



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:25 PM UTC

PDB ID : 5LZU / pdb_00005lzu
EMDB ID : EMD-4132
Title : Structure of the mammalian ribosomal termination complex with accommodated eRF1
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.75 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

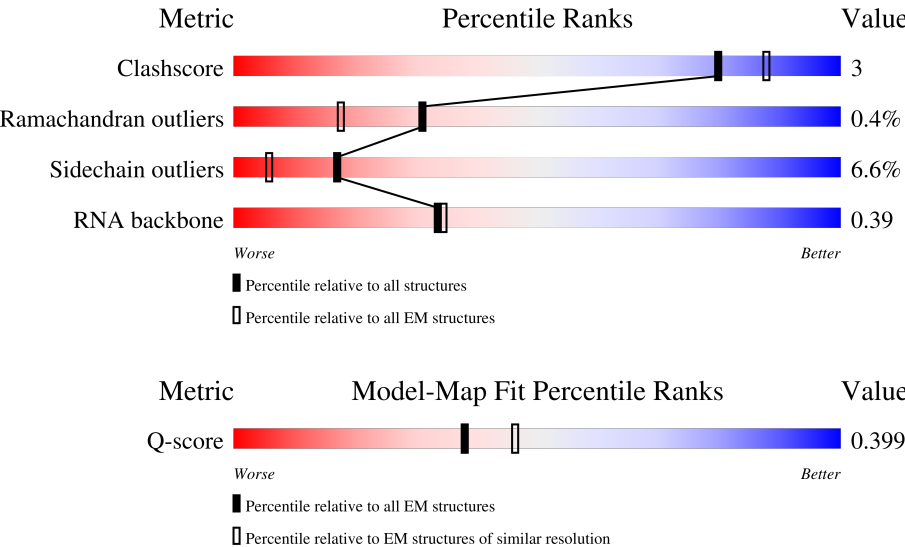
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.75 Å.

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



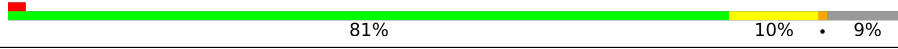
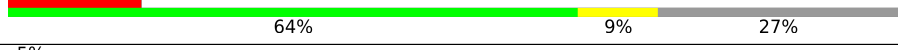
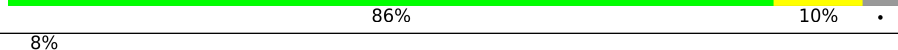
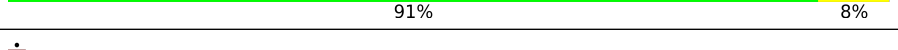
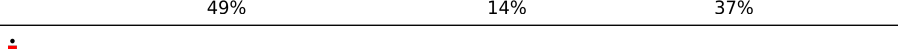
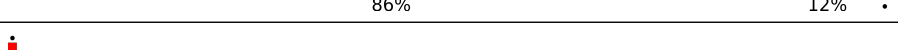
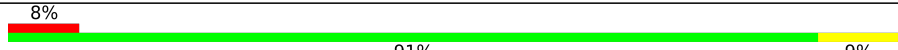
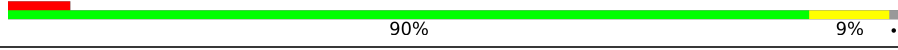
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10301 (3.25 - 4.25)

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

Mol	Chain	Length	Quality of chain
1	A	257	80% 14% . .
2	B	403	83% 14% .
3	C	425	73% 11% 15% .

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Mol	Chain	Length	Quality of chain
4	D	297	
5	E	291	
6	F	247	
7	G	319	
8	H	192	
9	I	214	
10	J	178	
11	L	211	
12	M	218	
13	N	204	
14	O	203	
15	P	184	
16	Q	188	
17	R	196	
18	S	176	
19	T	160	
20	U	128	
21	V	140	
22	W	157	
23	X	156	
24	Y	145	
25	Z	136	
26	a	148	
27	b	245	
28	c	115	

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Mol	Chain	Length	Quality of chain
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	2	76	
46	3	75	
47	5	3543	
48	7	120	
49	8	156	
50	9	1869	
51	AA	295	
52	BB	264	
53	CC	293	

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Mol	Chain	Length	Quality of chain
54	DD	243	
55	EE	263	
56	FF	204	
57	GG	249	
58	HH	194	
59	II	208	
60	JJ	194	
61	KK	165	
62	LL	158	
63	MM	132	
64	NN	151	
65	OO	168	
66	PP	145	
67	QQ	146	
68	RR	135	
69	SS	152	
70	TT	145	
71	UU	119	
72	VV	83	
73	WW	130	
74	XX	143	
75	YY	130	
76	ZZ	125	
77	aa	115	
78	bb	84	

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Mol	Chain	Length	Quality of chain
79	cc	69	
80	dd	56	
81	ee	133	
82	ff	156	
83	gg	317	
84	hh	15	
85	ii	459	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	ZN	dd	100	-	-	X	-

2 Entry composition

There are 87 unique types of molecules in this entry. The entry contains 219122 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 uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 2 is a protein called uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	394	Total	C	N	O	S	0	0
			3172	2020	597	542	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP G1TL06

- Molecule 3 is a protein called uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	362	Total	C	N	O	S	0	0
			2883	1812	577	480	14		

There are 47 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	379	VAL	-	expression tag	UNP G1SVW5
C	380	LYS	-	expression tag	UNP G1SVW5
C	381	LYS	-	expression tag	UNP G1SVW5
C	382	PRO	-	expression tag	UNP G1SVW5
C	383	ARG	-	expression tag	UNP G1SVW5
C	384	ALA	-	expression tag	UNP G1SVW5
C	385	VAL	-	expression tag	UNP G1SVW5
C	386	GLY	-	expression tag	UNP G1SVW5
C	387	ILE	-	expression tag	UNP G1SVW5
C	388	LYS	-	expression tag	UNP G1SVW5

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Chain	Residue	Modelled	Actual	Comment	Reference
C	389	GLN	-	expression tag	UNP G1SVW5
C	390	LYS	-	expression tag	UNP G1SVW5
C	391	LYS	-	expression tag	UNP G1SVW5
C	392	LYS	-	expression tag	UNP G1SVW5
C	393	PRO	-	expression tag	UNP G1SVW5
C	394	VAL	-	expression tag	UNP G1SVW5
C	395	VAL	-	expression tag	UNP G1SVW5
C	396	GLY	-	expression tag	UNP G1SVW5
C	397	ARG	-	expression tag	UNP G1SVW5
C	398	LYS	-	expression tag	UNP G1SVW5
C	399	ALA	-	expression tag	UNP G1SVW5
C	400	ALA	-	expression tag	UNP G1SVW5
C	401	ALA	-	expression tag	UNP G1SVW5
C	402	ALA	-	expression tag	UNP G1SVW5
C	403	LYS	-	expression tag	UNP G1SVW5
C	404	LYS	-	expression tag	UNP G1SVW5
C	405	PRO	-	expression tag	UNP G1SVW5
C	406	ALA	-	expression tag	UNP G1SVW5
C	407	ALA	-	expression tag	UNP G1SVW5
C	408	ASP	-	expression tag	UNP G1SVW5
C	409	LYS	-	expression tag	UNP G1SVW5
C	410	LYS	-	expression tag	UNP G1SVW5
C	411	ALA	-	expression tag	UNP G1SVW5
C	412	ALA	-	expression tag	UNP G1SVW5
C	413	ASP	-	expression tag	UNP G1SVW5
C	414	LYS	-	expression tag	UNP G1SVW5
C	415	ARG	-	expression tag	UNP G1SVW5
C	416	ALA	-	expression tag	UNP G1SVW5
C	417	GLY	-	expression tag	UNP G1SVW5
C	418	PRO	-	expression tag	UNP G1SVW5
C	419	GLU	-	expression tag	UNP G1SVW5
C	420	ASP	-	expression tag	UNP G1SVW5
C	421	LYS	-	expression tag	UNP G1SVW5
C	422	LYS	-	expression tag	UNP G1SVW5
C	423	PRO	-	expression tag	UNP G1SVW5
C	424	ALA	-	expression tag	UNP G1SVW5
C	425	ALA	-	expression tag	UNP G1SVW5

- Molecule 4 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	293	Total	C	N	O	S	0	0
			2391	1512	438	427	14		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	216	Total	C	N	O	S	0	0
			1729	1115	329	282	3		

- Molecule 6 is a protein called uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	225	Total	C	N	O	S	0	0
			1875	1205	358	303	9		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	1	MET	-	initiating methionine	UNP G1SV32
F	2	GLU	-	expression tag	UNP G1SV32
F	3	GLY	-	expression tag	UNP G1SV32
F	4	ALA	-	expression tag	UNP G1SV32
F	5	GLU	-	expression tag	UNP G1SV32

- Molecule 7 is a protein called eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	233	Total	C	N	O	S	0	0
			1879	1199	361	315	4		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	MET	-	initiating methionine	UNP G1STW0
G	2	SER	-	expression tag	UNP G1STW0
G	3	SER	-	expression tag	UNP G1STW0
G	4	TYR	-	expression tag	UNP G1STW0
G	5	ARG	-	expression tag	UNP G1STW0
G	6	LEU	-	expression tag	UNP G1STW0
G	7	GLY	-	expression tag	UNP G1STW0
G	8	TYR	-	expression tag	UNP G1STW0
G	9	CYS	-	expression tag	UNP G1STW0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	10	MET	-	expression tag	UNP G1STW0
G	11	LYS	-	expression tag	UNP G1STW0
G	12	GLU	-	expression tag	UNP G1STW0
G	13	GLU	-	expression tag	UNP G1STW0
G	14	ARG	-	expression tag	UNP G1STW0
G	15	HIS	-	expression tag	UNP G1STW0
G	16	ASN	-	expression tag	UNP G1STW0
G	17	LEU	-	expression tag	UNP G1STW0
G	18	VAL	-	expression tag	UNP G1STW0
G	19	LEU	-	expression tag	UNP G1STW0
G	20	CYS	-	expression tag	UNP G1STW0
G	21	LEU	-	expression tag	UNP G1STW0
G	22	TRP	-	expression tag	UNP G1STW0
G	23	SER	-	expression tag	UNP G1STW0
G	24	GLN	-	expression tag	UNP G1STW0
G	25	SER	-	expression tag	UNP G1STW0
G	26	PRO	-	expression tag	UNP G1STW0
G	27	GLY	-	expression tag	UNP G1STW0
G	28	ILE	-	expression tag	UNP G1STW0
G	29	LEU	-	expression tag	UNP G1STW0
G	30	ASN	-	expression tag	UNP G1STW0
G	31	SER	-	expression tag	UNP G1STW0
G	32	LYS	-	expression tag	UNP G1STW0
G	33	CYS	-	expression tag	UNP G1STW0
G	34	LEU	-	expression tag	UNP G1STW0
G	35	TRP	-	expression tag	UNP G1STW0
G	36	PRO	-	expression tag	UNP G1STW0
G	37	PHE	-	expression tag	UNP G1STW0
G	38	THR	-	expression tag	UNP G1STW0
G	39	ASN	-	expression tag	UNP G1STW0
G	40	ILE	-	expression tag	UNP G1STW0
G	41	HIS	-	expression tag	UNP G1STW0
G	42	LEU	-	expression tag	UNP G1STW0
G	43	LEU	-	expression tag	UNP G1STW0
G	44	VAL	-	expression tag	UNP G1STW0
G	45	GLY	-	expression tag	UNP G1STW0
G	46	ALA	-	expression tag	UNP G1STW0
G	47	LEU	-	expression tag	UNP G1STW0
G	48	PRO	-	expression tag	UNP G1STW0
G	49	ARG	-	expression tag	UNP G1STW0
G	50	GLU	-	expression tag	UNP G1STW0
G	51	GLY	-	expression tag	UNP G1STW0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	52	ALA	-	expression tag	UNP G1STW0
G	53	GLY	-	expression tag	UNP G1STW0
G	54	GLY	-	expression tag	UNP G1STW0
G	55	ALA	-	expression tag	UNP G1STW0
G	56	TRP	-	expression tag	UNP G1STW0
G	57	GLY	-	expression tag	UNP G1STW0
G	58	GLY	-	expression tag	UNP G1STW0
G	59	GLY	-	expression tag	UNP G1STW0
G	60	ARG	-	expression tag	UNP G1STW0
G	61	SER	-	expression tag	UNP G1STW0
G	62	GLU	-	expression tag	UNP G1STW0
G	63	GLN	-	expression tag	UNP G1STW0
G	64	LEU	-	expression tag	UNP G1STW0
G	65	PRO	-	expression tag	UNP G1STW0
G	66	THR	-	expression tag	UNP G1STW0
G	67	CYS	-	expression tag	UNP G1STW0
G	68	SER	-	expression tag	UNP G1STW0
G	69	THR	-	expression tag	UNP G1STW0
G	70	THR	-	expression tag	UNP G1STW0
G	71	HIS	-	expression tag	UNP G1STW0
G	72	HIS	-	expression tag	UNP G1STW0
G	73	ASP	-	expression tag	UNP G1STW0
G	74	PHE	-	expression tag	UNP G1STW0
G	75	THR	-	expression tag	UNP G1STW0
G	76	TRP	-	expression tag	UNP G1STW0
G	77	ASP	-	expression tag	UNP G1STW0
G	244	GLY	CYS	conflict	UNP G1STW0

- Molecule 8 is a protein called uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	190	Total	C	N	O	S	0	0
			1516	954	284	272	6		

- Molecule 9 is a protein called uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	205	Total	C	N	O	S	0	0
			1664	1056	321	274	13		

- Molecule 10 is a protein called uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 11 is a protein called eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	210	Total	C	N	O	S	0	0
			1702	1065	354	279	4		

- Molecule 12 is a protein called eL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	138	Total	C	N	O	S	0	0
			1137	727	221	182	7		

- Molecule 13 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 14 is a protein called uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	199	Total	C	N	O	S	0	0
			1630	1051	319	255	5		

- Molecule 15 is a protein called uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	153	Total	C	N	O	S	0	0
			1242	777	241	215	9		

- Molecule 16 is a protein called eL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	187	Total	C	N	O	S	0	0
			1515	946	315	250	4		

- Molecule 17 is a protein called eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	180	Total	C	N	O	S	0	0
			1508	933	328	238	9		

- Molecule 18 is a protein called eL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	176	Total	C	N	O	S	0	0
			1462	930	285	236	11		

- Molecule 19 is a protein called eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 20 is a protein called eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	99	Total	C	N	O	S	0	0
			809	519	141	147	2		

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 22 is a protein called eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	106	Total	C	N	O	S	0	0
			860	538	174	144	4		

- Molecule 23 is a protein called uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	118	Total	C	N	O	S	0	0
			967	618	181	167	1		

- Molecule 24 is a protein called uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 25 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 26 is a protein called uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	147	Total	C	N	O	S	0	0
			1162	734	239	185	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1	MET	GLN	conflict	UNP G1SNY0

- Molecule 27 is a protein called eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	104	Total	C	N	O	S	0	0
			848	527	189	129	3		

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
b	227	ALA	-	expression tag	UNP G1SGR6
b	228	PRO	-	expression tag	UNP G1SGR6
b	229	VAL	-	expression tag	UNP G1SGR6
b	230	PRO	-	expression tag	UNP G1SGR6
b	231	ALA	-	expression tag	UNP G1SGR6
b	232	GLN	-	expression tag	UNP G1SGR6
b	233	ALA	-	expression tag	UNP G1SGR6
b	234	PRO	-	expression tag	UNP G1SGR6
b	235	PRO	-	expression tag	UNP G1SGR6
b	236	LYS	-	expression tag	UNP G1SGR6
b	237	GLY	-	expression tag	UNP G1SGR6
b	238	ALA	-	expression tag	UNP G1SGR6
b	239	GLN	-	expression tag	UNP G1SGR6

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Chain	Residue	Modelled	Actual	Comment	Reference
b	240	PRO	-	expression tag	UNP G1SGR6
b	241	PRO	-	expression tag	UNP G1SGR6
b	242	ALA	-	expression tag	UNP G1SGR6
b	243	LYS	-	expression tag	UNP G1SGR6
b	244	ALA	-	expression tag	UNP G1SGR6
b	245	PRO	-	expression tag	UNP G1SGR6

- Molecule 28 is a protein called eL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	98	Total	C	N	O	S	0	0
			761	481	134	140	6		

- Molecule 29 is a protein called eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 30 is a protein called eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 31 is a protein called eL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	109	Total	C	N	O	S	0	0
			876	555	174	143	4		

- Molecule 32 is a protein called eL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
g	117	LYS	-	expression tag	UNP G1U945

- Molecule 33 is a protein called uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	122	Total	C	N	O	S	0	0
			1013	640	204	168	1		

- Molecule 34 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	102	Total	C	N	O	S	0	0
			830	520	176	129	5		

- Molecule 35 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 36 is a protein called eL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	24	LYS	ASN	conflict	UNP G1U001

- Molecule 37 is a protein called eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	50	Total	C	N	O	S	0	0
			447	286	96	64	1		

- Molecule 38 is a protein called eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 39 is a protein called 60s ribosomal protein l41.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	25	Total	C	N	O	S	0	0
			239	145	64	27	3		

- Molecule 40 is a protein called eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	104	Total	C	N	O	S	0	0
			851	533	174	138	6		

- Molecule 41 is a protein called eL43.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 42 is a protein called eL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	r	124	Total	C	N	O	S	0	0
			994	616	205	167	6		

- Molecule 43 is a protein called uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	s	196	Total	C	N	O	S	0	0
			1507	959	263	276	9		

- Molecule 44 is a protein called uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	153	Total	C	N	O	S	0	0
			1160	722	218	217	3		

- Molecule 45 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 46 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 47 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 48 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 49 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 50 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 51 is a protein called uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	AA	217	Total	C	N	O	S	0	0
			1710	1086	300	316	8		

- Molecule 52 is a protein called 40S ribosomal protein S3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	BB	213	Total	C	N	O	S	0	0
			1729	1098	309	308	14		

- Molecule 53 is a protein called uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	CC	221	Total	C	N	O	S	0	0
			1716	1111	295	301	9		

- Molecule 54 is a protein called uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	DD	228	Total	C	N	O	S	0	0
			1768	1126	318	316	8		

- Molecule 55 is a protein called 40S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	EE	262	Total	C	N	O	S	0	0
			2076	1324	386	358	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EE	25	GLY	SER	conflict	UNP G1TK17
EE	51	ARG	LYS	conflict	UNP G1TK17
EE	78	THR	ALA	conflict	UNP G1TK17
EE	156	VAL	MET	conflict	UNP G1TK17

- Molecule 56 is a protein called uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	FF	185	Total	C	N	O	S	0	0
			1471	921	277	266	7		

- Molecule 57 is a protein called 40S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	GG	237	Total	C	N	O	S	0	0
			1923	1200	387	329	7		

- Molecule 58 is a protein called eS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	HH	185	Total	C	N	O	S	0	0
			1488	952	271	264	1		

- Molecule 59 is a protein called 40S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	II	206	Total	C	N	O	S	0	0
			1686	1058	332	291	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
II	47	ARG	GLY	conflict	UNP G1TJW1

- Molecule 60 is a protein called Ribosomal protein S9 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
60	JJ	185	Total	C	N	O	S	0	0
			1525	969	306	248	2		

- Molecule 61 is a protein called eS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	KK	96	Total	C	N	O	S	0	0
			810	530	143	131	6		

- Molecule 62 is a protein called uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	LL	143	Total	C	N	O	S	0	0
			1175	749	222	198	6		

- Molecule 63 is a protein called 40S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	MM	117	Total	C	N	O	S	0	0
			908	570	161	169	8		

- Molecule 64 is a protein called uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
64	NN	149	Total	C	N	O	S	0	0
			1202	770	228	203	1		

- Molecule 65 is a protein called uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	OO	136	Total	C	N	O	S	0	0
			1016	621	199	190	6		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
OO	-16	MET	-	initiating methionine	UNP G1T1F0
OO	-15	LYS	-	expression tag	UNP G1T1F0
OO	-14	ALA	-	expression tag	UNP G1T1F0
OO	-13	ARG	-	expression tag	UNP G1T1F0
OO	-12	ALA	-	expression tag	UNP G1T1F0
OO	-11	LEU	-	expression tag	UNP G1T1F0
OO	-10	SER	-	expression tag	UNP G1T1F0
OO	-9	GLY	-	expression tag	UNP G1T1F0
OO	-8	SER	-	expression tag	UNP G1T1F0
OO	-7	GLY	-	expression tag	UNP G1T1F0
OO	-6	VAL	-	expression tag	UNP G1T1F0
OO	-5	ARG	-	expression tag	UNP G1T1F0

- Molecule 66 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	PP	120	Total	C	N	O	S	0	0
			997	635	187	168	7		

- Molecule 67 is a protein called uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
67	QQ	142	Total	C	N	O	S	0	0
			1128	717	213	195	3		

- Molecule 68 is a protein called eS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
68	RR	132	Total	C	N	O	S	0	0
			1068	670	199	195	4		

- Molecule 69 is a protein called uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
69	SS	144	Total	C	N	O	S	0	0
			1190	746	241	202	1		

- Molecule 70 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
70	TT	141	Total	C	N	O	S	0	0
			1097	688	211	195	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
TT	119	GLY	TRP	conflict	UNP G1TN62

- Molecule 71 is a protein called uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	UU	100	Total	C	N	O	S	0	0
			795	498	152	141	4		

- Molecule 72 is a protein called eS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
72	VV	83	Total	C	N	O	S	0	0
			636	393	117	121	5		

- Molecule 73 is a protein called uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
73	WW	129	Total	C	N	O	S	0	0
			1034	659	193	176	6		

- Molecule 74 is a protein called uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
74	XX	141	Total	C	N	O	S	0	0
			1098	693	219	183	3		

- Molecule 75 is a protein called eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
75	YY	124	Total	C	N	O	S	0	0
			1011	640	198	168	5		

- Molecule 76 is a protein called eS25.

Mol	Chain	Residues	Atoms					AltConf	Trace
76	ZZ	75	Total	C	N	O	S	0	0
			598	382	111	104	1		

- Molecule 77 is a protein called eS26.

Mol	Chain	Residues	Atoms					AltConf	Trace
77	aa	101	Total	C	N	O	S	0	0
			814	507	170	132	5		

- Molecule 78 is a protein called 40S ribosomal protein S27.

Mol	Chain	Residues	Atoms					AltConf	Trace
78	bb	83	Total	C	N	O	S	0	0
			651	408	121	115	7		

- Molecule 79 is a protein called eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
79	cc	62	Total	C	N	O	S	0	0
			488	297	97	92	2		

- Molecule 80 is a protein called uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
80	dd	55	Total	C	N	O	S	0	0
			459	286	94	74	5		

- Molecule 81 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	ee	55	Total	C	N	O	S	0	0
			443	274	97	71	1		

- Molecule 82 is a protein called eS31.

Mol	Chain	Residues	Atoms					AltConf	Trace
82	ff	68	Total	C	N	O	S	0	0
			555	351	103	94	7		

- Molecule 83 is a protein called RACK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
83	gg	313	Total	C	N	O	S	0	0
			2436	1535	424	465	12		

- Molecule 84 is a RNA chain called mRNA (UGA stop codon).

Mol	Chain	Residues	Atoms					AltConf	Trace
84	hh	15	Total	C	N	O	P	0	0
			317	142	54	106	15		

- Molecule 85 is a protein called Eukaryotic peptide chain release factor subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
85	ii	418	Total	C	N	O	S	0	0
			3295	2095	561	627	12		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
ii	-21	MET	-	initiating methionine	UNP P62495
ii	-20	ARG	-	expression tag	UNP P62495
ii	-19	GLY	-	expression tag	UNP P62495
ii	-18	SER	-	expression tag	UNP P62495
ii	-17	HIS	-	expression tag	UNP P62495
ii	-16	HIS	-	expression tag	UNP P62495
ii	-15	HIS	-	expression tag	UNP P62495
ii	-14	HIS	-	expression tag	UNP P62495
ii	-13	HIS	-	expression tag	UNP P62495
ii	-12	HIS	-	expression tag	UNP P62495
ii	-11	GLY	-	expression tag	UNP P62495
ii	-10	MET	-	expression tag	UNP P62495
ii	-9	ALA	-	expression tag	UNP P62495
ii	-8	SER	-	expression tag	UNP P62495
ii	-7	GLU	-	expression tag	UNP P62495
ii	-6	ASN	-	expression tag	UNP P62495
ii	-5	LEU	-	expression tag	UNP P62495
ii	-4	TYR	-	expression tag	UNP P62495
ii	-3	PHE	-	expression tag	UNP P62495
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495

- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	B	1	Total 1	Mg 1	0
86	I	1	Total 1	Mg 1	0
86	P	1	Total 1	Mg 1	0
86	Q	1	Total 1	Mg 1	0
86	V	1	Total 1	Mg 1	0
86	a	1	Total 1	Mg 1	0
86	e	1	Total 1	Mg 1	0
86	g	1	Total 1	Mg 1	0
86	j	1	Total 1	Mg 1	0
86	5	169	Total 169	Mg 169	0
86	7	5	Total 5	Mg 5	0
86	8	3	Total 3	Mg 3	0
86	9	71	Total 71	Mg 71	0
86	hh	1	Total 1	Mg 1	0

- Molecule 87 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
87	g	1	Total 1	Zn 1	0
87	j	1	Total 1	Zn 1	0
87	m	1	Total 1	Zn 1	0
87	o	1	Total 1	Zn 1	0
87	p	1	Total 1	Zn 1	0
87	aa	1	Total 1	Zn 1	0

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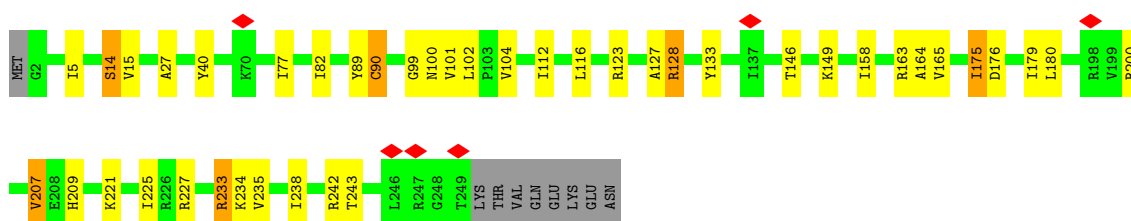
Mol	Chain	Residues	Atoms		AltConf
87	dd	1	Total 1	Zn 1	0
87	ff	1	Total 1	Zn 1	0

3 Residue-property plots [i](#)

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

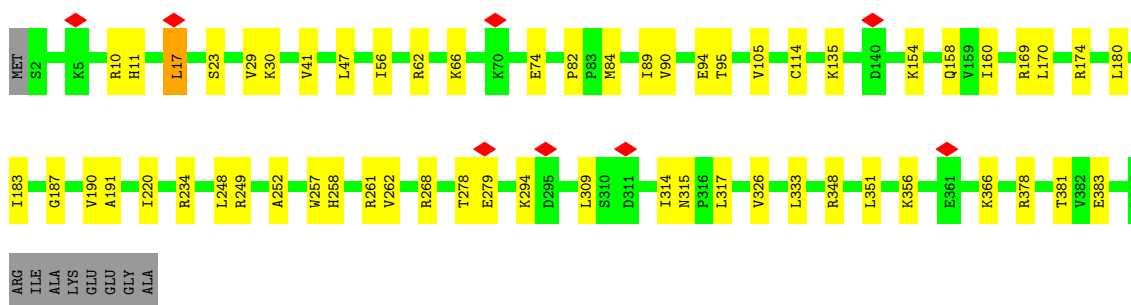
• Molecule 1: uL2

Chain A: 



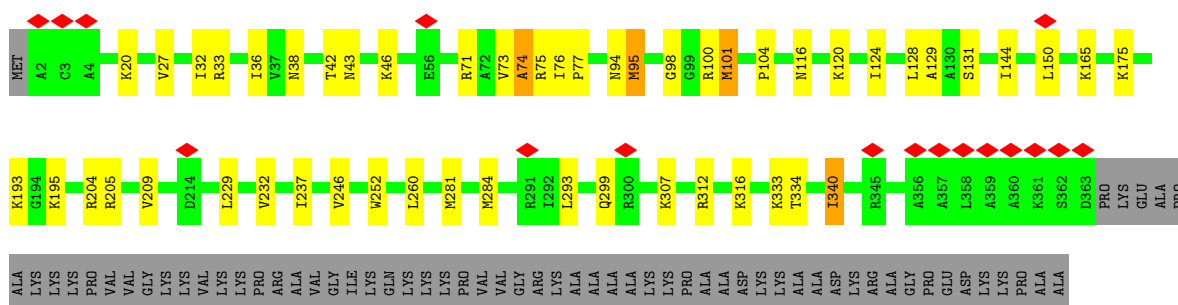
• Molecule 2: uL3

Chain B: 



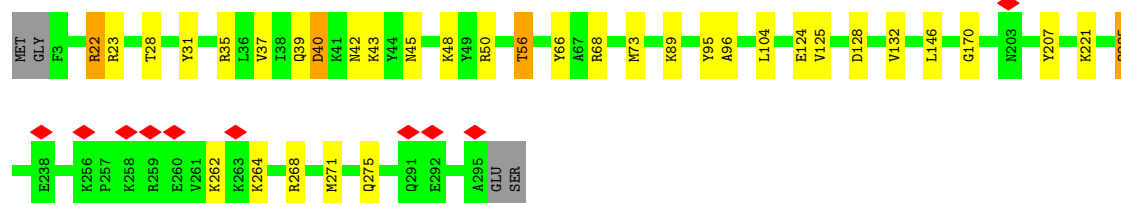
• Molecule 3: uL4

Chain C: 



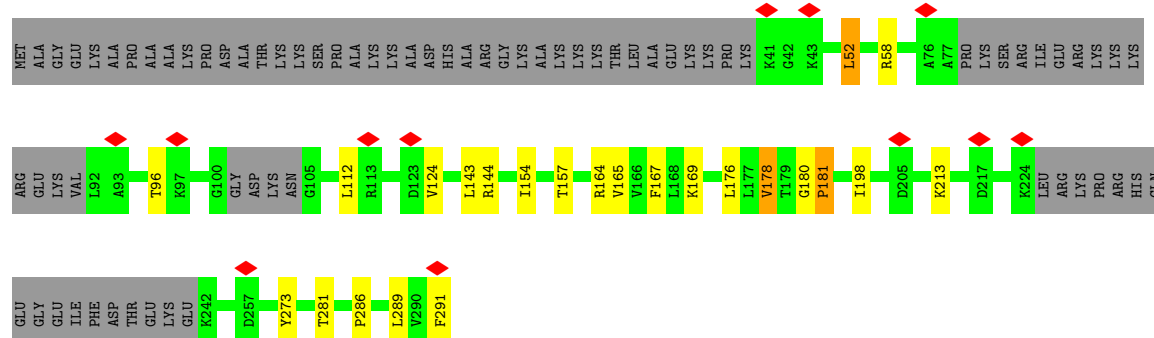
- Molecule 4: 60S ribosomal protein L5

Chain D:  87% 10% ..



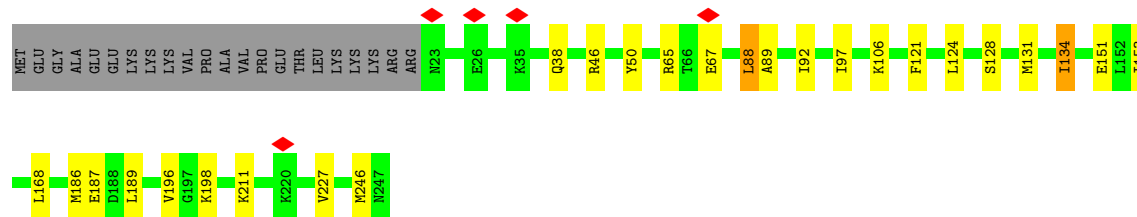
- Molecule 5: 60S ribosomal protein L6

Chain E:  66% 7% 26%



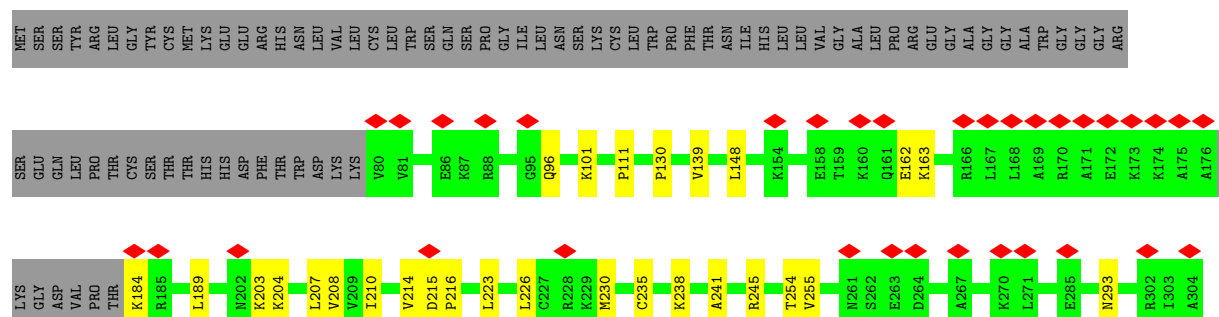
- Molecule 6: uL30

Chain F:  81% 10% 9%



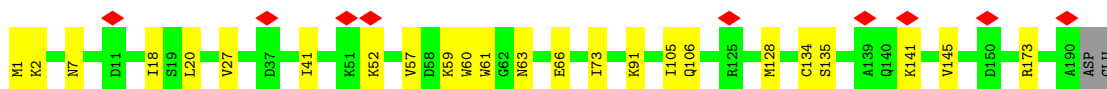
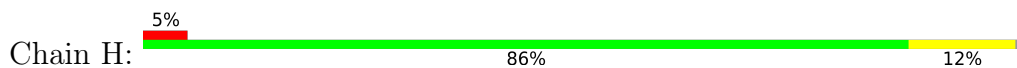
- Molecule 7: eL8

Chain G:  15% 64% 9% 27%

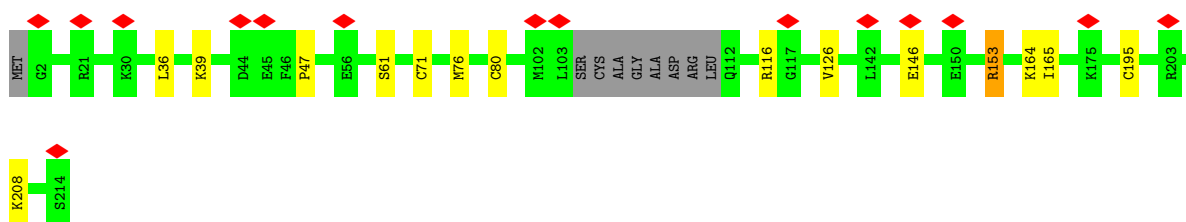
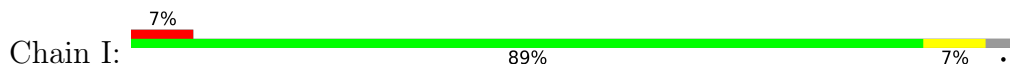




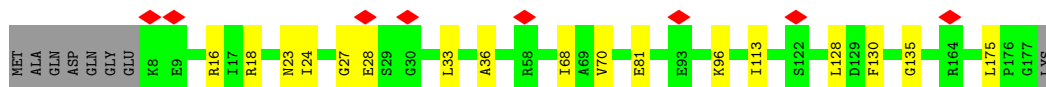
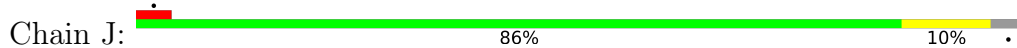
- Molecule 8: uL6



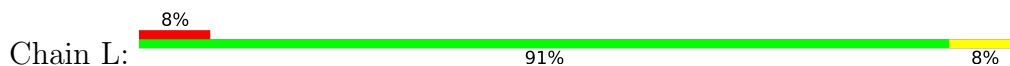
- Molecule 9: uL16



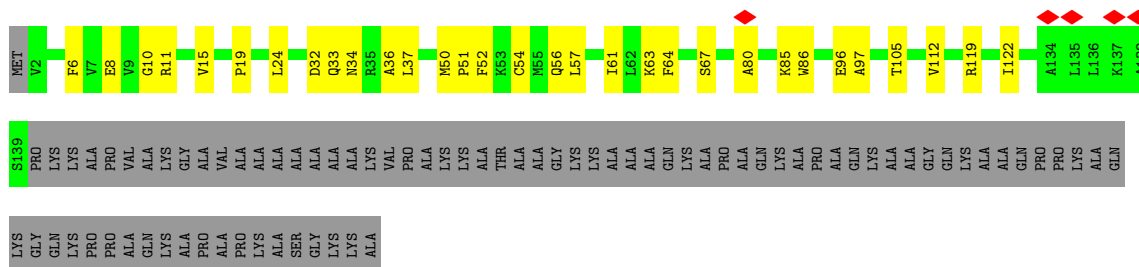
- Molecule 10: uL5



- Molecule 11: eL13



- Molecule 12: eL14



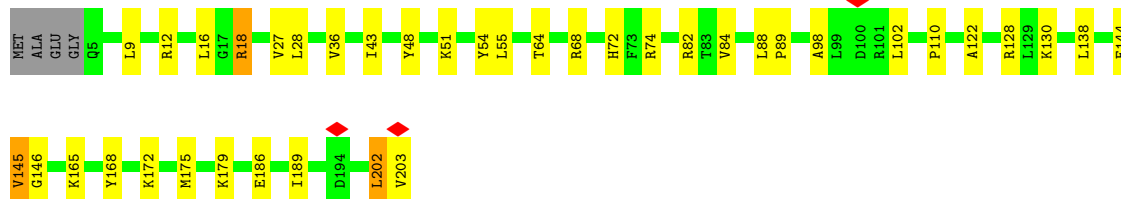
- Molecule 13: Ribosomal protein L15

Chain N:  86% 12% .



- Molecule 14: uL13

Chain O:  79% 18% ..



- Molecule 15: uL22

Chain P:  73% 9% 17% .



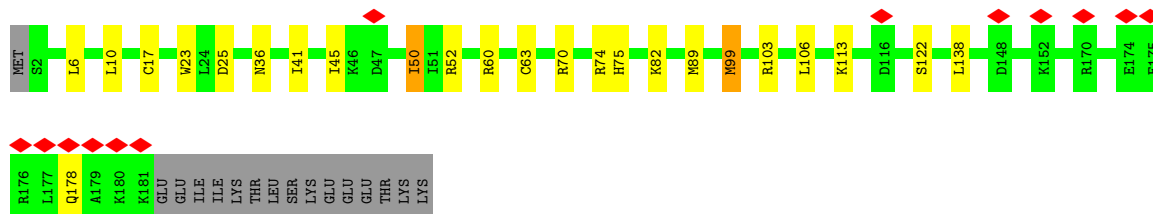
- Molecule 16: eL18

Chain Q:  87% 12% ..



- Molecule 17: eL19

Chain R:  7% 80% 11% 8% .



- Molecule 18: eL20

Chain S:  84% 15% .



