



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 04:28 PM UTC

PDB ID : 5LZS / pdb_00005lzs
EMDB ID : EMD-4130
Title : Structure of the mammalian ribosomal elongation complex with aminoacyl-tRNA, eEF1A, and didemnin B
Authors : Shao, S.; Murray, J.; Brown, A.; Taunton, J.; Ramakrishnan, V.; Hegde, R.S.
Deposited on : 2016-10-02
Resolution : 3.31 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

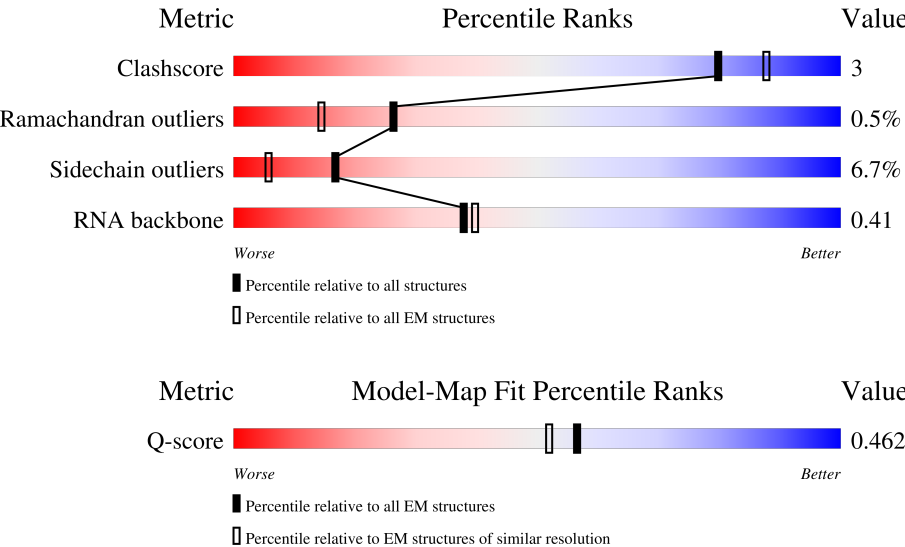
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.31 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	14550 (2.81 - 3.81)

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	116	
33	h	123	
34	i	105	
35	j	97	
36	k	70	
37	l	51	
38	m	102	
39	n	25	
40	o	106	
41	p	92	
42	r	137	
43	s	318	
44	t	165	
45	2	76	
45	ii	76	
46	3	75	
47	5	3543	
48	7	120	
49	8	156	
50	9	1869	
51	AA	295	
52	BB	264	

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

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Mol	Chain	Length	Quality of chain
78	bb	84	
79	cc	69	
80	dd	56	
81	ee	133	
82	ff	156	
83	gg	317	
84	hh	10	
85	jj	462	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
87	ZN	ff	200	-	-	X	-
87	ZN	j	101	-	-	X	-

2 Entry composition

There are 89 unique types of molecules in this entry. The entry contains 220934 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called uL2.

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

- Molecule 2 is a protein called uL3.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called uL4.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 6 is a protein called uL30.

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

There are 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 Ribosomal protein L10 (Predicted).

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

- Molecule 10 is a protein called uL5.

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

- Molecule 11 is a protein called eL13.

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

- Molecule 12 is a protein called eL14.

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

- Molecule 13 is a protein called Ribosomal protein L15.

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

- Molecule 14 is a protein called uL13.

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

- Molecule 15 is a protein called uL22.

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

- Molecule 16 is a protein called eL18.

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

- Molecule 17 is a protein called eL19.

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

- Molecule 18 is a protein called eL20.

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

- Molecule 19 is a protein called eL21.

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

- Molecule 20 is a protein called eL22.

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

- Molecule 21 is a protein called uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	139	Total	C	N	O	S	0	0
			1034	648	199	182	5		

- Molecule 22 is a protein called uL24.

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

- Molecule 23 is a protein called uL23.

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

- Molecule 24 is a protein called uL24.

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

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

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

- Molecule 26 is a protein called uL15.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 27 is a protein called eL29.

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

- 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		

- Molecule 33 is a protein called uL29.

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

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

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

- Molecule 35 is a protein called Ribosomal protein L37.

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

- Molecule 36 is a protein called eL38.

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

- Molecule 37 is a protein called eL39.

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

- Molecule 38 is a protein called eL40.

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

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

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

- Molecule 40 is a protein called eL42.

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

- Molecule 41 is a protein called eL43.

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

- Molecule 42 is a protein called eL28.

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

- Molecule 43 is a protein called uL10.

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

- Molecule 44 is a protein called uL11.

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

- Molecule 45 is a RNA chain called tRNA.

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	7	119	Total	C	N	O	P	0	0
			2538	1132	454	834	118		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	9	1697	Total	C	N	O	P	0	0
			36229	16171	6507	11855	1696		

- Molecule 51 is a protein called uS2.

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

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

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

- Molecule 53 is a protein called uS5.

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

- Molecule 54 is a protein called uS4.

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

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

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

- Molecule 56 is a protein called Uncharacterized protein.

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

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

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

- Molecule 58 is a protein called uS7.

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

- Molecule 61 is a protein called eS10.

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

- Molecule 62 is a protein called uS17.

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

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

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

- Molecule 64 is a protein called uS15.

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

- Molecule 65 is a protein called uS11.

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

- Molecule 66 is a protein called uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
66	PP	129	Total	C	N	O	S	0	0
			1058	670	201	180	7		

- Molecule 67 is a protein called uS9.

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

- Molecule 68 is a protein called eS17.

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

- Molecule 69 is a protein called uS13.

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

- Molecule 70 is a protein called eS19.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 71 is a protein called uS10.

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

- Molecule 72 is a protein called eS21.

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

- Molecule 73 is a protein called uS8.

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

- Molecule 74 is a protein called uS12.

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

- Molecule 75 is a protein called eS24.

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

- Molecule 76 is a protein called eS25.

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

- Molecule 77 is a protein called eS26.

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

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

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

- Molecule 79 is a protein called eS28.

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

- Molecule 80 is a protein called uS14.

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

- Molecule 81 is a protein called eS30.

Mol	Chain	Residues	Atoms					AltConf	Trace
81	ee	57	Total	C	N	O	S	0	0
			457	282	101	73	1		

- Molecule 82 is a protein called eS31.

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

- Molecule 83 is a protein called RACK1.

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

- Molecule 84 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
84	hh	10	Total	C	N	O	P	0	0
			210	94	33	73	10		

- Molecule 85 is a protein called Elongation factor 1-alpha 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
85	jj	441	Total	C	N	O	P	S	0	0
			3383	2148	581	636	1	17		

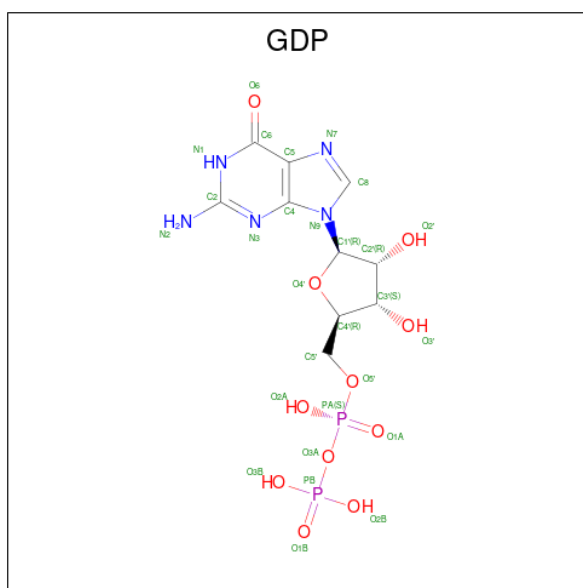
- Molecule 86 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
86	B	1	Total	Mg	0
			1	1	
86	I	1	Total	Mg	0
			1	1	
86	P	1	Total	Mg	0
			1	1	
86	Q	1	Total	Mg	0
			1	1	
86	V	1	Total	Mg	0
			1	1	
86	a	2	Total	Mg	0
			2	2	
86	g	1	Total	Mg	0
			1	1	
86	j	1	Total	Mg	0
			1	1	
86	5	185	Total	Mg	0
			185	185	
86	7	6	Total	Mg	0
			6	6	
86	8	5	Total	Mg	0
			5	5	
86	9	69	Total	Mg	0
			69	69	
86	aa	1	Total	Mg	0
			1	1	
86	jj	1	Total	Mg	0
			1	1	

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

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

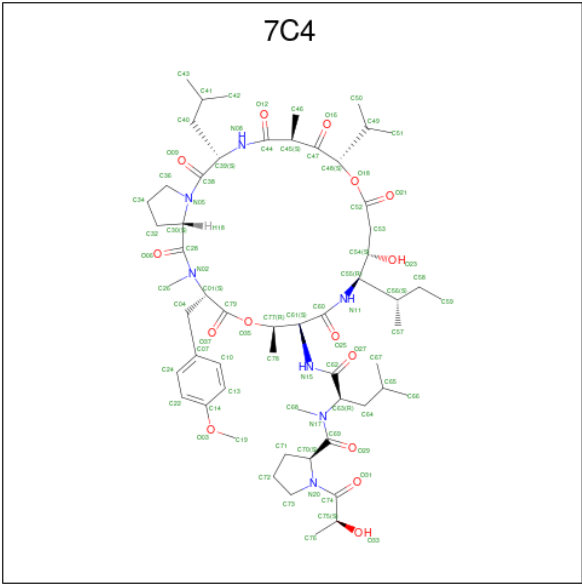
- Molecule 88 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
88	jj	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 89 is (2 {S})- {N}-[(2 {R})-1-[(3 {S},6 {S},8 {S},12 {S},13 {R},16 {S},17 {R},20 {S},23 {S})-13-[(2 {S})-butan-2-yl]-20-[(4-methoxyphenyl)methyl]-6,17,21-trimethyl-3-(2-methylpropyl)-12-oxidanyl-2,5,7,10,15,19,22-heptakis(oxidanylidene)-8-propan-2-yl-9,18-dioxo-1,4,14,21-tetrazabicyclo[21.3.0]hexacosan-16-yl]amino]-4-methyl-1-oxidanylidene-pentan-2-yl]- {N}-methyl-1-[(2 {S})-2-oxidanylpropanoyl]pyrrolidine-2-carboxamide (CCD ID: 7C4)

(formula: C₅₇H₈₉N₇O₁₅).

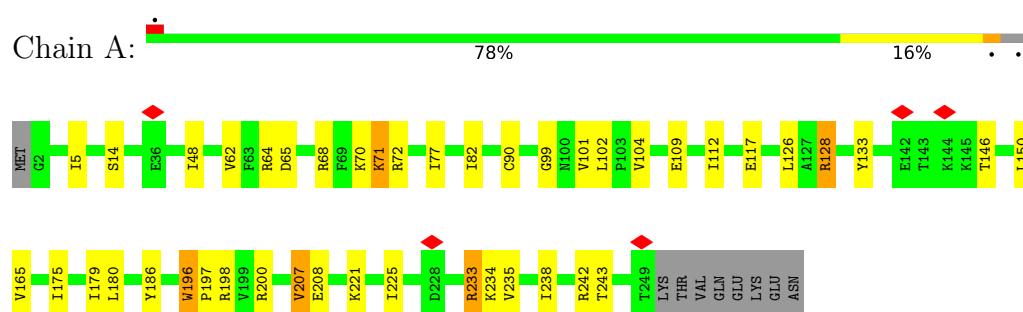


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
89	jj	1	79	57	7	15	0

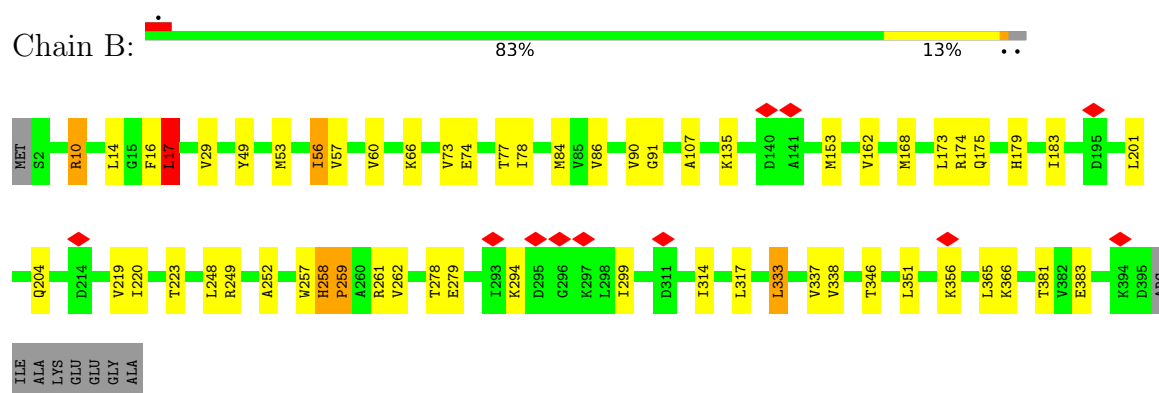
3 Residue-property plots [i](#)

