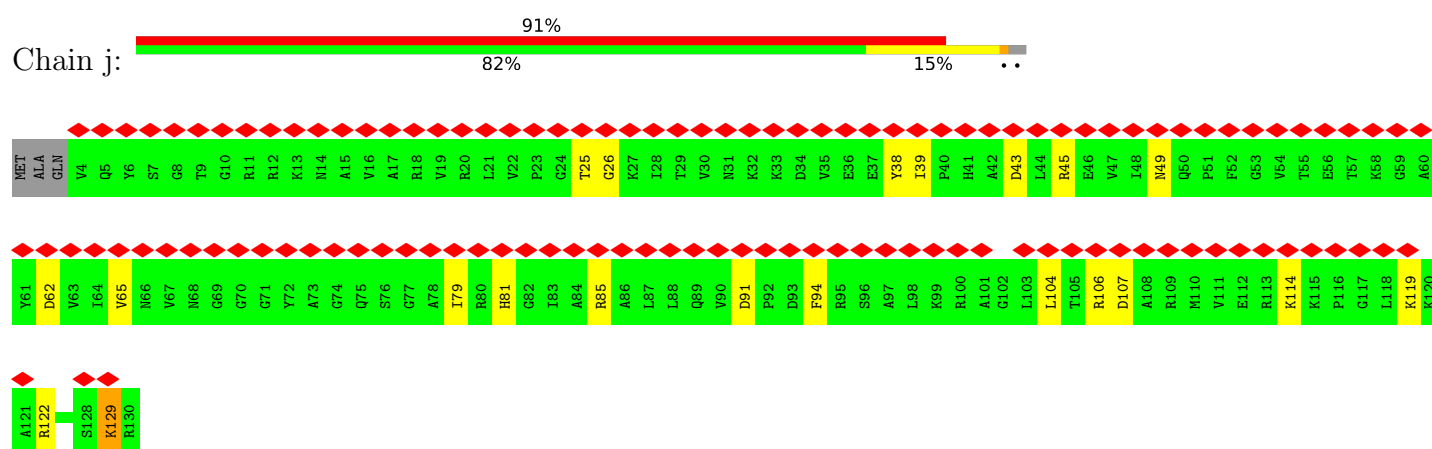
• Molecule 40: 30S ribosomal protein S7



• Molecule 41: 30S ribosomal protein S8



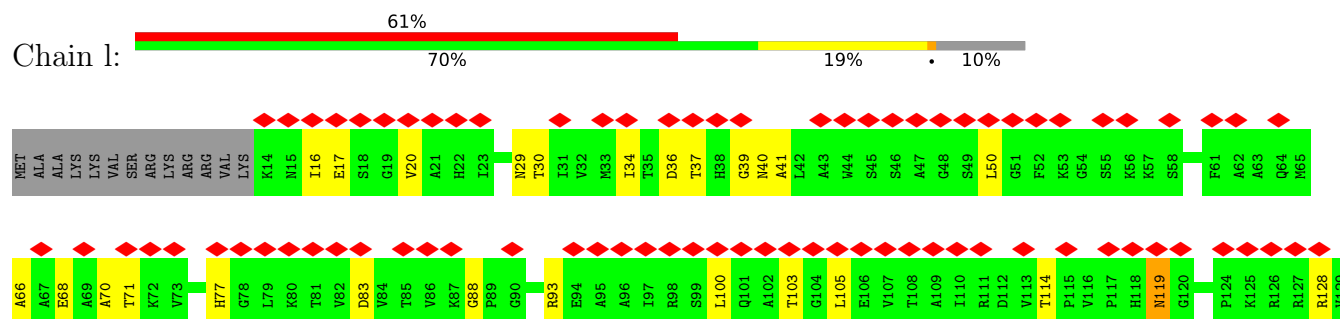
• Molecule 42: 30S ribosomal protein S9

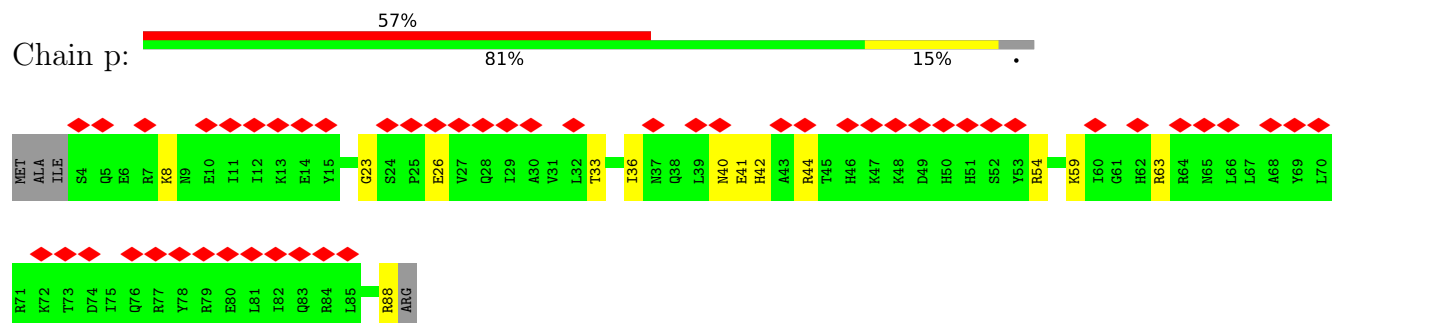


• Molecule 43: 30S ribosomal protein S10

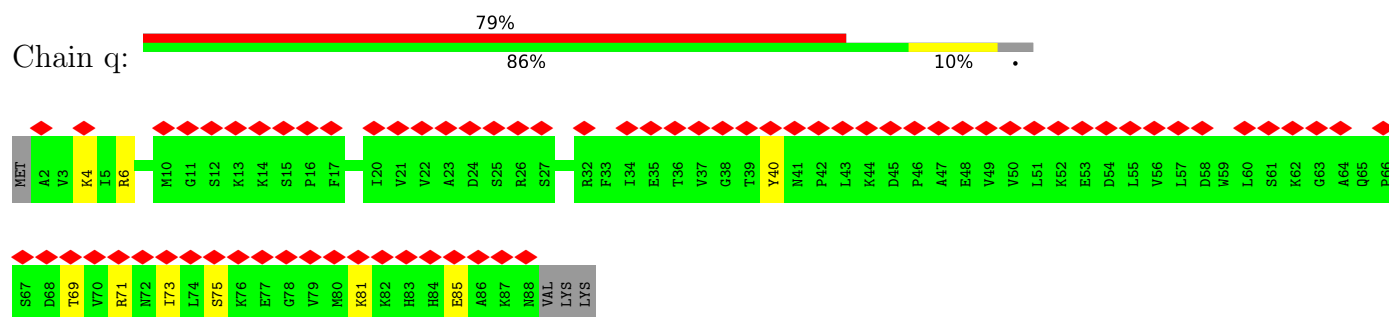


• Molecule 44: 30S ribosomal protein S11

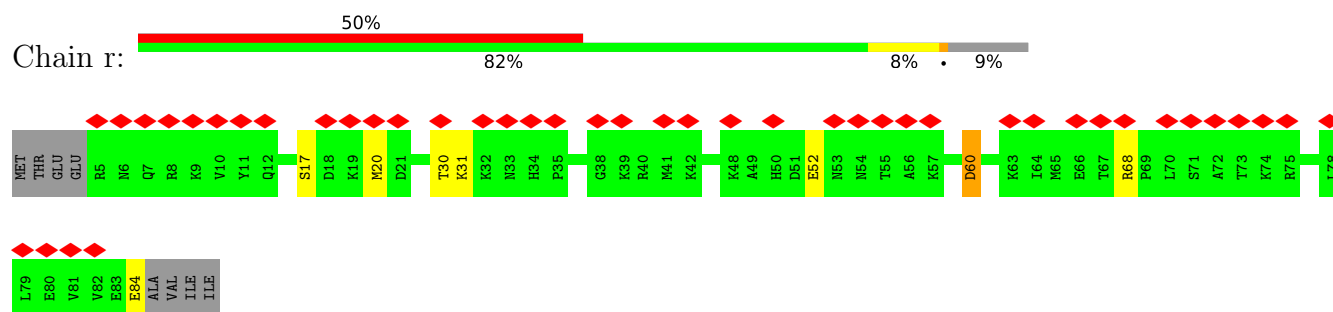




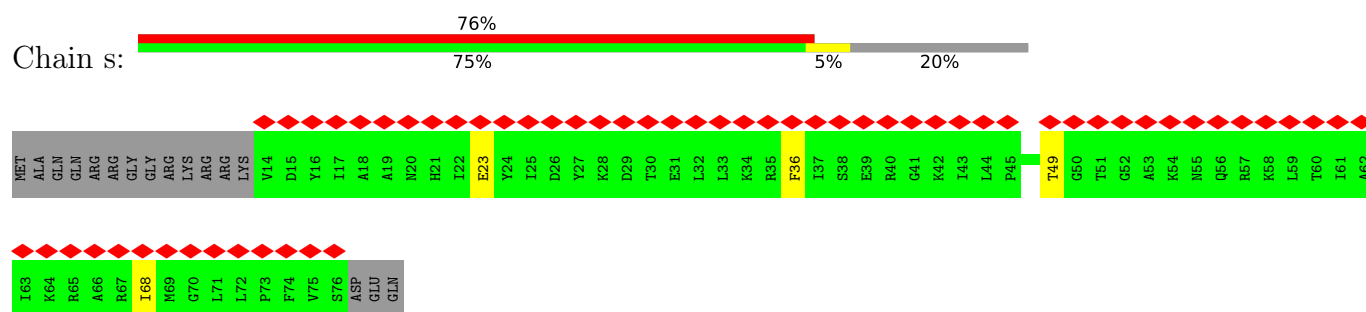
- Molecule 49: 30S ribosomal protein S16



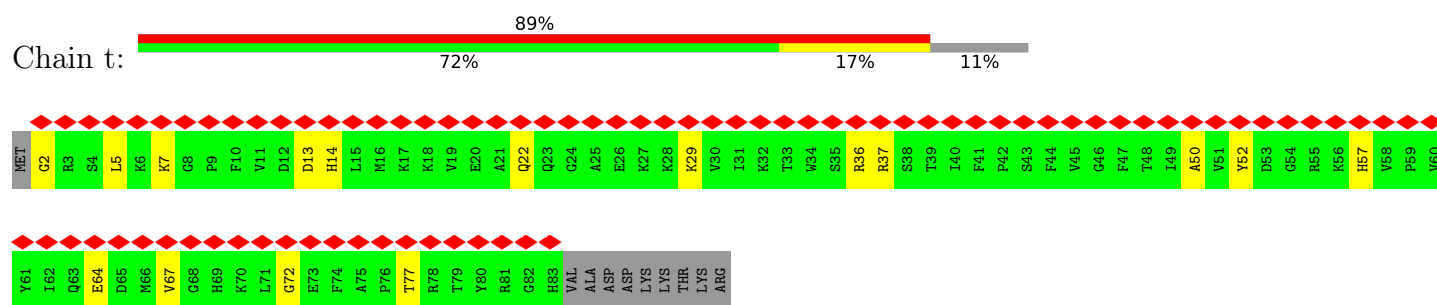
- Molecule 50: 30S ribosomal protein S17



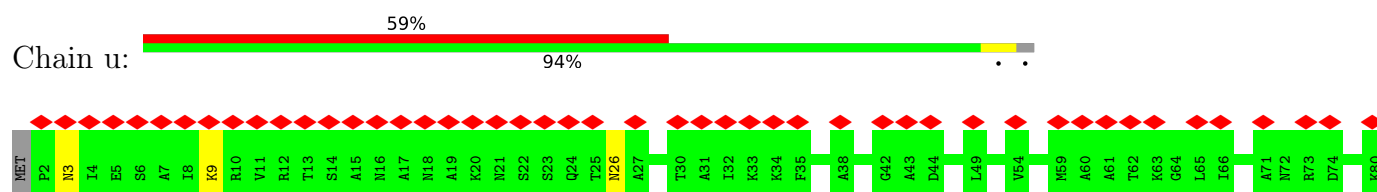
- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29581	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 ($e^-/\text{\AA}^2$)	30.255	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.064	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

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

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	0	0.15	0/4421	0.26	0/5951
2	1	0.16	0/492	0.21	0/654
3	2	0.19	0/430	0.25	0/579
4	3	0.13	0/664	0.26	0/896
5	4	0.19	0/413	0.27	0/549
6	5	0.21	0/415	0.25	0/552
7	6	0.22	0/377	0.32	0/491
8	7	0.21	0/529	0.28	0/689
9	8	0.20	0/310	0.24	0/409
10	A	0.25	0/69752	0.32	0/108803
11	B	0.18	0/2728	0.22	0/4252
12	D	0.20	0/1815	0.24	0/2828
13	F	0.10	0/1717	0.27	0/2318
14	G	0.21	0/2141	0.27	0/2881
15	H	0.21	0/1594	0.27	0/2140
16	I	0.20	0/1595	0.24	0/2157
17	J	0.13	0/1411	0.27	0/1897
18	K	0.14	0/1355	0.25	0/1825
19	M	0.21	0/1167	0.25	0/1576
20	N	0.21	0/930	0.24	0/1247
21	O	0.20	0/1106	0.26	0/1474
22	P	0.20	0/1093	0.27	0/1457
23	Q	0.21	0/1006	0.25	0/1349
24	R	0.17	0/917	0.26	0/1226
25	S	0.20	0/939	0.25	0/1262
26	T	0.22	0/963	0.27	0/1280
27	U	0.21	0/791	0.24	0/1061
28	V	0.21	0/850	0.25	0/1145
29	W	0.20	0/743	0.27	0/993
30	X	0.18	0/772	0.25	0/1035
31	Y	0.21	0/565	0.26	0/755
32	Z	0.17	0/486	0.23	0/648

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.20	0/36487	0.25	0/56905
34	b	0.15	0/319	0.32	0/494
35	c	0.14	0/1803	0.27	0/2430
36	d	0.16	0/1643	0.24	0/2208
37	e	0.15	0/1641	0.24	0/2206
38	f	0.17	0/1217	0.25	0/1641
39	g	0.14	0/799	0.25	0/1075
40	h	0.15	0/1238	0.24	0/1668
41	i	0.17	0/1054	0.27	0/1417
42	j	0.15	0/993	0.27	0/1331
43	k	0.15	0/785	0.26	0/1059
44	l	0.14	0/869	0.25	0/1174
45	m	0.16	0/1068	0.30	0/1435
46	n	0.13	0/908	0.25	0/1219
47	o	0.18	0/504	0.23	0/669
48	p	0.16	0/726	0.23	0/969
49	q	0.16	0/704	0.28	0/945
50	r	0.15	0/668	0.26	0/891
51	s	0.14	0/518	0.24	0/694
52	t	0.14	0/680	0.25	0/911
53	u	0.16	0/611	0.26	0/818
All	All	0.22	0/159722	0.28	0/238538

