



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:03 PM UTC

PDB ID : 5LZT / pdb_00005lzt
EMDB ID : EMD-4131
Title : Structure of the mammalian ribosomal termination complex with eRF1 and eRF3.
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.65 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

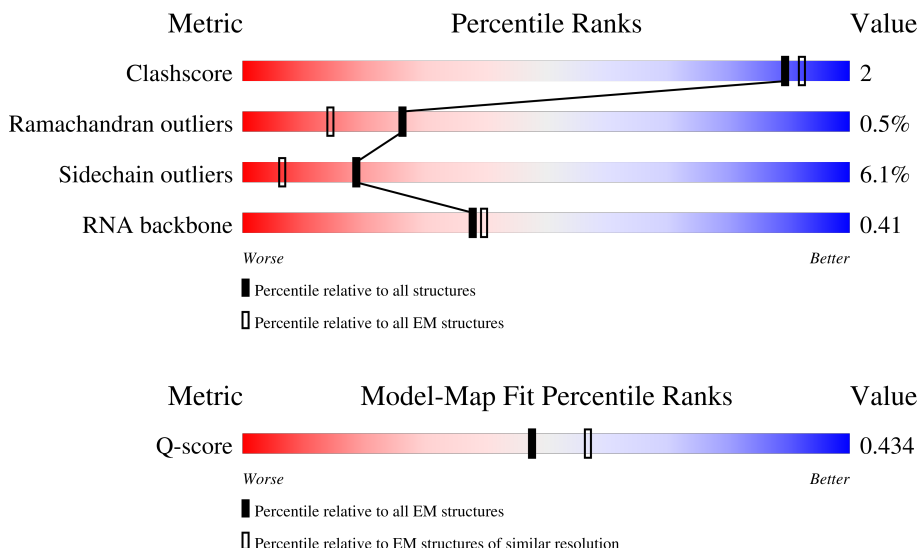
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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.



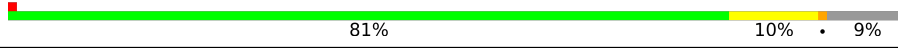
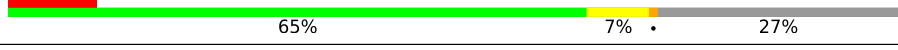
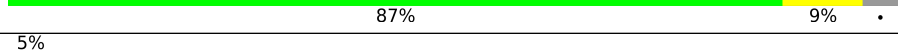
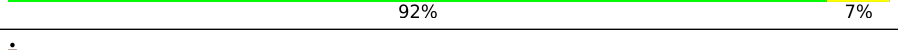
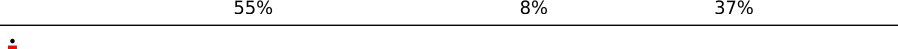
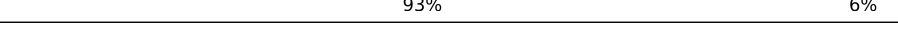
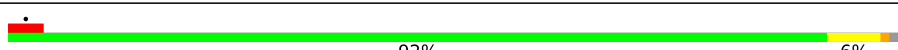
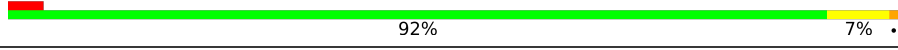
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11564 (3.15 - 4.15)

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	
2	B	403	
3	C	425	

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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	

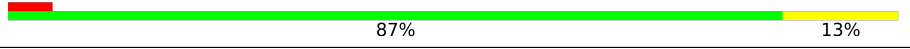
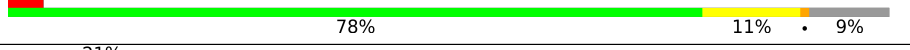
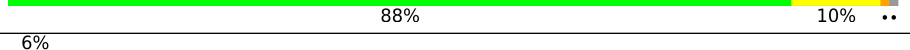
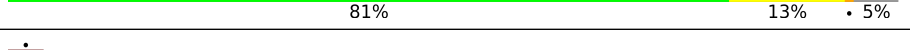
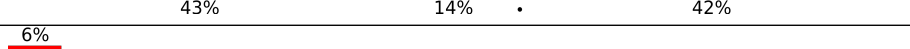
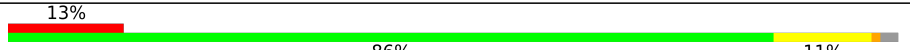
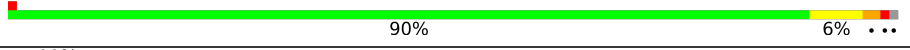
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Mol	Chain	Length	Quality of chain
29	d	125	
30	e	135	
31	f	110	
32	g	117	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	1	15	
46	2	76	
47	3	75	
48	5	3543	
49	7	120	
50	8	156	
51	9	1869	
52	AA	295	
53	BB	264	

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Mol	Chain	Length	Quality of chain
54	CC	293	
55	DD	243	
56	EE	263	
57	FF	204	
58	GG	249	
59	HH	194	
60	II	208	
61	JJ	194	
62	KK	165	
63	LL	158	
64	MM	132	
65	NN	151	
66	OO	168	
67	PP	145	
68	QQ	146	
69	RR	135	
70	SS	152	
71	TT	145	
72	UU	119	
73	VV	83	
74	WW	130	
75	XX	143	
76	YY	130	
77	ZZ	125	
78	aa	115	

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Mol	Chain	Length	Quality of chain
79	bb	84	
80	cc	69	
81	dd	56	
82	ee	133	
83	ff	156	
84	gg	317	
85	hh	15	
86	ii	459	
87	jj	637	

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
89	ZN	p	100	-	-	X	-

2 Entry composition [i](#)

There are 90 unique types of molecules in this entry. The entry contains 222683 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	GLN	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		

- Molecule 4 is a protein called uL18.

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	LYS	initiating methionine	UNP G1SYJ6

- Molecule 5 is a protein called eL6.

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 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	61	ARG	GLY	conflict	UNP G1TUB1
F	93	ARG	GLY	conflict	UNP G1TUB1
F	131	MET	VAL	conflict	UNP G1TUB1
F	153	ILE	VAL	conflict	UNP G1TUB1

- 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 is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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 eL15.

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 eL27.

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		

- 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	-	insertion	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 eL36.

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 eL37.

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		

- 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 eL41.

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 protein called Nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	15	Total	C	N	O	S	0	0
			125	82	20	22	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	76	Total	C	N	O	P	0	0
			1616	723	291	527	75		

- Molecule 47 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	3	75	Total	C	N	O	P	0	0
			1593	712	281	526	74		

- Molecule 48 is a RNA chain called 28S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	5	3543	Total	C	N	O	P	0	0
			75972	33833	13910	24686	3543		

- Molecule 49 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 50 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	8	151	Total	C	N	O	P	0	0
			3208	1432	564	1062	150		

- Molecule 51 is a RNA chain called 18S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	1698	Total	C	N	O	P	0	0
			36249	16180	6508	11864	1697		

- Molecule 52 is a protein called uS2.

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

- Molecule 53 is a protein called eS1.

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

- Molecule 54 is a protein called uS5.

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

- Molecule 55 is a protein called uS3.

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

- Molecule 56 is a protein called eS4.

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

- Molecule 57 is a protein called uS7.

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

- Molecule 58 is a protein called eS6.

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

- Molecule 59 is a protein called eS7.

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

- Molecule 60 is a protein called eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	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 61 is a protein called uS4.

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

- Molecule 62 is a protein called eS10.

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

- Molecule 63 is a protein called uS17.

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

- Molecule 64 is a protein called eS12.

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

- Molecule 65 is a protein called uS15.

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

- Molecule 66 is a protein called uS11.

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

- Molecule 67 is a protein called uS19.

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

- Molecule 68 is a protein called uS9.

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

- Molecule 69 is a protein called eS17.

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

- Molecule 70 is a protein called uS13.

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

- Molecule 71 is a protein called eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
71	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 72 is a protein called uS10.

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

- Molecule 73 is a protein called eS21.

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

- Molecule 74 is a protein called uS8.

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

- Molecule 75 is a protein called uS12.

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

- Molecule 76 is a protein called eS24.

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

- Molecule 77 is a protein called eS25.

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

- Molecule 78 is a protein called eS26.

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

- Molecule 79 is a protein called eS27.

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

- Molecule 80 is a protein called eS28.

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

- Molecule 81 is a protein called uS14.

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

- Molecule 82 is a protein called eS30.

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

- Molecule 83 is a protein called eS31.

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

- Molecule 84 is a protein called RACK1.

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

- Molecule 85 is a RNA chain called mRNA (UGA stop codon).

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

- Molecule 86 is a protein called eRF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
86	ii	419	Total	C	N	O	S	0	0
			3307	2104	562	629	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

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Chain	Residue	Modelled	Actual	Comment	Reference
ii	-2	GLN	-	expression tag	UNP P62495
ii	-1	GLY	-	expression tag	UNP P62495
ii	0	SER	-	expression tag	UNP P62495

- Molecule 87 is a protein called eRF3a.

Mol	Chain	Residues	Atoms					AltConf	Trace
87	jj	428	Total	C	N	O	S	0	0
			3368	2144	580	623	21		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
jj	100	ALA	VAL	conflict	UNP P15170

- Molecule 88 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
88	A	1	Total	Mg	0
			1	1	
88	B	1	Total	Mg	0
			1	1	
88	I	1	Total	Mg	0
			1	1	
88	P	3	Total	Mg	0
			3	3	
88	Q	1	Total	Mg	0
			1	1	
88	V	1	Total	Mg	0
			1	1	
88	a	1	Total	Mg	0
			1	1	
88	g	1	Total	Mg	0
			1	1	
88	j	1	Total	Mg	0
			1	1	
88	5	185	Total	Mg	0
			185	185	
88	7	5	Total	Mg	0
			5	5	
88	8	8	Total	Mg	0
			8	8	

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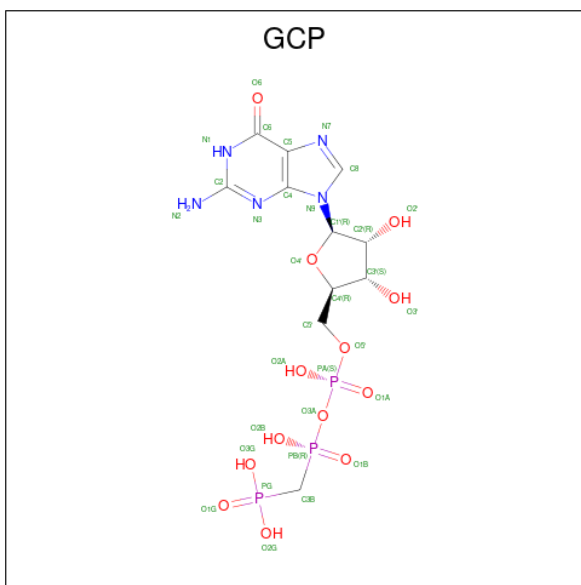
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Mol	Chain	Residues	Atoms		AltConf
88	9	71	Total 71	Mg 71	0
88	hh	1	Total 1	Mg 1	0
88	jj	1	Total 1	Mg 1	0

- Molecule 89 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
89	g	1	Total 1	Zn 1	0
89	j	1	Total 1	Zn 1	0
89	m	1	Total 1	Zn 1	0
89	o	1	Total 1	Zn 1	0
89	p	1	Total 1	Zn 1	0
89	aa	1	Total 1	Zn 1	0
89	dd	1	Total 1	Zn 1	0
89	ff	1	Total 1	Zn 1	0

- Molecule 90 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (CCD ID: GCP) (formula: C₁₁H₁₈N₅O₁₃P₃).



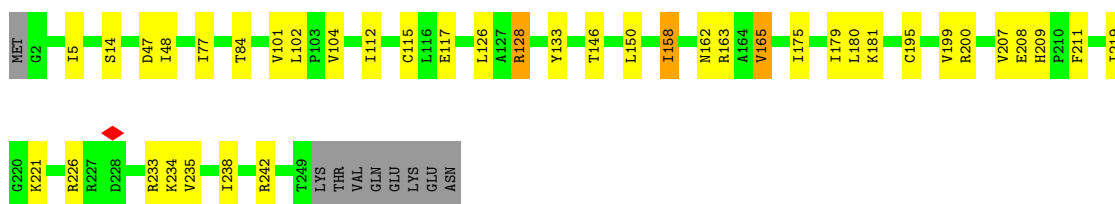
Mol	Chain	Residues	Atoms					AltConf
90	jj	1	Total	C	N	O	P	0
			32	11	5	13	3	

3 Residue-property plots

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

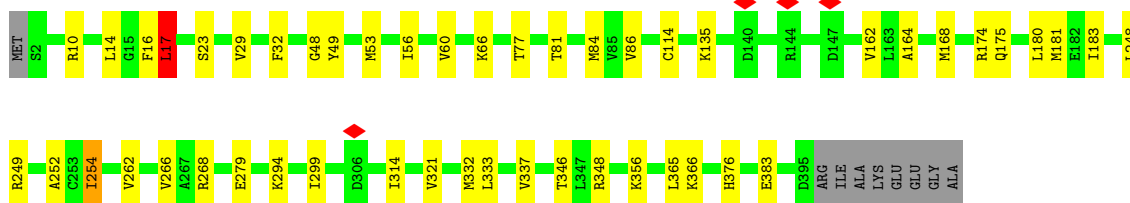
• Molecule 1: uL2

Chain A: 



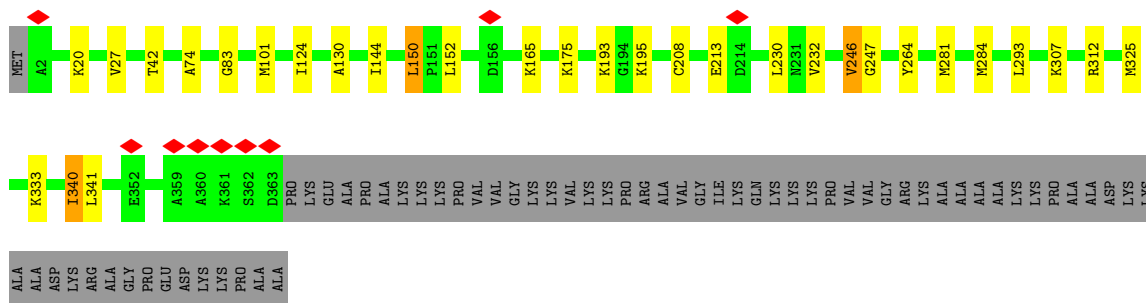
• Molecule 2: uL3

Chain B: 



• Molecule 3: uL4

Chain C: 



• Molecule 4: uL18

Two sequence logos for the 1000 Genomes Project. The top logo shows the top 1000 variants, and the bottom logo shows the bottom 1000 variants. Each logo has a y-axis from 0 to 10 and an x-axis with variant positions. The top logo has a red diamond at position 1000, and the bottom logo has a red diamond at position 1000.

A bar chart titled 'Amino acid types' showing the frequency of various amino acids across 1000 random sequences. The x-axis lists amino acid codes, and the y-axis represents their frequency. The bars are color-coded: grey for common, yellow for less common, and green for rare. MET is the most frequent, followed by GLY, ALA, and others. The chart is titled 'Amino acid types'.

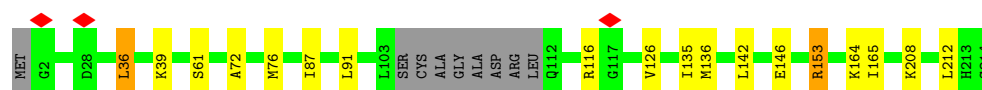
[illegible]

Chain H:  87% 11% ..



- Molecule 9: uL16

Chain I:  87% 7% ..

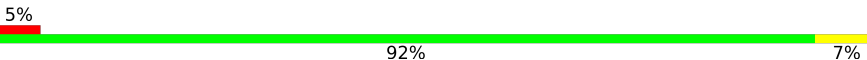


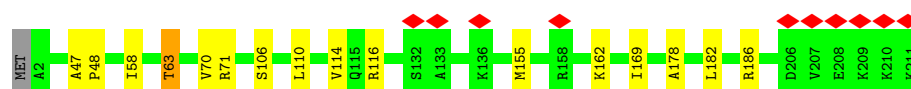
- Molecule 10: uL5

Chain J:  87% 9% .



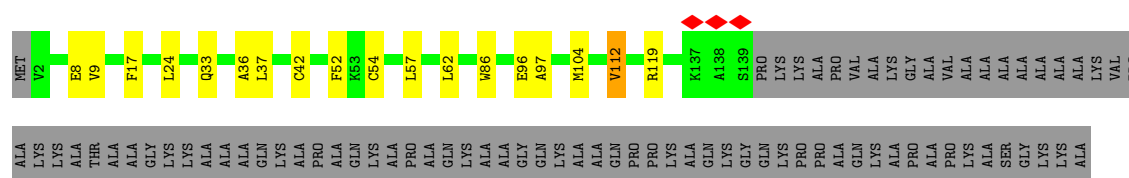
- Molecule 11: eL13

Chain L:  5% 92% 7%

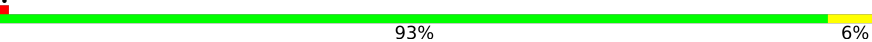


- Molecule 12: eL14

Chain M:  55% 8% 37%



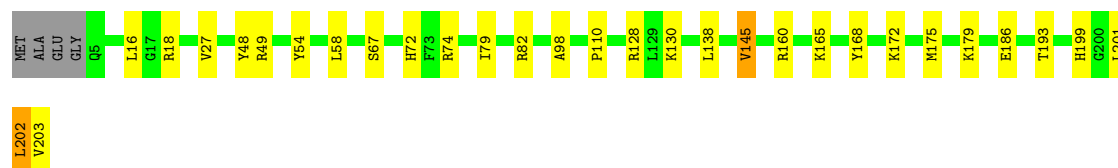
- Molecule 13: eL15

Chain N:  93% 6%

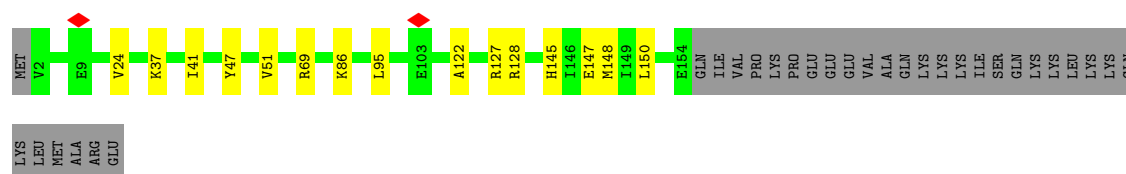
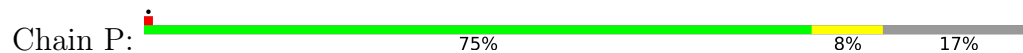


- Molecule 14: uL13

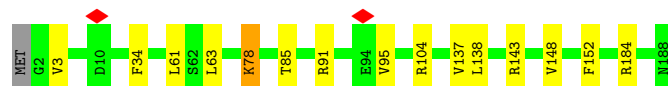
Chain O:  83% 14% ..



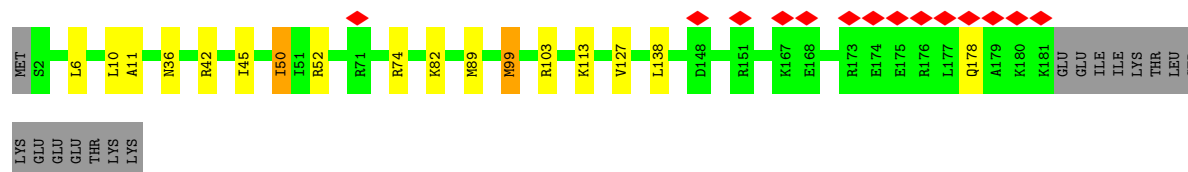
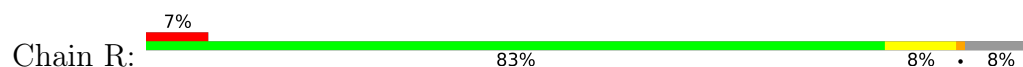
• Molecule 15: uL22



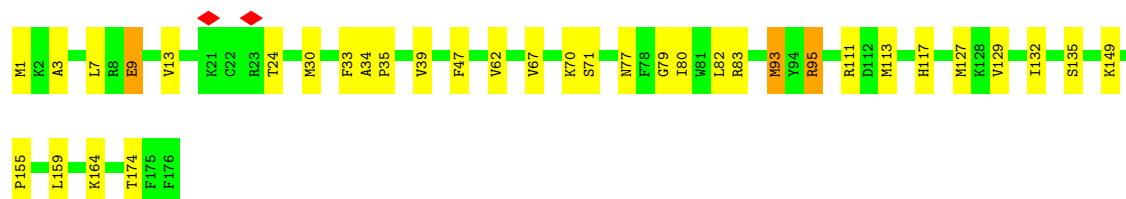
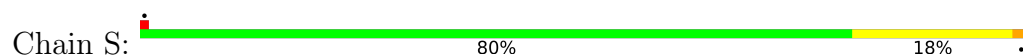
• Molecule 16: eL18



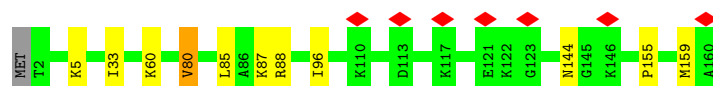
• Molecule 17: eL19



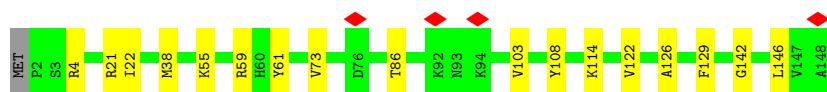
• Molecule 18: eL20



• Molecule 19: eL21

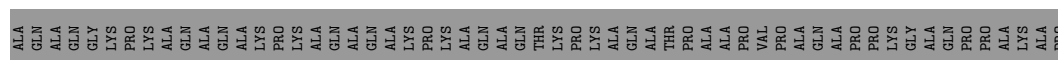
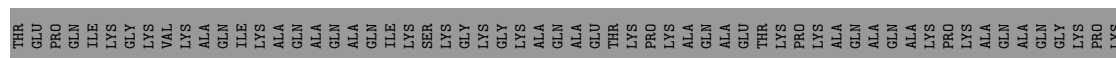
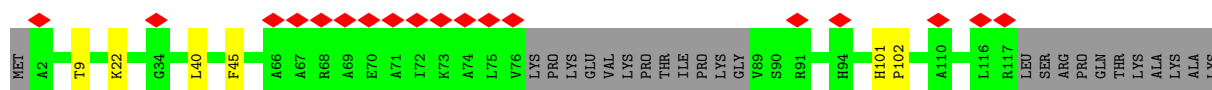


Chain a: 



• Molecule 27: eL29

Chain b: 



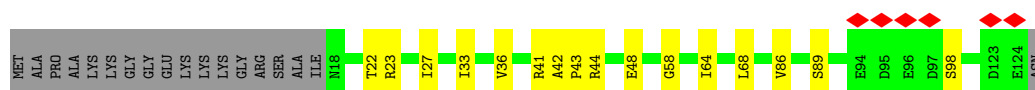
• Molecule 28: eL30

Chain c: 



• Molecule 29: eL31

Chain d: 



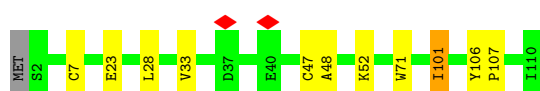
• Molecule 30: eL32

Chain e: 

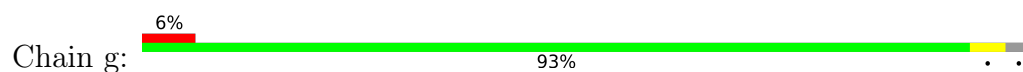


• Molecule 31: eL33

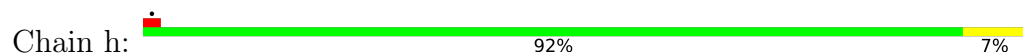
Chain f: 



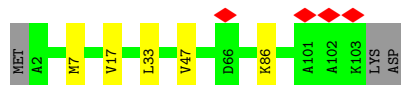
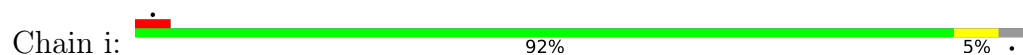
• Molecule 32: eL34



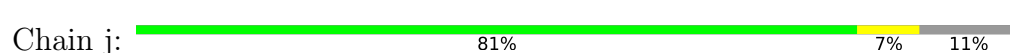
• Molecule 33: uL29



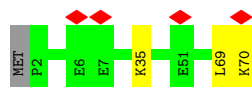
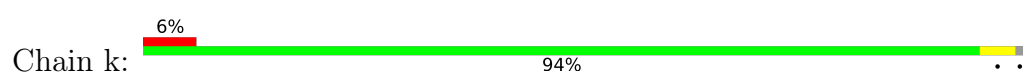
• Molecule 34: eL36



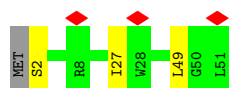
• Molecule 35: eL37



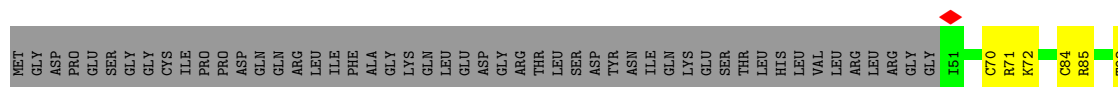
• Molecule 36: eL38



• Molecule 37: eL39

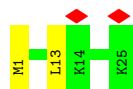


• Molecule 38: eL40

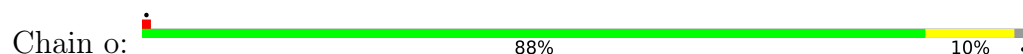




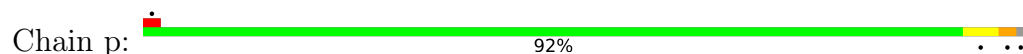
• Molecule 39: eL41



• Molecule 40: eL42



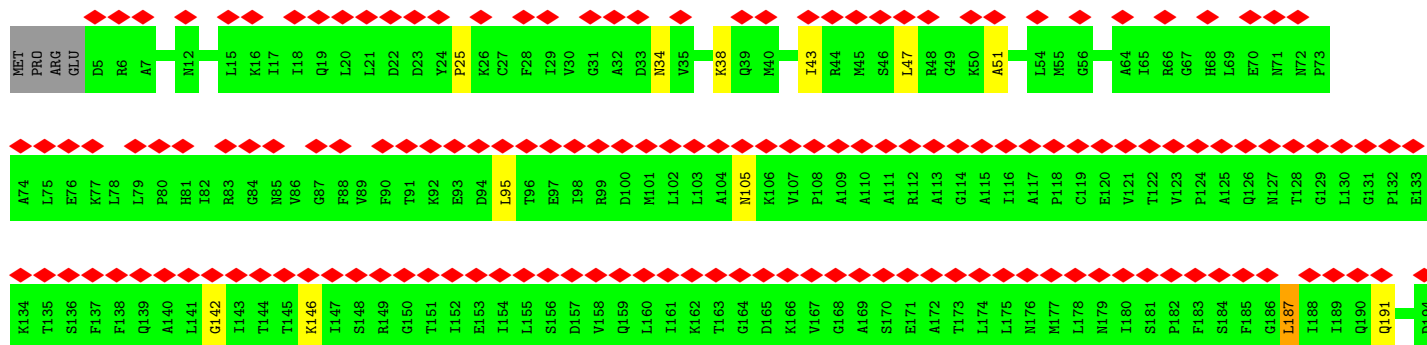
• Molecule 41: eL43

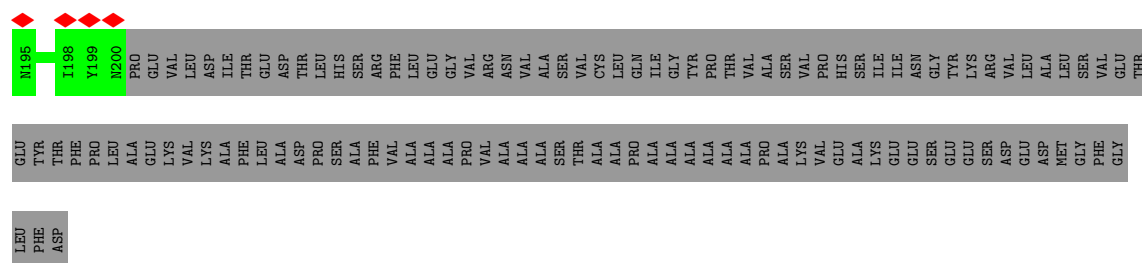


• Molecule 42: eL28

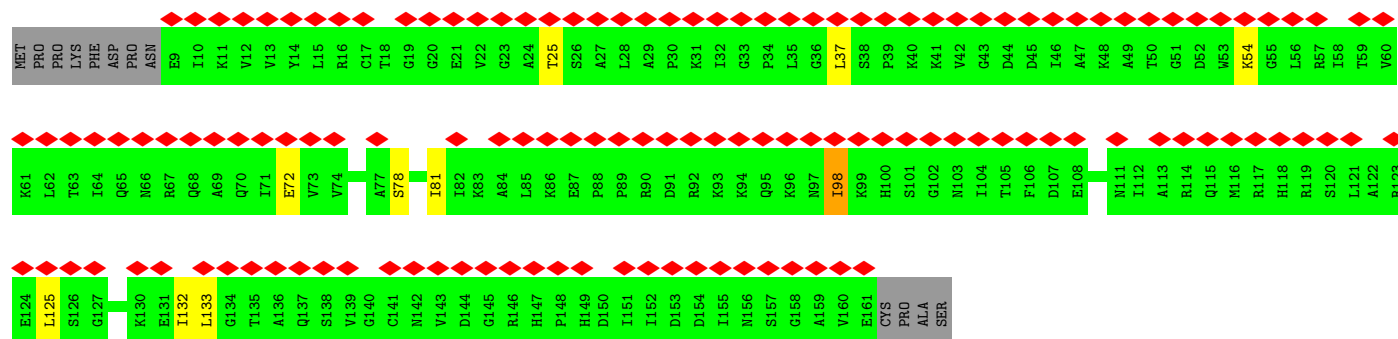
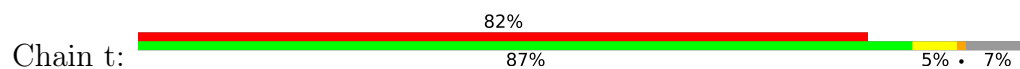


• Molecule 43: uL10

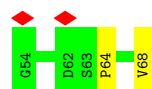
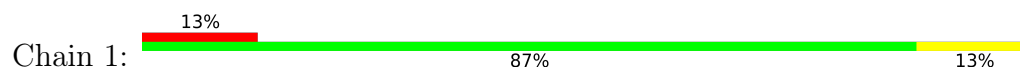




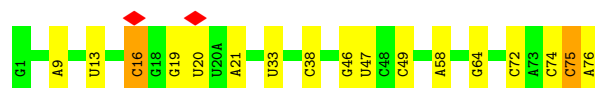
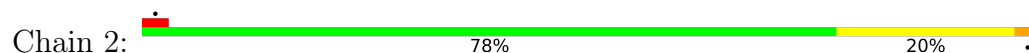
• Molecule 44: uL11