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

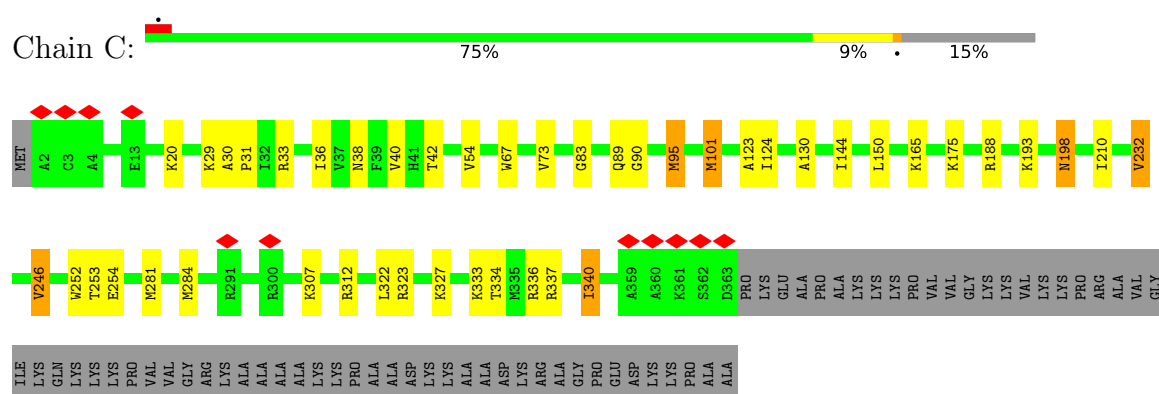
• Molecule 1: uL2



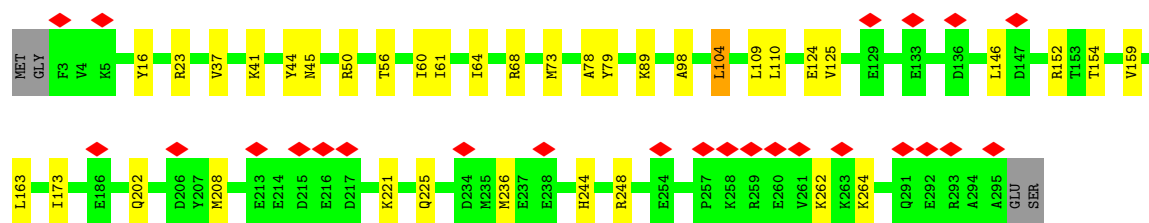
• Molecule 2: uL3



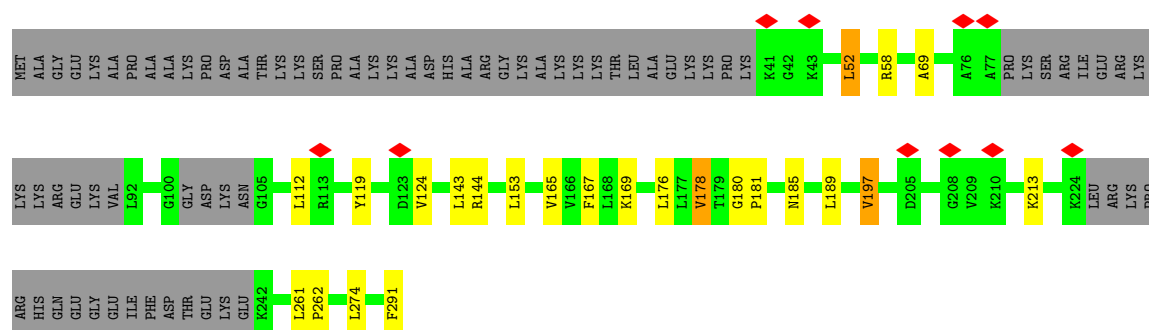
• Molecule 3: uL4



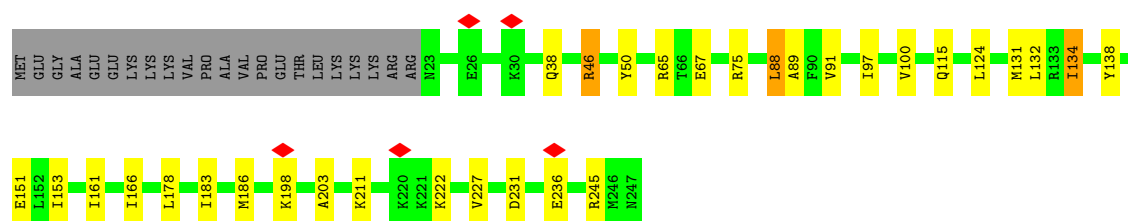
Chain D:



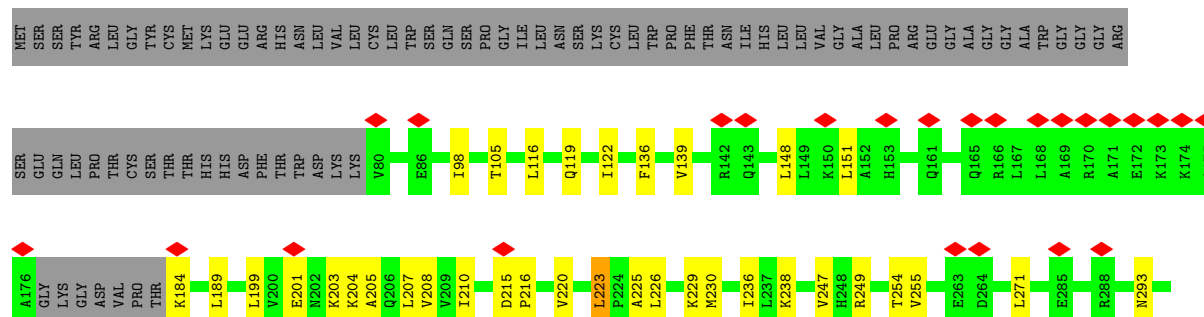
Chain E: 66% 7% 26%



Chain F: 78% 12% 9%

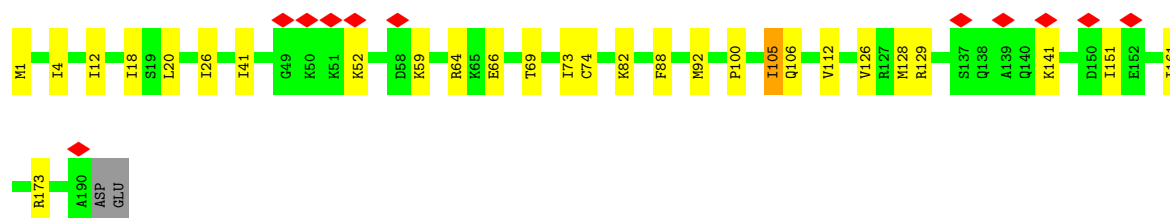
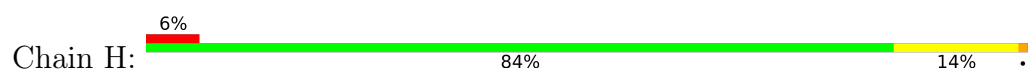


Chain G:

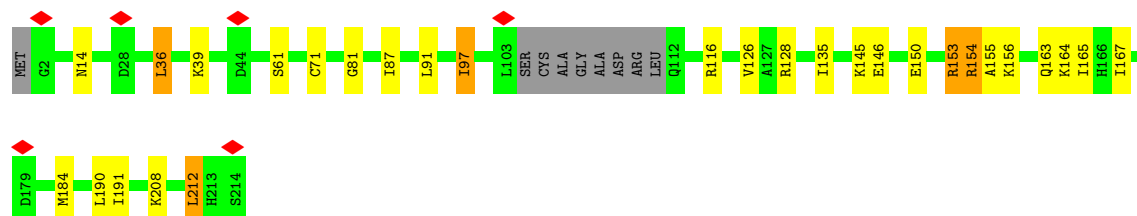
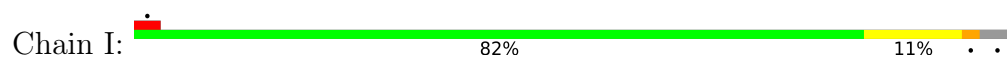




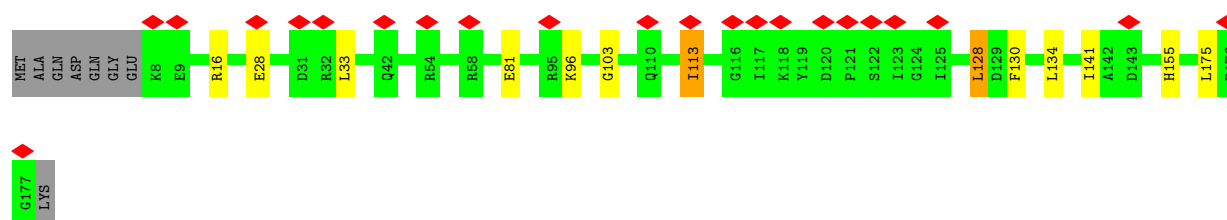
• Molecule 8: uL6



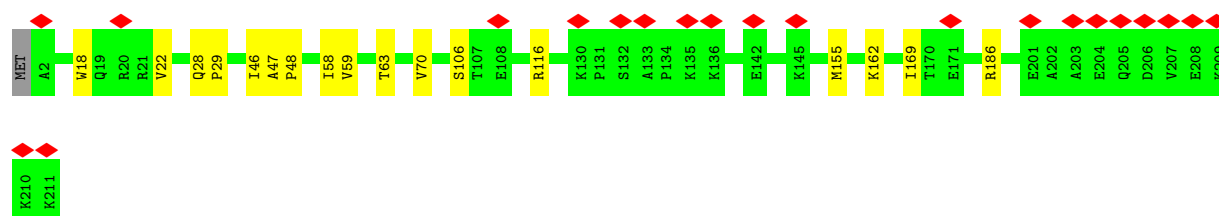
• Molecule 9: Ribosomal protein L10 (Predicted)



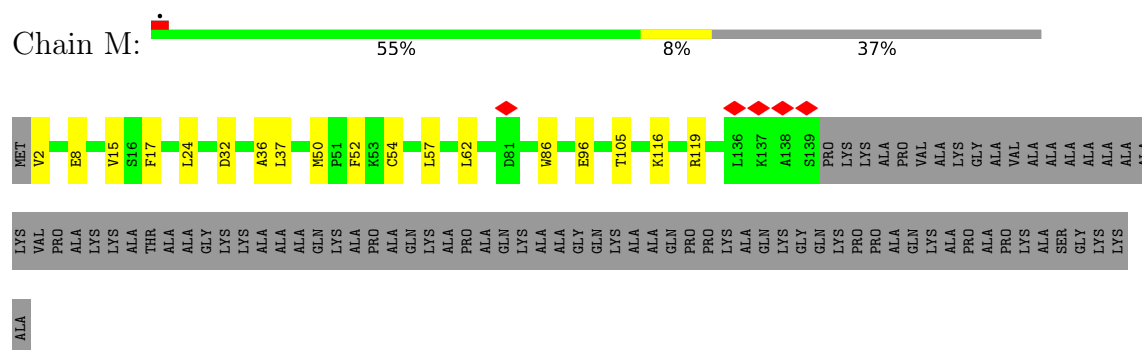
• Molecule 10: uL5

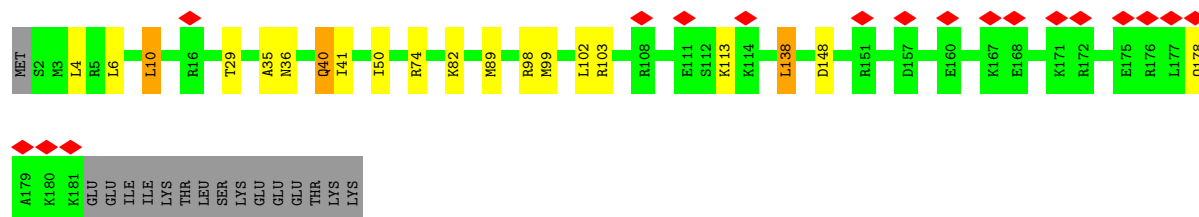


• Molecule 11: eL13

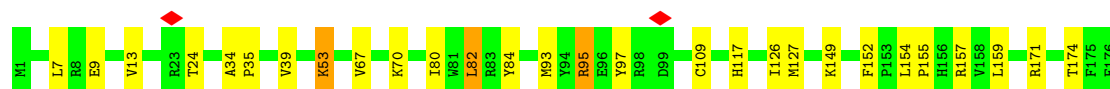
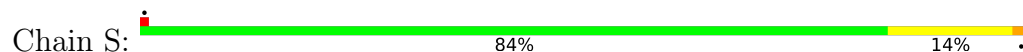