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	4347	0	4448	39	0
2	1	491	0	527	1	0
3	2	428	0	463	5	0
4	3	647	0	616	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	4	406	0	417	4	0
6	5	411	0	422	6	0
7	6	374	0	424	1	0
8	7	523	0	575	4	0
9	8	305	0	337	4	0
10	A	62268	0	31269	332	0
11	B	2439	0	1228	16	0
12	D	1624	0	824	14	0
13	F	1693	0	1751	41	0
14	G	2106	0	2189	27	0
15	H	1572	0	1654	19	0
16	I	1572	0	1614	14	0
17	J	1392	0	1454	25	0
18	K	1335	0	1369	23	0
19	M	1146	0	1191	7	0
20	N	923	0	985	13	0
21	O	1096	0	1149	10	0
22	P	1070	0	1136	11	0
23	Q	997	0	1033	9	0
24	R	908	0	944	10	0
25	S	925	0	979	5	0
26	T	950	0	1009	9	0
27	U	779	0	821	4	0
28	V	841	0	898	4	0
29	W	736	0	795	7	0
30	X	763	0	823	10	0
31	Y	559	0	568	9	0
32	Z	480	0	522	2	0
33	a	32595	0	16411	261	0
34	b	285	0	143	3	0
35	c	1773	0	1810	24	0
36	d	1618	0	1664	19	0
37	e	1611	0	1628	19	0
38	f	1204	0	1280	16	0
39	g	787	0	781	7	0
40	h	1218	0	1246	12	0
41	i	1041	0	1092	19	0
42	j	980	0	1027	14	0
43	k	773	0	814	21	0
44	l	854	0	869	20	0
45	m	1051	0	1115	14	0
46	n	902	0	956	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	o	492	0	508	12	0
48	p	716	0	727	11	0
49	q	692	0	724	6	0
50	r	660	0	699	8	0
51	s	511	0	549	4	0
52	t	663	0	675	12	0
53	u	608	0	635	3	0
54	0	62	0	23	3	0
55	0	2	0	0	0	0
55	A	139	0	0	0	0
55	B	1	0	0	0	0
55	G	1	0	0	0	0
55	Q	1	0	0	0	0
55	a	44	0	0	0	0
55	n	1	0	0	0	0
56	4	1	0	0	0	0
56	5	1	0	0	0	0
56	8	1	0	0	0	0
56	o	1	0	0	0	0
57	7	2	0	0	0	0
57	A	103	0	0	0	0
57	B	3	0	0	0	0
57	G	3	0	0	0	0
57	P	1	0	0	0	0
57	a	38	0	0	0	0
57	g	1	0	0	0	0
57	o	1	0	0	0	0
58	a	6	0	12	0	0
59	a	23	0	23	1	0
All	All	147576	0	99845	1072	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1072) 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)
10:A:572:U:O2'	26:T:49:ASP:OD2	1.93	0.87
36:d:25:GLU:OE2	43:k:11:LYS:NZ	2.09	0.85
33:a:849:G:HO2'	41:i:2:VAL:N	1.74	0.85
37:e:150:SER:OG	37:e:154:GLU:OE2	1.93	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:I:21:GLU:N	16:I:21:GLU:OE1	2.11	0.84
33:a:1386:A:OP2	47:o:35:ARG:NH2	2.10	0.83
10:A:2139:A:N1	10:A:2175:G:O2'	2.12	0.83
1:0:180:LEU:HB3	1:0:208:VAL:HG23	1.61	0.83
10:A:1936:U:HO2'	12:D:12:G:HO2'	1.18	0.83
37:e:183:ARG:NH2	37:e:187:TYR:O	2.12	0.82
33:a:917:G:O2'	33:a:933:G:O6	1.97	0.82
10:A:1105:U:N3	10:A:1108:A:OP2	2.12	0.82
11:B:41:C:O2	17:J:92:ARG:NH1	2.13	0.81
33:a:1013:A:N3	52:t:52:TYR:OH	2.13	0.81
50:r:52:GLU:N	50:r:52:GLU:OE1	2.14	0.81
33:a:159:G:O2'	33:a:228:A:N1	2.14	0.81
1:0:88:ARG:NH2	1:0:133:GLU:OE2	2.14	0.81
33:a:678:U:O4	33:a:778:G:O2'	1.99	0.81
33:a:227:A:O2'	33:a:228:A:O5'	1.97	0.80
14:G:274:ARG:O	14:G:275:THR:OG1	2.00	0.79
26:T:48:ARG:NH1	26:T:49:ASP:OD1	2.15	0.79
13:F:7:LYS:HD2	13:F:35:ILE:HG21	1.64	0.79
41:i:26:GLU:OE2	41:i:61:ARG:NH1	2.16	0.78
51:s:23:GLU:N	51:s:23:GLU:OE1	2.15	0.78
14:G:77:VAL:HG12	14:G:115:ARG:HG2	1.66	0.78
18:K:173:GLU:N	18:K:173:GLU:OE1	2.16	0.78
33:a:1104:G:N2	33:a:1107:A:OP2	2.15	0.78
33:a:1062:G:O2'	33:a:1063:A:O5'	2.00	0.78
10:A:1691:G:O2'	23:Q:116:ASP:OD2	2.01	0.78
33:a:1557:G:O2'	33:a:1558:A:OP2	2.00	0.77
41:i:79:ARG:NH1	41:i:81:SER:O	2.17	0.77
33:a:845:A:O2'	33:a:846:U:OP1	2.02	0.76
33:a:1392:C:OP1	42:j:119:LYS:NZ	2.19	0.76
15:H:90:GLU:O	15:H:95:LYS:NZ	2.19	0.76
10:A:319:U:O2'	10:A:321:U:OP2	2.02	0.76
33:a:1107:A:OP1	38:f:52:LYS:NZ	2.19	0.75
40:h:111:ARG:NH2	40:h:126:ASP:OD2	2.20	0.75
10:A:450:G:OP2	10:A:2419:C:O2'	2.03	0.75
33:a:1565:C:O2	34:b:2:G:N2	2.19	0.75
13:F:43:GLU:OE1	13:F:43:GLU:N	2.19	0.75
15:H:42:GLU:N	15:H:42:GLU:OE1	2.20	0.75
33:a:1286:U:OP1	33:a:1310:C:O2'	2.04	0.75
10:A:2216:G:O2'	10:A:2217:C:OP2	2.05	0.74
10:A:2496:C:N3	22:P:124:LYS:NZ	2.35	0.74
10:A:1003:C:O2'	10:A:2286:A:N3	2.18	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1083:A:O2'	10:A:1150:A:N1	2.19	0.74
35:c:75:GLN:OE1	35:c:75:GLN:N	2.19	0.74
33:a:1519:A:O2'	33:a:1520:A:O4'	2.04	0.74
33:a:1343:C:O2	52:t:37:ARG:NH2	2.20	0.74
10:A:2808:U:N3	10:A:2809:U:O2	2.21	0.74
36:d:90:LEU:O	36:d:94:THR:HG22	1.87	0.74
10:A:1108:A:O2'	10:A:1112:A:N7	2.18	0.74
10:A:2463:A:O2'	12:D:77:A:N1	2.20	0.74
4:3:36:GLU:N	4:3:36:GLU:OE1	2.21	0.74
41:i:110:GLU:N	41:i:110:GLU:OE1	2.20	0.74
45:m:75:GLU:N	45:m:75:GLU:OE1	2.20	0.73
35:c:34:GLU:N	35:c:34:GLU:OE1	2.20	0.73
10:A:1065:A:OP2	10:A:1173:C:O2'	2.04	0.73
50:r:84:GLU:N	50:r:84:GLU:OE1	2.22	0.73
33:a:1372:A:OP1	42:j:122:ARG:NH1	2.22	0.73
30:X:5:LYS:NZ	30:X:24:LEU:O	2.22	0.72
10:A:1311:G:OP2	10:A:1687:G:O2'	2.05	0.72
11:B:11:A:O2'	11:B:13:A:OP2	2.07	0.72
10:A:1263:G:N7	26:T:16:LYS:NZ	2.37	0.72
48:p:26:GLU:OE1	48:p:26:GLU:N	2.22	0.72
10:A:559:U:O2'	10:A:560:G:N7	2.20	0.71
10:A:1885:G:OP2	10:A:1885:G:N2	2.22	0.71
10:A:199:A:N6	10:A:2443:A:O2'	2.24	0.71
18:K:20:ASP:OD1	18:K:21:GLY:N	2.22	0.71
33:a:604:A:O2'	33:a:754:A:N3	2.23	0.71
33:a:1004:A:O2'	33:a:1006:C:OP2	2.08	0.71
22:P:51:ARG:HG3	22:P:66:ILE:HD11	1.73	0.71
15:H:58:GLU:N	15:H:58:GLU:OE1	2.23	0.71
33:a:1131:G:OP1	35:c:110:ARG:NE	2.24	0.70
40:h:113:GLU:N	40:h:113:GLU:OE1	2.23	0.70
46:n:107:ARG:NH1	46:n:111:GLY:O	2.25	0.70
10:A:2535:U:O2'	10:A:2660:U:OP1	2.08	0.70
33:a:1006:C:O2	47:o:19:GLN:NE2	2.25	0.70
43:k:45:GLU:OE2	43:k:71:LYS:NZ	2.16	0.70
33:a:1079:U:O2'	33:a:1082:A:OP2	2.03	0.70
33:a:427:C:O2'	33:a:647:A:N3	2.22	0.70
33:a:1295:A:N1	33:a:1338:G:O2'	2.22	0.70
43:k:36:VAL:HG12	43:k:76:ILE:CD1	2.22	0.70
29:W:19:ALA:HB1	29:W:24:LYS:HG3	1.74	0.69
41:i:109:SER:OG	41:i:110:GLU:OE1	2.08	0.69
29:W:52:ASN:OD1	29:W:53:VAL:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:1339:G:N7	52:t:2:GLY:N	2.39	0.69
10:A:2670:A:O3'	18:K:160:LYS:NZ	2.25	0.69
31:Y:42:GLY:N	31:Y:73:ASP:OD1	2.26	0.69
33:a:1178:G:OP1	43:k:70:HIS:ND1	2.25	0.69
33:a:690:G:H22	33:a:767:G:H1	1.39	0.69
33:a:868:U:O2'	33:a:871:C:N4	2.25	0.68
43:k:80:THR:OG1	43:k:83:THR:HG23	1.92	0.68
10:A:2349:A:H61	31:Y:52:THR:HG21	1.58	0.68
10:A:2147:A:N3	10:A:2172:G:O2'	2.26	0.68
18:K:8:VAL:HG12	18:K:51:THR:HG22	1.75	0.68
44:l:71:THR:OG1	44:l:100:LEU:HD23	1.94	0.68
10:A:2144:A:O4'	10:A:2171:A:N6	2.25	0.68
33:a:986:A:HO2'	33:a:1011:C:HO2'	1.39	0.68
10:A:2349:A:H61	31:Y:52:THR:CG2	2.06	0.68
19:M:42:LYS:NZ	19:M:51:THR:O	2.23	0.68
30:X:74:SER:OG	30:X:99:GLU:OE2	2.12	0.68
33:a:1209:U:O2'	33:a:1210:G:OP1	2.11	0.68
10:A:2815:A:O2'	10:A:2816:A:O5'	2.10	0.68
13:F:166:ASP:OD1	13:F:168:ALA:N	2.27	0.68
17:J:73:SER:OG	17:J:81:GLU:N	2.27	0.68
10:A:2356:U:HO2'	10:A:2386:A:HO2'	1.38	0.67
10:A:228:A:O2'	10:A:231:U:O4	2.10	0.67
13:F:29:LEU:O	13:F:33:THR:HG23	1.95	0.67
33:a:1292:G:N2	33:a:1295:A:OP2	2.23	0.67
10:A:83:G:H1	10:A:101:G:HO2'	1.43	0.67
10:A:2124:U:O2'	10:A:2158:C:O2	2.04	0.67
46:n:71:ARG:O	46:n:75:LEU:HD13	1.94	0.67
22:P:48:GLU:OE2	22:P:51:ARG:NH2	2.28	0.67
10:A:846:U:O2'	10:A:2073:A:N1	2.27	0.67
10:A:2577:A:OP1	10:A:2661:G:O2'	2.12	0.67
20:N:22:ILE:HD11	20:N:42:THR:OG1	1.95	0.67
44:l:36:ASP:OD1	44:l:40:ASN:N	2.28	0.67
33:a:1209:U:O2'	33:a:1211:G:OP2	2.12	0.67
18:K:89:LEU:O	18:K:89:LEU:HD12	1.95	0.66
46:n:23:TYR:CE1	46:n:69:LEU:HD23	2.30	0.66
33:a:1247:G:O3'	52:t:77:THR:HG21	1.95	0.66
36:d:35:ASP:OD1	36:d:58:ARG:NH2	2.28	0.66
24:R:95:ARG:NH1	24:R:98:TYR:O	2.28	0.66
10:A:1420:A:O2'	10:A:1431:U:O2	2.13	0.66
24:R:46:ASP:O	24:R:50:GLY:N	2.29	0.66
10:A:247:G:O2'	10:A:423:A:N1	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:544:C:O2'	33:a:556:G:N2	2.28	0.66
47:o:26:ARG:NH1	47:o:46:GLU:OE1	2.29	0.66
33:a:768:G:OP1	48:p:59:LYS:NZ	2.29	0.66
36:d:76:ILE:HA	36:d:83:VAL:HG13	1.78	0.66
42:j:45:ARG:O	42:j:49:ASN:ND2	2.28	0.66
33:a:1525:U:O2'	34:b:14:U:OP1	2.11	0.65
11:B:3:U:OP1	11:B:59:U:O2'	2.13	0.65
10:A:1758:G:O2'	10:A:1759:G:OP2	2.13	0.65
10:A:1792:U:O2	10:A:1796:A:N6	2.29	0.65
10:A:2482:A:N6	10:A:2494:G:O2'	2.28	0.65
13:F:49:ASN:ND2	13:F:205:LYS:O	2.29	0.65
13:F:161:VAL:HG11	13:F:173:VAL:HG23	1.78	0.65
33:a:868:U:N3	33:a:870:C:OP1	2.30	0.65
33:a:822:C:OP1	44:l:128:ARG:N	2.28	0.65
13:F:85:LYS:O	13:F:85:LYS:NZ	2.30	0.65
10:A:925:C:N4	10:A:932:G:O6	2.30	0.64
10:A:613:G:O2'	10:A:1290:A:OP1	2.16	0.64
10:A:1086:G:N2	10:A:1149:G:O2'	2.30	0.64
22:P:38:GLU:HB2	22:P:127:VAL:HG13	1.80	0.64
26:T:88:ILE:HG22	26:T:90:ILE:HG22	1.80	0.64
31:Y:81:LYS:N	31:Y:85:LYS:O	2.30	0.64
16:I:141:GLN:NE2	16:I:145:ASN:OD1	2.31	0.64
40:h:117:GLU:N	40:h:117:GLU:OE1	2.31	0.64
10:A:2867:G:N2	10:A:2870:A:OP2	2.31	0.63
17:J:140:GLU:OE1	17:J:140:GLU:N	2.32	0.63
15:H:55:ASP:OD1	15:H:77:LYS:NZ	2.24	0.63
36:d:205:GLU:N	36:d:205:GLU:OE1	2.28	0.63
10:A:2128:G:O2'	10:A:2180:U:O2	2.17	0.63
12:D:7:G:O2'	12:D:50:G:O4'	2.17	0.63
44:l:36:ASP:OD1	44:l:39:GLY:N	2.31	0.63
46:n:17:VAL:O	46:n:20:THR:OG1	2.16	0.63
10:A:2157:G:N2	10:A:2159:U:O2	2.32	0.63
13:F:181:ASP:OD1	13:F:182:ASN:N	2.32	0.63
33:a:272:A:N1	33:a:304:C:O2'	2.31	0.63
10:A:680:G:N2	10:A:683:U:OP2	2.25	0.62
10:A:2810:U:O2'	10:A:2811:A:OP2	2.10	0.62
33:a:139:C:OP1	33:a:337:C:O2'	2.17	0.62
10:A:1124:A:O2'	10:A:1125:A:O4'	2.17	0.62
11:B:12:U:OP2	11:B:68:C:O2'	2.17	0.62
10:A:502:G:N2	10:A:505:A:OP2	2.31	0.62
29:W:88:GLU:N	29:W:88:GLU:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:988:U:OP1	33:a:1249:C:O2'	2.11	0.62
33:a:1003:G:OP2	33:a:1384:U:O2'	2.18	0.62
41:i:48:ASP:OD1	41:i:49:VAL:N	2.30	0.62
10:A:2092:U:O2'	32:Z:23:ASN:OD1	2.17	0.62
33:a:1113:U:H3	33:a:1126:G:H22	1.48	0.62
39:g:87:ASN:OD1	39:g:89:ASP:N	2.33	0.62
10:A:1710:A:O2'	10:A:1716:G:N7	2.26	0.62
44:l:29:ASN:OD1	44:l:30:THR:N	2.33	0.61
33:a:48:G:O2'	33:a:391:U:O2	2.16	0.61
36:d:182:ASP:OD1	36:d:183:TYR:N	2.31	0.61
46:n:12:ASP:O	46:n:44:ARG:NH1	2.33	0.61
52:t:13:ASP:OD1	52:t:14:HIS:N	2.33	0.61
30:X:10:LYS:HB2	30:X:71:ILE:HD11	1.81	0.61
33:a:21:C:OP2	38:f:132:THR:OG1	2.16	0.61
4:3:14:PHE:HE1	4:3:46:LEU:HD23	1.66	0.61
10:A:965:U:O2'	10:A:966:C:OP1	2.18	0.61
10:A:1034:C:O2	19:M:4:THR:OG1	2.06	0.61
4:3:16:ASP:O	4:3:20:GLY:N	2.31	0.61
10:A:2191:C:O2'	13:F:170:ASN:ND2	2.32	0.61
1:0:450:GLU:OE2	54:0:602:ATP:O3'	2.19	0.61
18:K:60:GLU:OE1	18:K:60:GLU:N	2.30	0.61
32:Z:41:ASP:OD1	32:Z:43:LYS:NZ	2.25	0.61
33:a:872:G:O2'	33:a:873:C:OP1	2.18	0.61
33:a:1177:A:OP1	43:k:44:THR:HG22	2.01	0.61
10:A:281:A:O2'	10:A:282:G:O5'	2.17	0.61
17:J:54:VAL:HG13	17:J:65:PRO:CG	2.31	0.61
33:a:727:U:O2	33:a:729:G:N1	2.33	0.61
42:j:26:GLY:N	42:j:62:ASP:OD1	2.34	0.61
4:3:68:ASP:OD1	4:3:69:GLY:N	2.34	0.61
43:k:36:VAL:HG12	43:k:76:ILE:HD12	1.83	0.61
8:7:39:LYS:NZ	10:A:2378:G:N7	2.49	0.60
10:A:668:G:N2	10:A:671:A:OP2	2.31	0.60
38:f:148:LYS:NZ	41:i:75:THR:OG1	2.32	0.60
18:K:89:LEU:HD13	18:K:94:TYR:HB3	1.82	0.60
37:e:166:VAL:HG12	37:e:177:PHE:CE1	2.36	0.60
10:A:1537:A:N3	10:A:1622:C:O2'	2.31	0.60
33:a:323:G:N2	33:a:326:A:OP2	2.27	0.60
1:0:444:ASN:OD1	1:0:445:VAL:HG13	2.02	0.60
10:A:918:A:N6	10:A:939:G:O2'	2.34	0.60
33:a:795:G:H4'	33:a:1540:A:H4'	1.84	0.59
10:A:1189:U:O2'	10:A:1190:A:O5'	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:80:ILE:HD11	35:c:93:ASN:HB3	1.83	0.59
35:c:117:ILE:HD11	35:c:137:LEU:HB3	1.84	0.59
1:0:14:GLU:OE2	1:0:233:HIS:NE2	2.35	0.59
14:G:2:ALA:N	14:G:20:ASP:OD2	2.35	0.59
10:A:1302:G:O6	28:V:18:SER:OG	2.09	0.59
33:a:750:G:OP2	33:a:858:G:N2	2.36	0.59
23:Q:2:SER:OG	23:Q:3:TYR:N	2.36	0.59
31:Y:65:ASP:OD1	31:Y:67:THR:HG23	2.03	0.59
44:l:71:THR:HG23	44:l:105:LEU:CD1	2.32	0.59
8:7:13:ARG:NH2	10:A:252:G:OP1	2.35	0.59
10:A:2815:A:HO2'	10:A:2816:A:C5'	2.15	0.59
28:V:15:VAL:HG11	28:V:51:ILE:HG21	1.85	0.59
33:a:1563:C:O2'	33:a:1564:U:OP1	2.20	0.59
25:S:34:GLU:OE1	25:S:34:GLU:N	2.31	0.59
33:a:1402:U:O4	40:h:10:ARG:NH1	2.34	0.59
10:A:2263:G:O2'	10:A:2509:C:OP1	2.20	0.59
33:a:1001:A:OP2	47:o:32:SER:OG	2.20	0.59
33:a:1486:C:OP1	53:u:26:ASN:ND2	2.35	0.59
1:0:107:VAL:O	1:0:112:GLN:NE2	2.36	0.58
10:A:899:G:O2'	10:A:956:G:O6	2.20	0.58
46:n:37:VAL:HG12	46:n:39:VAL:HG23	1.85	0.58
10:A:281:A:HO2'	10:A:282:G:P	2.26	0.58
10:A:1067:A:N3	10:A:2499:G:O2'	2.26	0.58
13:F:10:GLU:OE1	13:F:14:LYS:NZ	2.35	0.58
17:J:136:LEU:HD22	17:J:143:TYR:HA	1.84	0.58
33:a:857:U:O2'	33:a:1566:C:OP1	2.19	0.58
33:a:1192:G:N1	33:a:1195:A:OP2	2.36	0.58
33:a:1170:G:N2	33:a:1172:A:H62	2.02	0.58
10:A:2318:U:O2'	10:A:2319:U:O5'	2.15	0.58
10:A:538:G:N1	10:A:541:A:OP2	2.37	0.58
33:a:301:G:O2'	50:r:20:MET:SD	2.60	0.58
1:0:187:ASN:OD1	1:0:188:HIS:N	2.37	0.58
12:D:39:A:O2'	33:a:816:A:OP1	2.21	0.58
33:a:358:G:OP2	53:u:3:ASN:N	2.37	0.58
42:j:65:VAL:HG11	42:j:79:ILE:HG12	1.86	0.58
3:2:11:SER:OG	10:A:1028:G:OP2	2.16	0.57
33:a:302:G:OP1	50:r:17:SER:OG	2.14	0.57
33:a:1002:A:H4'	33:a:1003:G:H5''	1.86	0.57
37:e:135:GLU:OE1	37:e:138:GLN:NE2	2.36	0.57
13:F:30:ALA:HB1	13:F:216:THR:HG23	1.86	0.57
17:J:73:SER:HG	17:J:81:GLU:H	1.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:176:ALA:HB3	35:c:183:ILE:HD11	1.86	0.57
33:a:74:C:O2'	33:a:75:U:O5'	2.22	0.57
12:D:31:G:OP1	33:a:1255:A:O2'	2.21	0.57
10:A:958:A:N3	11:B:78:U:O2'	2.33	0.57
38:f:82:PRO:HD2	38:f:147:LEU:HD22	1.86	0.57
10:A:520:G:O2'	10:A:545:A:N6	2.37	0.57
36:d:94:THR:HG23	36:d:96:LYS:H	1.69	0.57
40:h:65:ALA:HB1	40:h:127:ALA:HB3	1.87	0.57
40:h:94:GLU:OE1	40:h:94:GLU:N	2.34	0.57
44:l:71:THR:HG21	44:l:103:THR:OG1	2.04	0.57
10:A:509:A:OP1	16:I:79:ARG:NH2	2.30	0.57
10:A:1885:G:H21	10:A:1885:G:P	2.27	0.57
10:A:2841:G:O2'	10:A:2894:U:OP1	2.20	0.57
24:R:44:VAL:O	24:R:53:LEU:N	2.37	0.57
37:e:163:PRO:O	37:e:166:VAL:HG22	2.05	0.57
44:l:20:VAL:HG23	44:l:37:THR:HA	1.86	0.57
14:G:72:ASP:OD2	14:G:189:ARG:NH2	2.35	0.57
40:h:115:THR:OG1	40:h:117:GLU:OE2	2.22	0.57
41:i:76:ASN:OD1	41:i:77:LEU:N	2.37	0.57
10:A:782:A:O2'	10:A:1701:U:OP1	2.22	0.57
10:A:1310:A:N1	10:A:1330:C:O2'	2.37	0.57
13:F:98:ASP:O	13:F:101:VAL:HG22	2.04	0.57
22:P:109:VAL:HG13	22:P:110:PRO:HD2	1.86	0.57
13:F:77:VAL:HG11	13:F:149:VAL:HG11	1.87	0.56
44:l:20:VAL:HG22	44:l:83:ASP:OD1	2.05	0.56
1:0:351:PHE:HB3	1:0:521:ILE:HD11	1.87	0.56
22:P:75:THR:HG22	22:P:90:PRO:HA	1.87	0.56
33:a:64:U:O2'	33:a:405:C:O2	2.22	0.56
35:c:33:THR:HG22	35:c:34:GLU:H	1.70	0.56
38:f:39:VAL:HG12	38:f:67:ALA:HB1	1.87	0.56
10:A:622:A:N1	10:A:848:G:O2'	2.32	0.56
17:J:62:GLY:O	17:J:95:ARG:NH2	2.39	0.56
21:O:80:ASP:OD1	21:O:81:THR:N	2.38	0.56
37:e:53:GLU:HG3	37:e:194:LEU:HD12	1.86	0.56
33:a:1087:U:OP1	47:o:45:ARG:NH2	2.36	0.56
17:J:144:ASP:OD1	17:J:145:LEU:N	2.38	0.56
33:a:571:C:OP1	37:e:54:LYS:NZ	2.38	0.56
52:t:22:GLN:OE1	52:t:29:LYS:N	2.32	0.56
38:f:159:LYS:NZ	41:i:42:ARG:O	2.38	0.56
41:i:54:ASP:OD1	41:i:58:GLY:N	2.32	0.56
6:5:31:GLU:OE2	6:5:46:ARG:NE	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:491:U:O2'	33:a:493:A:N7	2.37	0.56
33:a:745:C:OP2	33:a:746:C:N4	2.38	0.56
33:a:1477:U:N3	33:a:1478:U:O3'	2.39	0.56
10:A:343:G:N1	10:A:346:A:OP2	2.37	0.56
14:G:71:LYS:NZ	14:G:98:ASP:OD2	2.26	0.56
30:X:72:ASP:O	30:X:76:GLY:N	2.34	0.56
33:a:685:C:OP2	48:p:8:LYS:NZ	2.33	0.56
4:3:12:VAL:HG23	4:3:44:PRO:O	2.06	0.56
33:a:37:G:O2'	45:m:128:SER:O	2.22	0.56
10:A:1106:A:N1	10:A:1134:A:O2'	2.28	0.55
33:a:1342:G:N7	52:t:7:LYS:NZ	2.54	0.55
6:5:30:LEU:HD11	6:5:32:LYS:HE2	1.87	0.55
10:A:519:A:O2'	30:X:42:LYS:O	2.24	0.55
35:c:130:PRO:O	35:c:132:LYS:N	2.38	0.55
17:J:54:VAL:HG13	17:J:65:PRO:HG2	1.88	0.55
45:m:26:LYS:O	45:m:72:ASN:ND2	2.38	0.55
10:A:2317:G:H22	10:A:2325:U:H3	1.54	0.55
10:A:2808:U:O2'	10:A:2809:U:OP1	2.23	0.55
38:f:76:MET:HE2	38:f:120:VAL:HG22	1.89	0.55
46:n:37:VAL:HG23	46:n:59:GLU:HG3	1.89	0.55
10:A:625:U:OP1	21:O:16:ARG:NH2	2.38	0.55
10:A:1180:U:H4'	10:A:1181:A:O4'	2.07	0.55
43:k:32:THR:OG1	43:k:83:THR:HG22	2.06	0.55
10:A:1583:G:HO2'	10:A:1584:U:P	2.30	0.55
10:A:2640:G:O2'	10:A:2794:A:N1	2.37	0.55
33:a:1176:U:O4	33:a:1177:A:N6	2.40	0.55
20:N:91:LYS:NZ	20:N:109:ASN:O	2.39	0.55
33:a:403:G:OP1	49:q:4:LYS:NZ	2.35	0.55
33:a:1150:A:O2'	43:k:39:PRO:O	2.24	0.55
35:c:73:LYS:NZ	35:c:205:ASP:OD1	2.31	0.55
14:G:43:ARG:NH2	14:G:49:ILE:HD11	2.22	0.55
33:a:369:U:O2'	33:a:372:G:O6	2.14	0.55
33:a:1330:G:N1	33:a:1358:A:OP2	2.40	0.55
33:a:1342:G:N1	33:a:1345:A:OP2	2.36	0.55
35:c:188:ASP:OD1	35:c:189:THR:N	2.36	0.55
41:i:50:GLU:OE2	41:i:61:ARG:NE	2.39	0.55
15:H:87:GLU:N	15:H:87:GLU:OE1	2.40	0.55
17:J:113:ASP:O	17:J:115:HIS:ND1	2.35	0.55
52:t:64:GLU:O	52:t:67:VAL:HG22	2.07	0.55
5:4:16:ARG:NH2	10:A:1300:G:OP1	2.38	0.54
10:A:299:G:O2'	10:A:460:C:OP2	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1376:U:OP1	10:A:1432:U:N3	2.40	0.54
33:a:994:C:OP2	33:a:995:A:O2'	2.17	0.54
35:c:33:THR:O	35:c:40:ILE:N	2.39	0.54
44:l:68:GLU:HA	44:l:103:THR:HG21	1.89	0.54
10:A:1376:U:OP2	10:A:1429:U:O2'	2.19	0.54
10:A:2890:C:O3'	23:Q:100:ARG:NH2	2.40	0.54
14:G:123:ASP:OD1	14:G:124:ILE:N	2.40	0.54
10:A:1755:U:O2	10:A:1758:G:N1	2.40	0.54
10:A:2128:G:H2'	10:A:2130:A:H62	1.71	0.54
41:i:42:ARG:NH1	41:i:117:GLU:OE2	2.40	0.54
42:j:43:ASP:OD1	42:j:43:ASP:N	2.39	0.54
10:A:1451:G:O2'	10:A:1452:U:O5'	2.24	0.54
33:a:1335:G:OP2	46:n:98:ARG:NH2	2.38	0.54
1:0:330:LEU:HD21	1:0:376:LEU:HD22	1.89	0.54
33:a:703:U:H3	33:a:739:G:H22	1.56	0.54
36:d:69:THR:HG22	36:d:71:LYS:H	1.73	0.54
43:k:24:LYS:HE3	43:k:90:LEU:HD11	1.90	0.54
1:0:317:MET:SD	1:0:484:ILE:HD13	2.48	0.54
13:F:75:VAL:HG22	13:F:156:VAL:HG11	1.89	0.54
35:c:117:ILE:HD11	35:c:137:LEU:HD13	1.90	0.54
1:0:104:LEU:HD11	1:0:119:MET:HE2	1.89	0.54
33:a:452:U:OP1	37:e:29:ARG:NH1	2.41	0.54
43:k:34:ALA:HB2	43:k:83:THR:HG21	1.90	0.54
10:A:1469:C:O2'	10:A:1614:A:OP2	2.19	0.54
33:a:1346:C:O2	52:t:36:ARG:NH2	2.40	0.54
17:J:104:VAL:HA	17:J:108:LEU:HD12	1.90	0.54
33:a:711:G:N1	33:a:730:A:OP2	2.39	0.54
43:k:36:VAL:HG12	43:k:76:ILE:HD13	1.90	0.54
44:l:71:THR:HG23	44:l:105:LEU:HD12	1.90	0.53
1:0:522:ASP:OD1	1:0:523:ASN:N	2.42	0.53
20:N:104:ARG:N	20:N:122:LEU:OXT	2.40	0.53
33:a:1218:C:N3	59:a:1675:SCM:O5	2.40	0.53
10:A:2304:U:OP1	10:A:2393:U:O2'	2.25	0.53