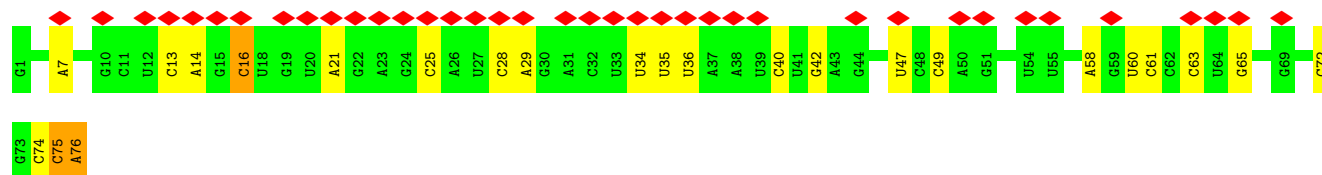
• Molecule 45: Nascent chain



• Molecule 46: P-site tRNA

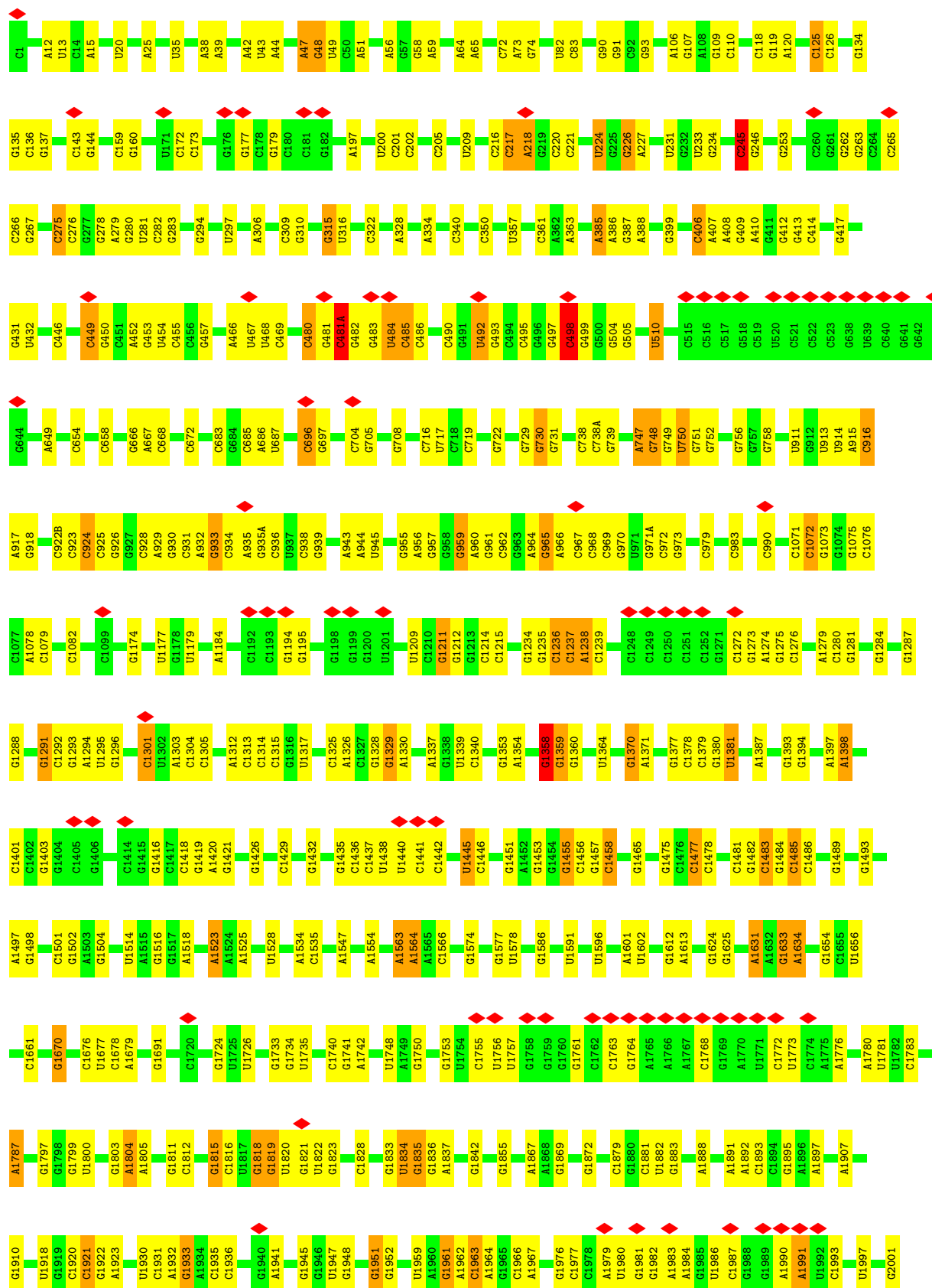


• Molecule 47: E-site tRNA

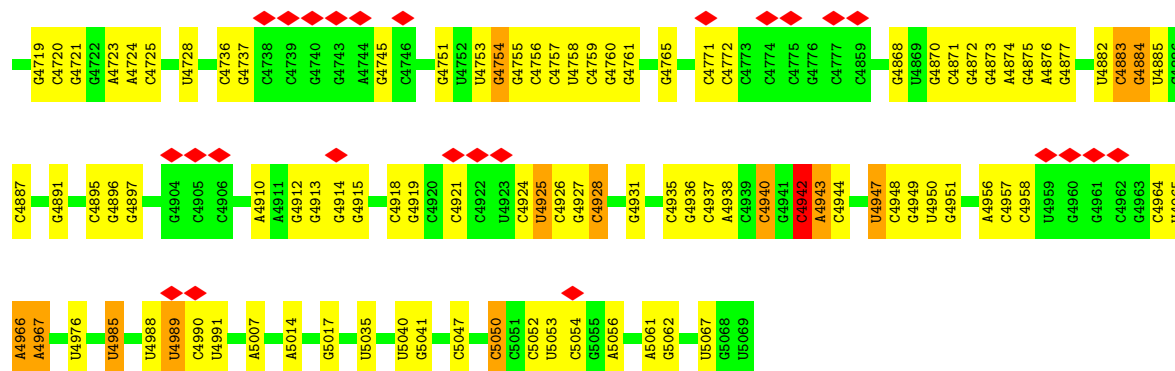


• Molecule 48: 28S ribosomal RNA

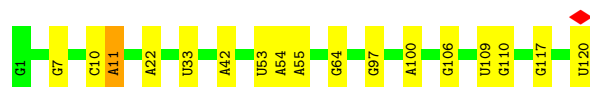
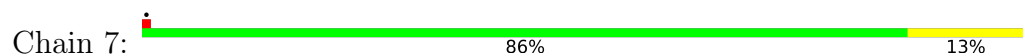




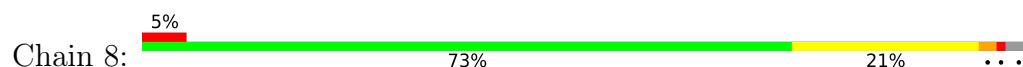




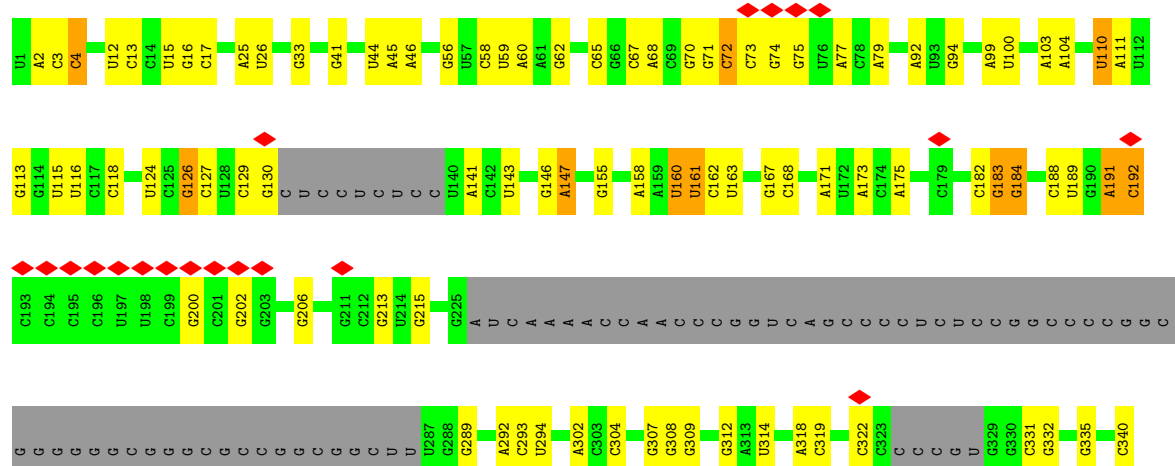
• Molecule 49: 5S ribosomal RNA



• Molecule 50: 5.8S ribosomal RNA

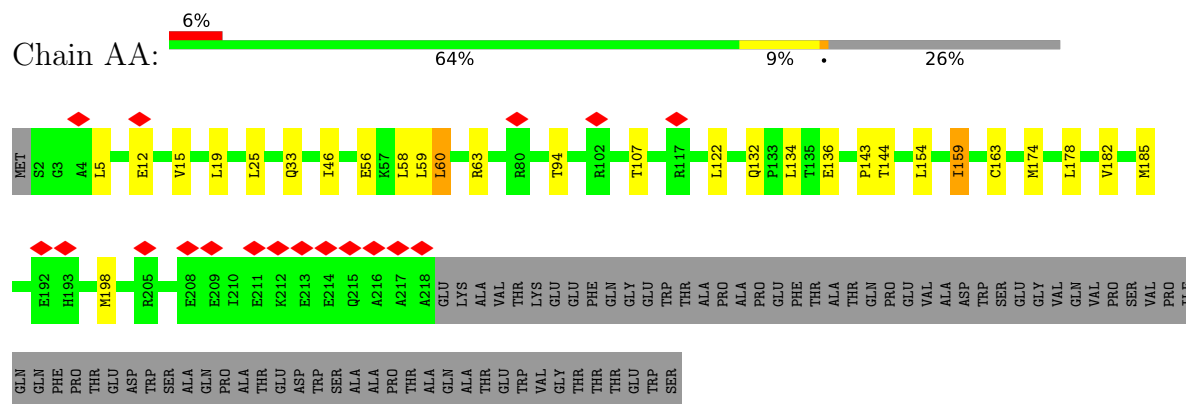


• Molecule 51: 18S ribosomal RNA

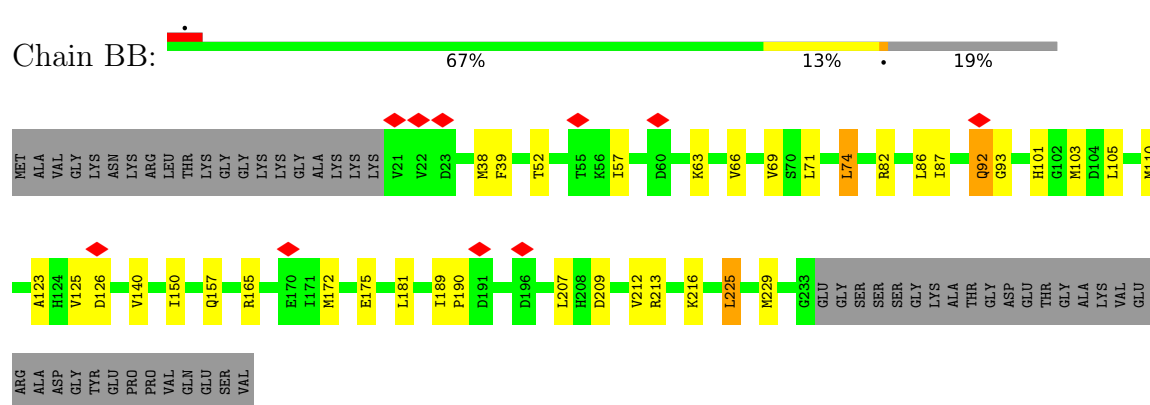




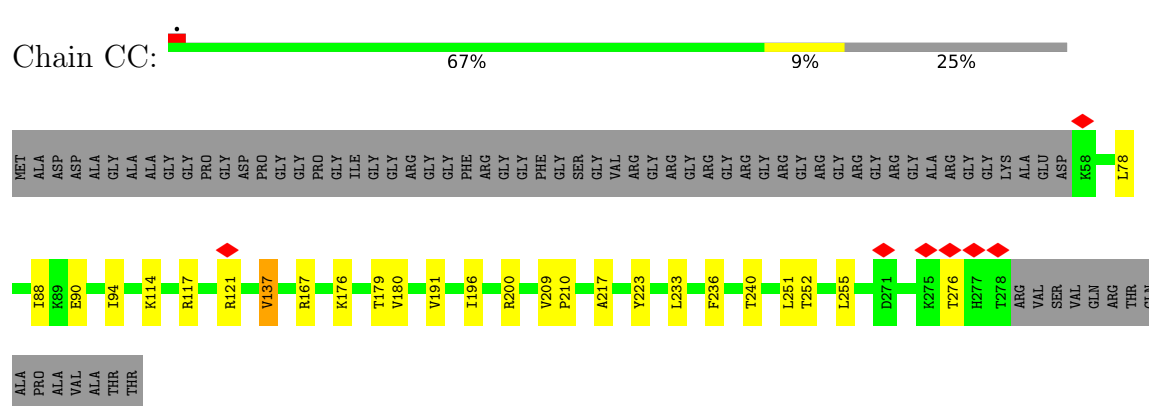
- Molecule 52: uS2



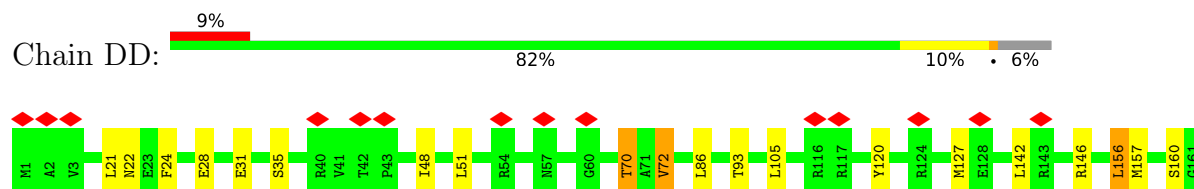
- Molecule 53: eS1

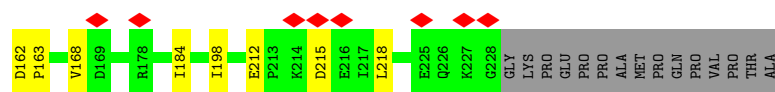


- Molecule 54: uS5

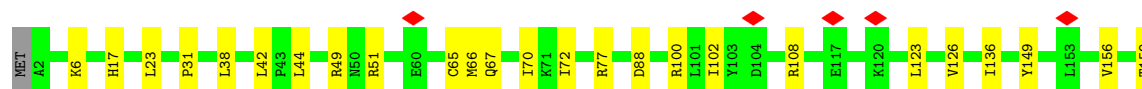
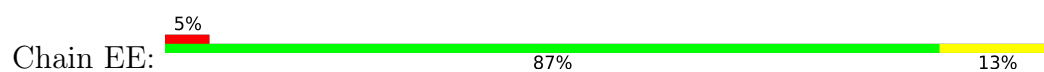


- Molecule 55: uS3

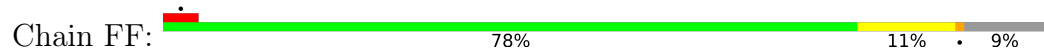




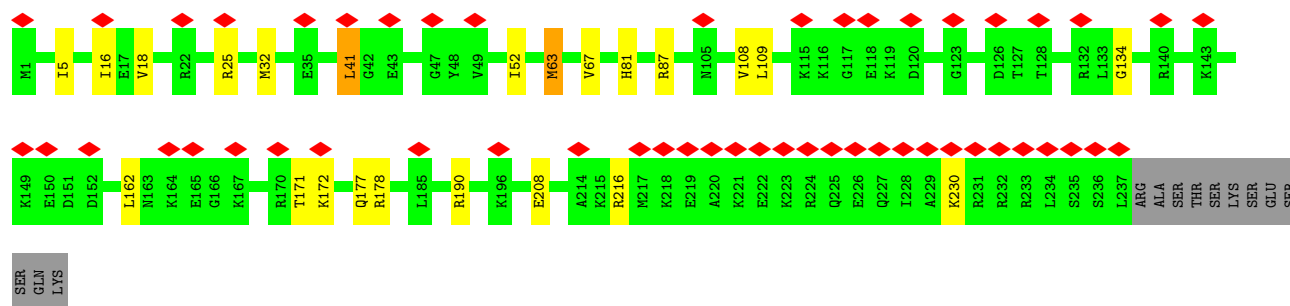
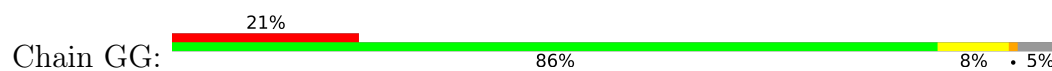
• Molecule 56: eS4



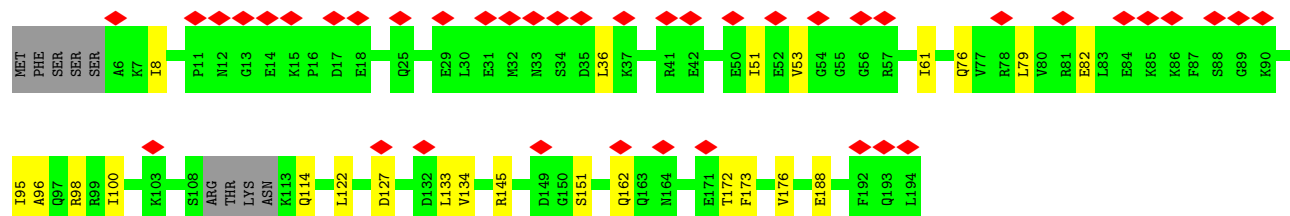
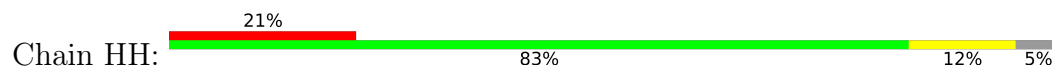
• Molecule 57: uS7



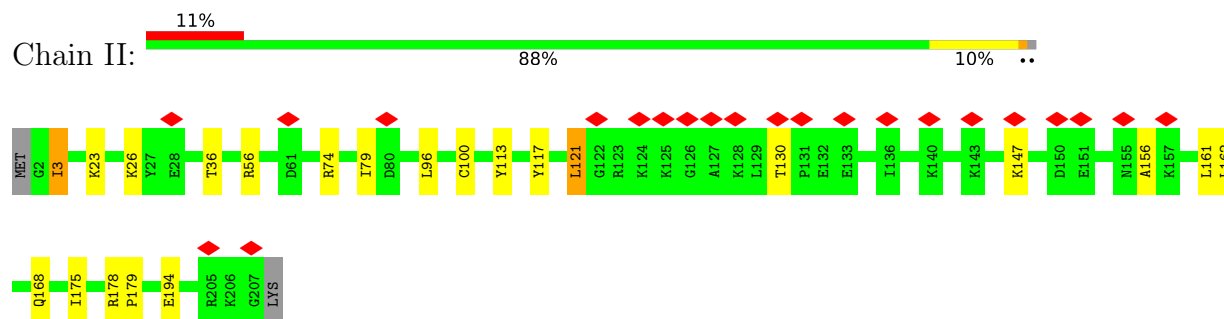
• Molecule 58: eS6



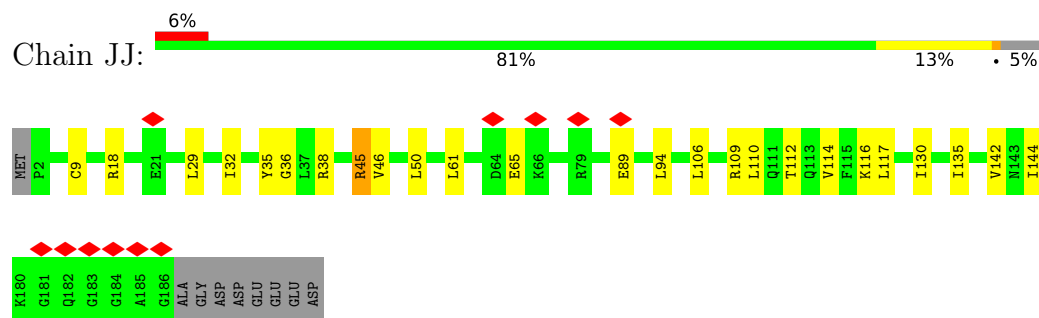
• Molecule 59: eS7



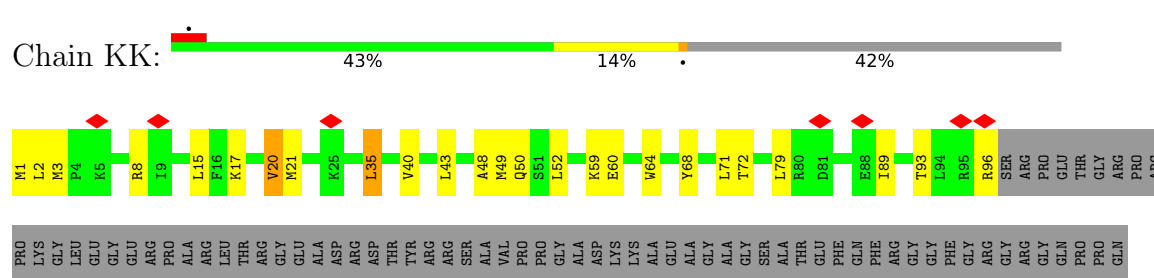
- Molecule 60: eS8



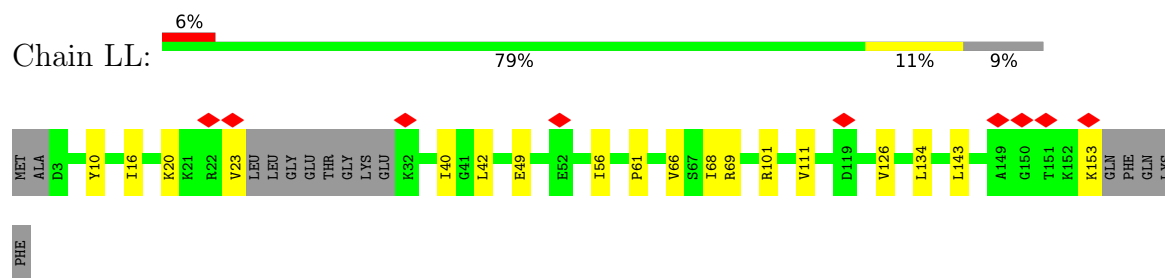
- Molecule 61: uS4



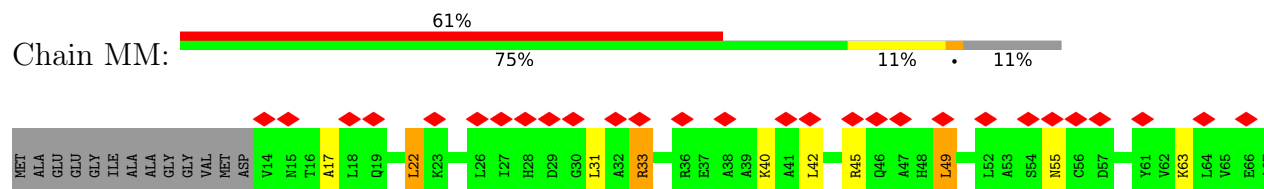
- Molecule 62: eS10

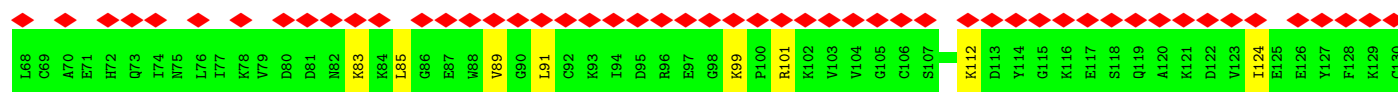


- Molecule 63: uS17



- Molecule 64: eS12

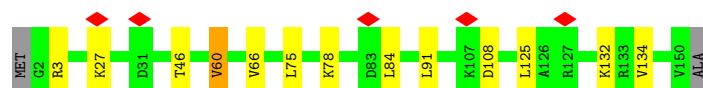




LYS
LYS

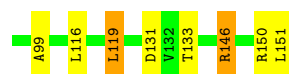
• Molecule 65: uS15

Chain NN: 90% 8% ..



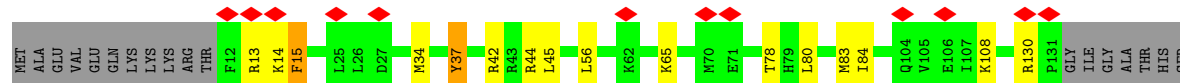
• Molecule 66: uS11

Chain OO: 69% 10% 19%



• Molecule 67: uS19

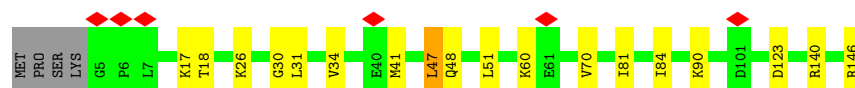
Chain PP: 8% 72% 10% 17%



SER
ARG
PHE
ILE
PRO
LEU
LYS

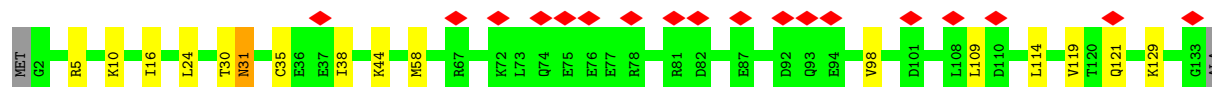
• Molecule 68: uS9

Chain QQ: 85% 12% ..



• Molecule 69: eS17

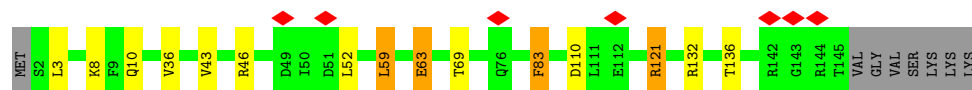
Chain RR: 13% 86% 11% ..



VAL

- Molecule 70: uS13

Chain SS: 



- Molecule 71: eS19

Chain TT: 

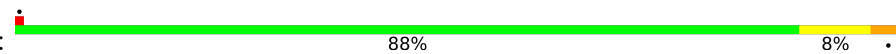


- Molecule 72: uS10

Chain UU: 



- Molecule 73: eS21

Chain VV: 



- Molecule 74: uS8

Chain WW: 



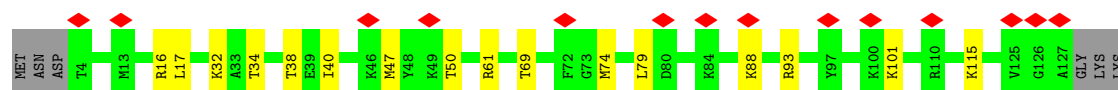
- Molecule 75: uS12

Chain XX: 

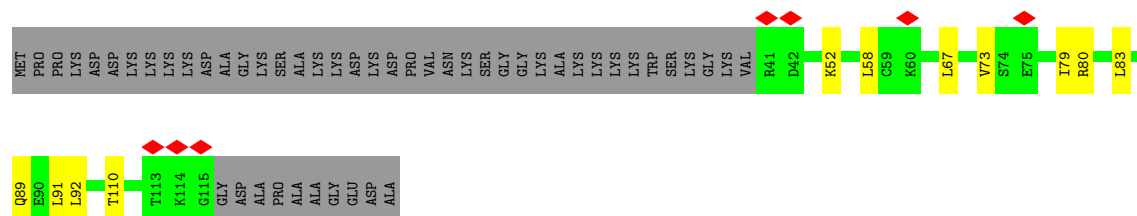


- Molecule 76: eS24

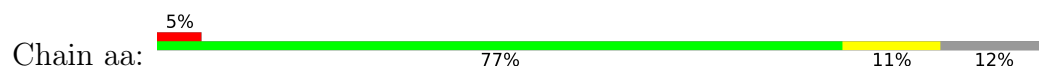
Chain YY: 



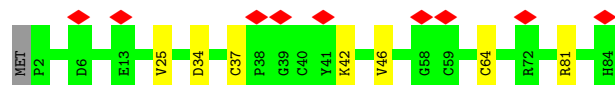
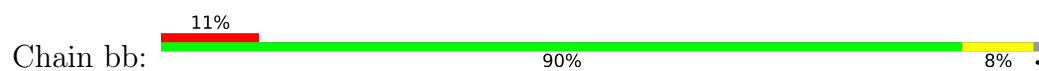
• Molecule 77: eS25



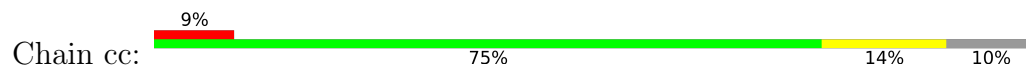
• Molecule 78: eS26



• Molecule 79: eS27



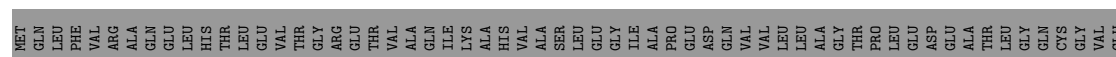
• Molecule 80: eS28

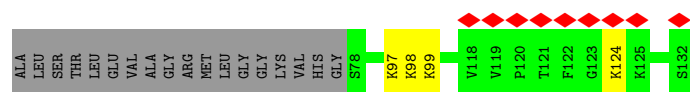


• Molecule 81: uS14

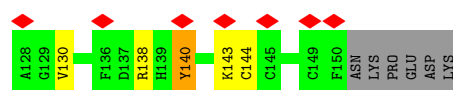
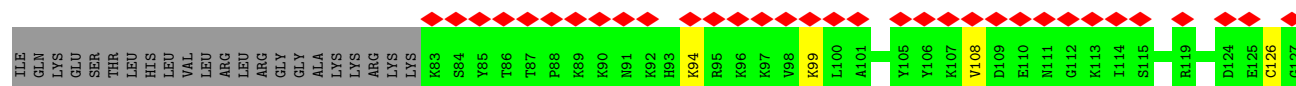
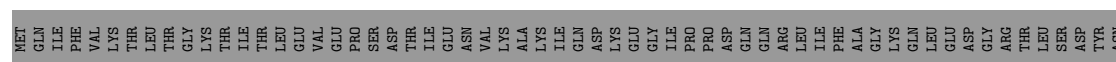
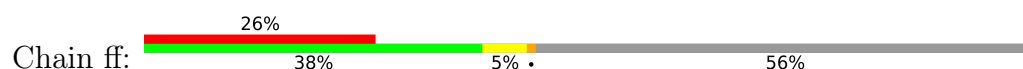


• Molecule 82: eS30

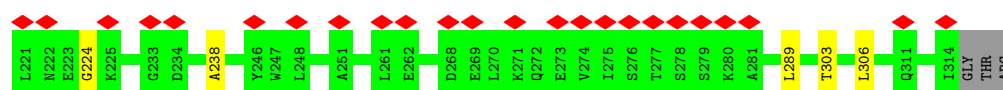
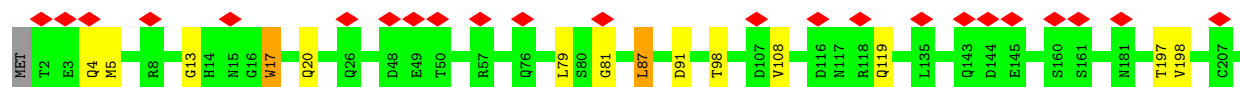




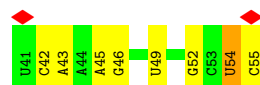
• Molecule 83: eS31



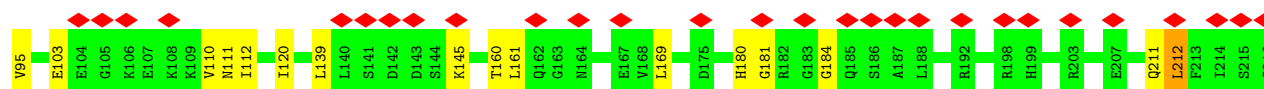
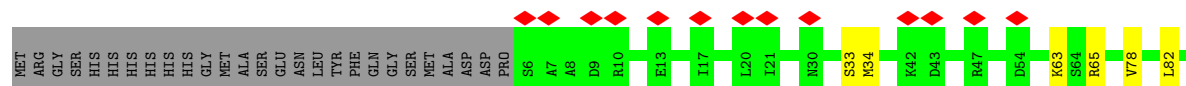
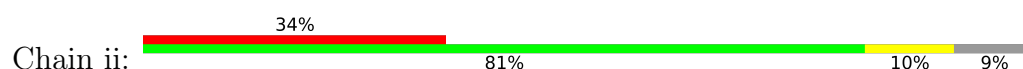
• Molecule 84: RACK1