• Molecule 12: eL14

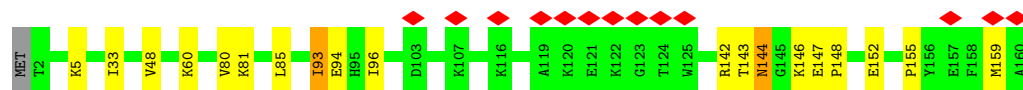
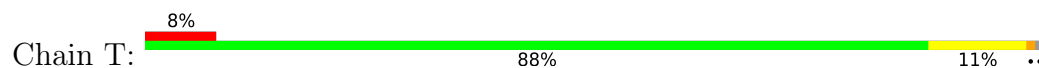




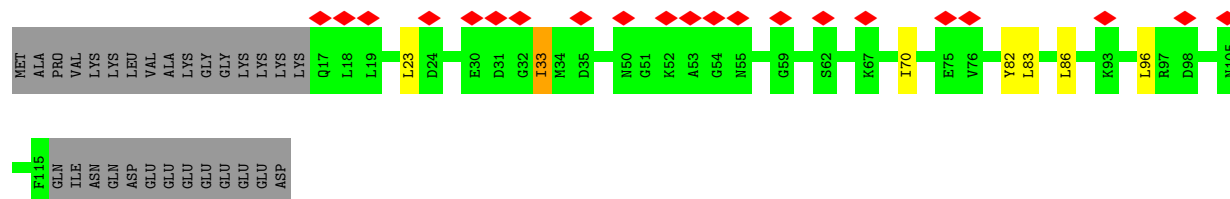
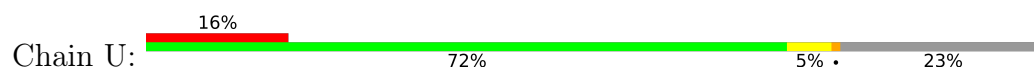
• Molecule 18: eL20



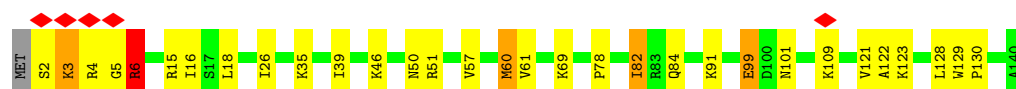
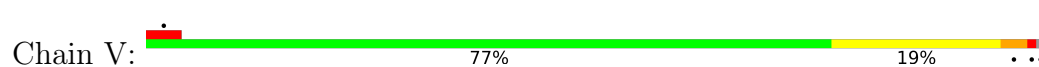
• Molecule 19: eL21



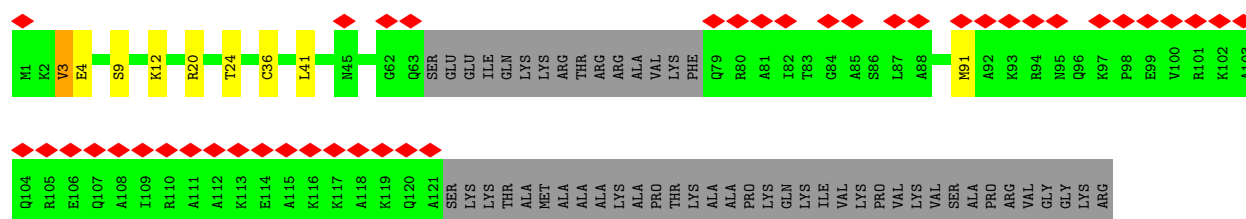
• Molecule 20: eL22

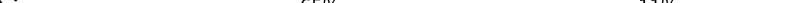


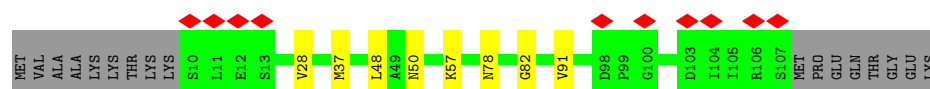
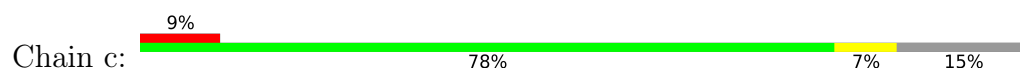
• Molecule 21: uL14



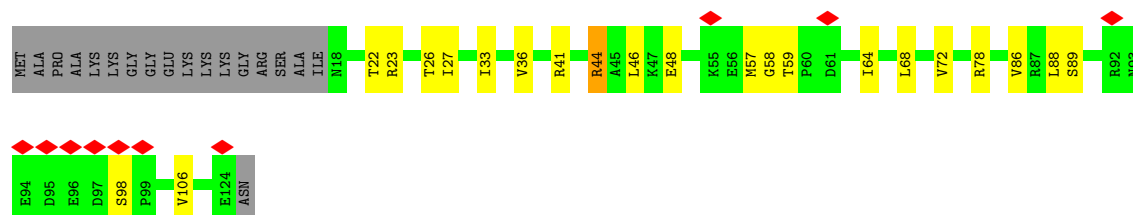
• Molecule 22: uL24



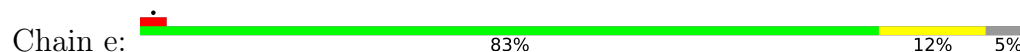
Chain X: 



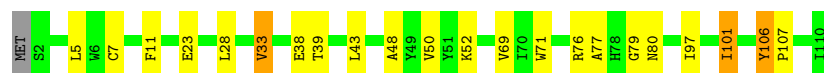
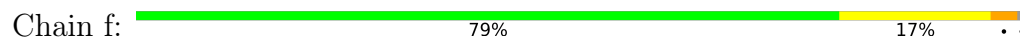
- Molecule 29: eL31



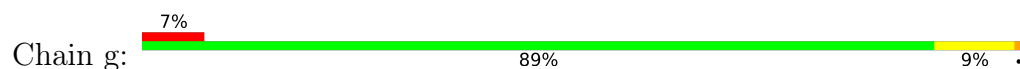
- Molecule 30: eL32



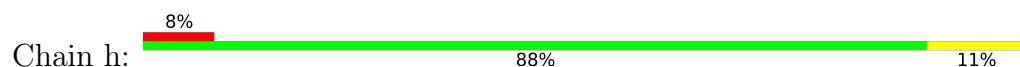
- Molecule 31: eL33



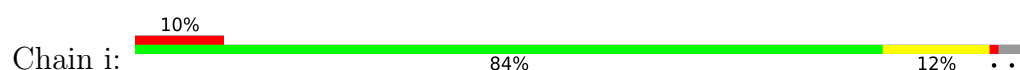
- Molecule 32: eL34

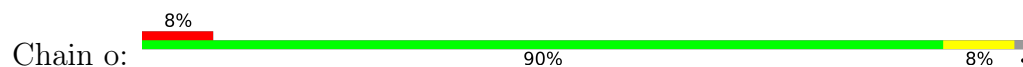


- Molecule 33: uL29



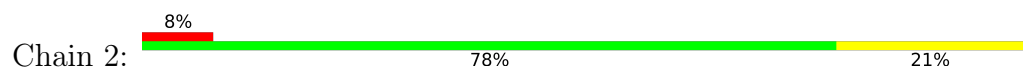
- Molecule 34: 60S ribosomal protein L36







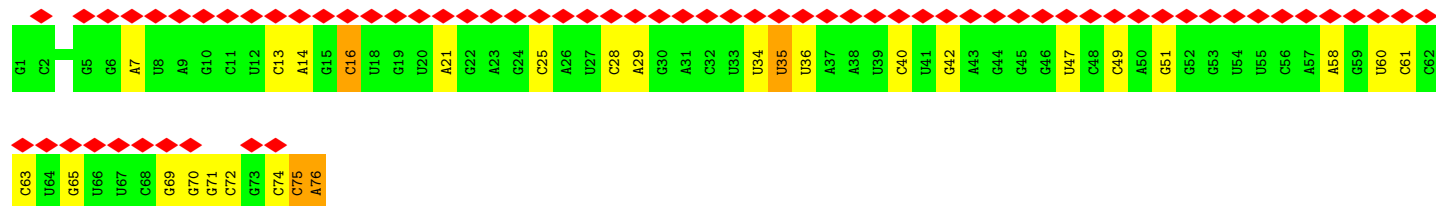
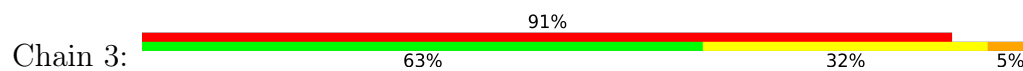
- Molecule 45: tRNA