12:D:7:G:H3'	12:D:8:U:C5'	2.39	0.53
13:F:40:ALA:O	13:F:178:VAL:HG13	2.08	0.53
33:a:710:U:O2'	44:l:41:ALA:O	2.22	0.53
10:A:32:C:N4	10:A:486:A:OP2	2.40	0.53
17:J:65:PRO:HA	17:J:89:VAL:HG22	1.91	0.53
36:d:187:GLU:OE1	36:d:194:LYS:NZ	2.30	0.53
10:A:846:U:OP2	21:O:41:ARG:NH2	2.40	0.53
33:a:399:A:O2'	33:a:477:A:N7	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:401:U:OP1	49:q:69:THR:OG1	2.16	0.53
13:F:166:ASP:OD2	13:F:170:ASN:N	2.41	0.53
10:A:515:G:N1	10:A:518:A:OP2	2.34	0.53
33:a:528:C:OP1	45:m:128:SER:N	2.35	0.53
10:A:1164:G:OP2	10:A:1165:A:O2'	2.23	0.53
17:J:36:ILE:HD11	17:J:152:MET:SD	2.48	0.53
33:a:802:G:N2	33:a:828:A:OP2	2.31	0.53
33:a:950:A:O2'	33:a:1425:C:OP2	2.18	0.53
33:a:1480:U:O2'	33:a:1481:G:O5'	2.26	0.53
37:e:184:ASP:OD1	37:e:184:ASP:N	2.42	0.53
43:k:73:LEU:O	43:k:74:ILE:HD13	2.09	0.53
50:r:30:THR:HG22	50:r:31:LYS:N	2.24	0.53
19:M:5:TYR:O	26:T:64:ARG:NH1	2.38	0.52
33:a:865:G:O2'	33:a:866:G:OP1	2.26	0.52
45:m:120:VAL:O	45:m:132:THR:HG21	2.10	0.52
33:a:601:G:O2'	33:a:847:G:OP2	2.23	0.52
21:O:87:ASP:OD1	21:O:120:LYS:N	2.42	0.52
33:a:1516:G:O2'	33:a:1517:U:O5'	2.25	0.52
2:1:29:ARG:NH2	29:W:7:ILE:O	2.43	0.52
10:A:2044:A:N3	10:A:2468:G:O2'	2.33	0.52
13:F:97:ASP:O	13:F:101:VAL:HG13	2.10	0.52
33:a:841:A:N7	33:a:1536:C:O2'	2.40	0.52
33:a:1461:G:H2'	33:a:1462:U:C6	2.45	0.52
10:A:230:A:H3'	10:A:231:U:O4'	2.10	0.52
39:g:38:ALA:HB1	39:g:68:VAL:CG2	2.40	0.52
33:a:1338:G:H5'	52:t:5:LEU:HD11	1.92	0.51
45:m:61:ALA:C	45:m:62:LEU:HD22	2.35	0.51
4:3:14:PHE:CE1	4:3:46:LEU:HD23	2.45	0.51
24:R:107:LEU:HD23	24:R:107:LEU:C	2.36	0.51
25:S:39:ARG:NH1	33:a:372:G:OP1	2.41	0.51
1:0:208:VAL:O	1:0:208:VAL:HG13	2.10	0.51
5:4:24:ILE:HG23	5:4:24:ILE:O	2.11	0.51
10:A:858:A:OP2	10:A:1224:G:N2	2.35	0.51
10:A:997:U:O2	11:B:87:U:O2'	2.22	0.51
12:D:22:A:H61	12:D:47:G:H2'	1.74	0.51
21:O:116:GLU:N	21:O:116:GLU:OE1	2.43	0.51
38:f:115:LEU:HD13	38:f:123:ILE:HG21	1.92	0.51
36:d:50:ALA:C	36:d:69:THR:HG23	2.36	0.51
9:8:12:GLU:OE1	9:8:12:GLU:N	2.34	0.51
10:A:309:G:O2'	10:A:310:A:OP2	2.22	0.51
23:Q:61:GLN:O	23:Q:64:THR:OG1	2.20	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:547:G:OP1	45:m:64:LYS:NZ	2.36	0.51
33:a:783:U:OP1	33:a:848:A:O2'	2.28	0.51
10:A:2217:C:OP1	14:G:147:LYS:NZ	2.42	0.51
10:A:1812:G:O2'	14:G:180:GLU:OE2	2.18	0.51
18:K:96:ALA:N	18:K:128:ASN:O	2.41	0.51
10:A:2148:G:O4'	10:A:2172:G:O2'	2.29	0.51
10:A:1355:G:C2	10:A:1364:U:H5'	2.47	0.51
26:T:37:GLU:O	26:T:41:ASN:ND2	2.44	0.51
33:a:872:G:O2'	33:a:873:C:P	2.68	0.51
33:a:1035:C:O2'	33:a:1036:U:P	2.69	0.51
10:A:2324:A:HO2'	10:A:2325:U:H6	1.54	0.50
13:F:183:GLU:O	13:F:186:VAL:HG12	2.12	0.50
33:a:391:U:H5'	33:a:392:C:OP1	2.11	0.50
10:A:1108:A:H4'	10:A:1109:A:H2'	1.94	0.50
10:A:2443:A:N3	10:A:2443:A:H2'	2.26	0.50
10:A:2770:A:N1	18:K:67:THR:OG1	2.35	0.50
12:D:59:A:O2'	12:D:61:U:OP2	2.29	0.50
17:J:130:LEU:HD21	17:J:132:ILE:HD11	1.93	0.50
17:J:160:ALA:O	24:R:1:MET:N	2.44	0.50
10:A:1373:G:O2'	10:A:1428:A:N1	2.44	0.50
10:A:2123:G:OP1	10:A:2131:U:N3	2.44	0.50
10:A:2275:U:OP2	31:Y:25:SER:OG	2.26	0.50
13:F:56:ASP:OD2	13:F:203:THR:HG21	2.12	0.50
15:H:16:PHE:O	25:S:12:GLN:NE2	2.39	0.50
10:A:64:A:C5	29:W:65:MET:HE2	2.47	0.50
10:A:1583:G:O2'	10:A:1584:U:P	2.69	0.50
22:P:127:VAL:HG12	22:P:128:LYS:O	2.11	0.50
42:j:38:TYR:HB3	42:j:39:ILE:HD12	1.92	0.50
10:A:33:U:HO2'	10:A:34:U:P	2.35	0.50
10:A:1026:C:O2'	10:A:1039:A:N3	2.39	0.50
10:A:1830:G:OP2	14:G:156:ARG:NH2	2.45	0.50
16:I:152:VAL:CG1	16:I:173:VAL:HG22	2.42	0.50
20:N:105:GLU:OE1	20:N:105:GLU:N	2.44	0.50
52:t:50:ALA:HB1	52:t:57:HIS:HB3	1.93	0.50
10:A:1811:U:O2'	10:A:1815:A:N3	2.42	0.50
10:A:2525:C:H2'	10:A:2526:G:O4'	2.12	0.50
3:2:6:ILE:HG12	3:2:56:VAL:HG12	1.94	0.49
18:K:79:VAL:HG22	18:K:136:ILE:HD11	1.94	0.49
28:V:85:PRO:O	28:V:105:THR:OG1	2.24	0.49
4:3:15:MET:HG2	4:3:45:LEU:HD21	1.94	0.49
10:A:2680:C:N3	18:K:110:SER:OG	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2815:A:HO2'	10:A:2816:A:P	2.33	0.49
17:J:50:LEU:HD13	17:J:50:LEU:C	2.37	0.49
18:K:10:VAL:C	18:K:11:LEU:HD12	2.37	0.49
13:F:77:VAL:CG1	13:F:149:VAL:HG11	2.42	0.49
33:a:1473:A:P	33:a:1474:C:H41	2.34	0.49
1:O:28:LYS:NZ	1:O:202:LYS:O	2.46	0.49
1:O:101:TYR:HA	1:O:104:LEU:HD12	1.94	0.49
10:A:33:U:O4	10:A:485:G:O2'	2.28	0.49
33:a:119:U:OP2	53:u:9:LYS:NZ	2.42	0.49
33:a:128:G:HO2'	33:a:380:G:HO2'	1.61	0.49
33:a:843:C:C4	33:a:845:A:H1'	2.47	0.49
33:a:1480:U:O2'	33:a:1481:G:P	2.70	0.49
41:i:25:LEU:C	41:i:25:LEU:HD12	2.37	0.49
10:A:1582:A:O2'	10:A:1584:U:O4'	2.24	0.49
45:m:112:ARG:NH1	45:m:118:ALA:O	2.45	0.49
10:A:59:G:O2'	10:A:74:U:OP2	2.26	0.49
10:A:932:G:H2'	10:A:933:G:C8	2.47	0.49
31:Y:48:ARG:HH11	31:Y:67:THR:HG21	1.78	0.49
35:c:126:PHE:HA	35:c:129:LEU:HD22	1.95	0.49
10:A:2299:A:H4'	10:A:2300:A:O4'	2.11	0.49
33:a:1171:C:H4'	33:a:1172:A:O5'	2.12	0.49
19:M:142:ASP:OD1	19:M:143:ILE:N	2.46	0.49
33:a:793:A:H2'	33:a:794:A:O4'	2.13	0.49
33:a:1281:G:H3'	33:a:1305:A:H61	1.77	0.49
44:l:34:ILE:HD13	44:l:70:ALA:HB1	1.94	0.49
10:A:2217:C:OP2	14:G:150:LYS:NZ	2.40	0.48
16:I:26:ILE:HG22	16:I:27:GLU:N	2.27	0.48
33:a:1152:U:O2'	33:a:1153:U:O5'	2.28	0.48
10:A:1029:A:O2'	10:A:1031:C:OP2	2.26	0.48
10:A:2318:U:H2'	10:A:2319:U:O4'	2.13	0.48
11:B:107:G:C2'	11:B:108:U:O5'	2.62	0.48
33:a:606:C:H2'	33:a:607:G:O4'	2.13	0.48
33:a:1563:C:O2'	33:a:1564:U:P	2.70	0.48
5:4:3:VAL:HG12	10:A:2028:A:C2	2.49	0.48
10:A:180:G:H2'	10:A:181:U:O4'	2.14	0.48
13:F:60:ARG:O	13:F:141:LYS:HG3	2.14	0.48
33:a:74:C:C2'	33:a:75:U:O5'	2.62	0.48
1:O:241:ASP:OD1	1:O:241:ASP:N	2.46	0.48
18:K:87:LEU:N	18:K:87:LEU:HD12	2.28	0.48
33:a:845:A:H4'	33:a:846:U:OP2	2.13	0.48
36:d:52:SER:OG	36:d:111:ASP:OD2	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2128:G:C2'	10:A:2130:A:H62	2.27	0.48
10:A:2658:G:H4'	10:A:2745:G:O2'	2.13	0.48
23:Q:26:ILE:O	23:Q:88:LYS:NZ	2.47	0.48
30:X:23:VAL:HG13	30:X:33:VAL:CG2	2.44	0.48
33:a:402:G:H5''	49:q:6:ARG:HB2	1.96	0.48
10:A:441:A:H2'	10:A:442:U:O4'	2.14	0.48
13:F:74:THR:OG1	13:F:111:PHE:HA	2.13	0.48
38:f:162:GLU:OE1	38:f:162:GLU:N	2.43	0.48
43:k:63:GLU:OE1	47:o:49:TYR:OH	2.31	0.48
50:r:60:ASP:N	50:r:60:ASP:OD1	2.46	0.48
10:A:1095:G:O2'	10:A:1142:A:N6	2.41	0.48
10:A:1591:G:OP2	10:A:1591:G:N2	2.37	0.48
10:A:1882:U:H2'	10:A:1885:G:H22	1.77	0.48
19:M:50:ASP:HB2	19:M:115:LEU:HD11	1.94	0.48
19:M:118:LYS:O	19:M:121:THR:OG1	2.29	0.48
33:a:276:A:N6	33:a:301:G:O6	2.47	0.48
33:a:607:G:N1	33:a:785:A:OP2	2.38	0.48
33:a:1425:C:O2	33:a:1529:A:N6	2.45	0.48
52:t:36:ARG:NH2	52:t:72:GLY:O	2.47	0.48
10:A:2111:U:O2'	10:A:2112:U:P	2.72	0.48
16:I:146:LEU:O	16:I:147:SER:OG	2.22	0.48
33:a:527:C:O2	33:a:575:C:O2'	2.30	0.48
10:A:231:U:O2'	10:A:232:U:OP2	2.25	0.48
10:A:1536:A:O2'	10:A:1537:A:P	2.71	0.48
33:a:1347:U:OP2	33:a:1348:C:O2'	2.32	0.48
35:c:129:LEU:HD21	35:c:137:LEU:HD12	1.96	0.48
1:0:369:LYS:N	54:0:601:ATP:O1B	2.43	0.47
10:A:2182:G:H2'	10:A:2183:G:O4'	2.14	0.47
14:G:45:ASN:OD1	14:G:46:ASN:N	2.47	0.47
14:G:129:ALA:C	14:G:130:LEU:HD12	2.38	0.47
27:U:57:THR:HG23	27:U:101:ASN:OD1	2.14	0.47
33:a:865:G:O2'	33:a:866:G:P	2.71	0.47
33:a:960:G:O6	40:h:3:ARG:NH1	2.46	0.47
33:a:1516:G:O2'	33:a:1517:U:P	2.72	0.47
13:F:41:THR:HG22	13:F:42:VAL:N	2.27	0.47
17:J:13:THR:HB	17:J:14:PRO:HD3	1.95	0.47
17:J:110:ARG:NH1	17:J:136:LEU:O	2.47	0.47
33:a:1313:A:N3	33:a:1379:G:O2'	2.39	0.47
37:e:179:ARG:NH2	37:e:185:GLU:OE2	2.39	0.47
8:7:23:LYS:NZ	10:A:668:G:OP1	2.37	0.47
10:A:1254:C:OP2	26:T:15:LYS:NZ	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:F:42:VAL:HG22	13:F:216:THR:HG22	1.95	0.47
13:F:76:LEU:HD12	13:F:114:VAL:HG13	1.96	0.47
20:N:105:GLU:O	20:N:109:ASN:ND2	2.45	0.47
23:Q:36:ARG:O	23:Q:40:VAL:HG23	2.15	0.47
44:l:50:LEU:HD11	44:l:66:ALA:HA	1.96	0.47
33:a:527:C:OP1	45:m:127:ARG:NH2	2.37	0.47
33:a:754:A:OP1	48:p:54:ARG:NH1	2.47	0.47
33:a:1392:C:O2'	43:k:62:ARG:NH2	2.38	0.47
4:3:38:GLU:O	4:3:39:ASP:HB2	2.14	0.47
10:A:641:G:N7	21:O:103:LYS:NZ	2.62	0.47
10:A:824:U:H2'	10:A:825:C:C6	2.49	0.47
24:R:27:GLU:OE1	24:R:27:GLU:N	2.38	0.47
33:a:1149:U:H2'	33:a:1150:A:O4'	2.15	0.47
10:A:832:A:OP2	10:A:2084:A:O2'	2.27	0.47
10:A:902:G:H2'	10:A:903:A:O4'	2.15	0.47
10:A:1116:A:H2'	10:A:1117:C:O4'	2.15	0.47
10:A:2318:U:O2'	10:A:2319:U:P	2.72	0.47
18:K:5:GLY:O	18:K:65:HIS:NE2	2.48	0.47
33:a:715:C:OP1	44:l:29:ASN:ND2	2.47	0.47
14:G:23:GLU:OE1	14:G:23:GLU:N	2.34	0.47
15:H:182:GLU:OE1	15:H:182:GLU:N	2.45	0.47
33:a:710:U:O2'	44:l:41:ALA:N	2.47	0.47
33:a:1322:C:H4'	33:a:1328:U:O4	2.14	0.47
33:a:1531:G:OP2	33:a:1534:A:O2'	2.26	0.47
35:c:33:THR:HG22	35:c:34:GLU:N	2.28	0.47
1:0:373:LEU:HD11	1:0:498:VAL:HG23	1.97	0.47
10:A:84:A:N1	10:A:98:U:O2'	2.45	0.47
12:D:17:C:OP1	12:D:61:U:O2'	2.28	0.47
13:F:104:ILE:HD13	13:F:108:TRP:HB2	1.95	0.47
18:K:54:ARG:NH2	18:K:57:ASP:OD1	2.44	0.47
42:j:25:THR:N	42:j:62:ASP:OD1	2.48	0.47
1:0:332:VAL:HG21	1:0:351:PHE:CZ	2.50	0.47
10:A:2320:G:O6	17:J:41:GLY:N	2.48	0.47
10:A:2877:G:O2'	10:A:2878:A:P	2.72	0.47
33:a:1013:A:H2'	33:a:1014:G:O4'	2.15	0.47
1:0:362:VAL:HG12	1:0:363:GLY:N	2.30	0.46
1:0:474:ASN:O	1:0:475:HIS:HB2	2.14	0.46
15:H:62:ASN:HB3	15:H:64:PRO:HD2	1.97	0.46
4:3:45:LEU:HD13	4:3:45:LEU:C	2.41	0.46
6:5:36:CYS:O	6:5:40:ARG:N	2.47	0.46
10:A:590:U:H2'	10:A:591:G:O4'	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1098:G:C8	10:A:1099:U:H2'	2.50	0.46
10:A:1107:G:H21	10:A:1135:A:H5'	1.80	0.46
10:A:1576:A:H2'	10:A:1577:A:C8	2.50	0.46
21:O:80:ASP:OD1	21:O:81:THR:HG23	2.15	0.46
3:2:28:LEU:HD21	3:2:35:VAL:HG12	1.97	0.46
10:A:1936:U:OP1	12:D:25:U:O2'	2.34	0.46
10:A:2907:U:O2'	19:M:137:GLN:NE2	2.47	0.46
17:J:43:ALA:HB2	17:J:50:LEU:HB2	1.97	0.46
33:a:355:A:O2'	33:a:358:G:N7	2.26	0.46
46:n:12:ASP:OD1	46:n:12:ASP:N	2.48	0.46
10:A:1792:U:H5	10:A:1797:A:N7	2.13	0.46
10:A:2304:U:H2'	10:A:2305:U:C6	2.50	0.46
33:a:1163:U:H2'	33:a:1164:A:O4'	2.15	0.46
48:p:33:THR:OG1	48:p:63:ARG:NH1	2.48	0.46
50:r:30:THR:HG22	50:r:31:LYS:H	1.79	0.46
18:K:4:ILE:HG22	18:K:69:ARG:HD2	1.96	0.46
33:a:699:G:H2'	33:a:700:G:C8	2.51	0.46
41:i:107:SER:HB2	41:i:128:ILE:HD11	1.96	0.46
43:k:35:ASP:OD1	43:k:36:VAL:N	2.47	0.46
46:n:53:THR:HG22	46:n:57:ARG:NH1	2.30	0.46
10:A:1236:U:H1'	26:T:4:VAL:HG22	1.97	0.46
14:G:121:GLU:N	14:G:121:GLU:OE1	2.49	0.46
20:N:24:VAL:HG13	20:N:33:ALA:HB2	1.97	0.46
37:e:165:PHE:CD1	37:e:166:VAL:HG13	2.51	0.46
39:g:68:VAL:HG22	39:g:69:THR:N	2.31	0.46
10:A:1536:A:H2'	10:A:1537:A:C8	2.50	0.46
10:A:1646:C:O2'	10:A:1652:A:N1	2.45	0.46
13:F:139:ASN:OD1	13:F:141:LYS:N	2.49	0.46
29:W:79:ILE:HD12	29:W:79:ILE:N	2.30	0.46
33:a:1334:U:OP1	46:n:97:THR:N	2.41	0.46
10:A:992:A:OP1	22:P:18:ARG:NH2	2.48	0.46
10:A:2736:C:OP2	15:H:115:LYS:NZ	2.49	0.46
10:A:2857:U:OP1	25:S:96:LYS:NZ	2.37	0.46
33:a:765:C:HO2'	48:p:42:HIS:CE1	2.31	0.46
33:a:1183:A:C2	33:a:1207:G:C4	3.04	0.46
43:k:78:ASN:O	43:k:78:ASN:ND2	2.48	0.46
10:A:1833:U:OP1	14:G:177:ASN:ND2	2.46	0.46
37:e:15:LEU:HD13	37:e:56:LYS:HA	1.97	0.46
10:A:1882:U:O3'	10:A:1883:U:O2	2.34	0.46
17:J:136:LEU:HD23	17:J:141:VAL:HG11	1.98	0.46
33:a:44:G:O2'	33:a:648:A:N1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:494:C:O2	33:a:494:C:O4'	2.34	0.46
9:8:32:LYS:NZ	10:A:2542:G:O6	2.49	0.45
33:a:865:G:HO2'	33:a:866:G:P	2.39	0.45
36:d:22:TRP:NE1	36:d:35:ASP:OD2	2.47	0.45
10:A:1212:U:O3'	10:A:1214:A:N6	2.49	0.45
13:F:38:PHE:O	13:F:40:ALA:N	2.46	0.45
33:a:131:G:O2'	33:a:132:A:N7	2.49	0.45
33:a:511:G:O2'	33:a:512:U:OP2	2.28	0.45
37:e:166:VAL:HG12	37:e:177:PHE:CD1	2.51	0.45
42:j:106:ARG:NH1	42:j:107:ASP:O	2.37	0.45
20:N:102:VAL:HG11	20:N:106:LEU:HD12	1.98	0.45
33:a:350:G:N1	33:a:353:A:OP2	2.50	0.45
37:e:37:GLY:N	37:e:38:PRO:HD2	2.32	0.45
10:A:572:U:H2'	10:A:573:C:C6	2.51	0.45
10:A:743:G:O2'	10:A:765:G:N2	2.44	0.45
10:A:1310:A:H4'	10:A:1311:G:OP1	2.17	0.45
10:A:1536:A:O2'	10:A:1537:A:OP1	2.33	0.45
21:O:71:ARG:NH2	21:O:73:ASP:OD1	2.50	0.45
33:a:760:G:H21	51:s:68:ILE:HD11	1.80	0.45
41:i:75:THR:N	41:i:132:TRP:OXT	2.49	0.45
44:l:88:GLY:H	44:l:114:THR:HG22	1.81	0.45
10:A:930:C:C2	10:A:931:G:N7	2.85	0.45
10:A:1125:A:N3	10:A:1125:A:H3'	2.32	0.45
10:A:1469:C:O2	10:A:1469:C:H2'	2.16	0.45
10:A:2802:C:O2'	10:A:2803:A:OP2	2.32	0.45
33:a:783:U:H2'	33:a:784:G:O4'	2.17	0.45
33:a:794:A:N3	33:a:1539:U:O2'	2.49	0.45
33:a:1341:U:O2'	33:a:1386:A:N3	2.44	0.45
1:0:169:PHE:CE2	1:0:173:LEU:HD11	2.52	0.45
10:A:693:G:N3	10:A:693:G:H2'	2.31	0.45
10:A:753:U:C4	48:p:88:ARG:NH2	2.85	0.45
10:A:2239:C:H2'	10:A:2240:A:O4'	2.17	0.45
10:A:2333:A:N3	10:A:2333:A:H2'	2.32	0.45
39:g:29:PHE:HA	39:g:32:ILE:HD12	1.97	0.45
1:0:327:ARG:NH1	40:h:110:LEU:O	2.50	0.45
10:A:2010:A:OP2	15:H:130:ARG:NH1	2.50	0.45
10:A:2109:U:H2'	10:A:2110:G:O4'	2.17	0.45
10:A:2487:C:O2	10:A:2487:C:O4'	2.32	0.45
33:a:445:U:OP1	33:a:539:A:O2'	2.26	0.45
33:a:866:G:H2'	33:a:867:U:O4'	2.17	0.45
10:A:1245:G:O2'	10:A:1273:A:N1	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2815:A:O2'	10:A:2816:A:P	2.74	0.45
13:F:78:PHE:CE1	13:F:101:VAL:HG12	2.52	0.45
33:a:75:U:O2	33:a:113:G:N2	2.50	0.45
4:3:66:GLN:O	4:3:67:ALA:HB3	2.17	0.45
16:I:149:ASP:OD1	16:I:149:ASP:N	2.49	0.45
17:J:156:ILE:N	17:J:156:ILE:HD12	2.32	0.45
33:a:1252:C:O2'	46:n:102:THR:O	2.29	0.45
42:j:81:HIS:NE2	42:j:104:LEU:O	2.46	0.45
14:G:130:LEU:HD13	14:G:192:ILE:HD11	1.99	0.45
18:K:35:ARG:NH1	18:K:71:ASN:OD1	2.50	0.45
33:a:53:A:N1	33:a:340:C:O2'	2.44	0.45
49:q:71:ARG:NH2	49:q:75:SER:OG	2.50	0.45
1:0:361:VAL:HB	1:0:498:VAL:HG22	1.99	0.44
8:7:28:PHE:O	8:7:36:LYS:NZ	2.48	0.44
10:A:1362:C:H2'	10:A:1363:G:O4'	2.17	0.44
17:J:74:ILE:N	17:J:79:LEU:O	2.50	0.44
33:a:131:G:O2'	33:a:132:A:C8	2.70	0.44
33:a:289:A:H2'	33:a:290:C:C6	2.52	0.44
33:a:846:U:H4'	33:a:847:G:OP2	2.16	0.44
35:c:80:ILE:HD11	35:c:93:ASN:CB	2.45	0.44
10:A:27:G:O2'	10:A:28:A:OP2	2.31	0.44
10:A:681:A:N1	10:A:2382:A:O2'	2.48	0.44
33:a:131:G:H5''	33:a:132:A:OP1	2.17	0.44
33:a:1477:U:C2	33:a:1478:U:O3'	2.71	0.44
49:q:81:LYS:NZ	49:q:85:GLU:OE2	2.37	0.44
10:A:856:C:O2'	10:A:878:U:OP1	2.35	0.44
10:A:1086:G:O2'	10:A:1087:A:OP2	2.34	0.44
11:B:28:C:O2	11:B:28:C:H2'	2.18	0.44
14:G:122:ALA:O	14:G:130:LEU:HD21	2.17	0.44
16:I:26:ILE:CG2	16:I:27:GLU:N	2.80	0.44
33:a:397:G:H2'	33:a:398:C:O4'	2.17	0.44
49:q:40:TYR:CD1	49:q:73:ILE:HD11	2.53	0.44
33:a:1205:A:H2'	33:a:1206:A:O4'	2.17	0.44
10:A:935:U:O2'	10:A:937:C:O4'	2.27	0.44
10:A:2279:A:H4'	10:A:2280:A:O5'	2.18	0.44
28:V:89:ARG:O	28:V:101:ILE:N	2.42	0.44
33:a:422:A:O2'	33:a:424:C:OP1	2.25	0.44
33:a:430:G:O2'	33:a:524:A:N1	2.48	0.44
34:b:3:A:H2'	34:b:4:G:C8	2.52	0.44
1:0:460:LEU:C	1:0:460:LEU:HD23	2.42	0.44
10:A:899:G:O2'	10:A:900:U:OP2	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:1758:G:O2'	10:A:1759:G:P	2.75	0.44
13:F:74:THR:N	13:F:112:ASP:OD1	2.47	0.44
33:a:1403:A:O2'	33:a:1404:C:OP2	2.32	0.44
33:a:1540:A:H2'	33:a:1541:U:C6	2.53	0.44
45:m:42:GLN:HB3	45:m:94:LEU:HD11	2.00	0.44
1:0:79:THR:HG22	1:0:80:VAL:N	2.31	0.44
1:0:173:LEU:HD21	1:0:200:TYR:CE2	2.52	0.44
10:A:712:C:OP1	16:I:54:ARG:NH1	2.40	0.44
10:A:2320:G:H4'	10:A:2321:G:O4'	2.18	0.44
20:N:97:ARG:NH2	33:a:364:A:OP1	2.51	0.44
33:a:1444:A:N6	33:a:1509:G:O2'	2.51	0.44
10:A:289:U:O2'	10:A:290:G:OP2	2.33	0.44
10:A:610:A:N6	10:A:2047:U:OP1	2.49	0.44
10:A:1814:A:OP2	14:G:150:LYS:NZ	2.46	0.44
10:A:2174:C:H2'	10:A:2175:G:O4'	2.17	0.44
16:I:123:LEU:C	16:I:123:LEU:HD13	2.43	0.44
29:W:61:LYS:H	29:W:72:THR:HG1	1.66	0.44
33:a:125:A:C6	33:a:352:G:C6	3.06	0.44
33:a:227:A:H2'	33:a:228:A:C8	2.53	0.44
33:a:543:G:N2	33:a:559:A:OP2	2.48	0.44
33:a:1165:G:H1'	33:a:1166:U:OP2	2.18	0.44
33:a:1457:C:H2'	33:a:1458:G:O4'	2.18	0.44
38:f:14:ARG:NH2	38:f:116:GLU:OE1	2.42	0.44
41:i:115:ASP:OD1	41:i:116:LYS:N	2.51	0.44
1:0:39:LYS:NZ	54:0:602:ATP:O1B	2.46	0.44
3:2:8:LEU:O	3:2:32:ASN:N	2.42	0.44
10:A:569:A:OP1	10:A:597:G:N1	2.50	0.44
10:A:2322:A:H2'	10:A:2323:A:O4'	2.17	0.44
13:F:209:ILE:HG21	13:F:212:ILE:HG12	1.99	0.44
33:a:164:G:H2'	33:a:165:G:C8	2.52	0.44
33:a:747:A:H4'	33:a:748:G:O4'	2.18	0.44
33:a:1183:A:N6	33:a:1206:A:N7	2.66	0.44
38:f:25:VAL:HG22	38:f:26:LYS:N	2.32	0.44
46:n:11:ARG:HA	46:n:45:VAL:CG2	2.48	0.44
10:A:1494:A:H62	10:A:1501:G:H22	1.64	0.43
39:g:12:ILE:HD12	39:g:55:MET:HE1	1.99	0.43
1:0:29:VAL:HB	1:0:209:LEU:HD22	2.00	0.43
10:A:138:U:N3	10:A:141:U:OP2	2.46	0.43
10:A:335:A:N3	10:A:355:U:O2'	2.49	0.43
10:A:2635:C:O2'	10:A:2835:G:N7	2.51	0.43
33:a:767:G:H2'	33:a:768:G:O4'	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:68:ASN:ND2	40:h:127:ALA:O	2.42	0.43
10:A:1189:U:O2'	10:A:1190:A:P	2.77	0.43
10:A:1792:U:OP2	10:A:1797:A:N6	2.38	0.43
10:A:2189:A:H4'	13:F:221:GLY:N	2.33	0.43
18:K:61:MET:HA	18:K:64:ILE:HG22	2.00	0.43
33:a:19:U:H2'	33:a:20:C:C6	2.54	0.43
33:a:146:A:N3	33:a:215:G:O2'	2.47	0.43
33:a:1076:U:OP1	47:o:2:ALA:N	2.52	0.43
41:i:10:PHE:CE1	41:i:14:ILE:HD11	2.53	0.43
45:m:94:LEU:C	45:m:95:LEU:HD22	2.43	0.43
10:A:1446:U:H2'	10:A:1447:U:O4'	2.18	0.43
10:A:1451:G:O2'	10:A:1452:U:O4'	2.33	0.43
10:A:2877:G:C2'	10:A:2878:A:OP2	2.66	0.43
11:B:26:C:H2'	11:B:27:A:O4'	2.18	0.43
11:B:104:G:H2'	11:B:105:A:O4'	2.18	0.43
13:F:192:ILE:O	13:F:195:VAL:HG12	2.18	0.43
18:K:89:LEU:HD13	18:K:94:TYR:CB	2.48	0.43
33:a:199:A:H1'	33:a:201:A:N7	2.34	0.43
44:l:16:ILE:HG22	44:l:17:GLU:N	2.33	0.43
10:A:2256:U:H2'	10:A:2257:U:C6	2.54	0.43
15:H:31:THR:O	15:H:32:PRO:C	2.61	0.43
33:a:395:C:OP2	33:a:414:G:N1	2.46	0.43
36:d:94:THR:HG21	36:d:98:VAL:CG2	2.49	0.43
47:o:24:CYS:O	47:o:28:GLY:N	2.43	0.43
10:A:309:G:O2'	10:A:310:A:P	2.76	0.43
14:G:69:ARG:O	14:G:189:ARG:NH1	2.51	0.43
33:a:23:G:H2'	33:a:24:G:C8	2.54	0.43
33:a:1002:A:H4'	33:a:1003:G:C5'	2.48	0.43
33:a:1563:C:HO2'	33:a:1564:U:P	2.42	0.43
10:A:793:U:O2'	10:A:1308:A:N1	2.52	0.43
10:A:2009:C:H4'	10:A:2010:A:OP1	2.19	0.43