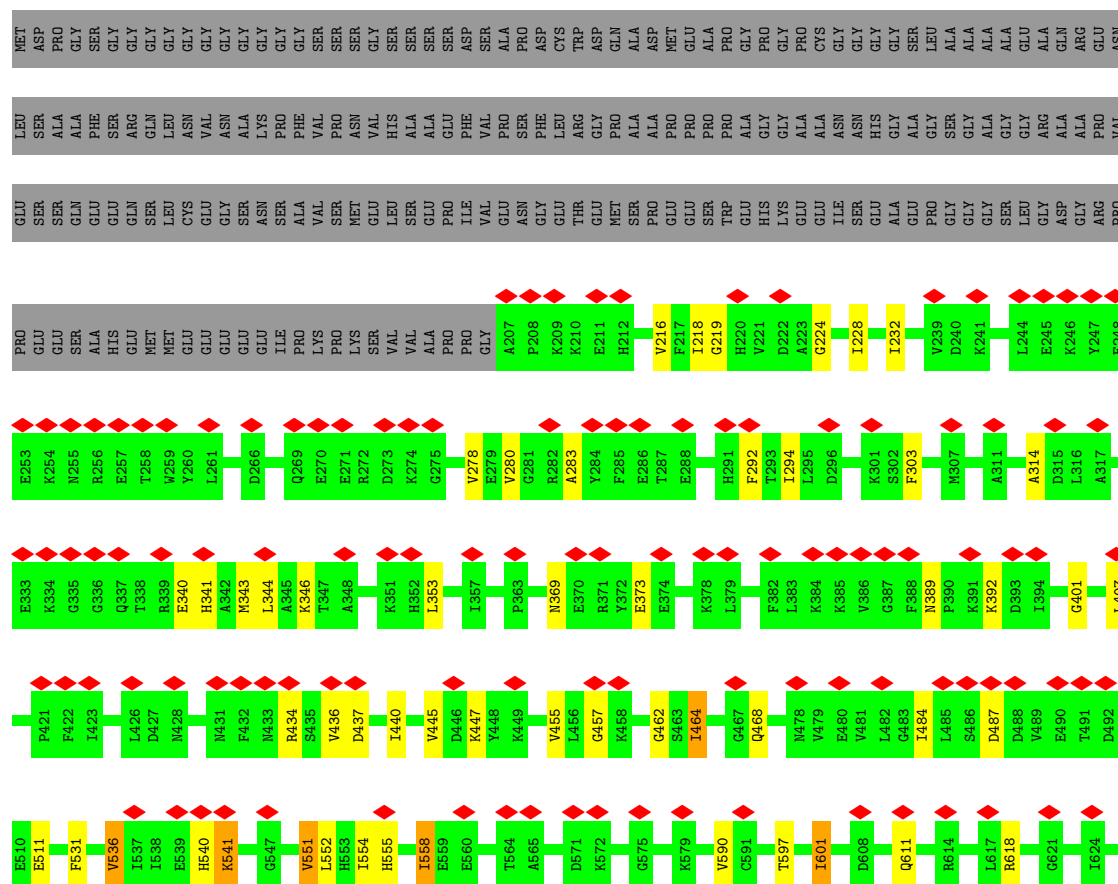


• Molecule 85: mRNA (UGA stop codon)



• Molecule 86: eRF1





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	61752	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	0.800	Depositor
Minimum map value	-0.493	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.023	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: ZN, GCP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.47	0/1936	0.78	0/2596
2	B	0.44	0/3240	0.76	0/4339
3	C	0.46	0/2937	0.79	2/3946 (0.1%)
4	D	0.45	0/2437	0.80	1/3264 (0.0%)
5	E	0.47	0/1762	0.78	1/2362 (0.0%)
6	F	0.48	0/1911	0.81	0/2549
7	G	0.48	0/1910	0.82	2/2569 (0.1%)
8	H	0.41	0/1535	0.69	0/2063
9	I	0.42	0/1702	0.74	0/2272
10	J	0.44	0/1385	0.75	0/1852
11	L	0.48	0/1733	0.81	0/2316
12	M	0.46	0/1158	0.82	0/1547
13	N	0.46	0/1746	0.78	0/2338
14	O	0.46	0/1662	0.83	1/2222 (0.0%)
15	P	0.48	0/1268	0.81	1/1700 (0.1%)
16	Q	0.46	0/1539	0.80	0/2054
17	R	0.47	0/1524	0.80	0/2013
18	S	0.48	0/1501	0.82	2/2012 (0.1%)
19	T	0.45	0/1326	0.72	0/1770
20	U	0.46	0/823	0.71	0/1104
21	V	0.45	0/993	0.77	0/1332
22	W	0.47	0/873	0.78	1/1158 (0.1%)
23	X	0.45	0/984	0.74	0/1323
24	Y	0.44	0/1132	0.77	0/1504
25	Z	0.46	0/1130	0.75	0/1507
26	a	0.43	0/1191	0.80	1/1590 (0.1%)
27	b	0.45	0/861	0.80	0/1138
28	c	0.45	0/771	0.78	0/1034
29	d	0.47	0/903	0.75	0/1216
30	e	0.45	0/1071	0.79	0/1429
31	f	0.47	0/895	0.77	0/1198
32	g	0.45	0/916	0.76	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.43	0/1021	0.81	0/1348
34	i	0.45	0/841	0.77	0/1112
35	j	0.47	0/720	0.81	0/952
36	k	0.44	0/575	0.72	0/761
37	l	0.46	0/459	0.78	0/608
38	m	0.46	0/435	0.78	0/575
39	n	0.41	0/240	0.83	0/305
40	o	0.44	0/864	0.71	0/1140
41	p	0.44	0/718	0.81	0/953
42	r	0.49	0/1010	0.86	1/1354 (0.1%)
43	s	0.54	0/1530	0.74	0/2064
44	t	0.57	0/1174	0.82	0/1582
45	1	0.51	0/129	0.86	0/173
46	2	0.35	0/1805	0.69	0/2809
47	3	0.37	0/1777	0.68	0/2763
48	5	0.37	0/84973	0.73	78/132508 (0.1%)
49	7	0.37	0/2858	0.71	0/4455
50	8	0.37	0/3581	0.71	2/5577 (0.0%)
51	9	0.37	1/40524 (0.0%)	0.73	30/63134 (0.0%)
52	AA	0.47	0/1747	0.80	0/2374
53	BB	0.43	0/1756	0.80	0/2350
54	CC	0.47	0/1753	0.83	0/2369
55	DD	0.50	0/1796	0.79	0/2417
56	EE	0.49	0/2118	0.78	1/2849 (0.0%)
57	FF	0.47	0/1492	0.87	0/2005
58	GG	0.51	0/1946	0.83	2/2590 (0.1%)
59	HH	0.51	0/1510	0.80	0/2022
60	II	0.47	0/1715	0.77	0/2287
61	JJ	0.45	0/1550	0.85	0/2069
62	KK	0.49	0/834	0.83	0/1125
63	LL	0.46	0/1195	0.76	0/1597
64	MM	0.53	0/918	0.87	0/1233
65	NN	0.46	0/1226	0.85	0/1649
66	OO	0.48	0/1029	0.93	1/1380 (0.1%)
67	PP	0.49	0/1017	0.83	0/1358
68	QQ	0.47	0/1146	0.76	0/1534
69	RR	0.48	0/1082	0.80	0/1452
70	SS	0.48	0/1208	0.82	0/1618
71	TT	0.49	0/1115	0.87	0/1493
72	UU	0.47	0/805	0.83	1/1081 (0.1%)
73	VV	0.49	0/643	0.83	1/860 (0.1%)
74	WW	0.46	0/1051	0.79	0/1406
75	XX	0.42	0/1116	0.79	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
76	YY	0.47	0/1028	0.77	0/1366
77	ZZ	0.48	0/604	0.81	0/810
78	aa	0.48	0/828	0.85	0/1109
79	bb	0.47	0/665	0.72	0/891
80	cc	0.46	0/490	0.76	0/656
81	dd	0.47	0/470	0.74	0/623
82	ee	0.46	0/447	0.85	0/587
83	ff	0.50	0/567	0.74	0/753
84	gg	0.46	0/2493	0.69	0/3394
85	hh	0.39	0/353	0.78	0/547
86	ii	0.50	0/3361	0.83	0/4519
87	jj	0.52	0/3435	0.78	0/4633
All	All	0.42	1/238498 (0.0%)	0.76	129/349206 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1
74	WW	0	1
75	XX	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	9	583	A	C1'-N9	-5.03	1.40	1.48

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	9	1835	A	C2'-C3'-O3'	12.62	128.43	109.50
48	5	2068	C	C4'-C3'-O3'	9.74	124.01	109.40
48	5	385	A	C4'-C3'-O3'	9.52	123.68	109.40
48	5	1818	G	C2'-C3'-O3'	9.31	123.47	109.50
48	5	2046	G	C2'-C3'-O3'	9.29	123.43	109.50
48	5	2695	A	C2'-C3'-O3'	9.22	123.34	109.50
48	5	1834	U	C2'-C3'-O3'	9.20	123.29	109.50
51	9	1664	A	C4'-C3'-O3'	9.07	123.01	109.40
48	5	47	A	C4'-C3'-O3'	8.85	122.68	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	48	G	C2'-C3'-O3'	8.70	122.54	109.50
51	9	1394	G	C2'-C3'-O3'	8.49	126.44	113.70
51	9	870	A	C4'-C3'-O3'	8.23	121.74	109.40
48	5	2474	G	C2'-C3'-O3'	8.04	121.56	109.50
48	5	2089	G	C2'-C3'-O3'	7.94	121.41	109.50
48	5	406	C	C2'-C3'-O3'	7.91	125.56	113.70
48	5	1370	G	C2'-C3'-O3'	7.80	121.20	109.50
48	5	4942	C	C4'-C3'-O3'	7.51	120.67	109.40
48	5	498	C	C4'-C3'-O3'	7.43	120.55	109.40
48	5	1477	C	C2'-C3'-O3'	7.41	124.81	113.70
48	5	3888	G	C2'-C3'-O3'	7.39	124.79	113.70
48	5	4448	G	C4'-C3'-O3'	7.31	123.97	113.00
48	5	1211	G	C2'-C3'-O3'	7.25	124.57	113.70
48	5	275	C	C2'-C3'-O3'	7.19	124.49	113.70
48	5	1670	G	C2'-C3'-O3'	-7.19	102.92	113.70
48	5	4170	A	C2'-C3'-O3'	7.12	120.18	109.50
51	9	1130	G	C4'-C3'-O3'	7.10	120.05	109.40
48	5	2468	U	C4'-C3'-O3'	7.09	120.03	109.40
51	9	72	C	C4'-C3'-O3'	6.93	119.79	109.40
26	a	22	ILE	N-CA-C	-6.88	104.48	110.74
48	5	1835	G	C2'-C3'-O3'	6.86	119.80	109.50
48	5	38	A	C4'-C3'-O3'	-6.86	102.71	113.00
3	C	340	ILE	N-CA-C	-6.83	106.22	111.62
51	9	1253	A	C2'-C3'-O3'	6.82	119.73	109.50
48	5	492	U	C2'-C3'-O3'	6.80	119.70	109.50
51	9	688	U	C2'-C3'-O3'	6.80	119.70	109.50
51	9	1646	C	C2'-C3'-O3'	6.70	123.75	113.70
48	5	3697	U	C2'-C3'-O3'	6.65	123.67	113.70
51	9	1061	U	C2'-C3'-O3'	-6.64	103.75	113.70
14	O	110	PRO	N-CA-C	6.54	118.68	110.70
51	9	1313	A	C4'-C3'-O3'	6.49	119.13	109.40
48	5	4925	U	C2'-C3'-O3'	6.41	119.11	109.50
51	9	160	U	C4'-C3'-O3'	6.38	118.97	109.40
48	5	1455	G	C2'-C3'-O3'	6.37	123.26	113.70
51	9	874	G	C2'-C3'-O3'	6.37	123.26	113.70
48	5	3876	A	C2'-C3'-O3'	6.37	119.05	109.50
48	5	696	C	C2'-C3'-O3'	6.36	119.04	109.50
48	5	4232	U	C4'-C3'-O3'	6.35	118.92	109.40
48	5	449	C	C2'-C3'-O3'	6.34	119.00	109.50
51	9	434	G	C2'-C3'-O3'	6.30	123.16	113.70
50	8	124	U	C4'-C3'-O3'	6.30	118.85	109.40
51	9	1520	G	C4'-C3'-O3'	6.29	122.44	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	4449	A	C4'-C3'-O3'	6.25	118.77	109.40
48	5	1072	C	C2'-C3'-O3'	6.18	118.76	109.50
48	5	1291	G	C2'-C3'-O3'	6.15	122.93	113.70
48	5	959	G	C2'-C3'-O3'	6.14	118.72	109.50
48	5	4075	U	C2'-C3'-O3'	6.12	118.68	109.50
48	5	4699	U	C4'-C3'-O3'	6.09	118.54	109.40
72	UU	72	GLU	N-CA-C	6.07	119.58	107.62
51	9	752	G	C2'-C3'-O3'	6.04	118.56	109.50
48	5	4947	U	C2'-C3'-O3'	6.03	122.75	113.70
48	5	245	C	C2'-C3'-O3'	6.00	122.69	113.70
50	8	94	G	C2'-C3'-O3'	5.98	118.47	109.50
48	5	1329	G	C2'-C3'-O3'	5.94	122.60	113.70
51	9	110	U	C2'-C3'-O3'	5.93	122.59	113.70
48	5	933	G	C2'-C3'-O3'	-5.91	104.84	113.70
51	9	642	U	C4'-C3'-O3'	5.91	121.86	113.00
48	5	2313	A	C2'-C3'-O3'	5.89	118.33	109.50
48	5	4378	A	C2'-C3'-O3'	5.83	118.25	109.50
48	5	924	C	C2'-C3'-O3'	-5.77	105.05	113.70
48	5	1209	U	C2'-C3'-O3'	-5.73	105.10	113.70
48	5	2661	U	C2'-C3'-O3'	5.69	118.04	109.50
48	5	48	G	C4'-C3'-O3'	5.64	117.86	109.40
48	5	3603	G	C4'-C3'-O3'	-5.63	104.55	113.00
48	5	4475	G	C4'-C3'-O3'	-5.60	104.60	113.00
51	9	532	C	C2'-C3'-O3'	5.56	122.04	113.70
51	9	501	C	N1-C1'-C2'	5.55	120.32	112.00
48	5	90	G	C4'-C3'-O3'	-5.54	104.69	113.00
42	r	10	VAL	N-CA-C	5.53	115.66	110.30
48	5	125	C	C2'-C3'-O3'	5.53	122.00	113.70
48	5	1445	U	C2'-C3'-O3'	5.53	121.99	113.70
58	GG	134	GLY	CA-C-N	5.47	126.68	119.84
58	GG	134	GLY	C-N-CA	5.47	126.68	119.84
48	5	1358	G	C2'-C3'-O3'	5.46	117.69	109.50
48	5	4884	G	C2'-C3'-O3'	5.43	121.84	113.70
15	P	37	LYS	N-CA-C	5.42	117.19	111.28
7	G	130	PRO	CA-C-N	5.42	125.24	119.28
7	G	130	PRO	C-N-CA	5.42	125.24	119.28
5	E	156	LEU	N-CA-C	5.41	117.25	111.36
48	5	1238	A	C3'-C2'-O2'	5.40	118.80	110.70
48	5	1393	G	C4'-C3'-O3'	-5.38	104.92	113.00
51	9	467	G	C3'-C2'-O2'	5.36	118.74	110.70
48	5	1485	C	C4'-C3'-O3'	5.36	117.44	109.40
48	5	1921	C	C2'-C3'-O3'	5.33	117.50	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	484	U	C4'-C3'-O3'	5.32	117.39	109.40
18	S	71	SER	CA-C-N	5.31	125.00	119.64
18	S	71	SER	C-N-CA	5.31	125.00	119.64
48	5	4241	C	C4'-C3'-O3'	-5.31	105.04	113.00
48	5	2266	C	C2'-C3'-O3'	5.30	117.46	109.50
48	5	481(A)	C	C2'-C3'-O3'	5.30	117.45	109.50
48	5	3625	G	C2'-C3'-O3'	5.28	121.62	113.70
48	5	480	C	C2'-C3'-O3'	5.25	121.58	113.70
48	5	231	U	C4'-C3'-O3'	-5.24	105.14	113.00
48	5	4529	G	C4'-C3'-O3'	-5.23	105.16	113.00
48	5	2349	A	C4'-C3'-O3'	-5.21	105.18	113.00
3	C	74	ALA	N-CA-C	5.21	119.12	112.87
48	5	90	G	C2'-C3'-O3'	5.18	121.47	113.70
51	9	1438	A	C4'-C3'-O3'	-5.17	105.25	113.00
51	9	873	G	C2'-C3'-O3'	5.15	117.23	109.50
48	5	1485	C	C2'-C3'-O3'	5.14	117.21	109.50
51	9	553	U	C2'-C3'-O3'	5.12	121.38	113.70
48	5	1804	A	C4'-C3'-O3'	5.12	117.07	109.40
51	9	1395	C	C4'-C3'-O3'	5.12	120.67	113.00
66	OO	146	ARG	N-CA-C	-5.11	105.79	111.36
4	D	22	ARG	CG-CD-NE	5.10	123.22	112.00
22	W	50	ASN	N-CA-C	5.10	116.53	111.07
51	9	1637	A	C2'-C3'-O3'	5.08	117.12	109.50
73	VV	23	ILE	N-CA-CB	5.08	116.45	110.82
48	5	1236	C	C4'-C3'-O3'	5.06	120.59	113.00
51	9	126	G	C4'-C3'-O3'	5.05	116.97	109.40
56	EE	108	ARG	N-CA-C	5.04	116.61	110.41
48	5	1445	U	C3'-C2'-O2'	5.04	118.26	110.70
51	9	1264	C	C4'-C3'-O3'	5.04	116.96	109.40
48	5	485	C	C3'-C2'-O2'	5.04	118.26	110.70
51	9	555	A	C2'-C3'-O3'	5.03	117.05	109.50
48	5	959	G	C4'-C3'-O3'	5.03	116.94	109.40
48	5	226	G	C4'-C3'-O3'	5.02	116.93	109.40
51	9	553	U	C3'-C2'-O2'	5.02	118.23	110.70
48	5	2088	A	C2'-C3'-O3'	5.01	117.01	109.50
48	5	2427	G	C4'-C3'-O3'	-5.00	105.49	113.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	PHE	Peptide

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Mol	Chain	Res	Type	Group
74	WW	27	ILE	Peptide
75	XX	61	GLN	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1898	0	1993	20	0
2	B	3172	0	3310	23	0
3	C	2883	0	3053	9	0
4	D	2391	0	2424	14	0
5	E	1729	0	1887	11	0
6	F	1875	0	1995	12	0
7	G	1879	0	2027	11	0
8	H	1516	0	1597	10	0
9	I	1664	0	1712	5	0
10	J	1362	0	1399	7	0
11	L	1702	0	1820	11	0
12	M	1137	0	1211	9	0
13	N	1701	0	1749	4	0
14	O	1630	0	1778	15	0
15	P	1242	0	1274	5	0
16	Q	1515	0	1634	6	0
17	R	1508	0	1664	5	0
18	S	1462	0	1508	16	0
19	T	1298	0	1366	5	0
20	U	809	0	833	1	0
21	V	979	0	1039	7	0
22	W	860	0	903	3	0
23	X	967	0	1040	3	0
24	Y	1115	0	1205	1	0
25	Z	1107	0	1182	4	0
26	a	1162	0	1209	11	0
27	b	848	0	920	1	0
28	c	761	0	794	0	0
29	d	888	0	930	9	0
30	e	1053	0	1147	5	0
31	f	876	0	912	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	g	906	0	999	0	0
33	h	1013	0	1147	4	0
34	i	830	0	916	3	0
35	j	705	0	737	2	0
36	k	569	0	637	1	0
37	l	447	0	480	1	0
38	m	429	0	465	2	0
39	n	239	0	289	0	0
40	o	851	0	920	5	0
41	p	708	0	758	6	0
42	r	994	0	1051	7	0
43	s	1507	0	1564	3	0
44	t	1160	0	1218	3	0
45	1	125	0	117	1	0
46	2	1616	0	824	5	0
47	3	1593	0	811	5	0
48	5	75972	0	38393	146	0
49	7	2558	0	1296	2	0
50	8	3208	0	1629	5	0
51	9	36249	0	18316	104	0
52	AA	1710	0	1708	12	0
53	BB	1729	0	1803	15	0
54	CC	1716	0	1806	10	0
55	DD	1768	0	1866	8	0
56	EE	2076	0	2177	8	0
57	FF	1471	0	1522	12	0
58	GG	1923	0	2089	9	0
59	HH	1488	0	1582	5	0
60	II	1686	0	1772	6	0
61	JJ	1525	0	1640	12	0
62	KK	810	0	836	9	0
63	LL	1175	0	1249	4	0
64	MM	908	0	939	8	0
65	NN	1202	0	1289	2	0
66	OO	1016	0	1039	9	0
67	PP	997	0	1045	6	0
68	QQ	1128	0	1195	8	0
69	RR	1068	0	1121	5	0
70	SS	1190	0	1249	3	0
71	TT	1097	0	1132	5	0
72	UU	795	0	862	4	0
73	VV	636	0	637	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
74	WW	1034	0	1080	9	0
75	XX	1098	0	1167	4	0
76	YY	1011	0	1083	1	0
77	ZZ	598	0	656	6	0
78	aa	814	0	864	4	0
79	bb	651	0	672	2	0
80	cc	488	0	514	6	0
81	dd	459	0	449	2	0
82	ee	443	0	492	0	0
83	ff	555	0	566	5	0
84	gg	2436	0	2393	7	0
85	hh	317	0	161	1	0
86	ii	3307	0	3346	16	0
87	jj	3368	0	3422	26	0
88	5	185	0	0	0	0
88	7	5	0	0	0	0
88	8	8	0	0	0	0
88	9	71	0	0	0	0
88	A	1	0	0	0	0
88	B	1	0	0	0	0
88	I	1	0	0	0	0
88	P	3	0	0	0	0
88	Q	1	0	0	0	0
88	V	1	0	0	0	0
88	a	1	0	0	0	0
88	g	1	0	0	0	0
88	hh	1	0	0	0	0
88	j	1	0	0	0	0
88	jj	1	0	0	0	0
89	aa	1	0	0	0	0
89	dd	1	0	0	0	0
89	ff	1	0	0	1	0
89	g	1	0	0	0	0
89	j	1	0	0	0	0
89	m	1	0	0	0	0
89	o	1	0	0	0	0
89	p	1	0	0	2	0
90	jj	32	0	14	0	0
All	All	222683	0	167519	689	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 2.