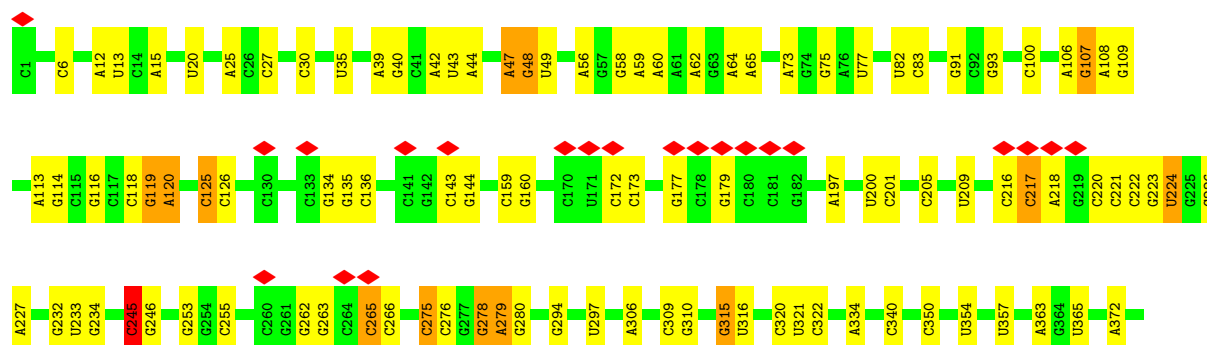
- Molecule 45: tRNA

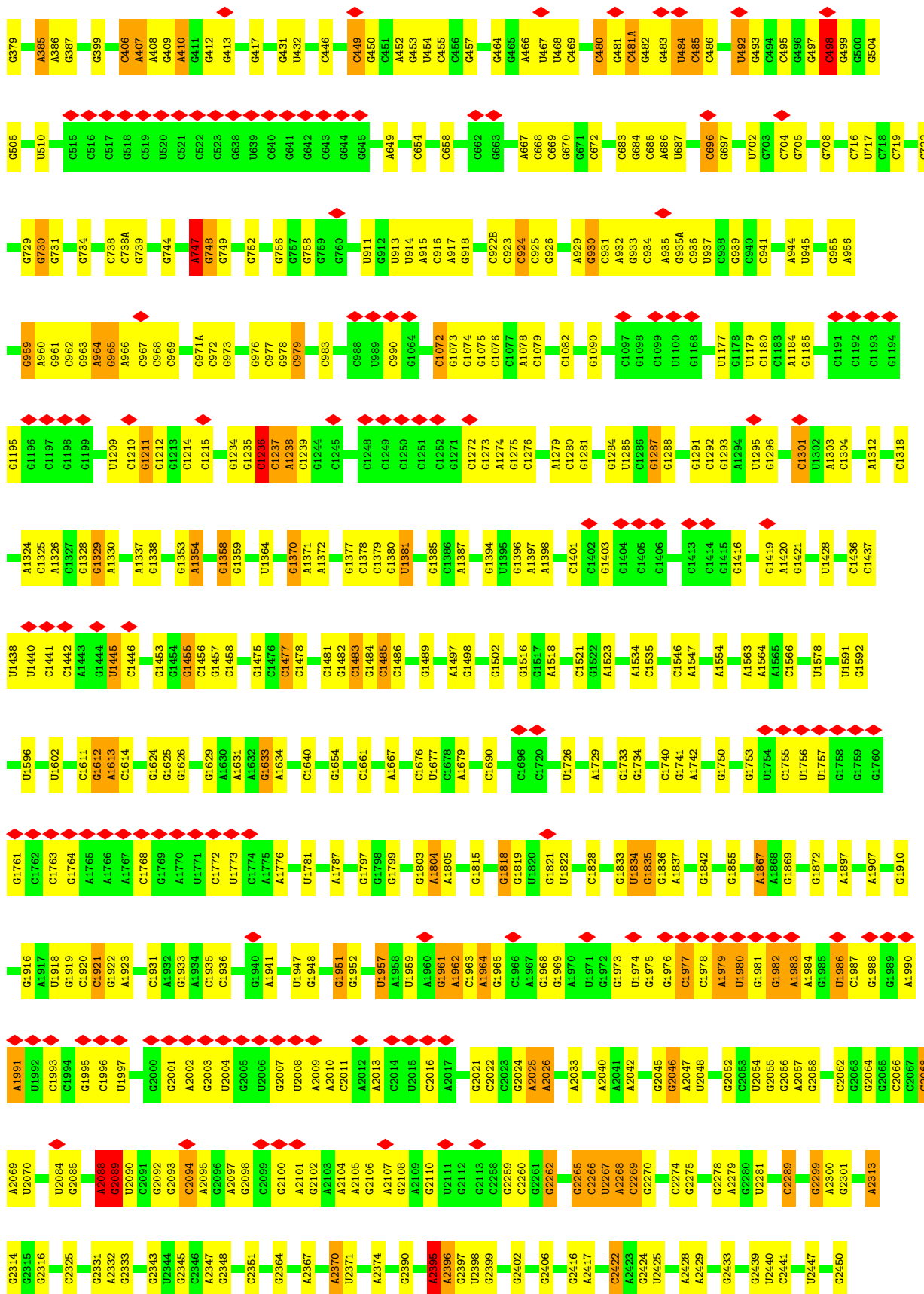


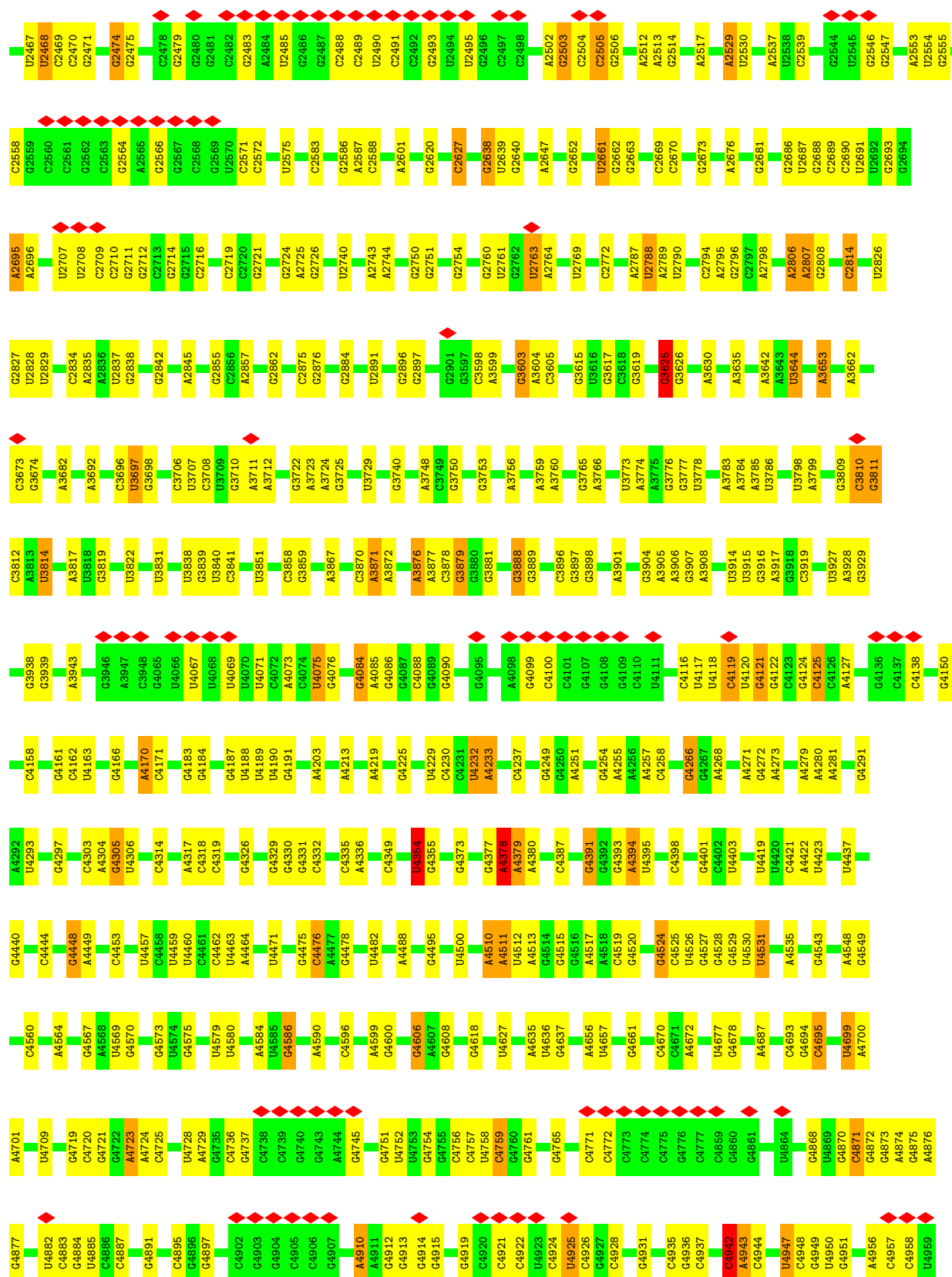
- Molecule 46: E-site tRNA



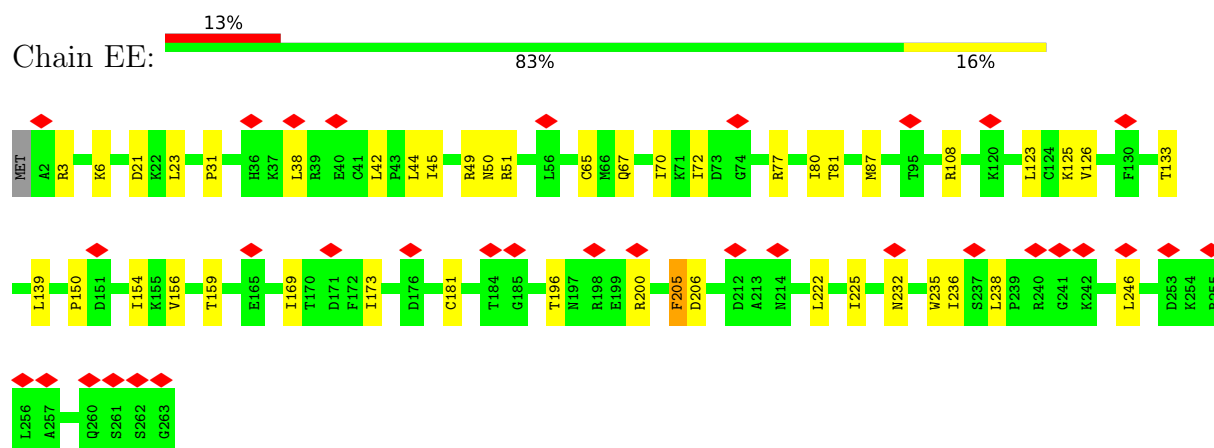
- Molecule 47: 28S ribosomal RNA



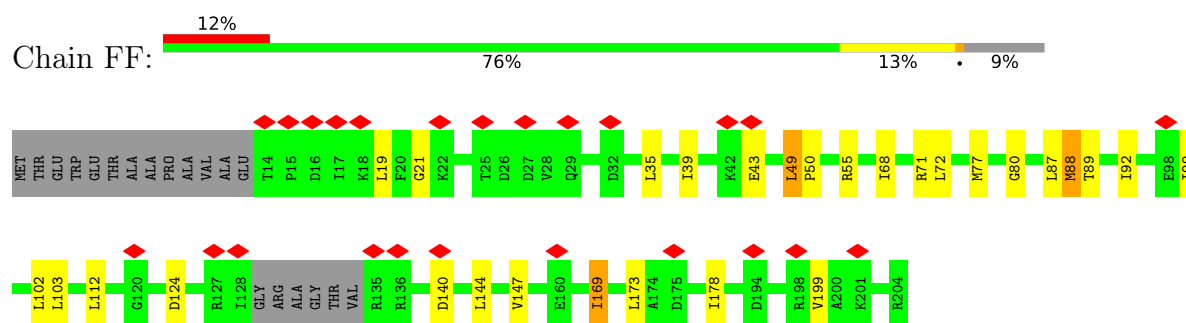




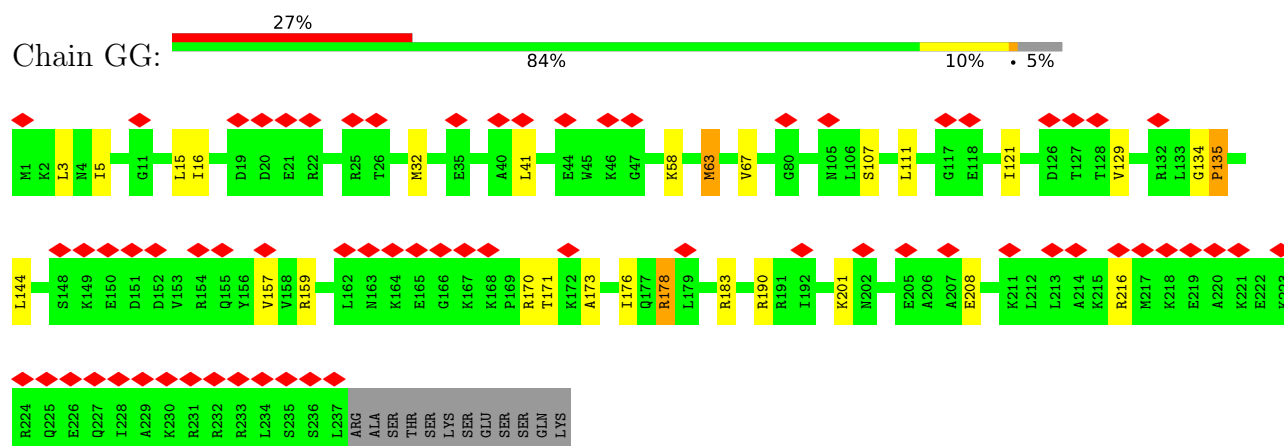
- Molecule 55: 40S ribosomal protein S4



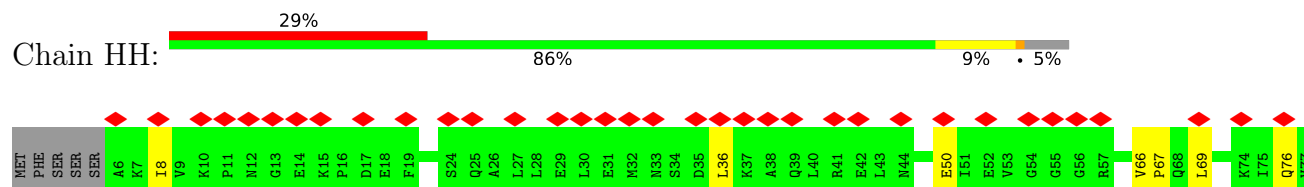
- Molecule 56: Uncharacterized protein

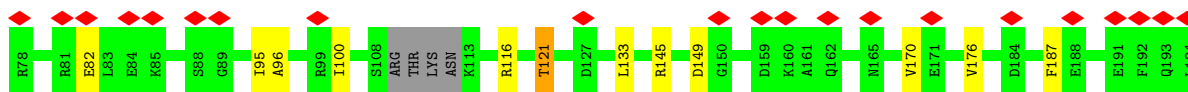


- Molecule 57: 40S ribosomal protein S6

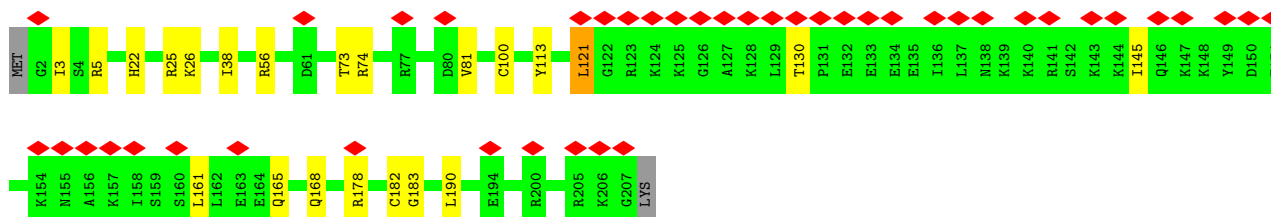
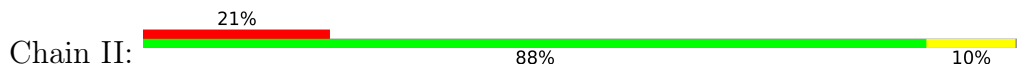