10:A:2348:A:HO2'	10:A:2349:A:H8	1.66	0.43
12:D:56:U:O2'	12:D:58:A:N7	2.36	0.43
13:F:76:LEU:HD13	13:F:76:LEU:C	2.44	0.43
15:H:14:GLN:HB2	15:H:22:LEU:HD11	2.01	0.43
16:I:177:THR:OG1	16:I:179:ASP:OD1	2.29	0.43
17:J:175:MET:O	17:J:177:PHE:N	2.51	0.43
33:a:1389:A:H2'	33:a:1389:A:N3	2.33	0.43
1:O:63:ARG:NH1	1:O:175:SER:O	2.44	0.43
1:O:456:LEU:HD13	1:O:484:ILE:HD11	1.99	0.43
11:B:13:A:O2'	11:B:14:G:H5'	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:P:109:VAL:HG11	22:P:113:VAL:HG12	2.01	0.43
33:a:62:A:H62	33:a:124:G:H4'	1.84	0.43
10:A:852:U:H2'	10:A:853:C:C6	2.53	0.43
10:A:2331:G:H5''	10:A:2332:A:OP2	2.18	0.43
33:a:908:G:H2'	33:a:909:C:O4'	2.19	0.43
35:c:186:MET:HE1	35:c:210:VAL:HG22	2.01	0.43
38:f:8:HIS:C	38:f:9:LEU:HD12	2.43	0.43
40:h:71:PRO:O	40:h:96:ARG:NE	2.52	0.43
10:A:2143:G:H2'	10:A:2171:A:H2	1.84	0.43
14:G:173:LEU:HD11	14:G:271:VAL:HG21	2.01	0.43
15:H:146:MET:HE1	15:H:160:LEU:HD11	2.00	0.43
20:N:97:ARG:NE	33:a:365:C:OP2	2.51	0.43
24:R:24:GLY:N	24:R:47:ASP:OD2	2.45	0.43
33:a:227:A:O2'	33:a:228:A:O4'	2.36	0.43
33:a:1028:U:H3	33:a:1065:A:H61	1.66	0.43
33:a:1121:G:O2'	33:a:1122:U:OP1	2.32	0.43
10:A:115:C:H2'	10:A:116:G:O4'	2.19	0.42
10:A:482:A:H1'	10:A:1238:U:O4'	2.19	0.42
10:A:1171:U:H3'	10:A:1172:A:H5''	2.01	0.42
10:A:2019:C:O2'	10:A:2833:A:N3	2.52	0.42
10:A:2608:G:N2	10:A:2611:A:OP2	2.41	0.42
10:A:2808:U:H3	10:A:2811:A:H62	1.67	0.42
22:P:109:VAL:CG1	22:P:110:PRO:HD2	2.49	0.42
33:a:1557:G:HO2'	33:a:1558:A:P	2.32	0.42
40:h:17:ILE:HD11	40:h:44:TYR:CD1	2.54	0.42
46:n:100:GLN:OE1	46:n:100:GLN:N	2.43	0.42
4:3:31:SER:OG	4:3:45:LEU:O	2.35	0.42
5:4:9:SER:HB3	10:A:2033:A:H5'	2.00	0.42
10:A:333:U:OP1	30:X:90:LYS:NZ	2.50	0.42
10:A:1165:A:H4'	10:A:1166:A:H5''	2.01	0.42
10:A:1583:G:O2'	10:A:1584:U:O5'	2.32	0.42
10:A:1673:G:N2	10:A:1676:U:OP2	2.49	0.42
10:A:2545:G:O2'	10:A:2670:A:N1	2.49	0.42
15:H:39:LYS:NZ	15:H:82:GLU:OE2	2.46	0.42
22:P:58:MET:HE3	22:P:109:VAL:HG21	2.01	0.42
33:a:993:G:O2'	42:j:129:LYS:O	2.36	0.42
33:a:1299:C:H2'	33:a:1300:A:O4'	2.19	0.42
33:a:1472:A:O2'	33:a:1473:A:H5'	2.19	0.42
46:n:23:TYR:HE1	46:n:69:LEU:HD23	1.80	0.42
10:A:261:G:O2'	10:A:659:A:O2'	2.36	0.42
10:A:1133:U:H2'	10:A:1135:A:N7	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:2034:G:N3	10:A:2034:G:H2'	2.34	0.42
10:A:2517:U:O2	10:A:2517:U:O5'	2.37	0.42
10:A:2700:U:H2'	10:A:2701:G:O4'	2.19	0.42
43:k:39:PRO:HA	43:k:74:ILE:HD13	2.00	0.42
1:0:101:TYR:HB3	13:F:122:ALA:HA	2.01	0.42
1:0:411:ILE:HD12	1:0:438:ASP:O	2.19	0.42
10:A:368:A:O2'	10:A:370:C:OP2	2.26	0.42
10:A:1392:C:H2'	10:A:1393:G:O4'	2.19	0.42
10:A:1566:C:O2'	10:A:1567:G:OP1	2.35	0.42
10:A:1810:C:O2'	14:G:259:THR:OG1	2.33	0.42
33:a:765:C:O2'	48:p:42:HIS:ND1	2.39	0.42
35:c:163:ILE:HD12	35:c:183:ILE:HG21	2.01	0.42
10:A:220:G:H22	10:A:237:U:H4'	1.84	0.42
10:A:1288:G:N2	26:T:37:GLU:OE2	2.45	0.42
14:G:108:LYS:N	14:G:194:SER:O	2.41	0.42
14:G:192:ILE:N	14:G:192:ILE:HD12	2.35	0.42
17:J:13:THR:O	17:J:17:VAL:HG23	2.19	0.42
25:S:2:ASN:HB3	25:S:3:PRO:HD3	2.01	0.42
33:a:849:G:O2'	41:i:2:VAL:N	2.43	0.42
51:s:49:THR:O	51:s:49:THR:HG22	2.20	0.42
9:8:7:VAL:O	9:8:7:VAL:HG23	2.19	0.42
10:A:311:U:O2	10:A:311:U:O4'	2.37	0.42
10:A:742:U:H2'	10:A:743:G:O4'	2.20	0.42
10:A:1870:G:C6	10:A:1871:G:C6	3.08	0.42
10:A:2184:A:H1'	10:A:2185:U:C2	2.55	0.42
10:A:2597:U:H5''	10:A:2598:U:OP2	2.19	0.42
10:A:2679:C:O2	10:A:2679:C:O4'	2.38	0.42
20:N:2:ILE:O	20:N:33:ALA:N	2.42	0.42
33:a:222:G:H2'	33:a:223:A:C8	2.54	0.42
33:a:439:G:N2	33:a:454:G:O3'	2.50	0.42
33:a:547:G:N7	45:m:63:ARG:NH1	2.62	0.42
10:A:8:U:H2'	10:A:9:G:O4'	2.19	0.42
10:A:214:C:H2'	10:A:215:A:O4'	2.20	0.42
10:A:624:U:H2'	10:A:625:U:C6	2.54	0.42
27:U:80:LYS:O	27:U:81:HIS:ND1	2.53	0.42
44:l:71:THR:HG23	44:l:105:LEU:HG	2.01	0.42
10:A:193:A:H2'	10:A:194:C:C6	2.55	0.42
10:A:342:U:H2'	10:A:343:G:O4'	2.20	0.42
10:A:1033:C:O2'	10:A:1035:A:OP1	2.33	0.42
10:A:2127:A:H2'	10:A:2128:G:O4'	2.20	0.42
33:a:370:A:H5''	33:a:371:C:H5	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:a:542:U:O2'	33:a:545:C:N3	2.51	0.42
35:c:27:MET:HE3	35:c:193:PRO:HD3	2.02	0.42
36:d:110:LEU:O	36:d:203:ARG:NH1	2.53	0.42
6:5:5:ILE:HD13	6:5:21:LYS:HG2	2.01	0.42
10:A:251:C:H4'	10:A:252:G:O5'	2.20	0.42
10:A:1758:G:N3	10:A:1758:G:C2'	2.82	0.42
36:d:111:ASP:OD1	36:d:114:LEU:N	2.38	0.42
38:f:5:ASP:OD1	38:f:5:ASP:O	2.37	0.42
38:f:74:VAL:O	38:f:74:VAL:HG23	2.20	0.42
1:0:30:GLY:N	1:0:222:ILE:HD12	2.34	0.42
1:0:415:VAL:O	1:0:415:VAL:HG12	2.20	0.42
18:K:86:ALA:C	18:K:87:LEU:HD12	2.45	0.42
35:c:131:LYS:O	35:c:134:VAL:HG12	2.20	0.42
10:A:1516:A:H2'	10:A:1517:U:O4'	2.20	0.41
10:A:2105:U:H4'	10:A:2106:G:H5'	2.02	0.41
11:B:27:A:H2'	11:B:28:C:C1'	2.50	0.41
33:a:227:A:HO2'	33:a:228:A:C5'	2.24	0.41
33:a:464:G:O2'	33:a:466:U:O4	2.25	0.41
33:a:895:C:H2'	33:a:896:A:O4'	2.20	0.41
33:a:987:U:O2'	33:a:1249:C:H4'	2.19	0.41
33:a:1062:G:HO2'	33:a:1063:A:P	2.40	0.41
33:a:1393:C:P	42:j:114:LYS:HZ1	2.42	0.41
35:c:101:LEU:HD11	35:c:161:MET:CE	2.50	0.41
10:A:58:G:O2'	10:A:73:A:N1	2.50	0.41
10:A:65:A:O2'	10:A:495:C:N3	2.47	0.41
10:A:249:G:OP2	10:A:251:C:N4	2.39	0.41
10:A:289:U:H1'	10:A:290:G:C8	2.55	0.41
10:A:2181:G:O2'	10:A:2183:G:N7	2.51	0.41
10:A:2336:G:H2'	10:A:2337:U:O4'	2.20	0.41
10:A:2859:G:O2'	10:A:2876:G:N2	2.53	0.41
11:B:29:C:O2'	11:B:51:A:N1	2.51	0.41
12:D:61:U:O5'	12:D:61:U:O2	2.39	0.41
18:K:96:ALA:HB2	18:K:105:LEU:HD23	2.00	0.41
33:a:24:G:O2'	33:a:940:A:N1	2.50	0.41
33:a:142:G:OP1	33:a:631:U:O2'	2.29	0.41
33:a:971:G:N1	33:a:1364:G:OP2	2.48	0.41
33:a:1020:G:O2'	33:a:1021:A:N7	2.53	0.41
6:5:19:THR:OG1	6:5:20:ASN:N	2.53	0.41
10:A:2517:U:O2	10:A:2517:U:O4'	2.37	0.41
33:a:33:G:O2'	33:a:50:C:N4	2.53	0.41
33:a:1164:A:N6	33:a:1166:U:O2'	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:33:HIS:NE2	47:o:38:HIS:HB2	2.36	0.41
10:A:723:G:C6	10:A:813:A:C4	3.08	0.41
10:A:2402:G:H5''	10:A:2403:U:O4'	2.21	0.41
10:A:2809:U:O2'	10:A:2810:U:O4'	2.32	0.41
16:I:153:LEU:HB2	16:I:189:ALA:HB2	2.01	0.41
30:X:74:SER:HG	30:X:99:GLU:CD	2.27	0.41
33:a:1027:U:H3'	33:a:1028:U:H5''	2.01	0.41
45:m:42:GLN:CB	45:m:94:LEU:HD11	2.50	0.41
10:A:2808:U:C2	10:A:2809:U:O2	2.74	0.41
10:A:2810:U:H1'	10:A:2811:A:P	2.60	0.41
10:A:2814:A:O2'	10:A:2815:A:H5'	2.20	0.41
15:H:18:GLU:O	15:H:19:SER:OG	2.21	0.41
16:I:126:VAL:HG11	16:I:146:LEU:HD11	2.02	0.41
27:U:80:LYS:C	27:U:81:HIS:CG	2.98	0.41
33:a:486:G:O2'	33:a:487:U:H5'	2.20	0.41
33:a:1094:A:N1	33:a:1135:G:O2'	2.48	0.41
33:a:1541:U:H2'	33:a:1542:C:C6	2.56	0.41
41:i:32:ILE:HD11	41:i:128:ILE:HD13	2.01	0.41
7:6:34:ARG:HD3	10:A:506:G:OP2	2.21	0.41
10:A:271:C:O2	10:A:271:C:H2'	2.20	0.41
10:A:333:U:P	30:X:90:LYS:HZ1	2.43	0.41
10:A:1021:C:O2	10:A:1021:C:O5'	2.38	0.41
10:A:1086:G:HO2'	10:A:1087:A:P	2.44	0.41
14:G:123:ASP:O	14:G:128:ASN:ND2	2.48	0.41
33:a:193:C:H2'	33:a:194:G:N3	2.35	0.41
33:a:408:A:H2'	33:a:409:A:C8	2.56	0.41
33:a:777:U:H2'	33:a:778:G:O4'	2.21	0.41
6:5:31:GLU:OE2	6:5:46:ARG:NH2	2.54	0.41
10:A:1211:A:H2'	10:A:1214:A:N6	2.36	0.41
10:A:1276:G:C8	10:A:1277:C:C6	3.09	0.41
10:A:1809:U:H2'	10:A:1810:C:C6	2.56	0.41
10:A:1965:A:OP1	20:N:42:THR:HG21	2.19	0.41
10:A:2174:C:C2	10:A:2175:G:C8	3.09	0.41
10:A:2272:G:C8	10:A:2440:C:C4	3.09	0.41
13:F:209:ILE:HG21	13:F:212:ILE:CG1	2.50	0.41
18:K:121:VAL:HG12	18:K:122:THR:N	2.35	0.41
24:R:11:ARG:HD2	24:R:98:TYR:CZ	2.56	0.41
33:a:1021:A:O2'	47:o:12:ARG:NH1	2.53	0.41
35:c:115:LYS:HE2	35:c:152:ALA:HB1	2.02	0.41
36:d:111:ASP:OD1	36:d:113:LYS:N	2.52	0.41
3:2:14:GLY:HA2	10:A:1008:G:O3'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:74:PHE:CE1	4:3:80:LEU:HD12	2.56	0.41
10:A:1885:G:O5'	10:A:1885:G:N3	2.54	0.41
10:A:2126:C:H2'	10:A:2127:A:O4'	2.21	0.41
10:A:2640:G:N2	10:A:2790:G:OP2	2.51	0.41
33:a:112:A:H3'	33:a:113:G:C8	2.55	0.41
33:a:290:C:O3'	50:r:68:ARG:NH1	2.53	0.41
33:a:350:G:N2	33:a:352:G:H3'	2.36	0.41
33:a:433:A:OP1	37:e:109:ARG:NH1	2.53	0.41
33:a:1006:C:O2	33:a:1006:C:H2'	2.19	0.41
33:a:1057:U:C4'	33:a:1058:C:OP1	2.69	0.41
35:c:32:PHE:N	35:c:40:ILE:O	2.39	0.41
43:k:29:ALA:HB3	43:k:36:VAL:HG11	2.02	0.41
48:p:41:GLU:OE2	48:p:44:ARG:NH1	2.54	0.41
1:0:107:VAL:HG11	1:0:111:LYS:H	1.85	0.41
1:0:362:VAL:HG12	1:0:363:GLY:H	1.86	0.41
10:A:74:U:H5''	10:A:75:G:O4'	2.21	0.41
10:A:390:C:H2'	10:A:391:A:O4'	2.21	0.41
10:A:518:A:H4'	10:A:519:A:OP1	2.20	0.41
10:A:667:C:O2	10:A:677:U:O2'	2.38	0.41
10:A:1018:A:H2'	10:A:1021:C:H41	1.84	0.41
10:A:1117:C:H1'	10:A:1127:A:H5''	2.03	0.41
10:A:1792:U:O2	10:A:1796:A:C6	2.74	0.41
10:A:2349:A:H61	31:Y:52:THR:HG22	1.83	0.41
12:D:64:U:H2'	12:D:65:G:O4'	2.21	0.41
13:F:96:GLY:HA3	13:F:100:MET:HE2	2.03	0.41
13:F:163:TYR:HB2	13:F:171:ILE:HD11	2.01	0.41
13:F:171:ILE:HG23	13:F:171:ILE:O	2.21	0.41
14:G:130:LEU:HD13	14:G:192:ILE:CD1	2.51	0.41
18:K:98:VAL:HB	18:K:125:VAL:HG21	2.03	0.41
33:a:212:C:O2	33:a:213:A:N6	2.49	0.41
33:a:346:G:H2'	33:a:347:A:O4'	2.20	0.41
33:a:695:G:O2'	33:a:696:A:H5'	2.20	0.41
33:a:703:U:O2	33:a:803:A:O2'	2.37	0.41
33:a:777:U:O4'	48:p:23:GLY:O	2.38	0.41
33:a:1007:C:H2'	33:a:1008:U:O4'	2.21	0.41
33:a:1300:A:H2'	33:a:1301:U:C6	2.55	0.41
33:a:1513:G:H2'	33:a:1514:G:C8	2.56	0.41
43:k:25:ILE:HD13	43:k:90:LEU:HD23	2.03	0.41
44:l:88:GLY:O	44:l:93:ARG:NH2	2.54	0.41
51:s:36:PHE:CD1	51:s:49:THR:HG21	2.56	0.41
10:A:207:G:HO2'	10:A:208:U:P	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:322:G:O6	10:A:389:A:N6	2.54	0.41
10:A:584:A:H4'	10:A:585:A:OP1	2.21	0.41
10:A:2064:A:N6	10:A:2627:A:O2'	2.45	0.41
10:A:2210:U:O2'	10:A:2211:A:C8	2.74	0.41
10:A:2558:G:H2'	10:A:2559:U:O4'	2.20	0.41
12:D:60:A:H3'	12:D:61:U:O2	2.21	0.41
15:H:63:LYS:N	15:H:64:PRO:HD2	2.36	0.41
16:I:179:ASP:OD1	16:I:180:ASN:N	2.55	0.41
23:Q:37:ALA:CB	23:Q:121:VAL:HG21	2.51	0.41
33:a:1330:G:N2	33:a:1358:A:OP2	2.54	0.41
36:d:72:PRO:HD3	36:d:104:GLU:OE1	2.21	0.41
1:0:469:LEU:HB3	1:0:472:PRO:HG3	2.03	0.40
9:8:2:LYS:NZ	10:A:2491:A:OP2	2.38	0.40
10:A:1259:G:N7	27:U:70:LYS:NZ	2.70	0.40
10:A:1541:U:H2'	10:A:1542:U:O4'	2.22	0.40
10:A:2051:G:H2'	10:A:2052:G:O4'	2.20	0.40
10:A:2089:U:O2	10:A:2089:U:O4'	2.38	0.40
10:A:2169:G:C6	10:A:2170:G:N1	2.89	0.40
10:A:2877:G:O2'	10:A:2878:A:H8	2.04	0.40
13:F:215:THR:OG1	13:F:219:GLY:O	2.38	0.40
14:G:130:LEU:HD12	14:G:130:LEU:N	2.36	0.40
15:H:54:GLN:O	15:H:55:ASP:C	2.64	0.40
15:H:56:LYS:N	15:H:76:PRO:O	2.47	0.40
20:N:12:ASP:OD1	20:N:14:SER:OG	2.28	0.40
21:O:120:LYS:O	21:O:121:LEU:HD23	2.21	0.40
33:a:453:C:OP2	33:a:454:G:O2'	2.31	0.40
33:a:478:A:H3'	33:a:479:C:H5''	2.03	0.40
33:a:535:A:N3	33:a:569:G:O2'	2.46	0.40
33:a:544:C:O3'	45:m:60:SER:OG	2.37	0.40
33:a:646:C:H1'	37:e:129:ILE:HG21	2.03	0.40
33:a:1213:G:N3	47:o:60:SER:OG	2.55	0.40
33:a:1254:C:H4'	46:n:114:LYS:O	2.19	0.40
33:a:1342:G:N2	33:a:1344:A:H3'	2.36	0.40
38:f:13:ASP:OD2	38:f:64:ILE:HD11	2.21	0.40
39:g:31:THR:HG22	39:g:35:ASP:OD2	2.20	0.40
10:A:844:G:N2	10:A:868:A:OP1	2.53	0.40
10:A:1178:G:O2'	10:A:1182:A:N1	2.50	0.40
10:A:1354:G:C5	10:A:1355:G:C6	3.09	0.40
10:A:2327:A:H2'	10:A:2328:U:C6	2.56	0.40
23:Q:59:ARG:HA	23:Q:90:PHE:CZ	2.56	0.40
24:R:60:ASP:OD2	24:R:82:ARG:NH1	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:65:VAL:O	30:X:68:VAL:HG22	2.21	0.40
33:a:1049:C:O3'	33:a:1050:U:O4'	2.40	0.40
33:a:1238:U:H5''	33:a:1239:A:O5'	2.22	0.40
39:g:51:LEU:HD12	39:g:58:PHE:O	2.20	0.40
10:A:1786:A:N7	10:A:1842:A:H1'	2.36	0.40
10:A:2271:C:O2'	10:A:2440:C:OP2	2.34	0.40
11:B:11:A:N1	11:B:67:G:O2'	2.41	0.40
11:B:38:U:N3	11:B:42:G:OP2	2.45	0.40
13:F:75:VAL:HG22	13:F:156:VAL:CG1	2.50	0.40
20:N:102:VAL:CG1	20:N:106:LEU:HD12	2.51	0.40
33:a:52:A:O2'	33:a:386:G:N2	2.53	0.40
33:a:1480:U:H2'	33:a:1481:G:O4'	2.21	0.40
35:c:86:ARG:NH1	35:c:219:ASP:OD1	2.49	0.40
36:d:33:HIS:CE1	47:o:25:GLU:HB2	2.56	0.40
37:e:13:ARG:NE	37:e:31:TYR:O	2.48	0.40
37:e:115:VAL:HG11	37:e:130:PRO:HA	2.03	0.40
10:A:346:A:O2'	10:A:347:A:OP2	2.33	0.40
10:A:1145:A:C4	10:A:1146:G:C8	3.09	0.40
10:A:1309:A:N6	10:A:1688:A:N3	2.69	0.40
10:A:2201:U:C2	10:A:2202:G:N7	2.89	0.40
10:A:2712:U:H2'	10:A:2713:C:C6	2.56	0.40
15:H:27:VAL:HG22	15:H:187:LEU:HD22	2.04	0.40
31:Y:52:THR:HG23	31:Y:52:THR:O	2.21	0.40
33:a:381:C:C4	33:a:382:A:N7	2.88	0.40
33:a:406:G:N2	33:a:409:A:OP2	2.47	0.40
33:a:605:G:H5'	33:a:754:A:H1'	2.03	0.40
33:a:690:G:H2'	33:a:692:G:OP1	2.22	0.40
38:f:41:ASP:OD1	38:f:41:ASP:O	2.38	0.40
42:j:91:ASP:OD1	42:j:94:PHE:N	2.54	0.40
48:p:36:ILE:O	48:p:40:ASN:ND2	2.49	0.40
1:O:198:THR:HG22	1:O:217:PHE:CD1	2.56	0.40
10:A:852:U:O5'	21:O:24:SER:OG	2.40	0.40
10:A:1108:A:OP1	10:A:1109:A:C8	2.75	0.40
10:A:1165:A:H4'	10:A:1166:A:C5'	2.52	0.40
10:A:1524:U:H2'	10:A:1525:G:O4'	2.21	0.40
10:A:2132:A:C2	10:A:2184:A:C4	3.09	0.40
11:B:35:C:O2	24:R:101:HIS:NE2	2.48	0.40
23:Q:113:ARG:O	23:Q:117:ALA:N	2.52	0.40
33:a:468:U:H2'	33:a:469:U:O4'	2.22	0.40
33:a:1018:U:O2'	33:a:1019:U:OP2	2.37	0.40
37:e:62:GLY:O	37:e:112:ARG:NH1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:j:107:ASP:OD1	42:j:107:ASP:C	2.64	0.40
43:k:10:LEU:HD12	43:k:10:LEU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	532/586 (91%)	522 (98%)	10 (2%)	0	100	100
2	1	57/62 (92%)	56 (98%)	1 (2%)	0	100	100
3	2	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	3	78/89 (88%)	75 (96%)	3 (4%)	0	100	100
5	4	51/59 (86%)	49 (96%)	2 (4%)	0	100	100
6	5	46/48 (96%)	46 (100%)	0	0	100	100
7	6	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
8	7	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
9	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
13	F	224/229 (98%)	219 (98%)	5 (2%)	0	100	100
14	G	272/276 (99%)	264 (97%)	7 (3%)	1 (0%)	30	59
15	H	204/209 (98%)	197 (97%)	7 (3%)	0	100	100
16	I	203/207 (98%)	201 (99%)	2 (1%)	0	100	100
17	J	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
18	K	172/178 (97%)	163 (95%)	9 (5%)	0	100	100
19	M	145/147 (99%)	143 (99%)	2 (1%)	0	100	100
20	N	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
21	O	144/146 (99%)	138 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	P	132/144 (92%)	129 (98%)	3 (2%)	0	100	100
23	Q	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
24	R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
25	S	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
26	T	116/119 (98%)	115 (99%)	1 (1%)	0	100	100
27	U	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
28	V	109/115 (95%)	109 (100%)	0	0	100	100
29	W	89/96 (93%)	87 (98%)	2 (2%)	0	100	100
30	X	99/103 (96%)	91 (92%)	8 (8%)	0	100	100
31	Y	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
32	Z	59/62 (95%)	59 (100%)	0	0	100	100
35	c	220/261 (84%)	210 (96%)	10 (4%)	0	100	100
36	d	203/218 (93%)	199 (98%)	4 (2%)	0	100	100
37	e	198/203 (98%)	193 (98%)	5 (2%)	0	100	100
38	f	161/166 (97%)	160 (99%)	1 (1%)	0	100	100
39	g	94/99 (95%)	93 (99%)	1 (1%)	0	100	100
40	h	151/156 (97%)	148 (98%)	3 (2%)	0	100	100
41	i	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
42	j	125/130 (96%)	118 (94%)	7 (6%)	0	100	100
43	k	94/102 (92%)	90 (96%)	4 (4%)	0	100	100
44	l	114/129 (88%)	110 (96%)	3 (3%)	1 (1%)	14	41
45	m	132/137 (96%)	124 (94%)	8 (6%)	0	100	100
46	n	112/121 (93%)	107 (96%)	5 (4%)	0	100	100
47	o	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
48	p	83/89 (93%)	81 (98%)	2 (2%)	0	100	100
49	q	85/91 (93%)	83 (98%)	2 (2%)	0	100	100
50	r	78/88 (89%)	74 (95%)	4 (5%)	0	100	100
51	s	61/79 (77%)	58 (95%)	3 (5%)	0	100	100
52	t	80/92 (87%)	77 (96%)	3 (4%)	0	100	100
53	u	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
All	All	6001/6376 (94%)	5824 (97%)	175 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	I	119	ASN
14	G	155	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	489/533 (92%)	485 (99%)	4 (1%)	73	90
2	1	54/56 (96%)	54 (100%)	0	100	100
3	2	48/50 (96%)	48 (100%)	0	100	100
4	3	72/79 (91%)	72 (100%)	0	100	100
5	4	43/47 (92%)	42 (98%)	1 (2%)	44	76
6	5	48/48 (100%)	47 (98%)	1 (2%)	47	77
7	6	39/39 (100%)	39 (100%)	0	100	100
8	7	51/52 (98%)	51 (100%)	0	100	100
9	8	35/35 (100%)	35 (100%)	0	100	100
13	F	181/183 (99%)	177 (98%)	4 (2%)	45	77
14	G	224/226 (99%)	224 (100%)	0	100	100
15	H	169/172 (98%)	169 (100%)	0	100	100
16	I	172/173 (99%)	172 (100%)	0	100	100
17	J	154/156 (99%)	154 (100%)	0	100	100
18	K	145/148 (98%)	145 (100%)	0	100	100
19	M	124/124 (100%)	123 (99%)	1 (1%)	73	90
20	N	98/98 (100%)	97 (99%)	1 (1%)	68	89
21	O	112/112 (100%)	112 (100%)	0	100	100
22	P	107/113 (95%)	106 (99%)	1 (1%)	70	90
23	Q	107/109 (98%)	107 (100%)	0	100	100
24	R	92/92 (100%)	92 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	S	97/98 (99%)	97 (100%)	0	100	100
26	T	94/95 (99%)	94 (100%)	0	100	100
27	U	83/83 (100%)	83 (100%)	0	100	100
28	V	94/98 (96%)	94 (100%)	0	100	100
29	W	82/85 (96%)	81 (99%)	1 (1%)	63	86
30	X	85/86 (99%)	85 (100%)	0	100	100
31	Y	59/75 (79%)	58 (98%)	1 (2%)	53	82
32	Z	54/55 (98%)	54 (100%)	0	100	100
35	c	187/220 (85%)	184 (98%)	3 (2%)	55	83
36	d	163/174 (94%)	163 (100%)	0	100	100
37	e	174/177 (98%)	172 (99%)	2 (1%)	65	88
38	f	126/128 (98%)	125 (99%)	1 (1%)	73	90
39	g	85/88 (97%)	85 (100%)	0	100	100
40	h	130/133 (98%)	130 (100%)	0	100	100
41	i	112/113 (99%)	110 (98%)	2 (2%)	51	80
42	j	100/102 (98%)	98 (98%)	2 (2%)	48	78
43	k	87/92 (95%)	87 (100%)	0	100	100
44	l	90/101 (89%)	88 (98%)	2 (2%)	45	77
45	m	117/119 (98%)	117 (100%)	0	100	100
46	n	98/102 (96%)	97 (99%)	1 (1%)	68	89
47	o	51/52 (98%)	51 (100%)	0	100	100
48	p	76/79 (96%)	76 (100%)	0	100	100
49	q	77/81 (95%)	77 (100%)	0	100	100
50	r	74/81 (91%)	73 (99%)	1 (1%)	59	85
51	s	54/67 (81%)	54 (100%)	0	100	100
52	t	70/79 (89%)	70 (100%)	0	100	100
53	u	62/64 (97%)	62 (100%)	0	100	100
All	All	5145/5372 (96%)	5116 (99%)	29 (1%)	76	93