All (689) 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)
87:jj:346:LYS:CD	87:jj:389:ASN:OD1	1.65	1.41
83:ff:144:CYS:SG	89:ff:200:ZN:ZN	1.24	1.26
48:5:2367:A:N1	48:5:2788:U:O4	1.66	1.25
51:9:1137:U:O4	51:9:1148:A:N1	1.68	1.23
87:jj:346:LYS:HD3	87:jj:389:ASN:OD1	1.01	1.18
51:9:1137:U:C4	51:9:1148:A:N1	2.11	1.18
87:jj:346:LYS:CG	87:jj:389:ASN:OD1	1.95	1.14
62:KK:15:LEU:HD22	62:KK:49:MET:HE1	1.43	1.00
51:9:1137:U:O4	51:9:1148:A:C2	2.17	0.98
51:9:1679:A:OP1	80:cc:20:ARG:NH2	2.03	0.92
86:ii:160:THR:HG23	86:ii:169:LEU:HD11	1.57	0.87
51:9:1137:U:O4	51:9:1148:A:C6	2.32	0.82
18:S:93:MET:HE3	18:S:113:MET:HE1	1.59	0.82
48:5:2367:A:N1	48:5:2788:U:C4	2.49	0.81
87:jj:484:ILE:HG22	87:jj:502:ILE:HG22	1.63	0.81
57:FF:99:ILE:HG23	77:ZZ:67:LEU:HD21	1.65	0.77
48:5:2367:A:N6	48:5:2788:U:N3	2.32	0.77
51:9:1137:U:C4	51:9:1148:A:C6	2.75	0.74
48:5:4579:U:H2'	48:5:4580:U:C6	2.23	0.72
2:B:254:ILE:HG23	2:B:266:VAL:HG11	1.71	0.72
48:5:3914:U:H3	48:5:4378:A:N6	1.87	0.71
62:KK:35:LEU:HD13	62:KK:40:VAL:HG21	1.72	0.70
48:5:3914:U:N3	48:5:4378:A:N6	2.40	0.69
48:5:4723:A:H2'	48:5:4724:A:C8	2.28	0.68
53:BB:66:VAL:HG22	53:BB:87:ILE:HG22	1.76	0.68
51:9:1407:U:H2'	51:9:1408:U:C6	2.29	0.68
87:jj:436:VAL:HG12	87:jj:437:ASP:N	2.09	0.67
87:jj:346:LYS:HG3	87:jj:389:ASN:OD1	1.92	0.66
67:PP:56:LEU:HD13	67:PP:78:THR:HG21	1.76	0.66
11:L:169:ILE:HD13	26:a:142:GLY:HA2	1.77	0.66
38:m:84:CYS:SG	38:m:85:ARG:N	2.69	0.65
48:5:2031:C:O3'	48:5:2032:U:P	2.55	0.65
42:r:98:ARG:NH2	48:5:2262:G:OP2	2.30	0.65
61:JJ:130:ILE:HG12	61:JJ:135:ILE:HD11	1.79	0.65
35:j:19:CYS:SG	35:j:20:ARG:N	2.71	0.64
71:TT:60:THR:HG23	71:TT:75:MET:HE2	1.79	0.64
1:A:126:LEU:HD13	1:A:150:LEU:HD21	1.79	0.64
51:9:1137:U:N3	51:9:1148:A:N6	2.45	0.64
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.80	0.63
48:5:747:A:H4'	48:5:748:G:OP1	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:45:GLN:HE22	40:o:51:GLN:HA	1.64	0.63
84:gg:87:LEU:HD21	84:gg:108:VAL:HG11	1.81	0.63
60:II:36:THR:HG21	60:II:179:PRO:HB2	1.80	0.63
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.80	0.62
4:D:23:ARG:NH2	48:5:4280:A:OP2	2.33	0.62
55:DD:72:VAL:HG23	62:KK:20:VAL:HG21	1.82	0.62
51:9:1438:A:H2'	51:9:1439:A:C8	2.35	0.62
18:S:95:ARG:NH2	48:5:1951:G:O2'	2.33	0.62
51:9:1091:C:HO2'	74:WW:2:VAL:N	1.98	0.61
41:p:60:CYS:SG	89:p:100:ZN:ZN	1.88	0.61
53:BB:69:VAL:HG11	53:BB:74:LEU:HD13	1.80	0.61
14:O:72:HIS:N	48:5:4586:G:OP1	2.28	0.61
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.35	0.60
52:AA:33:GLN:HB3	52:AA:154:LEU:HD12	1.83	0.60
74:WW:75:ILE:HD11	74:WW:93:LEU:HD11	1.83	0.60
15:P:41:ILE:HD12	15:P:150:LEU:HD13	1.83	0.60
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.65	0.60
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.82	0.60
64:MM:33:ARG:NH2	64:MM:91:LEU:HD21	2.16	0.60
58:GG:32:MET:HE2	58:GG:63:MET:HG2	1.83	0.59
17:R:74:ARG:NH2	48:5:2891:U:OP2	2.35	0.59
51:9:1130:G:H2'	51:9:1130:G:N3	2.17	0.59
52:AA:63:ARG:HG3	52:AA:185:MET:HE1	1.85	0.59
11:L:178:ALA:HB1	26:a:146:LEU:HD21	1.84	0.59
75:XX:51:VAL:HG13	75:XX:70:VAL:HG13	1.85	0.59
48:5:217:C:O2'	48:5:218:A:OP2	2.12	0.59
86:ii:78:VAL:HG23	86:ii:95:VAL:HG11	1.85	0.59
1:A:199:VAL:HG21	48:5:1631:A:C8	2.38	0.59
14:O:160:ARG:NH2	48:5:4760:G:OP1	2.35	0.58
51:9:1680:G:H4'	80:cc:20:ARG:HD2	1.84	0.58
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.85	0.58
86:ii:317:VAL:HG23	86:ii:387:ALA:HB2	1.85	0.58
40:o:81:ARG:NH2	48:5:4293:U:O2'	2.36	0.58
64:MM:22:LEU:HD21	64:MM:89:VAL:HG23	1.86	0.58
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.38	0.57
37:l:2:SER:N	48:5:2406:G:N7	2.52	0.57
51:9:980:A:H2'	51:9:981:A:C8	2.39	0.57
48:5:4942:C:H4'	48:5:4943:A:OP1	2.05	0.57
51:9:1611:G:OP2	70:SS:121:ARG:NH1	2.37	0.57
54:CC:209:VAL:HG21	54:CC:233:LEU:CD1	2.35	0.57
46:2:16:C:O4'	46:2:16:C:O2	2.24	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:127:MET:HE1	19:T:155:PRO:HA	1.87	0.56
47:3:16:C:O2	47:3:16:C:O4'	2.24	0.56
64:MM:22:LEU:HD11	64:MM:89:VAL:HA	1.87	0.56
48:5:2395:A:O2'	48:5:2806:A:H1'	2.05	0.56
48:5:4510:A:O2'	48:5:4511:A:O4'	2.24	0.56
41:p:60:CYS:HG	89:p:100:ZN:ZN	1.17	0.56
2:B:84:MET:HE1	2:B:183:ILE:HD11	1.86	0.56
81:dd:24:CYS:SG	81:dd:42:CYS:SG	3.04	0.56
52:AA:163:CYS:SG	52:AA:174:MET:HE2	2.46	0.56
86:ii:322:VAL:HG11	86:ii:375:LEU:HD13	1.88	0.56
44:t:81:ILE:HD11	44:t:132:ILE:HG23	1.87	0.55
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.88	0.55
29:d:27:ILE:HD12	29:d:86:VAL:HG21	1.88	0.55
48:5:3766:A:N1	51:9:1827:U:O2'	2.28	0.55
54:CC:88:ILE:HG21	54:CC:94:ILE:CD1	2.37	0.55
2:B:49:TYR:CE2	2:B:168:MET:HE1	2.41	0.55
69:RR:16:ILE:HG22	69:RR:24:LEU:HD11	1.89	0.55
86:ii:169:LEU:HD13	86:ii:212:LEU:HD12	1.87	0.55
51:9:1680:G:H1'	80:cc:20:ARG:NH1	2.20	0.55
19:T:80:VAL:CG2	19:T:85:LEU:HD12	2.36	0.55
87:jj:554:ILE:HG22	87:jj:555:HIS:CD2	2.41	0.55
52:AA:60:LEU:HD13	52:AA:159:ILE:HD11	1.89	0.55
14:O:18:ARG:NH2	48:5:2057:A:OP1	2.38	0.55
2:B:174:ARG:NH1	48:5:4985:U:O2	2.40	0.55
33:h:44:LEU:O	33:h:47:ILE:HG22	2.07	0.55
56:EE:44:LEU:HD13	56:EE:72:ILE:HD11	1.88	0.55
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.89	0.55
3:C:130:ALA:HB3	3:C:246:VAL:HG12	1.89	0.54
4:D:22:ARG:NH1	4:D:28:THR:OG1	2.41	0.54
5:E:159:ARG:NH1	48:5:4940:C:OP1	2.39	0.54
51:9:1274:G:N7	62:KK:43:LEU:HD13	2.22	0.54
87:jj:436:VAL:CG1	87:jj:437:ASP:N	2.69	0.54
29:d:33:ILE:O	29:d:36:VAL:HG22	2.07	0.54
87:jj:216:VAL:HG23	87:jj:314:ALA:HB2	1.89	0.54
51:9:945:U:H2'	51:9:946:U:C6	2.42	0.54
54:CC:176:LYS:O	54:CC:200:ARG:NH1	2.40	0.54
51:9:1351:G:O2'	51:9:1378:A:N1	2.34	0.54
51:9:501:C:H2'	51:9:501:C:O2	2.06	0.54
8:H:88:PHE:CE1	8:H:151:ILE:HD12	2.43	0.54
48:5:245:C:O4'	48:5:245:C:O2	2.24	0.54
48:5:2505:C:O2	48:5:2505:C:O4'	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:1139:C:O4'	51:9:1139:C:O2	2.21	0.54
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.90	0.54
48:5:1483:C:O2	48:5:1483:C:O4'	2.23	0.53
51:9:434:G:H2'	51:9:435:A:C8	2.43	0.53
51:9:1117:C:O2'	51:9:1118:C:O4'	2.27	0.53
57:FF:88:MET:HE1	57:FF:92:ILE:HD11	1.89	0.53
30:e:81:ASN:HA	30:e:111:ILE:HD11	1.90	0.53
51:9:94:G:O2'	51:9:508:A:O2'	2.25	0.53
51:9:1315:U:O2	51:9:1315:U:O4'	2.27	0.53
5:E:165:VAL:HG11	5:E:178:VAL:HG13	1.89	0.53
57:FF:39:ILE:HG23	57:FF:68:ILE:HD13	1.89	0.53
6:F:88:LEU:HD22	6:F:89:ALA:N	2.23	0.53
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.90	0.53
48:5:3723:A:H2'	48:5:3724:A:C8	2.42	0.53
48:5:4989:U:O2	48:5:4989:U:O4'	2.27	0.53
62:KK:35:LEU:CD1	62:KK:40:VAL:HG21	2.37	0.53
18:S:3:ALA:O	18:S:111:ARG:NH1	2.41	0.53
21:V:82:ILE:HD12	21:V:104:VAL:HG13	1.90	0.53
25:Z:11:VAL:HG11	25:Z:80:LEU:HD22	1.91	0.53
59:HH:61:ILE:HD11	59:HH:95:ILE:HD12	1.90	0.53
74:WW:3:ARG:HD3	74:WW:6:VAL:HG22	1.91	0.53
5:E:165:VAL:HG13	5:E:180:GLY:N	2.24	0.53
71:TT:104:LEU:HD22	71:TT:121:ARG:HG2	1.90	0.53
29:d:22:THR:HG22	29:d:89:SER:CB	2.39	0.52
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.91	0.52
48:5:3810:C:O4'	48:5:3810:C:O2	2.26	0.52
48:5:4467:A:O2'	48:5:4510:A:N3	2.42	0.52
80:cc:14:VAL:HG13	80:cc:30:VAL:HG13	1.92	0.52
83:ff:126:CYS:SG	83:ff:143:LYS:NZ	2.83	0.52
31:f:28:LEU:HG	31:f:101:ILE:HD11	1.92	0.52
8:H:12:ILE:HG22	8:H:81:ILE:HD11	1.90	0.52
45:1:68:VAL:C	46:2:76:A:O3'	2.53	0.52
58:GG:18:VAL:HG21	58:GG:41:LEU:HD23	1.90	0.52
58:GG:63:MET:SD	58:GG:63:MET:N	2.83	0.52
48:5:498:C:O2	48:5:498:C:O4'	2.28	0.52
5:E:281:THR:OG1	48:5:4754:G:N7	2.42	0.52
51:9:4:C:O2'	61:JJ:18:ARG:NH1	2.42	0.52
51:9:183:G:O2'	51:9:184:G:O5'	2.24	0.52
11:L:182:LEU:HD23	34:i:7:MET:HE2	1.91	0.51
51:9:1262:C:O2'	81:dd:12:ARG:NH1	2.44	0.51
51:9:1489:A:H4'	51:9:1490:G:OP2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:201:GLU:OE2	7:G:226:LEU:HD11	2.10	0.51
48:5:224:U:O2	48:5:224:U:O4'	2.28	0.51
51:9:1284:A:C6	64:MM:91:LEU:HD22	2.44	0.51
51:9:1364:U:O4'	51:9:1364:U:O2	2.29	0.51
43:s:43:ILE:HD13	43:s:187:LEU:HD21	1.92	0.51
47:3:75:C:O2	47:3:75:C:O4'	2.28	0.51
48:5:2627:C:O4'	48:5:2627:C:O2	2.27	0.51
51:9:824:C:C2	61:JJ:144:ILE:HD13	2.45	0.51
56:EE:31:PRO:HG2	56:EE:38:LEU:HD12	1.93	0.51
40:o:41:TYR:CD1	47:3:75:C:O2	2.63	0.51
52:AA:63:ARG:CG	52:AA:185:MET:HE1	2.41	0.51
18:S:93:MET:HE1	18:S:117:HIS:CE1	2.45	0.51
29:d:33:ILE:HD11	29:d:41:ARG:HB3	1.92	0.51
2:B:249:ARG:NH1	48:5:2837:U:OP1	2.43	0.51
74:WW:6:VAL:HG12	74:WW:34:ILE:HD11	1.93	0.51
50:8:125:C:O2	50:8:125:C:O4'	2.29	0.51
58:GG:5:ILE:HD12	58:GG:16:ILE:HD13	1.92	0.51
77:ZZ:73:VAL:HG12	77:ZZ:79:ILE:HD11	1.91	0.51
51:9:501:C:O2	51:9:501:C:C2'	2.57	0.51
76:YY:34:THR:HG23	76:YY:69:THR:HG21	1.92	0.51
56:EE:234:PRO:HG3	56:EE:238:LEU:HD11	1.92	0.50
48:5:2367:A:C2	48:5:2788:U:O4	2.53	0.50
1:A:179:ILE:O	48:5:3653:A:H4'	2.11	0.50
3:C:150:LEU:O	3:C:152:LEU:N	2.43	0.50
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.42	0.50
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.41	0.50
6:F:75:ARG:NE	48:5:730:G:OP2	2.36	0.50
7:G:98:ILE:HG21	48:5:4125:C:H4'	1.92	0.50
48:5:2763:U:O2	48:5:2763:U:O4'	2.29	0.50
7:G:139:VAL:HG11	7:G:238:LYS:HG3	1.93	0.50
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.92	0.50
18:S:79:GLY:HA3	18:S:132:ILE:HD12	1.92	0.50
87:jj:346:LYS:HG2	87:jj:389:ASN:OD1	2.02	0.50
1:A:77:ILE:HD12	1:A:115:CYS:SG	2.51	0.50
26:a:86:THR:HG22	48:5:510:U:H5''	1.94	0.50
48:5:1237:C:O4'	48:5:1237:C:O2	2.29	0.50
51:9:1624:U:O2	51:9:1624:U:O4'	2.30	0.50
54:CC:179:THR:HG23	54:CC:180:VAL:O	2.12	0.50
5:E:185:ASN:ND2	5:E:274:LEU:O	2.44	0.50
48:5:1426:G:N1	48:5:1458:C:OP2	2.35	0.50
57:FF:102:LEU:HD22	77:ZZ:110:THR:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
58:GG:52:ILE:HD11	58:GG:109:LEU:HD22	1.94	0.50
87:jj:219:GLY:O	87:jj:341:HIS:NE2	2.45	0.50
36:k:35:LYS:NZ	48:5:2693:G:OP1	2.41	0.50
51:9:1404:U:C6	72:UU:56:MET:HE2	2.47	0.50
64:MM:22:LEU:HD13	64:MM:22:LEU:C	2.37	0.50
21:V:99:GLU:HB3	22:W:24:THR:HG23	1.93	0.49
48:5:4378:A:O2'	48:5:4379:A:H2'	2.12	0.49
66:OO:99:ALA:H	66:OO:133:THR:HG22	1.77	0.49
4:D:140:GLY:O	48:5:1819:G:O2'	2.24	0.49
10:J:53:ALA:HB2	10:J:68:ILE:HD12	1.93	0.49
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.47	0.49
48:5:4758:U:O2	48:5:4758:U:O4'	2.30	0.49
51:9:853:C:O4'	51:9:853:C:O2	2.26	0.49
86:ii:33:SER:C	86:ii:34:MET:HE2	2.37	0.49
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.47	0.49
25:Z:11:VAL:CG1	25:Z:80:LEU:HD22	2.42	0.49
51:9:1543:U:OP2	71:TT:62:ARG:NH1	2.45	0.49
53:BB:103:MET:HE1	53:BB:212:VAL:HG23	1.94	0.49
3:C:42:THR:HG21	48:5:2340:C:H5'	1.93	0.49
4:D:106:ALA:HB1	4:D:171:LEU:HD13	1.95	0.49
11:L:106:SER:HB3	34:i:17:VAL:HG11	1.93	0.49
12:M:112:VAL:HG11	14:O:201:LEU:HD11	1.93	0.49
30:e:31:ILE:HD11	48:5:2347:A:C4	2.47	0.49
51:9:1374:C:H2'	51:9:1375:G:O4'	2.13	0.49
54:CC:209:VAL:HG21	54:CC:233:LEU:HD13	1.94	0.49
61:JJ:46:VAL:HG21	61:JJ:106:LEU:HD11	1.95	0.49
71:TT:39:LEU:HD11	71:TT:52:TRP:CZ3	2.47	0.49
80:cc:46:VAL:HG11	80:cc:50:VAL:CG2	2.43	0.49
87:jj:536:VAL:HG23	87:jj:590:VAL:HG22	1.94	0.49
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.94	0.49
16:Q:104:ARG:NH2	48:5:1353:G:N7	2.60	0.49
48:5:1381:U:O2	48:5:1381:U:O4'	2.30	0.49
48:5:4579:U:O2	48:5:4580:U:C2	2.66	0.49
51:9:1137:U:H3	51:9:1148:A:N6	2.08	0.49
69:RR:31:ASN:C	69:RR:31:ASN:HD22	2.20	0.49
12:M:97:ALA:HB2	14:O:203:VAL:HB	1.94	0.49
77:ZZ:58:LEU:HD21	77:ZZ:91:LEU:HD11	1.94	0.49
12:M:104:MET:HE2	14:O:199:HIS:HB3	1.94	0.49
51:9:1149:A:N3	51:9:1149:A:H2'	2.28	0.49
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.48	0.48
74:WW:55:ASP:O	74:WW:57:ARG:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:85:THR:HG22	16:Q:104:ARG:HB2	1.95	0.48
48:5:3724:A:N6	48:5:3725:G:C6	2.81	0.48
48:5:4966:A:H2'	48:5:4967:A:C8	2.48	0.48
57:FF:87:LEU:CD2	68:QQ:47:LEU:HD13	2.43	0.48
59:HH:134:VAL:HG12	59:HH:173:PHE:CE2	2.48	0.48
8:H:12:ILE:HG22	8:H:81:ILE:CD1	2.43	0.48
51:9:823:U:O2	51:9:823:U:O4'	2.30	0.48
17:R:42:ARG:HA	17:R:45:ILE:HD12	1.94	0.48
55:DD:105:LEU:HD23	55:DD:184:ILE:HG23	1.94	0.48
61:JJ:130:ILE:CG1	61:JJ:135:ILE:HD11	2.42	0.48
2:B:29:VAL:HG13	2:B:348:ARG:HD3	1.95	0.48
6:F:93:ARG:NH2	6:F:95:ARG:O	2.47	0.48
48:5:2097:A:OP1	48:5:2107:A:N6	2.46	0.48
48:5:4928:C:O4'	48:5:4928:C:O2	2.31	0.48
55:DD:24:PHE:CZ	55:DD:72:VAL:HG11	2.49	0.48
56:EE:100:ARG:HD2	56:EE:102:ILE:HD11	1.96	0.48
8:H:41:ILE:HG21	8:H:73:ILE:HD11	1.96	0.48
8:H:12:ILE:HG21	8:H:18:ILE:HD13	1.94	0.48
84:gg:17:TRP:CE3	84:gg:303:THR:HG22	2.48	0.48
87:jj:484:ILE:CG2	87:jj:502:ILE:HG22	2.40	0.48
48:5:4305:G:C2'	48:5:4305:G:N3	2.76	0.48
18:S:80:ILE:HG12	18:S:129:VAL:HG13	1.95	0.48
21:V:50:ASN:ND2	48:5:4457:U:OP1	2.47	0.48
67:PP:44:ARG:HD2	67:PP:84:ILE:HD13	1.96	0.48
86:ii:120:ILE:HG22	86:ii:139:LEU:HD13	1.96	0.48
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.49	0.48
48:5:4478:G:H2'	48:5:4479:A:O4'	2.13	0.48
1:A:207:VAL:HG12	48:5:3919:C:C5'	2.44	0.47
46:2:33:U:OP2	68:QQ:146:ARG:NH2	2.47	0.47
48:5:1872:G:O2'	48:5:4219:A:N3	2.43	0.47
51:9:1834:A:C2	51:9:1836:G:C4	3.02	0.47
54:CC:210:PRO:HA	54:CC:240:THR:HG21	1.96	0.47
67:PP:37:TYR:OH	67:PP:45:LEU:HD11	2.14	0.47
26:a:126:ALA:HB3	26:a:129:PHE:CE1	2.49	0.47
74:WW:55:ASP:HB3	79:bb:25:VAL:HG13	1.96	0.47
87:jj:369:ASN:OD1	87:jj:373:GLU:HG3	2.13	0.47
3:C:293:LEU:HD22	16:Q:34:PHE:CD2	2.49	0.47
57:FF:14:THR:HG23	57:FF:14:THR:O	2.14	0.47
26:a:21:ARG:NH1	48:5:1317:U:OP1	2.47	0.47
87:jj:440:ILE:HG22	87:jj:462:GLY:HA3	1.97	0.47
3:C:101:MET:HE2	48:5:2343:G:C4	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:148:VAL:HG12	16:Q:152:PHE:CZ	2.49	0.47
79:bb:46:VAL:HG11	79:bb:64:CYS:SG	2.55	0.47
51:9:1863:A:H1'	78:aa:79:ILE:HD13	1.96	0.47
2:B:48:GLY:HA3	2:B:81:THR:HG22	1.95	0.47
7:G:139:VAL:HG11	7:G:238:LYS:CG	2.45	0.47
8:H:128:MET:HE1	8:H:161:ILE:HG21	1.97	0.47
9:I:61:SER:HA	9:I:126:VAL:HG23	1.97	0.47
13:N:193:ARG:O	13:N:197:THR:HG23	2.15	0.47
14:O:74:ARG:NH1	48:5:4586:G:OP2	2.48	0.47
19:T:87:LYS:NZ	48:5:4301:U:OP2	2.47	0.47
48:5:964:A:H2'	48:5:965:G:O4'	2.15	0.47
57:FF:71:ARG:NH1	57:FF:148:ASN:OD1	2.45	0.47
44:t:98:ILE:HG23	44:t:98:ILE:O	2.14	0.47
48:5:82:U:H2'	48:5:83:C:O4'	2.15	0.47
51:9:161:U:O2'	58:GG:87:ARG:NH1	2.48	0.47
55:DD:21:LEU:HD21	55:DD:48:ILE:HD11	1.96	0.47
14:O:168:TYR:CE2	14:O:172:LYS:HD2	2.50	0.47
18:S:82:LEU:HB2	18:S:93:MET:HB2	1.97	0.47
51:9:146:G:O2'	51:9:147:A:O5'	2.33	0.47
51:9:1303:C:O2	51:9:1303:C:O4'	2.30	0.47
48:5:1964:A:C6	48:5:4694:G:C6	3.03	0.47
51:9:1291:A:N3	83:ff:140:TYR:OH	2.48	0.47
48:5:1358:G:H4'	48:5:1359:G:OP1	2.14	0.46
48:5:3617:G:O2'	48:5:3620:G:N7	2.48	0.46
42:r:46:ARG:HG2	42:r:70:GLN:HE22	1.80	0.46
48:5:1990:A:H3'	48:5:1991:A:H5''	1.97	0.46
51:9:183:G:O2'	51:9:183:G:N3	2.48	0.46
53:BB:39:PHE:CD1	53:BB:74:LEU:HD23	2.51	0.46
87:jj:343:MET:HE3	87:jj:344:LEU:HG	1.96	0.46
26:a:103:VAL:HG12	26:a:108:TYR:HB2	1.96	0.46
48:5:1358:G:O2'	48:5:1359:G:O5'	2.28	0.46
48:5:294:G:O6	48:5:315:G:H1'	2.16	0.46
48:5:4423:U:O2	48:5:4423:U:O4'	2.34	0.46
51:9:887:U:O2	51:9:887:U:O4'	2.31	0.46
53:BB:52:THR:HG23	53:BB:57:ILE:HA	1.97	0.46
70:SS:43:VAL:HG21	70:SS:83:PHE:CZ	2.50	0.46
84:gg:81:GLY:HA2	84:gg:87:LEU:HD23	1.98	0.46
11:L:71:ARG:NH2	48:5:74:G:O3'	2.49	0.46
16:Q:78:LYS:HG2	16:Q:137:VAL:HG23	1.97	0.46
51:9:1680:G:H1'	80:cc:20:ARG:HH11	1.81	0.46
63:LL:101:ARG:HB2	75:XX:10:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
75:XX:61:GLN:HB3	75:XX:62:PRO:CD	2.45	0.46
4:D:53:VAL:HG11	4:D:159:VAL:HA	1.98	0.46
48:5:2367:A:N6	48:5:2788:U:C4	2.80	0.46
68:QQ:47:LEU:HB3	68:QQ:81:ILE:HD13	1.97	0.46
73:VV:55:ILE:HD11	73:VV:69:ILE:HG12	1.97	0.46
13:N:135:ILE:HD13	13:N:151:ILE:HD13	1.97	0.46
40:o:41:TYR:CE1	47:3:75:C:O2	2.68	0.46
48:5:4723:A:C2	48:5:4724:A:C6	3.04	0.46
87:jj:283:ALA:HB3	87:jj:294:ILE:HG23	1.97	0.46
87:jj:540:HIS:N	87:jj:541:LYS:HA	2.31	0.46
15:P:95:LEU:HD12	15:P:148:MET:HE1	1.98	0.46
30:e:44:ARG:NH2	48:5:1312:A:O2'	2.49	0.46
48:5:716:C:H2'	48:5:717:U:O4'	2.16	0.46
48:5:2738:C:O2'	48:5:2740:U:OP2	2.25	0.46
48:5:4305:G:N3	48:5:4305:G:H2'	2.31	0.46
53:BB:110:MET:HE1	53:BB:140:VAL:HG21	1.97	0.46
18:S:35:PRO:HD2	18:S:39:VAL:HG21	1.98	0.46
48:5:3697:U:O2'	48:5:3698:G:OP2	2.27	0.46
51:9:1130:G:O2'	51:9:1131:G:P	2.74	0.46
18:S:80:ILE:HG23	18:S:129:VAL:HG22	1.96	0.45
58:GG:162:LEU:HD11	58:GG:172:LYS:HB2	1.97	0.45
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.46	0.45
15:P:127:ARG:NH2	48:5:2422:C:OP1	2.49	0.45
30:e:38:PRO:HD2	30:e:55:MET:HE3	1.98	0.45
46:2:74:C:H2'	46:2:75:C:H5'	1.99	0.45
51:9:1653:U:H2'	51:9:1654:G:C8	2.52	0.45
68:QQ:34:VAL:HG22	68:QQ:70:VAL:HB	1.98	0.45
48:5:4966:A:C2	48:5:5067:U:N3	2.85	0.45
51:9:92:A:C6	51:9:446:G:C6	3.04	0.45
57:FF:173:LEU:HD13	57:FF:177:LEU:HD12	1.98	0.45
86:ii:110:VAL:HG22	86:ii:112:ILE:HD11	1.98	0.45
2:B:252:ALA:HB1	48:5:4524:G:N3	2.31	0.45
3:C:341:LEU:HD21	5:E:52:LEU:HD21	1.97	0.45
48:5:1633:G:H5'	48:5:1634:A:OP1	2.15	0.45
51:9:183:G:N3	51:9:183:G:C2'	2.78	0.45
56:EE:136:ILE:HD12	56:EE:149:TYR:OH	2.16	0.45
48:5:1301:C:O2	48:5:1301:C:O4'	2.32	0.45
54:CC:196:ILE:HB	54:CC:223:TYR:HB2	1.98	0.45
72:UU:24:LEU:CD2	72:UU:112:VAL:HG22	2.46	0.45
72:UU:50:VAL:HG23	72:UU:91:LEU:HD23	1.99	0.45
84:gg:91:ASP:HB2	84:gg:98:THR:HG23	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
86:ii:145:LYS:HD3	86:ii:160:THR:HG21	1.98	0.45
41:p:8:VAL:HG22	48:5:2876:G:OP1	2.17	0.45
55:DD:70:THR:HG22	55:DD:86:LEU:HD13	1.98	0.45
62:KK:3:MET:HE1	62:KK:48:ALA:HB2	1.98	0.45
67:PP:56:LEU:HD13	67:PP:78:THR:CG2	2.43	0.45
6:F:158:TYR:CE2	6:F:167:ALA:HB2	2.52	0.45
86:ii:290:TYR:CE2	86:ii:294:ILE:HD11	2.51	0.45
86:ii:312:LEU:HD12	86:ii:317:VAL:HG21	1.98	0.45
2:B:168:MET:HE2	2:B:175:GLN:CG	2.47	0.45
8:H:128:MET:HE1	8:H:161:ILE:CG2	2.47	0.45
68:QQ:34:VAL:HG21	68:QQ:84:ILE:HD12	1.97	0.45
2:B:29:VAL:HG11	2:B:32:PHE:CD1	2.52	0.45
14:O:79:ILE:HG21	14:O:138:LEU:HD11	1.97	0.45
16:Q:184:ARG:NE	26:a:55:LYS:O	2.50	0.45
44:t:78:SER:HA	44:t:81:ILE:HD12	1.99	0.45
48:5:3928:A:H2'	48:5:3929:G:O4'	2.17	0.45
5:E:180:GLY:O	5:E:181:PRO:C	2.60	0.45
54:CC:191:VAL:HG11	54:CC:236:PHE:HA	1.99	0.45
59:HH:51:ILE:HD11	59:HH:176:VAL:HG22	1.98	0.45
60:II:113:TYR:CE1	60:II:121:LEU:HD23	2.51	0.45
66:OO:56:VAL:HG12	66:OO:81:VAL:HG23	1.99	0.45
4:D:64:ILE:HD12	4:D:109:LEU:HD22	1.99	0.44
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.99	0.44
12:M:17:PHE:CE1	12:M:54:CYS:HA	2.52	0.44
51:9:427:U:O4'	51:9:427:U:O2	2.31	0.44
51:9:1207:G:C6	51:9:1837:G:C6	3.05	0.44
2:B:86:VAL:HG13	2:B:162:VAL:HG22	1.99	0.44
51:9:1144:A:C6	51:9:1145:A:C6	3.05	0.44
1:A:48:ILE:HG22	41:p:54:ILE:HD12	1.98	0.44
10:J:135:GLY:O	10:J:157:ILE:HD11	2.16	0.44
17:R:45:ILE:HG12	17:R:50:ILE:HD11	1.99	0.44
54:CC:251:LEU:HD23	73:VV:23:ILE:HG23	2.00	0.44
62:KK:3:MET:HE3	62:KK:8:ARG:NH2	2.32	0.44
74:WW:11:LEU:HD22	74:WW:72:CYS:SG	2.58	0.44
86:ii:169:LEU:HD13	86:ii:212:LEU:CD1	2.46	0.44
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.99	0.44
68:QQ:51:LEU:HD22	68:QQ:84:ILE:HG13	1.99	0.44
7:G:215:ASP:HB3	7:G:216:PRO:HD3	1.98	0.44
15:P:122:ALA:HB2	15:P:145:HIS:CD2	2.52	0.44
51:9:12:U:H2'	51:9:13:C:C6	2.53	0.44
53:BB:92:GLN:CD	53:BB:229:MET:HE1	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:153:LEU:HB3	5:E:197:VAL:HG13	1.99	0.44
11:L:106:SER:CB	34:i:17:VAL:HG11	2.48	0.44
48:5:1961:G:O2'	48:5:2025:A:N6	2.50	0.44
53:BB:150:ILE:HD13	69:RR:129:LYS:HB2	1.99	0.44
55:DD:162:ASP:N	55:DD:163:PRO:CD	2.80	0.44
87:jj:531:PHE:CZ	87:jj:552:LEU:HD21	2.52	0.44
3:C:27:VAL:CG2	3:C:264:TYR:HB2	2.47	0.44
48:5:106:A:H2'	48:5:107:G:O4'	2.17	0.44
50:8:94:G:H5'	50:8:94:G:C8	2.52	0.44
51:9:929:G:H2'	51:9:930:C:O4'	2.18	0.44
57:FF:72:LEU:HD22	57:FF:112:LEU:HD11	1.99	0.44
1:A:180:LEU:HD22	41:p:18:TYR:CB	2.48	0.44
23:X:79:PHE:CD1	33:h:36:VAL:HG21	2.53	0.44
29:d:22:THR:HG22	29:d:89:SER:HB3	1.99	0.44
56:EE:126:VAL:HG23	56:EE:156:VAL:O	2.18	0.44
62:KK:71:LEU:HD21	62:KK:79:LEU:HD12	2.00	0.44
48:5:2367:A:C6	48:5:2788:U:C4	3.06	0.44
51:9:980:A:C2	51:9:981:A:C6	3.05	0.44
55:DD:72:VAL:HG13	62:KK:68:TYR:CD1	2.52	0.44
3:C:208:CYS:SG	3:C:230:LEU:HD12	2.58	0.43
14:O:48:TYR:CD2	48:5:1930:U:C6	3.06	0.43
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.99	0.43
51:9:15:U:H2'	51:9:16:G:O4'	2.18	0.43
51:9:1143:A:C2	51:9:1144:A:C2	3.06	0.43
57:FF:89:THR:HA	57:FF:92:ILE:HD12	2.00	0.43
61:JJ:114:VAL:HG21	61:JJ:135:ILE:CD1	2.48	0.43
7:G:189:LEU:HD22	7:G:255:VAL:HG12	2.00	0.43
48:5:1748:U:C2	48:5:1783:C:C2	3.06	0.43
51:9:1130:G:O2'	51:9:1131:G:O5'	2.36	0.43
52:AA:33:GLN:CB	52:AA:154:LEU:HD12	2.47	0.43
26:a:114:LYS:O	48:5:1398:A:OP1	2.36	0.43
51:9:1336:C:H2'	51:9:1337:C:O4'	2.19	0.43
52:AA:143:PRO:HA	73:VV:32:ILE:HD11	2.00	0.43
4:D:103:LEU:HD11	4:D:248:ARG:HD3	2.00	0.43
23:X:146:ALA:HA	23:X:149:VAL:HG12	2.00	0.43
51:9:1129:G:C6	51:9:1130:G:O6	2.71	0.43
8:H:61:TRP:CZ3	12:M:33:GLN:HG2	2.53	0.43
10:J:27:GLY:HA2	10:J:68:ILE:HG23	2.00	0.43
26:a:38:MET:HE1	48:5:4340:U:H1'	2.00	0.43
48:5:481(A):C:O2	48:5:481(A):C:O4'	2.37	0.43
48:5:1279:A:O2'	48:5:1281:G:N7	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:9:522:A:OP2	61:JJ:45:ARG:NH2	2.46	0.43
51:9:1238:U:H2'	51:9:1239:U:O4'	2.19	0.43
53:BB:123:ALA:HB2	53:BB:165:ARG:HG3	2.00	0.43
74:WW:52:ILE:HG22	74:WW:61:ILE:HG23	2.01	0.43
2:B:114:CYS:SG	2:B:180:LEU:HD11	2.58	0.43
51:9:1834:A:C2'	51:9:1834:A:N3	2.82	0.43
61:JJ:46:VAL:HG21	61:JJ:106:LEU:CD1	2.48	0.43
2:B:332:MET:HE1	2:B:365:LEU:HD11	2.00	0.43
17:R:99:MET:HE3	17:R:127:VAL:HG12	2.00	0.43
51:9:1674:G:N7	68:QQ:17:LYS:NZ	2.67	0.43
84:gg:81:GLY:CA	84:gg:87:LEU:HD23	2.49	0.43
2:B:168:MET:HE2	2:B:175:GLN:HG3	2.00	0.43
2:B:181:MET:HE1	2:B:346:THR:HG23	2.00	0.43
29:d:36:VAL:HG23	29:d:41:ARG:CG	2.49	0.43
48:5:2088:A:O2'	48:5:2089:G:OP2	2.32	0.43
51:9:914:U:O2	51:9:914:U:O4'	2.36	0.43
57:FF:99:ILE:CG2	77:ZZ:67:LEU:HD21	2.41	0.43
60:II:3:ILE:HG23	60:II:3:ILE:O	2.18	0.43
72:UU:29:VAL:HG22	72:UU:85:HIS:CE1	2.54	0.43
78:aa:45:VAL:HG11	78:aa:53:ILE:CD1	2.49	0.43
13:N:114:ARG:HD2	13:N:151:ILE:HG22	2.01	0.43
48:5:2367:A:N6	48:5:2788:U:H3	2.12	0.43
52:AA:94:THR:HG23	52:AA:182:VAL:HG21	2.00	0.43
63:LL:68:ILE:HG21	63:LL:143:LEU:HD21	2.01	0.43
14:O:193:THR:HG23	14:O:202:LEU:HD23	2.01	0.43
29:d:36:VAL:HG11	29:d:44:ARG:HG2	2.01	0.43
30:e:31:ILE:HD11	48:5:2347:A:C5	2.54	0.43
48:5:750:U:H2'	48:5:751:G:O4'	2.18	0.43
48:5:2094:C:O2	48:5:2094:C:O4'	2.34	0.43
51:9:1546:G:C5'	68:QQ:18:THR:HG21	2.48	0.43
4:D:66:TYR:OH	4:D:73:MET:HE3	2.19	0.42
7:G:210:ILE:HG12	7:G:254:THR:HG22	2.01	0.42
10:J:139:PHE:CE1	10:J:151:ILE:HD13	2.54	0.42
15:P:47:TYR:O	15:P:51:VAL:HG23	2.18	0.42
18:S:13:VAL:HG23	18:S:62:VAL:HB	2.01	0.42
48:5:1963:C:N4	48:5:4694:G:O6	2.52	0.42
48:5:2458:C:H2'	48:5:2459:G:O4'	2.18	0.42
51:9:1228:A:H2'	51:9:1229:G:C8	2.54	0.42
60:II:36:THR:HG23	60:II:96:LEU:HB2	2.00	0.42
74:WW:52:ILE:HG22	74:WW:61:ILE:HG12	2.00	0.42
86:ii:252:LYS:HD2	86:ii:274:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
87:jj:218:ILE:HD12	87:jj:341:HIS:HB3	2.01	0.42
51:9:1596:U:H2'	51:9:1597:C:O4'	2.19	0.42
59:HH:122:LEU:C	59:HH:122:LEU:HD13	2.44	0.42
42:r:97:ILE:HD13	42:r:107:ARG:HA	2.01	0.42
48:5:1787:A:N3	48:5:4210:U:O2'	2.53	0.42
48:5:2439:G:C6	48:5:2440:U:C4	3.06	0.42
66:OO:119:LEU:C	66:OO:119:LEU:HD12	2.44	0.42
51:9:1035:A:H2'	51:9:1036:A:O4'	2.20	0.42
66:OO:44:VAL:HG11	66:OO:85:CYS:SG	2.59	0.42
87:jj:597:THR:HG21	87:jj:601:ILE:HG21	2.00	0.42
1:A:211:PHE:CG	1:A:219:ILE:HG23	2.54	0.42
2:B:321:VAL:HA	48:5:5050:C:O2'	2.19	0.42
6:F:90:PHE:CE2	6:F:92:ILE:HD11	2.55	0.42
9:I:72:ALA:CB	9:I:136:MET:HE1	2.48	0.42
51:9:944:A:C5	51:9:945:U:C5	3.07	0.42
55:DD:156:LEU:HD12	55:DD:157:MET:N	2.35	0.42
65:NN:91:LEU:HD12	65:NN:125:LEU:HD12	2.00	0.42
6:F:89:ALA:CB	6:F:124:LEU:HD21	2.48	0.42
38:m:70:CYS:HA	38:m:95:LEU:HD23	2.01	0.42
48:5:686:A:N3	48:5:686:A:H2'	2.35	0.42
48:5:1888:A:N6	48:5:3873:G:O2'	2.52	0.42
48:5:1895:G:O2'	48:5:1907:A:N3	2.46	0.42
50:8:15:G:C6	50:8:16:G:N1	2.87	0.42
51:9:171:A:H5'	58:GG:177:GLN:HG2	2.02	0.42
52:AA:15:VAL:HG12	52:AA:19:LEU:HD12	2.00	0.42
52:AA:134:LEU:CD2	52:AA:144:THR:HG21	2.48	0.42
60:II:194:GLU:HG2	63:LL:10:TYR:CD2	2.55	0.42
64:MM:49:LEU:C	64:MM:49:LEU:HD13	2.44	0.42
87:jj:445:VAL:HG23	87:jj:457:GLY:HA2	2.01	0.42
9:I:153:ARG:HA	9:I:165:ILE:HD11	2.02	0.42
10:J:141:ILE:HD11	49:7:55:A:N3	2.35	0.42
18:S:9:GLU:CG	18:S:33:PHE:CE1	3.02	0.42
40:o:15:CYS:SG	40:o:19:GLN:NE2	2.93	0.42
48:5:51:A:N3	48:5:1528:U:O2'	2.52	0.42
51:9:958:G:N1	51:9:959:G:C6	2.88	0.42
56:EE:181:CYS:SG	56:EE:225:ILE:HG23	2.59	0.42
66:OO:95:ILE:HD13	66:OO:116:LEU:HG	2.02	0.42
6:F:222:LYS:HE3	48:5:1907:A:H4'	2.01	0.42
7:G:131:PRO:HA	7:G:134:ASN:HB3	2.01	0.42
51:9:1520:G:H2'	51:9:1520:G:N3	2.35	0.42
69:RR:119:VAL:HG13	69:RR:119:VAL:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:30:MET:HE1	18:S:47:PHE:CB	2.50	0.42
48:5:3656:A:O4'	48:5:3747:A:C2	2.72	0.42
48:5:4260:U:H2'	48:5:4261:C:C6	2.55	0.42
66:OO:75:MET:HE3	66:OO:79:GLN:NE2	2.35	0.42
67:PP:15:PHE:CD1	67:PP:15:PHE:C	2.97	0.42
70:SS:59:LEU:HD12	70:SS:63:GLU:OE2	2.20	0.42
2:B:14:LEU:O	2:B:17:LEU:HG	2.20	0.42
22:W:3:VAL:HG23	22:W:3:VAL:O	2.20	0.42
48:5:4724:A:C6	48:5:4725:C:C4	3.08	0.42
87:jj:228:ILE:HG22	87:jj:401:GLY:CA	2.50	0.42
10:J:53:ALA:HB2	10:J:68:ILE:CD1	2.50	0.41
11:L:58:ILE:HG23	11:L:70:VAL:HG11	2.00	0.41
33:h:21:LEU:HD21	33:h:58:LEU:HD21	2.02	0.41
48:5:1811:G:C2	48:5:1812:C:C2	3.08	0.41
51:9:356:C:O2	51:9:356:C:C2'	2.66	0.41
51:9:584:A:C6	51:9:585:C:C4	3.08	0.41
57:FF:73:THR:HG22	57:FF:89:THR:HG23	2.01	0.41
73:VV:32:ILE:HD12	73:VV:60:ARG:HD2	2.02	0.41
77:ZZ:79:ILE:HB	77:ZZ:83:LEU:HD12	2.02	0.41
87:jj:232:ILE:HG22	87:jj:407:LEU:HD22	2.02	0.41
18:S:83:ARG:CB	18:S:127:MET:HE3	2.50	0.41
23:X:65:ALA:HB2	33:h:69:LEU:HD11	2.02	0.41
26:a:59:ARG:NH2	26:a:61:TYR:OH	2.53	0.41
48:5:1932:A:C2'	48:5:1933:G:O5'	2.68	0.41
48:5:3765:G:O2'	48:5:3766:A:N7	2.53	0.41
52:AA:134:LEU:HD21	52:AA:144:THR:HG21	2.01	0.41
2:B:299:ILE:N	2:B:299:ILE:HD12	2.36	0.41
7:G:189:LEU:HD21	7:G:257:PHE:CE2	2.55	0.41
9:I:36:LEU:HD12	9:I:87:ILE:HB	2.02	0.41
20:U:23:LEU:HD11	20:U:83:LEU:CD2	2.50	0.41
42:r:18:ILE:HG23	42:r:25:TYR:HB2	2.02	0.41
48:5:2408:U:O4'	48:5:2409:U:C5	2.74	0.41
51:9:1834:A:N1	51:9:1836:G:C2	2.88	0.41
60:II:117:TYR:CD1	60:II:156:ALA:HB2	2.56	0.41
63:LL:61:PRO:HA	63:LL:66:VAL:HG13	2.01	0.41
67:PP:34:MET:HG2	67:PP:45:LEU:HD12	2.02	0.41
86:ii:262:ASN:HD22	87:jj:551:VAL:HG13	1.85	0.41
1:A:207:VAL:HG23	1:A:208:GLU:HG3	2.02	0.41
11:L:116:ARG:NH1	11:L:155:MET:O	2.53	0.41
13:N:158:HIS:HB3	13:N:161:MET:HG2	2.02	0.41
19:T:85:LEU:HD13	48:5:4305:G:C2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:4459:U:H2'	48:5:4460:U:C6	2.55	0.41
51:9:482:G:N1	51:9:485:A:OP2	2.51	0.41
53:BB:87:ILE:HG23	53:BB:101:HIS:CG	2.56	0.41
61:JJ:35:TYR:CD2	61:JJ:106:LEU:HD23	2.55	0.41
84:gg:197:THR:HG21	84:gg:238:ALA:HA	2.03	0.41
5:E:164:ARG:O	5:E:185:ASN:ND2	2.53	0.41
31:f:48:ALA:HB2	31:f:71:TRP:CZ3	2.56	0.41
42:r:37:SER:OG	48:5:2267:U:OP1	2.32	0.41
48:5:916:C:O2	48:5:916:C:O4'	2.38	0.41
48:5:3656:A:O2'	48:5:3747:A:O2'	2.32	0.41
51:9:1700:C:C2	51:9:1834:A:N6	2.88	0.41
51:9:1707:U:H2'	51:9:1708:C:O4'	2.21	0.41
4:D:50:ARG:NH2	4:D:72:ASP:OD2	2.53	0.41
51:9:1581:C:OP2	51:9:1582:C:N4	2.47	0.41
53:BB:189:ILE:HB	53:BB:190:PRO:HD3	2.02	0.41
61:JJ:149:VAL:HG11	61:JJ:157:ILE:HD11	2.02	0.41
65:NN:60:VAL:HG23	65:NN:66:VAL:HG21	2.02	0.41
2:B:29:VAL:HG23	2:B:346:THR:HG21	2.01	0.41
2:B:77:THR:HG21	2:B:337:VAL:HG22	2.02	0.41
2:B:164:ALA:HB3	2:B:183:ILE:HD12	2.03	0.41
4:D:64:ILE:CD1	4:D:109:LEU:HD22	2.49	0.41
21:V:20:LEU:HB2	21:V:55:ALA:O	2.21	0.41
42:r:33:LYS:NZ	48:5:2265:G:OP2	2.53	0.41
48:5:1523:A:N3	48:5:4389:C:O2'	2.51	0.41
48:5:1879:C:O2'	48:5:1891:A:N3	2.49	0.41
48:5:4896:G:N2	48:5:4927:G:O6	2.50	0.41
52:AA:60:LEU:HD13	52:AA:159:ILE:CD1	2.51	0.41
66:OO:116:LEU:HD22	78:aa:53:ILE:HD11	2.03	0.41
86:ii:338:THR:HG21	86:ii:362:THR:HG21	2.02	0.41
3:C:325:MET:HE1	6:F:154:TYR:CZ	2.56	0.41
8:H:41:ILE:HD11	8:H:69:THR:HB	2.03	0.41
48:5:1563:A:O2'	48:5:1564:A:O4'	2.38	0.41
50:8:137:A:H2'	50:8:138:C:C6	2.55	0.41
51:9:118:C:H1'	51:9:445:A:C5	2.56	0.41
51:9:958:G:C6	51:9:959:G:C6	3.08	0.41
75:XX:67:ARG:HG2	75:XX:115:ILE:HG23	2.03	0.41
1:A:47:ASP:HA	1:A:84:THR:HG22	2.02	0.41
1:A:180:LEU:HD11	41:p:26:VAL:HG21	2.03	0.41
1:A:181:LYS:HB2	48:5:1577:G:C5	2.56	0.41
2:B:86:VAL:HG13	2:B:162:VAL:CG2	2.51	0.41
5:E:201:SER:N	5:E:291:PHE:O	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:42:ALA:N	29:d:43:PRO:CD	2.84	0.41
35:j:17:THR:HG21	35:j:29:LEU:HD21	2.03	0.41
51:9:407:G:H3'	51:9:408:A:C5'	2.50	0.41
51:9:1530:U:H2'	51:9:1531:A:O4'	2.21	0.41
53:BB:103:MET:CE	53:BB:212:VAL:HG23	2.51	0.41
54:CC:137:VAL:HG21	54:CC:217:ALA:HB2	2.03	0.41
66:OO:99:ALA:N	66:OO:133:THR:HG22	2.36	0.41
71:TT:18:LEU:HB3	71:TT:58:ALA:HB1	2.03	0.41
6:F:124:LEU:HD12	6:F:129:ILE:HG12	2.01	0.41
7:G:220:VAL:O	7:G:221:VAL:C	2.64	0.41
11:L:110:LEU:O	11:L:114:VAL:HG23	2.20	0.41
22:W:3:VAL:HG21	22:W:12:LYS:HE3	2.02	0.41
25:Z:75:TYR:CD2	25:Z:80:LEU:HD21	2.56	0.41
42:r:97:ILE:HG21	42:r:107:ARG:HA	2.02	0.41
43:s:34:ASN:N	43:s:34:ASN:HD22	2.19	0.41
43:s:47:LEU:HB3	43:s:51:ALA:HB3	2.03	0.41
47:3:75:C:H2'	47:3:76:A:H4'	2.04	0.41
51:9:1551:U:O2	51:9:1551:U:O4'	2.38	0.41
51:9:1650:A:H2'	51:9:1651:A:O4'	2.21	0.41
64:MM:17:ALA:C	64:MM:124:ILE:HD11	2.46	0.41
86:ii:257:SER:O	86:ii:259:GLY:N	2.52	0.41
2:B:29:VAL:HG11	2:B:32:PHE:CE1	2.55	0.40
4:D:16:TYR:O	49:7:11:A:N6	2.54	0.40
14:O:58:LEU:HD11	14:O:145:VAL:HG22	2.02	0.40
17:R:11:ALA:HB1	17:R:50:ILE:HD13	2.02	0.40
27:b:45:PHE:CE1	48:5:1815:G:C6	3.09	0.40
53:BB:74:LEU:HD21	53:BB:86:LEU:HD11	2.03	0.40
59:HH:96:ALA:HB3	59:HH:98:ARG:NH1	2.36	0.40
69:RR:5:ARG:HB2	69:RR:10:LYS:HE2	2.03	0.40
73:VV:43:THR:HG22	73:VV:45:ARG:HG3	2.02	0.40
83:ff:130:VAL:HG21	83:ff:143:LYS:HE3	2.03	0.40
48:5:1325:C:O2	48:5:1325:C:O5'	2.39	0.40
51:9:1692:U:H2'	51:9:1693:G:C8	2.57	0.40
61:JJ:110:LEU:HD13	61:JJ:142:VAL:HG11	2.02	0.40
85:hh:54:U:O2	85:hh:54:U:C2'	2.69	0.40
5:E:184:LEU:O	48:5:4883:C:N4	2.54	0.40
8:H:104:VAL:HG13	8:H:113:GLU:HB2	2.02	0.40
12:M:119:ARG:HH11	14:O:202:LEU:HD21	1.87	0.40
21:V:22:VAL:HG23	21:V:53:PRO:O	2.21	0.40
48:5:282:C:H2'	48:5:283:G:O4'	2.21	0.40
48:5:1314:C:C2	48:5:1315:C:C5	3.08	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:5:1432:G:HO2'	48:5:1451:G:H22	1.68	0.40
51:9:1045:U:H2'	51:9:1046:U:O4'	2.21	0.40
1:A:117:GLU:HB2	1:A:162:ASN:HB2	2.03	0.40
1:A:199:VAL:HG21	48:5:1631:A:N7	2.37	0.40
48:5:1339:U:H2'	48:5:1340:C:C6	2.56	0.40
48:5:3690:U:H2'	48:5:3691:G:O4'	2.21	0.40
51:9:191:A:C2'	51:9:192:C:OP1	2.70	0.40
51:9:953:C:H2'	51:9:954:U:O4'	2.21	0.40
51:9:1130:G:HO2'	51:9:1131:G:C5'	2.34	0.40
51:9:1149:A:C4	51:9:1151:G:C8	3.10	0.40
51:9:1231:C:H2'	51:9:1232:U:O4'	2.21	0.40
51:9:1452:A:C6	51:9:1476:A:C6	3.09	0.40
53:BB:225:LEU:CD2	53:BB:229:MET:HE2	2.52	0.40
58:GG:16:ILE:HD12	58:GG:16:ILE:N	2.36	0.40
61:JJ:32:ILE:O	61:JJ:36:GLY:N	2.53	0.40
66:OO:116:LEU:HD22	78:aa:53:ILE:CD1	2.51	0.40
4:D:60:ILE:HD13	4:D:98:ALA:HB2	2.03	0.40
4:D:219:TYR:CE2	4:D:227:ILE:HD11	2.56	0.40
6:F:235:ARG:O	6:F:236:GLU:C	2.65	0.40
7:G:247:VAL:HG21	7:G:249:ARG:NH1	2.36	0.40
26:a:73:VAL:HB	26:a:108:TYR:CD1	2.56	0.40
29:d:64:ILE:HD11	29:d:68:LEU:HD23	2.04	0.40
46:2:38:C:O2'	51:9:1058:A:OP1	2.36	0.40
48:5:1305:C:OP1	50:8:7:U:O2'	2.40	0.40
48:5:2693:G:C6	48:5:2694:G:N1	2.90	0.40
48:5:3798:U:C2	48:5:3801:U:C5	3.09	0.40
51:9:488:U:O2	51:9:488:U:O4'	2.38	0.40
51:9:943:U:OP2	53:BB:216:LYS:NZ	2.48	0.40
51:9:962:A:N1	51:9:1055:A:O2'	2.54	0.40
51:9:1843:G:H2'	51:9:1844:U:O4'	2.21	0.40
56:EE:44:LEU:HD21	56:EE:70:ILE:HG21	2.03	0.40
64:MM:63:LYS:HD2	83:ff:108:VAL:HG21	2.02	0.40
84:gg:4:GLN:C	84:gg:5:MET:HE2	2.46	0.40
87:jj:278:VAL:HG12	87:jj:303:PHE:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	246/257 (96%)	218 (89%)	26 (11%)	2 (1%)	16	45
2	B	392/403 (97%)	360 (92%)	29 (7%)	3 (1%)	16	45
3	C	360/425 (85%)	337 (94%)	21 (6%)	2 (1%)	21	51
4	D	291/297 (98%)	275 (94%)	15 (5%)	1 (0%)	36	64
5	E	208/291 (72%)	191 (92%)	17 (8%)	0	100	100
6	F	223/247 (90%)	212 (95%)	10 (4%)	1 (0%)	30	58
7	G	229/319 (72%)	216 (94%)	11 (5%)	2 (1%)	14	43
8	H	188/192 (98%)	178 (95%)	10 (5%)	0	100	100
9	I	201/214 (94%)	185 (92%)	16 (8%)	0	100	100
10	J	168/178 (94%)	161 (96%)	7 (4%)	0	100	100
11	L	208/211 (99%)	196 (94%)	11 (5%)	1 (0%)	24	55
12	M	136/218 (62%)	123 (90%)	12 (9%)	1 (1%)	18	48
13	N	201/204 (98%)	187 (93%)	13 (6%)	1 (0%)	24	55
14	O	197/203 (97%)	188 (95%)	8 (4%)	1 (0%)	24	55
15	P	151/184 (82%)	142 (94%)	9 (6%)	0	100	100
16	Q	185/188 (98%)	173 (94%)	12 (6%)	0	100	100
17	R	178/196 (91%)	173 (97%)	5 (3%)	0	100	100
18	S	174/176 (99%)	159 (91%)	14 (8%)	1 (1%)	21	51
19	T	157/160 (98%)	147 (94%)	10 (6%)	0	100	100
20	U	97/128 (76%)	87 (90%)	10 (10%)	0	100	100
21	V	129/140 (92%)	120 (93%)	9 (7%)	0	100	100
22	W	102/157 (65%)	97 (95%)	4 (4%)	1 (1%)	12	41
23	X	116/156 (74%)	107 (92%)	9 (8%)	0	100	100
24	Y	132/145 (91%)	122 (92%)	10 (8%)	0	100	100
25	Z	133/136 (98%)	126 (95%)	5 (4%)	2 (2%)	8	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	a	145/148 (98%)	131 (90%)	14 (10%)	0	100	100
27	b	100/245 (41%)	94 (94%)	5 (5%)	1 (1%)	12	41
28	c	96/115 (84%)	93 (97%)	3 (3%)	0	100	100
29	d	105/125 (84%)	89 (85%)	15 (14%)	1 (1%)	12	41
30	e	126/135 (93%)	120 (95%)	6 (5%)	0	100	100
31	f	107/110 (97%)	97 (91%)	8 (8%)	2 (2%)	6	30
32	g	112/117 (96%)	105 (94%)	7 (6%)	0	100	100
33	h	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
34	i	100/105 (95%)	94 (94%)	5 (5%)	1 (1%)	12	41
35	j	84/97 (87%)	78 (93%)	6 (7%)	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%)	47 (94%)	3 (6%)	0	100	100
39	n	23/25 (92%)	23 (100%)	0	0	100	100
40	o	102/106 (96%)	98 (96%)	4 (4%)	0	100	100
41	p	89/92 (97%)	83 (93%)	5 (6%)	1 (1%)	11	39
42	r	122/137 (89%)	112 (92%)	9 (7%)	1 (1%)	16	45
43	s	194/318 (61%)	176 (91%)	16 (8%)	2 (1%)	12	41
44	t	151/165 (92%)	135 (89%)	14 (9%)	2 (1%)	9	36
45	l	13/15 (87%)	10 (77%)	2 (15%)	1 (8%)	1	7
52	AA	215/295 (73%)	203 (94%)	11 (5%)	1 (0%)	24	55
53	BB	211/264 (80%)	198 (94%)	12 (6%)	1 (0%)	24	55
54	CC	219/293 (75%)	206 (94%)	13 (6%)	0	100	100
55	DD	226/243 (93%)	213 (94%)	12 (5%)	1 (0%)	30	58
56	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
57	FF	181/204 (89%)	170 (94%)	9 (5%)	2 (1%)	11	39
58	GG	235/249 (94%)	224 (95%)	11 (5%)	0	100	100
59	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
60	II	204/208 (98%)	192 (94%)	11 (5%)	1 (0%)	24	55
61	JJ	183/194 (94%)	177 (97%)	6 (3%)	0	100	100
62	KK	94/165 (57%)	89 (95%)	4 (4%)	1 (1%)	11	39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	LL	139/158 (88%)	130 (94%)	9 (6%)	0	100	100
64	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
65	NN	147/151 (97%)	142 (97%)	4 (3%)	1 (1%)	18	48
66	OO	134/168 (80%)	123 (92%)	9 (7%)	2 (2%)	8	33
67	PP	118/145 (81%)	105 (89%)	12 (10%)	1 (1%)	16	45
68	QQ	140/146 (96%)	132 (94%)	7 (5%)	1 (1%)	18	48
69	RR	130/135 (96%)	120 (92%)	10 (8%)	0	100	100
70	SS	142/152 (93%)	135 (95%)	7 (5%)	0	100	100
71	TT	139/145 (96%)	130 (94%)	8 (6%)	1 (1%)	18	48
72	UU	98/119 (82%)	91 (93%)	7 (7%)	0	100	100
73	VV	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
74	WW	127/130 (98%)	120 (94%)	5 (4%)	2 (2%)	7	32
75	XX	139/143 (97%)	128 (92%)	8 (6%)	3 (2%)	5	27
76	YY	122/130 (94%)	115 (94%)	7 (6%)	0	100	100
77	ZZ	73/125 (58%)	70 (96%)	3 (4%)	0	100	100
78	aa	99/115 (86%)	93 (94%)	4 (4%)	2 (2%)	6	29
79	bb	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
80	cc	60/69 (87%)	58 (97%)	2 (3%)	0	100	100
81	dd	53/56 (95%)	48 (91%)	5 (9%)	0	100	100
82	ee	53/133 (40%)	51 (96%)	2 (4%)	0	100	100
83	ff	66/156 (42%)	59 (89%)	7 (11%)	0	100	100
84	gg	311/317 (98%)	285 (92%)	24 (8%)	2 (1%)	21	51
86	ii	417/459 (91%)	387 (93%)	24 (6%)	6 (1%)	9	34
87	jj	426/637 (67%)	371 (87%)	50 (12%)	5 (1%)	10	38
All	All	12375/14486 (85%)	11531 (93%)	780 (6%)	64 (0%)	26	55