- Molecule 58: uS7

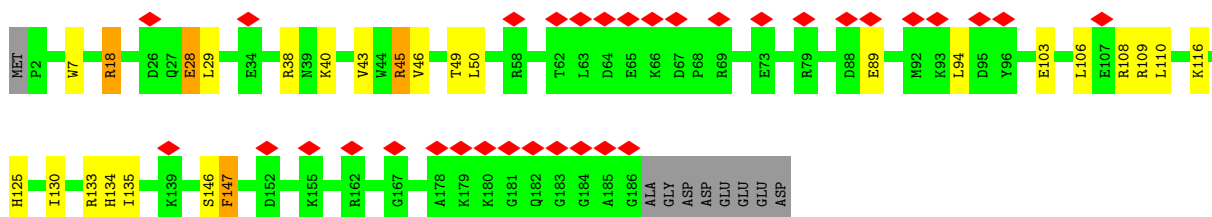
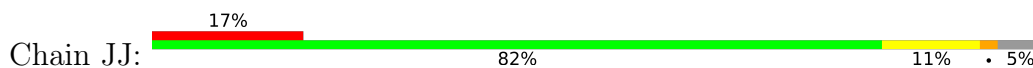




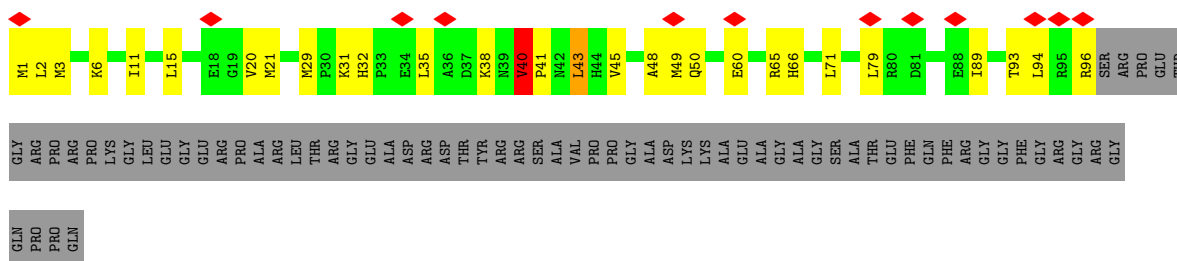
- Molecule 59: 40S ribosomal protein S8



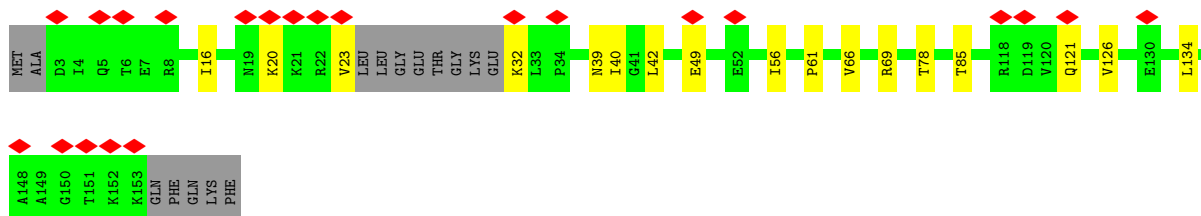
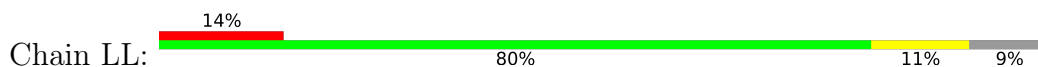
- Molecule 60: Ribosomal protein S9 (Predicted)



- Molecule 61: eS10



- Molecule 62: uS17



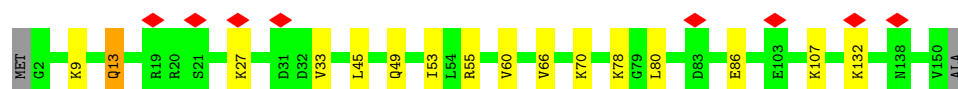
- Molecule 63: 40S ribosomal protein S12

Chain MM: 



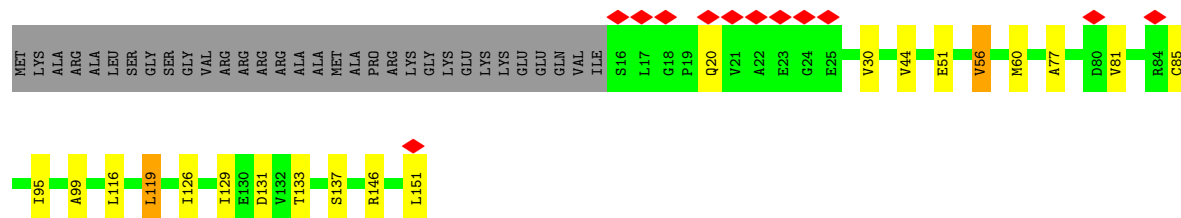
- Molecule 64: uS15

Chain NN: 



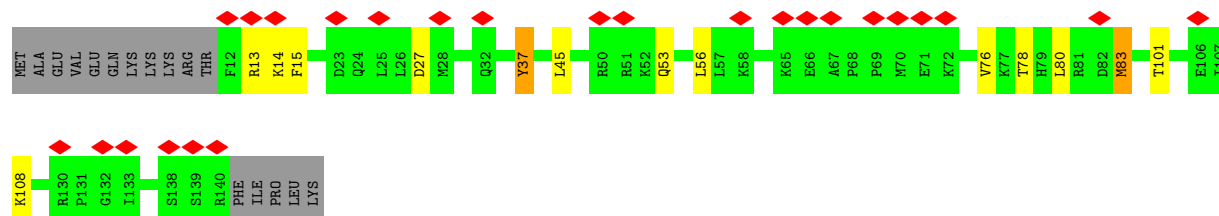
- Molecule 65: uS11

Chain OO: 



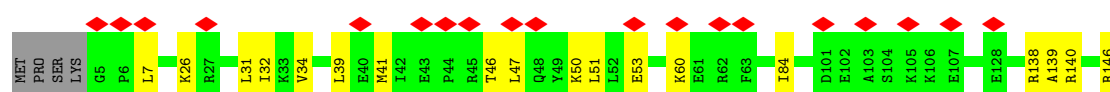
- Molecule 66: uS19

Chain PP: 

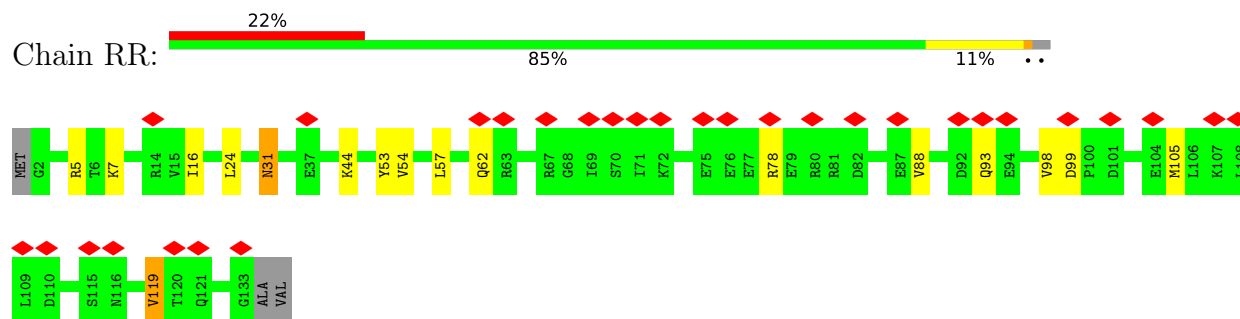


- Molecule 67: uS9

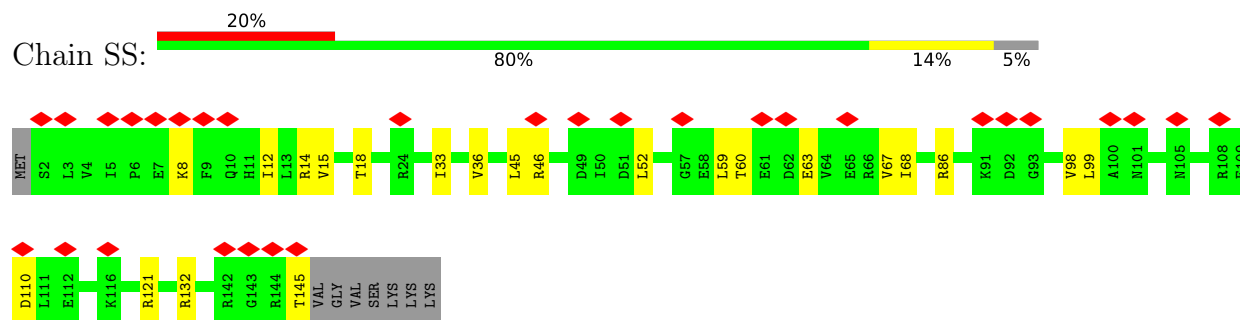
Chain QQ: 



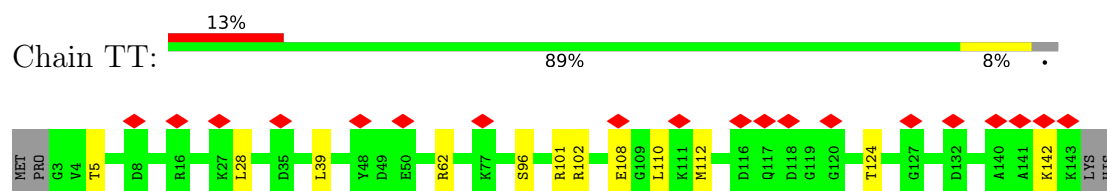
- Molecule 68: eS17



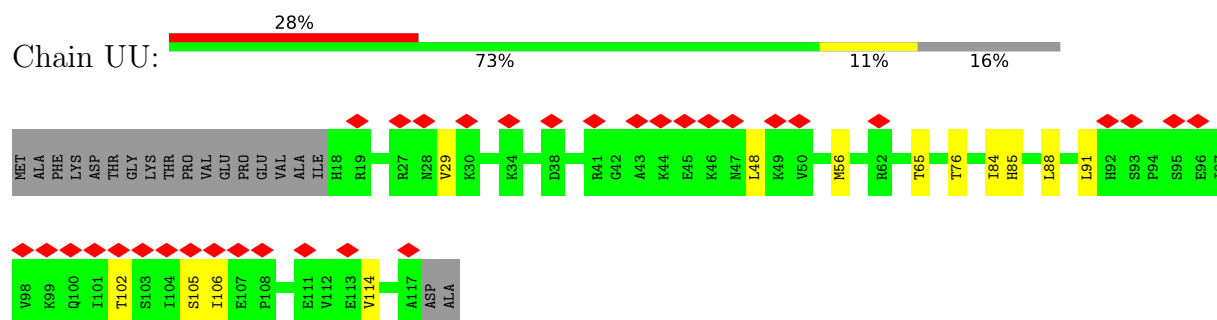
- Molecule 69: uS13



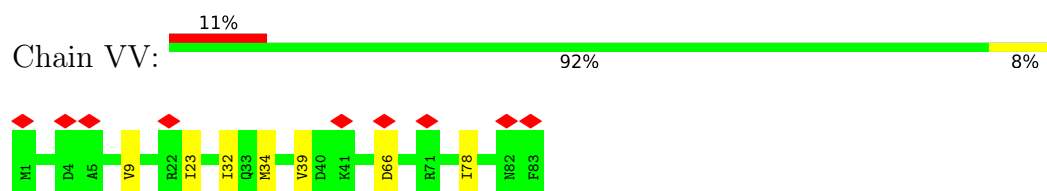
- Molecule 70: eS19



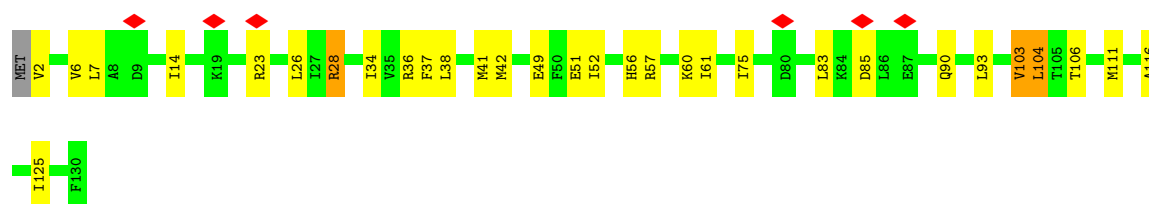
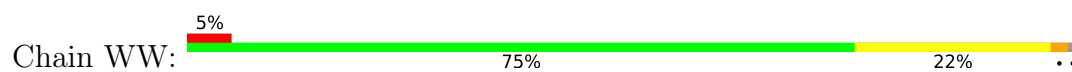
- Molecule 71: uS10