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	152	PHE

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Mol	Chain	Res	Type
1	0	245	TYR
1	0	289	ARG
1	0	346	TYR
5	4	22	LEU
6	5	21	LYS
13	F	83	LYS
13	F	109	PHE
13	F	166	ASP
13	F	170	ASN
19	M	53	ASP
20	N	34	ASN
22	P	56	ARG
29	W	56	LEU
31	Y	80	ARG
35	c	113	ARG
35	c	117	ILE
35	c	129	LEU
37	e	65	GLU
37	e	113	GLN
38	f	117	LEU
41	i	22	HIS
41	i	77	LEU
42	j	85	ARG
42	j	129	LYS
44	l	77	HIS
44	l	119	ASN
46	n	107	ARG
50	r	60	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	22	HIS
1	0	475	HIS
7	6	26	ASN
8	7	61	GLN
9	8	13	HIS
13	F	211	ASN
13	F	223	HIS
16	I	158	ASN
17	J	37	ASN
18	K	106	ASN

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Mol	Chain	Res	Type
18	K	111	HIS
19	M	137	GLN
20	N	3	GLN
21	O	17	ASN
22	P	35	GLN
23	Q	27	ASN
25	S	66	ASN
25	S	104	HIS
27	U	18	GLN
29	W	54	ASN
36	d	85	ASN
37	e	59	HIS
37	e	86	ASN
37	e	200	ASN
40	h	41	ASN
41	i	99	ASN
49	q	41	ASN
49	q	72	ASN
52	t	23	GLN
52	t	57	HIS
53	u	18	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2898/2912 (99%)	416 (14%)	16 (0%)
11	B	113/115 (98%)	20 (17%)	0
12	D	75/77 (97%)	15 (20%)	2 (2%)
33	a	1518/1558 (97%)	232 (15%)	0
34	b	11/19 (57%)	2 (18%)	0
All	All	4615/4681 (98%)	685 (14%)	18 (0%)

All (685) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	10	A
10	A	46	C
10	A	55	G
10	A	63	U
10	A	71	A
10	A	74	U

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Mol	Chain	Res	Type
10	A	75	G
10	A	93	U
10	A	101	G
10	A	117	A
10	A	118	A
10	A	119	U
10	A	150	A
10	A	161	A
10	A	164	A
10	A	169	G
10	A	177	G
10	A	198	A
10	A	201	A
10	A	215	A
10	A	218	A
10	A	224	A
10	A	225	A
10	A	230	A
10	A	231	U
10	A	247	G
10	A	250	G
10	A	251	C
10	A	252	G
10	A	257	A
10	A	271	C
10	A	282	G
10	A	289	U
10	A	290	G
10	A	297	U
10	A	298	U
10	A	299	G
10	A	300	U
10	A	301	A
10	A	308	C
10	A	309	G
10	A	310	A
10	A	311	U
10	A	312	A
10	A	317	A
10	A	318	G
10	A	320	C
10	A	321	U

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Mol	Chain	Res	Type
10	A	322	G
10	A	347	A
10	A	353	G
10	A	366	A
10	A	398	A
10	A	399	G
10	A	402	G
10	A	403	G
10	A	410	A
10	A	411	G
10	A	425	G
10	A	440	A
10	A	445	G
10	A	450	G
10	A	451	A
10	A	459	G
10	A	474	C
10	A	495	C
10	A	496	A
10	A	509	A
10	A	519	A
10	A	520	G
10	A	534	G
10	A	543	A
10	A	546	U
10	A	547	C
10	A	560	G
10	A	568	C
10	A	569	A
10	A	570	A
10	A	581	G
10	A	582	U
10	A	583	U
10	A	584	A
10	A	585	A
10	A	587	G
10	A	599	G
10	A	609	G
10	A	610	A
10	A	611	A
10	A	639	A
10	A	651	A

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Mol	Chain	Res	Type
10	A	665	A
10	A	675	A
10	A	683	U
10	A	684	A
10	A	691	A
10	A	692	U
10	A	694	A
10	A	724	A
10	A	725	U
10	A	768	G
10	A	769	A
10	A	786	U
10	A	796	G
10	A	803	A
10	A	814	G
10	A	821	A
10	A	823	U
10	A	829	A
10	A	831	G
10	A	844	G
10	A	851	C
10	A	858	A
10	A	866	U
10	A	867	U
10	A	885	U
10	A	886	G
10	A	899	G
10	A	906	A
10	A	921	G
10	A	922	G
10	A	926	A
10	A	928	C
10	A	929	U
10	A	931	G
10	A	933	G
10	A	935	U
10	A	936	A
10	A	950	A
10	A	952	C
10	A	954	C
10	A	957	A
10	A	965	U

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Mol	Chain	Res	Type
10	A	966	C
10	A	972	U
10	A	974	U
10	A	984	A
10	A	985	G
10	A	1000	G
10	A	1013	A
10	A	1022	A
10	A	1035	A
10	A	1051	U
10	A	1052	A
10	A	1064	G
10	A	1072	U
10	A	1086	G
10	A	1101	G
10	A	1109	A
10	A	1110	G
10	A	1111	C
10	A	1115	C
10	A	1117	C
10	A	1122	U
10	A	1123	A
10	A	1126	G
10	A	1127	A
10	A	1151	G
10	A	1155	C
10	A	1166	A
10	A	1167	A
10	A	1171	U
10	A	1172	A
10	A	1174	C
10	A	1175	G
10	A	1181	A
10	A	1182	A
10	A	1190	A
10	A	1196	G
10	A	1212	U
10	A	1213	U
10	A	1232	G
10	A	1248	G
10	A	1272	G
10	A	1274	G

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Mol	Chain	Res	Type
10	A	1286	G
10	A	1289	A
10	A	1292	G
10	A	1307	G
10	A	1308	A
10	A	1310	A
10	A	1311	G
10	A	1324	C
10	A	1335	U
10	A	1336	A
10	A	1338	G
10	A	1364	U
10	A	1380	C
10	A	1385	C
10	A	1387	U
10	A	1395	G
10	A	1400	A
10	A	1413	A
10	A	1414	U
10	A	1421	C
10	A	1430	A
10	A	1431	U
10	A	1451	G
10	A	1454	U
10	A	1455	G
10	A	1460	A
10	A	1461	U
10	A	1468	A
10	A	1469	C
10	A	1474	U
10	A	1495	U
10	A	1496	U
10	A	1497	G
10	A	1500	A
10	A	1503	G
10	A	1509	C
10	A	1511	A
10	A	1517	U
10	A	1520	G
10	A	1524	U
10	A	1526	A
10	A	1530	G

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Mol	Chain	Res	Type
10	A	1534	U
10	A	1535	A
10	A	1536	A
10	A	1537	A
10	A	1538	U
10	A	1544	A
10	A	1551	A
10	A	1564	G
10	A	1565	A
10	A	1567	G
10	A	1569	G
10	A	1575	A
10	A	1576	A
10	A	1583	G
10	A	1584	U
10	A	1611	A
10	A	1614	A
10	A	1621	U
10	A	1623	U
10	A	1627	G
10	A	1629	G
10	A	1649	U
10	A	1650	A
10	A	1652	A
10	A	1688	A
10	A	1689	G
10	A	1690	C
10	A	1691	G
10	A	1716	G
10	A	1742	A
10	A	1756	U
10	A	1757	C
10	A	1758	G
10	A	1759	G
10	A	1769	G
10	A	1775	A
10	A	1776	G
10	A	1777	G
10	A	1786	A
10	A	1795	C
10	A	1804	A
10	A	1813	C

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Mol	Chain	Res	Type
10	A	1814	A
10	A	1829	A
10	A	1830	G
10	A	1842	A
10	A	1855	G
10	A	1860	A
10	A	1873	U
10	A	1883	U
10	A	1884	C
10	A	1885	G
10	A	1919	G
10	A	1926	A
10	A	1927	C
10	A	1935	G
10	A	1942	G
10	A	1943	G
10	A	1950	A
10	A	1951	A
10	A	1953	U
10	A	1968	U
10	A	1976	C
10	A	1980	C
10	A	1983	A
10	A	1984	A
10	A	1985	G
10	A	2004	U
10	A	2006	U
10	A	2009	C
10	A	2010	A
10	A	2034	G
10	A	2035	U
10	A	2036	A
10	A	2044	A
10	A	2045	G
10	A	2046	A
10	A	2056	C
10	A	2068	C
10	A	2069	G
10	A	2073	A
10	A	2074	G
10	A	2075	A
10	A	2082	G

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Mol	Chain	Res	Type
10	A	2096	G
10	A	2108	G
10	A	2112	U
10	A	2120	C
10	A	2121	A
10	A	2124	U
10	A	2125	A
10	A	2129	G
10	A	2130	A
10	A	2145	U
10	A	2146	G
10	A	2158	C
10	A	2160	A
10	A	2161	G
10	A	2171	A
10	A	2172	G
10	A	2173	G
10	A	2185	U
10	A	2186	A
10	A	2191	C
10	A	2196	U
10	A	2201	U
10	A	2207	C
10	A	2211	A
10	A	2212	A
10	A	2216	G
10	A	2217	C
10	A	2224	A
10	A	2225	A
10	A	2227	C
10	A	2238	A
10	A	2251	G
10	A	2252	G
10	A	2259	G
10	A	2281	A
10	A	2292	G
10	A	2296	C
10	A	2300	A
10	A	2312	G
10	A	2318	U
10	A	2319	U
10	A	2321	G