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
75	XX	62	PRO
86	ii	258	TYR
86	ii	272	THR
87	jj	224	GLY
87	jj	280	VAL

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Mol	Chain	Res	Type
13	N	89	VAL
42	r	11	ARG
43	s	142	GLY
65	NN	108	ASP
66	OO	20	GLN
66	OO	30	VAL
67	PP	80	LEU
68	QQ	30	GLY
75	XX	61	GLN
75	XX	86	PRO
86	ii	181	GLY
1	A	14	SER
6	F	236	GLU
11	L	63	THR
18	S	155	PRO
25	Z	90	PRO
25	Z	91	LEU
27	b	102	PRO
31	f	107	PRO
44	t	125	LEU
55	DD	93	THR
60	II	3	ILE
62	KK	64	TRP
74	WW	56	HIS
86	ii	370	GLU
2	B	17	LEU
2	B	376	HIS
41	p	18	TYR
44	t	54	LYS
78	aa	15	ARG
86	ii	326	LEU
3	C	83	GLY
14	O	186	GLU
29	d	58	GLY
31	f	106	TYR
45	1	64	PRO
52	AA	159	ILE
57	FF	21	GLY
57	FF	80	GLY
74	WW	29	PRO
78	aa	47	ALA
86	ii	184	GLY

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Mol	Chain	Res	Type
87	jj	487	ASP
1	A	195	CYS
7	G	221	VAL
43	s	25	PRO
84	gg	224	GLY
87	jj	464	ILE
87	jj	558	ILE
7	G	216	PRO
22	W	3	VAL
53	BB	93	GLY
2	B	254	ILE
3	C	247	GLY
4	D	125	VAL
12	M	9	VAL
34	i	47	VAL
71	TT	109	GLY
84	gg	13	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	176 (93%)	14 (7%)	13	37
2	B	342/348 (98%)	324 (95%)	18 (5%)	20	45
3	C	302/347 (87%)	285 (94%)	17 (6%)	19	44
4	D	247/250 (99%)	235 (95%)	12 (5%)	22	47
5	E	190/251 (76%)	178 (94%)	12 (6%)	16	41
6	F	196/215 (91%)	185 (94%)	11 (6%)	19	44
7	G	200/272 (74%)	190 (95%)	10 (5%)	22	46
8	H	169/171 (99%)	158 (94%)	11 (6%)	15	40
9	I	175/181 (97%)	165 (94%)	10 (6%)	18	43
10	J	143/149 (96%)	137 (96%)	6 (4%)	26	49
11	L	175/176 (99%)	172 (98%)	3 (2%)	53	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	M	117/161 (73%)	110 (94%)	7 (6%)	17	42
13	N	171/172 (99%)	165 (96%)	6 (4%)	32	53
14	O	171/173 (99%)	160 (94%)	11 (6%)	16	41
15	P	134/163 (82%)	129 (96%)	5 (4%)	30	52
16	Q	164/165 (99%)	156 (95%)	8 (5%)	22	47
17	R	159/175 (91%)	147 (92%)	12 (8%)	12	37
18	S	157/157 (100%)	143 (91%)	14 (9%)	9	31
19	T	139/140 (99%)	131 (94%)	8 (6%)	18	43
20	U	89/114 (78%)	88 (99%)	1 (1%)	65	71
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%)	99 (93%)	7 (7%)	15	40
24	Y	124/135 (92%)	118 (95%)	6 (5%)	23	47
25	Z	117/118 (99%)	113 (97%)	4 (3%)	32	53
26	a	119/120 (99%)	117 (98%)	2 (2%)	53	65
27	b	84/184 (46%)	80 (95%)	4 (5%)	23	47
28	c	84/98 (86%)	81 (96%)	3 (4%)	31	53
29	d	98/110 (89%)	95 (97%)	3 (3%)	35	55
30	e	114/121 (94%)	104 (91%)	10 (9%)	9	31
31	f	88/89 (99%)	82 (93%)	6 (7%)	14	40
32	g	98/100 (98%)	93 (95%)	5 (5%)	21	46
33	h	109/110 (99%)	106 (97%)	3 (3%)	38	57
34	i	86/89 (97%)	84 (98%)	2 (2%)	44	61
35	j	73/80 (91%)	70 (96%)	3 (4%)	27	50
36	k	64/65 (98%)	62 (97%)	2 (3%)	35	55
37	l	47/48 (98%)	45 (96%)	2 (4%)	26	49
38	m	48/90 (53%)	45 (94%)	3 (6%)	16	41
39	n	24/24 (100%)	22 (92%)	2 (8%)	10	33
40	o	92/94 (98%)	87 (95%)	5 (5%)	20	45
41	p	74/75 (99%)	72 (97%)	2 (3%)	39	57
42	r	108/121 (89%)	100 (93%)	8 (7%)	13	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
43	s	164/258 (64%)	158 (96%)	6 (4%)	30	52
44	t	126/137 (92%)	121 (96%)	5 (4%)	28	50
45	1	13/13 (100%)	13 (100%)	0	100	100
52	AA	180/245 (74%)	166 (92%)	14 (8%)	11	36
53	BB	194/231 (84%)	177 (91%)	17 (9%)	9	31
54	CC	187/225 (83%)	177 (95%)	10 (5%)	20	45
55	DD	190/202 (94%)	172 (90%)	18 (10%)	8	30
56	EE	224/225 (100%)	205 (92%)	19 (8%)	10	32
57	FF	158/170 (93%)	147 (93%)	11 (7%)	14	39
58	GG	207/218 (95%)	195 (94%)	12 (6%)	18	43
59	HH	165/174 (95%)	150 (91%)	15 (9%)	9	31
60	II	178/180 (99%)	164 (92%)	14 (8%)	11	35
61	JJ	161/168 (96%)	148 (92%)	13 (8%)	11	34
62	KK	87/136 (64%)	73 (84%)	14 (16%)	2	13
63	LL	130/142 (92%)	118 (91%)	12 (9%)	8	30
64	MM	99/108 (92%)	86 (87%)	13 (13%)	4	19
65	NN	130/131 (99%)	121 (93%)	9 (7%)	14	39
66	OO	106/130 (82%)	96 (91%)	10 (9%)	8	30
67	PP	109/130 (84%)	100 (92%)	9 (8%)	10	33
68	QQ	117/121 (97%)	108 (92%)	9 (8%)	12	36
69	RR	119/121 (98%)	109 (92%)	10 (8%)	10	33
70	SS	125/132 (95%)	111 (89%)	14 (11%)	6	24
71	TT	111/115 (96%)	104 (94%)	7 (6%)	16	41
72	UU	92/107 (86%)	87 (95%)	5 (5%)	20	45
73	VV	67/67 (100%)	62 (92%)	5 (8%)	12	37
74	WW	112/113 (99%)	106 (95%)	6 (5%)	20	45
75	XX	113/115 (98%)	106 (94%)	7 (6%)	16	41
76	YY	107/112 (96%)	93 (87%)	14 (13%)	4	19
77	ZZ	66/103 (64%)	62 (94%)	4 (6%)	17	42
78	aa	88/98 (90%)	80 (91%)	8 (9%)	9	31
79	bb	75/76 (99%)	71 (95%)	4 (5%)	20	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
80	cc	55/62 (89%)	50 (91%)	5 (9%)	9	31
81	dd	48/49 (98%)	45 (94%)	3 (6%)	16	41
82	ee	46/106 (43%)	42 (91%)	4 (9%)	9	32
83	ff	61/140 (44%)	57 (93%)	4 (7%)	15	40
84	gg	272/275 (99%)	264 (97%)	8 (3%)	37	56
86	ii	361/394 (92%)	344 (95%)	17 (5%)	23	47
87	jj	372/520 (72%)	352 (95%)	20 (5%)	20	45
All	All	10789/12266 (88%)	10126 (94%)	663 (6%)	19	42

All (663) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	102	LEU
1	A	128	ARG
1	A	158	ILE
1	A	163	ARG
1	A	165	VAL
1	A	175	ILE
1	A	200	ARG
1	A	209	HIS
1	A	221	LYS
1	A	226	ARG
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
2	B	10	ARG
2	B	17	LEU
2	B	23	SER
2	B	53	MET
2	B	56	ILE
2	B	60	VAL
2	B	66	LYS
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	314	ILE

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Mol	Chain	Res	Type
2	B	333	LEU
2	B	356	LYS
2	B	366	LYS
2	B	383	GLU
3	C	20	LYS
3	C	124	ILE
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	193	LYS
3	C	195	LYS
3	C	213	GLU
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	33	ARG
4	D	37	VAL
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	124	GLU
4	D	202	GLN
4	D	225	GLN
4	D	262	LYS
4	D	264	LYS
5	E	52	LEU
5	E	58	ARG
5	E	112	LEU
5	E	123	ASP
5	E	143	LEU
5	E	169	LYS
5	E	178	VAL
5	E	182	LEU
5	E	197	VAL

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Mol	Chain	Res	Type
5	E	213	LYS
5	E	286	PRO
5	E	291	PHE
6	F	38	GLN
6	F	41	LEU
6	F	46	ARG
6	F	65	ARG
6	F	67	GLU
6	F	88	LEU
6	F	100	VAL
6	F	134	ILE
6	F	151	GLU
6	F	198	LYS
6	F	211	LYS
7	G	184	LYS
7	G	201	GLU
7	G	203	LYS
7	G	204	LYS
7	G	223	LEU
7	G	226	LEU
7	G	230	MET
7	G	273	GLU
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	76	MET
9	I	116	ARG
9	I	142	LEU
9	I	146	GLU
9	I	153	ARG

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Mol	Chain	Res	Type
9	I	164	LYS
9	I	208	LYS
9	I	212	LEU
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	81	GLU
10	J	96	LYS
10	J	113	ILE
11	L	63	THR
11	L	162	LYS
11	L	186	ARG
12	M	8	GLU
12	M	37	LEU
12	M	42	CYS
12	M	57	LEU
12	M	62	LEU
12	M	96	GLU
12	M	112	VAL
13	N	9	GLU
13	N	64	ILE
13	N	72	LYS
13	N	77	LYS
13	N	89	VAL
13	N	182	HIS
14	O	16	LEU
14	O	49	ARG
14	O	67	SER
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	24	VAL
15	P	69	ARG
15	P	86	LYS
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL

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Mol	Chain	Res	Type
16	Q	61	LEU
16	Q	63	LEU
16	Q	78	LYS
16	Q	91	ARG
16	Q	95	VAL
16	Q	138	LEU
16	Q	143	ARG
17	R	6	LEU
17	R	10	LEU
17	R	36	ASN
17	R	50	ILE
17	R	52	ARG
17	R	82	LYS
17	R	89	MET
17	R	99	MET
17	R	103	ARG
17	R	113	LYS
17	R	138	LEU
17	R	178	GLN
18	S	1	MET
18	S	7	LEU
18	S	9	GLU
18	S	24	THR
18	S	67	VAL
18	S	70	LYS
18	S	77	ASN
18	S	93	MET
18	S	95	ARG
18	S	135	SER
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	88	ARG
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	18	LEU
21	V	35	LYS
21	V	60	MET
21	V	69	LYS
21	V	82	ILE
21	V	91	LYS
21	V	99	GLU
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	91	GLU
23	X	111	GLN
24	Y	2	LYS
24	Y	8	THR
24	Y	28	LYS
24	Y	55	VAL
24	Y	72	GLN
24	Y	104	VAL
25	Z	3	LYS
25	Z	11	VAL
25	Z	33	THR
25	Z	42	LEU
26	a	4	ARG
26	a	122	VAL
27	b	9	THR
27	b	22	LYS
27	b	40	LEU
27	b	101	HIS
28	c	37	MET
28	c	55	LEU
28	c	78	ASN
29	d	23	ARG
29	d	48	GLU
29	d	98	SER
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE

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Mol	Chain	Res	Type
30	e	22	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	89	LEU
30	e	106	LYS
30	e	128	ARG
31	f	7	CYS
31	f	23	GLU
31	f	33	VAL
31	f	47	CYS
31	f	52	LYS
31	f	101	ILE
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	86	LYS
35	j	3	LYS
35	j	11	ARG
35	j	58	THR
36	k	69	LEU
36	k	70	LYS
37	l	27	ILE
37	l	49	LEU
38	m	71	ARG
38	m	72	LYS
38	m	92	THR
39	n	1	MET
39	n	13	LEU
40	o	17	LYS
40	o	18	HIS
40	o	28	LYS
40	o	36	GLN
40	o	61	LYS
41	p	8	VAL
41	p	84	ARG

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Mol	Chain	Res	Type
42	r	8	MET
42	r	32	LEU
42	r	39	ARG
42	r	60	VAL
42	r	67	ARG
42	r	80	THR
42	r	103	HIS
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	25	THR
44	t	37	LEU
44	t	72	GLU
44	t	98	ILE
44	t	133	LEU
52	AA	5	LEU
52	AA	12	GLU
52	AA	25	LEU
52	AA	46	ILE
52	AA	56	GLU
52	AA	58	LEU
52	AA	59	LEU
52	AA	60	LEU
52	AA	107	THR
52	AA	122	LEU
52	AA	132	GLN
52	AA	136	GLU
52	AA	178	LEU
52	AA	198	MET
53	BB	38	MET
53	BB	63	LYS
53	BB	71	LEU
53	BB	74	LEU
53	BB	82	ARG
53	BB	92	GLN
53	BB	105	LEU
53	BB	125	VAL
53	BB	126	ASP