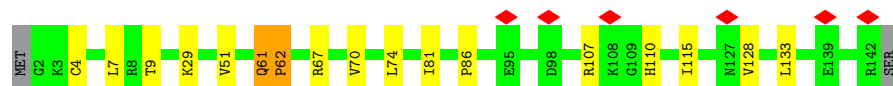
- Molecule 72: eS21



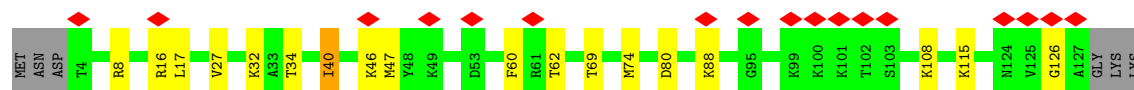
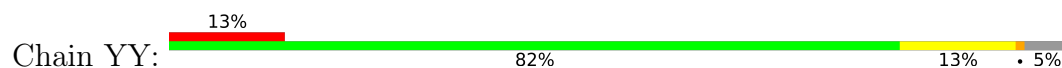
- Molecule 73: uS8



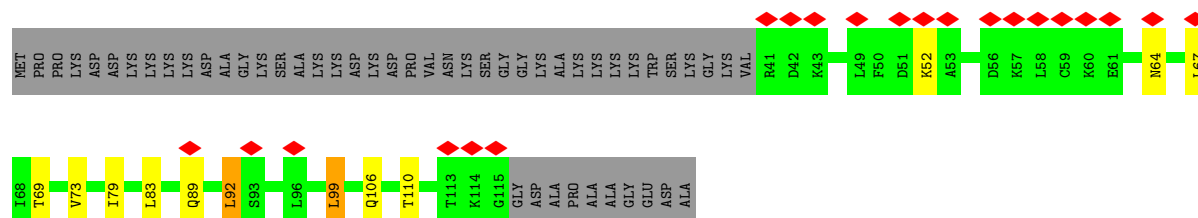
- Molecule 74: uS12



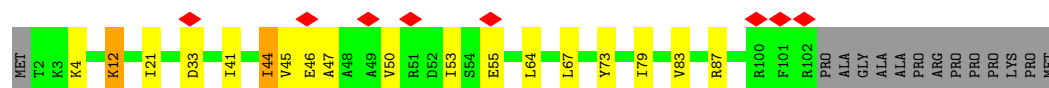
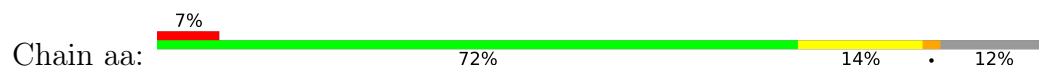
- Molecule 75: eS24



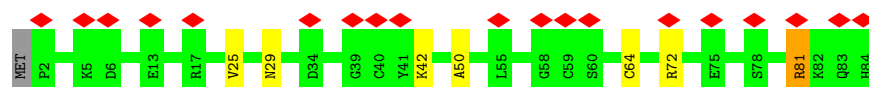
- Molecule 76: eS25



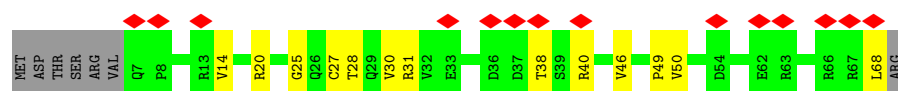
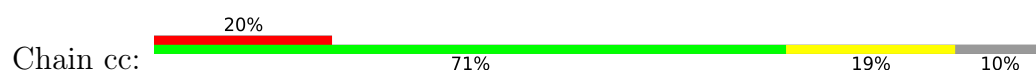
- Molecule 77: eS26



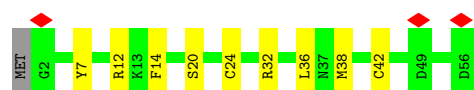
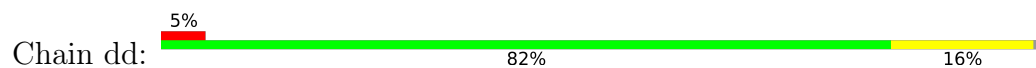
- Molecule 78: 40S ribosomal protein S27



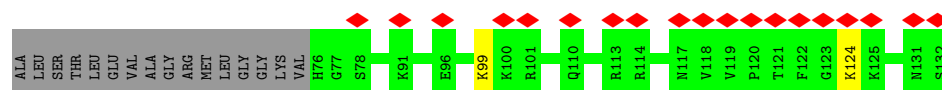
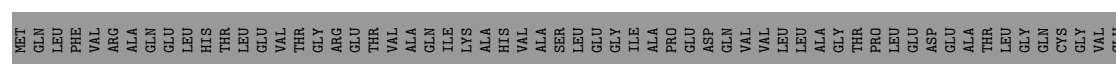
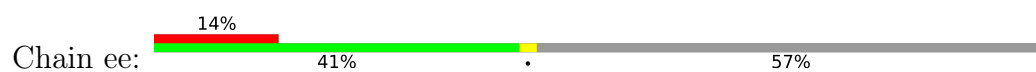
- Molecule 79: eS28



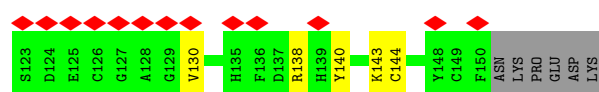
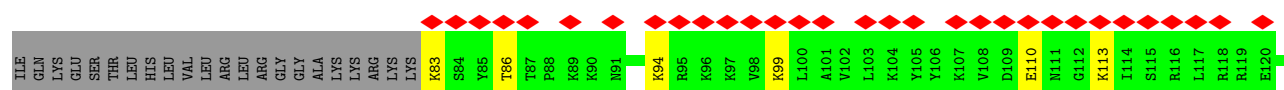
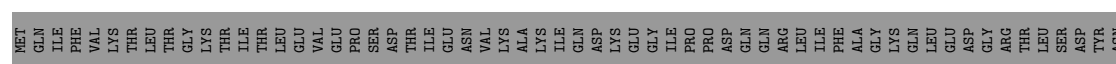
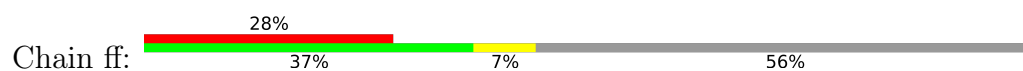
• Molecule 80: uS14



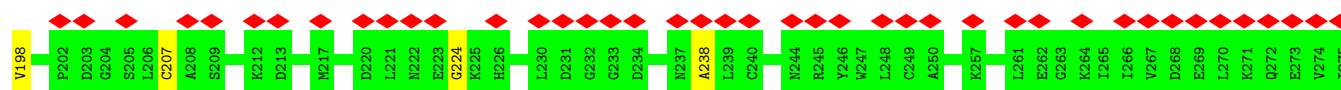
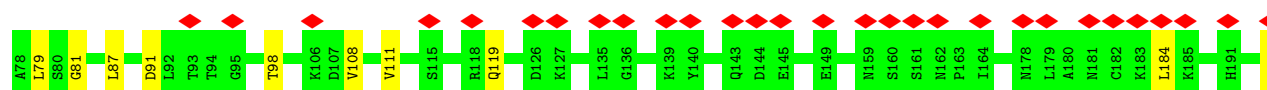
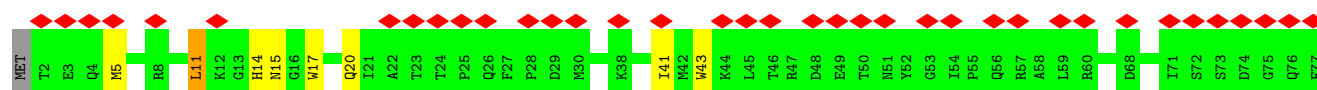
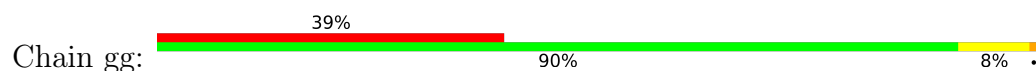
• Molecule 81: eS30

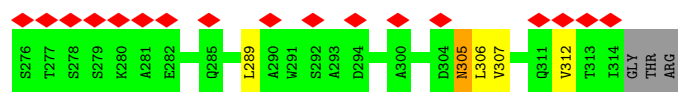


• Molecule 82: eS31



• Molecule 83: RACK1





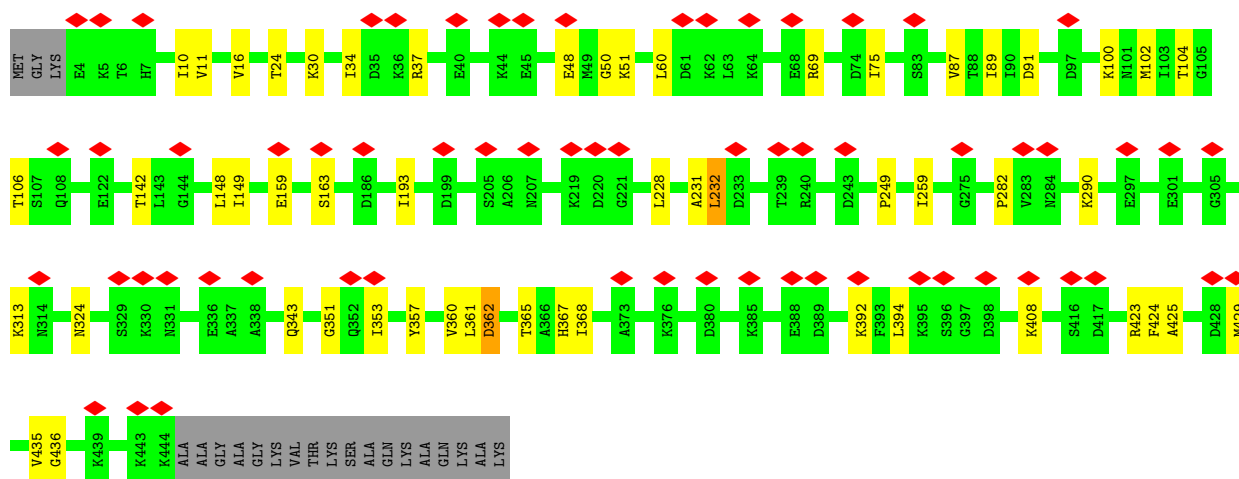
• Molecule 84: mRNA

Chain hh: 90% 10%



• Molecule 85: Elongation factor 1-alpha 1

Chain jj: 14% 84% 11% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	40347	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	134615	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.600	Depositor
Minimum map value	-0.346	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	499.19998, 499.19998, 499.19998	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 7C4, MG, SEP, GDP, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/1936	0.83	0/2596
2	B	0.49	0/3240	0.81	1/4339 (0.0%)
3	C	0.57	0/2937	0.92	2/3946 (0.1%)
4	D	0.50	0/2437	0.88	0/3264
5	E	0.49	0/1762	0.84	0/2362
6	F	0.56	0/1911	0.95	0/2549
7	G	0.57	0/1910	1.01	0/2569
8	H	0.46	0/1535	0.74	0/2063
9	I	0.47	0/1702	0.81	0/2272
10	J	0.46	0/1385	0.78	0/1852
11	L	0.57	0/1733	0.97	0/2316
12	M	0.54	0/1158	0.99	0/1547
13	N	0.56	0/1746	0.92	1/2338 (0.0%)
14	O	0.63	0/1662	1.07	1/2222 (0.0%)
15	P	0.54	0/1268	0.84	0/1700
16	Q	0.52	0/1539	0.90	0/2054
17	R	0.63	0/1524	1.07	0/2013
18	S	0.48	0/1501	0.82	0/2012
19	T	0.48	0/1326	0.78	1/1770 (0.1%)
20	U	0.47	0/823	0.72	0/1104
21	V	0.52	0/1048	0.89	1/1402 (0.1%)
22	W	0.48	0/873	0.83	0/1158
23	X	0.49	0/984	0.82	1/1323 (0.1%)
24	Y	0.45	0/1132	0.82	0/1504
25	Z	0.52	0/1130	0.84	0/1507
26	a	0.52	0/1191	0.88	2/1590 (0.1%)
27	b	0.53	0/861	0.95	0/1138
28	c	0.47	0/771	0.83	0/1034
29	d	0.53	0/903	0.79	0/1216
30	e	0.50	0/1071	0.80	0/1429
31	f	0.55	0/895	0.80	0/1198
32	g	0.46	0/916	0.81	0/1220