Protein	Number of Mutations
M1	1
K2	1
T8	2
V55	3
Q72	2
K77	2
Y78	2
V79	2
E83	3
H100	2
V104	3
D114	4
E120	4
E131	4
K132	4
G133	4
K134	4
TYR	4
LYS	4
GLU	4
GLU	4
THR	4
THR	4
ILE	4
GLU	4
LYS	4
MET	4
MET	4
GLN	4
GLU	4

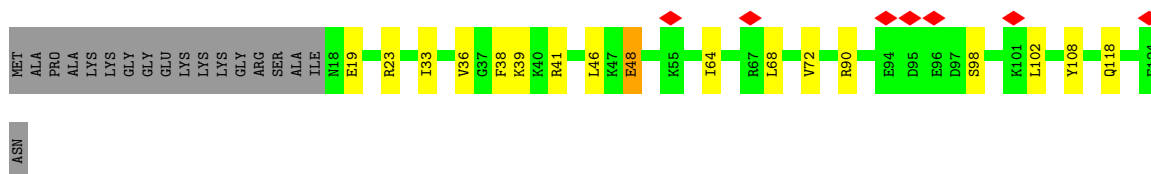
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G2	1
K3	1
V11	1
L14	1
D31	1
G32	1
T33	1
S34	1
D35	1
L42	1
R51	1
K52	1
A56	1
K60	1
R65	1
N76	1
Y77	1
N78	1
M81	1
P90	1
L91	1
D99	1
R102	1
F136	1

MET
P2
S3
R4
T8
L11
R12
I22
K27
A35
H41
H49
R59
H60
Y61
R65
D76
E84
G85
T86
K94
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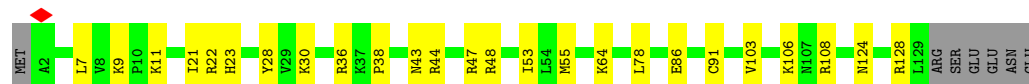
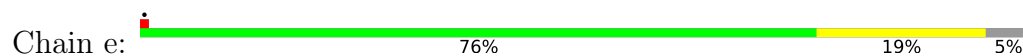
[illegible]

MET	VAL	ALA	ALA	LYS	LYS	LYS	LYS	S10	L11	E12	S13	R17	L29	K37	A64	K68	T69	G70	N78	K87	L94	G100	D103	S107	PRO	GLU	GLN	THR	GLY	GLU	LYS
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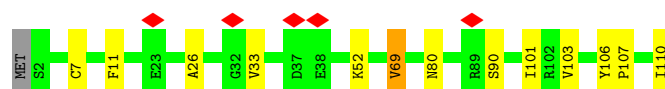
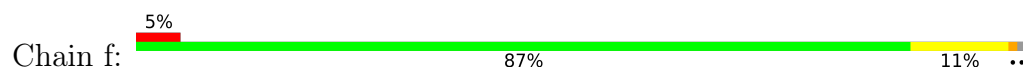
Chain d:



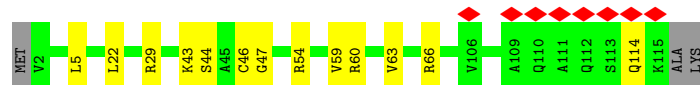
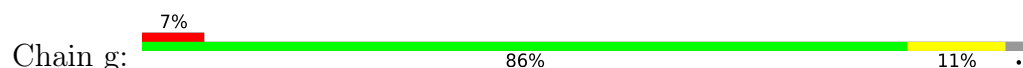
• Molecule 30: eL32



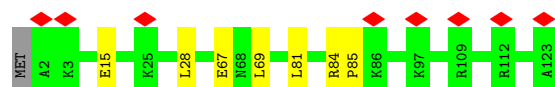
• Molecule 31: eL33



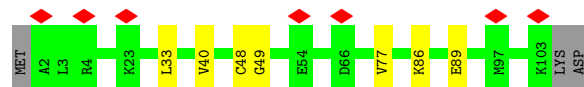
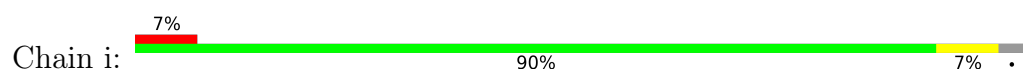
• Molecule 32: eL34



• Molecule 33: uL29



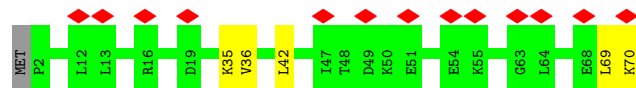
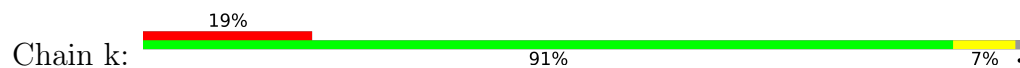
• Molecule 34: 60S ribosomal protein L36



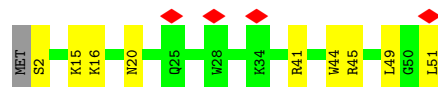
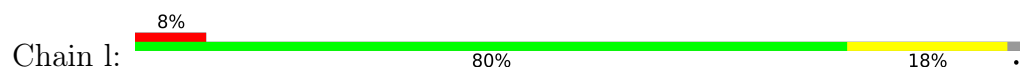
• Molecule 35: Ribosomal protein L37



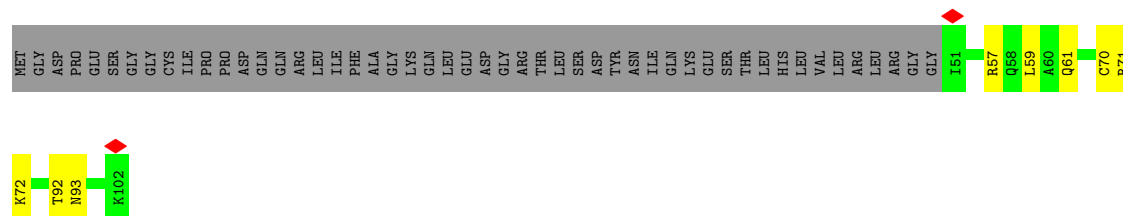
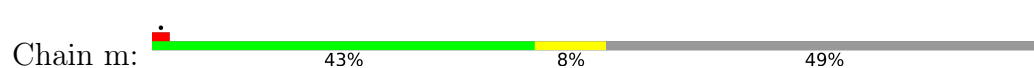
- Molecule 36: eL38



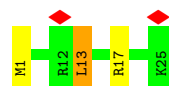
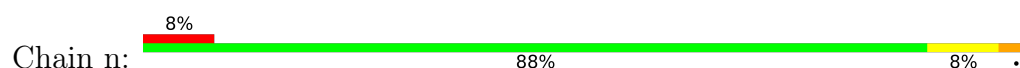
- Molecule 37: eL39



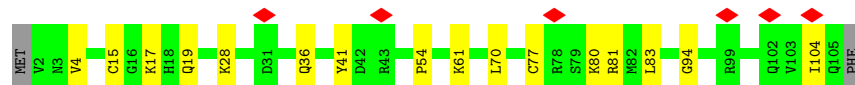
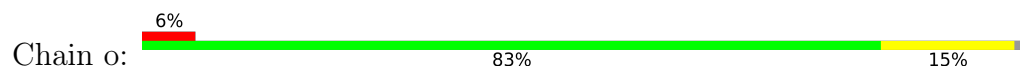
- Molecule 38: eL40



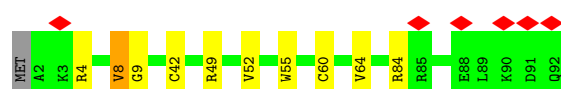
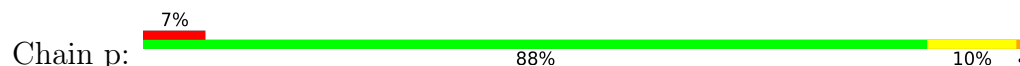
- Molecule 39: 60s ribosomal protein l41



- Molecule 40: eL42



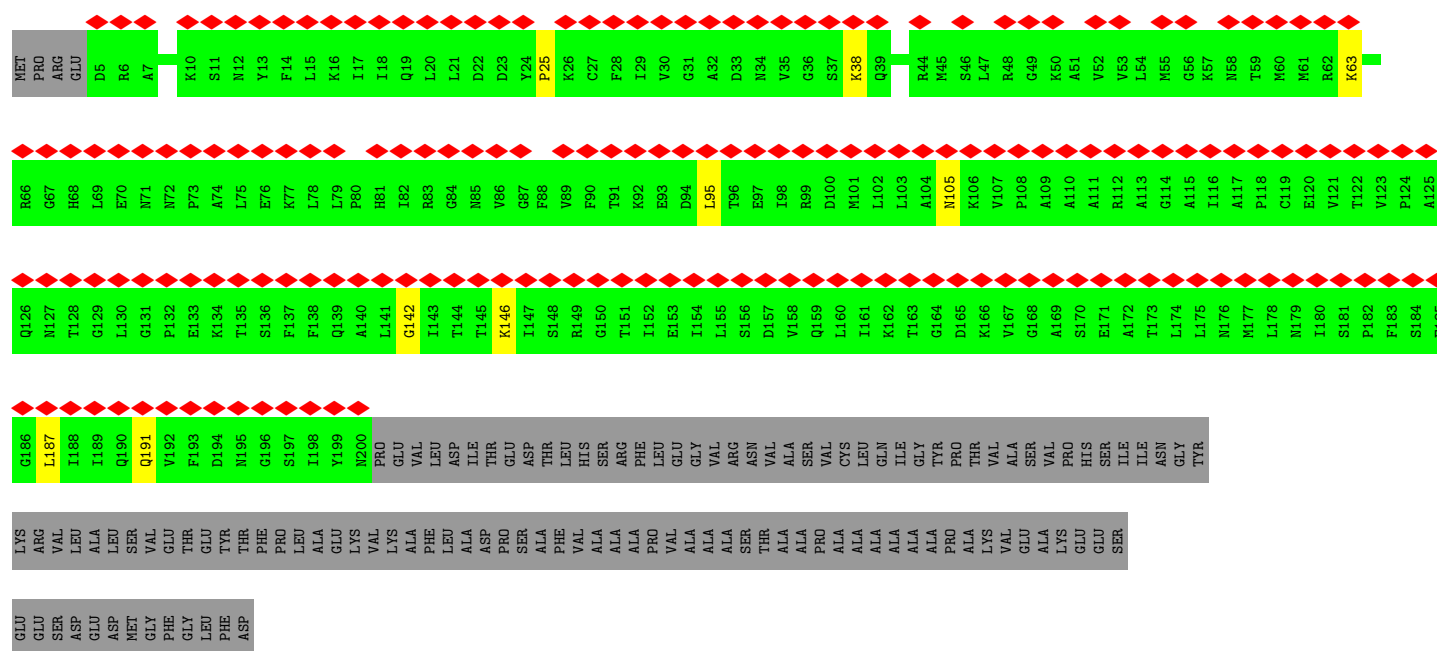
- Molecule 41: eL43



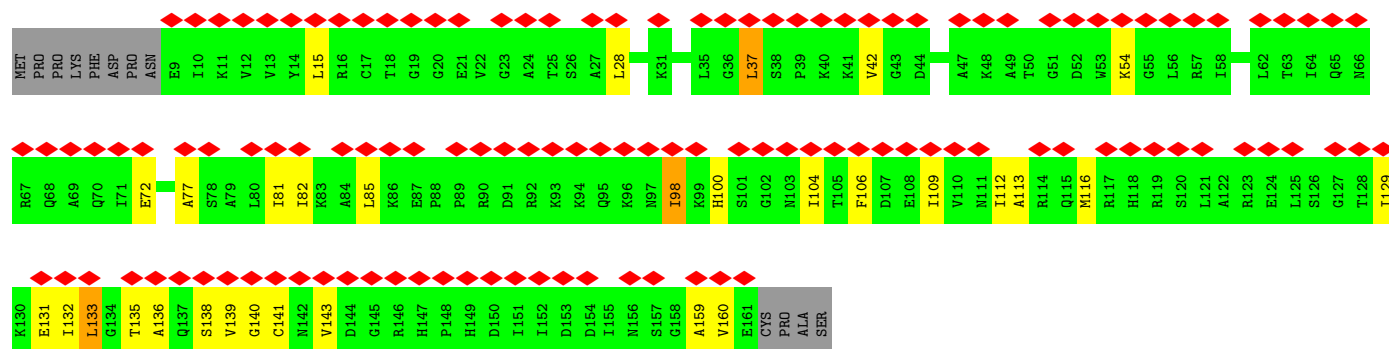
- Molecule 42: eL28



Chain s: 57% 59% 38%



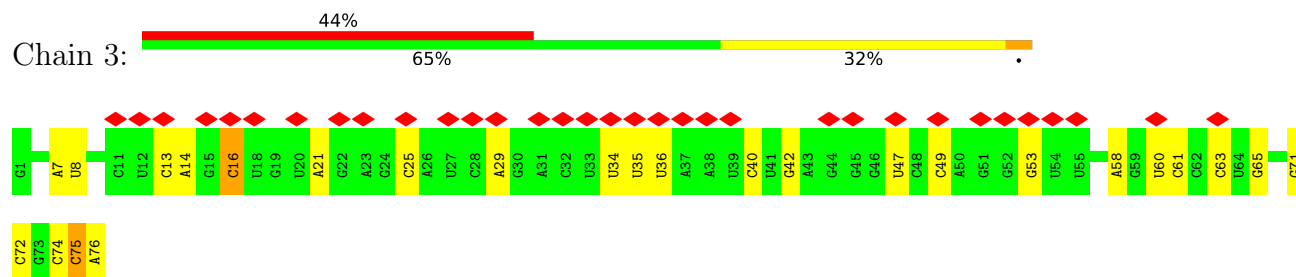
Chain t: 75% 74% 17% 7%



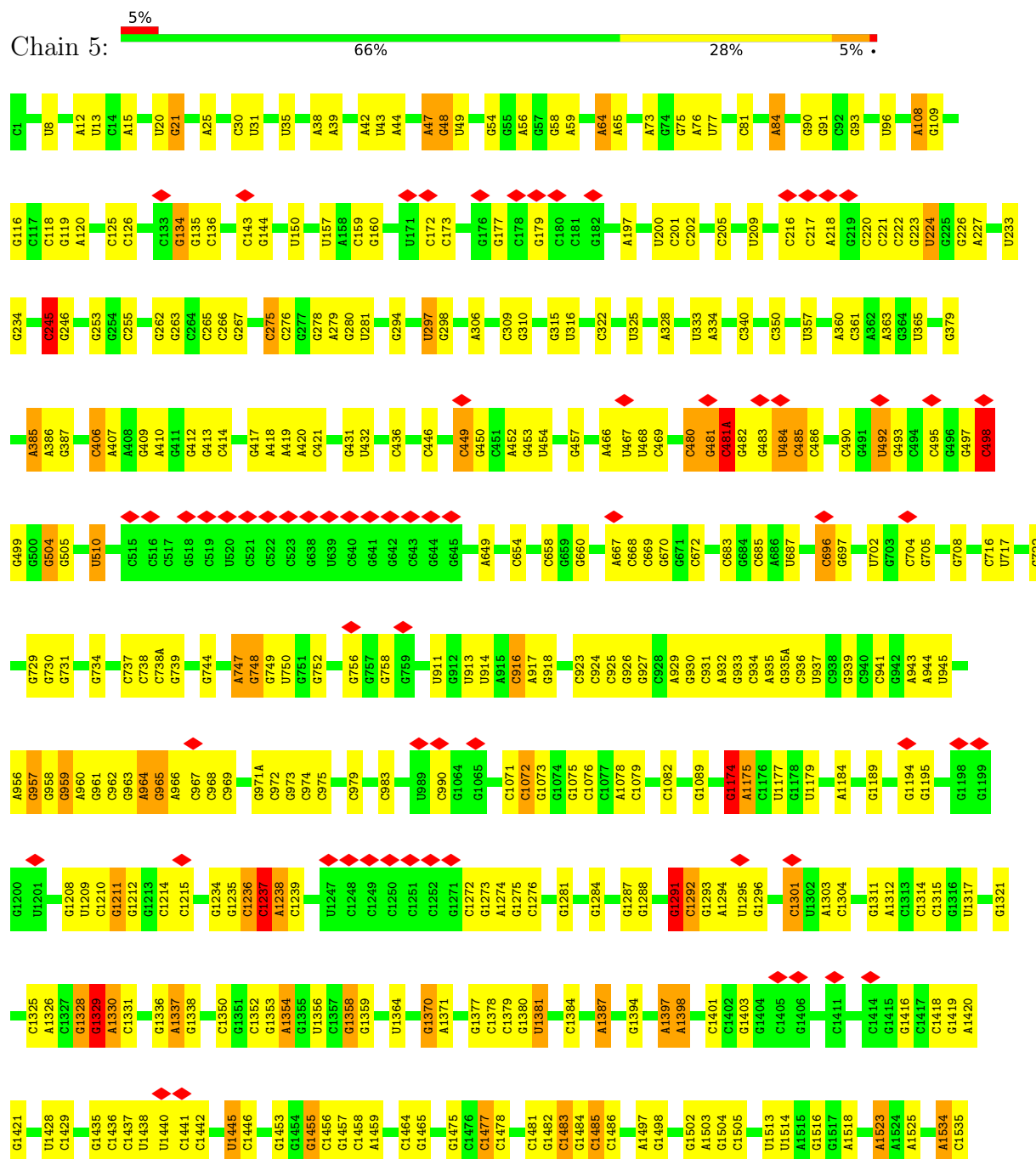
Chain 2: 24% 74% 21%



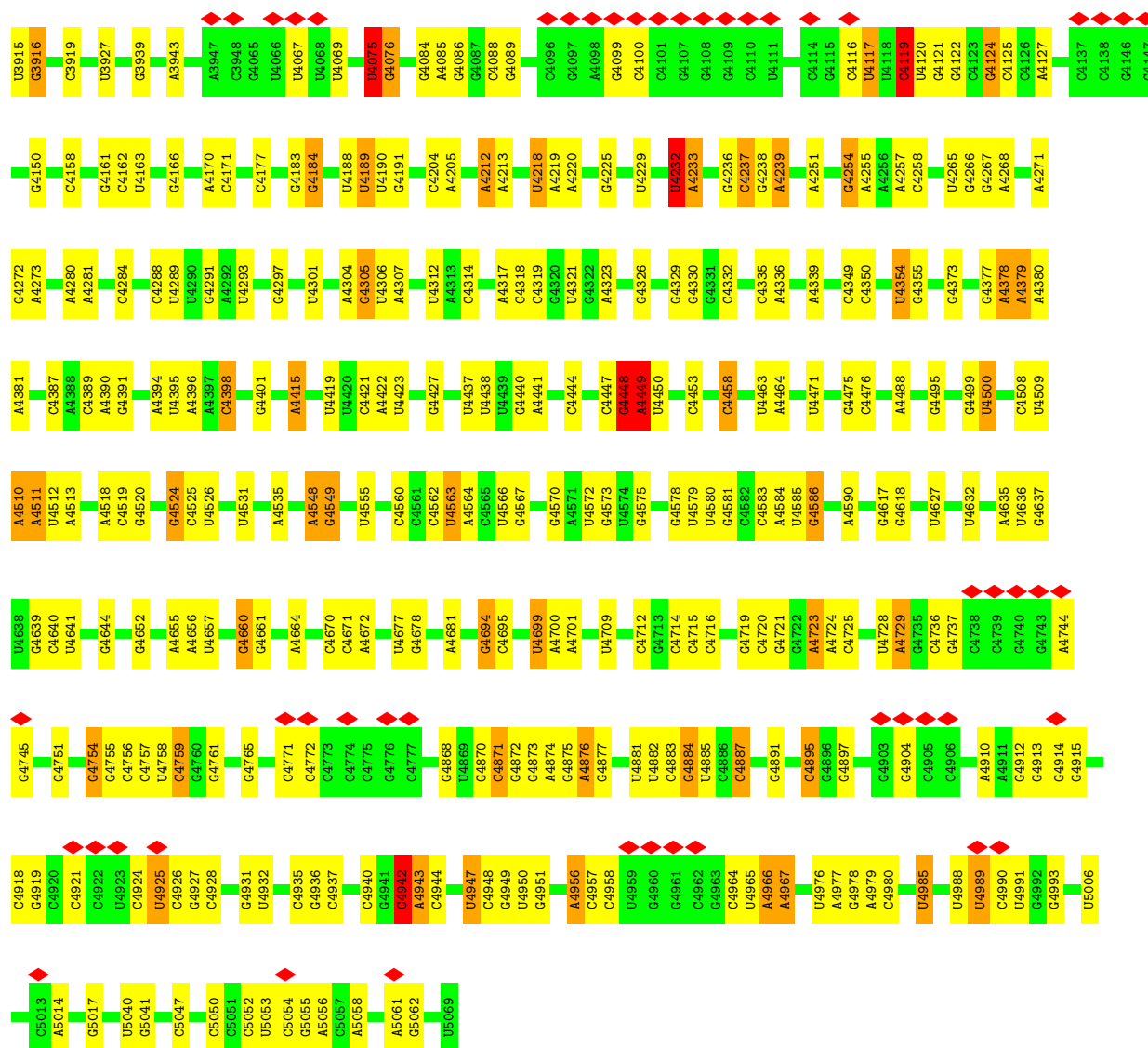
• Molecule 46: E-site tRNA



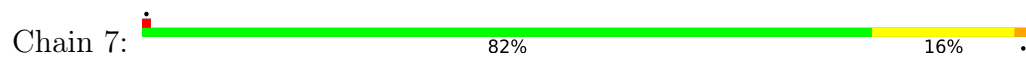
• Molecule 47: 28S ribosomal RNA



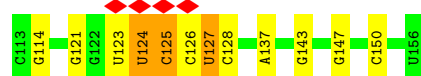
A3785	U3786	A3807	C3808	C3810	C3811	C3812	C3813	U3814	C3815	A3816	A3817	C3818	C3820	A3821	U3822	C3829	A3830	U3831	U3838	C3839	U3840	A3845	U3851	C3859	A3860	A3867	C3868	A3876	C3877	C3878	C3879	C3888	C3889	C3895	C3896	C3897	C3898	A3901	C3904	A3905	A3906	C3907	A3908	U3914								
G3691	A3692	U3693	C3696	C3697	C3698	C3699	C3700	C3703	U3704	G3710	A3711	A3712	C3722	A3723	A3724	C3725	U3729	U3730	C3731	A3732	A3733	C3739	C3740	A3746	A3747	A3748	C3749	C3750	C3753	C3754	C3755	A3759	A3760	A3763	A3766	U3772	U3773	A3774	C3775	C3776	C3777	A3778	A3779	C3780	A3783	A3784						
A2857	A2858	C2862	C2863	A2864	C2875	C2876	C2884	U2891	G2896	C2897	C3598	A3604	C3605	G3615	U3616	C3617	C3618	G3619	C3620	A3621	C3622	G3625	C3626	A3630	A3635	U3640	U3644	U3645	A3646	A3647	A3648	A3652	A3653	C3654	C3659	A3662	C3673	C3674	C3685	U3690												
C2733	U2734	C2735	C2739	U2740	A2743	A2744	A2745	C2754	A2755	U2760	U2761	C2762	U2763	A2764	U2769	C2772	C2786	A2787	U2788	A2789	U2790	C2794	A2795	A2798	A2806	A2807	C2808	C2814	U2819	C2823	U2826	C2827	U2828	U2829	A2835	C2838	G2841	C2842	G2855	C2856												
G2618	C2619	G2620	U2625	U2626	C2627	G2638	U2639	G2640	A2641	A2647	G2658	A2659	A2660	U2661	G2662	G2663	C2669	C2670	G2673	A2674	A2676	G2680	C2681	G2686	U2687	C2688	C2689	G2693	G2694	A2695	A2696	U2707	U2708	C2709	C2710	C2711	C2712	C2716	C2719	C2720	C2721	G2724	A2725	C2726								
G2483	A2484	U2485	C2486	C2487	C2488	C2489	U2490	C2491	C2492	C2493	U2494	U2495	A2502	C2503	C2504	C2505	C2506	A2513	C2521	C2522	C2523	U2524	A2529	U2530	A2537	C2544	U2545	C2546	C2547	A2553	U2554	C2555	C2560	C2561	C2562	C2563	C2564	C2565	C2566	C2571	U2575	C2583	A2587	A2601								
A2366	A2367	A2368	U2369	A2370	A2374	G2394	A2395	A2396	C2397	U2398	C2399	G2406	U2407	U2408	U2409	C2410	C2411	A2412	U2415	C2416	A2417	A2418	C2419	C2422	A2423	A2424	U2425	U2426	C2427	A2428	A2429	C2433	A2438	C2439	U2440	C2441	U2447	G2450	U2467	U2468	C2469	C2470	C2471	G2474	C2475	C2476	C2477					
A2104	A2105	A2106	A2107	C2108	C2109	G2110	G2259	A2260	C2261	G2262	G2265	C2266	U2267	A2268	C2269	G2270	C2274	G2275	A2276	C2277	G2278	A2279	C2280	U2281	A2282	G2287	C2288	C2289	C2290	A2300	G2301	A2313	C2314	G2321	G2322	G2331	A2332	C2333	G2345	G2348	A2349	U2350	C2351	U2359	C2363	A2364	C2365					
A2009	A2010	C2011	A2012	C2013	C2014	U2015	G2024	A2025	A2026	G2034	C2035	C2036	C2046	U2047	U2048	G2052	C2053	U2054	G2055	C2056	A2057	C2062	C2063	G2064	G2065	C2066	C2067	C2068	A2069	U2070	U2080	C2081	C2082	C2083	U2084	G2085	A2088	C2089	U2090	C2091	C2092	C2093	C2094	A2095	C2096	A2097	C2098	C2099	G2100	A2101	G2102	A2103
C1931	A1932	A1933	A1934	C1935	C1936	A1939	G1940	A1941	U1947	U1948	G1951	G1952	U1957	A1958	U1959	A1960	G1961	A1962	C1963	A1964	G1965	C1966	A1967	G1973	U1974	C1975	C1976	C1977	C1978	A1979	U1980	A1983	A1984	G1985	U1986	C1987	G1988	C1989	A1990	A1991	U1992	C1993	U1997	G2001	A2002	G2003	U2004	G2005	U2006	C2007	U2008	
A1805	G1815	A1818	C1819	U1820	G1821	U1822	G1823	C1828	G1833	U1834	G1835	G1836	A1837	G1840	C1841	G1842	U1852	G1855	C1856	A1867	U1868	G1869	G1880	C1881	U1882	G1883	U1889	A1892	C1893	A1897	A1907	A1908	G1909	G1910	C1911	G1916	A1917	U1918	G1919	C1920	C1921	G1922	A1923	U1930	G1759	U1800	A1801	G1802	G1803	A1804		
U1677	C1678	A1679	G1685	G1691	G1724	U1725	U1726	G1733	G1734	U1735	G1740	G1741	A1742	G1750	G1753	C1754	U1755	U1756	U1757	G1758	G1759	G1760	G1761	C1762	C1763	G1764	A1765	A1766	C1767	C1768	G1769	A1770	U1771	C1772	U1773	A1776	U1780	U1781	C1785	A1786	A1787	A1788	G1789	U1800	A1801	G1802	G1803	A1804				
A1547	A1554	A1563	A1564	A1565	C1566	C1567	C1568	G1574	U1578	G1586	C1590	U1591	U1592	U1596	G1612	A1613	G1617	G1624	G1625	G1626	C1628	A1631	A1632	G1633	A1634	C1635	C1640	G1641	A1653	G1654	C1655	U1656	U1660	C1661	C1662	C1663	A1667	A1668	A1669	G1670	C1676											



• Molecule 48: 5S ribosomal RNA



• Molecule 49: 5.8S ribosomal RNA



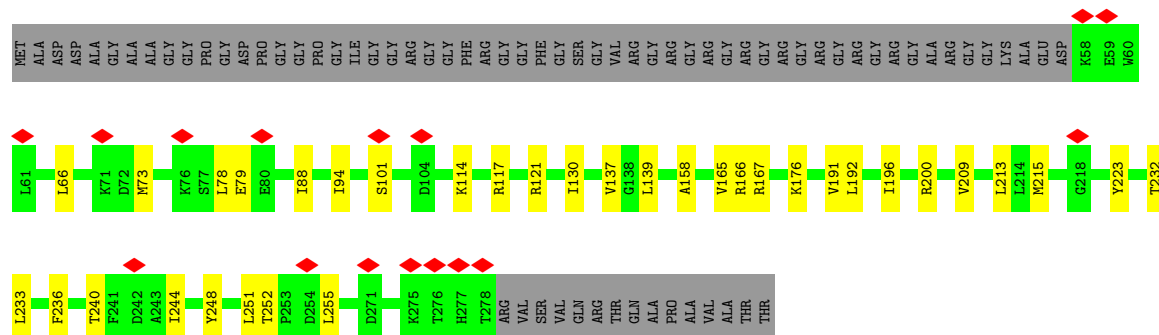
Chain 9: 6% 58% 27% 5% 9%



GLU
ARG
ALA
ASP
GLY
TYR
GLU
PRO
PRO
GLY
VAL
GLN
SER
VAL

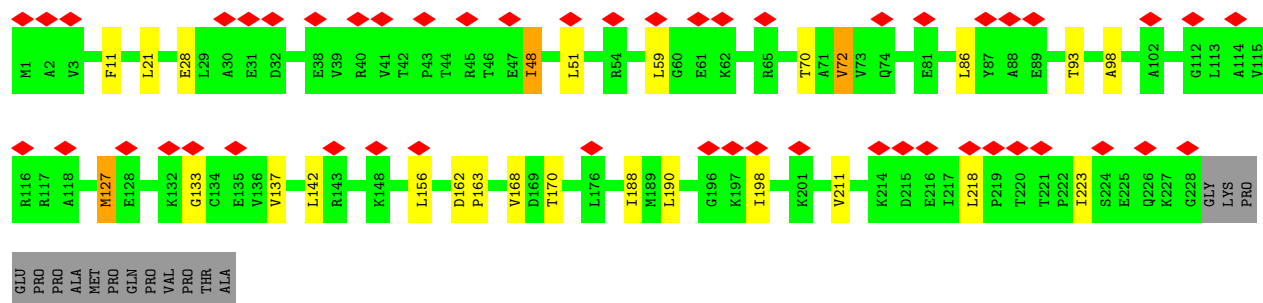
• Molecule 53: uS5

Chain CC:  5% 63% 12% 25%



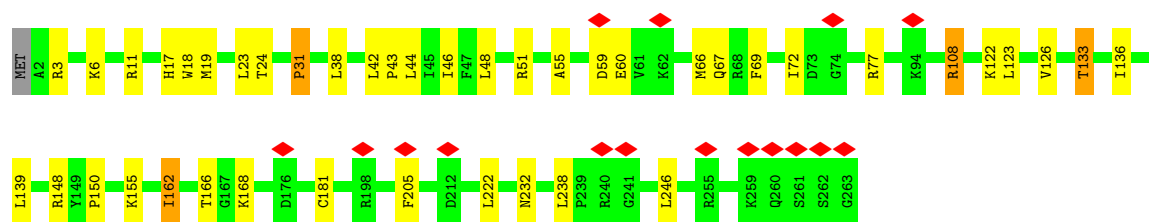
• Molecule 54: uS3

Chain DD:  21% 83% 9% 6%



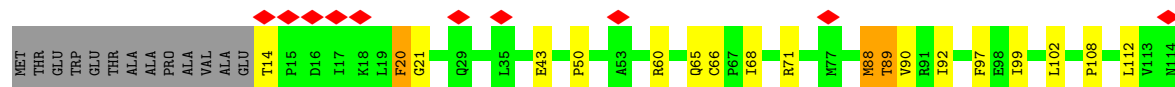
• Molecule 55: 40S ribosomal protein S4

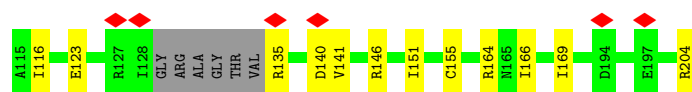
Chain EE:  6% 83% 15% 0%



• Molecule 56: uS7

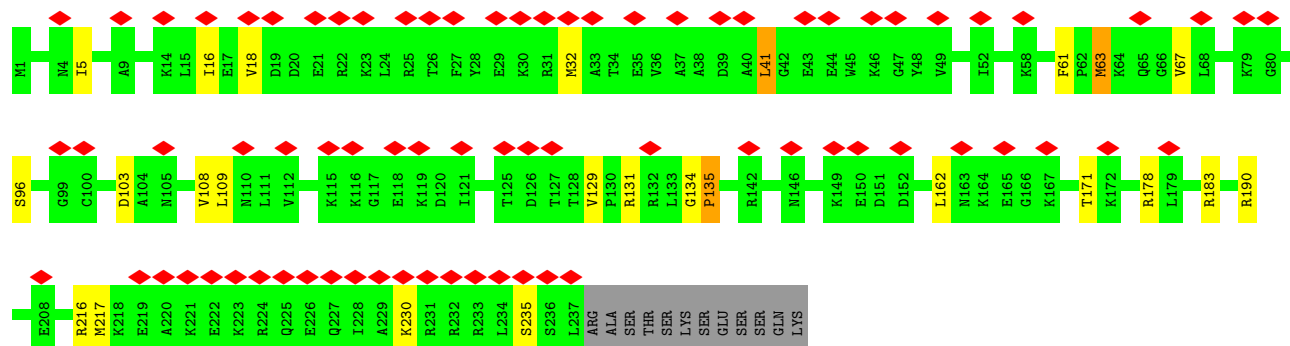
Chain FF:  8% 75% 14% 9%





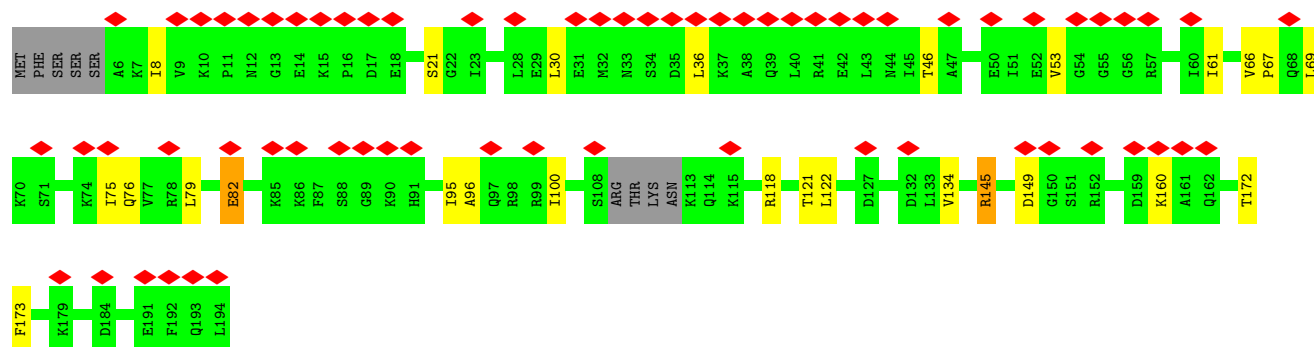
- Molecule 57: 40S ribosomal protein S6

Chain GG: 31% 85% 9% • 5%



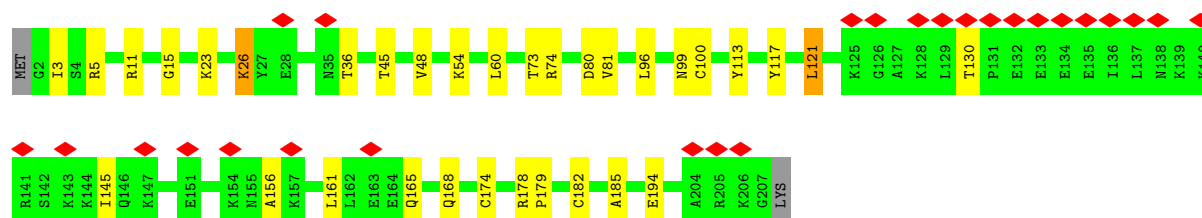
- Molecule 58: eS7

Chain HH: 34% 82% 12% • 5%



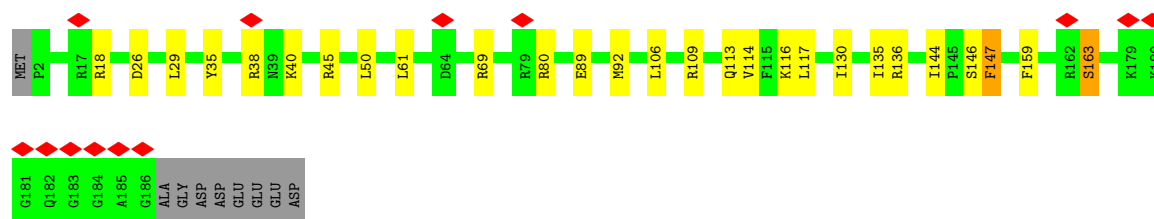
- Molecule 59: 40S ribosomal protein S8

Chain II: 12% 83% 15% ••

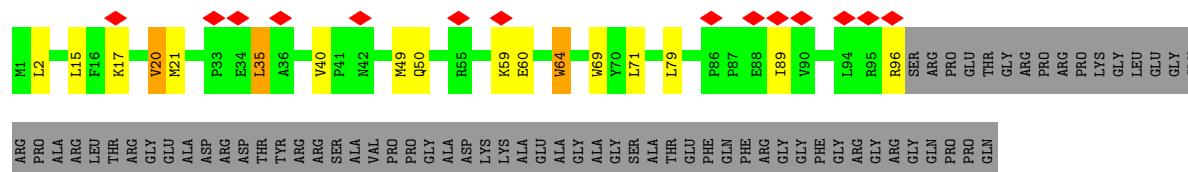


- Molecule 60: Ribosomal protein S9 (Predicted)

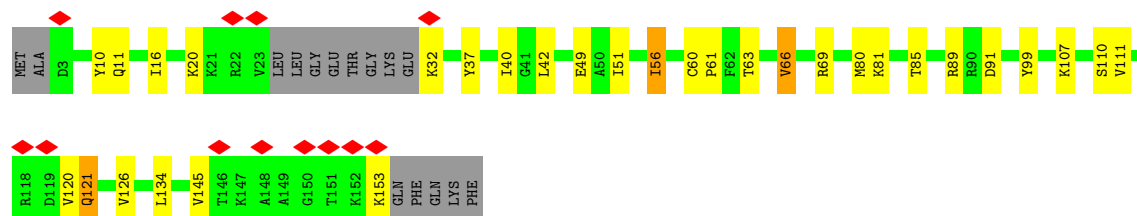
Chain JJ: 7% 81% 13% • 5%



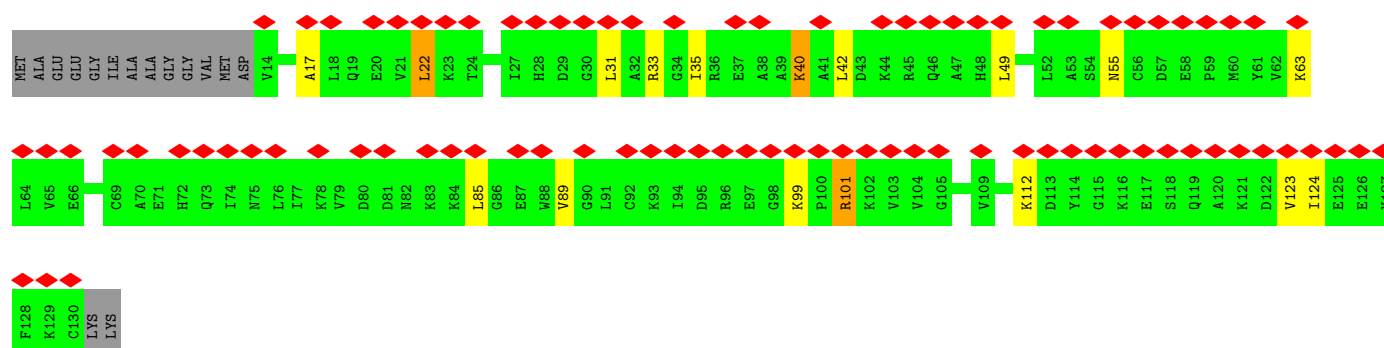
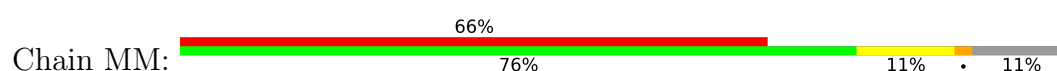
• Molecule 61: eS10