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Mol	Chain	Res	Type
10	A	2331	G
10	A	2333	A
10	A	2334	G
10	A	2335	A
10	A	2338	G
10	A	2347	G
10	A	2348	A
10	A	2360	C
10	A	2363	C
10	A	2396	G
10	A	2398	C
10	A	2415	U
10	A	2435	C
10	A	2437	C
10	A	2438	A
10	A	2442	G
10	A	2443	A
10	A	2448	A
10	A	2454	C
10	A	2461	A
10	A	2478	C
10	A	2489	A
10	A	2515	G
10	A	2518	G
10	A	2531	A
10	A	2533	C
10	A	2542	G
10	A	2548	G
10	A	2561	G
10	A	2567	U
10	A	2579	A
10	A	2580	G
10	A	2591	G
10	A	2597	U
10	A	2599	C
10	A	2615	A
10	A	2622	U
10	A	2623	C
10	A	2626	U
10	A	2628	U
10	A	2642	U
10	A	2674	G

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Mol	Chain	Res	Type
10	A	2695	G
10	A	2698	G
10	A	2702	U
10	A	2727	G
10	A	2739	U
10	A	2746	A
10	A	2761	A
10	A	2770	A
10	A	2778	A
10	A	2779	G
10	A	2791	A
10	A	2792	U
10	A	2793	G
10	A	2803	A
10	A	2804	U
10	A	2809	U
10	A	2810	U
10	A	2811	A
10	A	2812	A
10	A	2813	G
10	A	2816	A
10	A	2818	U
10	A	2830	G
10	A	2843	A
10	A	2845	A
10	A	2871	U
10	A	2877	G
10	A	2878	A
10	A	2882	G
10	A	2890	C
10	A	2893	A
10	A	2903	G
11	B	5	G
11	B	7	G
11	B	10	G
11	B	13	A
11	B	23	A
11	B	28	C
11	B	33	U
11	B	35	C
11	B	39	G
11	B	54	U

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Mol	Chain	Res	Type
11	B	55	A
11	B	64	A
11	B	65	G
11	B	87	U
11	B	88	C
11	B	97	A
11	B	101	U
11	B	107	G
11	B	108	U
11	B	115	G
12	D	6	G
12	D	8	U
12	D	11	A
12	D	14	A
12	D	16	U
12	D	17	C
12	D	18	A
12	D	19	G
12	D	21	U
12	D	22	A
12	D	23	G
12	D	47	G
12	D	48	U
12	D	50	G
12	D	68	C
33	a	10	A
33	a	11	G
33	a	34	A
33	a	41	G
33	a	49	C
33	a	50	C
33	a	53	A
33	a	57	A
33	a	74	C
33	a	75	U
33	a	117	A
33	a	118	G
33	a	132	A
33	a	135	A
33	a	136	A
33	a	137	C
33	a	146	A

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Mol	Chain	Res	Type
33	a	154	C
33	a	161	G
33	a	162	G
33	a	163	G
33	a	168	A
33	a	172	C
33	a	177	A
33	a	179	A
33	a	180	C
33	a	182	G
33	a	190	U
33	a	191	A
33	a	194	G
33	a	200	C
33	a	213	A
33	a	215	G
33	a	227	A
33	a	228	A
33	a	229	A
33	a	230	G
33	a	266	U
33	a	271	U
33	a	272	A
33	a	273	G
33	a	277	G
33	a	292	G
33	a	293	C
33	a	297	C
33	a	299	A
33	a	315	G
33	a	347	A
33	a	354	C
33	a	355	A
33	a	358	G
33	a	370	A
33	a	373	G
33	a	378	C
33	a	380	G
33	a	391	U
33	a	392	C
33	a	393	U
33	a	398	C

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Mol	Chain	Res	Type
33	a	399	A
33	a	418	G
33	a	423	A
33	a	432	G
33	a	438	A
33	a	439	G
33	a	440	A
33	a	441	A
33	a	442	G
33	a	447	U
33	a	448	C
33	a	451	A
33	a	455	U
33	a	465	U
33	a	470	A
33	a	471	G
33	a	473	G
33	a	478	A
33	a	479	C
33	a	485	C
33	a	488	U
33	a	494	C
33	a	495	U
33	a	502	C
33	a	510	G
33	a	511	G
33	a	524	A
33	a	535	A
33	a	537	C
33	a	539	A
33	a	540	C
33	a	544	C
33	a	547	G
33	a	553	G
33	a	556	G
33	a	557	U
33	a	558	A
33	a	573	A
33	a	585	A
33	a	588	U
33	a	590	U
33	a	598	A

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Mol	Chain	Res	Type
33	a	599	A
33	a	602	C
33	a	603	G
33	a	644	C
33	a	659	U
33	a	679	U
33	a	691	A
33	a	712	U
33	a	713	A
33	a	736	G
33	a	749	U
33	a	750	G
33	a	757	G
33	a	787	G
33	a	803	A
33	a	819	U
33	a	820	A
33	a	841	A
33	a	843	C
33	a	846	U
33	a	854	A
33	a	862	G
33	a	866	G
33	a	870	C
33	a	873	C
33	a	882	G
33	a	899	A
33	a	929	G
33	a	941	A
33	a	954	G
33	a	961	C
33	a	962	A
33	a	972	G
33	a	985	A
33	a	987	U
33	a	994	C
33	a	995	A
33	a	996	A
33	a	998	G
33	a	1002	A
33	a	1003	G
33	a	1004	A

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Mol	Chain	Res	Type
33	a	1019	U
33	a	1020	G
33	a	1026	C
33	a	1028	U
33	a	1030	G
33	a	1031	A
33	a	1032	C
33	a	1033	C
33	a	1036	U
33	a	1045	A
33	a	1050	U
33	a	1051	U
33	a	1052	U
33	a	1053	C
33	a	1055	C
33	a	1058	C
33	a	1059	G
33	a	1060	G
33	a	1063	A
33	a	1064	C
33	a	1065	A
33	a	1067	A
33	a	1073	A
33	a	1076	U
33	a	1077	G
33	a	1080	G
33	a	1081	C
33	a	1092	U
33	a	1121	G
33	a	1122	U
33	a	1128	A
33	a	1149	U
33	a	1159	C
33	a	1161	U
33	a	1163	U
33	a	1165	G
33	a	1166	U
33	a	1171	C
33	a	1172	A
33	a	1180	G
33	a	1183	A
33	a	1185	U

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Mol	Chain	Res	Type
33	a	1194	C
33	a	1210	G
33	a	1222	A
33	a	1223	A
33	a	1239	A
33	a	1240	U
33	a	1253	A
33	a	1264	A
33	a	1283	C
33	a	1286	U
33	a	1306	A
33	a	1307	U
33	a	1313	A
33	a	1319	U
33	a	1326	G
33	a	1328	U
33	a	1331	G
33	a	1340	C
33	a	1344	A
33	a	1348	C
33	a	1379	G
33	a	1390	C
33	a	1404	C
33	a	1415	C
33	a	1420	A
33	a	1423	C
33	a	1424	A
33	a	1445	G
33	a	1455	C
33	a	1466	U
33	a	1468	A
33	a	1472	A
33	a	1478	U
33	a	1479	U
33	a	1480	U
33	a	1481	G
33	a	1517	U
33	a	1519	A
33	a	1521	G
33	a	1524	G
33	a	1530	A
33	a	1533	U

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Mol	Chain	Res	Type
33	a	1544	G
33	a	1556	G
33	a	1557	G
33	a	1558	A
33	a	1564	U
34	b	6	U
34	b	16	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	9	G
10	A	227	A
10	A	251	C
10	A	288	U
10	A	297	U
10	A	1057	U
10	A	1189	U
10	A	1536	A
10	A	1583	G
10	A	1689	G
10	A	2111	U
10	A	2216	G
10	A	2318	U
10	A	2808	U
10	A	2810	U
10	A	2877	G
12	D	16	U
12	D	20	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

Of 349 ligands modelled in this entry, 345 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	SCM	a	1675	-	23,25,25	7.26	11 (47%)	27,39,39	1.45	4 (14%)
54	ATP	0	601	55	32,33,33	3.50	15 (46%)	48,52,52	2.18	14 (29%)
54	ATP	0	602	55	32,33,33	3.55	15 (46%)	48,52,52	2.21	15 (31%)
58	PUT	a	1664	-	5,5,5	0.24	0	4,4,4	0.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	SCM	a	1675	-	-	0/4/57/57	0/3/3/3
54	ATP	0	601	55	-	9/22/38/38	0/3/3/3
54	ATP	0	602	55	-	7/22/38/38	0/3/3/3
58	PUT	a	1664	-	-	0/3/3/3	-

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	a	1675	SCM	O2B-C12	-27.81	1.01	1.44
59	a	1675	SCM	O1-C2	-16.66	1.15	1.44
54	0	601	ATP	C2'-C3'	-10.66	1.24	1.53
54	0	602	ATP	C2'-C3'	-10.58	1.24	1.53
54	0	602	ATP	O4'-C4'	-6.79	1.29	1.45
54	0	601	ATP	O4'-C4'	-6.57	1.30	1.45
54	0	602	ATP	PA-O3A	6.00	1.66	1.59
54	0	602	ATP	PB-O3A	5.72	1.65	1.59
54	0	601	ATP	PA-O3A	5.55	1.65	1.59
54	0	601	ATP	C3'-C4'	5.54	1.67	1.53
59	a	1675	SCM	C2M-C2	5.53	1.72	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	0	602	ATP	C3'-C4'	5.48	1.66	1.53
54	0	601	ATP	PB-O3A	5.48	1.65	1.59
54	0	602	ATP	PB-O3B	5.41	1.65	1.59
54	0	601	ATP	PB-O3B	5.39	1.65	1.59
54	0	602	ATP	C1'-N9	-5.08	1.32	1.46
54	0	601	ATP	C1'-N9	-5.03	1.32	1.46
59	a	1675	SCM	C9-C8	4.65	1.61	1.53
54	0	602	ATP	C6-N6	4.52	1.45	1.34
59	a	1675	SCM	C8-N8	-4.48	1.39	1.47
54	0	601	ATP	C6-N6	4.47	1.45	1.34
59	a	1675	SCM	O1B-C7	4.02	1.50	1.44
59	a	1675	SCM	C11-C12	3.91	1.62	1.52
54	0	601	ATP	O4'-C1'	3.79	1.50	1.42
59	a	1675	SCM	C12-C7	-3.72	1.44	1.52
54	0	602	ATP	O4'-C1'	3.71	1.50	1.42
59	a	1675	SCM	C3-C2	-3.48	1.44	1.51
59	a	1675	SCM	O11-C11	-3.46	1.34	1.43
54	0	602	ATP	C5-C4	-3.20	1.33	1.39
54	0	602	ATP	O2'-C2'	3.09	1.50	1.43
54	0	601	ATP	O2'-C2'	3.06	1.50	1.43
54	0	601	ATP	C5-C4	-3.05	1.33	1.39
54	0	602	ATP	C5-N7	-2.58	1.34	1.39
54	0	601	ATP	C5-N7	-2.57	1.34	1.39
59	a	1675	SCM	C9-C10	-2.35	1.48	1.53
54	0	602	ATP	C8-N9	-2.24	1.33	1.37
54	0	601	ATP	C2'-C1'	2.23	1.60	1.53
54	0	602	ATP	C2'-C1'	2.22	1.60	1.53
54	0	601	ATP	C8-N9	-2.20	1.33	1.37
54	0	601	ATP	O3'-C3'	2.01	1.47	1.43
54	0	602	ATP	O3'-C3'	2.01	1.47	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	0	602	ATP	N3-C2-N1	-5.75	119.88	128.58
54	0	601	ATP	C1'-N9-C8	-5.74	114.36	127.09
54	0	602	ATP	C1'-N9-C8	-5.64	114.57	127.09
54	0	601	ATP	N3-C2-N1	-5.58	120.13	128.58
54	0	601	ATP	C5-C4-N3	-4.78	120.13	126.72
54	0	601	ATP	C4-N9-C1'	4.67	137.54	126.63
54	0	602	ATP	C5-C4-N3	-4.63	120.35	126.72
54	0	602	ATP	C4-N9-C1'	4.47	137.09	126.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	0	602	ATP	N9-C8-N7	-4.30	107.83	113.94
54	0	601	ATP	N6-C6-N1	-4.14	109.16	118.38
54	0	602	ATP	N6-C6-N1	-4.14	109.17	118.38
54	0	601	ATP	N9-C8-N7	-4.13	108.08	113.94
59	a	1675	SCM	C1M-N10-C10	-3.91	109.18	114.23
54	0	602	ATP	C4'-O4'-C1'	-3.45	101.85	109.47
54	0	602	ATP	C2-N3-C4	3.36	120.04	111.83
54	0	601	ATP	C2-N3-C4	3.33	119.97	111.83
54	0	601	ATP	C5-C6-N6	2.89	130.45	123.29
54	0	601	ATP	C2'-C3'-C4'	2.88	108.18	102.61
59	a	1675	SCM	C2M-C2-C3	-2.87	108.10	113.27
54	0	602	ATP	C5-C6-N6	2.86	130.36	123.29
54	0	601	ATP	N3-C4-N9	2.82	131.96	127.17
54	0	601	ATP	C5-N7-C8	2.78	107.81	103.45
54	0	602	ATP	C5-N7-C8	2.77	107.81	103.45
54	0	602	ATP	N3-C4-N9	2.76	131.86	127.17
59	a	1675	SCM	C8M-N8-C8	-2.52	110.98	114.23
54	0	602	ATP	C2'-C3'-C4'	2.51	107.46	102.61
54	0	602	ATP	C4-N9-C8	2.47	108.33	105.74
59	a	1675	SCM	O1-C2-C3	2.33	111.87	108.62
54	0	601	ATP	C3'-C2'-C1'	2.24	105.70	101.46
54	0	601	ATP	C4-N9-C8	2.23	108.08	105.74
54	0	601	ATP	C4-C5-N7	-2.16	108.11	110.58
54	0	602	ATP	C3'-C2'-C1'	2.15	105.52	101.46
54	0	602	ATP	C4-C5-N7	-2.06	108.23	110.58

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
54	0	601	ATP	PB-O3B-PG-O2G
54	0	601	ATP	C5'-O5'-PA-O1A
54	0	601	ATP	C5'-O5'-PA-O2A
54	0	601	ATP	O4'-C4'-C5'-O5'
54	0	601	ATP	C3'-C4'-C5'-O5'
54	0	602	ATP	O4'-C4'-C5'-O5'
54	0	601	ATP	C5'-O5'-PA-O3A
54	0	602	ATP	C5'-O5'-PA-O1A
54	0	602	ATP	C5'-O5'-PA-O2A
54	0	602	ATP	C5'-O5'-PA-O3A
54	0	601	ATP	PG-O3B-PB-O2B
54	0	602	ATP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
54	0	601	ATP	PB-O3B-PG-O1G
54	0	601	ATP	PG-O3B-PB-O1B
54	0	602	ATP	C3'-C4'-C5'-O5'
54	0	602	ATP	PA-O3A-PB-O1B

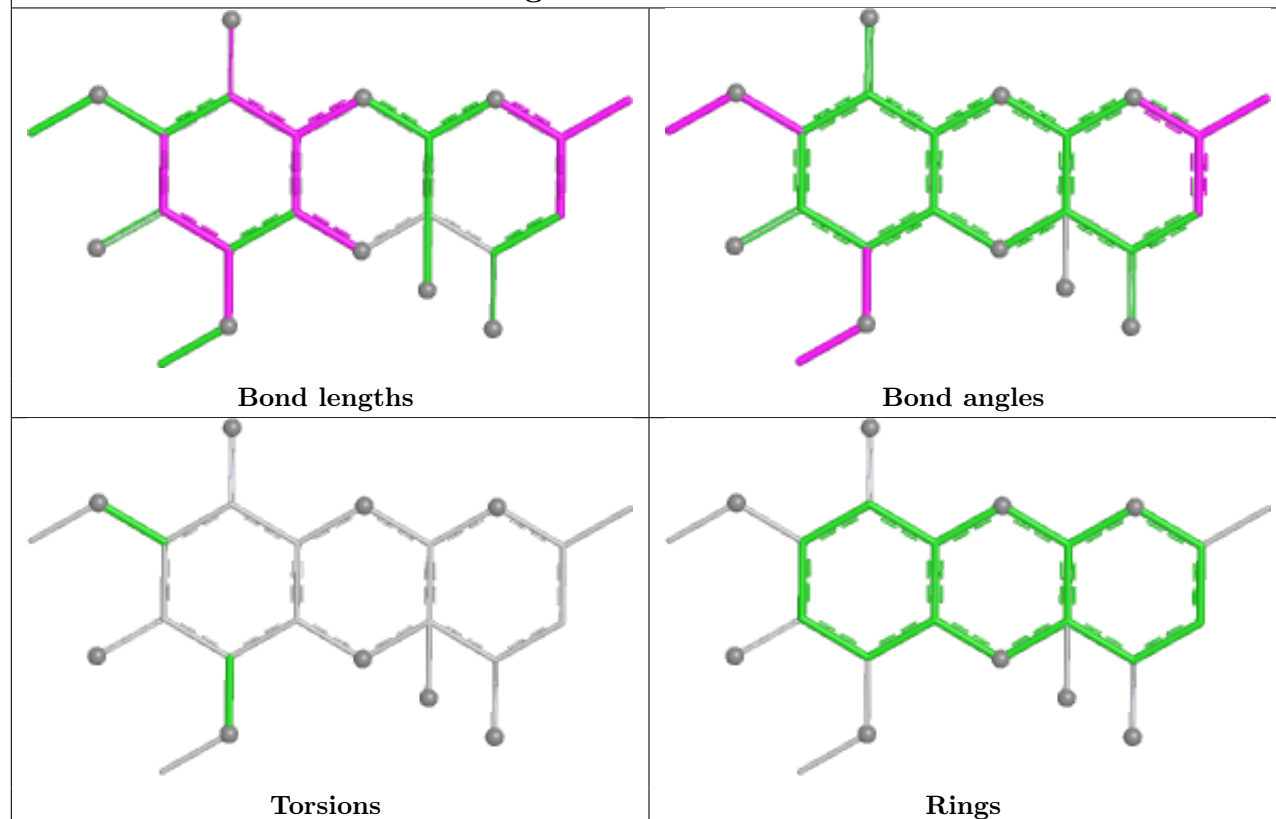
There are no ring outliers.

3 monomers are involved in 4 short contacts:

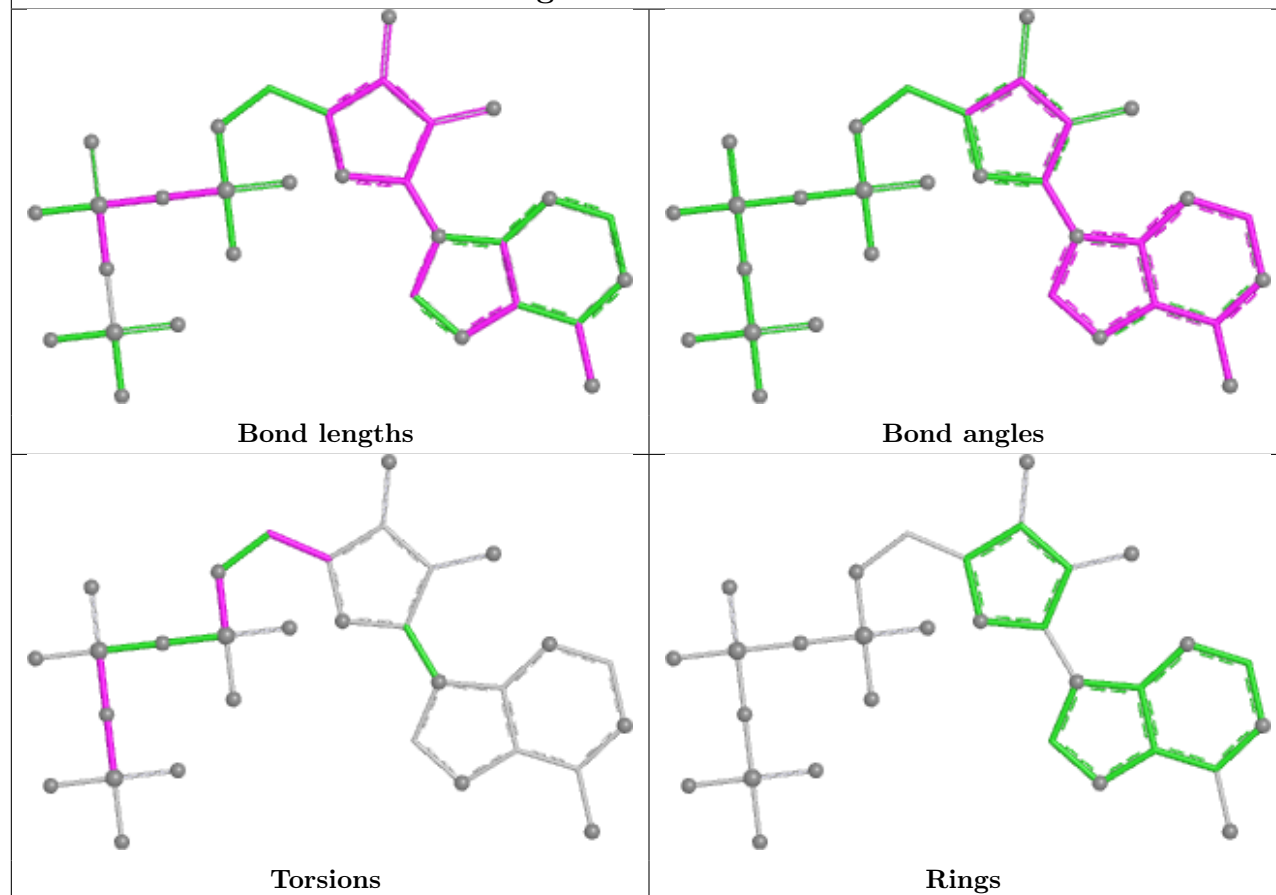
Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	a	1675	SCM	1	0
54	0	601	ATP	1	0
54	0	602	ATP	2	0

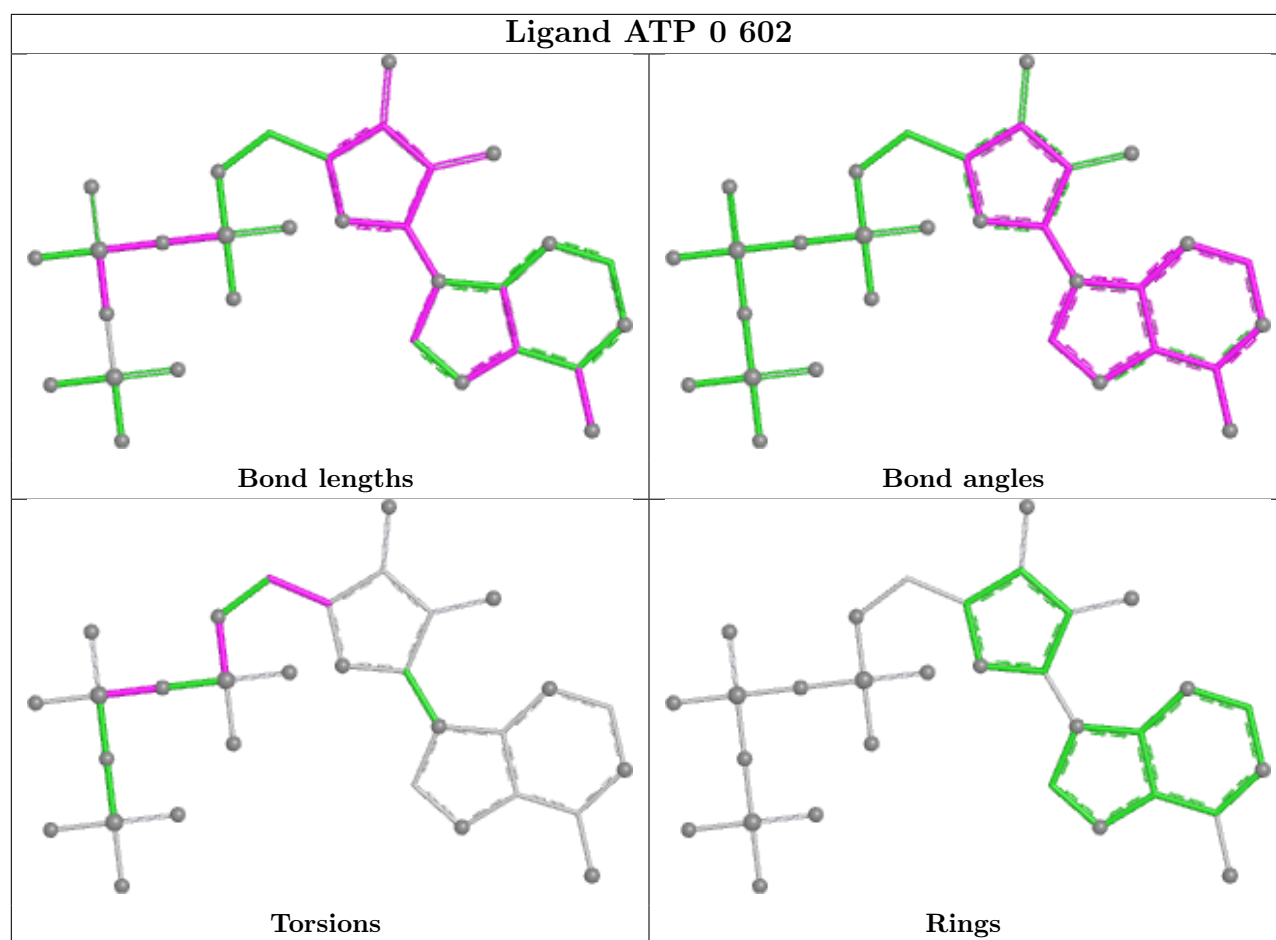
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand SCM a 1675



Ligand ATP 0 601





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

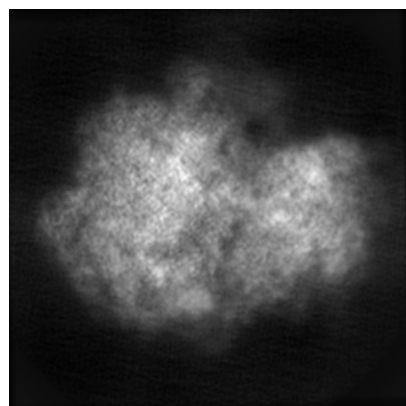
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13242. These allow visual inspection of the internal detail of the map and identification of artifacts.