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	h	0.65	0/1021	1.11	0/1348
34	i	0.64	0/841	1.10	1/1112 (0.1%)
35	j	0.55	0/720	0.91	0/952
36	k	0.54	0/575	0.89	0/761
37	l	0.60	0/459	0.96	0/608
38	m	0.53	0/435	0.86	0/575
39	n	0.67	0/240	1.22	0/305
40	o	0.48	0/864	0.82	0/1140
41	p	0.55	0/718	1.02	0/953
42	r	0.60	0/1010	0.99	0/1354
43	s	0.61	0/1530	0.92	0/2064
44	t	0.69	0/1174	1.03	0/1582
45	2	0.37	0/1803	0.69	0/2801
45	ii	0.37	0/1805	0.73	2/2809 (0.1%)
46	3	0.37	0/1777	0.68	0/2763
47	5	0.39	1/84973 (0.0%)	0.75	88/132508 (0.1%)
48	7	0.37	0/2836	0.69	0/4421
49	8	0.38	0/3581	0.72	2/5577 (0.0%)
50	9	0.37	1/40502 (0.0%)	0.74	39/63100 (0.1%)
51	AA	0.47	0/1747	0.80	1/2374 (0.0%)
52	BB	0.44	0/1756	0.80	0/2350
53	CC	0.46	0/1753	0.81	0/2369
54	DD	0.51	0/1796	0.86	0/2417
55	EE	0.50	0/2118	0.79	2/2849 (0.1%)
56	FF	0.48	0/1492	0.87	0/2005
57	GG	0.49	0/1946	0.81	2/2590 (0.1%)
58	HH	0.49	0/1510	0.83	0/2022
59	II	0.47	0/1715	0.78	0/2287
60	JJ	0.49	0/1550	0.88	0/2069
61	KK	0.49	0/834	0.83	2/1125 (0.2%)
62	LL	0.46	0/1195	0.71	0/1597
63	MM	0.52	0/918	0.85	0/1233
64	NN	0.47	0/1226	0.83	0/1649
65	OO	0.50	0/1029	0.92	1/1380 (0.1%)
66	PP	0.52	0/1079	0.84	0/1441
67	QQ	0.47	0/1146	0.75	0/1534
68	RR	0.49	0/1082	0.81	0/1452
69	SS	0.50	0/1208	0.81	0/1618
70	TT	0.51	0/1115	0.89	0/1493
71	UU	0.46	0/805	0.83	0/1081
72	VV	0.46	0/643	0.80	0/860
73	WW	0.51	0/1051	0.87	1/1406 (0.1%)
74	XX	0.47	0/1116	0.82	0/1490

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
75	YY	0.48	0/1028	0.79	0/1366
76	ZZ	0.48	0/604	0.88	0/810
77	aa	0.51	0/828	0.84	1/1109 (0.1%)
78	bb	0.50	0/665	0.83	1/891 (0.1%)
79	cc	0.48	0/490	0.81	0/656
80	dd	0.49	0/470	0.84	0/623
81	ee	0.47	0/462	0.88	0/607
82	ff	0.51	0/567	0.69	0/753
83	gg	0.47	0/2493	0.70	0/3394
84	hh	0.36	0/233	0.71	0/360
85	jj	0.54	0/3442	0.75	0/4656
All	All	0.45	2/236786 (0.0%)	0.79	153/347256 (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	3
21	V	0	1
31	f	0	1
74	XX	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	5	2025	A	O3'-P	-24.45	1.24	1.61
50	9	583	A	C1'-N9	-5.03	1.40	1.48

All (153) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	2025	A	OP1-P-O3'	-30.04	17.89	108.00
47	5	2025	A	P-O3'-C3'	-14.07	99.09	120.20
50	9	1835	A	C2'-C3'-O3'	12.49	128.24	109.50
47	5	47	A	C4'-C3'-O3'	10.06	124.50	109.40
47	5	2695	A	C2'-C3'-O3'	9.71	124.07	109.50
47	5	385	A	C4'-C3'-O3'	8.87	122.70	109.40
47	5	2046	G	C2'-C3'-O3'	8.86	122.79	109.50
47	5	1370	G	C2'-C3'-O3'	8.73	122.60	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	3888	G	C2'-C3'-O3'	8.39	126.28	113.70
50	9	1016	U	C4'-C3'-O3'	8.29	121.83	109.40
50	9	1664	A	C4'-C3'-O3'	8.26	121.79	109.40
50	9	870	A	C4'-C3'-O3'	8.24	121.77	109.40
50	9	553	U	C2'-C3'-O3'	8.21	121.82	109.50
14	O	110	PRO	N-CA-C	8.19	120.69	110.70
50	9	688	U	C2'-C3'-O3'	8.07	121.61	109.50
50	9	110	U	C2'-C3'-O3'	7.91	125.57	113.70
47	5	2474	G	C2'-C3'-O3'	7.67	121.00	109.50
47	5	2468	U	C4'-C3'-O3'	7.59	120.78	109.40
47	5	4170	A	C2'-C3'-O3'	7.59	120.88	109.50
21	V	4	ARG	N-CA-C	7.58	121.97	111.74
45	ii	7	G	C2'-C3'-O3'	7.58	120.86	109.50
50	9	72	C	C4'-C3'-O3'	7.54	120.70	109.40
50	9	581	U	N1-C1'-C2'	-7.48	100.77	112.00
47	5	498	C	C4'-C3'-O3'	7.42	120.54	109.40
50	9	581	U	C4'-C3'-O3'	7.38	124.07	113.00
47	5	2089	G	C2'-C3'-O3'	7.29	120.44	109.50
47	5	48	G	C2'-C3'-O3'	7.23	120.34	109.50
47	5	4232	U	C4'-C3'-O3'	7.22	120.23	109.40
47	5	2266	C	C2'-C3'-O3'	7.14	120.21	109.50
47	5	3697	U	C2'-C3'-O3'	7.14	124.40	113.70
47	5	1477	C	C2'-C3'-O3'	7.09	124.34	113.70
47	5	4942	C	C4'-C3'-O3'	7.09	120.03	109.40
47	5	4517	A	C4'-C3'-O3'	-7.03	102.45	113.00
61	KK	40	VAL	C-N-CD	-6.96	96.44	125.00
47	5	1329	G	C4'-C3'-O3'	6.87	123.31	113.00
47	5	1834	U	C2'-C3'-O3'	6.85	119.77	109.50
50	9	1061	U	C2'-C3'-O3'	-6.83	103.46	113.70
65	OO	137	SER	N-CA-C	-6.83	103.53	110.97
47	5	2661	U	C2'-C3'-O3'	6.76	119.64	109.50
47	5	959	G	C2'-C3'-O3'	6.75	119.63	109.50
47	5	4947	U	C2'-C3'-O3'	6.72	123.78	113.70
55	EE	205	PHE	N-CA-C	6.66	119.40	110.35
47	5	406	C	C2'-C3'-O3'	6.62	123.64	113.70
50	9	1489	A	C2'-C3'-O3'	6.61	119.42	109.50
50	9	582	U	N1-C1'-C2'	-6.61	102.09	112.00
47	5	492	U	C2'-C3'-O3'	6.58	119.38	109.50
50	9	464	A	C4'-C3'-O3'	6.57	119.25	109.40
47	5	1211	G	C2'-C3'-O3'	6.56	123.54	113.70
47	5	4925	U	C2'-C3'-O3'	6.51	119.27	109.50
47	5	2068	C	C4'-C3'-O3'	6.49	119.13	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	265	C	C4'-C3'-O3'	6.37	118.95	109.40
47	5	449	C	C2'-C3'-O3'	6.37	119.05	109.50
47	5	1072	C	C2'-C3'-O3'	6.36	119.04	109.50
47	5	275	C	C2'-C3'-O3'	6.34	123.21	113.70
47	5	1485	C	C2'-C3'-O3'	6.32	118.98	109.50
47	5	1455	G	C2'-C3'-O3'	6.31	123.16	113.70
57	GG	134	GLY	CA-C-N	6.27	127.67	119.84
57	GG	134	GLY	C-N-CA	6.27	127.67	119.84
47	5	3697	U	C4'-C3'-O3'	-6.25	103.62	113.00
23	X	153	ILE	N-CA-C	6.25	117.03	110.72
50	9	561	A	C2'-C3'-O3'	6.25	123.07	113.70
47	5	4075	U	C2'-C3'-O3'	6.25	118.87	109.50
61	KK	66	HIS	N-CA-C	6.21	119.03	108.90
51	AA	191	ARG	N-CA-C	6.21	119.33	111.69
47	5	4335	C	C4'-C3'-O3'	-6.16	103.77	113.00
47	5	1804	A	C2'-C3'-O3'	6.15	118.72	109.50
47	5	1329	G	C2'-C3'-O3'	6.10	122.86	113.70
47	5	4699	U	C4'-C3'-O3'	6.10	118.55	109.40
50	9	627	U	C2'-C3'-O3'	6.09	122.83	113.70
47	5	1916	G	C4'-C3'-O3'	-6.08	103.88	113.00
50	9	752	G	C2'-C3'-O3'	6.06	118.59	109.50
47	5	696	C	C2'-C3'-O3'	6.04	118.55	109.50
50	9	1679	A	C2'-C3'-O3'	6.04	118.55	109.50
47	5	2807	A	C4'-C3'-O3'	-6.00	104.00	113.00
47	5	1358	G	C4'-C3'-O3'	5.99	118.39	109.40
50	9	1313	A	C4'-C3'-O3'	5.90	118.24	109.40
47	5	1835	G	C2'-C3'-O3'	5.89	118.34	109.50
47	5	2395	A	C2'-C3'-O3'	5.88	118.32	109.50
47	5	217	C	C4'-C3'-O3'	5.86	118.20	109.40
26	a	22	ILE	N-CA-C	-5.82	106.14	111.67
77	aa	46	GLU	N-CA-C	5.82	117.49	111.03
13	N	90	ASN	N-CA-C	5.82	117.49	111.03
47	5	480	C	C2'-C3'-O3'	5.80	122.39	113.70
47	5	930	G	C2'-C3'-O3'	5.79	122.39	113.70
49	8	94	G	C2'-C3'-O3'	5.77	118.16	109.50
47	5	1818	G	C2'-C3'-O3'	5.77	122.35	113.70
47	5	2313	A	C2'-C3'-O3'	5.75	118.13	109.50
50	9	1255	G	C2'-C3'-O3'	5.75	122.32	113.70
50	9	561	A	C3'-C2'-O2'	5.74	119.31	110.70
47	5	4448	G	C4'-C3'-O3'	5.73	121.59	113.00
47	5	1236	C	C4'-C3'-O3'	5.70	121.55	113.00
50	9	1137	U	C2'-C3'-O3'	5.70	122.24	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	3876	A	C2'-C3'-O3'	5.66	117.99	109.50
47	5	4354	U	C4'-C3'-O3'	-5.65	104.52	113.00
47	5	4394	A	C4'-C3'-O3'	5.65	117.88	109.40
50	9	24	C	C2'-C3'-O3'	5.61	122.12	113.70
3	C	232	VAL	CB-CA-C	-5.60	104.74	112.24
50	9	555	A	C2'-C3'-O3'	5.60	117.89	109.50
34	i	77	VAL	N-CA-C	5.59	117.54	112.29
50	9	160	U	C4'-C3'-O3'	5.57	117.76	109.40
49	8	124	U	C4'-C3'-O3'	5.56	117.74	109.40
47	5	3603	G	C4'-C3'-O3'	-5.55	104.67	113.00
45	ii	61	A	C4'-C3'-O3'	-5.54	104.68	113.00
47	5	4378	A	C2'-C3'-O3'	5.52	117.78	109.50
50	9	1115	U	C2'-C3'-O3'	5.49	117.73	109.50
50	9	465	A	C2'-C3'-O3'	5.48	117.73	109.50
47	5	924	C	C2'-C3'-O3'	-5.48	105.48	113.70
50	9	1637	A	C4'-C3'-O3'	5.47	117.61	109.40
50	9	980	A	C4'-C3'-O3'	-5.42	104.87	113.00
3	C	340	ILE	N-CA-C	-5.41	106.53	111.67
47	5	1396	G	C4'-C3'-O3'	-5.40	104.90	113.00
47	5	4543	G	C4'-C3'-O3'	-5.38	104.94	113.00
26	a	61	TYR	N-CA-C	5.35	118.02	111.82
50	9	582	U	C3'-C2'-O2'	5.34	118.71	110.70
50	9	532	C	C2'-C3'-O3'	5.33	121.70	113.70
47	5	2089	G	C4'-C3'-O3'	5.31	117.37	109.40
19	T	93	ILE	CB-CA-C	-5.31	105.08	112.04
47	5	1445	U	C2'-C3'-O3'	5.30	121.65	113.70
47	5	2088	A	C2'-C3'-O3'	5.29	117.44	109.50
50	9	126	G	C4'-C3'-O3'	5.28	117.32	109.40
50	9	1837	G	C2'-C3'-O3'	-5.28	105.79	113.70
47	5	3625	G	C2'-C3'-O3'	5.27	121.61	113.70
55	EE	108	ARG	N-CA-C	5.25	117.11	110.33
47	5	484	U	C4'-C3'-O3'	5.25	117.27	109.40
47	5	3619	G	C4'-C3'-O3'	-5.25	105.13	113.00
47	5	1921	C	C2'-C3'-O3'	5.24	117.36	109.50
47	5	2266	C	C4'-C3'-O3'	5.24	117.25	109.40
47	5	1428	U	C4'-C3'-O3'	-5.23	105.15	113.00
50	9	627	U	C3'-C2'-O2'	5.22	118.53	110.70
47	5	278	G	C4'-C3'-O3'	5.21	117.22	109.40
47	5	245	C	C2'-C3'-O3'	5.20	121.50	113.70
47	5	2529	A	C2'-C3'-O3'	5.20	117.30	109.50
47	5	4119	C	C3'-C2'-O2'	5.19	118.48	110.70
47	5	1287	G	C4'-C3'-O3'	5.17	117.16	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	5	1818	G	C3'-C2'-O2'	5.16	118.44	110.70
47	5	4723	A	N9-C1'-C2'	5.15	119.73	112.00
73	WW	28	ARG	N-CA-C	5.14	119.24	112.35
2	B	259	PRO	N-CA-C	-5.10	101.96	112.47
47	5	4529	G	C4'-C3'-O3'	-5.10	105.35	113.00
50	9	1395	C	C3'-C2'-O2'	5.09	118.34	110.70
50	9	627	U	C4'-C3'-O3'	-5.08	105.38	113.00
47	5	3841	C	C3'-C2'-O2'	5.07	118.31	110.70
50	9	585	C	N1-C1'-C2'	-5.06	104.41	112.00
47	5	485	C	C3'-C2'-O2'	5.05	118.28	110.70
47	5	1445	U	C3'-C2'-O2'	5.04	118.27	110.70
78	bb	50	ALA	N-CA-C	5.04	116.86	111.36
47	5	125	C	C2'-C3'-O3'	5.04	121.25	113.70
47	5	747	A	C4'-C3'-O3'	5.03	116.94	109.40
47	5	3858	C	C4'-C3'-O3'	-5.02	105.47	113.00
50	9	1353	A	C4'-C3'-O3'	-5.01	105.49	113.00
50	9	1438	A	C4'-C3'-O3'	-5.01	105.49	113.00
47	5	5049	G	C4'-C3'-O3'	5.00	116.91	109.40
47	5	4121	G	C4'-C3'-O3'	5.00	116.90	109.40