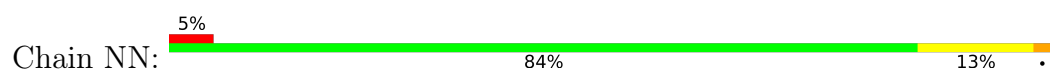
• Molecule 62: uS17



• Molecule 63: 40S ribosomal protein S12

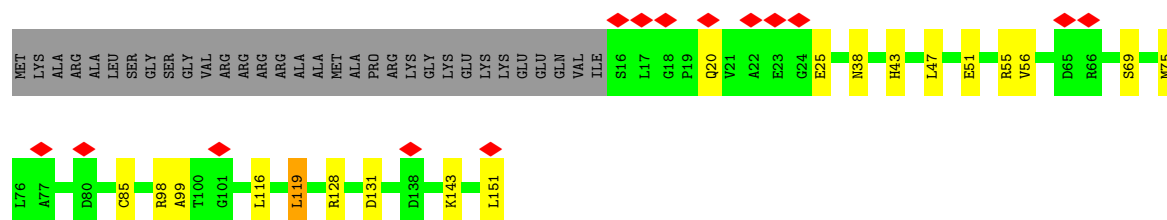


• Molecule 64: uS15



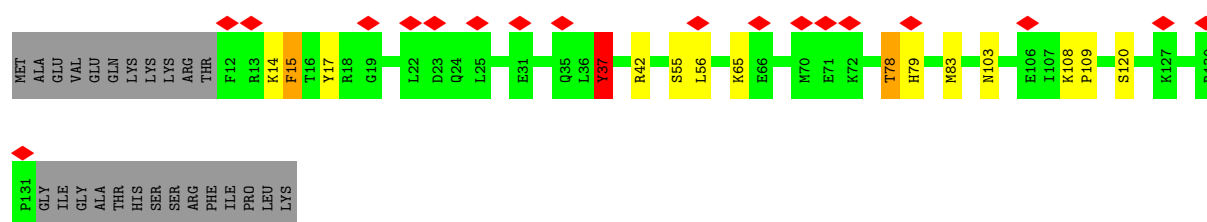
- Molecule 65: uS11

Chain OO: 



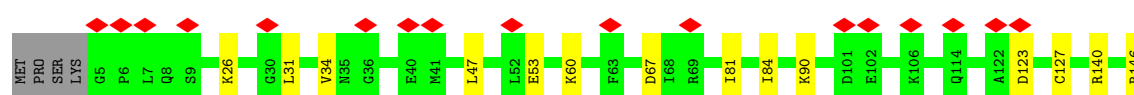
- Molecule 66: uS19

Chain PP: 



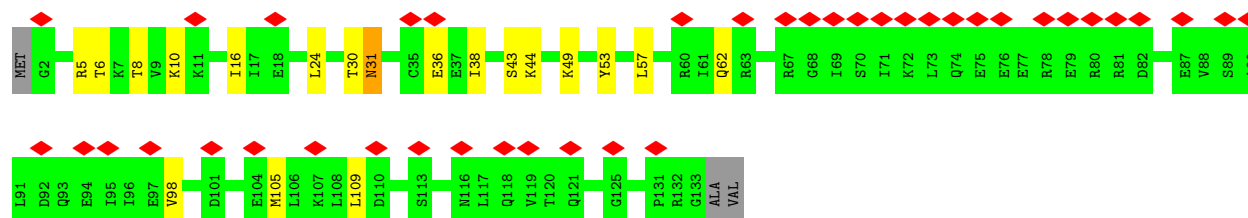
- Molecule 67: uS9

Chain QQ: 



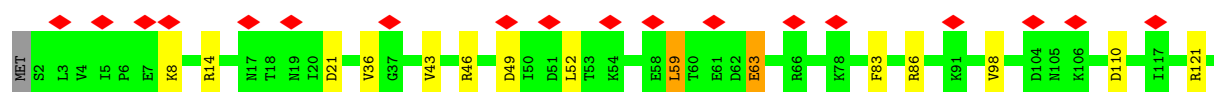
- Molecule 68: eS17

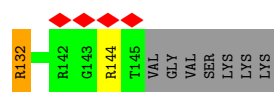
Chain RR: 



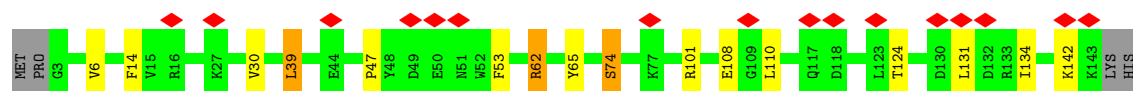
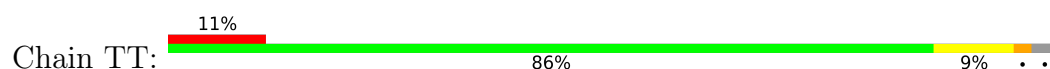
- Molecule 69: uS13

Chain SS: 

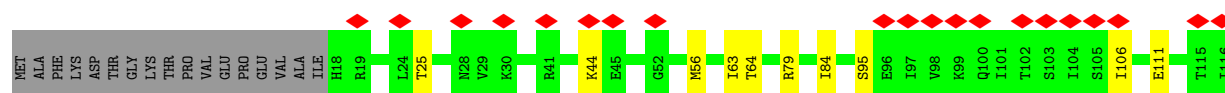
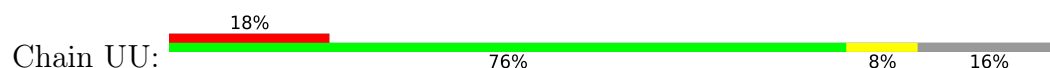




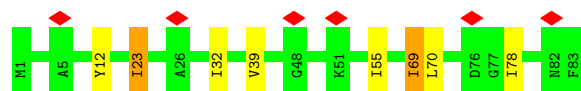
- Molecule 70: eS19



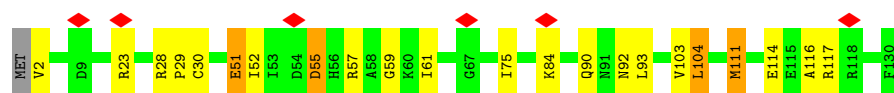
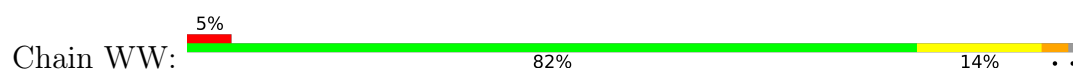
- Molecule 71: uS10



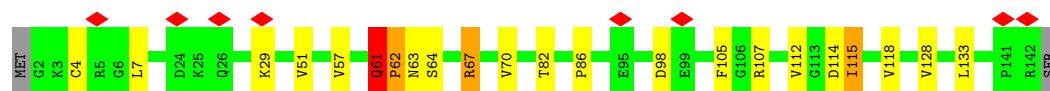
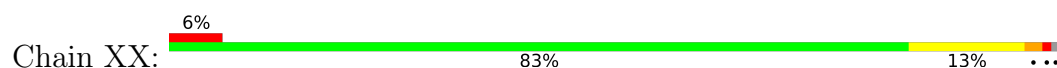
- Molecule 72: eS21



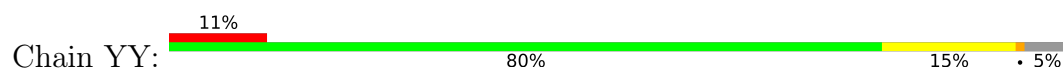
- Molecule 73: uS8

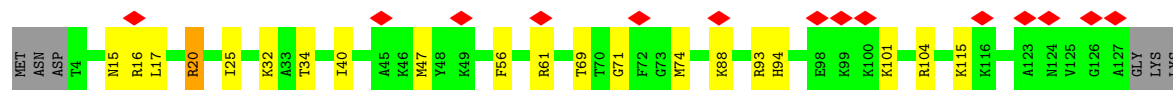


- Molecule 74: uS12

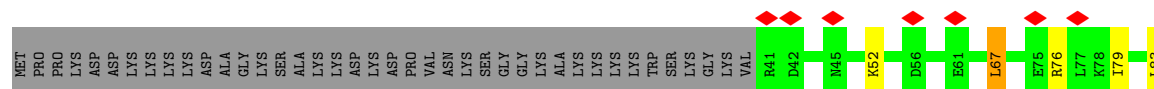


- Molecule 75: eS24

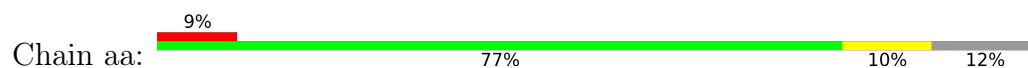




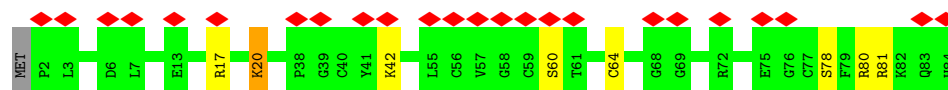
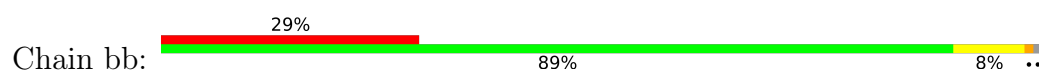
• Molecule 76: eS25



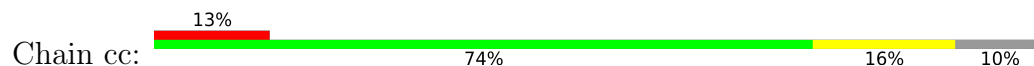
• Molecule 77: eS26



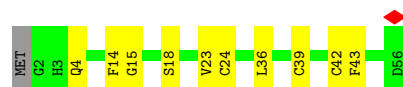
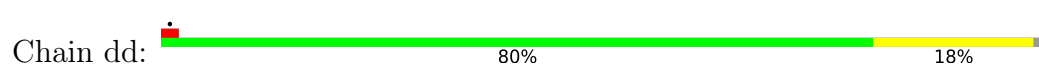
• Molecule 78: 40S ribosomal protein S27



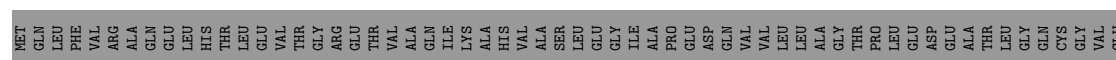
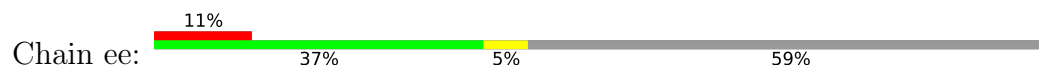
• Molecule 79: eS28

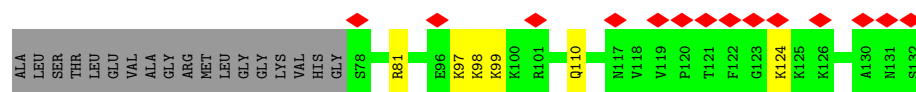


• Molecule 80: uS14

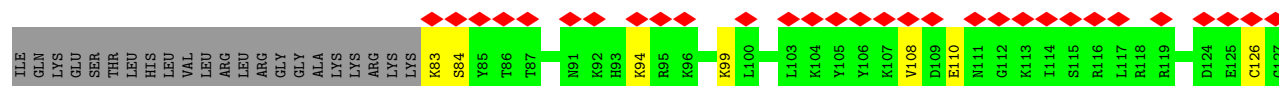
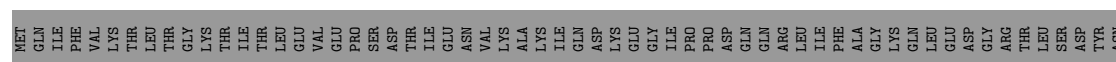
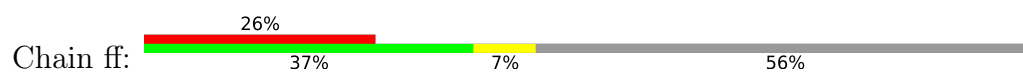


• Molecule 81: eS30

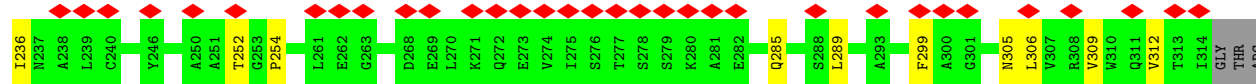
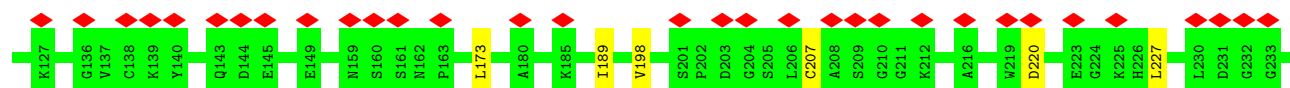
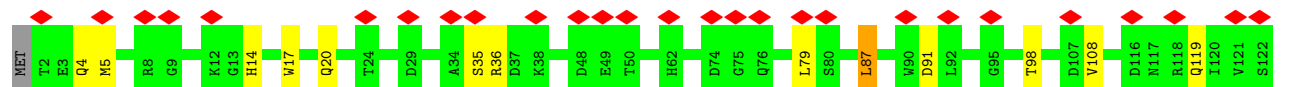
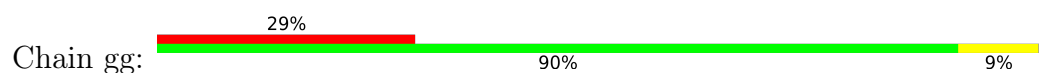




• Molecule 82: eS31



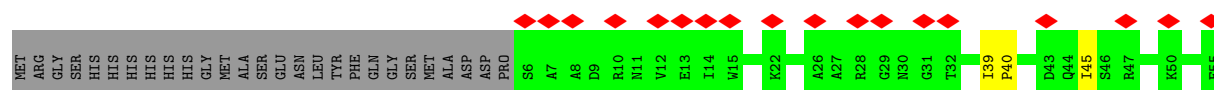
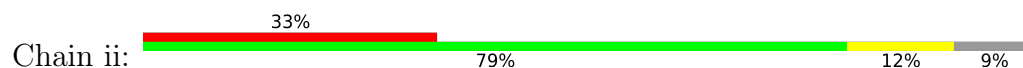
• Molecule 83: RACK1



• Molecule 84: mRNA (UGA stop codon)



• Molecule 85: Eukaryotic peptide chain release factor subunit 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	13852	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	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	104478	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.671	Depositor
Minimum map value	-0.487	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	562.8, 562.8, 562.8	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3399999, 1.3399999, 1.3399999	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 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	A	0.60	0/1936	0.89	1/2596 (0.0%)
2	B	0.64	0/3240	0.89	3/4339 (0.1%)
3	C	0.66	0/2937	0.96	2/3946 (0.1%)
4	D	0.65	0/2437	0.96	0/3264
5	E	0.54	0/1762	0.83	1/2362 (0.0%)
6	F	0.69	0/1911	0.98	0/2549
7	G	0.59	0/1910	0.96	1/2569 (0.0%)
8	H	0.50	0/1535	0.76	0/2063
9	I	0.59	0/1702	0.87	0/2272
10	J	0.52	0/1385	0.83	1/1852 (0.1%)
11	L	0.69	1/1733 (0.1%)	0.96	0/2316
12	M	0.73	0/1158	1.02	1/1547 (0.1%)
13	N	0.64	0/1746	0.97	2/2338 (0.1%)
14	O	0.71	0/1662	1.04	1/2222 (0.0%)
15	P	0.64	0/1268	0.91	2/1700 (0.1%)
16	Q	0.69	0/1539	0.96	0/2054
17	R	0.69	0/1524	1.00	0/2013
18	S	0.61	0/1501	0.86	0/2012
19	T	0.61	0/1326	0.82	1/1770 (0.1%)
20	U	0.51	0/823	0.75	0/1104
21	V	0.63	0/993	0.90	0/1332
22	W	0.53	0/873	0.82	0/1158
23	X	0.57	0/984	0.87	1/1323 (0.1%)
24	Y	0.50	0/1132	0.83	2/1504 (0.1%)
25	Z	0.55	0/1130	0.81	0/1507
26	a	0.67	0/1191	0.97	2/1590 (0.1%)
27	b	0.60	0/861	0.96	0/1138
28	c	0.54	0/771	0.85	0/1034
29	d	0.62	0/903	0.85	1/1216 (0.1%)
30	e	0.64	0/1071	0.87	0/1429
31	f	0.58	0/895	0.83	2/1198 (0.2%)
32	g	0.56	0/916	0.84	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.69	0/1021	1.04	0/1348
34	i	0.55	0/841	0.91	0/1112
35	j	0.73	0/720	0.98	0/952
36	k	0.56	0/575	0.84	0/761
37	l	0.70	0/459	0.96	0/608
38	m	0.64	0/435	0.94	0/575
39	n	0.71	0/240	1.16	0/305
40	o	0.61	0/864	0.85	0/1140
41	p	0.71	0/718	1.03	1/953 (0.1%)
42	r	0.61	0/1010	0.96	0/1354
43	s	0.59	0/1530	0.89	0/2064
44	t	0.66	0/1173	1.05	0/1579
45	2	0.46	1/1803 (0.1%)	0.78	4/2801 (0.1%)
46	3	0.38	0/1777	0.71	0/2763
47	5	0.44	0/84974	0.81	134/132512 (0.1%)
48	7	0.43	0/2858	0.76	2/4455 (0.0%)
49	8	0.44	0/3581	0.78	2/5577 (0.0%)
50	9	0.42	1/40516 (0.0%)	0.80	49/63102 (0.1%)
51	AA	0.56	0/1747	0.86	0/2374
52	BB	0.50	0/1756	0.85	0/2350
53	CC	0.54	0/1753	0.90	0/2369
54	DD	0.55	0/1796	0.89	0/2417
55	EE	0.57	0/2118	0.89	4/2849 (0.1%)
56	FF	0.56	0/1492	0.93	0/2005
57	GG	0.54	0/1946	0.87	2/2590 (0.1%)
58	HH	0.52	0/1510	0.87	0/2022
59	II	0.60	0/1715	0.88	0/2287
60	JJ	0.55	0/1550	0.96	1/2069 (0.0%)
61	KK	0.55	0/834	0.84	0/1125
62	LL	0.57	0/1195	0.89	2/1597 (0.1%)
63	MM	0.56	0/918	0.92	1/1233 (0.1%)
64	NN	0.56	0/1226	0.91	0/1649
65	OO	0.53	0/1029	0.93	0/1380
66	PP	0.53	0/1017	0.90	1/1358 (0.1%)
67	QQ	0.54	0/1146	0.84	0/1534
68	RR	0.55	0/1082	0.86	0/1452
69	SS	0.52	0/1208	0.85	0/1618
70	TT	0.55	0/1115	0.91	0/1493
71	UU	0.55	0/805	0.88	0/1081
72	VV	0.57	0/643	0.93	1/860 (0.1%)
73	WW	0.54	0/1051	0.90	1/1406 (0.1%)
74	XX	0.55	0/1116	0.90	0/1490
75	YY	0.49	0/1028	0.82	0/1366

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	ZZ	0.49	0/604	0.90	0/810
77	aa	0.57	0/828	0.92	0/1109
78	bb	0.49	0/665	0.85	0/891
79	cc	0.55	0/490	0.84	0/656
80	dd	0.58	0/470	0.92	0/623
81	ee	0.52	0/447	0.92	0/587
82	ff	0.49	0/567	0.71	0/753
83	gg	0.49	0/2493	0.75	0/3394
84	hh	0.39	0/353	0.78	0/547
85	ii	0.54	1/3345 (0.0%)	0.87	3/4492 (0.1%)
All	All	0.51	4/234908 (0.0%)	0.84	232/344334 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
12	M	0	1
51	AA	0	1
55	EE	0	1
74	XX	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
85	ii	144	SER	C-O	6.61	1.32	1.24
45	2	20	U	C5'-C4'	6.31	1.60	1.51
11	L	52	ALA	C-O	5.24	1.30	1.24
50	9	583	A	C1'-N9	-5.19	1.40	1.48

All (232) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	2068	C	C4'-C3'-O3'	12.36	127.94	109.40
50	9	1835	A	C2'-C3'-O3'	11.64	126.95	109.50
47	5	2695	A	C2'-C3'-O3'	10.49	125.23	109.50
47	5	47	A	C4'-C3'-O3'	9.79	124.09	109.40
47	5	385	A	C4'-C3'-O3'	9.61	123.81	109.40
50	9	870	A	C4'-C3'-O3'	9.13	123.09	109.40
47	5	2468	U	C4'-C3'-O3'	9.01	122.91	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1394	G	C2'-C3'-O3'	8.61	126.61	113.70
47	5	1477	C	C2'-C3'-O3'	8.31	126.16	113.70
47	5	1455	G	C2'-C3'-O3'	8.28	126.11	113.70
47	5	2046	G	C2'-C3'-O3'	8.19	121.78	109.50
50	9	1664	A	C4'-C3'-O3'	8.17	121.66	109.40
47	5	1329	G	C2'-C3'-O3'	7.90	125.55	113.70
47	5	1834	U	C2'-C3'-O3'	7.87	121.31	109.50
50	9	434	G	C4'-C3'-O3'	7.83	124.74	113.00
47	5	449	C	C2'-C3'-O3'	7.81	121.22	109.50
47	5	1174	G	C2'-C3'-O3'	7.72	125.28	113.70
50	9	1137	U	C2'-C3'-O3'	7.70	121.06	109.50
50	9	1061	U	C2'-C3'-O3'	-7.68	102.17	113.70
50	9	110	U	C2'-C3'-O3'	7.66	125.20	113.70
45	2	20(A)	U	C2'-C3'-O3'	7.64	120.96	109.50
50	9	688	U	C2'-C3'-O3'	7.63	120.95	109.50
47	5	4925	U	C2'-C3'-O3'	7.58	120.88	109.50
47	5	4239	A	C4'-C3'-O3'	-7.58	101.64	113.00
13	N	90	ASN	N-CA-C	7.54	119.28	111.14
47	5	959	G	C2'-C3'-O3'	7.53	120.79	109.50
47	5	1370	G	C2'-C3'-O3'	7.46	120.69	109.50
19	T	154	ILE	N-CA-C	7.25	115.76	109.02
47	5	498	C	C4'-C3'-O3'	7.24	120.26	109.40
55	EE	108	ARG	N-CA-C	7.24	119.67	110.33
47	5	4232	U	C4'-C3'-O3'	7.23	120.24	109.40
14	O	110	PRO	N-CA-C	7.18	119.46	110.70
15	P	126	ARG	N-CA-C	7.12	119.87	107.49
47	5	1485	C	C2'-C3'-O3'	7.11	120.16	109.50
50	9	874	G	C2'-C3'-O3'	7.09	124.34	113.70
47	5	1979	A	C2'-C3'-O3'	7.03	124.25	113.70
50	9	72	C	C4'-C3'-O3'	7.02	119.93	109.40
47	5	3859	G	C4'-C3'-O3'	-7.00	102.50	113.00
47	5	2521	G	C4'-C3'-O3'	-6.94	102.59	113.00
47	5	2025	A	C4'-C3'-O3'	6.91	119.76	109.40
26	a	22	ILE	N-CA-C	-6.88	103.95	110.42
72	VV	23	ILE	N-CA-C	6.83	117.86	108.84
47	5	2089	G	C2'-C3'-O3'	6.83	119.75	109.50
50	9	1115	U	C2'-C3'-O3'	6.73	119.60	109.50
47	5	48	G	C4'-C3'-O3'	6.72	119.48	109.40
47	5	406	C	C2'-C3'-O3'	6.69	123.73	113.70
47	5	1921	C	C2'-C3'-O3'	6.68	119.52	109.50
47	5	4699	U	C4'-C3'-O3'	6.68	119.42	109.40
47	5	4942	C	C4'-C3'-O3'	6.68	119.42	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	9	1837	G	C2'-C3'-O3'	-6.64	103.74	113.70
50	9	873	G	C2'-C3'-O3'	6.63	119.45	109.50
45	2	20	U	C5'-C4'-C3'	6.59	125.08	115.20
47	5	3888	G	C2'-C3'-O3'	6.58	123.58	113.70
49	8	124	U	C4'-C3'-O3'	6.58	119.27	109.40
47	5	48	G	C2'-C3'-O3'	6.57	119.35	109.50
47	5	1358	G	C4'-C3'-O3'	6.55	119.22	109.40
47	5	3816	A	C4'-C3'-O3'	-6.54	103.18	113.00
45	2	20(A)	U	C1'-C2'-O2'	6.52	121.58	111.80
47	5	3625	G	C2'-C3'-O3'	6.52	123.48	113.70
50	9	1646	C	C2'-C3'-O3'	6.52	123.48	113.70
50	9	1520	G	C4'-C3'-O3'	6.51	122.77	113.00
50	9	1864	U	C3'-C2'-O2'	6.50	120.45	110.70
50	9	24	C	C4'-C3'-O3'	-6.48	103.27	113.00
47	5	2661	U	C2'-C3'-O3'	6.47	119.20	109.50
47	5	1211	G	C2'-C3'-O3'	6.46	123.39	113.70
47	5	1072	C	C2'-C3'-O3'	6.43	119.15	109.50
29	d	38	PHE	N-CA-C	6.40	119.07	111.33
50	9	1679	A	C2'-C3'-O3'	6.33	119.00	109.50
47	5	1960	A	C4'-C3'-O3'	6.30	118.85	109.40
47	5	2359	U	C4'-C3'-O3'	-6.29	103.57	113.00
47	5	1445	U	C2'-C3'-O3'	6.19	122.98	113.70
50	9	160	U	C4'-C3'-O3'	6.19	118.68	109.40
47	5	4237	C	C1'-C2'-O2'	6.18	117.68	108.40
47	5	4448	G	C4'-C3'-O3'	6.18	122.27	113.00
47	5	4284	C	C4'-C3'-O3'	-6.18	103.73	113.00
50	9	752	G	C2'-C3'-O3'	6.17	118.75	109.50
47	5	2411	C	C4'-C3'-O3'	-6.17	103.75	113.00
60	JJ	163	SER	N-CA-C	6.15	113.75	108.22
47	5	4449	A	C4'-C3'-O3'	6.14	118.61	109.40
62	LL	99	TYR	N-CA-C	-6.13	99.25	109.24
63	MM	35	ILE	N-CA-C	6.09	116.75	110.36
47	5	3697	U	C2'-C3'-O3'	6.08	122.82	113.70
50	9	1130	G	C4'-C3'-O3'	6.08	122.12	113.00
50	9	640	A	C4'-C3'-O3'	-6.08	103.89	113.00
47	5	696	C	C2'-C3'-O3'	6.06	118.59	109.50
47	5	1317	U	C4'-C3'-O3'	-6.06	103.91	113.00
47	5	1960	A	C2'-C3'-O3'	-6.04	100.43	109.50
50	9	1438	A	C4'-C3'-O3'	-6.04	103.94	113.00
3	C	98	GLY	N-CA-C	-6.04	100.79	112.02
47	5	4947	U	C2'-C3'-O3'	6.03	122.74	113.70
47	5	492	U	C2'-C3'-O3'	6.02	118.53	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	1428	U	C4'-C3'-O3'	-6.00	104.00	113.00
47	5	4535	A	C4'-C3'-O3'	-5.99	104.01	113.00
47	5	1670	G	C2'-C3'-O3'	-5.96	104.76	113.70
50	9	1395	C	C4'-C3'-O3'	5.95	121.93	113.00
47	5	3876	A	C2'-C3'-O3'	5.94	118.40	109.50
47	5	3746	A	C4'-C3'-O3'	-5.91	104.14	113.00
47	5	480	C	C2'-C3'-O3'	5.89	122.53	113.70
47	5	3914	U	C2'-C3'-O3'	-5.88	104.88	113.70
47	5	4655	A	C4'-C3'-O3'	-5.88	104.18	113.00
47	5	2587	A	C2'-C3'-O3'	-5.88	104.89	113.70
47	5	1916	G	C4'-C3'-O3'	-5.88	104.19	113.00
47	5	90	G	C4'-C3'-O3'	-5.87	104.19	113.00
47	5	3619	G	C4'-C3'-O3'	-5.87	104.20	113.00
50	9	642	U	C4'-C3'-O3'	5.86	121.80	113.00
31	f	69	VAL	N-CA-C	5.85	116.78	108.42
15	P	37	LYS	N-CA-C	5.85	117.65	111.28
50	9	23	G	C4'-C3'-O3'	-5.84	104.23	113.00
47	5	2067	C	C4'-C3'-O3'	-5.84	104.24	113.00
47	5	4312	U	C4'-C3'-O3'	-5.83	104.25	113.00
50	9	1646	C	C4'-C3'-O3'	-5.83	104.25	113.00
50	9	1313	A	C4'-C3'-O3'	5.82	118.14	109.40
47	5	47	A	C2'-C3'-O3'	-5.82	100.77	109.50
57	GG	134	GLY	CA-C-N	5.79	127.08	119.84
57	GG	134	GLY	C-N-CA	5.79	127.08	119.84
47	5	2080	U	C3'-C2'-O2'	5.76	119.35	110.70
47	5	4660	G	C4'-C3'-O3'	-5.75	104.37	113.00
47	5	504	G	C2'-C3'-O3'	5.75	122.33	113.70
47	5	1921	C	C4'-C3'-O3'	5.74	118.02	109.40
47	5	4632	U	C1'-C2'-O2'	5.73	117.00	108.40
50	9	532	C	C2'-C3'-O3'	5.73	122.30	113.70
50	9	1264	C	C4'-C3'-O3'	5.73	118.00	109.40
47	5	1685	G	C1'-C2'-O2'	5.69	116.93	108.40
50	9	642	U	C2'-C3'-O3'	5.69	122.23	113.70
50	9	1637	A	C2'-C3'-O3'	5.66	117.99	109.50
50	9	1253	A	C2'-C3'-O3'	5.66	117.99	109.50
47	5	1291	G	C3'-C2'-O2'	5.64	119.16	110.70
47	5	1889	U	C2'-C3'-O3'	-5.64	105.24	113.70
47	5	1880	G	C4'-C3'-O3'	-5.63	104.56	113.00
47	5	1236	C	C4'-C3'-O3'	5.62	121.44	113.00
47	5	421	C	C3'-C2'-O2'	5.62	119.13	110.70
47	5	2474	G	C3'-C2'-O2'	5.62	119.13	110.70
47	5	481	G	C4'-C3'-O3'	-5.59	104.61	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	1237	C	C2'-C3'-O3'	-5.58	105.33	113.70
50	9	1489	A	C4'-C3'-O3'	5.56	121.34	113.00
48	7	55	A	C3'-C2'-O2'	5.54	119.01	110.70
47	5	1291	G	C2'-C3'-O3'	5.54	122.00	113.70
50	9	1620	A	C4'-C3'-O3'	-5.53	101.10	109.40
47	5	3673	C	C2'-C3'-O3'	5.53	117.79	109.50
47	5	4189	U	C1'-C2'-O2'	5.52	116.68	108.40
55	EE	133	THR	N-CA-C	5.52	119.50	112.87
47	5	275	C	C2'-C3'-O3'	5.50	121.96	113.70
47	5	1350	C	C3'-C2'-O2'	5.50	118.95	110.70
47	5	4381	A	C4'-C3'-O3'	-5.50	104.75	113.00
47	5	2423	A	C4'-C3'-O3'	-5.48	104.78	113.00
5	E	157	THR	N-CA-C	5.48	117.06	111.14
47	5	2089	G	C4'-C3'-O3'	5.48	117.62	109.40
47	5	4447	C	C2'-C3'-O3'	-5.46	105.52	113.70
47	5	2313	A	C2'-C3'-O3'	5.45	117.67	109.50
45	2	20(A)	U	N1-C1'-C2'	5.42	122.13	114.00
47	5	2524	U	C4'-C3'-O3'	-5.42	104.88	113.00
47	5	3916	G	C4'-C3'-O3'	-5.42	104.87	113.00
13	N	185	GLY	N-CA-C	-5.41	104.60	112.17
47	5	1356	U	C4'-C3'-O3'	-5.41	104.89	113.00
47	5	1818	G	C2'-C3'-O3'	5.40	121.80	113.70
47	5	916	C	C4'-C3'-O3'	5.40	117.50	109.40
55	EE	136	ILE	CA-C-N	-5.39	114.41	119.85
55	EE	136	ILE	C-N-CA	-5.39	114.41	119.85
2	B	258	HIS	N-CA-C	5.38	121.70	109.81
47	5	3895	G	C2'-C3'-O3'	-5.36	105.67	113.70
47	5	2287	G	C4'-C3'-O3'	-5.35	104.98	113.00
50	9	1130	G	C3'-C2'-O2'	5.34	118.71	110.70
47	5	2471	G	C2'-C3'-O3'	5.33	117.50	109.50
47	5	1485	C	C4'-C3'-O3'	5.33	117.39	109.40
47	5	245	C	C2'-C3'-O3'	5.33	121.69	113.70
47	5	4458	C	C3'-C2'-O2'	5.32	118.68	110.70
1	A	90	CYS	N-CA-C	5.32	116.49	108.46
50	9	980	A	C4'-C3'-O3'	-5.32	105.03	113.00
47	5	4254	G	C4'-C3'-O3'	5.31	117.37	109.40
47	5	134	G	C2'-C3'-O3'	5.31	117.47	109.50
50	9	553	U	C2'-C3'-O3'	5.31	121.66	113.70
73	WW	55	ASP	N-CA-C	-5.30	102.20	110.42
7	G	130	PRO	O-C-N	5.29	123.64	121.15
47	5	4876	A	C2'-C3'-O3'	5.29	117.43	109.50
47	5	3807	A	C4'-C3'-O3'	-5.28	105.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	M	63	LYS	N-CA-C	5.28	117.33	108.73
50	9	555	A	C2'-C3'-O3'	5.27	117.40	109.50
47	5	2278	G	C4'-C3'-O3'	5.27	117.30	109.40
10	J	23	ASN	N-CA-C	5.26	117.08	108.76
47	5	484	U	C4'-C3'-O3'	5.25	117.28	109.40
47	5	4884	G	C2'-C3'-O3'	5.25	121.57	113.70
47	5	1815	G	C2'-C3'-O3'	5.24	117.36	109.50
50	9	417	C	C4'-C3'-O3'	-5.22	105.17	113.00
47	5	2266	C	C2'-C3'-O3'	5.21	117.32	109.50
47	5	38	A	C4'-C3'-O3'	-5.20	105.20	113.00
50	9	99	A	C1'-C2'-O2'	5.20	116.20	108.40
50	9	501	C	N1-C1'-C2'	5.20	119.80	112.00
47	5	1983	A	C4'-C3'-O3'	5.20	120.79	113.00
85	ii	370	GLU	N-CA-C	5.19	116.99	110.24
47	5	4723	A	N9-C1'-C2'	5.19	119.78	112.00
47	5	2398	U	C4'-C3'-O3'	5.18	117.17	109.40
47	5	2055	G	C4'-C3'-O3'	-5.18	101.64	109.40
50	9	687	C	C2'-C3'-O3'	5.17	117.26	109.50
47	5	1238	A	C3'-C2'-O2'	5.17	118.46	110.70
47	5	4075	U	C2'-C3'-O3'	5.17	117.25	109.50
2	B	82	PRO	O-C-N	5.16	123.57	121.15
85	ii	40	PRO	CA-C-N	5.15	124.76	119.05
85	ii	40	PRO	C-N-CA	5.15	124.76	119.05
47	5	485	C	C3'-C2'-O2'	5.14	118.41	110.70
49	8	45	C	C3'-C2'-O2'	5.14	118.40	110.70
3	C	74	ALA	N-CA-C	5.13	119.39	113.18
47	5	3690	U	C1'-C2'-O2'	5.13	116.09	108.40
47	5	4119	C	C3'-C2'-O2'	5.13	118.39	110.70
47	5	481(A)	C	C2'-C3'-O3'	5.12	117.18	109.50
23	X	79	PHE	N-CA-C	5.11	114.70	108.11
31	f	103	VAL	N-CA-CB	5.10	116.09	110.53
47	5	1336	G	C2'-C3'-O3'	-5.10	106.05	113.70
50	9	1129	G	C4'-C3'-O3'	-5.10	105.36	113.00
47	5	4448	G	C2'-C3'-O3'	-5.09	106.06	113.70
47	5	325	U	C1'-C2'-O2'	5.09	116.03	108.40
47	5	4184	G	C3'-C2'-O2'	5.09	118.33	110.70
47	5	2266	C	C4'-C3'-O3'	5.08	117.02	109.40
50	9	91	A	C4'-C3'-O3'	-5.08	105.38	113.00
41	p	64	VAL	CB-CA-C	-5.08	103.21	110.12
47	5	1633	G	C1'-C2'-O2'	5.08	116.01	108.40
66	PP	37	TYR	CA-CB-CG	5.07	123.03	113.90
62	LL	107	LYS	N-CA-C	-5.07	101.84	109.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	2546	G	C3'-C2'-O2'	5.07	118.30	110.70
47	5	3640	U	C3'-C2'-O2'	5.06	118.29	110.70
50	9	1852	C	C4'-C3'-O3'	-5.05	105.42	113.00
24	Y	100	HIS	CA-C-N	5.05	125.08	119.32
24	Y	100	HIS	C-N-CA	5.05	125.08	119.32
47	5	81	C	C3'-C2'-O2'	5.04	118.27	110.70
47	5	365	U	C4'-C3'-O3'	-5.04	105.44	113.00
50	9	13	C	C4'-C3'-O3'	-5.04	105.44	113.00
48	7	4	U	C3'-C2'-O2'	5.03	118.25	110.70
47	5	64	A	C4'-C3'-O3'	5.03	116.94	109.40
2	B	47	LEU	N-CA-C	5.02	118.34	107.49
47	5	1464	C	C4'-C3'-O3'	-5.02	105.47	113.00
26	a	27	LYS	N-CA-C	5.01	116.55	111.14
47	5	2823	G	C3'-C2'-O2'	5.01	118.21	110.70
50	9	454	U	C4'-C3'-O3'	-5.00	105.50	113.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
51	AA	42	LYS	Peptide
55	EE	155	LYS	Peptide
12	M	67	SER	Peptide
74	XX	61	GLN	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	19	0
2	B	3172	0	3310	23	0
3	C	2883	0	3053	25	0
4	D	2391	0	2424	17	0
5	E	1729	0	1887	10	0
6	F	1875	0	1995	11	0
7	G	1879	0	2027	11	0
8	H	1516	0	1597	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1664	0	1712	2	0
10	J	1362	0	1399	5	0
11	L	1702	0	1820	8	0
12	M	1137	0	1211	15	0
13	N	1701	0	1749	11	0
14	O	1630	0	1778	22	0
15	P	1242	0	1274	5	0
16	Q	1515	0	1634	9	0
17	R	1508	0	1664	7	0
18	S	1462	0	1508	16	0
19	T	1298	0	1366	5	0
20	U	809	0	833	5	0
21	V	979	0	1039	7	0
22	W	860	0	903	4	0
23	X	967	0	1040	4	0
24	Y	1115	0	1205	2	0
25	Z	1107	0	1182	3	0
26	a	1162	0	1209	18	0
27	b	848	0	920	1	0
28	c	761	0	794	2	0
29	d	888	0	930	10	0
30	e	1053	0	1147	11	0
31	f	876	0	912	3	0
32	g	906	0	998	4	0
33	h	1013	0	1147	3	0
34	i	830	0	916	2	0
35	j	705	0	737	8	0
36	k	569	0	637	2	0
37	l	447	0	480	7	0
38	m	429	0	466	2	0
39	n	239	0	289	1	0
40	o	851	0	920	9	0
41	p	708	0	758	5	0
42	r	994	0	1051	3	0
43	s	1507	0	1564	3	0
44	t	1160	0	1217	40	0
45	2	1616	0	826	37	0
46	3	1593	0	811	5	0
47	5	75972	0	38391	280	0
48	7	2558	0	1296	4	0
49	8	3208	0	1629	10	0
50	9	36249	0	18324	160	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	AA	1710	0	1708	17	0
52	BB	1729	0	1803	8	0
53	CC	1716	0	1806	10	0
54	DD	1768	0	1866	13	0
55	EE	2076	0	2177	19	0
56	FF	1471	0	1522	15	0
57	GG	1923	0	2089	9	0
58	HH	1488	0	1582	9	0
59	II	1686	0	1772	17	0
60	JJ	1525	0	1640	9	0
61	KK	810	0	836	7	0
62	LL	1175	0	1249	11	0
63	MM	908	0	939	8	0
64	NN	1202	0	1289	8	0
65	OO	1016	0	1039	5	0
66	PP	997	0	1045	6	0
67	QQ	1128	0	1195	2	0
68	RR	1068	0	1121	5	0
69	SS	1190	0	1249	4	0
70	TT	1097	0	1132	9	0
71	UU	795	0	862	3	0
72	VV	636	0	637	6	0
73	WW	1034	0	1080	10	0
74	XX	1098	0	1167	12	0
75	YY	1011	0	1083	5	0
76	ZZ	598	0	656	6	0
77	aa	814	0	865	4	0
78	bb	651	0	672	1	0
79	cc	488	0	514	10	0
80	dd	459	0	450	7	0
81	ee	443	0	492	1	0
82	ff	555	0	566	4	0
83	gg	2436	0	2393	10	0
84	hh	317	0	161	2	0
85	ii	3295	0	3334	26	0
86	5	169	0	0	0	0
86	7	5	0	0	0	0
86	8	3	0	0	0	0
86	9	71	0	0	0	0
86	B	1	0	0	0	0
86	I	1	0	0	0	0
86	P	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	Q	1	0	0	0	0
86	V	1	0	0	0	0
86	a	1	0	0	0	0
86	e	1	0	0	0	0
86	g	1	0	0	0	0
86	hh	1	0	0	0	0
86	j	1	0	0	0	0
87	aa	1	0	0	0	0
87	dd	1	0	0	2	0
87	ff	1	0	0	0	0
87	g	1	0	0	0	0
87	j	1	0	0	0	0
87	m	1	0	0	0	0
87	o	1	0	0	0	0
87	p	1	0	0	1	0
All	All	219122	0	163963	1004	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 3.