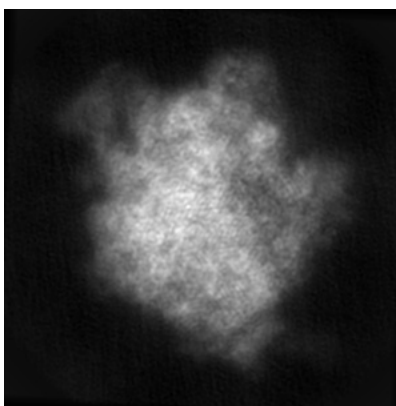
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

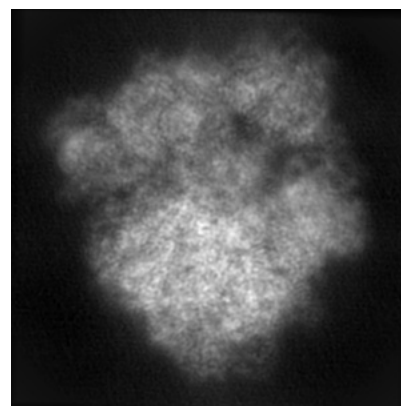
6.1.1 Primary map



X

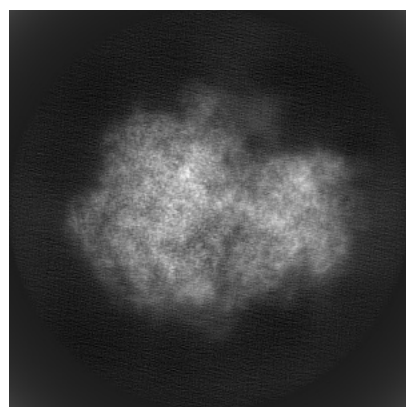


Y

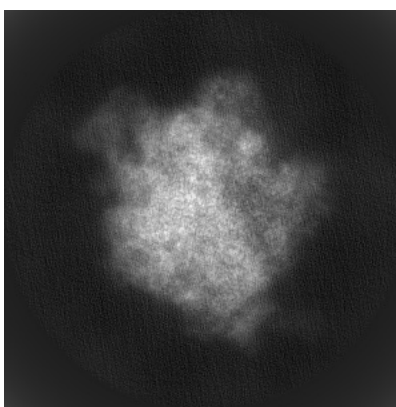


Z

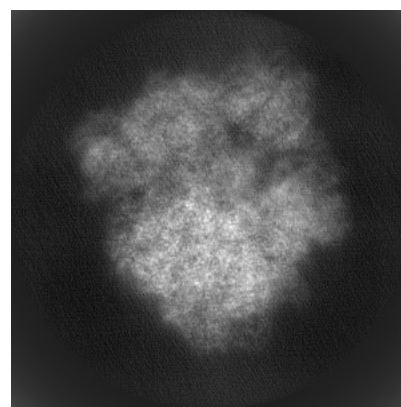
6.1.2 Raw map



X



Y

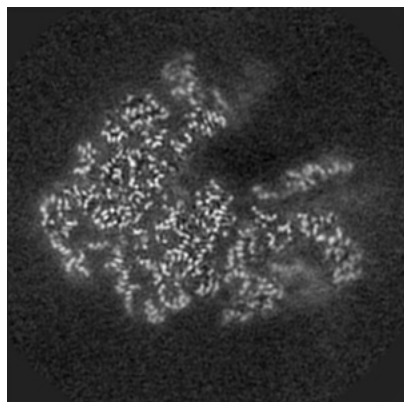


Z

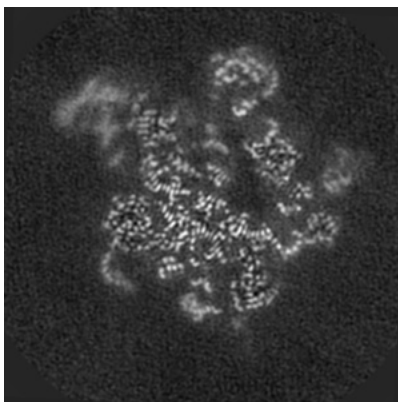
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

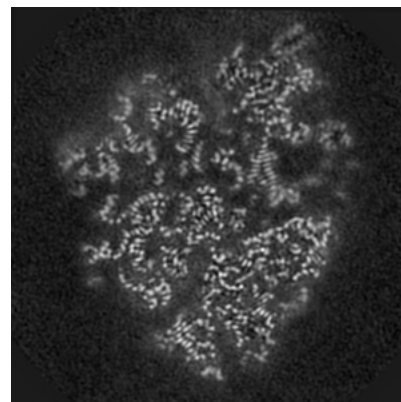
6.2.1 Primary map



X Index: 180

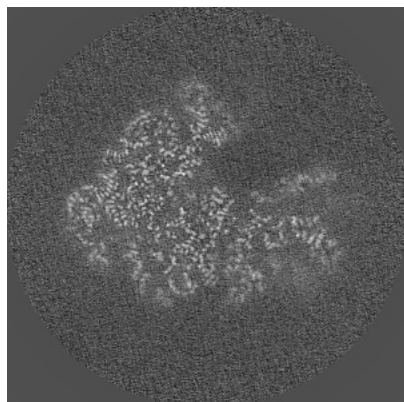


Y Index: 180

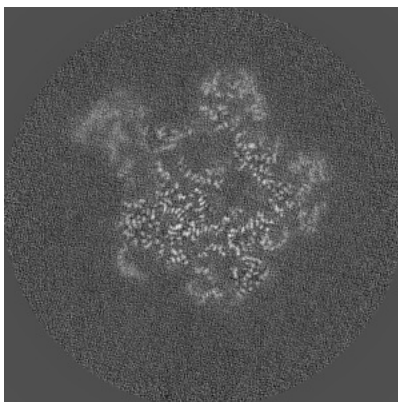


Z Index: 180

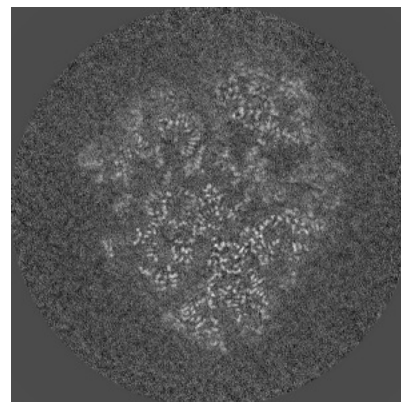
6.2.2 Raw map



X Index: 210



Y Index: 210

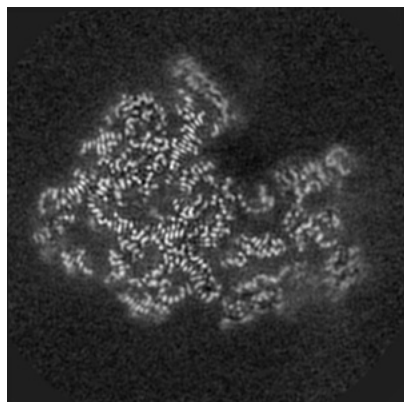


Z Index: 210

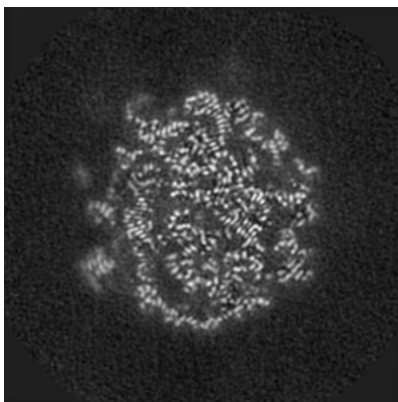
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

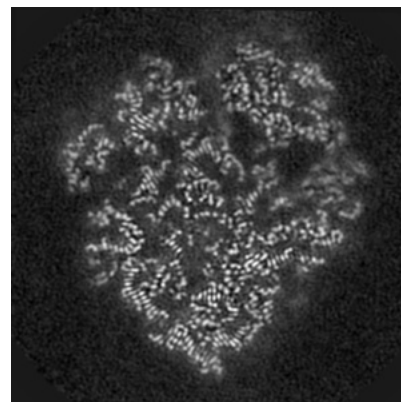
6.3.1 Primary map



X Index: 171

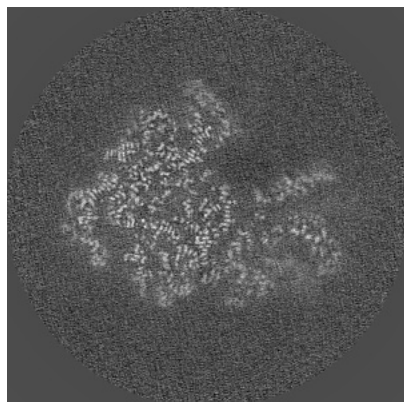


Y Index: 130

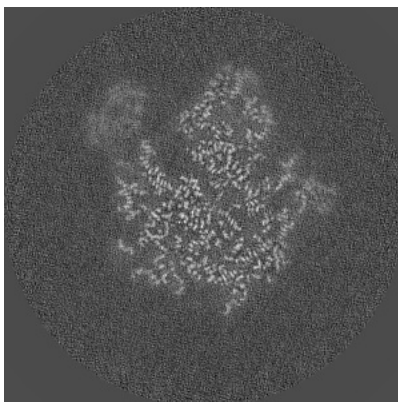


Z Index: 188

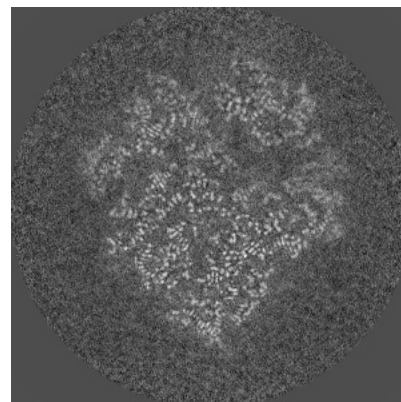
6.3.2 Raw map



X Index: 207



Y Index: 191

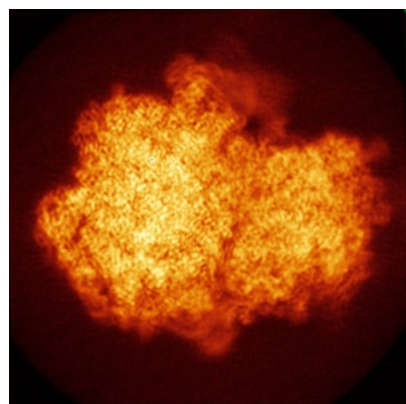


Z Index: 217

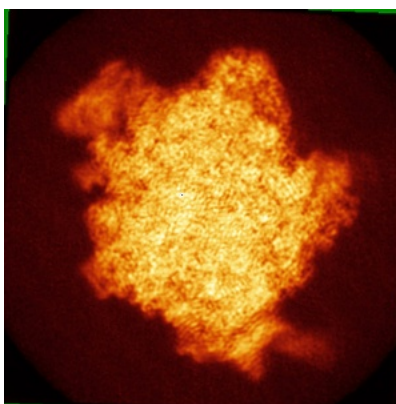
The images above show the largest variance slices of the map in three orthogonal directions.

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

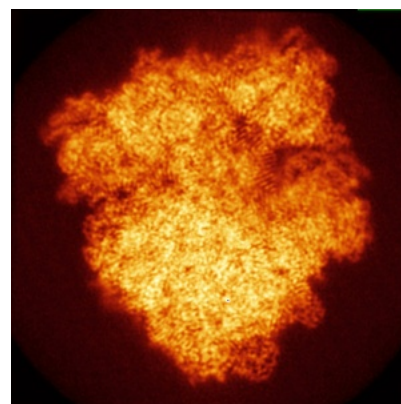
6.4.1 Primary map



X

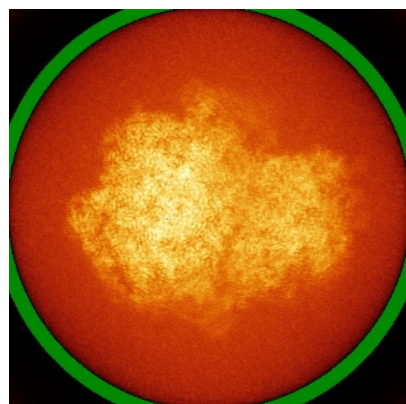


Y

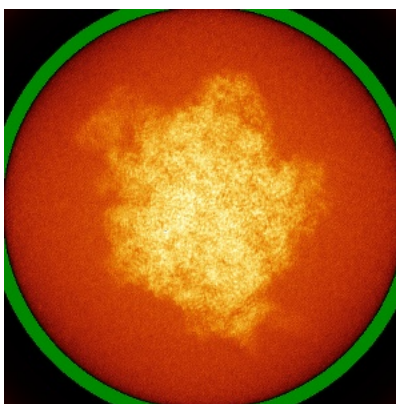


Z

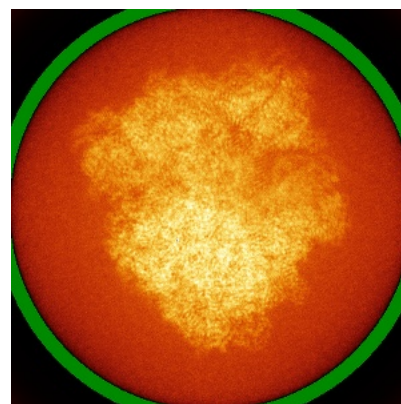
6.4.2 Raw map



X



Y

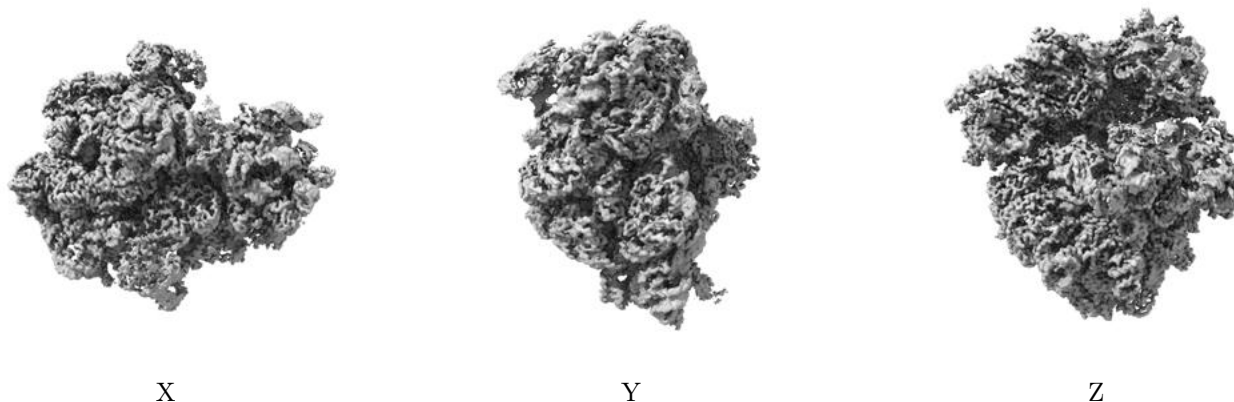


Z

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

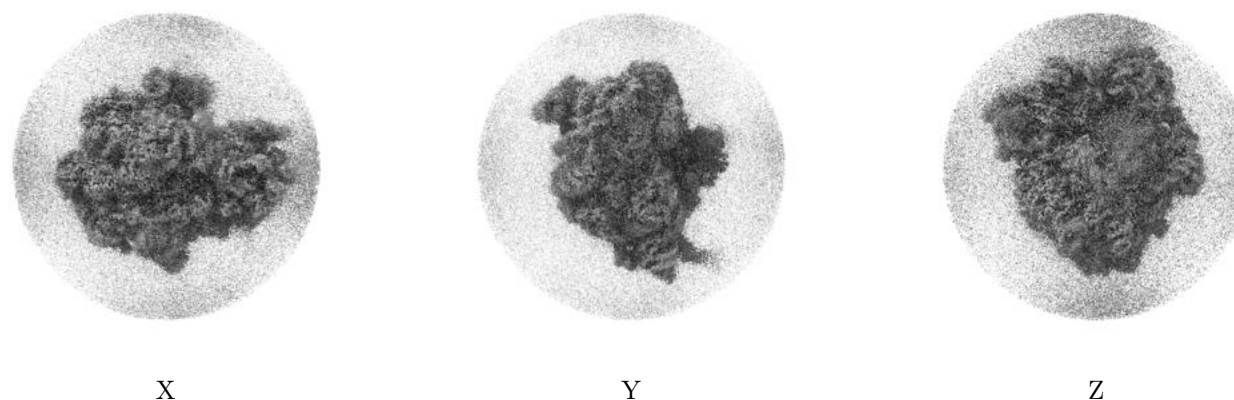
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

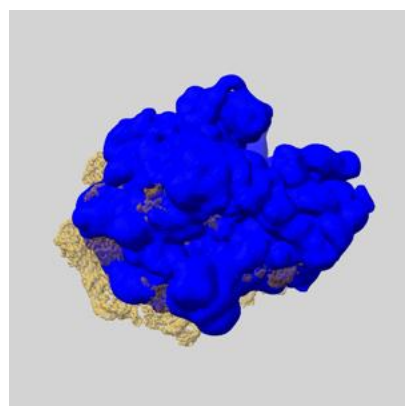
6.6 Mask visualisation [i](#)

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

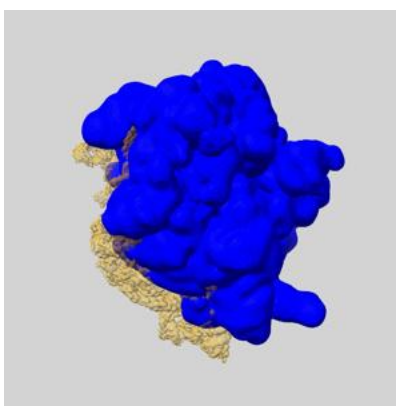
A mask typically either:

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

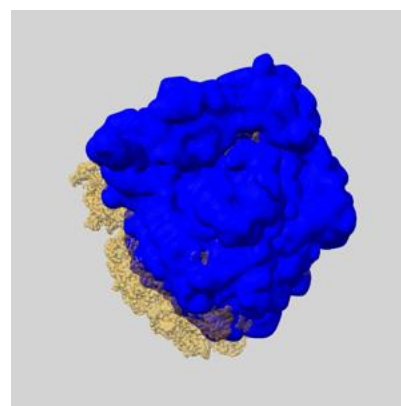
6.6.1 emd_13242_msk_1.map [i](#)