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Mol	Chain	Res	Type
53	BB	157	GLN
53	BB	172	MET
53	BB	175	GLU
53	BB	181	LEU
53	BB	207	LEU
53	BB	209	ASP
53	BB	213	ARG
53	BB	225	LEU
54	CC	78	LEU
54	CC	90	GLU
54	CC	114	LYS
54	CC	117	ARG
54	CC	121	ARG
54	CC	137	VAL
54	CC	167	ARG
54	CC	252	THR
54	CC	255	LEU
54	CC	276	THR
55	DD	22	ASN
55	DD	28	GLU
55	DD	31	GLU
55	DD	35	SER
55	DD	51	LEU
55	DD	70	THR
55	DD	72	VAL
55	DD	120	TYR
55	DD	127	MET
55	DD	142	LEU
55	DD	146	ARG
55	DD	156	LEU
55	DD	160	SER
55	DD	168	VAL
55	DD	198	ILE
55	DD	212	GLU
55	DD	215	ASP
55	DD	218	LEU
56	EE	6	LYS
56	EE	17	HIS
56	EE	23	LEU
56	EE	42	LEU
56	EE	49	ARG
56	EE	51	ARG

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Mol	Chain	Res	Type
56	EE	65	CYS
56	EE	66	MET
56	EE	67	GLN
56	EE	77	ARG
56	EE	88	ASP
56	EE	123	LEU
56	EE	159	THR
56	EE	162	ILE
56	EE	177	THR
56	EE	222	LEU
56	EE	232	ASN
56	EE	238	LEU
56	EE	246	LEU
57	FF	35	LEU
57	FF	36	GLN
57	FF	71	ARG
57	FF	88	MET
57	FF	89	THR
57	FF	91	ARG
57	FF	122	ARG
57	FF	168	THR
57	FF	169	ILE
57	FF	175	ASP
57	FF	204	ARG
58	GG	25	ARG
58	GG	41	LEU
58	GG	63	MET
58	GG	67	VAL
58	GG	81	HIS
58	GG	108	VAL
58	GG	171	THR
58	GG	178	ARG
58	GG	190	ARG
58	GG	208	GLU
58	GG	216	ARG
58	GG	230	LYS
59	HH	8	ILE
59	HH	36	LEU
59	HH	53	VAL
59	HH	76	GLN
59	HH	79	LEU
59	HH	82	GLU

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Mol	Chain	Res	Type
59	HH	100	ILE
59	HH	114	GLN
59	HH	127	ASP
59	HH	133	LEU
59	HH	145	ARG
59	HH	151	SER
59	HH	162	GLN
59	HH	172	THR
59	HH	188	GLU
60	II	23	LYS
60	II	26	LYS
60	II	56	ARG
60	II	74	ARG
60	II	79	ILE
60	II	100	CYS
60	II	121	LEU
60	II	130	THR
60	II	147	LYS
60	II	161	LEU
60	II	162	LEU
60	II	168	GLN
60	II	175	ILE
60	II	178	ARG
61	JJ	9	CYS
61	JJ	29	LEU
61	JJ	38	ARG
61	JJ	45	ARG
61	JJ	50	LEU
61	JJ	61	LEU
61	JJ	65	GLU
61	JJ	89	GLU
61	JJ	94	LEU
61	JJ	109	ARG
61	JJ	112	THR
61	JJ	116	LYS
61	JJ	117	LEU
62	KK	1	MET
62	KK	2	LEU
62	KK	17	LYS
62	KK	20	VAL
62	KK	21	MET
62	KK	35	LEU

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Mol	Chain	Res	Type
62	KK	50	GLN
62	KK	52	LEU
62	KK	59	LYS
62	KK	60	GLU
62	KK	72	THR
62	KK	89	ILE
62	KK	93	THR
62	KK	96	ARG
63	LL	16	ILE
63	LL	20	LYS
63	LL	23	VAL
63	LL	40	ILE
63	LL	42	LEU
63	LL	49	GLU
63	LL	56	ILE
63	LL	69	ARG
63	LL	111	VAL
63	LL	126	VAL
63	LL	134	LEU
63	LL	153	LYS
64	MM	22	LEU
64	MM	31	LEU
64	MM	33	ARG
64	MM	40	LYS
64	MM	42	LEU
64	MM	45	ARG
64	MM	49	LEU
64	MM	55	ASN
64	MM	83	LYS
64	MM	85	LEU
64	MM	99	LYS
64	MM	101	ARG
64	MM	112	LYS
65	NN	3	ARG
65	NN	27	LYS
65	NN	46	THR
65	NN	60	VAL
65	NN	75	LEU
65	NN	78	LYS
65	NN	84	LEU
65	NN	132	LYS
65	NN	134	VAL

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Mol	Chain	Res	Type
66	OO	38	ASN
66	OO	51	GLU
66	OO	56	VAL
66	OO	76	LEU
66	OO	85	CYS
66	OO	119	LEU
66	OO	131	ASP
66	OO	146	ARG
66	OO	150	ARG
66	OO	151	LEU
67	PP	13	ARG
67	PP	14	LYS
67	PP	15	PHE
67	PP	37	TYR
67	PP	42	ARG
67	PP	65	LYS
67	PP	83	MET
67	PP	108	LYS
67	PP	130	ARG
68	QQ	26	LYS
68	QQ	31	LEU
68	QQ	41	MET
68	QQ	47	LEU
68	QQ	48	GLN
68	QQ	60	LYS
68	QQ	90	LYS
68	QQ	123	ASP
68	QQ	140	ARG
69	RR	30	THR
69	RR	31	ASN
69	RR	35	CYS
69	RR	38	ILE
69	RR	44	LYS
69	RR	58	MET
69	RR	98	VAL
69	RR	109	LEU
69	RR	114	LEU
69	RR	121	GLN
70	SS	3	LEU
70	SS	8	LYS
70	SS	10	GLN
70	SS	36	VAL

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Mol	Chain	Res	Type
70	SS	46	ARG
70	SS	52	LEU
70	SS	59	LEU
70	SS	63	GLU
70	SS	69	THR
70	SS	83	PHE
70	SS	110	ASP
70	SS	121	ARG
70	SS	132	ARG
70	SS	136	THR
71	TT	62	ARG
71	TT	75	MET
71	TT	103	VAL
71	TT	108	GLU
71	TT	110	LEU
71	TT	124	THR
71	TT	142	LYS
72	UU	56	MET
72	UU	79	ARG
72	UU	88	LEU
72	UU	106	ILE
72	UU	111	GLU
73	VV	12	TYR
73	VV	32	ILE
73	VV	66	ASP
73	VV	68	SER
73	VV	69	ILE
74	WW	28	ARG
74	WW	51	GLU
74	WW	92	ASN
74	WW	103	VAL
74	WW	104	LEU
74	WW	117	ARG
75	XX	7	LEU
75	XX	29	LYS
75	XX	67	ARG
75	XX	82	THR
75	XX	112	VAL
75	XX	115	ILE
75	XX	129	SER
76	YY	16	ARG
76	YY	17	LEU

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Mol	Chain	Res	Type
76	YY	32	LYS
76	YY	38	THR
76	YY	40	ILE
76	YY	47	MET
76	YY	50	THR
76	YY	61	ARG
76	YY	74	MET
76	YY	79	LEU
76	YY	88	LYS
76	YY	93	ARG
76	YY	101	LYS
76	YY	115	LYS
77	ZZ	52	LYS
77	ZZ	80	ARG
77	ZZ	89	GLN
77	ZZ	92	LEU
78	aa	12	LYS
78	aa	21	ILE
78	aa	34	LYS
78	aa	41	ILE
78	aa	44	ILE
78	aa	55	GLU
78	aa	87	ARG
78	aa	100	ARG
79	bb	34	ASP
79	bb	37	CYS
79	bb	42	LYS
79	bb	81	ARG
80	cc	27	CYS
80	cc	28	THR
80	cc	31	ARG
80	cc	40	ARG
80	cc	44	ARG
81	dd	6	LEU
81	dd	20	SER
81	dd	54	LYS
82	ee	97	LYS
82	ee	98	LYS
82	ee	99	LYS
82	ee	124	LYS
83	ff	94	LYS
83	ff	99	LYS

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Mol	Chain	Res	Type
83	ff	138	ARG
83	ff	140	TYR
84	gg	17	TRP
84	gg	20	GLN
84	gg	79	LEU
84	gg	87	LEU
84	gg	119	GLN
84	gg	198	VAL
84	gg	289	LEU
84	gg	306	LEU
86	ii	63	LYS
86	ii	65	ARG
86	ii	82	LEU
86	ii	103	GLU
86	ii	111	ASN
86	ii	161	LEU
86	ii	180	HIS
86	ii	211	GLN
86	ii	212	LEU
86	ii	241	MET
86	ii	291	PHE
86	ii	300	LYS
86	ii	330	ARG
86	ii	341	GLU
86	ii	368	LEU
86	ii	381	ASN
86	ii	417	VAL
87	jj	249	ARG
87	jj	292	PHE
87	jj	340	GLU
87	jj	353	LEU
87	jj	392	LYS
87	jj	434	ARG
87	jj	447	LYS
87	jj	455	VAL
87	jj	464	ILE
87	jj	468	GLN
87	jj	502	ILE
87	jj	509	GLU
87	jj	511	GLU
87	jj	536	VAL
87	jj	541	LYS

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Mol	Chain	Res	Type
87	jj	551	VAL
87	jj	558	ILE
87	jj	601	ILE
87	jj	611	GLN
87	jj	618	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (151) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	158	GLN
2	B	271	GLN
2	B	354	GLN
3	C	41	HIS
3	C	310	HIS
3	C	347	HIS
4	D	191	ASN
4	D	229	ASN
4	D	250	ASN
5	E	160	HIS
5	E	185	ASN
5	E	269	GLN
6	F	55	HIS
6	F	204	ASN
7	G	147	GLN
7	G	161	GLN
7	G	206	GLN
7	G	293	ASN
8	H	8	GLN
8	H	78	GLN
8	H	98	HIS
9	I	100	ASN
9	I	144	ASN
11	L	27	ASN
11	L	87	HIS
13	N	8	GLN
13	N	15	GLN
13	N	32	GLN
13	N	182	HIS
14	O	26	GLN
14	O	50	ASN
14	O	167	HIS
15	P	56	GLN

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Mol	Chain	Res	Type
15	P	75	GLN
15	P	137	ASN
16	Q	44	ASN
16	Q	45	GLN
16	Q	162	HIS
17	R	34	ASN
17	R	36	ASN
18	S	125	GLN
18	S	163	HIS
19	T	49	GLN
19	T	90	ASN
21	V	27	ASN
22	W	30	GLN
23	X	57	GLN
23	X	105	ASN
23	X	111	GLN
24	Y	20	ASN
24	Y	56	GLN
27	b	49	HIS
27	b	60	ASN
28	c	15	ASN
28	c	78	ASN
29	d	30	HIS
29	d	121	ASN
31	f	99	HIS
32	g	14	ASN
32	g	28	ASN
33	h	65	GLN
33	h	107	GLN
40	o	19	GLN
40	o	51	GLN
42	r	12	ASN
42	r	70	GLN
42	r	103	HIS
42	r	121	GLN
43	s	34	ASN
43	s	39	GLN
43	s	42	GLN
43	s	126	GLN
43	s	179	ASN
44	t	65	GLN
44	t	95	GLN

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Mol	Chain	Res	Type
44	t	103	ASN
52	AA	36	GLN
52	AA	81	ASN
52	AA	111	GLN
52	AA	132	GLN
53	BB	75	GLN
53	BB	95	ASN
53	BB	158	HIS
53	BB	163	GLN
53	BB	186	ASN
55	DD	22	ASN
55	DD	226	GLN
56	EE	17	HIS
56	EE	67	GLN
56	EE	161	GLN
56	EE	188	ASN
56	EE	209	HIS
56	EE	260	GLN
57	FF	29	GLN
57	FF	101	HIS
57	FF	118	ASN
58	GG	197	GLN
58	GG	202	ASN
59	HH	91	HIS
59	HH	97	GLN
59	HH	162	GLN
59	HH	193	GLN
60	II	7	ASN
60	II	146	GLN
62	KK	32	HIS
62	KK	42	ASN
62	KK	44	HIS
63	LL	18	GLN
63	LL	39	ASN
63	LL	65	ASN
64	MM	55	ASN
65	NN	62	GLN
66	OO	20	GLN
66	OO	94	HIS
67	PP	98	ASN
68	QQ	8	GLN
68	QQ	24	HIS

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Mol	Chain	Res	Type
69	RR	127	ASN
70	SS	11	HIS
70	SS	73	ASN
71	TT	83	GLN
73	VV	47	ASN
74	WW	15	ASN
74	WW	92	ASN
75	XX	16	HIS
75	XX	97	ASN
76	YY	19	GLN
76	YY	85	ASN
77	ZZ	103	HIS
77	ZZ	112	ASN
78	aa	86	ASN
79	bb	26	GLN
80	cc	29	GLN
80	cc	45	ASN
84	gg	196	ASN
84	gg	222	ASN
84	gg	305	ASN
86	ii	79	GLN
86	ii	238	GLN
86	ii	266	GLN
86	ii	380	ASN
86	ii	401	GLN
87	jj	214	ASN
87	jj	313	GLN
87	jj	428	ASN
87	jj	469	GLN
87	jj	477	HIS
87	jj	499	ASN
87	jj	523	ASN
87	jj	555	HIS
87	jj	611	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
46	2	74/76 (97%)	13 (17%)	0
47	3	72/75 (96%)	24 (33%)	2 (2%)
48	5	3519/3543 (99%)	893 (25%)	169 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
49	7	119/120 (99%)	14 (11%)	2 (1%)
50	8	149/156 (95%)	32 (21%)	6 (4%)
51	9	1682/1869 (89%)	431 (25%)	71 (4%)
85	hh	14/15 (93%)	8 (57%)	0
All	All	5629/5854 (96%)	1415 (25%)	250 (4%)

All (1415) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
46	2	9	A
46	2	13	U
46	2	16	C
46	2	19	G
46	2	20	U
46	2	21	A
46	2	46	G
46	2	47	U
46	2	49	C
46	2	58	A
46	2	64	G
46	2	72	C
46	2	75	C
47	3	7	A
47	3	13	C
47	3	14	A
47	3	16	C
47	3	21	A
47	3	25	C
47	3	28	C
47	3	29	A
47	3	34	U
47	3	35	U
47	3	36	U
47	3	40	C
47	3	42	G
47	3	47	U
47	3	49	C
47	3	58	A
47	3	60	U
47	3	61	C
47	3	63	C
47	3	65	G

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Mol	Chain	Res	Type
47	3	72	C
47	3	74	C
47	3	75	C
47	3	76	A
48	5	12	A
48	5	13	U
48	5	15	A
48	5	25	A
48	5	35	U
48	5	39	A
48	5	42	A
48	5	43	U
48	5	44	A
48	5	48	G
48	5	49	U
48	5	56	A
48	5	58	G
48	5	59	A
48	5	64	A
48	5	65	A
48	5	72	C
48	5	73	A
48	5	91	G
48	5	93	G
48	5	109	G
48	5	110	C
48	5	118	C
48	5	119	G
48	5	120	A
48	5	126	C
48	5	134	G
48	5	135	G
48	5	136	C
48	5	137	G
48	5	143	C
48	5	144	G
48	5	159	C
48	5	160	G
48	5	172	C
48	5	173	C
48	5	177	G
48	5	179	G

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Mol	Chain	Res	Type
48	5	197	A
48	5	200	U
48	5	201	C
48	5	202	C
48	5	205	C
48	5	209	U
48	5	216	C
48	5	217	C
48	5	218	A
48	5	220	C
48	5	221	C
48	5	224	U
48	5	226	G
48	5	227	A
48	5	233	U
48	5	234	G
48	5	245	C
48	5	246	G
48	5	253	G
48	5	262	G
48	5	263	G
48	5	266	C
48	5	267	G
48	5	276	C
48	5	279	A
48	5	280	G
48	5	281	U
48	5	297	U
48	5	306	A
48	5	309	C
48	5	310	G
48	5	315	G
48	5	316	U
48	5	322	C
48	5	328	A
48	5	334	A
48	5	340	C
48	5	350	C
48	5	357	U
48	5	361	C
48	5	363	A
48	5	386	A

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Mol	Chain	Res	Type
48	5	387	G
48	5	388	A
48	5	399	G
48	5	406	C
48	5	407	A
48	5	408	A
48	5	409	G
48	5	410	A
48	5	412	G
48	5	413	G
48	5	414	C
48	5	431	G
48	5	432	U
48	5	446	C
48	5	449	C
48	5	450	G
48	5	452	A
48	5	453	G
48	5	454	U
48	5	455	C
48	5	457	G
48	5	466	A
48	5	467	U
48	5	468	U
48	5	469	C
48	5	481	G
48	5	481(A)	C
48	5	482	G
48	5	483	G
48	5	484	U
48	5	485	C
48	5	486	C
48	5	490	C
48	5	492	U
48	5	493	G
48	5	495	C
48	5	497	G
48	5	498	C
48	5	499	G
48	5	505	G
48	5	510	U
48	5	649	A

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Mol	Chain	Res	Type
48	5	654	C
48	5	658	C
48	5	666	G
48	5	667	A
48	5	668	C
48	5	672	C
48	5	683	C
48	5	685	C
48	5	687	U
48	5	696	C
48	5	697	G
48	5	704	C
48	5	705	G
48	5	708	G
48	5	719	C
48	5	722	G
48	5	729	G
48	5	730	G
48	5	731	G
48	5	738	C
48	5	738(A)	C
48	5	739	G
48	5	747	A
48	5	748	G
48	5	749	G
48	5	750	U
48	5	752	G
48	5	756	G
48	5	758	G
48	5	911	U
48	5	913	U
48	5	914	U
48	5	915	A
48	5	916	C
48	5	917	A
48	5	918	G
48	5	923	C
48	5	924	C
48	5	925	C
48	5	926	G
48	5	928	C
48	5	929	A

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Mol	Chain	Res	Type
48	5	931	C
48	5	932	A
48	5	933	G
48	5	934	C
48	5	935	A
48	5	935(A)	G
48	5	936	C
48	5	938	C
48	5	939	G
48	5	943	A
48	5	944	A
48	5	945	U
48	5	955	G
48	5	956	A
48	5	957	G
48	5	959	G
48	5	960	A
48	5	961	G
48	5	962	C
48	5	965	G
48	5	966	A
48	5	967	C
48	5	968	C
48	5	969	C
48	5	970	G
48	5	972	C
48	5	973	G
48	5	979	C
48	5	983	C
48	5	990	C
48	5	1071	C
48	5	1072	C
48	5	1073	G
48	5	1075	G
48	5	1076	C
48	5	1078	A
48	5	1079	C
48	5	1082	C
48	5	1174	G
48	5	1177	U
48	5	1179	U
48	5	1184	A

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Mol	Chain	Res	Type
48	5	1194	G
48	5	1195	G
48	5	1211	G
48	5	1212	G
48	5	1214	C
48	5	1215	C
48	5	1234	G
48	5	1235	G
48	5	1236	C
48	5	1237	C
48	5	1238	A
48	5	1239	C
48	5	1272	C
48	5	1273	G
48	5	1274	A
48	5	1275	G
48	5	1276	C
48	5	1280	C
48	5	1284	G
48	5	1287	G
48	5	1288	G
48	5	1291	G
48	5	1292	C
48	5	1293	G
48	5	1295	U
48	5	1296	G
48	5	1301	C
48	5	1303	A
48	5	1304	C
48	5	1313	C
48	5	1326	A
48	5	1328	G
48	5	1329	G
48	5	1330	A
48	5	1337	A
48	5	1354	A
48	5	1359	G
48	5	1360	G
48	5	1364	U
48	5	1370	G
48	5	1371	A
48	5	1377	G

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Mol	Chain	Res	Type
48	5	1378	C
48	5	1379	C
48	5	1380	G
48	5	1381	U
48	5	1387	A
48	5	1394	G
48	5	1397	A
48	5	1398	A
48	5	1401	C
48	5	1403	G
48	5	1416	G
48	5	1418	C
48	5	1419	G
48	5	1420	A
48	5	1421	G
48	5	1429	C
48	5	1435	G
48	5	1436	C
48	5	1437	C
48	5	1438	U
48	5	1440	U
48	5	1441	C
48	5	1442	C
48	5	1445	U
48	5	1446	C
48	5	1453	G
48	5	1455	G
48	5	1456	C
48	5	1457	G
48	5	1458	C
48	5	1465	G
48	5	1475	G
48	5	1477	C
48	5	1478	C
48	5	1481	C
48	5	1482	G
48	5	1483	C
48	5	1484	G
48	5	1485	C
48	5	1486	C
48	5	1489	G
48	5	1493	G

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Mol	Chain	Res	Type
48	5	1497	A
48	5	1498	G
48	5	1501	C
48	5	1502	G
48	5	1504	G
48	5	1514	U
48	5	1516	G
48	5	1518	A
48	5	1523	A
48	5	1525	A
48	5	1534	A
48	5	1535	C
48	5	1547	A
48	5	1554	A
48	5	1563	A
48	5	1564	A
48	5	1566	C
48	5	1574	G
48	5	1578	U
48	5	1586	G
48	5	1591	U
48	5	1596	U
48	5	1601	A
48	5	1602	U
48	5	1612	G
48	5	1613	A
48	5	1624	G
48	5	1625	G
48	5	1631	A
48	5	1633	G
48	5	1634	A
48	5	1654	G
48	5	1656	U
48	5	1661	C
48	5	1670	G
48	5	1676	C
48	5	1677	U
48	5	1679	A
48	5	1691	G
48	5	1724	G
48	5	1726	U
48	5	1733	G

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Mol	Chain	Res	Type
48	5	1734	G
48	5	1735	U
48	5	1740	C
48	5	1741	G
48	5	1742	A
48	5	1750	G
48	5	1753	G
48	5	1755	C
48	5	1756	U
48	5	1757	U
48	5	1761	G
48	5	1763	C
48	5	1764	G
48	5	1768	C
48	5	1772	C
48	5	1773	U
48	5	1776	A
48	5	1780	A
48	5	1781	U
48	5	1787	A
48	5	1797	G
48	5	1799	G
48	5	1800	U
48	5	1803	G
48	5	1804	A
48	5	1805	A
48	5	1815	G
48	5	1816	C
48	5	1819	G
48	5	1820	U
48	5	1821	G
48	5	1822	U
48	5	1823	G
48	5	1828	C
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1837	A
48	5	1842	G
48	5	1855	G
48	5	1867	A

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Mol	Chain	Res	Type
48	5	1869	G
48	5	1882	U
48	5	1883	G
48	5	1892	A
48	5	1893	C
48	5	1897	A
48	5	1910	G
48	5	1918	U
48	5	1920	C
48	5	1921	C
48	5	1922	G
48	5	1923	A
48	5	1931	C
48	5	1933	G
48	5	1935	C
48	5	1936	C
48	5	1941	A
48	5	1945	G
48	5	1948	G
48	5	1951	G
48	5	1952	G
48	5	1959	U
48	5	1961	G
48	5	1962	A
48	5	1963	C
48	5	1966	C
48	5	1967	A
48	5	1976	G
48	5	1977	C
48	5	1979	A
48	5	1980	U
48	5	1981	G
48	5	1982	G
48	5	1983	A
48	5	1984	A
48	5	1986	U
48	5	1987	C
48	5	1991	A
48	5	1993	C
48	5	1997	U
48	5	2001	G
48	5	2002	A

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Mol	Chain	Res	Type
48	5	2003	G
48	5	2004	U
48	5	2005	G
48	5	2008	U
48	5	2011	C
48	5	2024	G
48	5	2025	A
48	5	2026	A
48	5	2044	U
48	5	2046	G
48	5	2047	A
48	5	2048	U
48	5	2052	G
48	5	2055	G
48	5	2056	G
48	5	2062	C
48	5	2064	G
48	5	2069	A
48	5	2070	U
48	5	2084	U
48	5	2085	G
48	5	2089	G
48	5	2090	U
48	5	2092	G
48	5	2093	G
48	5	2094	C
48	5	2095	A
48	5	2097	A
48	5	2098	G
48	5	2100	G
48	5	2101	A
48	5	2102	G
48	5	2104	A
48	5	2105	A
48	5	2106	G
48	5	2107	A
48	5	2108	G
48	5	2110	G
48	5	2259	G
48	5	2260	C
48	5	2262	G
48	5	2266	C

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Mol	Chain	Res	Type
48	5	2267	U
48	5	2268	A
48	5	2269	C
48	5	2270	G
48	5	2275	G
48	5	2278	G
48	5	2279	A
48	5	2288	G
48	5	2289	C
48	5	2300	A
48	5	2301	G
48	5	2313	A
48	5	2314	G
48	5	2322	G
48	5	2331	G
48	5	2333	G
48	5	2348	G
48	5	2351	C
48	5	2357	G
48	5	2364	G
48	5	2370	A
48	5	2395	A
48	5	2396	A
48	5	2399	G
48	5	2402	G
48	5	2416	G
48	5	2417	A
48	5	2422	C
48	5	2424	G
48	5	2425	U
48	5	2428	A
48	5	2429	A
48	5	2433	G
48	5	2441	C
48	5	2450	G
48	5	2467	U
48	5	2468	U
48	5	2469	C
48	5	2470	C
48	5	2471	G
48	5	2475	G
48	5	2479	G

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Mol	Chain	Res	Type
48	5	2483	G
48	5	2485	U
48	5	2488	C
48	5	2489	C
48	5	2490	U
48	5	2491	C
48	5	2493	G
48	5	2495	U
48	5	2503	G
48	5	2504	C
48	5	2505	C
48	5	2506	G
48	5	2513	A
48	5	2521	G
48	5	2530	U
48	5	2537	A
48	5	2546	G
48	5	2547	G
48	5	2554	U
48	5	2555	G
48	5	2564	G
48	5	2566	G
48	5	2571	C
48	5	2575	U
48	5	2583	C
48	5	2586	G
48	5	2587	A
48	5	2601	A
48	5	2618	G
48	5	2620	G
48	5	2623	A
48	5	2627	C
48	5	2638	G
48	5	2640	G
48	5	2647	A
48	5	2661	U
48	5	2662	G
48	5	2663	G
48	5	2669	C
48	5	2670	C
48	5	2673	G
48	5	2676	A

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Mol	Chain	Res	Type
48	5	2681	G
48	5	2686	G
48	5	2687	U
48	5	2688	G
48	5	2689	C
48	5	2695	A
48	5	2696	A
48	5	2707	U
48	5	2708	U
48	5	2709	C
48	5	2710	C
48	5	2711	G
48	5	2712	G
48	5	2714	G
48	5	2716	C
48	5	2719	C
48	5	2721	G
48	5	2725	A
48	5	2726	G
48	5	2740	U
48	5	2743	A
48	5	2744	A
48	5	2754	G
48	5	2755	A
48	5	2760	G
48	5	2761	U
48	5	2763	U
48	5	2764	A
48	5	2769	U
48	5	2772	C
48	5	2787	A
48	5	2788	U
48	5	2789	A
48	5	2790	U
48	5	2794	C
48	5	2795	A
48	5	2796	G
48	5	2798	A
48	5	2806	A
48	5	2807	A
48	5	2808	G
48	5	2814	C

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Mol	Chain	Res	Type
48	5	2826	U
48	5	2827	G
48	5	2828	U
48	5	2829	U
48	5	2835	A
48	5	2838	G
48	5	2839	U
48	5	2842	G
48	5	2845	A
48	5	2855	G
48	5	2864	A
48	5	2875	C
48	5	2884	G
48	5	2896	G
48	5	2897	G
48	5	3598	C
48	5	3599	A
48	5	3604	A
48	5	3605	C
48	5	3615	G
48	5	3625	G
48	5	3626	G
48	5	3635	A
48	5	3644	U
48	5	3653	A
48	5	3662	A
48	5	3671	G
48	5	3673	C
48	5	3674	G
48	5	3692	A
48	5	3696	C
48	5	3698	G
48	5	3711	A
48	5	3712	A
48	5	3722	G
48	5	3729	U
48	5	3733	A
48	5	3740	G
48	5	3748	A
48	5	3750	G
48	5	3753	G
48	5	3756	A

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Mol	Chain	Res	Type
48	5	3759	A
48	5	3760	A
48	5	3765	G
48	5	3766	A
48	5	3773	U
48	5	3774	A
48	5	3776	G
48	5	3777	G
48	5	3778	U
48	5	3783	A
48	5	3784	A
48	5	3785	A
48	5	3786	U
48	5	3799	A
48	5	3809	G
48	5	3810	C
48	5	3811	G
48	5	3812	C
48	5	3814	U
48	5	3817	A
48	5	3819	G
48	5	3822	U
48	5	3831	U
48	5	3838	U
48	5	3839	G
48	5	3840	U
48	5	3851	U
48	5	3859	G
48	5	3867	A
48	5	3876	A
48	5	3877	A
48	5	3878	C
48	5	3879	G
48	5	3889	G
48	5	3892	U
48	5	3897	G
48	5	3901	A
48	5	3905	A
48	5	3906	A
48	5	3907	G
48	5	3915	U
48	5	3916	G

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Mol	Chain	Res	Type
48	5	3917	A
48	5	3927	U
48	5	3939	G
48	5	3943	A
48	5	4067	U
48	5	4069	U
48	5	4071	U
48	5	4076	G
48	5	4084	G
48	5	4085	A
48	5	4086	G
48	5	4088	C
48	5	4099	G
48	5	4100	C
48	5	4116	C
48	5	4117	U
48	5	4118	U
48	5	4119	C
48	5	4120	U
48	5	4121	G
48	5	4122	G
48	5	4125	C
48	5	4127	A
48	5	4150	G
48	5	4158	C
48	5	4162	C
48	5	4163	U
48	5	4164	C
48	5	4166	G
48	5	4168	G
48	5	4171	C
48	5	4183	G
48	5	4184	G
48	5	4190	U
48	5	4191	G
48	5	4203	A
48	5	4212	A
48	5	4213	A
48	5	4218	U
48	5	4219	A
48	5	4225	G
48	5	4229	U

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Mol	Chain	Res	Type
48	5	4232	U
48	5	4233	A
48	5	4249	G
48	5	4251	A
48	5	4255	A
48	5	4257	A
48	5	4258	C
48	5	4265	U
48	5	4268	A
48	5	4271	A
48	5	4273	A
48	5	4281	A
48	5	4291	G
48	5	4297	G
48	5	4304	A
48	5	4305	G
48	5	4306	U
48	5	4314	C
48	5	4317	A
48	5	4318	C
48	5	4319	C
48	5	4326	G
48	5	4329	G
48	5	4330	G
48	5	4335	C
48	5	4336	A
48	5	4339	A
48	5	4349	C
48	5	4350	C
48	5	4354	U
48	5	4355	G
48	5	4373	G
48	5	4376	A
48	5	4377	G
48	5	4378	A
48	5	4379	A
48	5	4380	A
48	5	4387	C
48	5	4391	G
48	5	4393	G
48	5	4394	A
48	5	4395	U

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Mol	Chain	Res	Type
48	5	4398	C
48	5	4401	G
48	5	4415	A
48	5	4419	U
48	5	4421	C
48	5	4422	A
48	5	4440	G
48	5	4444	C
48	5	4448	G
48	5	4449	A
48	5	4450	U
48	5	4453	C
48	5	4464	A
48	5	4471	U
48	5	4475	G
48	5	4476	C
48	5	4488	A
48	5	4495	G
48	5	4500	U
48	5	4510	A
48	5	4511	A
48	5	4512	U
48	5	4513	A
48	5	4519	C
48	5	4520	G
48	5	4524	G
48	5	4527	G
48	5	4528	G
48	5	4531	U
48	5	4548	A
48	5	4549	G
48	5	4560	C
48	5	4567	G
48	5	4570	G
48	5	4573	G
48	5	4575	G
48	5	4578	G
48	5	4584	A
48	5	4586	G
48	5	4590	A
48	5	4618	G
48	5	4627	U