All (1004) 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)
45:2:20:U:C1'	45:2:20(A):U:H1'	1.32	1.56
45:2:20:U:C2'	45:2:20(A):U:C1'	1.75	1.55
45:2:20:U:H2'	45:2:20(A):U:C2'	1.34	1.50
45:2:20:U:C3'	45:2:20(A):U:C3'	1.77	1.50
45:2:20:U:C2'	45:2:20(A):U:H1'	1.09	1.39
47:5:3914:U:O4	47:5:4378:A:N1	1.56	1.38
45:2:20:U:H3'	45:2:20(A):U:C3'	0.85	1.33
50:9:1137:U:O4	50:9:1148:A:N1	1.65	1.29
45:2:20:U:H2'	45:2:20(A):U:O2'	1.33	1.28
45:2:20:U:C2'	45:2:20(A):U:C2'	1.95	1.27
47:5:2367:A:N1	47:5:2788:U:O4	1.71	1.22
50:9:1137:U:C4	50:9:1148:A:N1	2.09	1.20
45:2:20:U:C3'	45:2:20(A):U:O3'	1.91	1.17
45:2:20:U:H2'	45:2:20(A):U:C1'	1.57	1.13
45:2:20:U:H3'	45:2:20(A):U:C2'	1.66	1.11
45:2:20:U:C3'	45:2:20(A):U:C2'	2.07	1.10
45:2:20:U:O4'	45:2:20(A):U:O2	1.73	1.06
41:p:60:CYS:SG	87:p:100:ZN:ZN	1.51	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:2:20:U:H3'	45:2:20(A):U:O3'	1.57	0.98
50:9:1680:G:H4'	79:cc:20:ARG:HD2	1.45	0.97
45:2:20:U:O3'	45:2:20(A):U:O3'	1.82	0.96
50:9:1137:U:O4	50:9:1148:A:C2	2.18	0.95
45:2:20:U:C2'	45:2:20(A):U:O2'	2.04	0.92
45:2:20:U:O4'	45:2:20(A):U:C2	2.24	0.91
44:t:81:ILE:HG21	44:t:136:ALA:HB2	1.54	0.90
44:t:81:ILE:HG21	44:t:136:ALA:CB	2.02	0.89
45:2:20:U:C1'	45:2:20(A):U:C1'	2.26	0.86
47:5:3914:U:H3	47:5:4378:A:N6	1.74	0.85
44:t:104:ILE:HB	44:t:143:VAL:HG22	1.60	0.82
80:dd:39:CYS:HG	87:dd:100:ZN:ZN	0.52	0.82
47:5:2367:A:N6	47:5:2788:U:N3	2.26	0.82
47:5:3914:U:C4	47:5:4378:A:N1	2.48	0.80
44:t:81:ILE:HD11	44:t:132:ILE:O	1.81	0.79
47:5:3914:U:O4	47:5:4378:A:C2	2.35	0.79
79:cc:20:ARG:HH11	79:cc:28:THR:HG23	1.45	0.79
80:dd:39:CYS:SG	87:dd:100:ZN:ZN	1.71	0.78
47:5:4579:U:H2'	47:5:4580:U:C6	2.18	0.78
45:2:20:U:H2'	45:2:20(A):U:HO2'	1.48	0.77
1:A:225:ILE:HD12	1:A:233:ARG:CZ	2.14	0.77
44:t:81:ILE:CD1	44:t:132:ILE:O	2.32	0.77
50:9:1407:U:H2'	50:9:1408:U:C6	2.20	0.77
44:t:112:ILE:HG22	44:t:132:ILE:HD13	1.67	0.76
44:t:104:ILE:O	44:t:143:VAL:HG13	1.84	0.76
50:9:1137:U:O4	50:9:1148:A:C6	2.38	0.76
47:5:3914:U:N3	47:5:4378:A:N6	2.31	0.76
61:KK:15:LEU:HD22	61:KK:49:MET:HE1	1.69	0.75
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.19	0.74
50:9:1680:G:O2'	79:cc:20:ARG:HD3	1.86	0.74
47:5:2395:A:O2'	47:5:2806:A:N3	2.17	0.74
85:ii:78:VAL:HG23	85:ii:95:VAL:HG11	1.69	0.73
47:5:2367:A:H61	47:5:2788:U:H3	1.34	0.73
44:t:82:ILE:HG12	44:t:139:VAL:CG1	2.19	0.73
47:5:2367:A:N1	47:5:2788:U:C4	2.57	0.71
17:R:74:ARG:NH2	47:5:2891:U:OP2	2.23	0.71
47:5:2367:A:N6	47:5:2788:U:H3	1.86	0.71
26:a:59:ARG:NH2	47:5:294:G:O2'	2.23	0.70
61:KK:35:LEU:HD13	61:KK:40:VAL:HG21	1.72	0.70
37:l:20:ASN:O	37:l:41:ARG:NE	2.25	0.70
3:C:101:MET:SD	3:C:104:PRO:HA	2.31	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:t:131:GLU:O	44:t:135:THR:HG23	1.91	0.70
55:EE:122:LYS:HG2	55:EE:162:ILE:HD11	1.73	0.69
44:t:82:ILE:HG12	44:t:139:VAL:HG11	1.73	0.69
45:2:20:U:C6	45:2:20(A):U:C6	2.81	0.69
44:t:81:ILE:CD1	44:t:135:THR:OG1	2.40	0.69
47:5:1986:U:C2	47:5:2006:U:O4	2.46	0.69
14:O:18:ARG:NH1	47:5:2053:C:O3'	2.26	0.69
47:5:1986:U:O2	47:5:2006:U:O4	2.11	0.68
50:9:1438:A:H2'	50:9:1439:A:C8	2.29	0.68
47:5:3654:G:O2'	47:5:3693:U:OP1	2.11	0.68
47:5:1986:U:O2	47:5:2006:U:C4	2.47	0.68
47:5:1986:U:H2'	47:5:2007:G:O6	1.94	0.68
47:5:3766:A:N1	50:9:1827:U:O2'	2.23	0.68
55:EE:122:LYS:CG	55:EE:162:ILE:HD11	2.25	0.67
60:JJ:35:TYR:CD2	60:JJ:106:LEU:HD23	2.29	0.67
50:9:1137:U:C4	50:9:1148:A:C6	2.83	0.67
85:ii:374:LEU:C	85:ii:375:LEU:N	2.52	0.66
50:9:980:A:H2'	50:9:981:A:C8	2.31	0.66
47:5:4579:U:O2	47:5:4580:U:C2	2.49	0.66
4:D:146:LEU:HD12	47:5:4323:A:C2	2.31	0.65
47:5:2013:A:C2	47:5:2014:C:C2	2.85	0.65
50:9:945:U:H2'	50:9:946:U:C6	2.31	0.65
45:2:20:U:C2	45:2:20(A):U:C2	2.85	0.65
14:O:72:HIS:N	47:5:4586:G:OP1	2.24	0.65
44:t:100:HIS:HB2	44:t:140:GLY:O	1.96	0.65
50:9:1533:A:OP2	56:FF:164:ARG:NH2	2.30	0.65
56:FF:68:ILE:HD12	56:FF:112:LEU:HD22	1.78	0.65
76:ZZ:79:ILE:HB	76:ZZ:83:LEU:HD12	1.79	0.64
26:a:86:THR:HG22	47:5:510:U:H5''	1.78	0.64
50:9:1130:G:H2'	50:9:1130:G:N3	2.11	0.64
35:j:19:CYS:SG	35:j:20:ARG:N	2.71	0.64
1:A:27:ALA:O	1:A:128:ARG:NH2	2.31	0.63
3:C:38:ASN:O	3:C:42:THR:HG23	1.99	0.63
5:E:124:VAL:HG13	30:e:7:LEU:HD11	1.80	0.63
50:9:298:G:OP1	55:EE:133:THR:O	2.16	0.63
18:S:82:LEU:HG	18:S:113:MET:HE2	1.79	0.63
35:j:12:ARG:NH2	47:5:1617:G:O3'	2.32	0.62
47:5:4398:C:OP1	85:ii:189:ARG:NH2	2.33	0.62
50:9:1611:G:OP2	69:SS:121:ARG:NH1	2.32	0.62
50:9:384:U:O4	59:II:5:ARG:NH2	2.33	0.62
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:r:18:ILE:HD11	42:r:20:ARG:NH2	2.13	0.62
36:k:35:LYS:NZ	47:5:2693:G:OP1	2.32	0.62
47:5:1986:U:C4	47:5:2013:A:N6	2.68	0.61
2:B:174:ARG:NH1	47:5:4985:U:O2	2.33	0.61
47:5:1964:A:C6	47:5:4694:G:C6	2.89	0.61
85:ii:39:ILE:HD12	85:ii:93:LEU:HD23	1.83	0.61
44:t:113:ALA:CB	44:t:129:ILE:HG13	2.30	0.61
47:5:4723:A:H2'	47:5:4724:A:C8	2.35	0.61
50:9:640:A:H2'	50:9:641:A:C8	2.36	0.61
50:9:124:U:OP1	55:EE:148:ARG:NE	2.34	0.60
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.37	0.60
44:t:100:HIS:HB2	44:t:140:GLY:C	2.26	0.60
40:o:81:ARG:NH2	47:5:4293:U:O2'	2.34	0.60
83:gg:91:ASP:HB2	83:gg:98:THR:HG23	1.83	0.60
50:9:1091:C:HO2'	73:WW:2:VAL:N	1.99	0.60
55:EE:55:ALA:HB1	55:EE:60:GLU:HB2	1.84	0.60
51:AA:60:LEU:HD13	51:AA:159:ILE:HD11	1.84	0.60
50:9:1016:U:OP2	78:bb:20:LYS:NZ	2.34	0.59
26:a:114:LYS:O	47:5:1398:A:OP1	2.20	0.59
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.38	0.59
47:5:3811:G:O2'	47:5:3814:U:OP2	2.21	0.59
63:MM:22:LEU:HD11	63:MM:89:VAL:HA	1.85	0.59
21:V:98:PHE:CD1	22:W:22:ALA:HB3	2.37	0.58
47:5:747:A:H4'	47:5:748:G:OP1	2.03	0.58
47:5:4887:C:H5''	47:5:4887:C:H6	1.68	0.58
65:OO:116:LEU:HD22	77:aa:53:ILE:HD11	1.85	0.58
44:t:113:ALA:HB2	44:t:129:ILE:HG13	1.85	0.58
3:C:334:THR:HG21	6:F:50:TYR:OH	2.03	0.58
75:YY:34:THR:HG23	75:YY:69:THR:HG21	1.85	0.58
51:AA:104:THR:O	51:AA:107:THR:HG23	2.02	0.58
54:DD:11:PHE:CE2	71:UU:84:ILE:HD11	2.39	0.58
11:L:55:ILE:HG21	11:L:155:MET:HE2	1.84	0.58
4:D:39:GLN:HG2	4:D:48:LYS:HB2	1.86	0.58
3:C:73:VAL:O	47:5:2350:U:C4	2.57	0.57
11:L:169:ILE:HD13	26:a:142:GLY:HA2	1.85	0.57
52:BB:66:VAL:HG22	52:BB:87:ILE:HG22	1.86	0.57
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.86	0.57
5:E:144:ARG:NH1	31:f:110:ILE:OXT	2.38	0.57
14:O:12:ARG:O	18:S:171:ARG:NH2	2.37	0.57
50:9:1220:A:N6	50:9:1221:G:C6	2.73	0.57
73:WW:75:ILE:HD11	73:WW:93:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:164:LYS:HB3	18:S:165:PRO:HD3	1.87	0.57
47:5:2007:G:C2	47:5:2013:A:N6	2.73	0.57
63:MM:22:LEU:HD21	63:MM:89:VAL:HG23	1.85	0.57
40:o:15:CYS:SG	40:o:19:GLN:NE2	2.77	0.57
50:9:925:G:N2	64:NN:48:SER:OG	2.37	0.57
53:CC:251:LEU:HD23	72:VV:23:ILE:HG23	1.87	0.57
19:T:87:LYS:NZ	47:5:4301:U:OP2	2.38	0.57
47:5:1964:A:C5	47:5:4694:G:C6	2.93	0.56
55:EE:31:PRO:HG2	55:EE:38:LEU:HD12	1.87	0.56
8:H:61:TRP:CZ3	12:M:33:GLN:HG2	2.39	0.56
50:9:1117:C:O2'	50:9:1118:C:O4'	2.24	0.56
45:2:20:U:N1	45:2:20(A):U:C2	2.74	0.56
50:9:507:G:OP2	75:YY:104:ARG:NH2	2.38	0.56
71:UU:63:ILE:HG21	80:dd:43:PHE:CE2	2.40	0.56
34:i:48:CYS:SG	34:i:49:GLY:N	2.79	0.56
44:t:135:THR:HG22	47:5:1974:U:C5	2.41	0.56
47:5:3690:U:O2'	47:5:3817:A:N3	2.32	0.56
51:AA:33:GLN:HB3	51:AA:154:LEU:HD12	1.87	0.56
44:t:81:ILE:HD13	44:t:132:ILE:O	2.05	0.56
44:t:138:SER:HB2	47:5:1976:G:N3	2.20	0.56
44:t:116:MET:HG3	44:t:132:ILE:HD11	1.87	0.56
45:2:20:U:C1'	45:2:20(A):U:N1	2.69	0.56
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.86	0.56
45:2:16:C:O4'	45:2:16:C:O2	2.24	0.56
47:5:4548:A:H5'	47:5:4549:G:OP1	2.05	0.56
50:9:1599:U:H2'	56:FF:166:ILE:HD11	1.87	0.55
68:RR:16:ILE:HG22	68:RR:24:LEU:HD11	1.87	0.55
50:9:183:G:O2'	50:9:184:G:O5'	2.23	0.55
44:t:135:THR:O	44:t:138:SER:OG	2.20	0.55
47:5:1483:C:O2	47:5:1483:C:O4'	2.22	0.55
5:E:281:THR:OG1	47:5:4754:G:N7	2.40	0.55
18:S:97:TYR:CZ	18:S:109:CYS:HA	2.42	0.55
50:9:115:U:H2'	50:9:116:U:C6	2.41	0.55
1:A:14:SER:OG	1:A:15:VAL:N	2.39	0.55
47:5:21:G:O6	49:8:36:G:C6	2.60	0.55
47:5:222:C:H2'	47:5:223:G:O4'	2.06	0.55
50:9:1589:A:N3	50:9:1653:U:O2'	2.36	0.55
50:9:1593:C:OP2	76:ZZ:104:ARG:NH2	2.40	0.55
56:FF:102:LEU:HD22	76:ZZ:110:THR:HG21	1.89	0.55
15:P:70:CYS:SG	15:P:73:ALA:N	2.80	0.55
57:GG:63:MET:SD	57:GG:63:MET:N	2.75	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:82:ILE:HD12	21:V:104:VAL:HG13	1.87	0.55
30:e:36:ARG:NH1	47:5:2322:G:OP1	2.40	0.55
47:5:2505:C:O2	47:5:2505:C:O4'	2.24	0.55
50:9:616:A:H4'	81:ee:81:ARG:O	2.07	0.55
47:5:1381:U:H5''	47:5:1381:U:O2	2.07	0.55
18:S:3:ALA:O	18:S:111:ARG:NH1	2.40	0.55
62:LL:37:TYR:CE2	62:LL:51:ILE:HG23	2.41	0.54
4:D:42:ASN:HD21	19:T:69:GLN:HE22	1.54	0.54
85:ii:314:MET:HE1	85:ii:417:VAL:HG11	1.89	0.54
47:5:4942:C:H4'	47:5:4943:A:OP1	2.08	0.54
50:9:1489:A:H4'	50:9:1490:G:OP2	2.07	0.54
72:VV:55:ILE:HD11	72:VV:69:ILE:CG1	2.38	0.54
74:XX:128:VAL:HG11	74:XX:133:LEU:HD21	1.90	0.54
50:9:501:C:O2	50:9:501:C:C2'	2.56	0.54
51:AA:58:LEU:CD1	51:AA:174:MET:HE1	2.37	0.54
85:ii:305:VAL:CG1	85:ii:328:ILE:HD13	2.36	0.54
12:M:97:ALA:HB2	14:O:203:VAL:HB	1.89	0.54
32:g:59:VAL:HG21	32:g:63:VAL:HG11	1.89	0.54
52:BB:38:MET:HE3	52:BB:185:VAL:HG11	1.89	0.54
32:g:44:SER:OG	32:g:46:CYS:SG	2.66	0.54
47:5:2627:C:O4'	47:5:2627:C:O2	2.24	0.54
50:9:427:U:O4'	50:9:427:U:O2	2.26	0.54
50:9:1351:G:O2'	50:9:1378:A:N1	2.29	0.54
51:AA:63:ARG:HG2	51:AA:185:MET:HE1	1.88	0.54
7:G:189:LEU:HD22	7:G:255:VAL:CG1	2.38	0.54
24:Y:55:VAL:HG13	24:Y:104:VAL:HG13	1.90	0.54
47:5:3810:C:O4'	47:5:3810:C:O2	2.25	0.54
6:F:153:ILE:HG22	6:F:186:MET:HE3	1.90	0.54
49:8:102:G:OP2	49:8:104:A:O2'	2.24	0.54
16:Q:67:ILE:HD12	16:Q:96:PRO:HD2	1.88	0.53
47:5:224:U:O2	47:5:224:U:O4'	2.26	0.53
50:9:1315:U:O2	50:9:1315:U:O4'	2.26	0.53
18:S:93:MET:HE3	18:S:113:MET:HE1	1.90	0.53
43:s:63:LYS:HG3	47:5:1960:A:C8	2.43	0.53
50:9:1139:C:O4'	50:9:1139:C:O2	2.24	0.53
1:A:207:VAL:HG11	47:5:1633:G:C6	2.44	0.53
47:5:4989:U:O2	47:5:4989:U:O4'	2.27	0.53
50:9:823:U:O4'	50:9:823:U:O2	2.26	0.53
54:DD:11:PHE:CZ	71:UU:84:ILE:HD11	2.43	0.53
11:L:7:GLY:O	26:a:49:HIS:NE2	2.39	0.53
54:DD:72:VAL:HG23	61:KK:20:VAL:HG21	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:FF:112:LEU:HD23	56:FF:112:LEU:C	2.34	0.53
26:a:12:ARG:NH2	47:5:1338:G:OP2	2.39	0.53
45:2:20:U:C4'	45:2:20(A):U:O2	2.56	0.53
50:9:501:C:O2	50:9:501:C:H2'	2.08	0.53
50:9:1137:U:N3	50:9:1148:A:N6	2.56	0.53
54:DD:70:THR:HG22	54:DD:86:LEU:HD13	1.90	0.53
45:2:20:U:O2'	45:2:20(A):U:O2'	2.26	0.53
47:5:2408:U:O4'	47:5:2409:U:C5	2.62	0.53
51:AA:63:ARG:CG	51:AA:185:MET:HE1	2.39	0.53
47:5:245:C:O4'	47:5:245:C:O2	2.25	0.52
82:ff:126:CYS:SG	82:ff:143:LYS:NZ	2.81	0.52
85:ii:324:GLU:C	85:ii:325:ASN:N	2.67	0.52
2:B:41:VAL:HA	2:B:187:GLY:HA3	1.91	0.52
2:B:252:ALA:HB1	47:5:4524:G:N3	2.25	0.52
50:9:1364:U:O4'	50:9:1364:U:O2	2.28	0.52
47:5:2265:G:O2'	47:5:2266:C:OP1	2.24	0.52
47:5:3724:A:N6	47:5:3725:G:C6	2.77	0.52
50:9:1653:U:H2'	50:9:1654:G:C8	2.45	0.52
5:E:180:GLY:O	5:E:181:PRO:C	2.52	0.52
45:2:74:C:OP2	47:5:4548:A:N3	2.43	0.52
53:CC:196:ILE:HB	53:CC:223:TYR:HB2	1.90	0.52
14:O:84:VAL:HG11	14:O:102:LEU:HD22	1.92	0.52
85:ii:144:SER:C	85:ii:145:LYS:N	2.68	0.52
37:l:16:LYS:HG3	37:l:49:LEU:HD21	1.92	0.52
40:o:41:TYR:CD1	46:3:75:C:O2	2.62	0.52
44:t:85:LEU:HD13	44:t:141:CYS:CB	2.40	0.52
50:9:1129:G:C6	50:9:1130:G:O6	2.63	0.52
12:M:51:PRO:HG2	12:M:54:CYS:SG	2.50	0.52
62:LL:60:CYS:SG	62:LL:63:THR:N	2.79	0.52
47:5:2733:C:H2'	47:5:2734:U:O4'	2.09	0.52
55:EE:44:LEU:HD13	55:EE:72:ILE:HD11	1.92	0.52
54:DD:21:LEU:HD21	54:DD:48:ILE:HD11	1.92	0.51
37:l:44:TRP:CH2	37:l:45:ARG:HD3	2.45	0.51
44:t:112:ILE:CG2	44:t:132:ILE:HD13	2.39	0.51
46:3:16:C:O2	46:3:16:C:O4'	2.24	0.51
50:9:92:A:C6	50:9:446:G:C6	2.97	0.51
58:HH:69:LEU:HG	58:HH:96:ALA:HB2	1.91	0.51
64:NN:125:LEU:HD22	64:NN:129:TYR:CE2	2.45	0.51
76:ZZ:99:LEU:HD23	76:ZZ:100:VAL:N	2.25	0.51
12:M:11:ARG:HD2	12:M:57:LEU:HD12	1.91	0.51
2:B:249:ARG:NH2	47:5:3845:A:OP2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:48:ARG:O	47:5:1883:G:O2'	2.26	0.51
47:5:2412:A:C2	47:5:2433:G:C2	2.99	0.51
50:9:887:U:O2	50:9:887:U:O4'	2.28	0.51
56:FF:99:ILE:HG23	76:ZZ:67:LEU:HD21	1.92	0.51
50:9:146:G:O2'	50:9:147:A:O5'	2.24	0.51
3:C:299:GLN:NE2	47:5:2089:G:OP1	2.44	0.51
12:M:15:VAL:HG22	12:M:50:MET:HE1	1.93	0.51
13:N:6:TYR:CZ	34:i:40:VAL:HG22	2.45	0.51
54:DD:21:LEU:CD2	54:DD:48:ILE:HD11	2.41	0.51
41:p:42:CYS:HA	47:5:2674:A:N6	2.26	0.51
47:5:1802:A:O2'	47:5:1837:A:OP1	2.28	0.51
74:XX:61:GLN:HB3	74:XX:62:PRO:CD	2.40	0.51
37:l:44:TRP:CZ3	37:l:45:ARG:HD3	2.46	0.51
49:8:125:C:O2	49:8:125:C:O4'	2.28	0.51
50:9:1680:G:H4'	79:cc:20:ARG:CD	2.31	0.51
73:WW:30:CYS:N	73:WW:59:GLY:O	2.44	0.51
50:9:1036:A:N3	50:9:1844:U:O2'	2.40	0.51
56:FF:89:THR:HA	56:FF:92:ILE:HD12	1.93	0.51
61:KK:64:TRP:CD2	80:dd:23:VAL:HG22	2.46	0.51
44:t:113:ALA:HB2	44:t:129:ILE:CG1	2.41	0.51
50:9:1272:C:O2'	50:9:1274:G:N2	2.44	0.51
59:II:117:TYR:CD1	59:II:156:ALA:HB2	2.45	0.51
3:C:316:LYS:NZ	47:5:1281:G:OP1	2.41	0.50
14:O:18:ARG:NH2	47:5:2057:A:OP1	2.44	0.50
47:5:4978:G:O2'	47:5:4980:C:OP2	2.19	0.50
45:2:20:U:C1'	45:2:20(A):U:C2	2.94	0.50
85:ii:183:GLY:O	85:ii:187:ALA:HB2	2.11	0.50
45:2:20:U:C5'	45:2:20(A):U:O2	2.60	0.50
50:9:1587:G:H1	70:TT:74:SER:HG	1.55	0.50
62:LL:37:TYR:CG	62:LL:51:ILE:HG12	2.46	0.50
63:MM:40:LYS:CE	82:ff:130:VAL:HG22	2.41	0.50
5:E:154:ILE:HB	5:E:198:ILE:HB	1.93	0.50
47:5:2763:U:O2	47:5:2763:U:O4'	2.29	0.50
47:5:3648:A:C4	47:5:3785:A:C6	2.99	0.50
73:WW:104:LEU:O	73:WW:104:LEU:HD12	2.12	0.50
22:W:9:SER:OG	22:W:36:CYS:SG	2.68	0.50
50:9:943:U:OP2	52:BB:216:LYS:NZ	2.40	0.50
85:ii:327:ASP:HB3	85:ii:348:PRO:HG3	1.93	0.50
15:P:127:ARG:NH2	47:5:2422:C:OP1	2.45	0.50
1:A:89:TYR:HB2	1:A:100:ASN:HD21	1.75	0.50
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:88:LEU:HD22	6:F:89:ALA:N	2.26	0.50
30:e:38:PRO:HD2	30:e:55:MET:HE3	1.93	0.50
47:5:1634:A:C6	47:5:1635:C:C4	2.99	0.50
47:5:2368:A:C2	47:5:2788:U:C5	3.00	0.50
47:5:3648:A:H1'	47:5:3785:A:N6	2.26	0.50
59:II:113:TYR:CE2	59:II:121:LEU:HD23	2.46	0.50
62:LL:120:VAL:HG22	62:LL:145:VAL:HG11	1.94	0.50
10:J:33:LEU:HD21	10:J:70:VAL:HB	1.94	0.50
25:Z:51:ARG:HB2	25:Z:65:ARG:HD2	1.94	0.50
85:ii:160:THR:HG23	85:ii:169:LEU:HD11	1.93	0.50
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.51	0.50
50:9:443:U:H2'	50:9:444:G:O4'	2.12	0.49
50:9:1444:U:O2'	50:9:1580:A:N1	2.44	0.49
50:9:1860:A:OP2	77:aa:10:ARG:NH2	2.42	0.49
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.47	0.49
4:D:56:THR:HG22	48:7:27:G:P	2.52	0.49
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.47	0.49
13:N:120:TRP:NE1	13:N:123:GLU:OE1	2.45	0.49
36:k:36:VAL:O	36:k:42:LEU:HD12	2.12	0.49
47:5:498:C:O2	47:5:498:C:O4'	2.27	0.49
50:9:1719:A:N6	50:9:1814:G:O2'	2.44	0.49
51:AA:89:LYS:HB3	51:AA:202:TYR:CZ	2.47	0.49
75:YY:15:ASN:HB2	75:YY:20:ARG:HG3	1.94	0.49
21:V:82:ILE:HG22	21:V:83:ARG:HG3	1.95	0.49
50:9:1714:U:H2'	50:9:1715:A:C8	2.47	0.49
64:NN:33:VAL:HG21	64:NN:66:VAL:HG11	1.93	0.49
66:PP:56:LEU:HD13	66:PP:78:THR:HG21	1.93	0.49
47:5:2439:G:C6	47:5:2440:U:C4	3.01	0.49
47:5:3653:A:N6	47:5:3691:G:O2'	2.46	0.49
53:CC:176:LYS:O	53:CC:200:ARG:NH1	2.45	0.49
44:t:85:LEU:HD13	44:t:141:CYS:SG	2.52	0.49
47:5:4525:C:H2'	47:5:4526:U:O4'	2.12	0.49
51:AA:180:ARG:HG2	51:AA:195:TRP:CE3	2.47	0.49
54:DD:98:ALA:HA	54:DD:188:ILE:HD12	1.94	0.49
5:E:167:PHE:CE1	5:E:176:LEU:HD22	2.48	0.49
13:N:76:PRO:O	13:N:79:ALA:HB3	2.12	0.49
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.43	0.49
47:5:3816:A:O2'	47:5:3819:G:N3	2.46	0.49
50:9:56:G:C6	50:9:57:U:C4	3.01	0.49
50:9:1298:G:C4	66:PP:79:HIS:CE1	3.00	0.49
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:209:VAL:HB	3:C:229:LEU:HD13	1.95	0.49
9:I:61:SER:HA	9:I:126:VAL:HG23	1.94	0.49
47:5:1311:G:H2'	47:5:1312:A:O4'	2.13	0.49
50:9:830:A:H2'	50:9:831:G:O4'	2.12	0.49
73:WW:52:ILE:HG22	73:WW:61:ILE:HG12	1.95	0.49
50:9:314:U:O2	50:9:314:U:H2'	2.13	0.49
50:9:439:A:O2'	50:9:1799:G:H4'	2.13	0.49
74:XX:51:VAL:HG13	74:XX:70:VAL:CG1	2.42	0.49
47:5:4236:G:C2	47:5:4289:U:O2	2.65	0.49
59:II:36:THR:HG21	59:II:179:PRO:HB2	1.95	0.49
15:P:54:LYS:HA	15:P:83:TRP:CD1	2.47	0.49
47:5:1662:C:H2'	47:5:1663:C:C6	2.48	0.49
50:9:853:C:O4'	50:9:853:C:O2	2.26	0.49
51:AA:161:ILE:HG22	51:AA:163:CYS:SG	2.53	0.49
75:YY:56:PHE:CD1	75:YY:94:HIS:NE2	2.81	0.49
3:C:95:MET:SD	3:C:95:MET:N	2.74	0.48
50:9:1700:C:C2	50:9:1834:A:N6	2.80	0.48
32:g:29:ARG:NH1	47:5:2522:G:OP2	2.45	0.48
47:5:2367:A:C2	47:5:2788:U:O4	2.58	0.48
50:9:1020:A:N7	64:NN:70:LYS:NZ	2.60	0.48
69:SS:43:VAL:HG21	69:SS:83:PHE:CZ	2.48	0.48
50:9:1667:U:H2'	50:9:1668:U:C6	2.48	0.48
51:AA:162:PRO:C	51:AA:163:CYS:SG	2.96	0.48
55:EE:139:LEU:HD12	55:EE:150:PRO:HB3	1.95	0.48
47:5:2009:A:C8	85:ii:415:TYR:CD2	3.01	0.48
70:TT:39:LEU:HD13	70:TT:47:PRO:CG	2.44	0.48
79:cc:20:ARG:HH11	79:cc:28:THR:CG2	2.21	0.48
7:G:139:VAL:HG11	7:G:238:LYS:HG3	1.96	0.48
13:N:158:HIS:HB3	13:N:161:MET:HG2	1.95	0.48
50:9:67:C:C6	57:GG:162:LEU:HD23	2.48	0.48
50:9:1587:G:N1	70:TT:74:SER:OG	2.43	0.48
58:HH:134:VAL:HG12	58:HH:173:PHE:CE2	2.49	0.48
83:gg:4:GLN:C	83:gg:5:MET:HE2	2.38	0.48
47:5:1960:A:C8	47:5:1960:A:OP1	2.67	0.48
47:5:4723:A:C2	47:5:4724:A:C6	3.02	0.48
56:FF:14:THR:HG23	56:FF:14:THR:O	2.14	0.48
3:C:116:ASN:O	3:C:120:LYS:HG3	2.13	0.48
37:l:2:SER:N	47:5:2406:G:N7	2.61	0.48
47:5:1986:U:H2'	47:5:2007:G:C6	2.48	0.48
47:5:1990:A:H3'	47:5:1991:A:H5''	1.96	0.48
4:D:39:GLN:OE1	4:D:43:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:R:70:ARG:HE	17:R:75:HIS:HB2	1.79	0.48
32:g:46:CYS:SG	32:g:47:GLY:N	2.87	0.48
47:5:3652:A:C2	47:5:3653:A:N1	2.82	0.48
50:9:4:C:O2'	60:JJ:18:ARG:NH1	2.46	0.48
50:9:1228:A:H2'	50:9:1229:G:C8	2.47	0.48
58:HH:145:ARG:HA	73:WW:51:GLU:HB2	1.95	0.48
47:5:3723:A:C2	47:5:3724:A:C6	3.01	0.48
50:9:1551:U:O2	50:9:1551:U:O4'	2.30	0.48
6:F:131:MET:O	6:F:134:ILE:HG22	2.14	0.47
26:a:59:ARG:NH2	26:a:61:TYR:OH	2.46	0.47
28:c:64:ALA:O	28:c:68:LYS:N	2.47	0.47
42:r:10:VAL:O	42:r:12:ASN:N	2.47	0.47
47:5:1352:C:H2'	47:5:1353:G:O4'	2.14	0.47
50:9:846:G:H2'	55:EE:19:MET:HE2	1.96	0.47
50:9:1707:U:H2'	50:9:1708:C:O4'	2.14	0.47
55:EE:18:TRP:CE3	55:EE:46:ILE:CD1	2.97	0.47
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.95	0.47
21:V:99:GLU:HB3	22:W:24:THR:HG23	1.96	0.47
79:cc:20:ARG:O	79:cc:21:THR:HG23	2.14	0.47
10:J:27:GLY:HA2	10:J:68:ILE:HG23	1.95	0.47
45:2:74:C:OP2	47:5:4548:A:C4	2.66	0.47
47:5:1590:C:H3'	47:5:1591:U:H4'	1.96	0.47
58:HH:118:ARG:O	58:HH:121:THR:HG22	2.15	0.47
80:dd:15:GLY:O	80:dd:18:SER:OG	2.27	0.47
8:H:134:CYS:SG	8:H:135:SER:N	2.88	0.47
50:9:1624:U:O2	50:9:1624:U:O4'	2.32	0.47
48:7:16:A:C2	48:7:64:G:C2	3.02	0.47
50:9:1834:A:H2'	50:9:1834:A:N3	2.29	0.47
51:AA:147:LEU:HD13	51:AA:161:ILE:HB	1.96	0.47
14:O:51:LYS:O	14:O:55:LEU:HG	2.14	0.47
44:t:77:ALA:HB1	44:t:132:ILE:HG12	1.97	0.47
44:t:131:GLU:HB2	47:5:1973:G:H1'	1.96	0.47
47:5:957:G:N7	47:5:958:G:C6	2.83	0.47
47:5:1237:C:O4'	47:5:1237:C:O2	2.33	0.47
47:5:1667:A:N1	47:5:2281:U:OP2	2.48	0.47
47:5:1840:G:O2'	47:5:1841:C:H5'	2.14	0.47
47:5:2268:A:H4'	47:5:2269:C:H5'	1.96	0.47
47:5:3696:C:C4	47:5:3697:U:C4	3.03	0.47
47:5:3723:A:H2'	47:5:3724:A:C8	2.49	0.47
50:9:944:A:C5	50:9:945:U:C5	3.03	0.47
50:9:1012:A:H2'	50:9:1013:U:O4'	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:DD:162:ASP:N	54:DD:163:PRO:CD	2.78	0.47
3:C:76:ILE:HG22	3:C:77:PRO:HD2	1.96	0.47
26:a:121:PRO:HA	26:a:141:GLY:O	2.15	0.47
30:e:44:ARG:HD2	47:5:1315:C:OP2	2.14	0.47
44:t:100:HIS:CD2	44:t:139:VAL:O	2.68	0.47
50:9:1834:A:C2	50:9:1836:G:C4	3.03	0.47
62:LL:80:MET:HE1	62:LL:121:GLN:HA	1.97	0.47
14:O:68:ARG:NH2	47:5:4564:A:OP1	2.48	0.47
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.97	0.47
53:CC:166:ARG:HB2	53:CC:248:TYR:CG	2.49	0.47
65:OO:98:ARG:NH1	65:OO:99:ALA:O	2.48	0.47
83:gg:173:LEU:HD22	83:gg:189:ILE:HG12	1.97	0.47
12:M:34:ASN:N	12:M:34:ASN:OD1	2.48	0.47
44:t:106:PHE:HE2	44:t:159:ALA:HB3	1.80	0.47
47:5:1804:A:N6	47:5:1833:G:O4'	2.47	0.47
50:9:1190:A:H2'	50:9:1191:C:O4'	2.14	0.47
74:XX:82:THR:O	74:XX:118:VAL:HG13	2.15	0.47
53:CC:66:LEU:C	53:CC:66:LEU:HD13	2.40	0.46
74:XX:105:PHE:CG	74:XX:112:VAL:HG21	2.50	0.46
76:ZZ:83:LEU:C	76:ZZ:83:LEU:HD13	2.40	0.46
2:B:378:ARG:HD3	22:W:11:TYR:CD2	2.50	0.46
8:H:18:ILE:HG22	8:H:27:VAL:HG22	1.98	0.46
13:N:198:LEU:HD13	13:N:200:LEU:HD21	1.97	0.46
31:f:11:PHE:CE1	31:f:26:ALA:HB1	2.50	0.46
63:MM:17:ALA:C	63:MM:124:ILE:HD11	2.40	0.46
85:ii:327:ASP:HB3	85:ii:348:PRO:CG	2.45	0.46
11:L:60:ARG:NH1	11:L:70:VAL:HG22	2.30	0.46
47:5:2035:C:C4	47:5:2036:C:C4	3.04	0.46
47:5:3749:C:C5	47:5:3750:G:C8	3.03	0.46
49:8:10:G:C6	49:8:11:C:C4	3.02	0.46
50:9:183:G:O2'	50:9:183:G:N3	2.48	0.46
50:9:1190:A:N3	50:9:1714:U:O2'	2.44	0.46
50:9:1303:C:O2	50:9:1303:C:O4'	2.30	0.46
50:9:1530:U:H2'	50:9:1531:A:O4'	2.15	0.46
50:9:1834:A:N3	50:9:1834:A:C2'	2.78	0.46
16:Q:13:VAL:HG23	47:5:1691:G:C8	2.50	0.46
40:o:54:PRO:HB3	47:5:4379:A:C8	2.51	0.46
40:o:104:ILE:HG21	45:2:56:C:N4	2.30	0.46
50:9:584:A:C6	50:9:585:C:C4	3.03	0.46
50:9:1046:U:H2'	50:9:1047:C:O4'	2.15	0.46
14:O:43:ILE:HD11	14:O:138:LEU:HD13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:1978:C:H3'	47:5:1979:A:H5''	1.97	0.46
51:AA:63:ARG:HE	72:VV:78:ILE:HG23	1.80	0.46
58:HH:30:LEU:HD22	58:HH:82:GLU:HG2	1.97	0.46
50:9:1581:C:OP2	50:9:1582:C:N4	2.47	0.46
4:D:207:TYR:CE1	48:7:33:U:C6	3.04	0.46
6:F:97:ILE:HD11	16:Q:4:ASP:CG	2.41	0.46
6:F:168:LEU:HB2	6:F:186:MET:HE1	1.97	0.46
18:S:164:LYS:HB3	18:S:165:PRO:CD	2.45	0.46
47:5:716:C:H2'	47:5:717:U:O4'	2.16	0.46
47:5:1337:A:C2	47:5:2349:A:C2	3.04	0.46
47:5:3621:A:H2'	47:5:3622:C:O4'	2.16	0.46
53:CC:130:ILE:HG22	53:CC:158:ALA:HB1	1.96	0.46
56:FF:116:ILE:HD12	56:FF:151:ILE:HG13	1.98	0.46
44:t:98:ILE:HG23	44:t:98:ILE:O	2.16	0.46
47:5:1612:G:C2'	47:5:1612:G:N3	2.79	0.46
47:5:1889:U:O4	47:5:1939:A:N6	2.49	0.46
55:EE:67:GLN:HB3	55:EE:69:PHE:CZ	2.50	0.46
74:XX:4:CYS:O	74:XX:4:CYS:SG	2.74	0.46
74:XX:67:ARG:NH2	74:XX:114:ASP:OD2	2.49	0.46
2:B:257:TRP:CE2	47:5:4518:A:N7	2.84	0.46
17:R:23:TRP:CH2	17:R:25:ASP:HA	2.51	0.46
18:S:9:GLU:HB3	18:S:67:VAL:HG13	1.98	0.46
21:V:13:LYS:O	47:5:4617:G:O2'	2.33	0.46
28:c:29:LEU:HD23	28:c:94:LEU:HD13	1.97	0.46
31:f:80:ASN:OD1	47:5:2065:G:O2'	2.34	0.46
37:l:15:LYS:NZ	49:8:46:G:OP2	2.38	0.46
47:5:4966:A:H2'	47:5:4967:A:C8	2.51	0.46
50:9:980:A:C2	50:9:981:A:C6	3.04	0.46
4:D:68:ARG:HG3	4:D:73:MET:HE2	1.97	0.46
4:D:271:MET:HE2	4:D:275:GLN:HB3	1.98	0.46
14:O:18:ARG:HH11	47:5:2054:U:P	2.39	0.46
14:O:144:GLU:OE2	47:5:4681:A:O2'	2.24	0.46
47:5:2744:A:C6	47:5:2745:A:C6	3.04	0.46
49:8:10:G:C5	49:8:11:C:C5	3.03	0.46
50:9:17:C:H2'	50:9:18:C:C6	2.50	0.46
50:9:168:C:OP1	57:GG:131:ARG:NH2	2.49	0.46
50:9:1021:U:O4'	50:9:1022:U:C2	2.69	0.46
57:GG:41:LEU:C	57:GG:41:LEU:HD22	2.41	0.46
4:D:31:TYR:CE1	4:D:35:ARG:NH2	2.84	0.45
13:N:108:ARG:NH2	47:5:54:G:O2'	2.47	0.45
23:X:65:ALA:HB2	33:h:69:LEU:HD11	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:33:ILE:HD11	29:d:41:ARG:HB3	1.97	0.45
44:t:129:ILE:CD1	44:t:160:VAL:HG22	2.47	0.45
52:BB:30:TRP:CH2	52:BB:48:LEU:HD23	2.51	0.45
59:II:11:ARG:NH1	59:II:15:GLY:O	2.49	0.45
68:RR:31:ASN:C	68:RR:31:ASN:HD22	2.24	0.45
68:RR:53:TYR:CE2	68:RR:57:LEU:HD11	2.52	0.45
30:e:23:HIS:HA	30:e:53:ILE:HD12	1.96	0.45
33:h:84:ARG:HB3	33:h:85:PRO:HD2	1.98	0.45
39:n:13:LEU:HD12	39:n:17:ARG:CZ	2.46	0.45
47:5:4232:U:H4'	47:5:4233:A:O5'	2.17	0.45
50:9:874:G:N2	50:9:875:A:C4	2.84	0.45
50:9:1149:A:N3	50:9:1149:A:H2'	2.32	0.45
54:DD:48:ILE:HG23	54:DD:86:LEU:HD12	1.98	0.45
79:cc:46:VAL:HG11	79:cc:50:VAL:CG2	2.46	0.45
85:ii:305:VAL:HG13	85:ii:328:ILE:HD13	1.98	0.45
18:S:95:ARG:NH2	47:5:1951:G:O2'	2.48	0.45
47:5:4724:A:C6	47:5:4725:C:C4	3.04	0.45
47:5:4758:U:O2	47:5:4758:U:O4'	2.33	0.45
54:DD:211:VAL:HG22	68:RR:38:ILE:O	2.17	0.45
56:FF:97:PHE:CD2	56:FF:108:PRO:HB2	2.51	0.45
47:5:1960:A:H4'	47:5:1961:G:OP2	2.17	0.45
4:D:40:ASP:OD1	4:D:40:ASP:N	2.50	0.45
14:O:168:TYR:CE2	14:O:172:LYS:HD2	2.50	0.45
40:o:41:TYR:CE1	46:3:75:C:O2	2.70	0.45
47:5:4510:A:C6	47:5:4511:A:C2	3.04	0.45
52:BB:69:VAL:HG11	52:BB:74:LEU:HD13	1.99	0.45
7:G:207:LEU:HD23	7:G:208:VAL:N	2.31	0.45
11:L:116:ARG:NH1	11:L:155:MET:O	2.50	0.45
30:e:103:VAL:O	30:e:108:ARG:NH2	2.49	0.45
47:5:419:A:C6	47:5:420:A:C6	3.05	0.45
47:5:4238:G:H2'	47:5:4239:A:C8	2.51	0.45
47:5:4966:A:C2	47:5:4967:A:C2	3.05	0.45
50:9:442:C:C2	50:9:452:G:N2	2.85	0.45
50:9:658:U:O4	50:9:1165:G:H2'	2.17	0.45
50:9:1543:U:OP2	70:TT:62:ARG:NH1	2.49	0.45
56:FF:20:PHE:CD1	56:FF:20:PHE:C	2.94	0.45
2:B:11:HIS:NE2	47:5:4458:C:OP1	2.50	0.45
47:5:1964:A:N7	47:5:4694:G:C4	2.84	0.45