X



Y

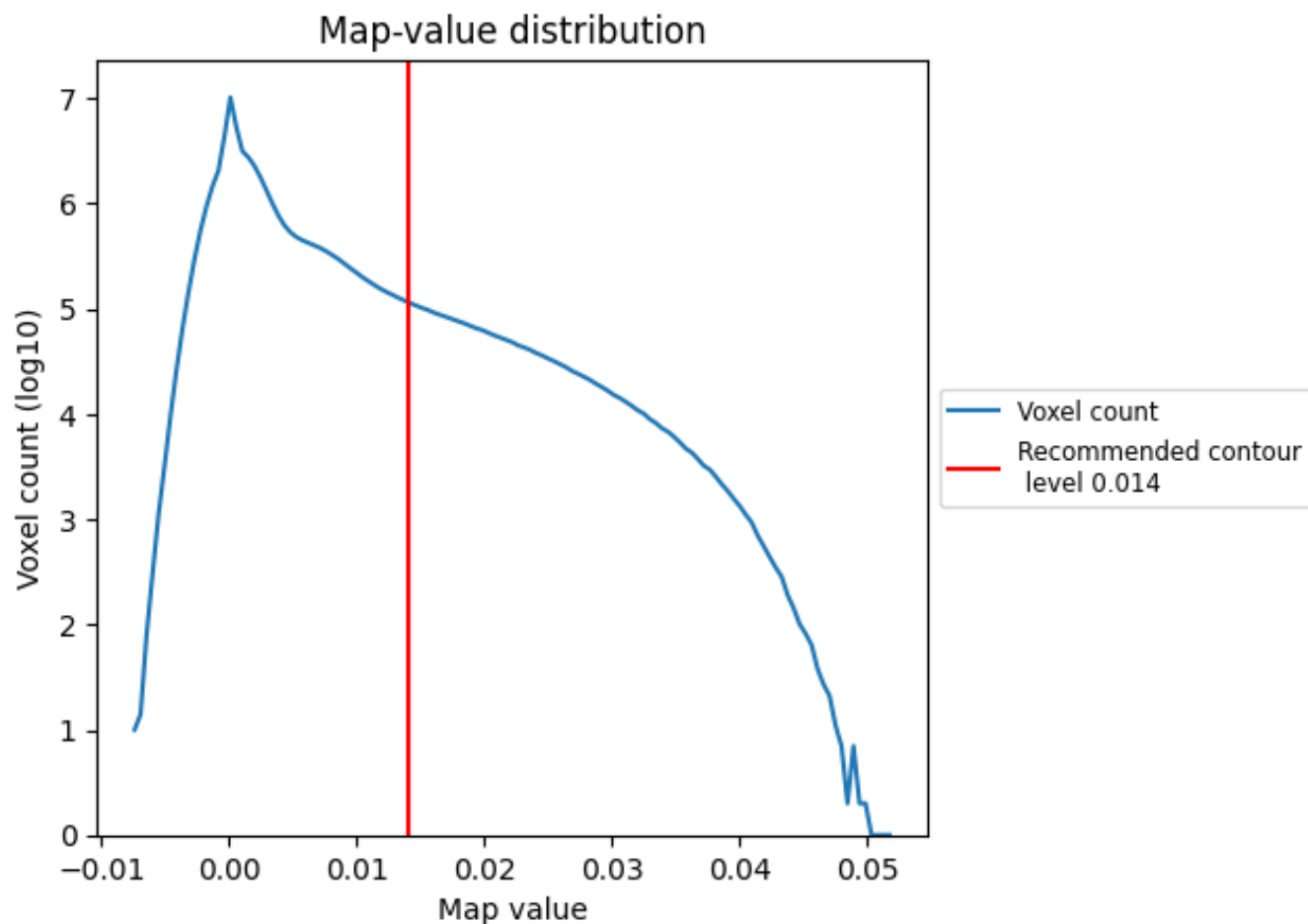


Z

7 Map analysis [i](#)

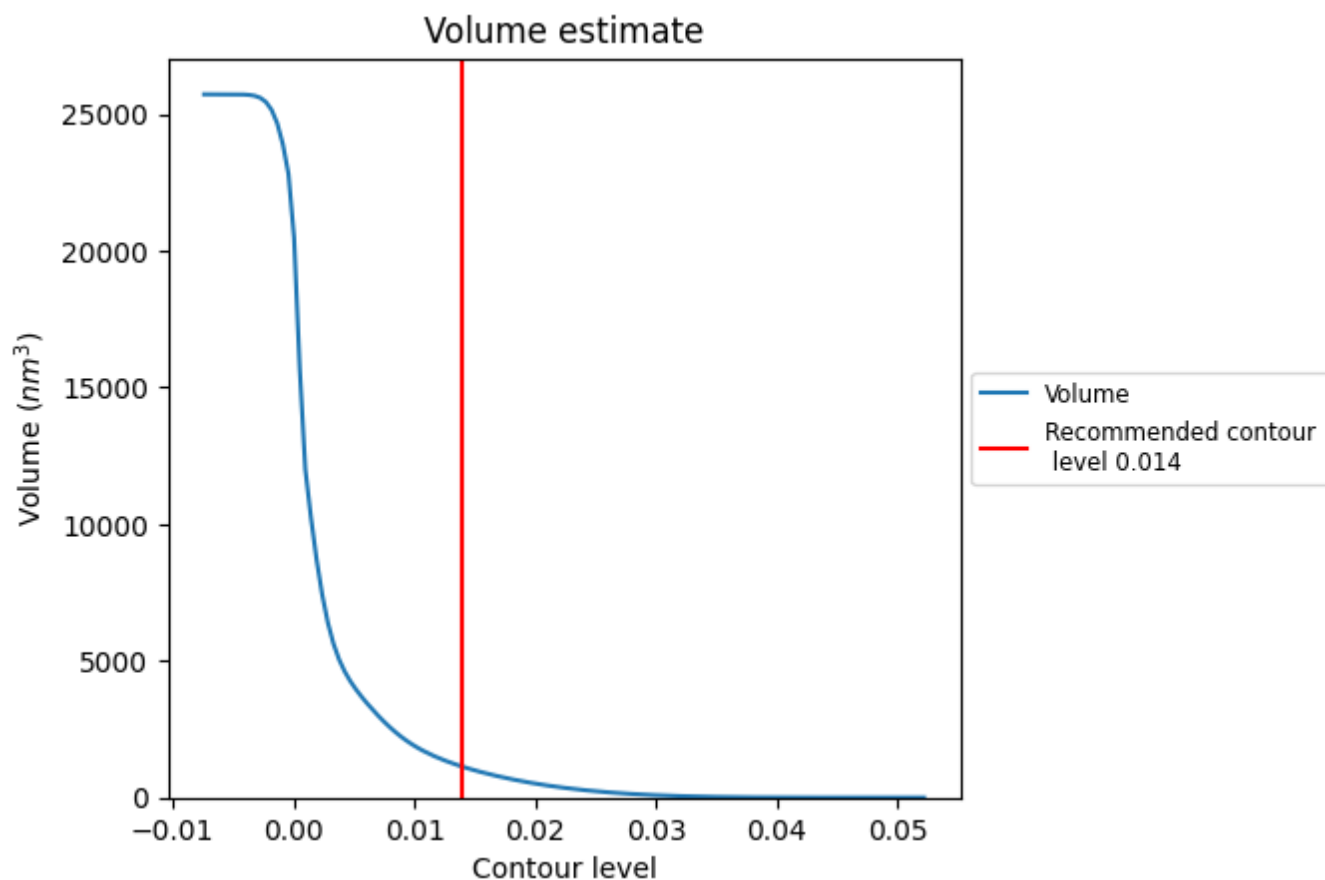
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

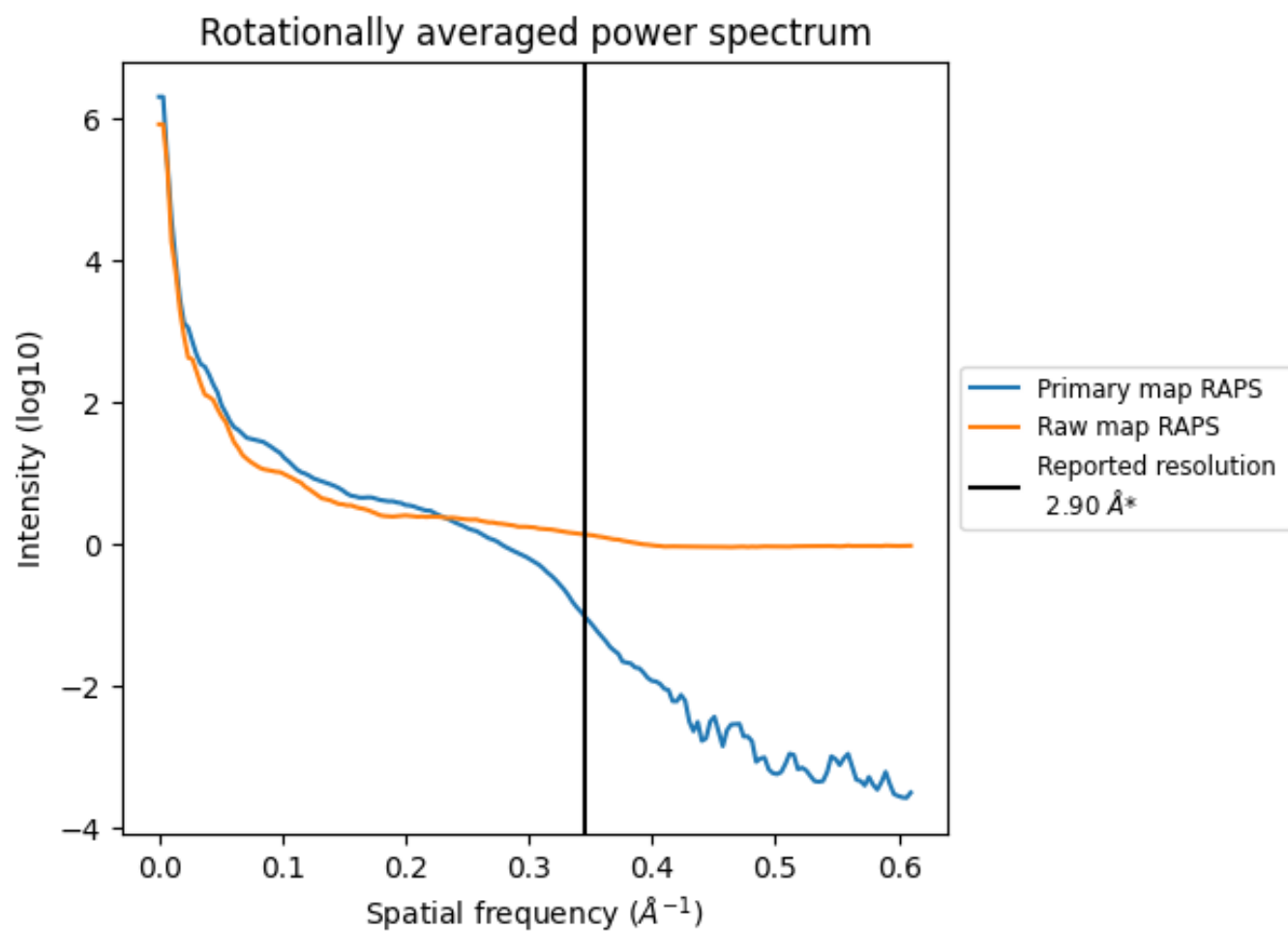
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1128 nm³; this corresponds to an approximate mass of 1019 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 ⓘ

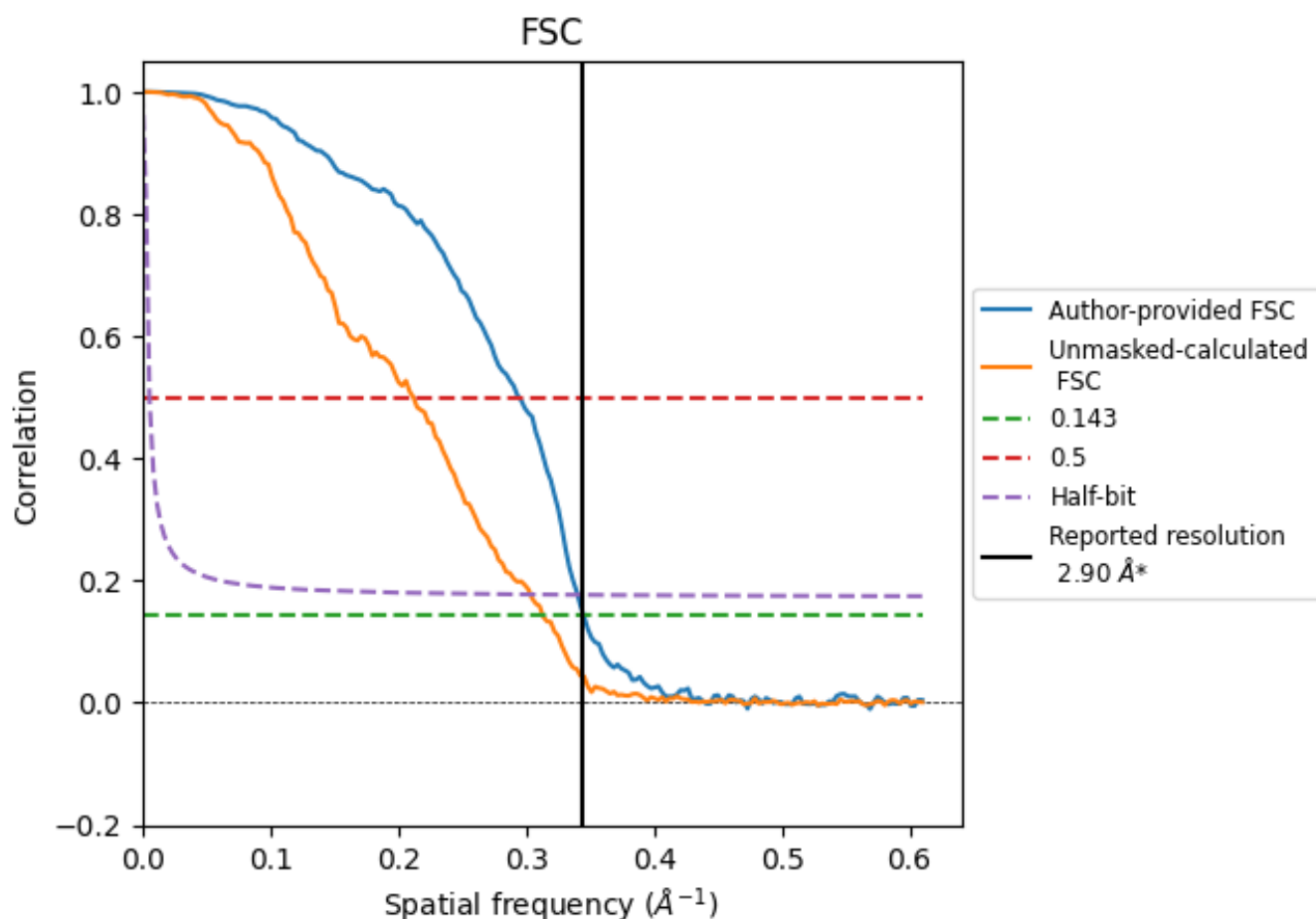


*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.345 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

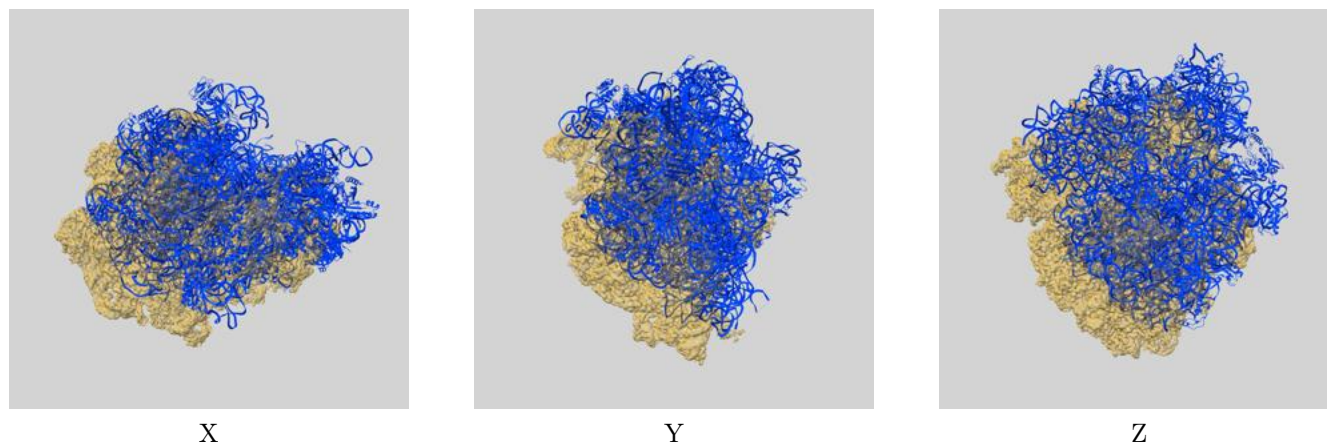
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.39	2.94
Unmasked-calculated*	3.19	4.72	3.29

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.19 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

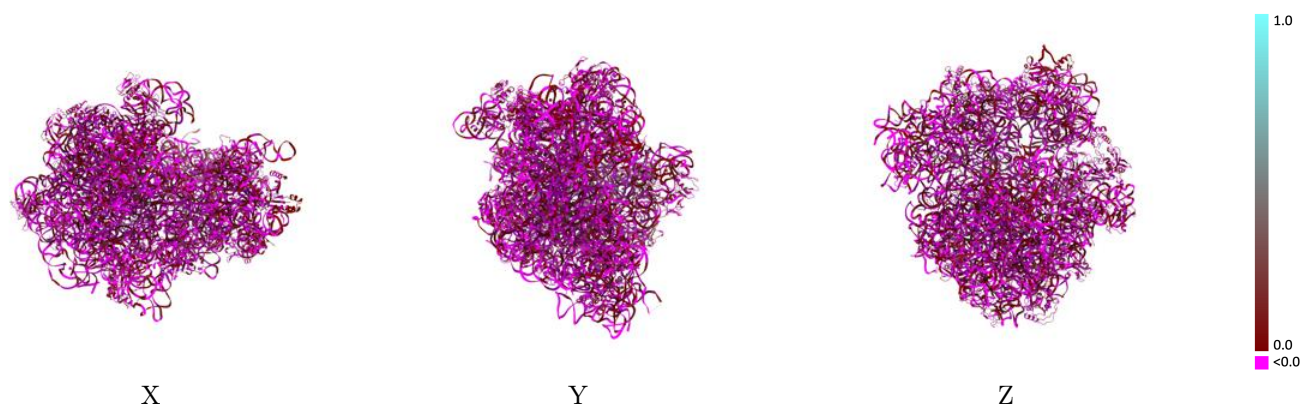
This section contains information regarding the fit between EMDB map EMD-13242 and PDB model 7P7R. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



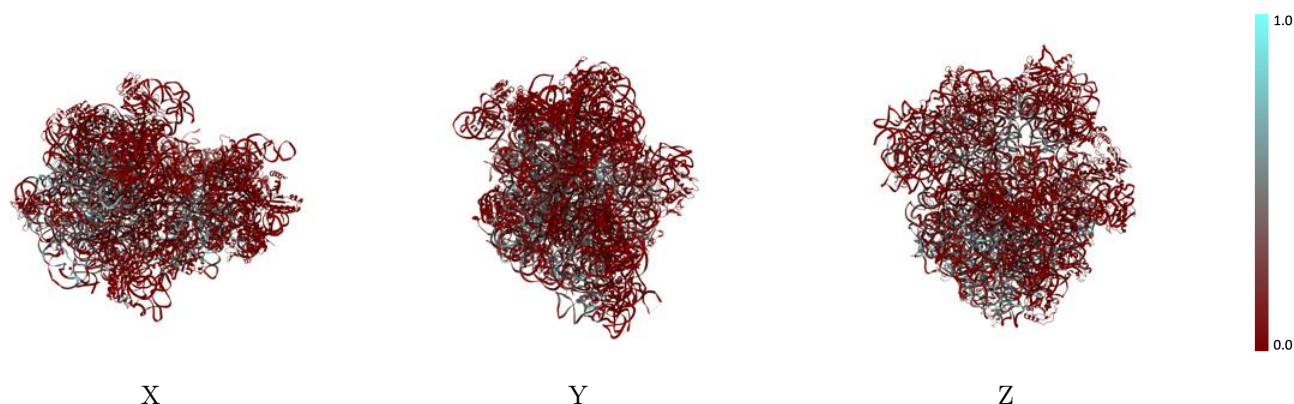
The images above show the 3D surface view of the map at the recommended contour level 0.014 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



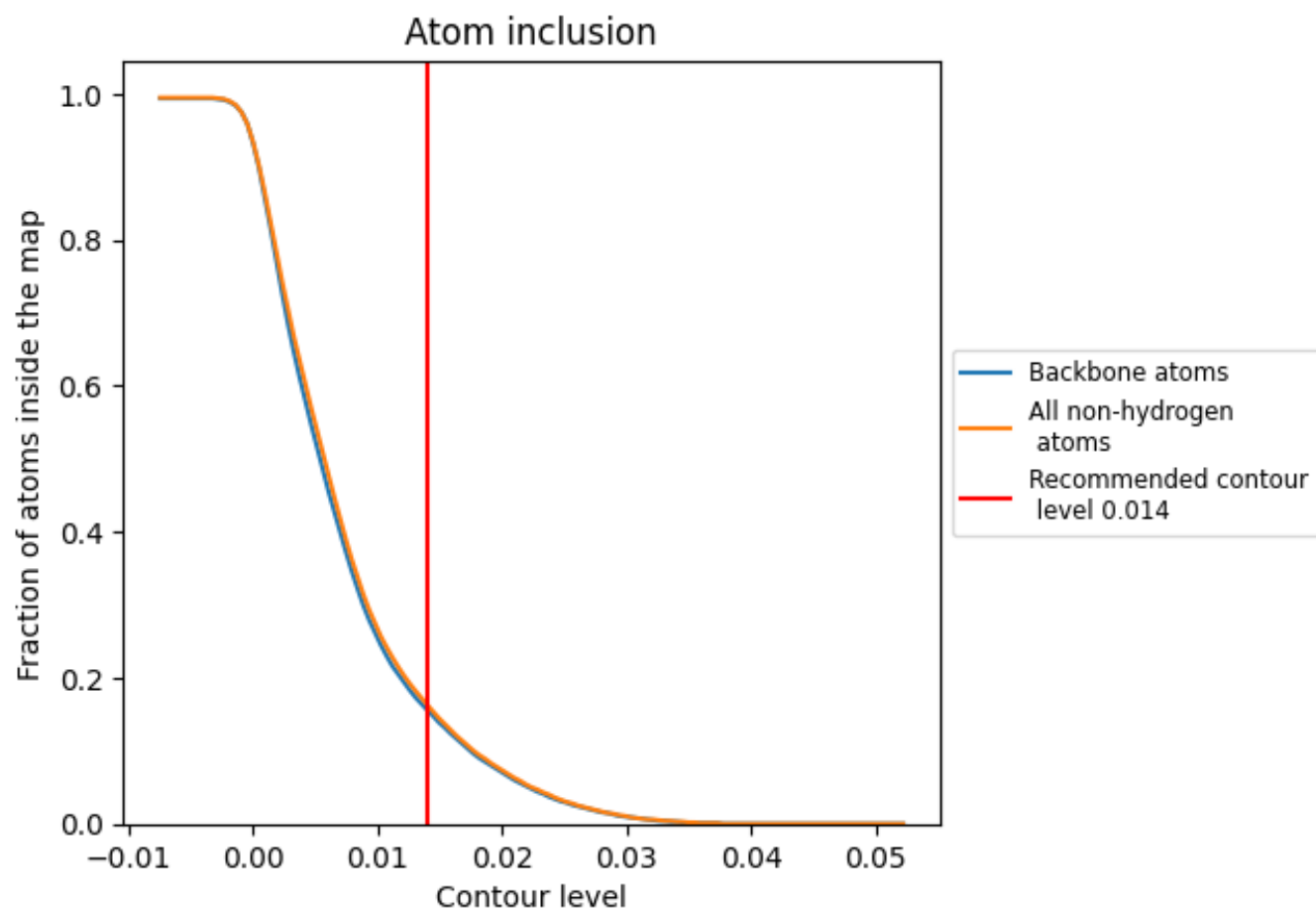
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion ⓘ



At the recommended contour level, 16% of all backbone atoms, 16% 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 (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.1630	 -0.0170
0	 0.0670	 -0.0160
1	 0.3360	 -0.0030
2	 0.0590	 -0.0070
3	 0.0000	 0.0100
4	 0.3600	 -0.0180
5	 0.2750	 -0.0260
6	 0.3850	 -0.0310
7	 0.2660	 -0.0410
8	 0.0340	 -0.0140
A	 0.2050	 -0.0230
B	 0.0000	 -0.0110
D	 0.1600	 -0.0250
F	 0.0530	 0.0040
G	 0.2690	 -0.0200
H	 0.1970	 -0.0050
I	 0.1180	 -0.0270
J	 0.0070	 0.0060
K	 0.0000	 0.0040
M	 0.1180	 -0.0350
N	 0.0300	 0.0190
O	 0.1940	 -0.0100
P	 0.0150	 -0.0070
Q	 0.3790	 -0.0260
R	 0.0020	 -0.0120
S	 0.0110	 -0.0190
T	 0.0900	 0.0010
U	 0.0690	 -0.0100
V	 0.3390	 -0.0280
W	 0.3560	 -0.0220
X	 0.3630	 -0.0430
Y	 0.3100	 -0.0000
Z	 0.1480	 -0.0460
a	 0.1480	 -0.0160
b	 0.3930	 -0.0220



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Chain	Atom inclusion	Q-score
c	 0.0300	 0.0000
d	 0.0250	 -0.0010
e	 0.0040	 0.0240
f	 0.0270	 0.0140
g	 0.1330	 0.0050
h	 0.2190	 0.0010
i	 0.0810	 -0.0270
j	 0.0550	 -0.0000
k	 0.0000	 0.0090
l	 0.2780	 -0.0010
m	 0.0520	 -0.0380
n	 0.0180	 -0.0050
o	 0.0000	 0.0180
p	 0.3520	 -0.0130
q	 0.1640	 -0.0090
r	 0.3630	 -0.0090
s	 0.0440	 -0.0130
t	 0.0000	 -0.0110
u	 0.3120	 -0.0310