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Mol	Chain	Res	Type
48	5	4636	U
48	5	4637	G
48	5	4639	G
48	5	4656	A
48	5	4657	U
48	5	4661	G
48	5	4667	C
48	5	4670	C
48	5	4672	A
48	5	4677	U
48	5	4678	G
48	5	4687	A
48	5	4694	G
48	5	4700	A
48	5	4701	A
48	5	4709	U
48	5	4719	G
48	5	4720	C
48	5	4721	G
48	5	4728	U
48	5	4736	C
48	5	4737	G
48	5	4745	G
48	5	4751	G
48	5	4754	G
48	5	4755	G
48	5	4756	C
48	5	4757	C
48	5	4759	C
48	5	4761	G
48	5	4765	G
48	5	4771	C
48	5	4772	C
48	5	4868	G
48	5	4870	G
48	5	4871	C
48	5	4872	G
48	5	4873	G
48	5	4874	A
48	5	4875	G
48	5	4876	A
48	5	4877	G

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Mol	Chain	Res	Type
48	5	4882	U
48	5	4883	C
48	5	4885	U
48	5	4887	C
48	5	4891	G
48	5	4895	C
48	5	4897	G
48	5	4910	A
48	5	4912	G
48	5	4913	G
48	5	4914	G
48	5	4915	G
48	5	4918	C
48	5	4919	G
48	5	4921	C
48	5	4924	C
48	5	4925	U
48	5	4926	C
48	5	4928	C
48	5	4931	G
48	5	4935	C
48	5	4937	C
48	5	4938	A
48	5	4940	C
48	5	4943	A
48	5	4944	C
48	5	4948	C
48	5	4949	G
48	5	4950	U
48	5	4951	G
48	5	4956	A
48	5	4957	C
48	5	4958	C
48	5	4964	C
48	5	4965	U
48	5	4966	A
48	5	4967	A
48	5	4976	U
48	5	4985	U
48	5	4988	U
48	5	4989	U
48	5	4990	C

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Mol	Chain	Res	Type
48	5	4991	U
48	5	5007	A
48	5	5014	A
48	5	5017	G
48	5	5035	U
48	5	5040	U
48	5	5041	G
48	5	5047	C
48	5	5050	C
48	5	5052	C
48	5	5053	U
48	5	5054	C
48	5	5056	A
48	5	5061	A
48	5	5062	G
49	7	7	G
49	7	11	A
49	7	22	A
49	7	33	U
49	7	42	A
49	7	53	U
49	7	54	A
49	7	64	G
49	7	97	G
49	7	100	A
49	7	106	G
49	7	110	G
49	7	117	G
49	7	120	U
50	8	2	G
50	8	3	A
50	8	32	C
50	8	34	U
50	8	35	C
50	8	49	G
50	8	59	A
50	8	62	A
50	8	63	U
50	8	75	G
50	8	79	G
50	8	86	U
50	8	87	G

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Mol	Chain	Res	Type
50	8	94	G
50	8	95	A
50	8	103	A
50	8	104	A
50	8	105	C
50	8	107	C
50	8	109	C
50	8	110	U
50	8	111	U
50	8	112	G
50	8	114	G
50	8	121	G
50	8	123	U
50	8	124	U
50	8	125	C
50	8	126	C
50	8	127	U
50	8	137	A
50	8	143	G
51	9	2	A
51	9	3	C
51	9	4	C
51	9	17	C
51	9	25	A
51	9	26	U
51	9	33	G
51	9	41	G
51	9	44	U
51	9	45	A
51	9	46	A
51	9	56	G
51	9	58	C
51	9	59	U
51	9	60	A
51	9	62	G
51	9	65	C
51	9	67	C
51	9	68	A
51	9	70	G
51	9	71	G
51	9	73	C
51	9	74	G

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Mol	Chain	Res	Type
51	9	75	G
51	9	77	A
51	9	79	A
51	9	99	A
51	9	100	U
51	9	103	A
51	9	104	A
51	9	110	U
51	9	111	A
51	9	113	G
51	9	115	U
51	9	116	U
51	9	124	U
51	9	126	G
51	9	127	C
51	9	129	C
51	9	130	G
51	9	141	A
51	9	143	U
51	9	147	A
51	9	155	G
51	9	158	A
51	9	161	U
51	9	162	C
51	9	163	U
51	9	167	G
51	9	168	C
51	9	173	A
51	9	175	A
51	9	182	C
51	9	183	G
51	9	184	G
51	9	188	C
51	9	189	U
51	9	191	A
51	9	192	C
51	9	200	G
51	9	202	G
51	9	206	G
51	9	213	G
51	9	215	G
51	9	289	G

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Mol	Chain	Res	Type
51	9	292	A
51	9	293	C
51	9	294	U
51	9	302	A
51	9	304	C
51	9	307	G
51	9	308	G
51	9	309	G
51	9	312	G
51	9	314	U
51	9	318	A
51	9	319	C
51	9	322	C
51	9	331	C
51	9	332	G
51	9	335	G
51	9	340	C
51	9	347	G
51	9	351	G
51	9	360	A
51	9	362	C
51	9	364	A
51	9	368	U
51	9	370	G
51	9	371	A
51	9	372	U
51	9	381	C
51	9	382	C
51	9	383	G
51	9	384	U
51	9	385	G
51	9	386	C
51	9	400	C
51	9	407	G
51	9	409	C
51	9	417	C
51	9	418	A
51	9	434	G
51	9	435	A
51	9	438	G
51	9	448	A
51	9	449	A

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Mol	Chain	Res	Type
51	9	450	C
51	9	459	C
51	9	460	A
51	9	462	C
51	9	464	A
51	9	465	A
51	9	466	G
51	9	472	C
51	9	473	A
51	9	474	G
51	9	476	A
51	9	482	G
51	9	487	U
51	9	492	C
51	9	496	C
51	9	507	G
51	9	508	A
51	9	512	A
51	9	516	A
51	9	525	A
51	9	531	A
51	9	532	C
51	9	533	A
51	9	544	G
51	9	545	A
51	9	546	G
51	9	548	C
51	9	549	C
51	9	550	C
51	9	551	U
51	9	554	A
51	9	555	A
51	9	556	U
51	9	557	U
51	9	559	G
51	9	563	G
51	9	564	A
51	9	568	C
51	9	576	A
51	9	583	A
51	9	587	A
51	9	588	G

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Mol	Chain	Res	Type
51	9	589	G
51	9	590	A
51	9	591	U
51	9	592	C
51	9	597	G
51	9	598	G
51	9	604	A
51	9	606	G
51	9	607	U
51	9	608	C
51	9	614	C
51	9	620	G
51	9	621	C
51	9	629	A
51	9	631	U
51	9	637	U
51	9	643	A
51	9	644	G
51	9	655	A
51	9	659	G
51	9	660	C
51	9	663	C
51	9	664	A
51	9	668	A
51	9	669	A
51	9	670	A
51	9	671	A
51	9	672	A
51	9	684	G
51	9	688	U
51	9	689	U
51	9	732	U
51	9	733	C
51	9	752	G
51	9	753	C
51	9	754	G
51	9	810	A
51	9	811	A
51	9	812	A
51	9	821	G
51	9	822	U
51	9	830	A

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Mol	Chain	Res	Type
51	9	834	C
51	9	847	A
51	9	861	A
51	9	868	G
51	9	869	A
51	9	870	A
51	9	871	U
51	9	872	A
51	9	873	G
51	9	874	G
51	9	875	A
51	9	877	C
51	9	878	G
51	9	885	U
51	9	887	U
51	9	890	U
51	9	892	U
51	9	913	A
51	9	914	U
51	9	920	A
51	9	922	A
51	9	930	C
51	9	933	G
51	9	934	G
51	9	943	U
51	9	955	A
51	9	971	G
51	9	985	G
51	9	990	A
51	9	992	A
51	9	999	G
51	9	1002	U
51	9	1016	U
51	9	1017	U
51	9	1023	A
51	9	1041	G
51	9	1045	U
51	9	1060	A
51	9	1061	U
51	9	1062	A
51	9	1078	C
51	9	1083	A

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Mol	Chain	Res	Type
51	9	1085	C
51	9	1089	G
51	9	1096	G
51	9	1099	G
51	9	1100	A
51	9	1113	A
51	9	1114	U
51	9	1115	U
51	9	1116	C
51	9	1117	C
51	9	1118	C
51	9	1120	U
51	9	1121	G
51	9	1131	G
51	9	1133	A
51	9	1138	C
51	9	1139	C
51	9	1148	A
51	9	1149	A
51	9	1150	A
51	9	1153	C
51	9	1154	U
51	9	1165	G
51	9	1166	G
51	9	1195	A
51	9	1197	G
51	9	1207	G
51	9	1208	A
51	9	1211	G
51	9	1213	C
51	9	1215	C
51	9	1216	C
51	9	1221	G
51	9	1223	A
51	9	1224	G
51	9	1240	A
51	9	1242	U
51	9	1251	A
51	9	1253	A
51	9	1254	C
51	9	1256	G
51	9	1257	G

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Mol	Chain	Res	Type
51	9	1259	A
51	9	1260	A
51	9	1265	A
51	9	1266	C
51	9	1270	G
51	9	1271	C
51	9	1274	G
51	9	1275	G
51	9	1281	G
51	9	1284	A
51	9	1285	G
51	9	1286	G
51	9	1287	A
51	9	1289	U
51	9	1293	A
51	9	1298	G
51	9	1299	A
51	9	1300	U
51	9	1301	A
51	9	1302	G
51	9	1307	U
51	9	1308	U
51	9	1313	A
51	9	1314	U
51	9	1316	C
51	9	1330	G
51	9	1331	C
51	9	1342	U
51	9	1348	G
51	9	1354	G
51	9	1369	A
51	9	1371	U
51	9	1372	U
51	9	1378	A
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1397	U
51	9	1401	A
51	9	1402	A
51	9	1404	U
51	9	1410	C

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Mol	Chain	Res	Type
51	9	1412	C
51	9	1424	G
51	9	1428	G
51	9	1439	A
51	9	1449	G
51	9	1452	A
51	9	1454	A
51	9	1458	G
51	9	1459	G
51	9	1462	U
51	9	1463	U
51	9	1466	G
51	9	1473	G
51	9	1476	A
51	9	1477	U
51	9	1478	U
51	9	1490	G
51	9	1493	C
51	9	1494	U
51	9	1497	G
51	9	1498	A
51	9	1507	G
51	9	1509	U
51	9	1510	G
51	9	1519	U
51	9	1520	G
51	9	1521	C
51	9	1522	A
51	9	1531	A
51	9	1533	A
51	9	1535	U
51	9	1536	G
51	9	1544	C
51	9	1545	A
51	9	1548	G
51	9	1552	G
51	9	1553	C
51	9	1555	U
51	9	1556	A
51	9	1557	C
51	9	1560	U
51	9	1570	G

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Mol	Chain	Res	Type
51	9	1574	C
51	9	1575	G
51	9	1580	A
51	9	1581	C
51	9	1582	C
51	9	1585	U
51	9	1586	U
51	9	1587	G
51	9	1588	A
51	9	1589	A
51	9	1600	G
51	9	1601	A
51	9	1602	U
51	9	1604	G
51	9	1621	U
51	9	1623	A
51	9	1625	U
51	9	1637	A
51	9	1638	G
51	9	1639	G
51	9	1641	A
51	9	1647	A
51	9	1648	G
51	9	1654	G
51	9	1664	A
51	9	1665	G
51	9	1671	G
51	9	1680	G
51	9	1682	C
51	9	1683	C
51	9	1686	G
51	9	1689	C
51	9	1695	A
51	9	1698	C
51	9	1699	A
51	9	1700	C
51	9	1703	C
51	9	1715	A
51	9	1721	U
51	9	1722	G
51	9	1726	G
51	9	1728	U

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Mol	Chain	Res	Type
51	9	1729	U
51	9	1730	U
51	9	1737	G
51	9	1744	G
51	9	1745	A
51	9	1753	C
51	9	1758	G
51	9	1760	G
51	9	1772	C
51	9	1783	C
51	9	1785	C
51	9	1800	A
51	9	1823	A
51	9	1825	A
51	9	1826	G
51	9	1829	G
51	9	1831	A
51	9	1835	A
51	9	1836	G
51	9	1838	U
51	9	1849	G
51	9	1851	A
51	9	1861	G
51	9	1862	G
51	9	1863	A
51	9	1865	C
51	9	1866	A
51	9	1867	U
51	9	1868	U
51	9	1869	A
85	hh	42	C
85	hh	43	A
85	hh	45	A
85	hh	46	G
85	hh	49	U
85	hh	52	G
85	hh	54	U
85	hh	55	C

All (250) RNA pucker outliers are listed below:

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Mol	Chain	Res	Type
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Mol	Chain	Res	Type
47	3	7	A
47	3	74	C
48	5	12	A
48	5	20	U
48	5	47	A
48	5	48	G
48	5	64	A
48	5	125	C
48	5	134	G
48	5	143	C
48	5	159	C
48	5	217	C
48	5	226	G
48	5	234	G
48	5	245	C
48	5	265	C
48	5	275	C
48	5	278	G
48	5	385	A
48	5	387	G
48	5	406	C
48	5	408	A
48	5	409	G
48	5	417	G
48	5	449	C
48	5	480	C
48	5	481(A)	C
48	5	482	G
48	5	484	U
48	5	485	C
48	5	492	U
48	5	497	G
48	5	498	C
48	5	504	G
48	5	696	C
48	5	729	G
48	5	738(A)	C
48	5	747	A
48	5	748	G
48	5	915	A
48	5	916	C

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Mol	Chain	Res	Type
48	5	922(B)	C
48	5	930	G
48	5	935(A)	G
48	5	936	C
48	5	955	G
48	5	956	A
48	5	959	G
48	5	965	G
48	5	966	A
48	5	969	C
48	5	971(A)	G
48	5	1071	C
48	5	1072	C
48	5	1211	G
48	5	1214	C
48	5	1236	C
48	5	1238	A
48	5	1287	G
48	5	1291	G
48	5	1294	A
48	5	1295	U
48	5	1329	G
48	5	1358	G
48	5	1359	G
48	5	1370	G
48	5	1378	C
48	5	1380	G
48	5	1420	A
48	5	1440	U
48	5	1445	U
48	5	1455	G
48	5	1477	C
48	5	1481	C
48	5	1484	G
48	5	1485	C
48	5	1497	A
48	5	1563	A
48	5	1633	G
48	5	1678	C
48	5	1733	G
48	5	1734	G
48	5	1740	C

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Mol	Chain	Res	Type
48	5	1804	A
48	5	1815	G
48	5	1818	G
48	5	1833	G
48	5	1834	U
48	5	1835	G
48	5	1836	G
48	5	1881	C
48	5	1892	A
48	5	1921	C
48	5	1935	C
48	5	1947	U
48	5	1979	A
48	5	1983	A
48	5	1986	U
48	5	2001	G
48	5	2003	G
48	5	2046	G
48	5	2068	C
48	5	2088	A
48	5	2089	G
48	5	2100	G
48	5	2265	G
48	5	2266	C
48	5	2278	G
48	5	2313	A
48	5	2398	U
48	5	2428	A
48	5	2467	U
48	5	2468	U
48	5	2474	G
48	5	2475	G
48	5	2490	U
48	5	2502	A
48	5	2546	G
48	5	2587	A
48	5	2661	U
48	5	2695	A
48	5	2741	U
48	5	2754	G
48	5	2794	C
48	5	2806	A

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Mol	Chain	Res	Type
48	5	3625	G
48	5	3673	C
48	5	3697	U
48	5	3710	G
48	5	3809	G
48	5	3876	A
48	5	3888	G
48	5	3904	G
48	5	4075	U
48	5	4076	G
48	5	4084	G
48	5	4116	C
48	5	4119	C
48	5	4121	G
48	5	4124	G
48	5	4162	C
48	5	4170	A
48	5	4221	C
48	5	4232	U
48	5	4254	G
48	5	4257	A
48	5	4266	G
48	5	4331	G
48	5	4378	A
48	5	4379	A
48	5	4395	U
48	5	4448	G
48	5	4449	A
48	5	4510	A
48	5	4527	G
48	5	4572	U
48	5	4626	A
48	5	4699	U
48	5	4719	G
48	5	4753	U
48	5	4871	C
48	5	4872	G
48	5	4876	A
48	5	4884	G
48	5	4925	U
48	5	4936	G
48	5	4942	C

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Mol	Chain	Res	Type
48	5	4947	U
48	5	4949	G
48	5	4965	U
48	5	4966	A
49	7	10	C
49	7	109	U
50	8	2	G
50	8	51	U
50	8	86	U
50	8	94	G
50	8	110	U
50	8	124	U
51	9	2	A
51	9	3	C
51	9	72	C
51	9	110	U
51	9	126	G
51	9	127	C
51	9	160	U
51	9	182	C
51	9	293	C
51	9	308	G
51	9	369	C
51	9	370	G
51	9	434	G
51	9	448	A
51	9	465	A
51	9	473	A
51	9	487	U
51	9	500	A
51	9	532	C
51	9	550	C
51	9	553	U
51	9	555	A
51	9	563	G
51	9	591	U
51	9	606	G
51	9	620	G
51	9	642	U
51	9	656	G
51	9	670	A
51	9	688	U

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Mol	Chain	Res	Type
51	9	752	G
51	9	821	G
51	9	869	A
51	9	870	A
51	9	872	A
51	9	874	G
51	9	1016	U
51	9	1114	U
51	9	1115	U
51	9	1120	U
51	9	1137	U
51	9	1165	G
51	9	1215	C
51	9	1253	A
51	9	1264	C
51	9	1284	A
51	9	1286	G
51	9	1313	A
51	9	1330	G
51	9	1394	G
51	9	1395	C
51	9	1396	A
51	9	1476	A
51	9	1489	A
51	9	1493	C
51	9	1519	U
51	9	1520	G
51	9	1535	U
51	9	1585	U
51	9	1636	G
51	9	1637	A
51	9	1646	C
51	9	1664	A
51	9	1679	A
51	9	1721	U
51	9	1744	G
51	9	1824	A
51	9	1826	G
51	9	1835	A
51	9	1867	U
51	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 291 ligands modelled in this entry, 290 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
90	GCP	jj	700	88	32,34,34	1.74	7 (21%)	49,54,54	1.82	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
90	GCP	jj	700	88	-	6/19/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
90	jj	700	GCP	PG-O1G	5.58	1.61	1.50
90	jj	700	GCP	C5-C4	3.20	1.47	1.38
90	jj	700	GCP	PG-O2G	2.96	1.61	1.55
90	jj	700	GCP	PG-O3G	-2.96	1.48	1.55
90	jj	700	GCP	PB-O3A	2.16	1.60	1.58
90	jj	700	GCP	C6-N1	-2.14	1.34	1.38
90	jj	700	GCP	C5-N7	-2.09	1.34	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
90	jj	700	GCP	C5-C4-N3	-6.00	118.84	128.39
90	jj	700	GCP	C2-N3-C4	5.23	121.32	112.30
90	jj	700	GCP	N9-C4-N3	4.57	135.08	125.95
90	jj	700	GCP	PB-O3A-PA	-3.63	120.51	132.37
90	jj	700	GCP	C6-C5-N7	3.55	136.75	130.29
90	jj	700	GCP	C4-C5-N7	-2.52	106.68	110.67
90	jj	700	GCP	O6-C6-C5	-2.23	120.66	126.53
90	jj	700	GCP	C5-C6-N1	2.21	118.89	113.25

There are no chirality outliers.

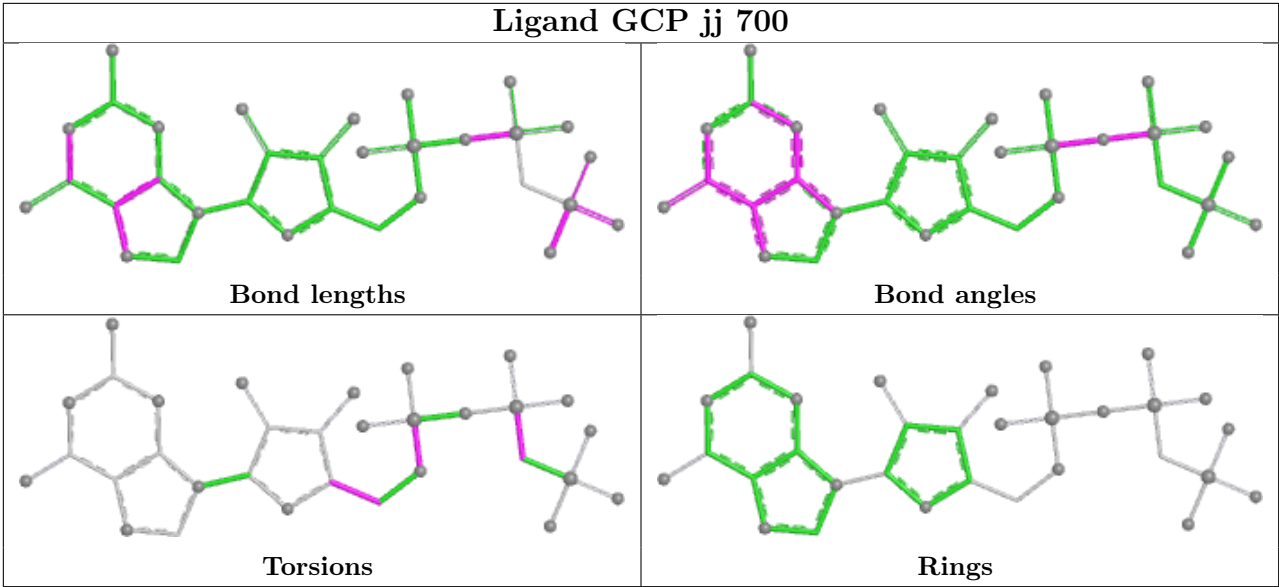
All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
90	jj	700	GCP	PG-C3B-PB-O1B
90	jj	700	GCP	PG-C3B-PB-O2B
90	jj	700	GCP	PG-C3B-PB-O3A
90	jj	700	GCP	C5'-O5'-PA-O3A
90	jj	700	GCP	C5'-O5'-PA-O1A
90	jj	700	GCP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
48	5	30
51	9	7
47	3	2
46	2	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	41.06
1	5	1252:C	O3'	1271:G	P	35.64
1	5	1219:G	O3'	1233:G	P	22.79
1	5	3948:C	O3'	4065:G	P	19.75
1	5	1406(C):G	O3'	1411:C	P	18.65
1	5	990:C	O3'	1064:G	P	18.31
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	17.52
1	5	4777:C	O3'	4859:C	P	16.78
1	5	760:G	O3'	904:C	P	15.07

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	1696:C	O3'	1720:C	P	14.63
1	5	5022:U	O3'	5028:G	P	14.63
1	5	182:G	O3'	189:G	P	14.05
1	5	1364:U	O3'	1368:A	P	13.97
1	5	2901:G	O3'	3597:G	P	13.29
1	5	512:U	O3'	515:C	P	9.99
1	5	4729:A	O3'	4735:G	P	9.79
1	5	1180:C	O3'	1183:C	P	9.09
1	5	500:G	O3'	504:G	P	6.73
1	5	1100:U	O3'	1168:G	P	5.98
1	3	19:G	O3'	20:U	P	5.77
1	5	1239:C	O3'	1244:G	P	5.36
1	9	322:C	O3'	323:C	P	5.19
1	5	4740:G	O3'	4743:G	P	4.87
1	3	16:C	O3'	18:U	P	4.79
1	2	16:C	O3'	18:G	P	4.35
1	9	309:G	O3'	310:C	P	4.34
1	9	798:G	O3'	799:U	P	4.27
1	9	304:C	O3'	305:U	P	4.18
1	5	170:C	O3'	171:U	P	3.77
1	9	902:G	O3'	903:A	P	3.43
1	5	1438:U	O3'	1440:U	P	3.34
1	9	903:A	O3'	904:A	P	3.33
1	5	4899:G	O3'	4902:C	P	3.32
1	9	1295:A	O3'	1296:U	P	3.24
1	5	5020:G	O3'	5021:C	P	3.16
1	5	267:G	O3'	268:G	P	3.15
1	5	751:G	O3'	752:G	P	3.15
1	5	2031:C	O3'	2032:U	P	2.55

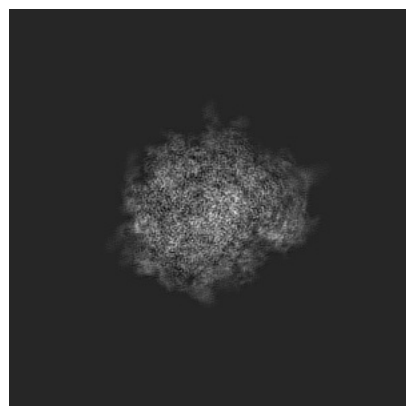
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4131. These allow visual inspection of the internal detail of the map and identification of artifacts.

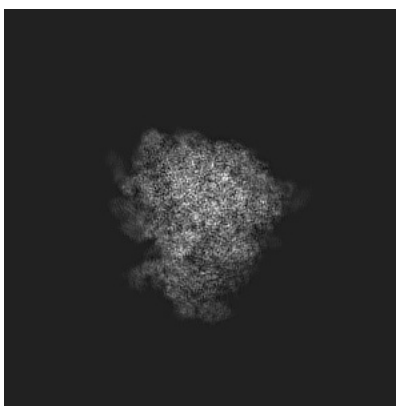
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

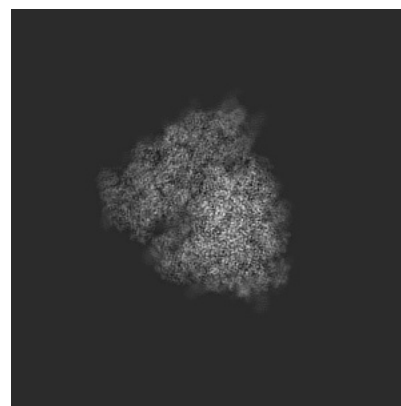
6.1.1 Primary map



X

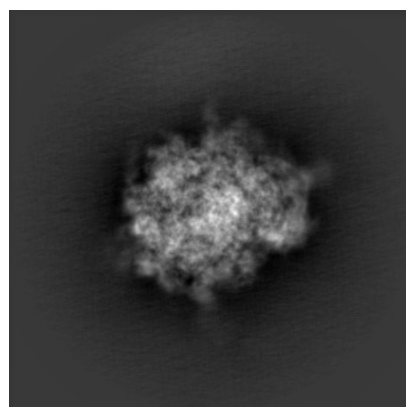


Y

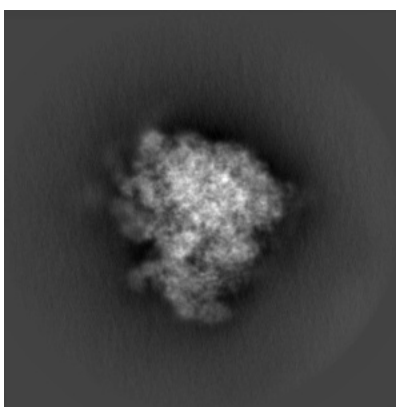


Z

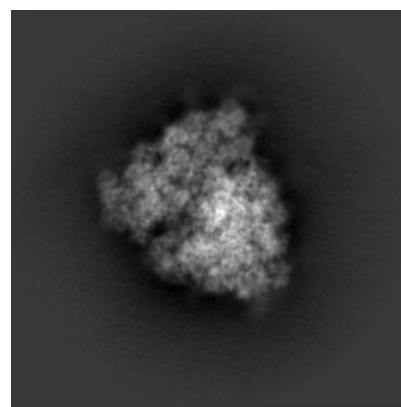
6.1.2 Raw map



X



Y

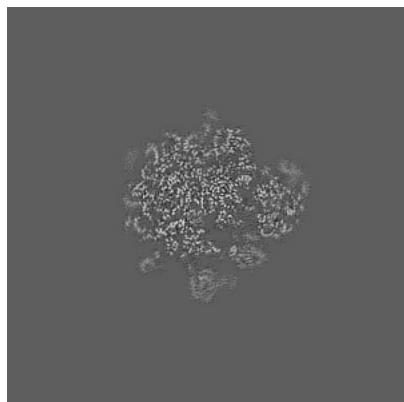


Z

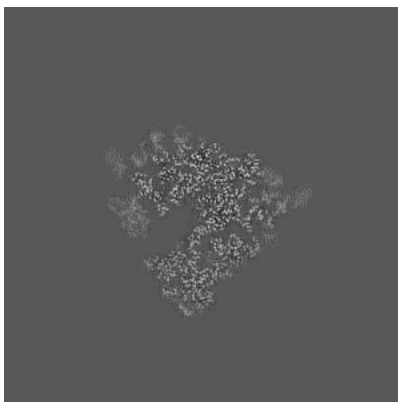
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

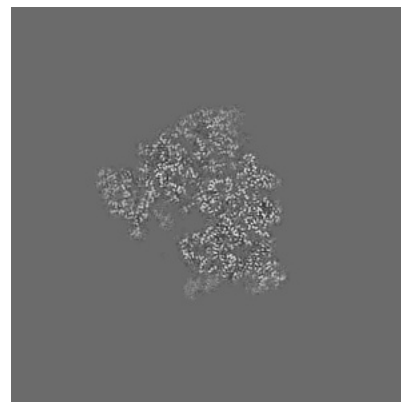
6.2.1 Primary map



X Index: 210

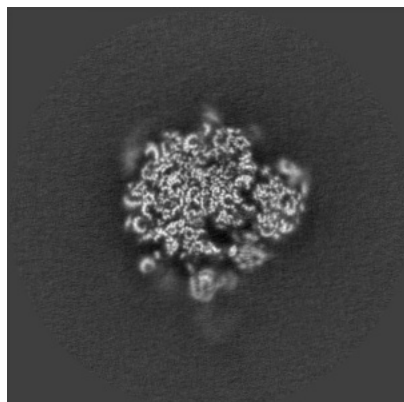


Y Index: 210

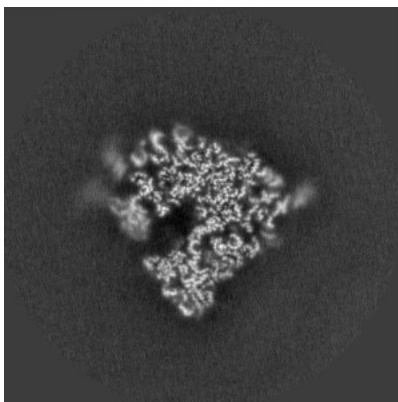


Z Index: 210

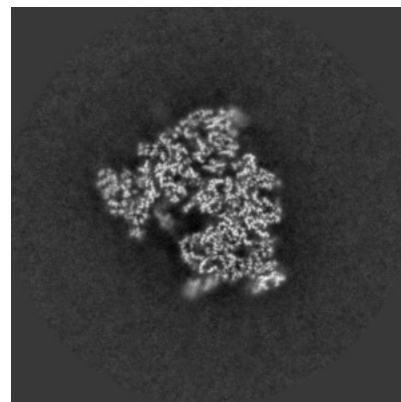
6.2.2 Raw map



X Index: 210



Y Index: 210

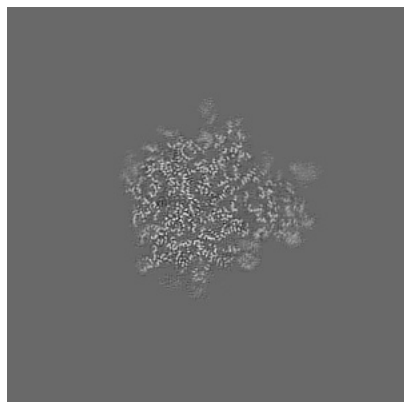


Z Index: 210

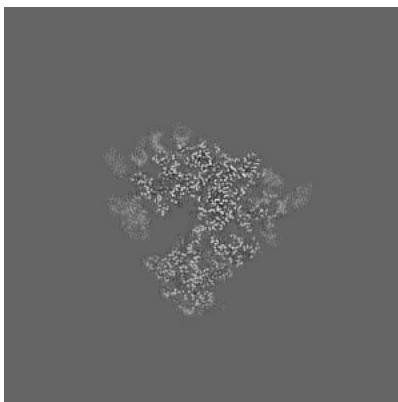
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

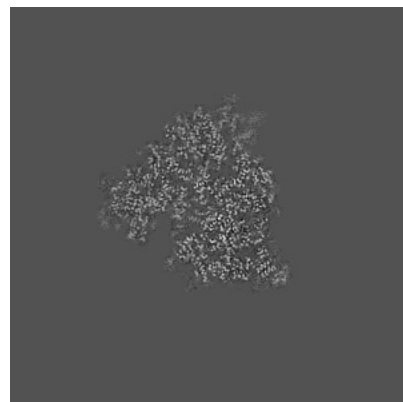
6.3.1 Primary map



X Index: 222

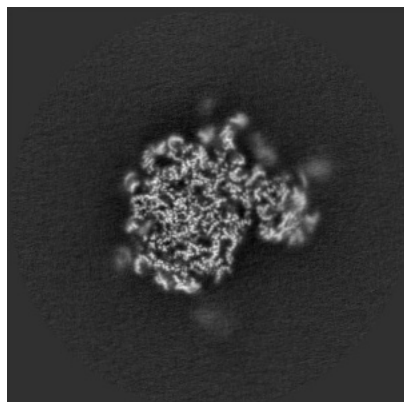


Y Index: 211

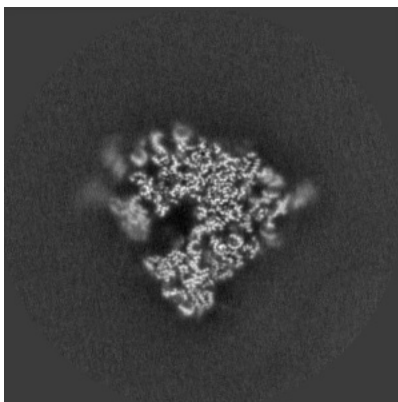


Z Index: 202

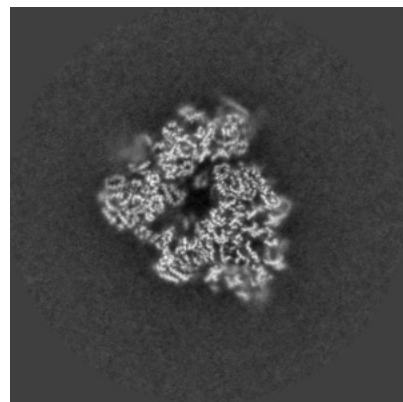
6.3.2 Raw map



X Index: 233



Y Index: 211

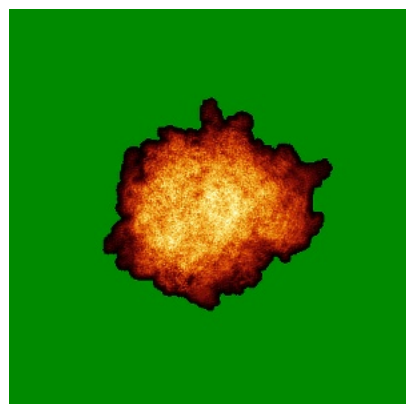


Z Index: 186

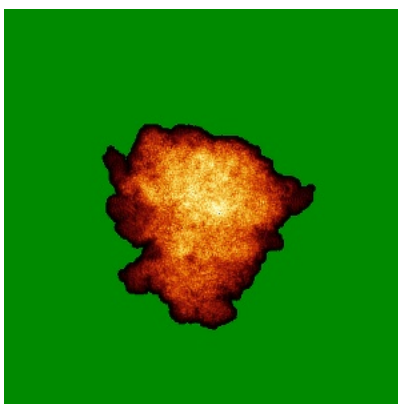
The images above show the largest variance slices of the map in three orthogonal directions.