50:9:980:A:O2'	50:9:981:A:O4'	2.31	0.45
50:9:1661:A:C8	80:dd:14:PHE:CD1	3.05	0.45
74:XX:57:VAL:HG11	74:XX:115:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:60:TRP:CD2	18:S:153:PRO:CD	3.00	0.45
17:R:60:ARG:NH1	17:R:63:CYS:SG	2.90	0.45
29:d:48:GLU:N	29:d:48:GLU:OE1	2.50	0.45
29:d:118:GLN:OE1	47:5:5055:G:N2	2.48	0.45
47:5:2363:A:C2	47:5:3860:A:C4	3.05	0.45
47:5:4398:C:OP1	85:ii:189:ARG:CZ	2.65	0.45
47:5:4398:C:P	85:ii:189:ARG:HH22	2.39	0.45
50:9:1045:U:H2'	50:9:1046:U:O4'	2.16	0.45
50:9:1374:C:O2'	50:9:1464:C:O2	2.34	0.45
50:9:1742:C:H2'	50:9:1743:G:O4'	2.17	0.45
65:OO:116:LEU:HD22	77:aa:53:ILE:CD1	2.47	0.45
85:ii:305:VAL:HG11	85:ii:328:ILE:HD13	1.98	0.45
2:B:160:ILE:HD12	2:B:190:VAL:HG13	1.98	0.45
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.52	0.45
47:5:1387:A:C6	47:5:1397:A:C8	3.04	0.45
47:5:4390:A:H2'	47:5:4391:G:O4'	2.17	0.45
50:9:183:G:N3	50:9:183:G:C2'	2.79	0.45
59:II:99:ASN:HA	59:II:174:CYS:SG	2.56	0.45
15:P:24:VAL:HG23	15:P:144:CYS:SG	2.57	0.45
26:a:61:TYR:N	47:5:4354:U:O4	2.50	0.45
45:2:20:U:C5'	45:2:20(A):U:C2	3.00	0.45
47:5:2088:A:O2'	47:5:2089:G:OP2	2.28	0.45
47:5:4744:A:N1	47:5:4956:A:N1	2.64	0.45
50:9:1610:G:OP2	69:SS:132:ARG:NH1	2.48	0.45
83:gg:87:LEU:HD21	83:gg:108:VAL:HG11	1.99	0.45
47:5:1669:A:N3	47:5:1852:U:O2'	2.47	0.44
47:5:3829:G:C2	47:5:3830:A:C8	3.05	0.44
50:9:363:A:N1	50:9:397:G:O2'	2.45	0.44
50:9:932:G:C2'	50:9:934:G:OP2	2.65	0.44
50:9:973:C:C5	50:9:974:C:C5	3.05	0.44
50:9:1130:G:O2'	50:9:1131:G:P	2.75	0.44
50:9:1605:G:C6	50:9:1606:G:N1	2.85	0.44
51:AA:145:ILE:HG12	51:AA:159:ILE:CG2	2.47	0.44
44:t:116:MET:CG	44:t:132:ILE:HD11	2.47	0.44
47:5:1986:U:N3	47:5:2013:A:N6	2.65	0.44
50:9:378:U:H2'	50:9:379:C:O4'	2.17	0.44
50:9:1735:A:C4	50:9:1800:A:C2	3.04	0.44
2:B:84:MET:HE1	2:B:183:ILE:HD11	1.99	0.44
3:C:73:VAL:O	47:5:2350:U:C5	2.70	0.44
20:U:63:LEU:HD23	20:U:64:GLU:N	2.32	0.44
26:a:12:ARG:NH1	47:5:2345:G:OP2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:1869:G:C4	47:5:3877:A:C2	3.05	0.44
47:5:2006:U:C4	47:5:2007:G:C8	3.05	0.44
47:5:4212:A:C2	47:5:4218:U:C5	3.05	0.44
50:9:846:G:C8	55:EE:19:MET:HE1	2.52	0.44
57:GG:5:ILE:HD12	57:GG:16:ILE:HD13	1.98	0.44
58:HH:122:LEU:C	58:HH:122:LEU:HD13	2.42	0.44
59:II:80:ASP:OD1	59:II:81:VAL:N	2.51	0.44
2:B:234:ARG:NH2	47:5:4566:U:O2'	2.50	0.44
2:B:249:ARG:N	47:5:2838:G:OP1	2.42	0.44
4:D:23:ARG:NH2	47:5:4280:A:OP2	2.48	0.44
44:t:81:ILE:HG21	44:t:136:ALA:CA	2.48	0.44
44:t:109:ILE:HG22	44:t:129:ILE:HG23	2.00	0.44
45:2:20:U:N1	45:2:20(A):U:N1	2.64	0.44
47:5:4635:A:C2	47:5:4664:A:C5	3.05	0.44
47:5:4759:C:O4'	47:5:4759:C:O2	2.36	0.44
50:9:360:A:C2	50:9:363:A:C8	3.05	0.44
2:B:317:LEU:HD21	2:B:381:THR:HA	1.99	0.44
13:N:64:ILE:HD11	13:N:102:ALA:HA	1.99	0.44
30:e:47:ARG:NH1	47:5:1883:G:OP1	2.51	0.44
47:5:2841:G:H3'	47:5:2842:G:H5''	2.00	0.44
62:LL:11:GLN:C	62:LL:56:ILE:HD12	2.42	0.44
1:A:90:CYS:HB2	1:A:101:VAL:HG13	1.99	0.44
10:J:24:ILE:HG21	10:J:36:ALA:HB1	2.00	0.44
12:M:24:LEU:HD11	12:M:86:TRP:CD2	2.52	0.44
47:5:2428:A:C6	47:5:2789:A:C5	3.05	0.44
49:8:94:G:H5'	49:8:94:G:C8	2.52	0.44
50:9:302:A:H1'	59:II:73:THR:HG23	2.00	0.44
50:9:1678:A:C6	50:9:1679:A:N6	2.86	0.44
26:a:117:LEU:HD12	26:a:118:PRO:HD2	2.00	0.44
38:m:70:CYS:SG	38:m:72:LYS:N	2.89	0.44
47:5:2397:G:C8	47:5:2399:G:C8	3.05	0.44
50:9:5:U:C2	50:9:20:G:N2	2.86	0.44
58:HH:61:ILE:HD11	58:HH:95:ILE:HD12	1.98	0.44
59:II:113:TYR:OH	59:II:156:ALA:O	2.34	0.44
72:VV:55:ILE:HD11	72:VV:69:ILE:HG12	1.99	0.44
30:e:38:PRO:HB2	30:e:43:ASN:ND2	2.33	0.44
47:5:1632:A:H2'	47:5:1632:A:N3	2.33	0.44
50:9:26:U:C2	50:9:27:A:C8	3.06	0.44
50:9:1130:G:O2'	50:9:1131:G:O5'	2.35	0.44
47:5:1174:G:C2'	47:5:1175:A:O5'	2.66	0.44
47:5:1965:G:H4'	47:5:4695:C:H1'	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:2625:U:C4	47:5:2626:U:C4	3.06	0.44
50:9:16:G:H2'	50:9:17:C:C6	2.52	0.44
50:9:448:A:C2	59:II:26:LYS:HG3	2.53	0.44
50:9:943:U:H2'	50:9:944:A:O4'	2.18	0.44
21:V:30:ASP:N	21:V:30:ASP:OD1	2.50	0.43
25:Z:14:LEU:HD22	25:Z:81:MET:HB2	2.00	0.43
33:h:81:LEU:HD23	33:h:84:ARG:HD2	1.99	0.43
47:5:1089:G:C4	47:5:1208:G:N2	2.86	0.43
47:5:1964:A:N7	47:5:4694:G:C5	2.86	0.43
47:5:2046:G:O2'	47:5:2047:A:OP2	2.34	0.43
47:5:2090:U:C4	47:5:2265:G:C5	3.05	0.43
50:9:824:C:C2	60:JJ:144:ILE:HD13	2.52	0.43
63:MM:22:LEU:HD13	63:MM:22:LEU:C	2.43	0.43
69:SS:59:LEU:HD12	69:SS:63:GLU:OE2	2.18	0.43
83:gg:220:ASP:HB2	83:gg:227:LEU:HD21	1.99	0.43
4:D:95:TYR:O	4:D:96:ALA:C	2.60	0.43
16:Q:33:ARG:HG2	16:Q:48:LEU:HD11	1.99	0.43
47:5:1563:A:O2'	47:5:1564:A:O4'	2.36	0.43
47:5:1907:A:N6	47:5:1908:A:N1	2.66	0.43
47:5:4288:C:O2'	47:5:4321:U:OP1	2.32	0.43
50:9:600:G:C2	50:9:601:G:C8	3.06	0.43
50:9:1673:U:H2'	50:9:1674:G:O4'	2.17	0.43
60:JJ:136:ARG:NH1	60:JJ:159:PHE:O	2.47	0.43
79:cc:46:VAL:HG11	79:cc:50:VAL:HG21	2.00	0.43
3:C:43:ASN:O	3:C:46:LYS:HB2	2.19	0.43
47:5:4871:C:O2	47:5:4871:C:O4'	2.36	0.43
53:CC:88:ILE:HG21	53:CC:94:ILE:CD1	2.48	0.43
60:JJ:146:SER:O	60:JJ:147:PHE:C	2.61	0.43
84:hh:49:U:O2	85:ii:62:ILE:HA	2.19	0.43
4:D:42:ASN:HD21	19:T:69:GLN:NE2	2.16	0.43
14:O:48:TYR:CD2	47:5:1930:U:C6	3.06	0.43
16:Q:67:ILE:HD13	16:Q:98:LEU:HD11	1.99	0.43
26:a:109:TYR:CD2	26:a:127:LYS:HD3	2.54	0.43
26:a:134:GLU:O	26:a:138:LYS:HG2	2.19	0.43
47:5:2094:C:O2	47:5:2094:C:O4'	2.33	0.43
53:CC:191:VAL:HG11	53:CC:236:PHE:HA	2.01	0.43
16:Q:186:TYR:CD2	47:5:4307:A:H4'	2.54	0.43
20:U:27:HIS:N	20:U:28:PRO:HD2	2.34	0.43
43:s:63:LYS:CG	47:5:1960:A:C8	3.02	0.43
44:t:143:VAL:HG12	44:t:143:VAL:O	2.18	0.43
47:5:2640:G:N2	47:5:2641:A:N3	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:2786:C:H5'	47:5:2787:A:C8	2.54	0.43
50:9:1096:G:C6	50:9:1097:G:C5	3.06	0.43
52:BB:52:THR:HG23	52:BB:57:ILE:HA	2.01	0.43
60:JJ:130:ILE:HG12	60:JJ:135:ILE:HD11	2.01	0.43
3:C:33:ARG:HD2	3:C:36:ILE:HD12	2.00	0.43
4:D:225:GLN:OE1	4:D:225:GLN:N	2.52	0.43
9:I:153:ARG:HA	9:I:165:ILE:HD11	2.00	0.43
14:O:122:ALA:HB2	18:S:162:GLN:HB3	1.99	0.43
30:e:124:ASN:N	30:e:124:ASN:OD1	2.52	0.43
44:t:81:ILE:HD12	44:t:135:THR:OG1	2.15	0.43
47:5:1330:A:C6	47:5:1331:C:C4	3.06	0.43
47:5:3867:A:C6	47:5:3868:G:C6	3.07	0.43
47:5:4640:C:C4	47:5:4641:U:C4	3.07	0.43
47:5:4714:C:C5	47:5:4715:C:C5	3.07	0.43
47:5:4729:A:O4'	47:5:4966:A:C8	2.72	0.43
50:9:1123:C:C4	50:9:1124:C:C5	3.07	0.43
50:9:1207:G:C6	50:9:1837:G:C6	3.06	0.43
79:cc:14:VAL:HG13	79:cc:30:VAL:HG13	2.01	0.43
2:B:29:VAL:HG13	2:B:348:ARG:HD3	2.01	0.43
6:F:92:ILE:HG21	6:F:246:MET:HE1	2.00	0.43
7:G:96:GLN:O	47:5:4124:G:N2	2.51	0.43
10:J:18:ARG:HG3	10:J:135:GLY:HA3	2.01	0.43
13:N:115:VAL:HG22	13:N:134:LEU:HD21	2.01	0.43
35:j:18:LEU:HD11	37:l:51:LEU:HD21	2.00	0.43
41:p:4:ARG:NH1	47:5:1554:A:OP2	2.52	0.43
42:r:60:VAL:HG22	42:r:117:ILE:HG21	2.01	0.43
46:3:75:C:O2	46:3:75:C:O4'	2.32	0.43
73:WW:111:MET:HE3	73:WW:116:ALA:HA	2.00	0.43
83:gg:299:PHE:CD2	83:gg:309:VAL:HG12	2.53	0.43
85:ii:200:ASN:C	85:ii:200:ASN:HD22	2.26	0.43
1:A:175:ILE:HD12	1:A:176:ASP:N	2.34	0.43
3:C:204:ARG:NH1	3:C:205:ARG:O	2.52	0.43
25:Z:76:ASN:HB3	25:Z:78:ASN:OD1	2.19	0.43
29:d:39:LYS:NZ	47:5:2370:A:N7	2.64	0.43
35:j:13:ASN:OD1	35:j:13:ASN:N	2.49	0.43
35:j:33:THR:HG22	35:j:40:PRO:HG2	1.99	0.43
47:5:1291:G:O2'	47:5:1292:C:OP1	2.27	0.43
74:XX:51:VAL:HG22	74:XX:70:VAL:HG11	2.01	0.43
2:B:261:ARG:HB2	14:O:64:THR:HG21	2.01	0.43
3:C:128:LEU:O	3:C:131:SER:OG	2.23	0.43
7:G:241:ALA:O	7:G:245:ARG:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:33:ILE:HD12	20:U:96:LEU:HD22	2.01	0.43
47:5:1381:U:O2	47:5:1381:U:O4'	2.36	0.43
50:9:86:C:N4	50:9:87:U:C4	2.87	0.43
50:9:1298:G:O2'	50:9:1299:A:O5'	2.37	0.43
50:9:1718:G:C6	50:9:1814:G:C6	3.07	0.43
56:FF:88:MET:CE	56:FF:92:ILE:HD11	2.48	0.43
57:GG:61:PHE:CE1	57:GG:96:SER:HB3	2.54	0.43
66:PP:103:ASN:HB2	66:PP:120:SER:HB2	2.00	0.43
73:WW:55:ASP:O	73:WW:57:ARG:N	2.52	0.43
84:hh:54:U:O2	84:hh:54:U:C2'	2.67	0.43
7:G:214:VAL:HG23	47:5:150:U:C4	2.54	0.43
8:H:7:ASN:OD1	8:H:7:ASN:N	2.52	0.43
12:M:80:ALA:O	12:M:85:LYS:NZ	2.52	0.43
13:N:11:TRP:CE3	13:N:44:ARG:NH2	2.87	0.43
29:d:64:ILE:HD11	29:d:68:LEU:CD2	2.49	0.43
47:5:1786:A:O2'	47:5:1788:A:OP2	2.34	0.43
47:5:4423:U:O2	47:5:4423:U:O4'	2.35	0.43
50:9:1144:A:H2'	50:9:1145:A:C8	2.54	0.43
80:dd:24:CYS:SG	80:dd:42:CYS:SG	3.13	0.43
2:B:56:ILE:HG22	2:B:74:GLU:HB3	2.01	0.42
13:N:65:ARG:HD3	13:N:127:TYR:CD1	2.54	0.42
14:O:9:LEU:O	14:O:36:VAL:HG12	2.19	0.42
27:b:17:HIS:NE2	27:b:21:ILE:HD12	2.34	0.42
44:t:15:LEU:HD13	44:t:28:LEU:HD22	2.01	0.42
56:FF:50:PRO:HG2	56:FF:90:VAL:HG13	2.01	0.42
57:GG:108:VAL:HG12	57:GG:109:LEU:N	2.33	0.42
79:cc:46:VAL:HG12	79:cc:47:LYS:O	2.19	0.42
5:E:164:ARG:HD2	5:E:273:TYR:CZ	2.53	0.42
11:L:169:ILE:HD11	26:a:123:ILE:HG13	2.00	0.42
29:d:64:ILE:HD11	29:d:68:LEU:HD23	2.01	0.42
50:9:92:A:O4'	55:EE:3:ARG:NH1	2.52	0.42
50:9:688:U:O2	58:HH:122:LEU:HG	2.19	0.42
50:9:1407:U:O2	50:9:1408:U:C2	2.72	0.42
63:MM:63:LYS:HD2	82:ff:108:VAL:HG21	2.01	0.42
68:RR:5:ARG:HB2	68:RR:10:LYS:HE2	2.01	0.42
83:gg:254:PRO:HA	83:gg:285:GLN:HA	2.00	0.42
12:M:122:ILE:HD13	14:O:189:ILE:HG22	2.01	0.42
13:N:93:LYS:NZ	47:5:4177:C:OP1	2.47	0.42
20:U:84:LYS:HA	20:U:87:THR:HG22	2.00	0.42
45:2:20:U:H5'	45:2:20(A):U:O2	2.19	0.42
47:5:737:C:C2	47:5:927:G:C2	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:1818:G:O2'	47:5:1819:G:OP1	2.21	0.42
47:5:2097:A:OP1	47:5:2107:A:N6	2.52	0.42
47:5:4075:U:O2'	47:5:4076:G:P	2.77	0.42
50:9:1395:C:O2'	50:9:1396:A:OP1	2.33	0.42
50:9:1518:C:O4'	50:9:1518:C:O2	2.35	0.42
53:CC:209:VAL:HG21	53:CC:233:LEU:HD13	2.01	0.42
55:EE:31:PRO:HG3	55:EE:43:PRO:HG3	2.01	0.42
60:JJ:114:VAL:HG21	60:JJ:135:ILE:CD1	2.49	0.42
75:YY:25:ILE:N	75:YY:71:GLY:O	2.52	0.42
85:ii:120:ILE:HG22	85:ii:139:LEU:HD13	2.01	0.42
2:B:315:ASN:OD1	2:B:326:VAL:N	2.52	0.42
6:F:88:LEU:HD21	6:F:121:PHE:CD1	2.54	0.42
11:L:77:SER:HB3	11:L:80:GLU:CD	2.44	0.42
47:5:974:C:C4	47:5:975:C:C4	3.08	0.42
47:5:1668:A:C4	47:5:2282:A:C2	3.07	0.42
47:5:4378:A:O2'	47:5:4379:A:H2'	2.20	0.42
29:d:68:LEU:HA	29:d:108:TYR:HB2	2.02	0.42
35:j:2:THR:O	35:j:7:SER:OG	2.29	0.42
44:t:109:ILE:HD13	44:t:133:LEU:CD1	2.49	0.42
47:5:1089:G:C2	47:5:1208:G:C2	3.07	0.42
47:5:1328:G:C6	47:5:1329:G:C6	3.08	0.42
50:9:1459:G:C6	50:9:1460:C:C4	3.07	0.42
1:A:179:ILE:O	1:A:180:LEU:C	2.62	0.42
6:F:189:LEU:HD23	6:F:189:LEU:O	2.19	0.42
7:G:111:PRO:CD	23:X:46:PHE:HD2	2.33	0.42
18:S:158:VAL:HG13	18:S:158:VAL:O	2.18	0.42
26:a:65:ARG:NH2	47:5:84:A:OP2	2.53	0.42
40:o:41:TYR:CG	46:3:75:C:O2	2.72	0.42
44:t:81:ILE:HD11	44:t:132:ILE:HG23	2.00	0.42
47:5:297:U:C2	47:5:298:G:C8	3.06	0.42
47:5:481(A):C:O2	47:5:481(A):C:O4'	2.38	0.42
47:5:2013:A:N3	47:5:2014:C:C6	2.88	0.42
52:BB:71:LEU:HD12	52:BB:82:ARG:HB3	2.02	0.42
57:GG:18:VAL:HG21	57:GG:41:LEU:HD23	2.01	0.42
64:NN:110:ASP:O	64:NN:114:ARG:HG2	2.20	0.42
2:B:94:GLU:HB2	2:B:158:GLN:HG3	2.02	0.42
2:B:220:ILE:HG12	2:B:278:THR:HG23	2.02	0.42
6:F:89:ALA:HB2	6:F:124:LEU:HD21	2.01	0.42
29:d:19:GLU:O	29:d:90:ARG:NH2	2.50	0.42
29:d:46:LEU:CD2	29:d:72:VAL:HG11	2.50	0.42
47:5:1957:U:O4	47:5:2026:A:N1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:4305:G:N3	47:5:4305:G:C2'	2.82	0.42
50:9:953:C:H2'	50:9:954:U:O4'	2.19	0.42
59:II:194:GLU:HA	62:LL:10:TYR:CE2	2.55	0.42
60:JJ:113:GLN:O	60:JJ:117:LEU:HD13	2.19	0.42
64:NN:67:THR:OG1	64:NN:69:ASN:O	2.37	0.42
83:gg:236:ILE:HG12	83:gg:252:THR:HG22	2.02	0.42
1:A:225:ILE:HD12	1:A:233:ARG:NH1	2.35	0.42
1:A:234:LYS:HG2	1:A:238:ILE:HD12	2.01	0.42
2:B:169:ARG:HH12	2:B:170:LEU:HD21	1.85	0.42
29:d:33:ILE:O	29:d:36:VAL:HG22	2.20	0.42
47:5:1321:G:C6	47:5:3876:A:C2	3.08	0.42
47:5:2368:A:N1	47:5:2788:U:C5	2.87	0.42
47:5:2438:A:C2	47:5:2441:C:C5	3.07	0.42
47:5:4895:C:O2	47:5:4895:C:C2'	2.68	0.42
50:9:15:U:H2'	50:9:16:G:O4'	2.20	0.42
50:9:979:C:C4	50:9:980:A:N7	2.88	0.42
62:LL:89:ARG:NH1	62:LL:91:ASP:OD2	2.49	0.42
70:TT:30:VAL:HG12	70:TT:53:PHE:CD1	2.54	0.42
85:ii:346:LEU:HD23	85:ii:351:GLU:HA	2.01	0.42
12:M:6:PHE:O	12:M:11:ARG:NE	2.53	0.42
47:5:1301:C:O2	47:5:1301:C:O4'	2.34	0.42
47:5:1563:A:O2'	47:5:1564:A:O5'	2.34	0.42
47:5:1633:G:H5'	47:5:1634:A:OP1	2.19	0.42
47:5:4119:C:O2	47:5:4119:C:O4'	2.37	0.42
50:9:1566:G:N7	70:TT:101:ARG:NH2	2.67	0.42
54:DD:72:VAL:HG23	61:KK:20:VAL:CG2	2.50	0.42
64:NN:3:ARG:CB	64:NN:6:ALA:HB3	2.50	0.42
7:G:101:LYS:HB3	23:X:42:THR:HG23	2.02	0.42
7:G:111:PRO:HD3	23:X:46:PHE:HD2	1.85	0.42
47:5:1855:G:C6	47:5:1856:C:C4	3.08	0.42
50:9:107:A:C2	50:9:355:G:C2	3.08	0.42
50:9:1336:C:H2'	50:9:1337:C:O4'	2.20	0.42
55:EE:166:THR:HG23	55:EE:168:LYS:HB2	2.02	0.42
59:II:48:VAL:HG11	59:II:54:LYS:HG3	2.01	0.42
16:Q:85:THR:HA	16:Q:104:ARG:O	2.19	0.41
47:5:1961:G:O2'	47:5:2025:A:N6	2.53	0.41
47:5:1986:U:C2'	47:5:2007:G:O6	2.67	0.41
47:5:2418:A:C5	47:5:2419:C:C5	3.08	0.41
47:5:4887:C:H6	47:5:4887:C:C5'	2.32	0.41
51:AA:57:LYS:HE2	72:VV:70:LEU:HD23	2.02	0.41
55:EE:122:LYS:O	55:EE:162:ILE:HD12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:ii:264:PHE:CZ	85:ii:268:ILE:HD11	2.55	0.41
3:C:252:TRP:CZ3	3:C:260:LEU:HD11	2.55	0.41
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.02	0.41
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.54	0.41
12:M:119:ARG:HH11	14:O:202:LEU:HD21	1.86	0.41
18:S:13:VAL:HA	18:S:28:TYR:O	2.20	0.41
19:T:2:THR:N	47:5:4220:A:OP2	2.53	0.41
47:5:1964:A:C6	47:5:4694:G:O6	2.73	0.41
50:9:35:C:H2'	50:9:36:U:C6	2.55	0.41
50:9:380:G:H1'	59:II:5:ARG:NE	2.36	0.41
3:C:252:TRP:CH2	3:C:260:LEU:HD11	2.55	0.41
8:H:91:LYS:HG2	8:H:145:VAL:HG22	2.03	0.41
26:a:8:THR:HA	26:a:11:LEU:HD12	2.02	0.41
30:e:28:TYR:HB3	30:e:30:LYS:HG2	2.01	0.41
41:p:52:VAL:HG21	47:5:2739:C:H4'	2.03	0.41
45:2:20(A):U:O2'	45:2:21:A:H5''	2.20	0.41
47:5:3700:C:O2'	47:5:3774:A:N3	2.50	0.41
47:5:4089:G:C2	47:5:4161:G:C2	3.08	0.41
50:9:1118:C:H2'	50:9:1119:A:C8	2.55	0.41
59:II:194:GLU:HA	62:LL:10:TYR:CD2	2.55	0.41
62:LL:61:PRO:HA	62:LL:66:VAL:HG13	2.02	0.41
66:PP:15:PHE:CD1	66:PP:15:PHE:C	2.98	0.41
77:aa:26:CYS:SG	77:aa:77:CYS:SG	3.17	0.41
83:gg:14:HIS:CE1	83:gg:35:SER:HB2	2.55	0.41
26:a:12:ARG:HD3	47:5:1660:U:H2'	2.02	0.41
26:a:35:ALA:O	26:a:41:HIS:ND1	2.52	0.41
45:2:33:U:OP2	67:QQ:146:ARG:NH2	2.53	0.41
45:2:74:C:OP2	47:5:4548:A:C2	2.73	0.41
47:5:1835:G:O2'	47:5:1836:G:OP2	2.32	0.41
50:9:845:G:H2'	50:9:846:G:O4'	2.20	0.41
51:AA:61:ALA:CB	51:AA:161:ILE:HD11	2.51	0.41
54:DD:127:MET:HE1	54:DD:133:GLY:HA2	2.02	0.41
74:XX:67:ARG:HG2	74:XX:115:ILE:HD12	2.02	0.41
3:C:27:VAL:HG11	3:C:128:LEU:HD13	2.03	0.41
4:D:132:VAL:HG21	4:D:170:GLY:C	2.45	0.41
14:O:28:LEU:HD11	14:O:88:LEU:HD23	2.01	0.41
35:j:63:ARG:NH2	49:8:58:G:N7	2.69	0.41
41:p:49:ARG:HB2	41:p:55:TRP:CZ3	2.55	0.41
47:5:1314:C:C2	47:5:1315:C:C5	3.08	0.41
47:5:1523:A:N3	47:5:4389:C:O2'	2.49	0.41
47:5:1627:G:C5	47:5:1628:C:C4	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:2046:G:C2	47:5:2047:A:C2	3.08	0.41
59:II:60:LEU:HD23	59:II:185:ALA:HB2	2.02	0.41
61:KK:49:MET:HB3	61:KK:69:TRP:CE2	2.55	0.41
66:PP:17:TYR:CE1	66:PP:37:TYR:HB3	2.55	0.41
1:A:40:TYR:CE1	47:5:4117:U:C4	3.08	0.41
49:8:68:G:H2'	49:8:69:U:O4'	2.21	0.41
49:8:127:U:C4	49:8:128:C:C5	3.08	0.41
50:9:1596:U:H2'	50:9:1597:C:O4'	2.20	0.41
51:AA:24:HIS:HB3	51:AA:51:LEU:HD11	2.02	0.41
52:BB:103:MET:CE	52:BB:212:VAL:HG23	2.51	0.41
59:II:36:THR:HG23	59:II:96:LEU:HB2	2.03	0.41
3:C:94:ASN:HA	3:C:100:ARG:O	2.20	0.41
4:D:66:TYR:OH	4:D:73:MET:HE3	2.20	0.41
18:S:53:LYS:NZ	48:7:74:A:O2'	2.53	0.41
47:5:2290:C:O4'	47:5:2321:G:C2	2.74	0.41
50:9:1391:C:H2'	50:9:1392:U:O4'	2.21	0.41
50:9:1679:A:H3'	56:FF:60:ARG:HD2	2.03	0.41
65:OO:119:LEU:HD12	65:OO:119:LEU:C	2.46	0.41
85:ii:322:VAL:HG21	85:ii:389:LEU:HD11	2.03	0.41
1:A:116:LEU:HA	1:A:164:ALA:HB2	2.03	0.41
3:C:32:ILE:HD13	3:C:129:ALA:HB3	2.02	0.41
11:L:90:VAL:O	11:L:93:THR:OG1	2.30	0.41
47:5:76:A:H2'	47:5:77:U:O4'	2.21	0.41
47:5:1354:A:N6	47:5:1503:A:O4'	2.54	0.41
47:5:3703:G:C6	47:5:3704:U:C4	3.09	0.41
50:9:302:A:H1'	59:II:73:THR:CG2	2.50	0.41
50:9:1130:G:N3	50:9:1130:G:C2'	2.82	0.41
56:FF:123:GLU:OE1	56:FF:204:ARG:NH1	2.54	0.41
57:GG:32:MET:HE2	57:GG:63:MET:HG2	2.03	0.41
73:WW:90:GLN:OE1	73:WW:117:ARG:NH2	2.54	0.41
1:A:227:ARG:NH2	47:5:3659:G:O2'	2.53	0.41
2:B:89:ILE:HD11	2:B:105:VAL:HB	2.03	0.41
3:C:237:ILE:HD12	3:C:237:ILE:H	1.86	0.41
3:C:340:ILE:HG21	5:E:52:LEU:HD12	2.03	0.41
17:R:45:ILE:HG12	17:R:50:ILE:HD11	2.01	0.41
17:R:99:MET:N	17:R:99:MET:SD	2.94	0.41
35:j:14:LYS:HA	47:5:1534:A:C5	2.56	0.41
47:5:108:A:N1	47:5:333:U:O2'	2.50	0.41
47:5:297:U:H2'	47:5:298:G:O4'	2.21	0.41
47:5:1384:C:O2'	47:5:1505:C:OP1	2.37	0.41
47:5:1591:U:N3	47:5:4555:U:OP1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:2081:C:H2'	47:5:2082:G:O4'	2.21	0.41
47:5:2395:A:C4'	47:5:2395:A:OP1	2.67	0.41
47:5:2415:U:C4	47:5:2416:G:C6	3.09	0.41
47:5:4499:G:N1	47:5:4500:U:O2	2.53	0.41
50:9:604:A:C6	50:9:605:A:N1	2.89	0.41
50:9:1057:C:O2	50:9:1057:C:O4'	2.38	0.41
50:9:1078:C:O2	50:9:1078:C:H2'	2.21	0.41
50:9:1095:U:O2	50:9:1151:G:N2	2.54	0.41
50:9:1260:A:C6	50:9:1619:A:C6	3.08	0.41
53:CC:166:ARG:HB2	53:CC:248:TYR:CD1	2.56	0.41
54:DD:48:ILE:CG2	54:DD:86:LEU:HD12	2.51	0.41
60:JJ:135:ILE:HG22	60:JJ:159:PHE:HA	2.03	0.41
62:LL:37:TYR:CD2	62:LL:51:ILE:HG23	2.56	0.41
63:MM:40:LYS:HE3	82:ff:130:VAL:HG22	2.02	0.41
63:MM:101:ARG:HA	63:MM:101:ARG:CZ	2.50	0.41
64:NN:98:VAL:HG11	64:NN:115:LEU:HB2	2.03	0.41
70:TT:6:VAL:HG22	70:TT:65:TYR:CE1	2.55	0.41
74:XX:51:VAL:HG13	74:XX:70:VAL:HG13	2.03	0.41
83:gg:5:MET:HE1	83:gg:312:VAL:HG13	2.03	0.41
85:ii:316:ALA:HB2	85:ii:415:TYR:CE1	2.56	0.41
7:G:210:ILE:HG12	7:G:254:THR:HG22	2.03	0.41
8:H:2:LYS:NZ	8:H:63:ASN:OD1	2.53	0.41
19:T:62:GLY:HA3	19:T:76:VAL:HG12	2.03	0.41
44:t:106:PHE:CE2	44:t:159:ALA:HB3	2.56	0.41
47:5:1513:U:H2'	47:5:1514:U:O4'	2.21	0.41
47:5:2809:G:O2'	47:5:4644:G:OP1	2.34	0.41
47:5:3732:A:C2	47:5:3733:A:C4	3.09	0.41
50:9:1444:U:H2'	50:9:1445:U:C6	2.56	0.41
55:EE:19:MET:HE3	55:EE:108:ARG:HD3	2.02	0.41
70:TT:14:PHE:CZ	70:TT:134:ILE:HD11	2.56	0.41
74:XX:61:GLN:O	74:XX:63:ASN:N	2.54	0.41
2:B:30:LYS:HG3	47:5:4716:C:OP2	2.21	0.40
2:B:154:LYS:HD2	2:B:191:ALA:CB	2.52	0.40
5:E:165:VAL:HG11	5:E:178:VAL:HG13	2.03	0.40
17:R:17:CYS:HB3	17:R:52:ARG:CZ	2.52	0.40
40:o:4:VAL:O	40:o:94:GLY:N	2.54	0.40
47:5:964:A:H2'	47:5:965:G:O4'	2.21	0.40
47:5:4562:C:H2'	47:5:4563:U:O4'	2.22	0.40
15:P:108:ASP:N	15:P:152:GLU:OE2	2.54	0.40
40:o:70:LEU:O	40:o:80:LYS:HA	2.21	0.40
43:s:63:LYS:HD2	47:5:1960:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:t:37:LEU:HD12	44:t:42:VAL:HG23	2.04	0.40
47:5:419:A:N1	47:5:420:A:C2	2.90	0.40
47:5:1337:A:C2	47:5:2349:A:N1	2.88	0.40
47:5:4508:C:H2'	47:5:4509:U:O4'	2.21	0.40
47:5:4579:U:H2'	47:5:4580:U:N1	2.34	0.40
47:5:4977:A:H2'	47:5:4978:G:O4'	2.21	0.40
61:KK:71:LEU:HD21	61:KK:79:LEU:HD12	2.03	0.40
70:TT:39:LEU:HD13	70:TT:47:PRO:HG2	2.03	0.40
85:ii:91:ASN:HA	85:ii:119:PRO:HA	2.03	0.40
1:A:82:ILE:HD11	1:A:99:GLY:CA	2.51	0.40
5:E:286:PRO:HA	5:E:289:LEU:CD2	2.52	0.40
12:M:10:GLY:HA2	12:M:64:PHE:CE1	2.56	0.40
14:O:74:ARG:NH2	47:5:4712:C:OP1	2.54	0.40
16:Q:89:ASP:OD1	16:Q:91:ARG:N	2.54	0.40
20:U:70:ILE:N	20:U:70:ILE:HD12	2.36	0.40
47:5:1653:A:H2'	47:5:1655:C:C4	2.57	0.40
47:5:1964:A:C5	47:5:4694:G:C5	3.09	0.40
47:5:3729:U:H2'	47:5:3730:U:C6	2.56	0.40
47:5:4415:A:N6	47:5:4427:G:O2'	2.53	0.40
50:9:1034:A:C6	50:9:1082:A:C4	3.09	0.40
50:9:1121:G:C6	50:9:1122:A:C5	3.10	0.40
55:EE:122:LYS:HG3	55:EE:162:ILE:HD11	1.99	0.40
66:PP:15:PHE:CE1	66:PP:109:PRO:HB3	2.56	0.40
3:C:33:ARG:CD	3:C:36:ILE:HD12	2.51	0.40
47:5:4188:U:H2'	47:5:4189:U:C6	2.57	0.40
51:AA:185:MET:HE3	72:VV:39:VAL:CG2	2.52	0.40
67:QQ:34:VAL:HG21	67:QQ:84:ILE:HD12	2.03	0.40
1:A:90:CYS:CB	1:A:101:VAL:HG13	2.51	0.40
1:A:207:VAL:HG12	47:5:3919:C:C5'	2.52	0.40
3:C:74:ALA:O	3:C:75:ARG:CB	2.70	0.40
24:Y:77:LYS:HB2	24:Y:79:VAL:HG12	2.03	0.40
38:m:57:ARG:O	38:m:61:GLN:HG2	2.22	0.40
47:5:30:C:C4	47:5:31:U:C4	3.10	0.40
47:5:3820:G:C6	47:5:3821:A:C5	3.10	0.40
47:5:3876:A:O2'	47:5:3877:A:P	2.80	0.40
47:5:4448:G:H4'	47:5:4449:A:OP2	2.22	0.40
50:9:1056:U:H2'	50:9:1057:C:O4'	2.21	0.40
50:9:1146:C:O2'	50:9:1150:A:N1	2.54	0.40
55:EE:11:ARG:NH2	55:EE:24:THR:OG1	2.50	0.40
58:HH:66:VAL:N	58:HH:67:PRO:CD	2.84	0.40
65:OO:43:HIS:CD2	65:OO:55:ARG:HB2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
73:WW:28:ARG:HB2	73:WW:29:PRO:HD3	2.03	0.40
85:ii:120:ILE:CG2	85:ii:139:LEU:HD13	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	216 (88%)	28 (11%)	2 (1%)	16	47
2	B	392/403 (97%)	364 (93%)	27 (7%)	1 (0%)	36	66
3	C	360/425 (85%)	335 (93%)	24 (7%)	1 (0%)	36	66
4	D	291/297 (98%)	277 (95%)	13 (4%)	1 (0%)	36	66
5	E	208/291 (72%)	194 (93%)	13 (6%)	1 (0%)	24	56
6	F	223/247 (90%)	213 (96%)	9 (4%)	1 (0%)	30	61
7	G	229/319 (72%)	216 (94%)	13 (6%)	0	100	100
8	H	188/192 (98%)	174 (93%)	14 (7%)	0	100	100
9	I	201/214 (94%)	185 (92%)	15 (8%)	1 (0%)	24	56
10	J	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
11	L	208/211 (99%)	198 (95%)	8 (4%)	2 (1%)	12	42
12	M	136/218 (62%)	123 (90%)	12 (9%)	1 (1%)	18	50
13	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	24	56
14	O	197/203 (97%)	186 (94%)	8 (4%)	3 (2%)	8	35
15	P	151/184 (82%)	141 (93%)	10 (7%)	0	100	100
16	Q	185/188 (98%)	172 (93%)	12 (6%)	1 (0%)	24	56
17	R	178/196 (91%)	170 (96%)	8 (4%)	0	100	100
18	S	174/176 (99%)	164 (94%)	9 (5%)	1 (1%)	21	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	T	157/160 (98%)	143 (91%)	13 (8%)	1 (1%)	21	52
20	U	97/128 (76%)	88 (91%)	9 (9%)	0	100	100
21	V	129/140 (92%)	114 (88%)	15 (12%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	12	42
23	X	116/156 (74%)	109 (94%)	7 (6%)	0	100	100
24	Y	132/145 (91%)	124 (94%)	8 (6%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	4 (3%)	3 (2%)	5	29
26	a	145/148 (98%)	133 (92%)	12 (8%)	0	100	100
27	b	100/245 (41%)	94 (94%)	5 (5%)	1 (1%)	12	42
28	c	96/115 (84%)	90 (94%)	6 (6%)	0	100	100
29	d	105/125 (84%)	92 (88%)	13 (12%)	0	100	100
30	e	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
31	f	107/110 (97%)	99 (92%)	6 (6%)	2 (2%)	6	32
32	g	112/117 (96%)	104 (93%)	8 (7%)	0	100	100
33	h	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
34	i	100/105 (95%)	93 (93%)	7 (7%)	0	100	100
35	j	84/97 (87%)	74 (88%)	10 (12%)	0	100	100
36	k	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
37	l	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
38	m	50/102 (49%)	48 (96%)	2 (4%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	99 (97%)	2 (2%)	1 (1%)	12	42
41	p	89/92 (97%)	80 (90%)	7 (8%)	2 (2%)	5	29
42	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	16	47
43	s	194/318 (61%)	177 (91%)	15 (8%)	2 (1%)	12	42
44	t	149/165 (90%)	135 (91%)	13 (9%)	1 (1%)	18	50
51	AA	215/295 (73%)	196 (91%)	18 (8%)	1 (0%)	24	56
52	BB	211/264 (80%)	202 (96%)	9 (4%)	0	100	100
53	CC	219/293 (75%)	206 (94%)	12 (6%)	1 (0%)	24	56
54	DD	226/243 (93%)	213 (94%)	11 (5%)	2 (1%)	14	43
55	EE	260/263 (99%)	239 (92%)	21 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
56	FF	181/204 (89%)	169 (93%)	11 (6%)	1 (1%)	21	52
57	GG	235/249 (94%)	226 (96%)	8 (3%)	1 (0%)	30	61
58	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
59	II	204/208 (98%)	186 (91%)	17 (8%)	1 (0%)	24	56
60	JJ	183/194 (94%)	175 (96%)	6 (3%)	2 (1%)	11	40
61	KK	94/165 (57%)	88 (94%)	5 (5%)	1 (1%)	11	40
62	LL	139/158 (88%)	126 (91%)	12 (9%)	1 (1%)	18	50
63	MM	115/132 (87%)	105 (91%)	10 (9%)	0	100	100
64	NN	147/151 (97%)	136 (92%)	11 (8%)	0	100	100
65	OO	134/168 (80%)	122 (91%)	10 (8%)	2 (2%)	8	35
66	PP	118/145 (81%)	109 (92%)	9 (8%)	0	100	100
67	QQ	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
68	RR	130/135 (96%)	122 (94%)	8 (6%)	0	100	100
69	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
70	TT	139/145 (96%)	130 (94%)	9 (6%)	0	100	100
71	UU	98/119 (82%)	87 (89%)	11 (11%)	0	100	100
72	VV	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
73	WW	127/130 (98%)	119 (94%)	8 (6%)	0	100	100
74	XX	139/143 (97%)	130 (94%)	6 (4%)	3 (2%)	5	29
75	YY	122/130 (94%)	113 (93%)	9 (7%)	0	100	100
76	ZZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
77	aa	99/115 (86%)	88 (89%)	11 (11%)	0	100	100
78	bb	81/84 (96%)	73 (90%)	7 (9%)	1 (1%)	10	39
79	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
80	dd	53/56 (95%)	52 (98%)	1 (2%)	0	100	100
81	ee	53/133 (40%)	50 (94%)	3 (6%)	0	100	100
82	ff	66/156 (42%)	60 (91%)	6 (9%)	0	100	100
83	gg	311/317 (98%)	286 (92%)	25 (8%)	0	100	100
85	ii	410/459 (89%)	394 (96%)	16 (4%)	0	100	100
All	All	11927/13834 (86%)	11108 (93%)	770 (6%)	49 (0%)	31	61

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	r	11	ARG
74	XX	61	GLN
74	XX	62	PRO
11	L	17	ASP
18	S	155	PRO
25	Z	52	LYS
25	Z	91	LEU
27	b	102	PRO
43	s	142	GLY
51	AA	159	ILE
54	DD	48	ILE
56	FF	21	GLY
59	II	3	ILE
62	LL	66	VAL
65	OO	20	GLN
74	XX	86	PRO
1	A	14	SER
11	L	63	THR
16	Q	14	ARG
25	Z	90	PRO
1	A	127	ALA
2	B	17	LEU
14	O	186	GLU
40	o	77	CYS
44	t	54	LYS
54	DD	93	THR
61	KK	64	TRP
9	I	47	PRO
13	N	89	VAL
14	O	89	PRO
31	f	106	TYR
41	p	9	GLY
57	GG	135	PRO
60	JJ	92	MET
60	JJ	147	PHE
65	OO	143	LYS
3	C	71	ARG
5	E	181	PRO
41	p	8	VAL
53	CC	232	THR
78	bb	20	LYS
22	W	3	VAL
6	F	196	VAL

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Mol	Chain	Res	Type
14	O	146	GLY
31	f	107	PRO
43	s	25	PRO
12	M	19	PRO
4	D	125	VAL
19	T	74	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	A	190/199 (96%)	173 (91%)	17 (9%)	9	32
2	B	342/348 (98%)	322 (94%)	20 (6%)	18	43
3	C	302/347 (87%)	284 (94%)	18 (6%)	17	43
4	D	247/250 (99%)	232 (94%)	15 (6%)	17	42
5	E	190/251 (76%)	181 (95%)	9 (5%)	23	47
6	F	196/215 (91%)	184 (94%)	12 (6%)	17	42
7	G	200/272 (74%)	188 (94%)	12 (6%)	17	43
8	H	169/171 (99%)	158 (94%)	11 (6%)	15	41
9	I	175/181 (97%)	164 (94%)	11 (6%)	16	42
10	J	143/149 (96%)	137 (96%)	6 (4%)	26	50
11	L	175/176 (99%)	171 (98%)	4 (2%)	44	62
12	M	117/161 (73%)	109 (93%)	8 (7%)	14	40
13	N	171/172 (99%)	164 (96%)	7 (4%)	27	51
14	O	171/173 (99%)	161 (94%)	10 (6%)	18	43
15	P	134/163 (82%)	126 (94%)	8 (6%)	17	43
16	Q	164/165 (99%)	153 (93%)	11 (7%)	15	40
17	R	159/175 (91%)	145 (91%)	14 (9%)	9	33
18	S	157/157 (100%)	147 (94%)	10 (6%)	16	41
19	T	139/140 (99%)	132 (95%)	7 (5%)	22	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	U	89/114 (78%)	88 (99%)	1 (1%)	65	72
21	V	101/107 (94%)	91 (90%)	10 (10%)	7	29
22	W	86/126 (68%)	86 (100%)	0	100	100
23	X	106/134 (79%)	100 (94%)	6 (6%)	18	44
24	Y	124/135 (92%)	119 (96%)	5 (4%)	28	51
25	Z	117/118 (99%)	114 (97%)	3 (3%)	40	59
26	a	119/120 (99%)	115 (97%)	4 (3%)	32	54
27	b	84/184 (46%)	82 (98%)	2 (2%)	43	61
28	c	84/98 (86%)	82 (98%)	2 (2%)	43	61
29	d	98/110 (89%)	94 (96%)	4 (4%)	27	51
30	e	114/121 (94%)	104 (91%)	10 (9%)	9	33
31	f	88/89 (99%)	82 (93%)	6 (7%)	14	40
32	g	98/100 (98%)	91 (93%)	7 (7%)	13	39
33	h	109/110 (99%)	106 (97%)	3 (3%)	38	57
34	i	86/89 (97%)	82 (95%)	4 (5%)	23	47
35	j	73/80 (91%)	68 (93%)	5 (7%)	14	40
36	k	64/65 (98%)	62 (97%)	2 (3%)	35	56
37	l	47/48 (98%)	47 (100%)	0	100	100
38	m	48/90 (53%)	44 (92%)	4 (8%)	10	34
39	n	24/24 (100%)	22 (92%)	2 (8%)	10	34
40	o	92/94 (98%)	87 (95%)	5 (5%)	20	45
41	p	74/75 (99%)	72 (97%)	2 (3%)	39	58
42	r	108/121 (89%)	101 (94%)	7 (6%)	15	41
43	s	164/258 (64%)	158 (96%)	6 (4%)	30	52
44	t	126/137 (92%)	122 (97%)	4 (3%)	34	55
51	AA	180/245 (74%)	162 (90%)	18 (10%)	7	28
52	BB	194/231 (84%)	173 (89%)	21 (11%)	6	25
53	CC	187/225 (83%)	169 (90%)	18 (10%)	8	30
54	DD	190/202 (94%)	176 (93%)	14 (7%)	13	38
55	EE	224/225 (100%)	205 (92%)	19 (8%)	10	33
56	FF	158/170 (93%)	145 (92%)	13 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	GG	207/218 (95%)	193 (93%)	14 (7%)	14	40
58	HH	165/174 (95%)	151 (92%)	14 (8%)	10	33
59	II	178/180 (99%)	165 (93%)	13 (7%)	13	38
60	JJ	161/168 (96%)	148 (92%)	13 (8%)	11	35
61	KK	87/136 (64%)	77 (88%)	10 (12%)	5	22
62	LL	130/142 (92%)	114 (88%)	16 (12%)	4	21
63	MM	99/108 (92%)	87 (88%)	12 (12%)	5	21
64	NN	130/131 (99%)	119 (92%)	11 (8%)	10	33
65	OO	106/130 (82%)	94 (89%)	12 (11%)	5	23
66	PP	109/130 (84%)	100 (92%)	9 (8%)	10	34
67	QQ	117/121 (97%)	106 (91%)	11 (9%)	8	30
68	RR	119/121 (98%)	107 (90%)	12 (10%)	7	27
69	SS	125/132 (95%)	111 (89%)	14 (11%)	6	24
70	TT	111/115 (96%)	103 (93%)	8 (7%)	13	39
71	UU	92/107 (86%)	84 (91%)	8 (9%)	9	33
72	VV	67/67 (100%)	64 (96%)	3 (4%)	24	48
73	WW	112/113 (99%)	104 (93%)	8 (7%)	13	39
74	XX	113/115 (98%)	106 (94%)	7 (6%)	16	42
75	YY	107/112 (96%)	95 (89%)	12 (11%)	6	24
76	ZZ	66/103 (64%)	61 (92%)	5 (8%)	12	37
77	aa	88/98 (90%)	80 (91%)	8 (9%)	9	32
78	bb	75/76 (99%)	68 (91%)	7 (9%)	8	31
79	cc	55/62 (89%)	52 (94%)	3 (6%)	19	44
80	dd	48/49 (98%)	46 (96%)	2 (4%)	26	50
81	ee	46/106 (43%)	41 (89%)	5 (11%)	6	25
82	ff	61/140 (44%)	54 (88%)	7 (12%)	5	22
83	gg	272/275 (99%)	261 (96%)	11 (4%)	28	51
85	ii	360/394 (91%)	341 (95%)	19 (5%)	20	45
All	All	10403/11733 (89%)	9712 (93%)	691 (7%)	17	41

All (691) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	102	LEU
1	A	123	ARG
1	A	128	ARG
1	A	149	LYS
1	A	158	ILE
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE
1	A	200	ARG
1	A	207	VAL
1	A	209	HIS
1	A	221	LYS
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
1	A	243	THR
2	B	10	ARG
2	B	17	LEU
2	B	23	SER
2	B	62	ARG
2	B	66	LYS
2	B	90	VAL
2	B	95	THR
2	B	135	LYS
2	B	248	LEU
2	B	262	VAL
2	B	268	ARG
2	B	279	GLU
2	B	294	LYS
2	B	309	LEU
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	356	LYS
2	B	366	LYS
2	B	383	GLU
3	C	20	LYS
3	C	95	MET
3	C	101	MET
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU

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Mol	Chain	Res	Type
3	C	165	LYS
3	C	175	LYS
3	C	193	LYS
3	C	195	LYS
3	C	232	VAL
3	C	246	VAL
3	C	281	MET
3	C	284	MET
3	C	307	LYS
3	C	312	ARG
3	C	333	LYS
3	C	340	ILE
4	D	22	ARG
4	D	37	VAL
4	D	40	ASP
4	D	45	ASN
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	128	ASP
4	D	221	LYS
4	D	225	GLN
4	D	262	LYS
4	D	264	LYS
4	D	268	ARG
5	E	52	LEU
5	E	58	ARG
5	E	96	THR
5	E	112	LEU
5	E	143	LEU
5	E	169	LYS
5	E	178	VAL
5	E	213	LYS
5	E	291	PHE
6	F	38	GLN
6	F	46	ARG
6	F	65	ARG
6	F	67	GLU
6	F	88	LEU
6	F	106	LYS

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Mol	Chain	Res	Type
6	F	128	SER
6	F	134	ILE
6	F	151	GLU
6	F	187	GLU
6	F	198	LYS
6	F	211	LYS
7	G	148	LEU
7	G	162	GLU
7	G	163	LYS
7	G	184	LYS
7	G	203	LYS
7	G	204	LYS
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	235	CYS
7	G	293	ASN
7	G	312	LYS
8	H	1	MET
8	H	20	LEU
8	H	52	LYS
8	H	57	VAL
8	H	59	LYS
8	H	66	GLU
8	H	105	ILE
8	H	106	GLN
8	H	128	MET
8	H	141	LYS
8	H	173	ARG
9	I	36	LEU
9	I	39	LYS
9	I	71	CYS
9	I	76	MET
9	I	80	CYS
9	I	116	ARG
9	I	146	GLU
9	I	153	ARG
9	I	164	LYS
9	I	195	CYS
9	I	208	LYS
10	J	16	ARG
10	J	28	GLU

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Mol	Chain	Res	Type
10	J	81	GLU
10	J	96	LYS
10	J	113	ILE
10	J	175	LEU
11	L	46	ILE
11	L	63	THR
11	L	162	LYS
11	L	186	ARG
12	M	8	GLU
12	M	32	ASP
12	M	37	LEU
12	M	56	GLN
12	M	61	ILE
12	M	96	GLU
12	M	105	THR
12	M	112	VAL
13	N	9	GLU
13	N	32	GLN
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	89	VAL
13	N	197	THR
14	O	16	LEU
14	O	18	ARG
14	O	82	ARG
14	O	128	ARG
14	O	130	LYS
14	O	145	VAL
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	202	LEU
15	P	10	ASN
15	P	24	VAL
15	P	36	ILE
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL

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Mol	Chain	Res	Type
16	Q	5	ILE
16	Q	20	SER
16	Q	42	THR
16	Q	61	LEU
16	Q	63	LEU
16	Q	91	ARG
16	Q	95	VAL
16	Q	115	LYS
16	Q	126	LEU
16	Q	143	ARG
17	R	6	LEU
17	R	10	LEU
17	R	36	ASN
17	R	41	ILE
17	R	50	ILE
17	R	82	LYS
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	106	LEU
17	R	113	LYS
17	R	122	SER
17	R	138	LEU
17	R	178	GLN
18	S	1	MET
18	S	7	LEU
18	S	9	GLU
18	S	70	LYS
18	S	84	TYR
18	S	95	ARG
18	S	149	LYS
18	S	159	LEU
18	S	164	LYS
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	60	LYS
19	T	80	VAL
19	T	96	ILE
19	T	144	ASN
19	T	159	MET
20	U	33	ILE

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Mol	Chain	Res	Type
21	V	15	ARG
21	V	16	ILE
21	V	18	LEU
21	V	35	LYS
21	V	60	MET
21	V	69	LYS
21	V	82	ILE
21	V	91	LYS
21	V	109	LYS
21	V	123	LYS
23	X	39	LYS
23	X	52	LEU
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	55	VAL
24	Y	72	GLN
24	Y	104	VAL
25	Z	11	VAL
25	Z	33	THR
25	Z	42	LEU
26	a	4	ARG
26	a	84	GLU
26	a	122	VAL
26	a	132	ARG
27	b	9	THR
27	b	22	LYS
28	c	37	MET
28	c	78	ASN
29	d	23	ARG
29	d	48	GLU
29	d	98	SER
29	d	102	LEU
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	64	LYS
30	e	78	LEU

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Mol	Chain	Res	Type
30	e	86	GLU
30	e	91	CYS
30	e	106	LYS
30	e	128	ARG
31	f	7	CYS
31	f	33	VAL
31	f	52	LYS
31	f	69	VAL
31	f	90	SER
31	f	101	ILE
32	g	5	LEU
32	g	22	LEU
32	g	43	LYS
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN
33	h	15	GLU
33	h	28	LEU
33	h	67	GLU
34	i	33	LEU
34	i	77	VAL
34	i	86	LYS
34	i	89	GLU
35	j	3	LYS
35	j	11	ARG
35	j	20	ARG
35	j	58	THR
35	j	59	THR
36	k	69	LEU
36	k	70	LYS
38	m	59	LEU
38	m	71	ARG
38	m	92	THR
38	m	93	ASN
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	28	LYS
40	o	36	GLN
40	o	61	LYS
40	o	83	LEU

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Mol	Chain	Res	Type
41	p	8	VAL
41	p	84	ARG
42	r	8	MET
42	r	20	ARG
42	r	32	LEU
42	r	67	ARG
42	r	80	THR
42	r	115	SER
42	r	118	LEU
43	s	38	LYS
43	s	95	LEU
43	s	105	ASN
43	s	146	LYS
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	72	GLU
44	t	98	ILE
44	t	133	LEU
51	AA	5	LEU
51	AA	12	GLU
51	AA	25	LEU
51	AA	46	ILE
51	AA	50	ASN
51	AA	56	GLU
51	AA	58	LEU
51	AA	59	LEU
51	AA	60	LEU
51	AA	122	LEU
51	AA	124	VAL
51	AA	132	GLN
51	AA	135	THR
51	AA	136	GLU
51	AA	170	SER
51	AA	173	LEU
51	AA	178	LEU
51	AA	198	MET
52	BB	38	MET
52	BB	47	THR
52	BB	63	LYS
52	BB	71	LEU
52	BB	74	LEU

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Mol	Chain	Res	Type
52	BB	82	ARG
52	BB	86	LEU
52	BB	105	LEU
52	BB	125	VAL
52	BB	157	GLN
52	BB	175	GLU
52	BB	179	ASN
52	BB	181	LEU
52	BB	184	VAL
52	BB	207	LEU
52	BB	209	ASP
52	BB	213	ARG
52	BB	217	MET
52	BB	225	LEU
52	BB	229	MET
52	BB	231	LEU
53	CC	73	MET
53	CC	78	LEU
53	CC	79	GLU
53	CC	101	SER
53	CC	114	LYS
53	CC	117	ARG
53	CC	121	ARG
53	CC	137	VAL
53	CC	139	LEU
53	CC	165	VAL
53	CC	167	ARG
53	CC	192	LEU
53	CC	213	LEU
53	CC	215	MET
53	CC	240	THR
53	CC	244	ILE
53	CC	252	THR
53	CC	255	LEU
54	DD	28	GLU
54	DD	51	LEU
54	DD	59	LEU
54	DD	72	VAL
54	DD	127	MET
54	DD	137	VAL
54	DD	142	LEU
54	DD	156	LEU

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Mol	Chain	Res	Type
54	DD	168	VAL
54	DD	170	THR
54	DD	190	LEU
54	DD	198	ILE
54	DD	218	LEU
54	DD	223	ILE
55	EE	6	LYS
55	EE	17	HIS
55	EE	23	LEU
55	EE	31	PRO
55	EE	42	LEU
55	EE	48	LEU
55	EE	51	ARG
55	EE	59	ASP
55	EE	66	MET
55	EE	77	ARG
55	EE	123	LEU
55	EE	126	VAL
55	EE	162	ILE
55	EE	181	CYS
55	EE	205	PHE
55	EE	222	LEU
55	EE	232	ASN
55	EE	238	LEU
55	EE	246	LEU
56	FF	20	PHE
56	FF	43	GLU
56	FF	65	GLN
56	FF	66	CYS
56	FF	71	ARG
56	FF	88	MET
56	FF	89	THR
56	FF	135	ARG
56	FF	140	ASP
56	FF	141	VAL
56	FF	146	ARG
56	FF	155	CYS
56	FF	169	ILE
57	GG	41	LEU
57	GG	63	MET
57	GG	67	VAL
57	GG	103	ASP

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Mol	Chain	Res	Type
57	GG	129	VAL
57	GG	135	PRO
57	GG	171	THR
57	GG	178	ARG
57	GG	183	ARG
57	GG	190	ARG
57	GG	216	ARG
57	GG	217	MET
57	GG	230	LYS
57	GG	235	SER
58	HH	8	ILE
58	HH	21	SER
58	HH	36	LEU
58	HH	46	THR
58	HH	53	VAL
58	HH	75	ILE
58	HH	76	GLN
58	HH	79	LEU
58	HH	82	GLU
58	HH	100	ILE
58	HH	145	ARG
58	HH	149	ASP
58	HH	160	LYS
58	HH	172	THR
59	II	23	LYS
59	II	26	LYS
59	II	45	THR
59	II	74	ARG
59	II	100	CYS
59	II	121	LEU
59	II	130	THR
59	II	145	ILE
59	II	161	LEU
59	II	165	GLN
59	II	168	GLN
59	II	178	ARG
59	II	182	CYS
60	JJ	26	ASP
60	JJ	29	LEU
60	JJ	38	ARG
60	JJ	40	LYS
60	JJ	45	ARG

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Mol	Chain	Res	Type
60	JJ	50	LEU
60	JJ	61	LEU
60	JJ	69	ARG
60	JJ	80	ARG
60	JJ	89	GLU
60	JJ	109	ARG
60	JJ	116	LYS
60	JJ	163	SER
61	KK	2	LEU
61	KK	17	LYS
61	KK	20	VAL
61	KK	21	MET
61	KK	35	LEU
61	KK	50	GLN
61	KK	59	LYS
61	KK	60	GLU
61	KK	89	ILE
61	KK	96	ARG
62	LL	16	ILE
62	LL	20	LYS
62	LL	32	LYS
62	LL	40	ILE
62	LL	42	LEU
62	LL	49	GLU
62	LL	56	ILE
62	LL	69	ARG
62	LL	81	LYS
62	LL	85	THR
62	LL	110	SER
62	LL	111	VAL
62	LL	121	GLN
62	LL	126	VAL
62	LL	134	LEU
62	LL	153	LYS
63	MM	22	LEU
63	MM	31	LEU
63	MM	33	ARG
63	MM	40	LYS
63	MM	42	LEU
63	MM	49	LEU
63	MM	55	ASN
63	MM	85	LEU

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Mol	Chain	Res	Type
63	MM	99	LYS
63	MM	101	ARG
63	MM	112	LYS
63	MM	123	VAL
64	NN	3	ARG
64	NN	27	LYS
64	NN	55	ARG
64	NN	60	VAL
64	NN	75	LEU
64	NN	78	LYS
64	NN	84	LEU
64	NN	110	ASP
64	NN	120	SER
64	NN	125	LEU
64	NN	132	LYS
65	OO	25	GLU
65	OO	38	ASN
65	OO	47	LEU
65	OO	51	GLU
65	OO	56	VAL
65	OO	69	SER
65	OO	75	MET
65	OO	85	CYS
65	OO	119	LEU
65	OO	128	ARG
65	OO	131	ASP
65	OO	151	LEU
66	PP	14	LYS
66	PP	15	PHE
66	PP	37	TYR
66	PP	42	ARG
66	PP	55	SER
66	PP	65	LYS
66	PP	78	THR
66	PP	83	MET
66	PP	108	LYS
67	QQ	26	LYS
67	QQ	31	LEU
67	QQ	47	LEU
67	QQ	53	GLU
67	QQ	60	LYS
67	QQ	67	ASP

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Mol	Chain	Res	Type
67	QQ	81	ILE
67	QQ	90	LYS
67	QQ	123	ASP
67	QQ	127	CYS
67	QQ	140	ARG
68	RR	6	THR
68	RR	8	THR
68	RR	30	THR
68	RR	31	ASN
68	RR	36	GLU
68	RR	43	SER
68	RR	44	LYS
68	RR	49	LYS
68	RR	62	GLN
68	RR	98	VAL
68	RR	105	MET
68	RR	109	LEU
69	SS	8	LYS
69	SS	14	ARG
69	SS	21	ASP
69	SS	36	VAL
69	SS	46	ARG
69	SS	49	ASP
69	SS	52	LEU
69	SS	59	LEU
69	SS	63	GLU
69	SS	86	ARG
69	SS	98	VAL
69	SS	110	ASP
69	SS	132	ARG
69	SS	144	ARG
70	TT	39	LEU
70	TT	62	ARG
70	TT	74	SER
70	TT	108	GLU
70	TT	110	LEU
70	TT	124	THR
70	TT	131	LEU
70	TT	142	LYS
71	UU	25	THR
71	UU	44	LYS
71	UU	56	MET

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Mol	Chain	Res	Type
71	UU	64	THR
71	UU	79	ARG
71	UU	95	SER
71	UU	106	ILE
71	UU	111	GLU
72	VV	12	TYR
72	VV	32	ILE
72	VV	69	ILE
73	WW	23	ARG
73	WW	51	GLU
73	WW	84	LYS
73	WW	92	ASN
73	WW	103	VAL
73	WW	104	LEU
73	WW	111	MET
73	WW	114	GLU
74	XX	7	LEU
74	XX	29	LYS
74	XX	64	SER
74	XX	67	ARG
74	XX	98	ASP
74	XX	107	ARG
74	XX	115	ILE
75	YY	16	ARG
75	YY	17	LEU
75	YY	20	ARG
75	YY	32	LYS
75	YY	40	ILE
75	YY	47	MET
75	YY	61	ARG
75	YY	74	MET
75	YY	88	LYS
75	YY	93	ARG
75	YY	101	LYS
75	YY	115	LYS
76	ZZ	52	LYS
76	ZZ	67	LEU
76	ZZ	76	ARG
76	ZZ	89	GLN
76	ZZ	92	LEU
77	aa	12	LYS
77	aa	21	ILE

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Mol	Chain	Res	Type
77	aa	23	CYS
77	aa	41	ILE
77	aa	44	ILE
77	aa	55	GLU
77	aa	57	SER
77	aa	67	LEU
78	bb	17	ARG
78	bb	42	LYS
78	bb	60	SER
78	bb	64	CYS
78	bb	78	SER
78	bb	80	ARG
78	bb	81	ARG
79	cc	26	GLN
79	cc	27	CYS
79	cc	40	ARG
80	dd	4	GLN
80	dd	36	LEU
81	ee	97	LYS
81	ee	98	LYS
81	ee	99	LYS
81	ee	110	GLN
81	ee	124	LYS
82	ff	83	LYS
82	ff	84	SER
82	ff	94	LYS
82	ff	99	LYS
82	ff	110	GLU
82	ff	138	ARG
82	ff	140	TYR
83	gg	17	TRP
83	gg	20	GLN
83	gg	36	ARG
83	gg	79	LEU
83	gg	87	LEU
83	gg	119	GLN
83	gg	198	VAL
83	gg	207	CYS
83	gg	289	LEU
83	gg	305	ASN
83	gg	306	LEU
85	ii	45	ILE

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Mol	Chain	Res	Type
85	ii	63	LYS
85	ii	68	ARG
85	ii	86	ASN
85	ii	103	GLU
85	ii	111	ASN
85	ii	134	GLU
85	ii	185	GLN
85	ii	193	LEU
85	ii	207	GLU
85	ii	211	GLN
85	ii	212	LEU
85	ii	231	ASP
85	ii	232	PHE
85	ii	241	MET
85	ii	246	LEU
85	ii	340	GLU
85	ii	368	LEU
85	ii	417	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	95	GLN
1	A	97	ASN
1	A	100	ASN
1	A	140	ASN
1	A	194	ASN
1	A	205	ASN
1	A	217	GLN
2	B	245	HIS
3	C	38	ASN
3	C	203	GLN
3	C	310	HIS
3	C	329	ASN
4	D	191	ASN
4	D	229	ASN
5	E	194	GLN
6	F	79	ASN
7	G	143	GLN
7	G	161	GLN
7	G	248	HIS

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Mol	Chain	Res	Type
8	H	42	ASN
8	H	78	GLN
8	H	98	HIS
8	H	162	GLN
9	I	59	GLN
9	I	100	ASN
9	I	144	ASN
10	J	71	HIS
11	L	27	ASN
11	L	113	ASN
12	M	33	GLN
12	M	48	GLN
14	O	180	GLN
14	O	184	ASN
15	P	21	ASN
15	P	56	GLN
15	P	137	ASN
17	R	34	ASN
17	R	75	HIS
18	S	162	GLN
18	S	163	HIS
19	T	49	GLN
19	T	69	GLN
19	T	144	ASN
22	W	59	HIS
22	W	79	GLN
23	X	69	ASN
23	X	94	ASN
24	Y	56	GLN
24	Y	61	HIS
26	a	44	ASN
26	a	60	HIS
28	c	15	ASN
31	f	65	ASN
33	h	108	GLN
35	j	48	ASN
37	l	38	ASN
38	m	94	ASN
40	o	102	GLN
41	p	72	ASN
42	r	12	ASN
42	r	103	HIS

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Mol	Chain	Res	Type
42	r	121	GLN
43	s	68	HIS
43	s	179	ASN
44	t	65	GLN
44	t	95	GLN
44	t	100	HIS
44	t	115	GLN
51	AA	24	HIS
51	AA	111	GLN
51	AA	132	GLN
52	BB	179	ASN
53	CC	272	HIS
55	EE	17	HIS
55	EE	36	HIS
55	EE	197	ASN
56	FF	83	ASN
58	HH	39	GLN
58	HH	91	HIS
58	HH	97	GLN
58	HH	193	GLN
59	II	7	ASN
59	II	35	ASN
59	II	116	HIS
60	JJ	156	HIS
61	KK	44	HIS
61	KK	84	HIS
62	LL	5	GLN
62	LL	65	ASN
62	LL	100	ASN
63	MM	55	ASN
63	MM	72	HIS
64	NN	62	GLN
64	NN	69	ASN
65	OO	20	GLN
66	PP	79	HIS
67	QQ	24	HIS
67	QQ	142	GLN
69	SS	125	HIS
74	XX	23	HIS
74	XX	61	GLN
74	XX	77	ASN
77	aa	80	HIS

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Mol	Chain	Res	Type
78	bb	51	GLN
79	cc	29	GLN
79	cc	45	ASN
80	dd	41	GLN
81	ee	88	GLN
83	gg	159	ASN
83	gg	196	ASN
83	gg	215	GLN
83	gg	222	ASN
85	ii	61	ASN
85	ii	79	GLN
85	ii	80	GLN
85	ii	132	HIS
85	ii	170	HIS
85	ii	185	GLN
85	ii	200	ASN
85	ii	381	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	2	73/76 (96%)	15 (20%)	1 (1%)
46	3	72/75 (96%)	26 (36%)	2 (2%)
47	5	3519/3543 (99%)	910 (25%)	175 (4%)
48	7	119/120 (99%)	18 (15%)	2 (1%)
49	8	150/156 (96%)	36 (24%)	8 (5%)
50	9	1678/1869 (89%)	442 (26%)	70 (4%)
84	hh	14/15 (93%)	8 (57%)	0
All	All	5625/5854 (96%)	1455 (25%)	258 (4%)

All (1455) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	2	8	U
45	2	9	A
45	2	13	U
45	2	16	C
45	2	19	G
45	2	21	A
45	2	46	G
45	2	47	U

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Mol	Chain	Res	Type
45	2	49	C
45	2	60	A
45	2	61	C
45	2	64	G
45	2	67	G
45	2	72	C
45	2	75	C
46	3	7	A
46	3	8	U
46	3	13	C
46	3	14	A
46	3	16	C
46	3	21	A
46	3	25	C
46	3	29	A
46	3	34	U
46	3	35	U
46	3	36	U
46	3	40	C
46	3	42	G
46	3	47	U
46	3	49	C
46	3	53	G
46	3	58	A
46	3	60	U
46	3	61	C
46	3	63	C
46	3	65	G
46	3	71	G
46	3	72	C
46	3	74	C
46	3	75	C
46	3	76	A
47	5	8	U
47	5	12	A
47	5	13	U
47	5	15	A
47	5	20	U
47	5	21	G
47	5	25	A
47	5	35	U
47	5	39	A

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Mol	Chain	Res	Type
47	5	42	A
47	5	43	U
47	5	44	A
47	5	48	G
47	5	49	U
47	5	56	A
47	5	58	G
47	5	59	A
47	5	64	A
47	5	65	A
47	5	73	A
47	5	75	G
47	5	84	A
47	5	91	G
47	5	93	G
47	5	96	U
47	5	108	A
47	5	109	G
47	5	116	G
47	5	118	C
47	5	119	G
47	5	120	A
47	5	126	C
47	5	134	G
47	5	135	G
47	5	136	C
47	5	143	C
47	5	144	G
47	5	157	U
47	5	159	C
47	5	160	G
47	5	172	C
47	5	173	C
47	5	177	G
47	5	179	G
47	5	197	A
47	5	200	U
47	5	201	C
47	5	202	C
47	5	205	C
47	5	209	U
47	5	216	C

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Mol	Chain	Res	Type
47	5	217	C
47	5	218	A
47	5	220	C
47	5	221	C
47	5	224	U
47	5	226	G
47	5	227	A
47	5	233	U
47	5	234	G
47	5	245	C
47	5	246	G
47	5	253	G
47	5	255	C
47	5	262	G
47	5	263	G
47	5	266	C
47	5	267	G
47	5	276	C
47	5	279	A
47	5	280	G
47	5	281	U
47	5	297	U
47	5	306	A
47	5	309	C
47	5	310	G
47	5	315	G
47	5	316	U
47	5	322	C
47	5	328	A
47	5	334	A
47	5	340	C
47	5	350	C
47	5	357	U
47	5	360	A
47	5	361	C
47	5	363	A
47	5	379	G
47	5	386	A
47	5	387	G
47	5	407	A
47	5	409	G
47	5	410	A

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Mol	Chain	Res	Type
47	5	412	G
47	5	413	G
47	5	414	C
47	5	418	A
47	5	431	G
47	5	432	U
47	5	436	C
47	5	446	C
47	5	449	C
47	5	450	G
47	5	452	A
47	5	453	G
47	5	454	U
47	5	457	G
47	5	466	A
47	5	467	U
47	5	468	U
47	5	469	C
47	5	481	G
47	5	481(A)	C
47	5	482	G
47	5	483	G
47	5	484	U
47	5	485	C
47	5	486	C
47	5	490	C
47	5	492	U
47	5	493	G
47	5	495	C
47	5	497	G
47	5	498	C
47	5	499	G
47	5	505	G
47	5	510	U
47	5	649	A
47	5	654	C
47	5	658	C
47	5	660	G
47	5	667	A
47	5	668	C
47	5	669	C
47	5	670	G