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

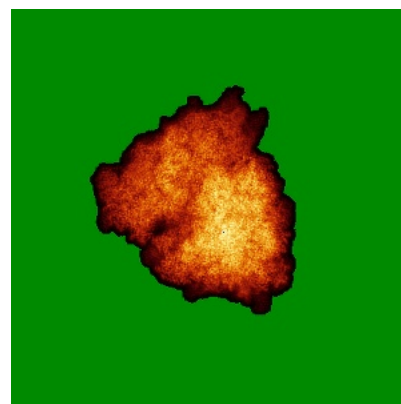
6.4.1 Primary map



X

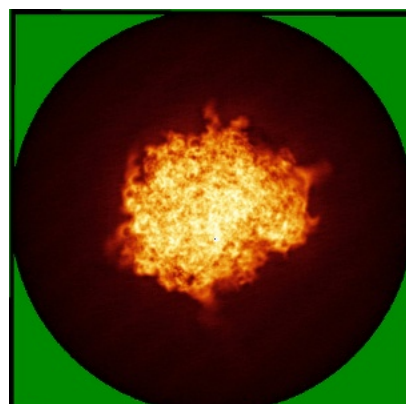


Y

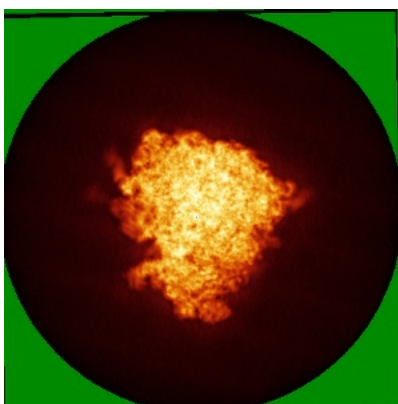


Z

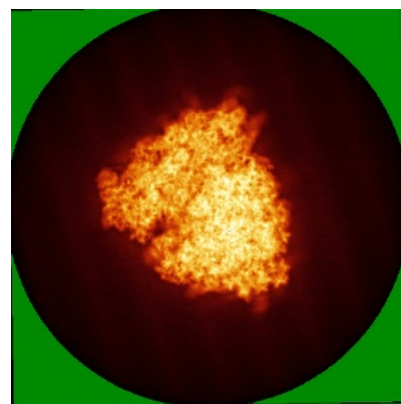
6.4.2 Raw map



X



Y

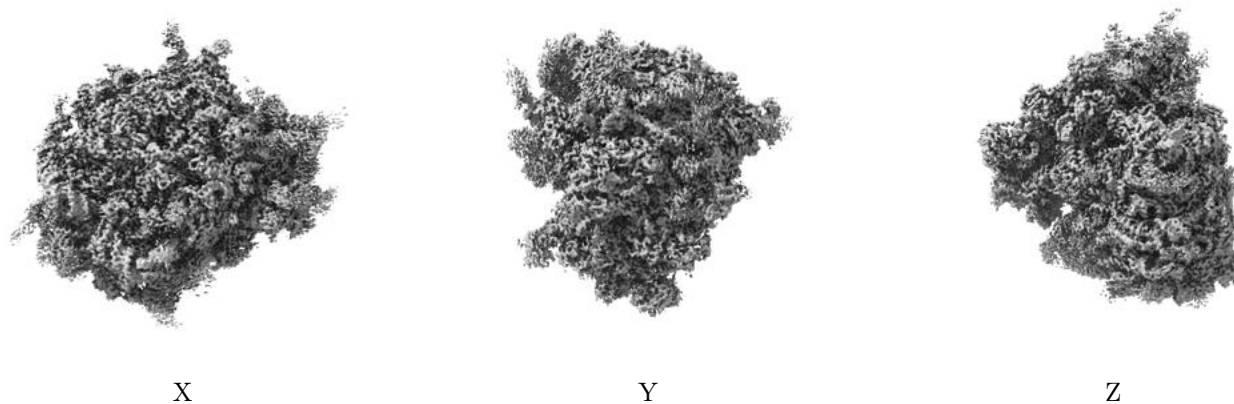


Z

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.

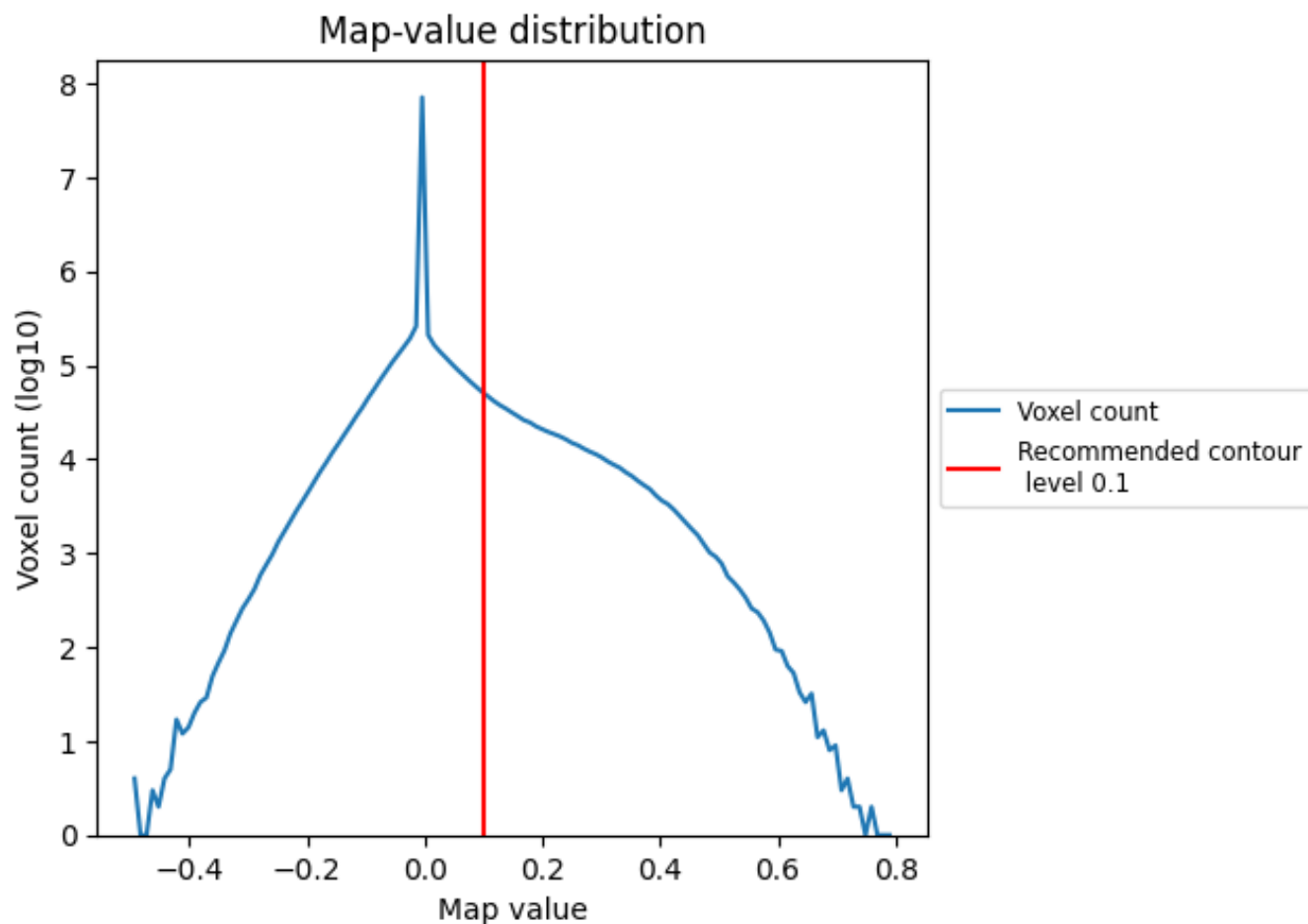
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

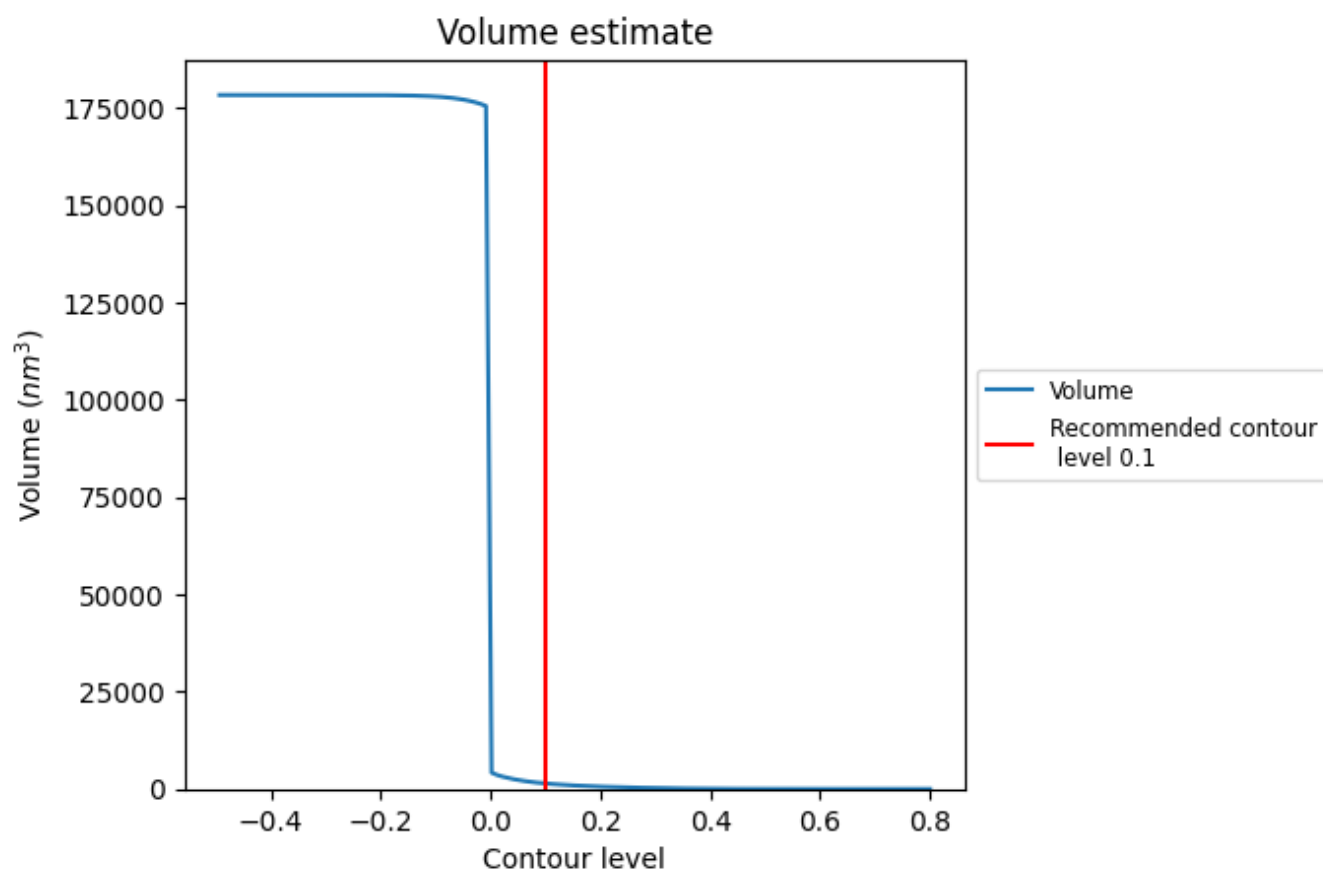
This section contains the results of statistical analysis of the map.

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.

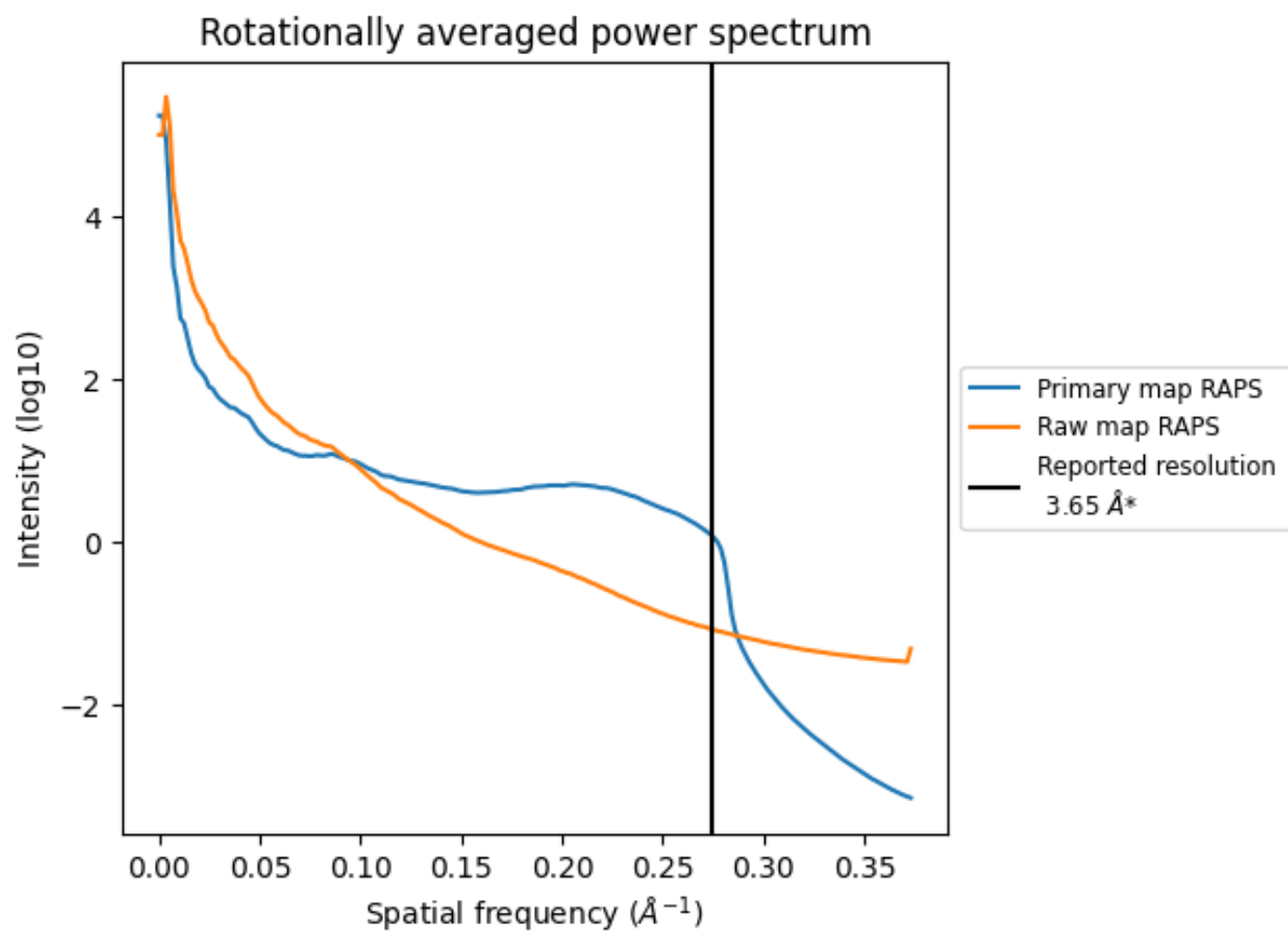
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1409 nm³; this corresponds to an approximate mass of 1273 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

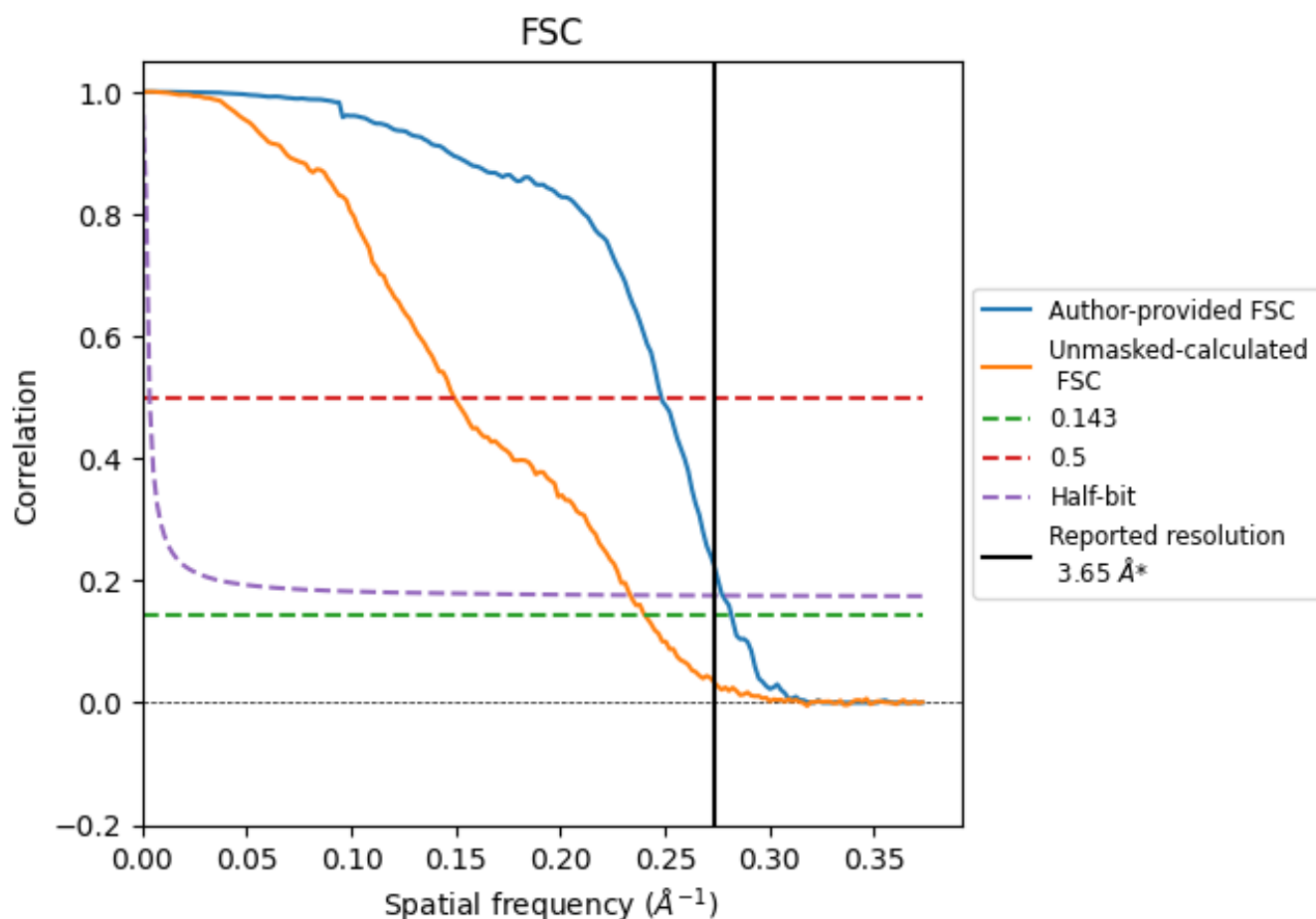


*Reported resolution corresponds to spatial frequency of $0.274 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.274 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

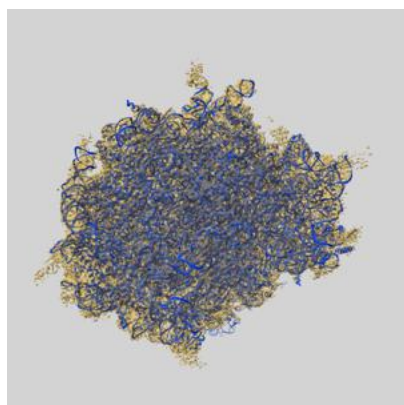
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.55	4.03	3.60
Unmasked-calculated*	4.16	6.71	4.28

*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 4.16 differs from the reported value 3.65 by more than 10 %

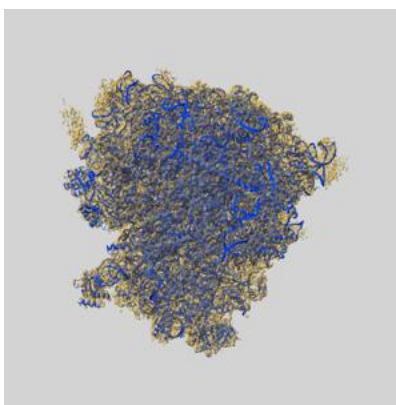
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4131 and PDB model 5LZT. Per-residue inclusion information can be found in [section 3](#) on [page 24](#).

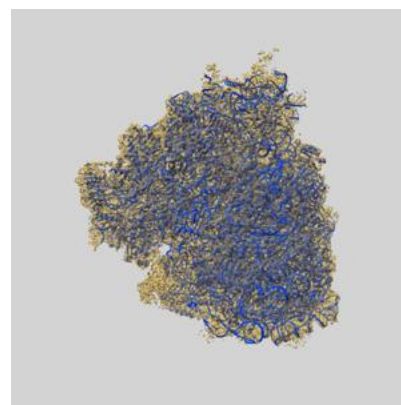
9.1 Map-model overlay [i](#)



X



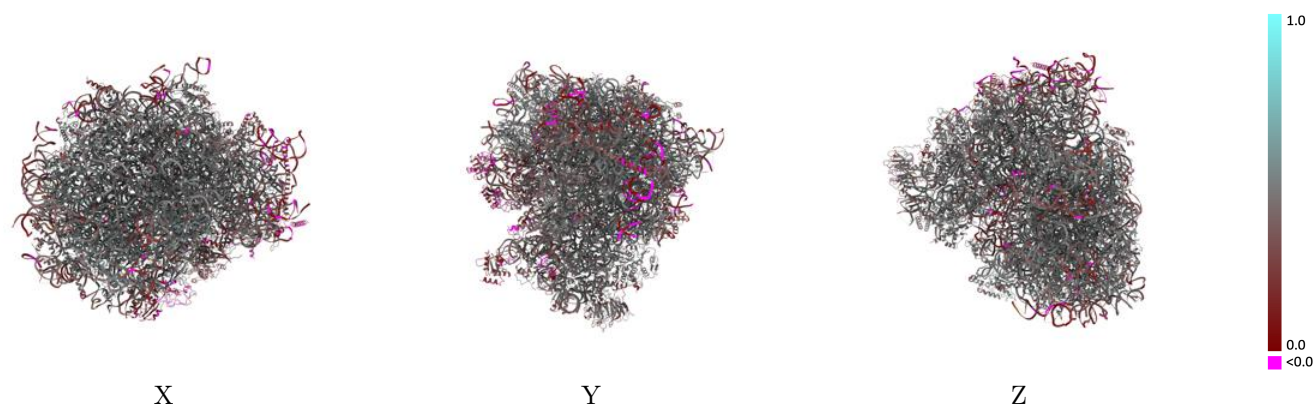
Y



Z

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](#)

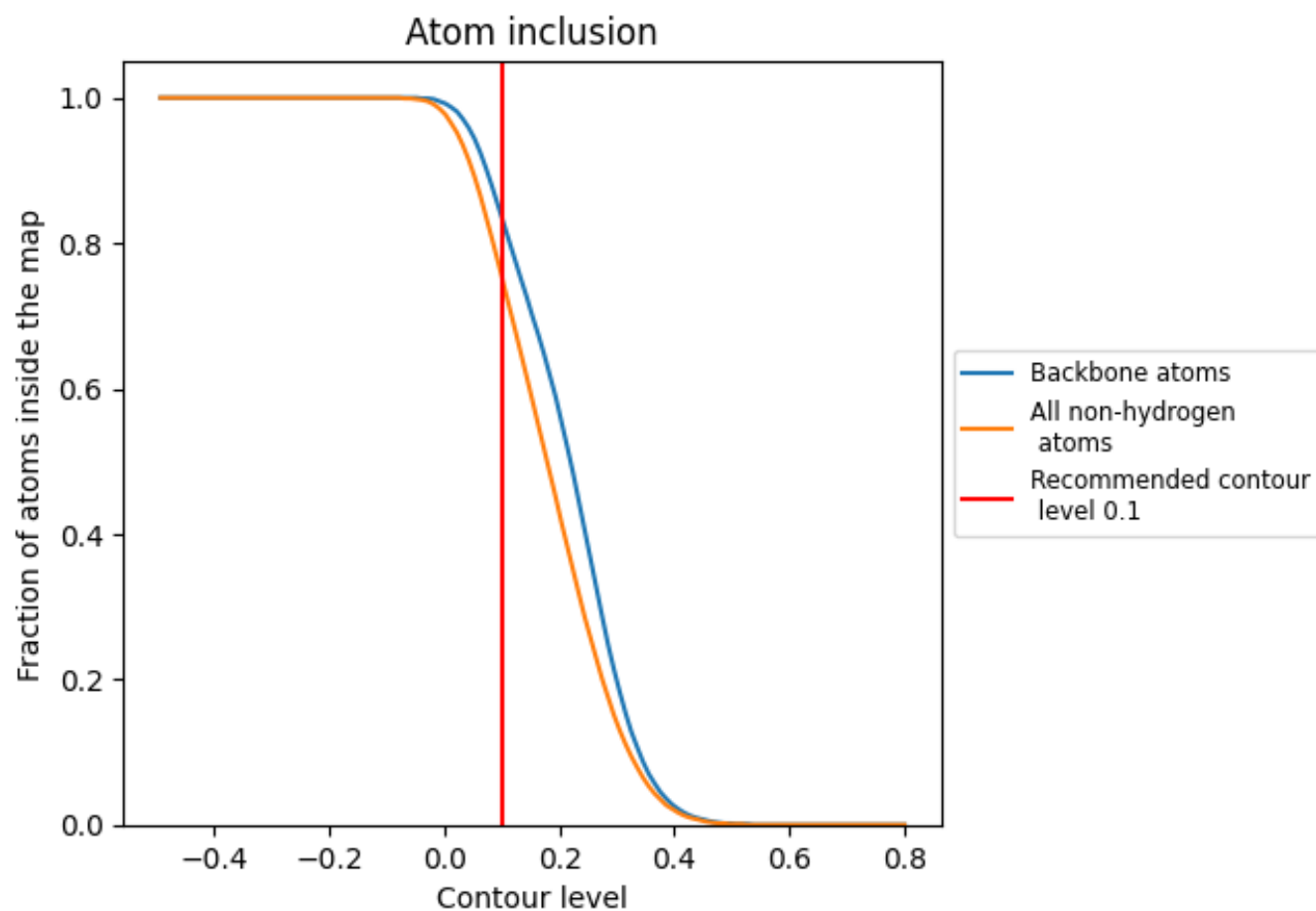


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 75% 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	 0.7540	 0.4340
1	 0.5870	 0.4450
2	 0.8010	 0.4240
3	 0.3870	 0.2490
5	 0.8250	 0.4360
7	 0.8970	 0.4710
8	 0.8440	 0.4440
9	 0.8020	 0.4180
A	 0.7740	 0.5010
AA	 0.6790	 0.4470
B	 0.7740	 0.4950
BB	 0.6940	 0.4600
C	 0.7680	 0.4960
CC	 0.7050	 0.4700
D	 0.7590	 0.4590
DD	 0.6270	 0.4280
E	 0.7780	 0.4740
EE	 0.7000	 0.4420
F	 0.7800	 0.4950
FF	 0.6900	 0.4530
G	 0.6600	 0.4150
GG	 0.5670	 0.3460
H	 0.7340	 0.4830
HH	 0.5440	 0.3770
I	 0.7350	 0.4830
II	 0.6720	 0.4350
J	 0.7210	 0.4550
JJ	 0.7220	 0.4450
KK	 0.6900	 0.4260
L	 0.7310	 0.4700
LL	 0.7130	 0.4710
M	 0.7750	 0.4910
MM	 0.2950	 0.1990
N	 0.7890	 0.5040
NN	 0.7080	 0.4680



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Chain	Atom inclusion	Q-score
O	 0.7680	 0.4900
OO	 0.7260	 0.4750
P	 0.7890	 0.5070
PP	 0.6530	 0.4130
Q	 0.7550	 0.4990
QQ	 0.7160	 0.4610
R	 0.7040	 0.4490
RR	 0.6170	 0.4240
S	 0.8000	 0.5060
SS	 0.7120	 0.4390
T	 0.7410	 0.4810
TT	 0.7170	 0.4410
U	 0.6710	 0.4040
UU	 0.6270	 0.4200
V	 0.7260	 0.4940
VV	 0.7110	 0.4640
W	 0.4900	 0.3390
WW	 0.7280	 0.4950
X	 0.7180	 0.4680
XX	 0.7110	 0.4900
Y	 0.7430	 0.4720
YY	 0.6440	 0.4110
Z	 0.7610	 0.4560
ZZ	 0.6550	 0.4160
a	 0.7870	 0.4970
aa	 0.7240	 0.4650
b	 0.6470	 0.4110
bb	 0.6590	 0.4280
c	 0.7140	 0.4630
cc	 0.6320	 0.4530
d	 0.7360	 0.4790
dd	 0.7380	 0.4740
e	 0.7640	 0.4960
ee	 0.6380	 0.4120
f	 0.8040	 0.5170
ff	 0.3600	 0.2610
g	 0.7060	 0.4670
gg	 0.6080	 0.3930
h	 0.7170	 0.4600
hh	 0.7140	 0.3910
i	 0.7120	 0.4560
ii	 0.4620	 0.3240

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Chain	Atom inclusion	Q-score
j	 0.7880	 0.4990
jj	 0.5020	 0.3280
k	 0.6660	 0.4320
l	 0.7260	 0.4840
m	 0.7620	 0.4750
n	 0.6650	 0.4660
o	 0.7410	 0.4870
p	 0.7500	 0.4860
r	 0.8120	 0.5060
s	 0.2030	 0.1760
t	 0.1480	 0.1400