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Mol	Chain	Res	Type
47	5	672	C
47	5	683	C
47	5	685	C
47	5	687	U
47	5	696	C
47	5	697	G
47	5	702	U
47	5	704	C
47	5	705	G
47	5	708	G
47	5	722	G
47	5	729	G
47	5	730	G
47	5	731	G
47	5	734	G
47	5	738	C
47	5	738(A)	C
47	5	739	G
47	5	744	G
47	5	747	A
47	5	748	G
47	5	749	G
47	5	750	U
47	5	752	G
47	5	756	G
47	5	758	G
47	5	911	U
47	5	913	U
47	5	914	U
47	5	917	A
47	5	918	G
47	5	923	C
47	5	924	C
47	5	925	C
47	5	926	G
47	5	929	A
47	5	931	C
47	5	932	A
47	5	933	G
47	5	934	C
47	5	935	A
47	5	935(A)	G

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Mol	Chain	Res	Type
47	5	936	C
47	5	937	U
47	5	939	G
47	5	941	C
47	5	943	A
47	5	944	A
47	5	945	U
47	5	956	A
47	5	957	G
47	5	959	G
47	5	960	A
47	5	961	G
47	5	962	C
47	5	963	G
47	5	964	A
47	5	965	G
47	5	966	A
47	5	967	C
47	5	968	C
47	5	969	C
47	5	972	C
47	5	973	G
47	5	979	C
47	5	983	C
47	5	990	C
47	5	1071	C
47	5	1072	C
47	5	1073	G
47	5	1075	G
47	5	1076	C
47	5	1078	A
47	5	1079	C
47	5	1082	C
47	5	1174	G
47	5	1175	A
47	5	1177	U
47	5	1179	U
47	5	1184	A
47	5	1189	G
47	5	1194	G
47	5	1195	G
47	5	1209	U

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Mol	Chain	Res	Type
47	5	1210	C
47	5	1211	G
47	5	1212	G
47	5	1214	C
47	5	1215	C
47	5	1234	G
47	5	1235	G
47	5	1236	C
47	5	1237	C
47	5	1238	A
47	5	1239	C
47	5	1272	C
47	5	1273	G
47	5	1274	A
47	5	1275	G
47	5	1276	C
47	5	1284	G
47	5	1287	G
47	5	1288	G
47	5	1292	C
47	5	1293	G
47	5	1295	U
47	5	1296	G
47	5	1301	C
47	5	1303	A
47	5	1304	C
47	5	1326	A
47	5	1328	G
47	5	1329	G
47	5	1330	A
47	5	1337	A
47	5	1354	A
47	5	1359	G
47	5	1364	U
47	5	1370	G
47	5	1371	A
47	5	1377	G
47	5	1378	C
47	5	1379	C
47	5	1381	U
47	5	1387	A
47	5	1394	G

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Mol	Chain	Res	Type
47	5	1397	A
47	5	1398	A
47	5	1401	C
47	5	1403	G
47	5	1416	G
47	5	1418	C
47	5	1419	G
47	5	1420	A
47	5	1421	G
47	5	1429	C
47	5	1435	G
47	5	1436	C
47	5	1437	C
47	5	1438	U
47	5	1440	U
47	5	1441	C
47	5	1442	C
47	5	1445	U
47	5	1446	C
47	5	1453	G
47	5	1456	C
47	5	1457	G
47	5	1458	C
47	5	1459	A
47	5	1465	G
47	5	1475	G
47	5	1477	C
47	5	1478	C
47	5	1481	C
47	5	1482	G
47	5	1483	C
47	5	1484	G
47	5	1485	C
47	5	1486	C
47	5	1497	A
47	5	1498	G
47	5	1502	G
47	5	1504	G
47	5	1516	G
47	5	1518	A
47	5	1523	A
47	5	1525	A

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Mol	Chain	Res	Type
47	5	1534	A
47	5	1535	C
47	5	1547	A
47	5	1554	A
47	5	1563	A
47	5	1564	A
47	5	1566	C
47	5	1568	C
47	5	1574	G
47	5	1578	U
47	5	1586	G
47	5	1591	U
47	5	1592	G
47	5	1596	U
47	5	1612	G
47	5	1613	A
47	5	1624	G
47	5	1625	G
47	5	1628	C
47	5	1631	A
47	5	1633	G
47	5	1634	A
47	5	1640	C
47	5	1641	G
47	5	1654	G
47	5	1655	C
47	5	1656	U
47	5	1661	C
47	5	1670	G
47	5	1676	C
47	5	1677	U
47	5	1678	C
47	5	1679	A
47	5	1691	G
47	5	1724	G
47	5	1726	U
47	5	1734	G
47	5	1735	U
47	5	1740	C
47	5	1741	G
47	5	1742	A
47	5	1750	G

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Mol	Chain	Res	Type
47	5	1753	G
47	5	1755	C
47	5	1756	U
47	5	1757	U
47	5	1760	G
47	5	1761	G
47	5	1763	C
47	5	1764	G
47	5	1768	C
47	5	1772	C
47	5	1773	U
47	5	1776	A
47	5	1780	A
47	5	1781	U
47	5	1785	C
47	5	1787	A
47	5	1799	G
47	5	1800	U
47	5	1804	A
47	5	1805	A
47	5	1818	G
47	5	1819	G
47	5	1821	G
47	5	1822	U
47	5	1823	G
47	5	1828	C
47	5	1833	G
47	5	1834	U
47	5	1835	G
47	5	1836	G
47	5	1837	A
47	5	1842	G
47	5	1855	G
47	5	1867	A
47	5	1869	G
47	5	1882	U
47	5	1893	C
47	5	1897	A
47	5	1910	G
47	5	1911	C
47	5	1918	U
47	5	1920	C

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Mol	Chain	Res	Type
47	5	1921	C
47	5	1922	G
47	5	1923	A
47	5	1931	C
47	5	1933	G
47	5	1935	C
47	5	1936	C
47	5	1941	A
47	5	1948	G
47	5	1952	G
47	5	1957	U
47	5	1959	U
47	5	1960	A
47	5	1961	G
47	5	1962	A
47	5	1963	C
47	5	1967	A
47	5	1976	G
47	5	1977	C
47	5	1978	C
47	5	1979	A
47	5	1980	U
47	5	1983	A
47	5	1984	A
47	5	1986	U
47	5	1987	C
47	5	1988	G
47	5	1991	A
47	5	1993	C
47	5	1997	U
47	5	2001	G
47	5	2002	A
47	5	2003	G
47	5	2004	U
47	5	2005	G
47	5	2007	G
47	5	2008	U
47	5	2011	C
47	5	2024	G
47	5	2026	A
47	5	2034	G
47	5	2046	G

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Mol	Chain	Res	Type
47	5	2047	A
47	5	2048	U
47	5	2052	G
47	5	2055	G
47	5	2056	G
47	5	2062	C
47	5	2064	G
47	5	2069	A
47	5	2070	U
47	5	2084	U
47	5	2085	G
47	5	2089	G
47	5	2090	U
47	5	2092	G
47	5	2093	G
47	5	2094	C
47	5	2095	A
47	5	2097	A
47	5	2098	G
47	5	2100	G
47	5	2101	A
47	5	2102	G
47	5	2104	A
47	5	2105	A
47	5	2106	G
47	5	2107	A
47	5	2108	G
47	5	2110	G
47	5	2259	G
47	5	2260	C
47	5	2262	G
47	5	2266	C
47	5	2267	U
47	5	2268	A
47	5	2269	C
47	5	2270	G
47	5	2274	C
47	5	2275	G
47	5	2277	C
47	5	2278	G
47	5	2279	A
47	5	2289	C

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Mol	Chain	Res	Type
47	5	2300	A
47	5	2301	G
47	5	2313	A
47	5	2314	G
47	5	2331	G
47	5	2333	G
47	5	2348	G
47	5	2351	C
47	5	2364	G
47	5	2366	A
47	5	2370	A
47	5	2374	A
47	5	2395	A
47	5	2396	A
47	5	2399	G
47	5	2416	G
47	5	2417	A
47	5	2422	C
47	5	2424	G
47	5	2425	U
47	5	2426	U
47	5	2428	A
47	5	2429	A
47	5	2433	G
47	5	2441	C
47	5	2447	U
47	5	2450	G
47	5	2467	U
47	5	2468	U
47	5	2469	C
47	5	2471	G
47	5	2475	G
47	5	2479	G
47	5	2483	G
47	5	2485	U
47	5	2488	C
47	5	2489	C
47	5	2490	U
47	5	2491	C
47	5	2493	G
47	5	2495	U
47	5	2503	G

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Mol	Chain	Res	Type
47	5	2504	C
47	5	2505	C
47	5	2506	G
47	5	2513	A
47	5	2521	G
47	5	2530	U
47	5	2537	A
47	5	2546	G
47	5	2547	G
47	5	2553	A
47	5	2554	U
47	5	2555	G
47	5	2564	G
47	5	2566	G
47	5	2571	C
47	5	2575	U
47	5	2583	C
47	5	2587	A
47	5	2601	A
47	5	2618	G
47	5	2620	G
47	5	2627	C
47	5	2638	G
47	5	2640	G
47	5	2647	A
47	5	2658	G
47	5	2660	A
47	5	2661	U
47	5	2662	G
47	5	2663	G
47	5	2669	C
47	5	2670	C
47	5	2673	G
47	5	2676	A
47	5	2680	G
47	5	2681	G
47	5	2686	G
47	5	2687	U
47	5	2688	G
47	5	2689	C
47	5	2694	G
47	5	2695	A

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Mol	Chain	Res	Type
47	5	2696	A
47	5	2707	U
47	5	2708	U
47	5	2709	C
47	5	2710	C
47	5	2711	G
47	5	2712	G
47	5	2716	C
47	5	2719	C
47	5	2721	G
47	5	2725	A
47	5	2726	G
47	5	2735	G
47	5	2740	U
47	5	2743	A
47	5	2754	G
47	5	2755	A
47	5	2760	G
47	5	2761	U
47	5	2763	U
47	5	2764	A
47	5	2769	U
47	5	2772	C
47	5	2787	A
47	5	2788	U
47	5	2789	A
47	5	2790	U
47	5	2794	C
47	5	2795	A
47	5	2798	A
47	5	2806	A
47	5	2807	A
47	5	2814	C
47	5	2819	U
47	5	2826	U
47	5	2827	G
47	5	2828	U
47	5	2829	U
47	5	2835	A
47	5	2838	G
47	5	2842	G
47	5	2855	G

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Mol	Chain	Res	Type
47	5	2857	A
47	5	2858	A
47	5	2862	G
47	5	2864	A
47	5	2875	C
47	5	2876	G
47	5	2884	G
47	5	2896	G
47	5	2897	G
47	5	3598	C
47	5	3604	A
47	5	3605	C
47	5	3615	G
47	5	3617	G
47	5	3625	G
47	5	3626	G
47	5	3630	A
47	5	3635	A
47	5	3644	U
47	5	3646	A
47	5	3662	A
47	5	3673	C
47	5	3674	G
47	5	3685	C
47	5	3692	A
47	5	3696	C
47	5	3698	G
47	5	3711	A
47	5	3712	A
47	5	3722	G
47	5	3729	U
47	5	3733	A
47	5	3739	C
47	5	3740	G
47	5	3748	A
47	5	3750	G
47	5	3753	G
47	5	3755	G
47	5	3759	A
47	5	3760	A
47	5	3763	A
47	5	3772	U

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Mol	Chain	Res	Type
47	5	3773	U
47	5	3774	A
47	5	3776	G
47	5	3777	G
47	5	3778	U
47	5	3780	G
47	5	3783	A
47	5	3784	A
47	5	3786	U
47	5	3810	C
47	5	3811	G
47	5	3812	C
47	5	3814	U
47	5	3817	A
47	5	3819	G
47	5	3822	U
47	5	3831	U
47	5	3838	U
47	5	3839	G
47	5	3840	U
47	5	3851	U
47	5	3859	G
47	5	3867	A
47	5	3876	A
47	5	3877	A
47	5	3878	C
47	5	3879	G
47	5	3889	G
47	5	3897	G
47	5	3898	G
47	5	3901	A
47	5	3905	A
47	5	3906	A
47	5	3907	G
47	5	3908	A
47	5	3915	U
47	5	3916	G
47	5	3927	U
47	5	3939	G
47	5	3943	A
47	5	4067	U
47	5	4069	U

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Mol	Chain	Res	Type
47	5	4076	G
47	5	4084	G
47	5	4085	A
47	5	4086	G
47	5	4088	C
47	5	4099	G
47	5	4100	C
47	5	4116	C
47	5	4117	U
47	5	4119	C
47	5	4120	U
47	5	4121	G
47	5	4122	G
47	5	4125	C
47	5	4127	A
47	5	4150	G
47	5	4158	C
47	5	4162	C
47	5	4163	U
47	5	4166	G
47	5	4171	C
47	5	4183	G
47	5	4184	G
47	5	4190	U
47	5	4191	G
47	5	4205	A
47	5	4212	A
47	5	4213	A
47	5	4218	U
47	5	4219	A
47	5	4225	G
47	5	4229	U
47	5	4232	U
47	5	4233	A
47	5	4237	C
47	5	4251	A
47	5	4255	A
47	5	4257	A
47	5	4258	C
47	5	4265	U
47	5	4267	G
47	5	4268	A

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Mol	Chain	Res	Type
47	5	4271	A
47	5	4272	G
47	5	4273	A
47	5	4281	A
47	5	4291	G
47	5	4297	G
47	5	4304	A
47	5	4305	G
47	5	4306	U
47	5	4314	C
47	5	4317	A
47	5	4318	C
47	5	4319	C
47	5	4326	G
47	5	4329	G
47	5	4330	G
47	5	4332	C
47	5	4335	C
47	5	4336	A
47	5	4339	A
47	5	4349	C
47	5	4350	C
47	5	4354	U
47	5	4355	G
47	5	4373	G
47	5	4377	G
47	5	4378	A
47	5	4379	A
47	5	4380	A
47	5	4387	C
47	5	4394	A
47	5	4395	U
47	5	4396	A
47	5	4398	C
47	5	4401	G
47	5	4415	A
47	5	4419	U
47	5	4421	C
47	5	4422	A
47	5	4437	U
47	5	4438	U
47	5	4440	G

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Mol	Chain	Res	Type
47	5	4441	A
47	5	4444	C
47	5	4448	G
47	5	4449	A
47	5	4450	U
47	5	4453	C
47	5	4463	U
47	5	4464	A
47	5	4471	U
47	5	4475	G
47	5	4476	C
47	5	4488	A
47	5	4495	G
47	5	4500	U
47	5	4510	A
47	5	4511	A
47	5	4512	U
47	5	4513	A
47	5	4519	C
47	5	4520	G
47	5	4524	G
47	5	4531	U
47	5	4548	A
47	5	4549	G
47	5	4560	C
47	5	4563	U
47	5	4567	G
47	5	4570	G
47	5	4573	G
47	5	4575	G
47	5	4578	G
47	5	4581	G
47	5	4584	A
47	5	4585	U
47	5	4586	G
47	5	4590	A
47	5	4618	G
47	5	4627	U
47	5	4636	U
47	5	4637	G
47	5	4639	G
47	5	4652	G

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Mol	Chain	Res	Type
47	5	4656	A
47	5	4657	U
47	5	4660	G
47	5	4661	G
47	5	4670	C
47	5	4671	C
47	5	4672	A
47	5	4677	U
47	5	4678	G
47	5	4694	G
47	5	4700	A
47	5	4701	A
47	5	4709	U
47	5	4719	G
47	5	4720	C
47	5	4721	G
47	5	4728	U
47	5	4729	A
47	5	4736	C
47	5	4737	G
47	5	4745	G
47	5	4751	G
47	5	4754	G
47	5	4755	G
47	5	4756	C
47	5	4757	C
47	5	4759	C
47	5	4761	G
47	5	4765	G
47	5	4771	C
47	5	4772	C
47	5	4868	G
47	5	4870	G
47	5	4871	C
47	5	4872	G
47	5	4873	G
47	5	4874	A
47	5	4875	G
47	5	4876	A
47	5	4877	G
47	5	4881	U
47	5	4882	U

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Mol	Chain	Res	Type
47	5	4883	C
47	5	4885	U
47	5	4887	C
47	5	4891	G
47	5	4895	C
47	5	4897	G
47	5	4904	G
47	5	4910	A
47	5	4912	G
47	5	4913	G
47	5	4914	G
47	5	4915	G
47	5	4918	C
47	5	4919	G
47	5	4921	C
47	5	4924	C
47	5	4925	U
47	5	4926	C
47	5	4927	G
47	5	4928	C
47	5	4931	G
47	5	4932	U
47	5	4935	C
47	5	4937	C
47	5	4940	C
47	5	4943	A
47	5	4944	C
47	5	4947	U
47	5	4948	C
47	5	4949	G
47	5	4950	U
47	5	4951	G
47	5	4956	A
47	5	4957	C
47	5	4958	C
47	5	4964	C
47	5	4965	U
47	5	4966	A
47	5	4967	A
47	5	4976	U
47	5	4979	A
47	5	4985	U

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Mol	Chain	Res	Type
47	5	4988	U
47	5	4989	U
47	5	4990	C
47	5	4991	U
47	5	4993	G
47	5	5006	U
47	5	5014	A
47	5	5017	G
47	5	5040	U
47	5	5041	G
47	5	5047	C
47	5	5050	C
47	5	5052	C
47	5	5053	U
47	5	5054	C
47	5	5056	A
47	5	5058	A
47	5	5061	A
47	5	5062	G
48	7	7	G
48	7	13	A
48	7	22	A
48	7	25	G
48	7	33	U
48	7	38	U
48	7	42	A
48	7	53	U
48	7	54	A
48	7	64	G
48	7	74	A
48	7	97	G
48	7	100	A
48	7	109	U
48	7	110	G
48	7	111	C
48	7	117	G
48	7	120	U
49	8	2	G
49	8	3	A
49	8	32	C
49	8	34	U
49	8	35	C

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Mol	Chain	Res	Type
49	8	38	U
49	8	49	G
49	8	52	A
49	8	59	A
49	8	62	A
49	8	63	U
49	8	75	G
49	8	79	G
49	8	86	U
49	8	87	G
49	8	90	C
49	8	94	G
49	8	95	A
49	8	103	A
49	8	105	C
49	8	107	C
49	8	109	C
49	8	110	U
49	8	111	U
49	8	112	G
49	8	114	G
49	8	121	G
49	8	123	U
49	8	124	U
49	8	125	C
49	8	126	C
49	8	127	U
49	8	137	A
49	8	143	G
49	8	147	G
49	8	150	C
50	9	2	A
50	9	3	C
50	9	4	C
50	9	17	C
50	9	25	A
50	9	26	U
50	9	33	G
50	9	44	U
50	9	45	A
50	9	46	A
50	9	56	G

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Mol	Chain	Res	Type
50	9	58	C
50	9	62	G
50	9	65	C
50	9	67	C
50	9	68	A
50	9	70	G
50	9	71	G
50	9	73	C
50	9	74	G
50	9	75	G
50	9	77	A
50	9	79	A
50	9	99	A
50	9	100	U
50	9	103	A
50	9	104	A
50	9	110	U
50	9	111	A
50	9	113	G
50	9	115	U
50	9	116	U
50	9	124	U
50	9	126	G
50	9	127	C
50	9	128	U
50	9	129	C
50	9	130	G
50	9	141	A
50	9	143	U
50	9	147	A
50	9	155	G
50	9	158	A
50	9	161	U
50	9	162	C
50	9	163	U
50	9	167	G
50	9	168	C
50	9	173	A
50	9	175	A
50	9	180	G
50	9	182	C
50	9	183	G

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Mol	Chain	Res	Type
50	9	184	G
50	9	188	C
50	9	189	U
50	9	191	A
50	9	192	C
50	9	200	G
50	9	202	G
50	9	206	G
50	9	213	G
50	9	215	G
50	9	292	A
50	9	293	C
50	9	294	U
50	9	302	A
50	9	304	C
50	9	307	G
50	9	308	G
50	9	309	G
50	9	312	G
50	9	314	U
50	9	318	A
50	9	319	C
50	9	322	C
50	9	331	C
50	9	332	G
50	9	340	C
50	9	343	A
50	9	347	G
50	9	351	G
50	9	360	A
50	9	362	C
50	9	364	A
50	9	368	U
50	9	370	G
50	9	379	C
50	9	381	C
50	9	382	C
50	9	383	G
50	9	384	U
50	9	385	G
50	9	386	C
50	9	400	C

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Mol	Chain	Res	Type
50	9	408	A
50	9	409	C
50	9	410	G
50	9	417	C
50	9	418	A
50	9	434	G
50	9	435	A
50	9	438	G
50	9	448	A
50	9	449	A
50	9	450	C
50	9	454	U
50	9	460	A
50	9	464	A
50	9	465	A
50	9	466	G
50	9	472	C
50	9	473	A
50	9	474	G
50	9	475	C
50	9	476	A
50	9	482	G
50	9	487	U
50	9	492	C
50	9	496	C
50	9	500	A
50	9	501	C
50	9	508	A
50	9	512	A
50	9	532	C
50	9	533	A
50	9	544	G
50	9	545	A
50	9	546	G
50	9	548	C
50	9	549	C
50	9	550	C
50	9	551	U
50	9	554	A
50	9	555	A
50	9	556	U
50	9	557	U

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Mol	Chain	Res	Type
50	9	559	G
50	9	560	A
50	9	562	U
50	9	563	G
50	9	564	A
50	9	568	C
50	9	576	A
50	9	583	A
50	9	587	A
50	9	588	G
50	9	589	G
50	9	590	A
50	9	591	U
50	9	592	C
50	9	595	U
50	9	597	G
50	9	598	G
50	9	604	A
50	9	606	G
50	9	607	U
50	9	608	C
50	9	614	C
50	9	620	G
50	9	621	C
50	9	628	A
50	9	629	A
50	9	631	U
50	9	637	U
50	9	643	A
50	9	644	G
50	9	659	G
50	9	660	C
50	9	663	C
50	9	664	A
50	9	668	A
50	9	669	A
50	9	670	A
50	9	671	A
50	9	672	A
50	9	673	G
50	9	678	U
50	9	684	G

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Mol	Chain	Res	Type
50	9	688	U
50	9	689	U
50	9	732	U
50	9	733	C
50	9	752	G
50	9	753	C
50	9	754	G
50	9	798	G
50	9	811	A
50	9	812	A
50	9	821	G
50	9	822	U
50	9	830	A
50	9	834	C
50	9	847	A
50	9	861	A
50	9	868	G
50	9	869	A
50	9	870	A
50	9	871	U
50	9	872	A
50	9	873	G
50	9	874	G
50	9	875	A
50	9	877	C
50	9	878	G
50	9	885	U
50	9	887	U
50	9	890	U
50	9	892	U
50	9	902	G
50	9	913	A
50	9	914	U
50	9	920	A
50	9	922	A
50	9	930	C
50	9	933	G
50	9	934	G
50	9	943	U
50	9	955	A
50	9	971	G
50	9	985	G

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Mol	Chain	Res	Type
50	9	990	A
50	9	992	A
50	9	999	G
50	9	1016	U
50	9	1017	U
50	9	1023	A
50	9	1030	A
50	9	1041	G
50	9	1044	G
50	9	1060	A
50	9	1061	U
50	9	1062	A
50	9	1067	C
50	9	1078	C
50	9	1083	A
50	9	1085	C
50	9	1089	G
50	9	1099	G
50	9	1100	A
50	9	1111	U
50	9	1114	U
50	9	1115	U
50	9	1116	C
50	9	1117	C
50	9	1118	C
50	9	1120	U
50	9	1121	G
50	9	1131	G
50	9	1132	C
50	9	1133	A
50	9	1138	C
50	9	1139	C
50	9	1144	A
50	9	1148	A
50	9	1149	A
50	9	1150	A
50	9	1153	C
50	9	1154	U
50	9	1165	G
50	9	1166	G
50	9	1195	A
50	9	1207	G

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Mol	Chain	Res	Type
50	9	1208	A
50	9	1211	G
50	9	1213	C
50	9	1215	C
50	9	1221	G
50	9	1224	G
50	9	1227	G
50	9	1240	A
50	9	1242	U
50	9	1251	A
50	9	1253	A
50	9	1254	C
50	9	1256	G
50	9	1257	G
50	9	1259	A
50	9	1265	A
50	9	1266	C
50	9	1268	C
50	9	1271	C
50	9	1274	G
50	9	1275	G
50	9	1281	G
50	9	1284	A
50	9	1285	G
50	9	1286	G
50	9	1287	A
50	9	1289	U
50	9	1293	A
50	9	1298	G
50	9	1299	A
50	9	1300	U
50	9	1301	A
50	9	1302	G
50	9	1303	C
50	9	1307	U
50	9	1308	U
50	9	1313	A
50	9	1314	U
50	9	1316	C
50	9	1321	G
50	9	1322	G
50	9	1330	G

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Mol	Chain	Res	Type
50	9	1331	C
50	9	1341	C
50	9	1342	U
50	9	1348	G
50	9	1354	G
50	9	1369	A
50	9	1371	U
50	9	1372	U
50	9	1375	G
50	9	1376	A
50	9	1378	A
50	9	1382	A
50	9	1394	G
50	9	1395	C
50	9	1396	A
50	9	1397	U
50	9	1401	A
50	9	1402	A
50	9	1404	U
50	9	1406	G
50	9	1410	C
50	9	1424	G
50	9	1428	G
50	9	1429	G
50	9	1439	A
50	9	1449	G
50	9	1454	A
50	9	1458	G
50	9	1459	G
50	9	1462	U
50	9	1463	U
50	9	1466	G
50	9	1473	G
50	9	1475	G
50	9	1476	A
50	9	1477	U
50	9	1478	U
50	9	1480	A
50	9	1490	G
50	9	1494	U
50	9	1495	G
50	9	1497	G

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Mol	Chain	Res	Type
50	9	1498	A
50	9	1509	U
50	9	1510	G
50	9	1521	C
50	9	1522	A
50	9	1531	A
50	9	1533	A
50	9	1536	G
50	9	1539	U
50	9	1544	C
50	9	1545	A
50	9	1548	G
50	9	1552	G
50	9	1553	C
50	9	1555	U
50	9	1556	A
50	9	1557	C
50	9	1560	U
50	9	1570	G
50	9	1574	C
50	9	1575	G
50	9	1580	A
50	9	1581	C
50	9	1582	C
50	9	1585	U
50	9	1586	U
50	9	1587	G
50	9	1588	A
50	9	1589	A
50	9	1600	G
50	9	1601	A
50	9	1602	U
50	9	1604	G
50	9	1621	U
50	9	1623	A
50	9	1625	U
50	9	1637	A
50	9	1638	G
50	9	1639	G
50	9	1641	A
50	9	1647	A
50	9	1648	G

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Mol	Chain	Res	Type
50	9	1654	G
50	9	1661	A
50	9	1664	A
50	9	1665	G
50	9	1671	G
50	9	1680	G
50	9	1682	C
50	9	1683	C
50	9	1686	G
50	9	1689	C
50	9	1695	A
50	9	1698	C
50	9	1699	A
50	9	1703	C
50	9	1715	A
50	9	1721	U
50	9	1722	G
50	9	1726	G
50	9	1728	U
50	9	1729	U
50	9	1730	U
50	9	1737	G
50	9	1744	G
50	9	1745	A
50	9	1753	C
50	9	1757	G
50	9	1758	G
50	9	1760	G
50	9	1772	C
50	9	1783	C
50	9	1785	C
50	9	1800	A
50	9	1801	A
50	9	1823	A
50	9	1824	A
50	9	1825	A
50	9	1826	G
50	9	1829	G
50	9	1831	A
50	9	1835	A
50	9	1836	G
50	9	1838	U

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Mol	Chain	Res	Type
50	9	1849	G
50	9	1851	A
50	9	1852	C
50	9	1861	G
50	9	1862	G
50	9	1863	A
50	9	1865	C
50	9	1866	A
50	9	1867	U
50	9	1868	U
50	9	1869	A
84	hh	42	C
84	hh	43	A
84	hh	45	A
84	hh	46	G
84	hh	49	U
84	hh	52	G
84	hh	54	U
84	hh	55	C

All (258) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	2	20(A)	U
46	3	7	A
46	3	74	C
47	5	12	A
47	5	20	U
47	5	47	A
47	5	48	G
47	5	64	A
47	5	119	G
47	5	125	C
47	5	134	G
47	5	135	G
47	5	143	C
47	5	159	C
47	5	209	U
47	5	217	C
47	5	226	G
47	5	245	C
47	5	265	C

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Mol	Chain	Res	Type
47	5	275	C
47	5	278	G
47	5	385	A
47	5	406	C
47	5	409	G
47	5	417	G
47	5	449	C
47	5	453	G
47	5	466	A
47	5	480	C
47	5	481(A)	C
47	5	484	U
47	5	485	C
47	5	492	U
47	5	497	G
47	5	498	C
47	5	504	G
47	5	669	C
47	5	696	C
47	5	729	G
47	5	738(A)	C
47	5	747	A
47	5	748	G
47	5	913	U
47	5	916	C
47	5	924	C
47	5	930	G
47	5	933	G
47	5	935(A)	G
47	5	936	C
47	5	956	A
47	5	959	G
47	5	963	G
47	5	966	A
47	5	968	C
47	5	969	C
47	5	971(A)	G
47	5	1071	C
47	5	1072	C
47	5	1174	G
47	5	1209	U
47	5	1211	G

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Mol	Chain	Res	Type
47	5	1214	C
47	5	1236	C
47	5	1238	A
47	5	1287	G
47	5	1291	G
47	5	1294	A
47	5	1295	U
47	5	1325	C
47	5	1329	G
47	5	1358	G
47	5	1370	G
47	5	1378	C
47	5	1380	G
47	5	1420	A
47	5	1440	U
47	5	1445	U
47	5	1455	G
47	5	1477	C
47	5	1481	C
47	5	1484	G
47	5	1485	C
47	5	1534	A
47	5	1563	A
47	5	1633	G
47	5	1654	G
47	5	1678	C
47	5	1733	G
47	5	1734	G
47	5	1740	C
47	5	1804	A
47	5	1818	G
47	5	1833	G
47	5	1834	U
47	5	1835	G
47	5	1892	A
47	5	1910	G
47	5	1921	C
47	5	1935	C
47	5	1947	U
47	5	1960	A
47	5	1979	A
47	5	1983	A

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Mol	Chain	Res	Type
47	5	1986	U
47	5	2001	G
47	5	2025	A
47	5	2046	G
47	5	2068	C
47	5	2088	A
47	5	2089	G
47	5	2100	G
47	5	2265	G
47	5	2266	C
47	5	2278	G
47	5	2313	A
47	5	2369	U
47	5	2394	G
47	5	2396	A
47	5	2398	U
47	5	2425	U
47	5	2428	A
47	5	2467	U
47	5	2468	U
47	5	2474	G
47	5	2475	G
47	5	2490	U
47	5	2502	A
47	5	2529	A
47	5	2546	G
47	5	2661	U
47	5	2695	A
47	5	2724	G
47	5	2754	G
47	5	2794	C
47	5	3625	G
47	5	3673	C
47	5	3697	U
47	5	3710	G
47	5	3809	G
47	5	3876	A
47	5	3878	C
47	5	3888	G
47	5	3904	G
47	5	4075	U
47	5	4076	G

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Mol	Chain	Res	Type
47	5	4084	G
47	5	4119	C
47	5	4121	G
47	5	4124	G
47	5	4162	C
47	5	4170	A
47	5	4204	C
47	5	4232	U
47	5	4254	G
47	5	4266	G
47	5	4272	G
47	5	4378	A
47	5	4395	U
47	5	4448	G
47	5	4449	A
47	5	4463	U
47	5	4488	A
47	5	4572	U
47	5	4583	C
47	5	4656	A
47	5	4671	C
47	5	4699	U
47	5	4719	G
47	5	4871	C
47	5	4872	G
47	5	4876	A
47	5	4884	G
47	5	4925	U
47	5	4936	G
47	5	4942	C
47	5	4947	U
47	5	4965	U
47	5	4966	A
48	7	13	A
48	7	109	U
49	8	2	G
49	8	34	U
49	8	51	U
49	8	85	U
49	8	86	U
49	8	94	G
49	8	110	U

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Mol	Chain	Res	Type
49	8	124	U
50	9	2	A
50	9	72	C
50	9	110	U
50	9	126	G
50	9	160	U
50	9	182	C
50	9	293	C
50	9	369	C
50	9	434	G
50	9	447	A
50	9	448	A
50	9	465	A
50	9	473	A
50	9	474	G
50	9	500	A
50	9	532	C
50	9	553	U
50	9	555	A
50	9	559	G
50	9	563	G
50	9	591	U
50	9	620	G
50	9	642	U
50	9	656	G
50	9	670	A
50	9	688	U
50	9	752	G
50	9	821	G
50	9	861	A
50	9	868	G
50	9	869	A
50	9	870	A
50	9	872	A
50	9	874	G
50	9	1016	U
50	9	1114	U
50	9	1115	U
50	9	1137	U
50	9	1138	C
50	9	1165	G
50	9	1253	A

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Mol	Chain	Res	Type
50	9	1264	C
50	9	1274	G
50	9	1284	A
50	9	1286	G
50	9	1313	A
50	9	1330	G
50	9	1394	G
50	9	1395	C
50	9	1396	A
50	9	1476	A
50	9	1489	A
50	9	1493	C
50	9	1497	G
50	9	1519	U
50	9	1520	G
50	9	1585	U
50	9	1636	G
50	9	1637	A
50	9	1646	C
50	9	1664	A
50	9	1665	G
50	9	1679	A
50	9	1721	U
50	9	1744	G
50	9	1824	A
50	9	1835	A
50	9	1837	G
50	9	1867	U
50	9	1868	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 266 ligands modelled in this entry, 266 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	5	29
50	9	15
45	2	3
85	ii	3
46	3	2
44	t	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2113:G	O3'	2258:C	P	41.35
1	5	1252:C	O3'	1271:G	P	35.75
1	5	1219:G	O3'	1233:G	P	22.89
1	5	3948:C	O3'	4065:G	P	19.77
1	5	1406(C):G	O3'	1411:C	P	18.60
1	5	990:C	O3'	1064:G	P	18.45
1	5	523:C	O3'	638:G	P	18.02
1	5	4138:C	O3'	4146:G	P	18.00
1	5	4101:C	O3'	4107:G	P	17.49
1	5	4777:C	O3'	4859:C	P	16.69
1	5	760:G	O3'	904:C	P	15.23
1	5	5022:U	O3'	5028:G	P	14.88
1	5	1696:C	O3'	1720:C	P	14.26
1	5	182:G	O3'	189:G	P	13.98
1	5	1364:U	O3'	1368:A	P	13.96

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	2901:G	O3'	3597:G	P	13.23
1	5	4729:A	O3'	4735:G	P	10.07
1	5	512:U	O3'	515:C	P	9.81
1	5	1180:C	O3'	1183:C	P	8.91
1	2	19:G	O3'	20:U	P	7.20
1	2	20:U	O3'	20(A):U	P	6.67
1	5	500:G	O3'	504:G	P	6.41
1	5	1100:U	O3'	1168:G	P	5.86
1	3	19:G	O3'	20:U	P	5.64
1	5	1239:C	O3'	1244:G	P	5.34
1	9	689:U	O3'	690:G	P	5.09
1	9	322:C	O3'	323:C	P	5.07
1	9	1412:C	O3'	1413:G	P	5.02
1	9	1410:C	O3'	1411:G	P	4.96
1	9	1411:G	O3'	1412:C	P	4.83
1	5	4740:G	O3'	4743:G	P	4.80
1	3	16:C	O3'	18:U	P	4.79
1	9	798:G	O3'	799:U	P	4.51
1	9	304:C	O3'	305:U	P	4.34
1	9	309:G	O3'	310:C	P	4.34
1	2	16:C	O3'	18:G	P	4.32
1	5	170:C	O3'	171:U	P	3.68
1	9	902:G	O3'	903:A	P	3.46
1	5	4899:G	O3'	4902:C	P	3.43
1	9	886:A	O3'	887:U	P	3.35
1	5	1438:U	O3'	1440:U	P	3.31
1	9	1295:A	O3'	1296:U	P	3.30
1	9	903:A	O3'	904:A	P	3.26
1	5	267:G	O3'	268:G	P	3.23
1	9	1413:G	O3'	1414:A	P	3.16
1	9	1414:A	O3'	1415:C	P	3.14
1	5	751:G	O3'	752:G	P	3.13
1	9	1406:G	O3'	1407:U	P	3.09
1	t	124:GLU	C	125:LEU	N	3.07
1	5	5020:G	O3'	5021:C	P	3.06
1	ii	144:SER	C	145:LYS	N	2.68
1	ii	324:GLU	C	325:ASN	N	2.67
1	ii	374:LEU	C	375:LEU	N	2.52

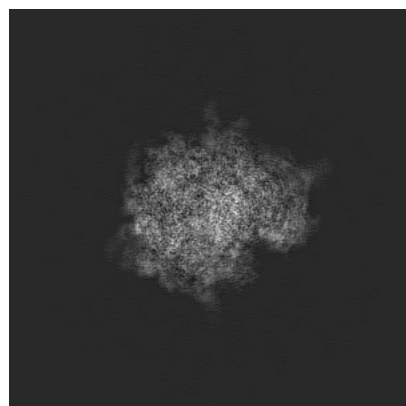
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4132. These allow visual inspection of the internal detail of the map and identification of artifacts.

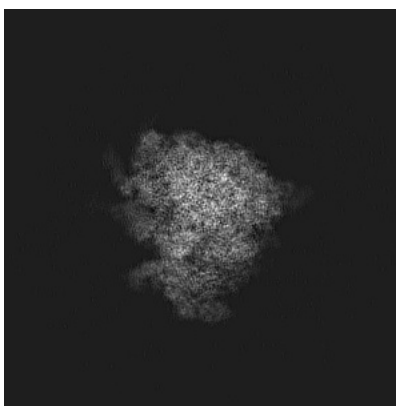
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

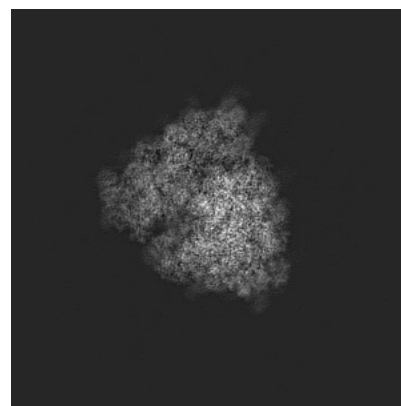
6.1.1 Primary map



X

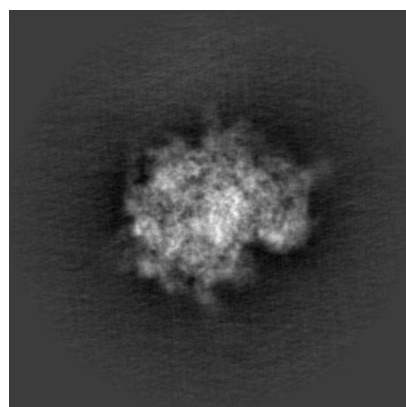


Y

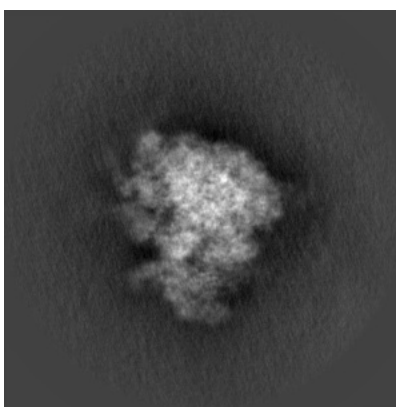


Z

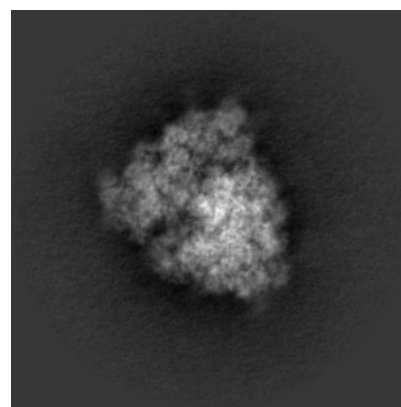
6.1.2 Raw map



X



Y

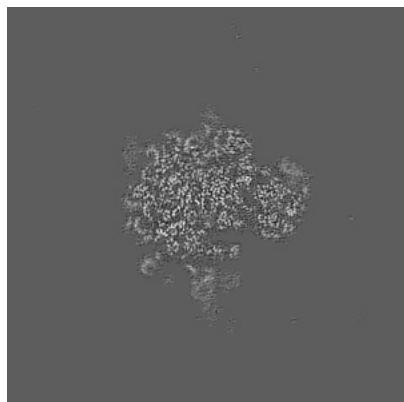


Z

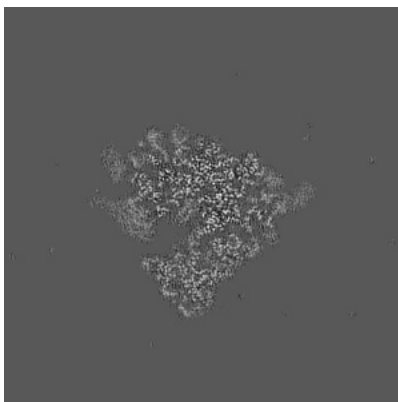
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

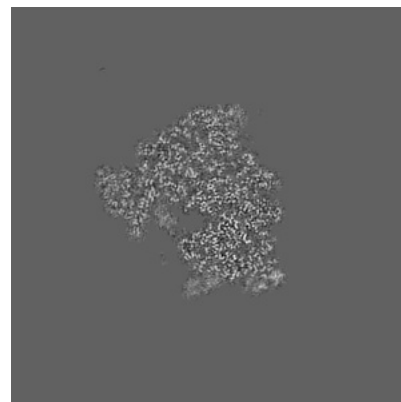
6.2.1 Primary map



X Index: 210

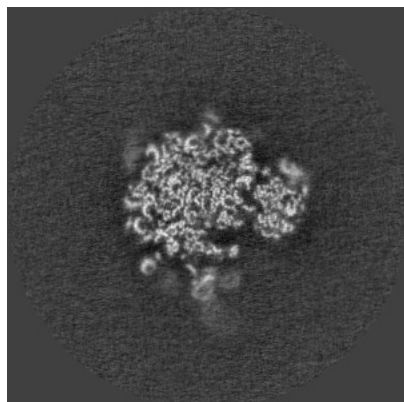


Y Index: 210

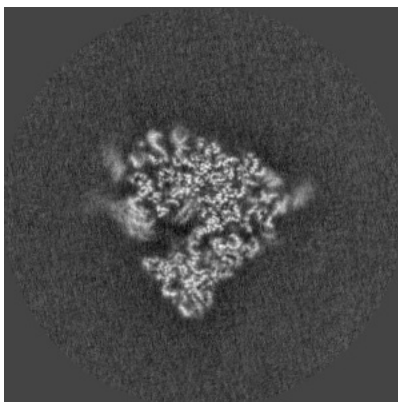


Z Index: 210

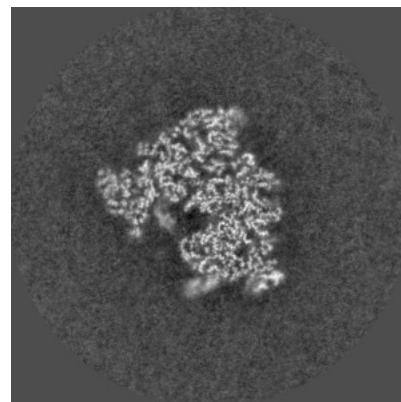
6.2.2 Raw map



X Index: 210



Y Index: 210

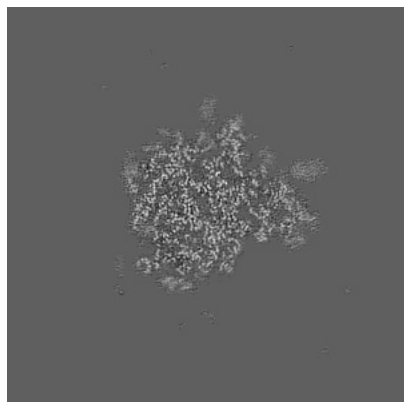


Z Index: 210

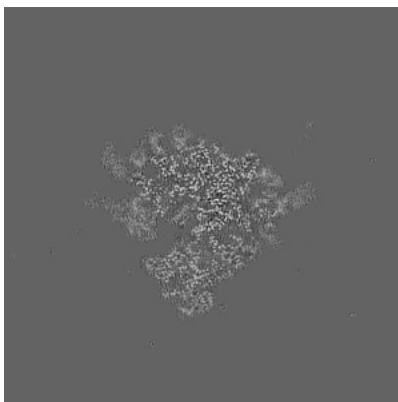
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

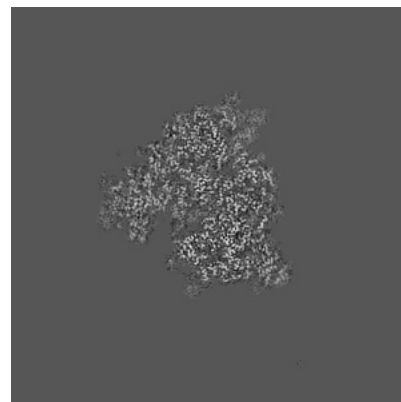
6.3.1 Primary map



X Index: 225

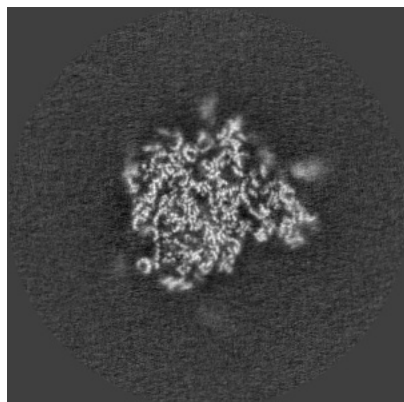


Y Index: 212

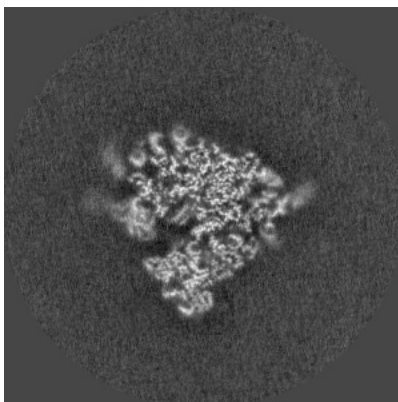


Z Index: 202

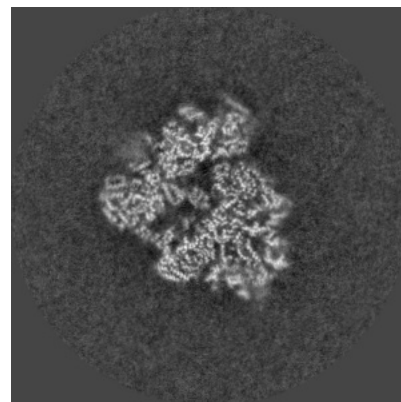
6.3.2 Raw map



X Index: 225



Y Index: 212

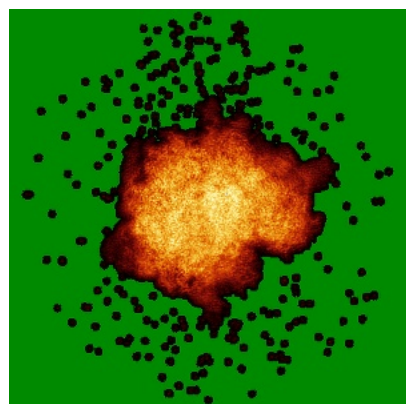


Z Index: 186

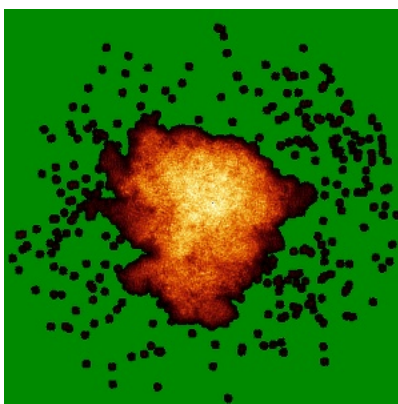
The images above show the largest variance slices of the map in three orthogonal directions.

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

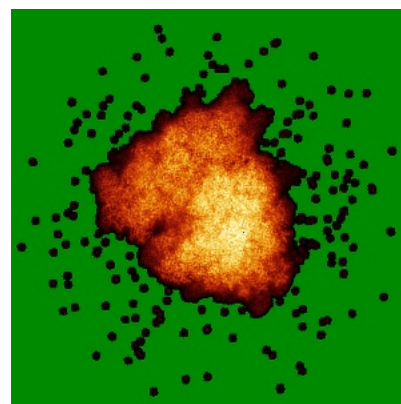
6.4.1 Primary map



X

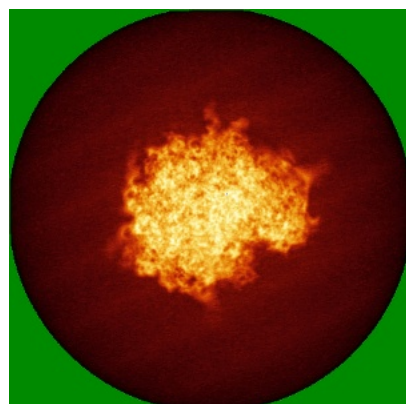


Y

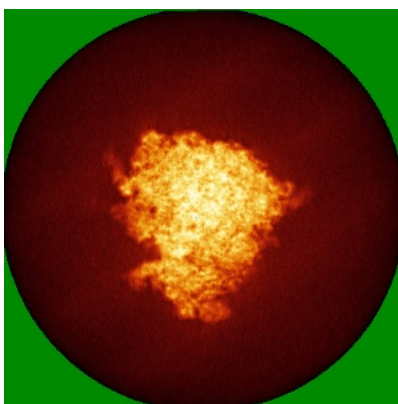


Z

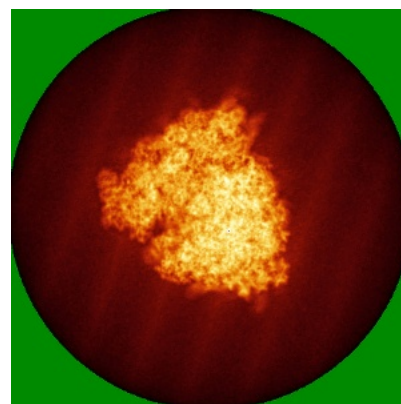
6.4.2 Raw map



X



Y

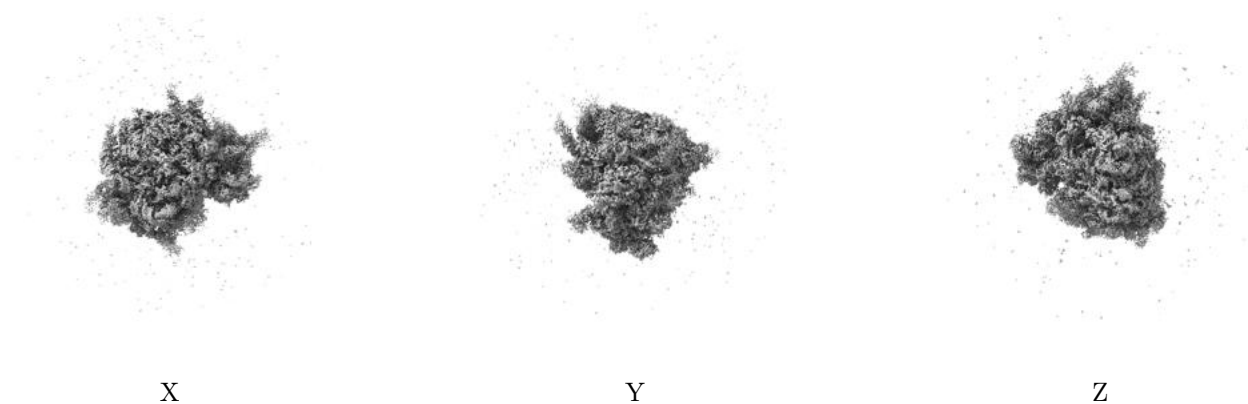


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. 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.

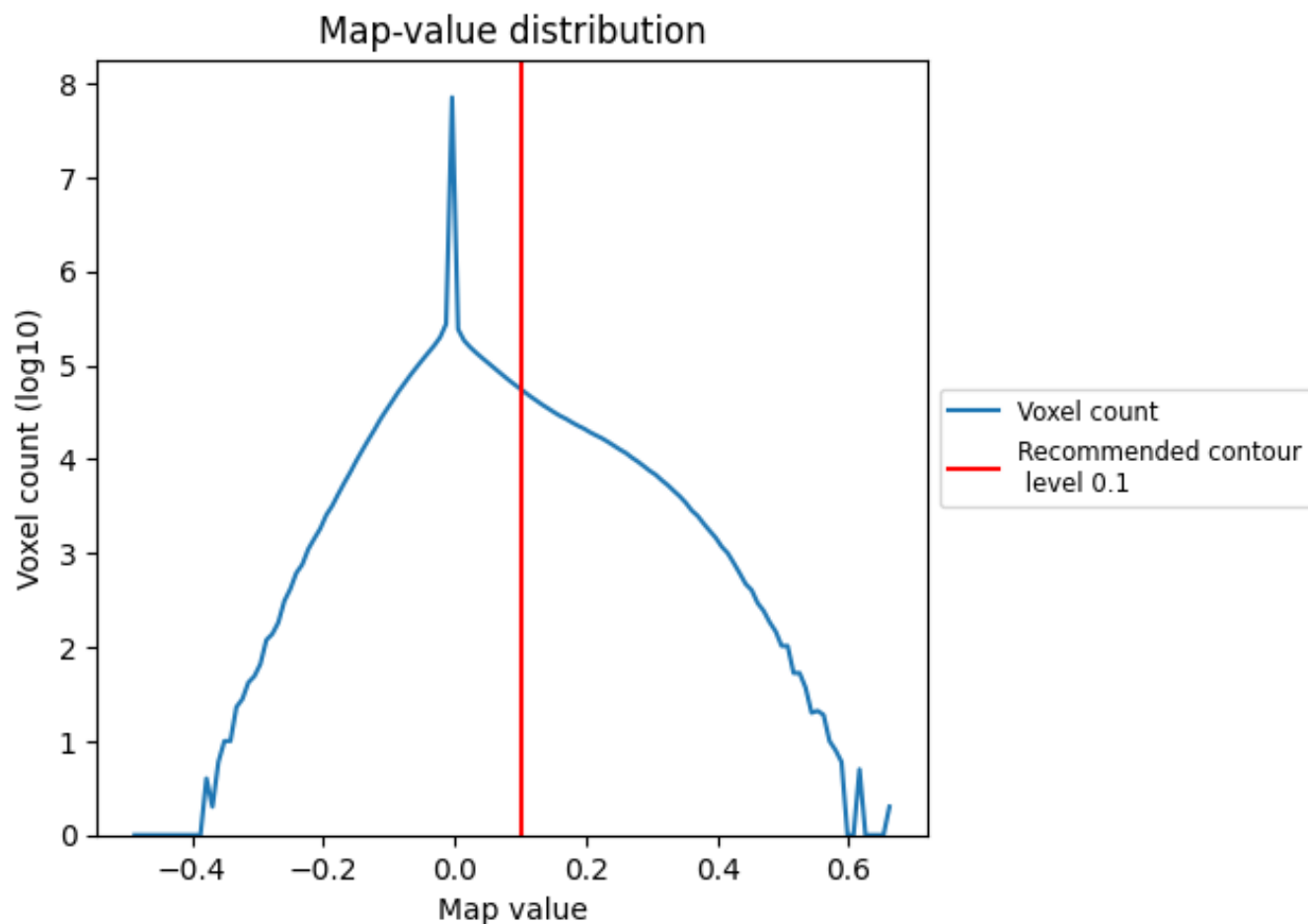
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

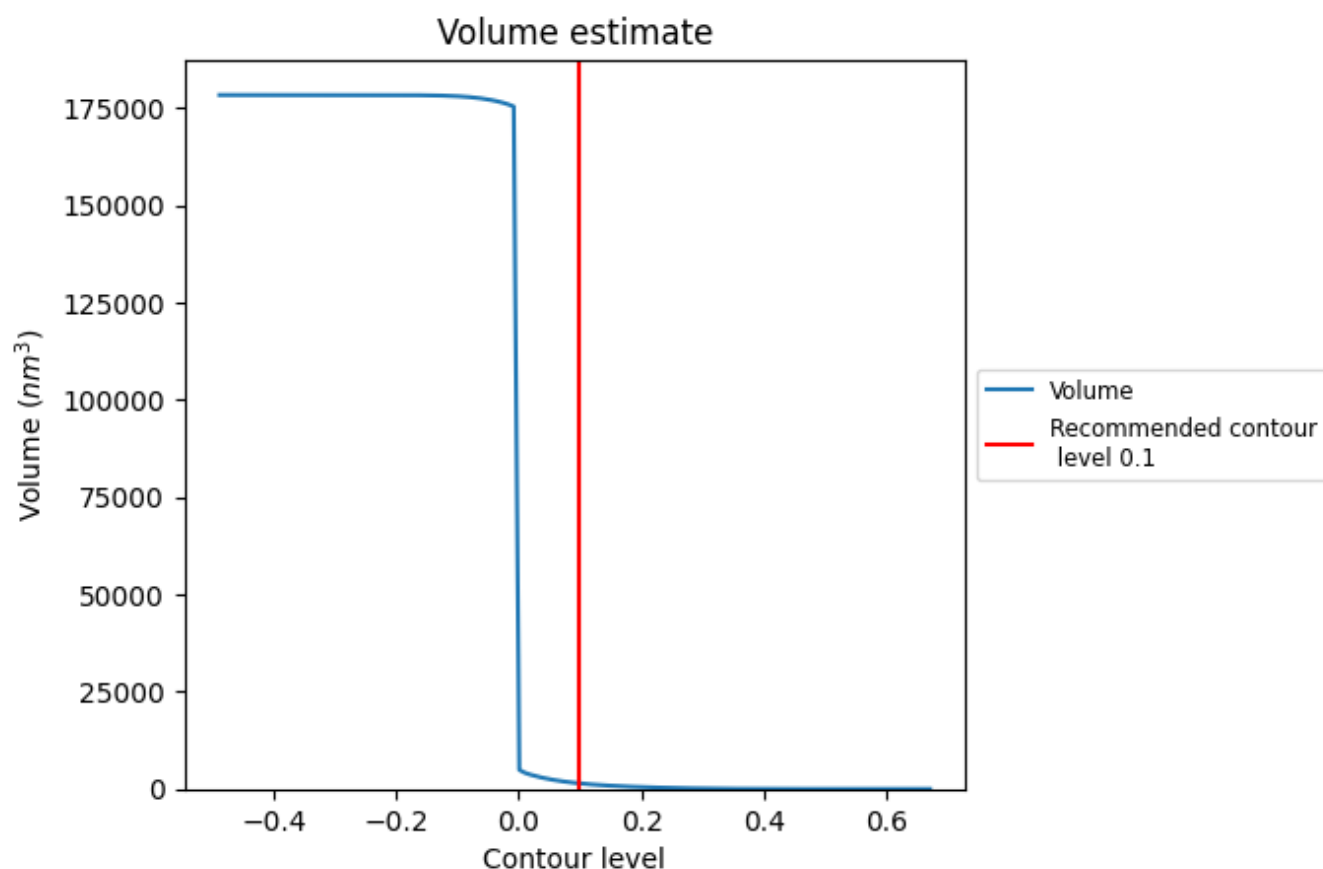
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

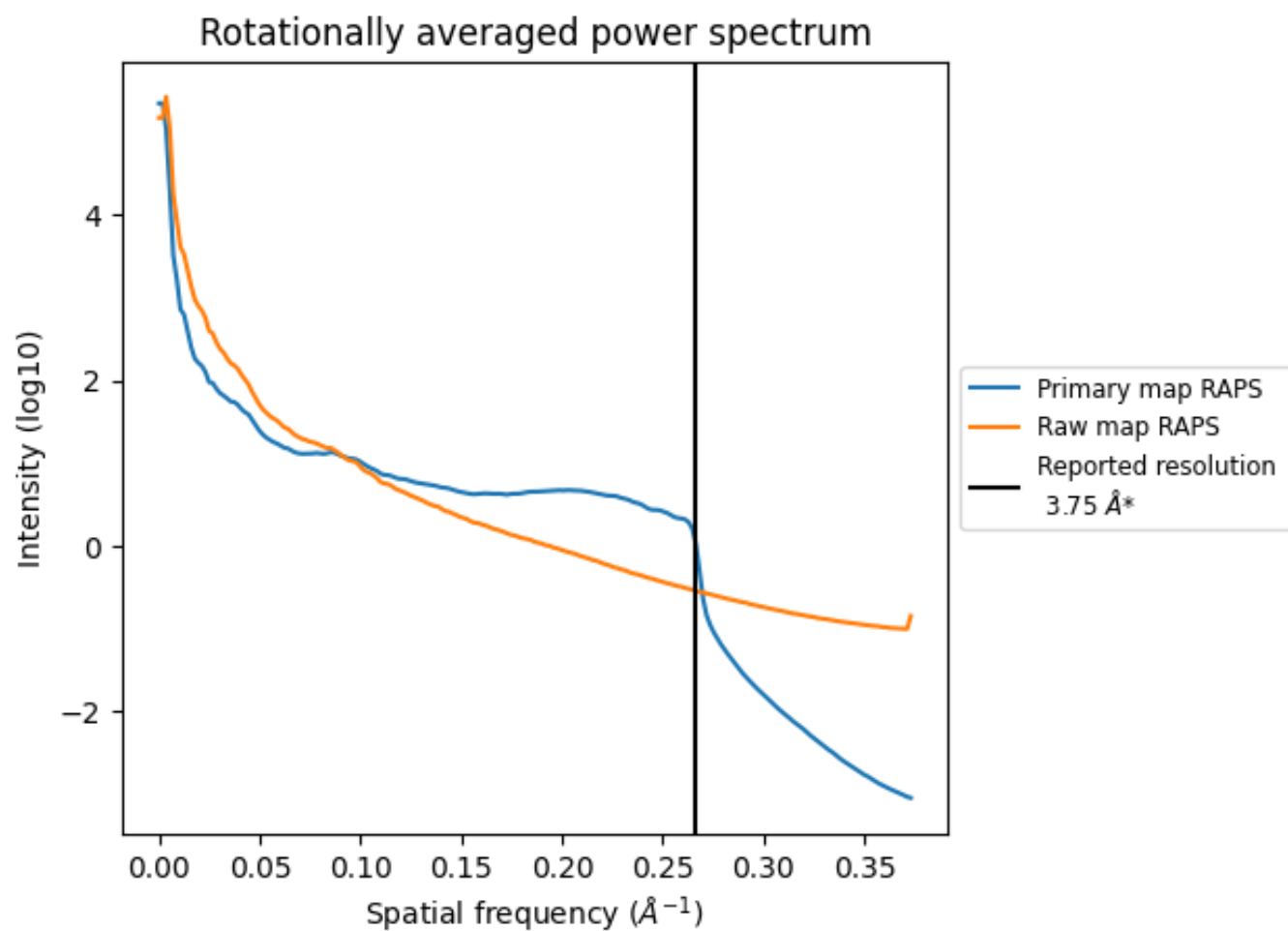
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1430 nm³; this corresponds to an approximate mass of 1291 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 ⓘ

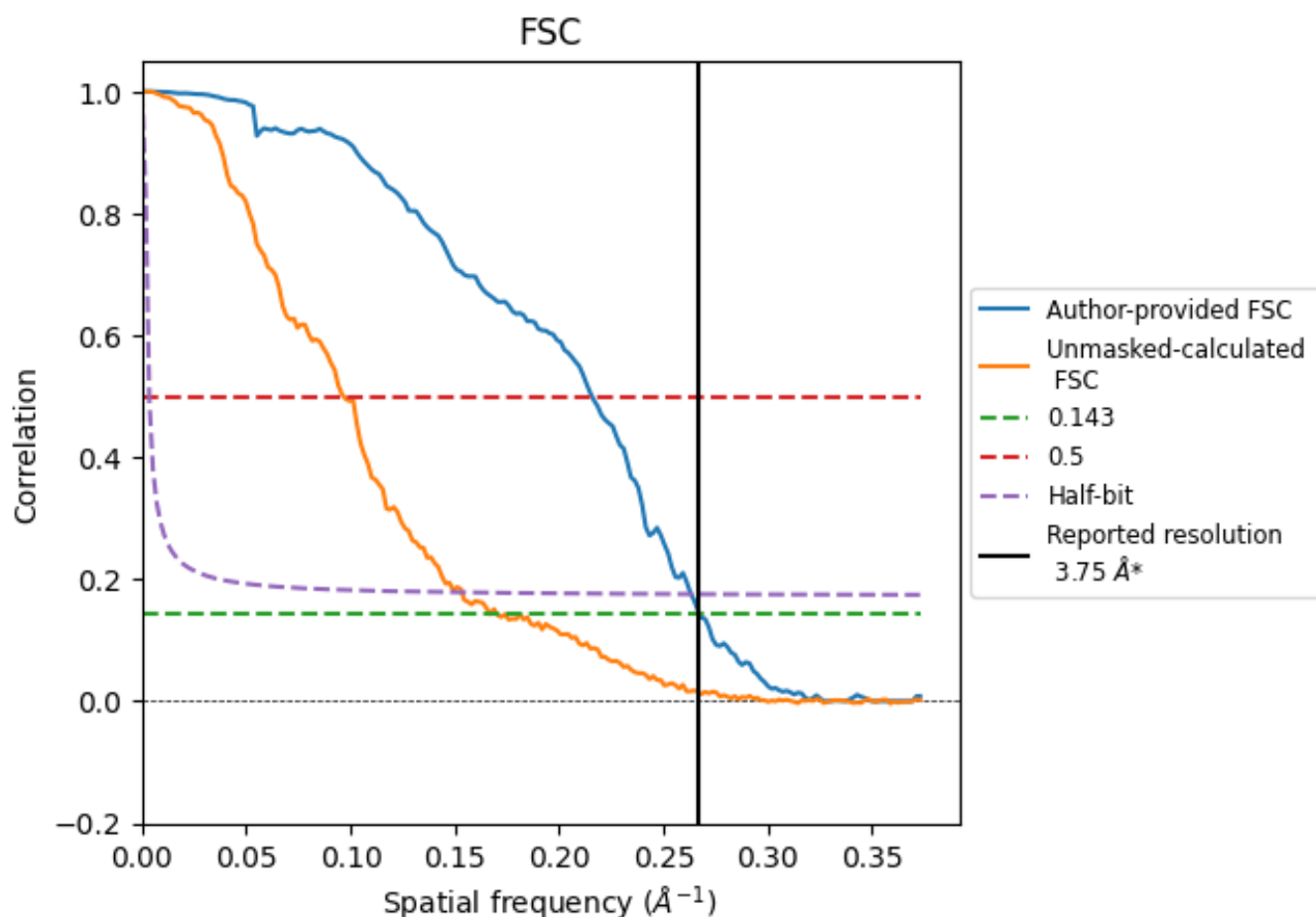


*Reported resolution corresponds to spatial frequency of 0.267 Å⁻¹

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 0.267 Å⁻¹

8.2 Resolution estimates [i](#)

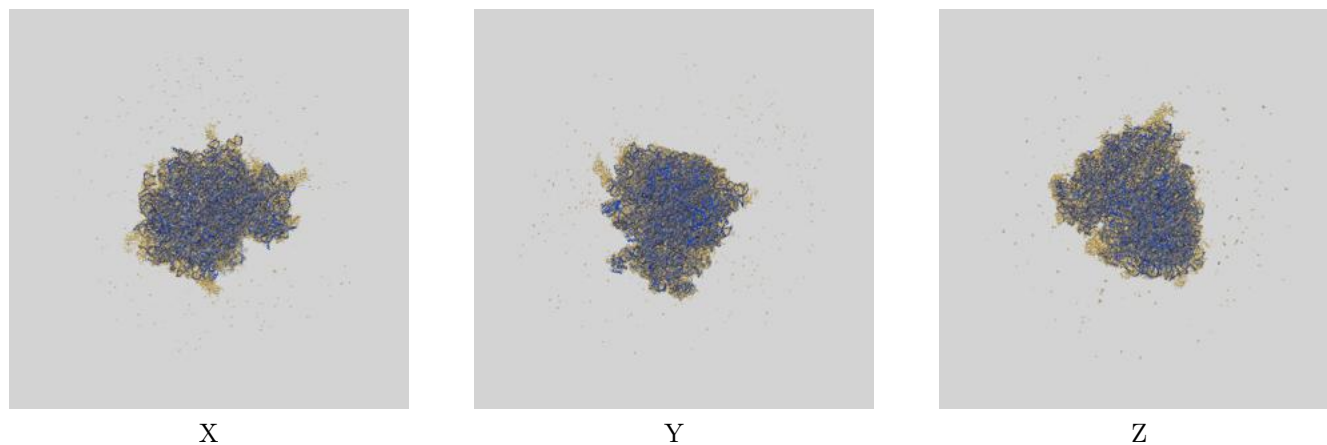
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.75	-	-
Author-provided FSC curve	3.74	4.63	3.80
Unmasked-calculated*	5.99	10.34	6.52

*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 5.99 differs from the reported value 3.75 by more than 10 %

9 Map-model fit [i](#)

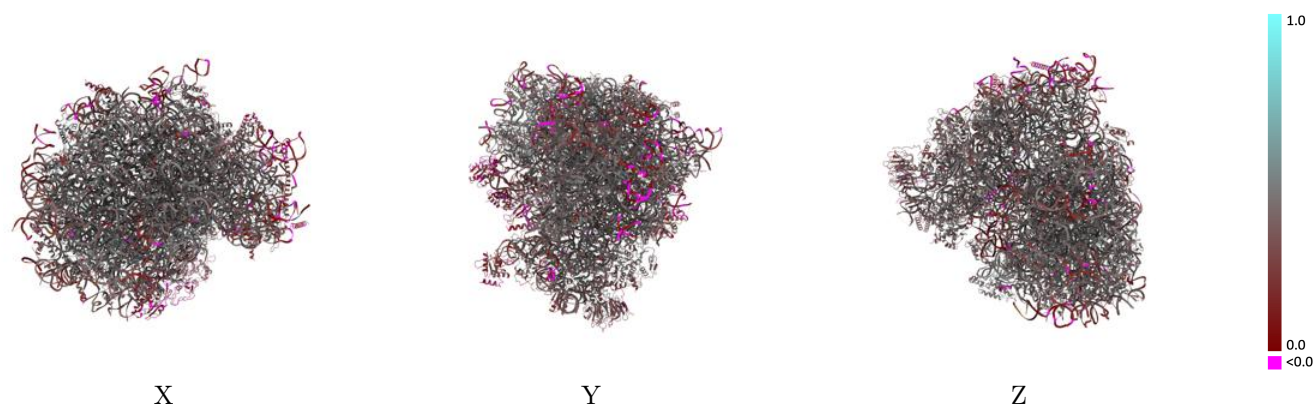
This section contains information regarding the fit between EMDB map EMD-4132 and PDB model 5LZU. Per-residue inclusion information can be found in section [3](#) on page [27](#).

9.1 Map-model overlay [i](#)



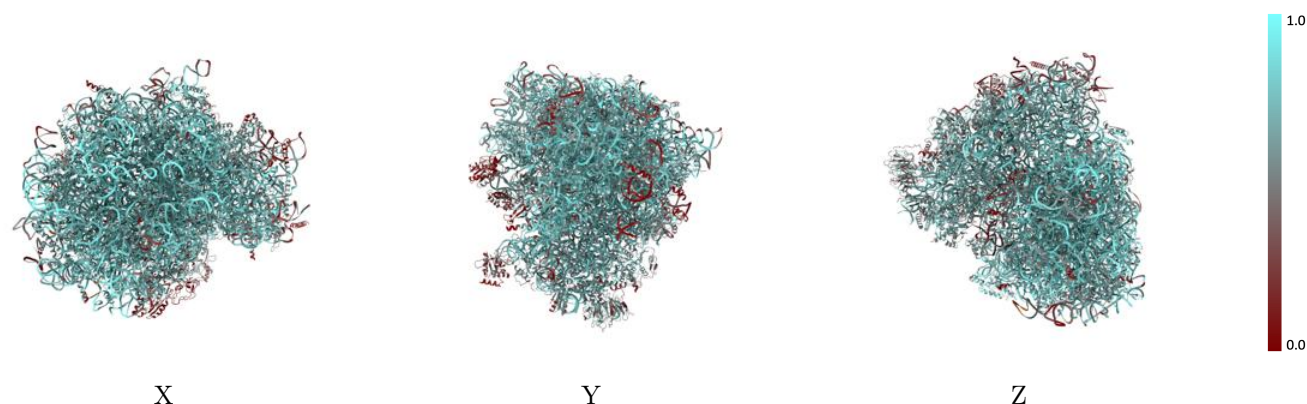
The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



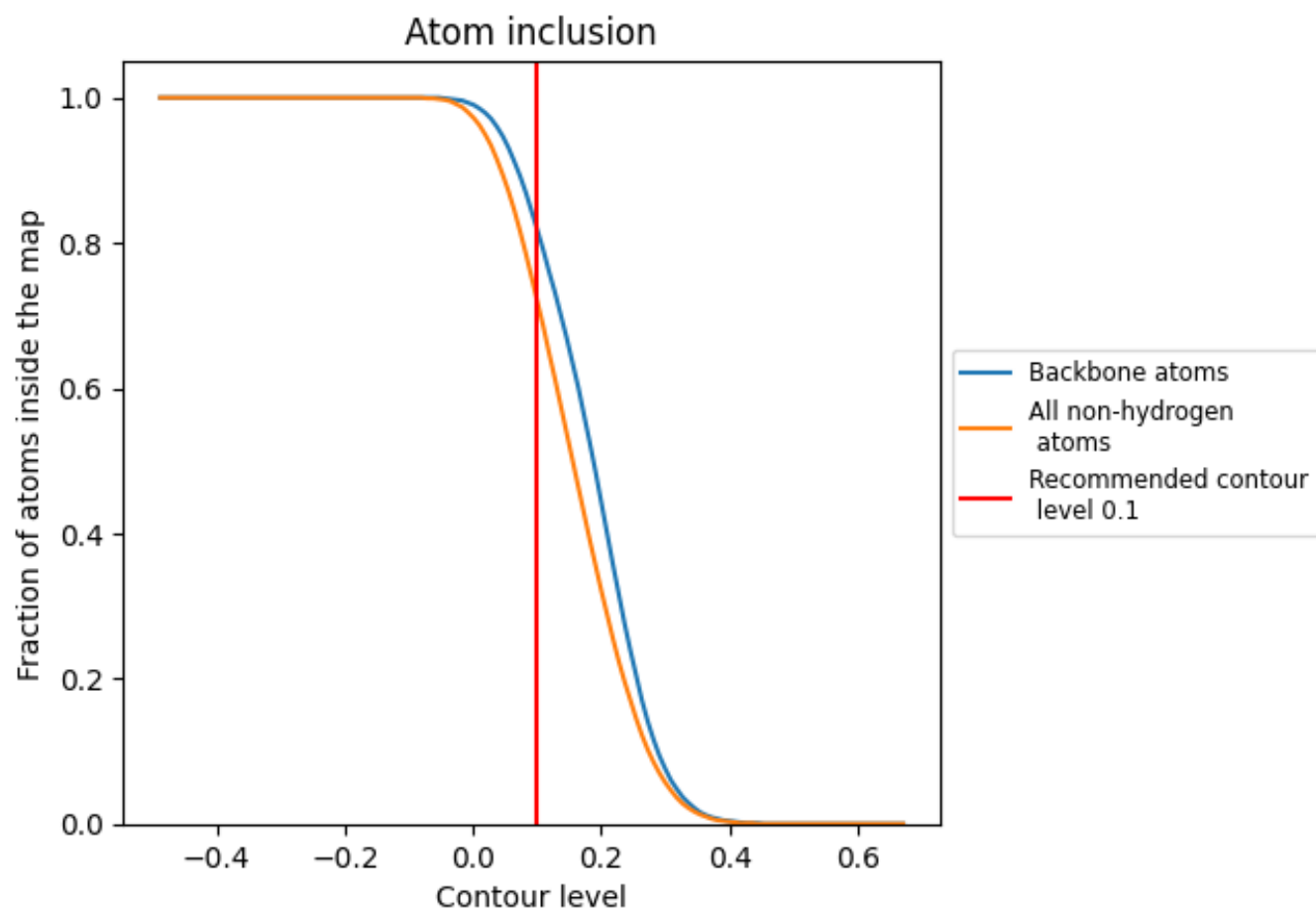
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 72% 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 (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7220	 0.3990
2	 0.5490	 0.3150
3	 0.4100	 0.2080
5	 0.8030	 0.4030
7	 0.8760	 0.4430
8	 0.8260	 0.4050
9	 0.7770	 0.3870
A	 0.7160	 0.4600
AA	 0.6290	 0.4090
B	 0.7400	 0.4630
BB	 0.6200	 0.4160
C	 0.7140	 0.4540
CC	 0.6480	 0.4300
D	 0.7440	 0.4330
DD	 0.5680	 0.3760
E	 0.6940	 0.4230
EE	 0.6790	 0.4280
F	 0.7230	 0.4560
FF	 0.6300	 0.4070
G	 0.6010	 0.3820
GG	 0.5150	 0.2950
H	 0.6800	 0.4300
HH	 0.4880	 0.3330
I	 0.7000	 0.4450
II	 0.6390	 0.4110
J	 0.6580	 0.4150
JJ	 0.6720	 0.4040
KK	 0.5910	 0.3600
L	 0.7040	 0.4280
LL	 0.6860	 0.4380
M	 0.7270	 0.4350
MM	 0.2420	 0.1550
N	 0.7460	 0.4710
NN	 0.6610	 0.4250
O	 0.7320	 0.4510



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Chain	Atom inclusion	Q-score
OO	 0.6270	 0.4250
P	 0.7280	 0.4630
PP	 0.6180	 0.3660
Q	 0.7350	 0.4670
QQ	 0.6350	 0.4060
R	 0.6880	 0.4230
RR	 0.5180	 0.3790
S	 0.7400	 0.4690
SS	 0.6050	 0.3750
T	 0.7150	 0.4500
TT	 0.6370	 0.3820
U	 0.6520	 0.3720
UU	 0.5520	 0.3790
V	 0.6930	 0.4670
VV	 0.6290	 0.4180
W	 0.5140	 0.3420
WW	 0.6580	 0.4490
X	 0.6890	 0.4220
XX	 0.6690	 0.4460
Y	 0.6980	 0.4360
YY	 0.6430	 0.3940
Z	 0.6710	 0.4130
ZZ	 0.5900	 0.3520
a	 0.7800	 0.4810
aa	 0.6670	 0.4270
b	 0.5800	 0.3680
bb	 0.5410	 0.3860
c	 0.6420	 0.4130
cc	 0.5830	 0.3990
d	 0.6970	 0.4420
dd	 0.6950	 0.4220
e	 0.7310	 0.4700
ee	 0.5680	 0.3560
f	 0.7410	 0.4870
ff	 0.3350	 0.1910
g	 0.6770	 0.4300
gg	 0.5100	 0.3200
h	 0.6900	 0.4300
hh	 0.6570	 0.3770
i	 0.6560	 0.3950
ii	 0.4750	 0.3040
j	 0.8000	 0.4800

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Chain	Atom inclusion	Q-score
k	 0.5980	 0.3670
l	 0.7330	 0.4430
m	 0.7140	 0.4490
n	 0.6380	 0.4390
o	 0.7070	 0.4550
p	 0.6860	 0.4430
r	 0.7250	 0.4590
s	 0.1240	 0.1220
t	 0.2290	 0.1310