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	16	PHE	Peptide
2	B	257	TRP	Peptide
2	B	258	HIS	Peptide
21	V	6	ARG	Sidechain
74	XX	61	GLN	Peptide
31	f	106	TYR	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	30	0
2	B	3172	0	3310	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	2883	0	3053	20	0
4	D	2391	0	2424	15	0
5	E	1729	0	1887	11	0
6	F	1875	0	1995	19	0
7	G	1879	0	2027	19	0
8	H	1516	0	1597	11	0
9	I	1664	0	1712	18	0
10	J	1362	0	1399	5	0
11	L	1702	0	1820	11	0
12	M	1137	0	1211	7	0
13	N	1701	0	1749	16	0
14	O	1630	0	1778	21	0
15	P	1242	0	1274	12	0
16	Q	1515	0	1634	9	0
17	R	1508	0	1664	5	0
18	S	1462	0	1508	14	0
19	T	1298	0	1366	18	0
20	U	809	0	833	5	0
21	V	1034	0	1097	25	0
22	W	860	0	903	6	0
23	X	967	0	1040	6	0
24	Y	1115	0	1205	5	0
25	Z	1107	0	1182	7	0
26	a	1162	0	1209	8	0
27	b	848	0	920	0	0
28	c	761	0	794	2	0
29	d	888	0	930	13	0
30	e	1053	0	1147	5	0
31	f	876	0	912	8	0
32	g	906	0	1000	4	0
33	h	1013	0	1147	9	0
34	i	830	0	916	8	0
35	j	705	0	738	5	0
36	k	569	0	637	1	0
37	l	447	0	480	3	0
38	m	429	0	465	1	0
39	n	239	0	289	2	0
40	o	851	0	921	4	0
41	p	708	0	756	7	0
42	r	994	0	1051	8	0
43	s	1507	0	1564	25	0
44	t	1160	0	1218	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	2	1616	0	826	3	0
45	ii	1616	0	824	24	0
46	3	1593	0	811	5	0
47	5	75972	0	38391	272	0
48	7	2538	0	1286	5	0
49	8	3208	0	1629	4	0
50	9	36229	0	18306	121	0
51	AA	1710	0	1708	32	0
52	BB	1729	0	1803	11	0
53	CC	1716	0	1806	11	0
54	DD	1768	0	1866	12	0
55	EE	2076	0	2177	13	0
56	FF	1471	0	1522	14	0
57	GG	1923	0	2089	8	0
58	HH	1488	0	1582	7	0
59	II	1686	0	1772	7	0
60	JJ	1525	0	1640	9	0
61	KK	810	0	836	15	0
62	LL	1175	0	1249	1	0
63	MM	908	0	939	5	0
64	NN	1202	0	1289	4	0
65	OO	1016	0	1039	9	0
66	PP	1058	0	1104	4	0
67	QQ	1128	0	1195	7	0
68	RR	1068	0	1121	6	0
69	SS	1190	0	1249	4	0
70	TT	1097	0	1132	2	0
71	UU	795	0	862	5	0
72	VV	636	0	637	6	0
73	WW	1034	0	1080	15	0
74	XX	1098	0	1167	7	0
75	YY	1011	0	1083	6	0
76	ZZ	598	0	656	6	0
77	aa	814	0	864	11	0
78	bb	651	0	672	0	0
79	cc	488	0	514	7	0
80	dd	459	0	449	5	0
81	ee	457	0	502	0	0
82	ff	555	0	565	3	0
83	gg	2436	0	2393	32	0
84	hh	210	0	106	0	0
85	jj	3383	0	3431	60	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
86	5	185	0	0	0	0
86	7	6	0	0	0	0
86	8	5	0	0	0	0
86	9	69	0	0	0	0
86	B	1	0	0	0	0
86	I	1	0	0	0	0
86	P	1	0	0	0	0
86	Q	1	0	0	0	0
86	V	1	0	0	0	0
86	a	2	0	0	0	0
86	aa	1	0	0	0	0
86	g	1	0	0	0	0
86	j	1	0	0	0	0
86	jj	1	0	0	0	0
87	aa	1	0	0	0	0
87	dd	1	0	0	0	0
87	ff	1	0	0	2	0
87	g	1	0	0	1	0
87	j	1	0	0	2	0
87	m	1	0	0	0	0
87	o	1	0	0	0	0
87	p	1	0	0	0	0
88	jj	28	0	12	0	0
89	jj	79	0	0	6	0
All	All	220934	0	164939	1027	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (1027) 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)
83:gg:14:HIS:CE1	83:gg:41:ILE:HG12	1.51	1.44
83:gg:14:HIS:CE1	83:gg:41:ILE:CG1	2.00	1.43
47:5:1962:A:H2	47:5:2026:A:N3	1.15	1.38
47:5:3914:U:O4	47:5:4378:A:N1	1.62	1.32
47:5:1962:A:C2	47:5:2026:A:N3	1.97	1.32
47:5:1979:A:C2	47:5:1980:U:O2	1.84	1.28
47:5:1962:A:N1	47:5:2026:A:H1'	1.48	1.26
47:5:2367:A:N1	47:5:2788:U:O4	1.66	1.26
51:AA:189:ILE:HD11	51:AA:195:TRP:NE1	1.57	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AA:189:ILE:CD1	51:AA:195:TRP:CD1	2.28	1.17
51:AA:189:ILE:HD11	51:AA:195:TRP:CD1	1.84	1.13
43:s:6:ARG:NH2	47:5:1957:U:H3'	1.68	1.08
1:A:68:ARG:NH2	47:5:4084:G:C2	2.22	1.07
9:I:150:GLU:OE2	9:I:154:ARG:NH2	1.85	1.07
82:ff:144:CYS:SG	87:ff:200:ZN:ZN	1.44	1.06
51:AA:181:GLU:O	51:AA:185:MET:HG3	1.54	1.06
79:cc:20:ARG:NH1	79:cc:25:GLY:O	1.87	1.06
55:EE:200:ARG:HA	55:EE:206:ASP:OD2	1.56	1.05
61:KK:15:LEU:HD22	61:KK:49:MET:HE1	1.37	1.05
85:jj:249:PRO:HB2	85:jj:365:THR:HG22	1.36	1.04
50:9:1473:G:OP1	83:gg:15:ASN:ND2	1.90	1.03
19:T:142:ARG:NH1	47:5:1090:G:OP1	1.92	1.02
21:V:3:LYS:HG3	21:V:128:LEU:HD11	1.37	1.02
83:gg:14:HIS:CE1	83:gg:41:ILE:HG13	1.94	0.99
43:s:6:ARG:NH2	47:5:1957:U:O5'	1.96	0.98
21:V:130:PRO:CB	85:jj:48:GLU:OE1	2.11	0.98
85:jj:249:PRO:HB2	85:jj:365:THR:CG2	1.94	0.97
51:AA:189:ILE:HD13	51:AA:195:TRP:CD1	2.01	0.96
32:g:49:CYS:HG	87:g:201:ZN:ZN	0.64	0.95
21:V:6:ARG:HH21	21:V:6:ARG:HG3	1.32	0.94
50:9:583:A:H2'	50:9:584:A:H5'	1.49	0.94
47:5:1962:A:N1	47:5:2026:A:C1'	2.30	0.94
1:A:68:ARG:HH21	47:5:4084:G:N2	1.64	0.94
50:9:568:C:N4	50:9:582:U:O2	2.01	0.94
47:5:1979:A:C2	47:5:1980:U:C2	2.56	0.94
50:9:1473:G:P	83:gg:15:ASN:ND2	2.42	0.92
21:V:130:PRO:HB2	85:jj:48:GLU:OE1	1.69	0.92
43:s:6:ARG:HH22	47:5:1957:U:P	1.92	0.92
45:ii:57:C:H2'	45:ii:57:C:O2	1.70	0.91
9:I:154:ARG:HG2	9:I:154:ARG:HH21	1.36	0.91
47:5:1979:A:N1	47:5:1980:U:O2	2.03	0.90
82:ff:144:CYS:HG	87:ff:200:ZN:ZN	0.59	0.90
45:ii:68:G:OP1	85:jj:408:LYS:NZ	2.05	0.89
83:gg:14:HIS:CE1	83:gg:41:ILE:CB	2.54	0.89
47:5:1981:G:C6	45:ii:57:C:C4	2.60	0.89
21:V:6:ARG:O	47:5:4596:C:OP1	1.90	0.88
43:s:34:ASN:CB	47:5:1968:G:O3'	2.20	0.88
47:5:1981:G:O6	45:ii:57:C:N4	2.06	0.88
44:t:16:ARG:HD3	47:5:1975:G:N2	1.89	0.87
21:V:3:LYS:CG	21:V:128:LEU:HD11	2.03	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:34:ASN:HB2	47:5:1968:G:O3'	1.74	0.87
43:s:34:ASN:HA	47:5:1968:G:O2'	1.75	0.86
34:i:72:PHE:O	34:i:76:ARG:HG2	1.77	0.84
19:T:147:GLU:HB3	19:T:148:PRO:CD	2.06	0.84
44:t:16:ARG:HB2	47:5:1975:G:N1	1.92	0.84
50:9:584:A:C6	50:9:585:C:C4	2.67	0.82
50:9:1473:G:P	83:gg:15:ASN:HD21	2.02	0.82
43:s:34:ASN:HB2	47:5:1969:G:P	2.20	0.82
47:5:1962:A:C2	47:5:2026:A:H1'	2.14	0.81
50:9:566:U:O2	50:9:584:A:N1	2.13	0.81
51:AA:185:MET:HE1	72:VV:39:VAL:HG21	1.62	0.81
47:5:2395:A:O2'	47:5:2806:A:H1'	1.81	0.81
43:s:84:GLY:C	47:5:2021:G:H4'	2.06	0.80
83:gg:14:HIS:NE2	83:gg:41:ILE:HB	1.97	0.79
47:5:1982:G:P	47:5:1982:G:H3'	2.23	0.79
47:5:1981:G:C6	45:ii:57:C:N4	2.51	0.79
52:BB:66:VAL:HG22	52:BB:87:ILE:HG22	1.63	0.78
47:5:2367:A:N1	47:5:2788:U:C4	2.51	0.78
50:9:582:U:O2'	50:9:583:A:O4'	2.01	0.78
19:T:147:GLU:HB3	19:T:148:PRO:HD2	1.64	0.78
83:gg:14:HIS:HE1	83:gg:41:ILE:CG1	1.67	0.78
44:t:121:LEU:HD13	47:5:1973:G:H5''	1.66	0.77
66:PP:56:LEU:HD13	66:PP:78:THR:HG21	1.67	0.77
47:5:1963:C:C5	47:5:1964:A:H2	2.01	0.77
50:9:584:A:N6	50:9:585:C:N4	2.33	0.77
83:gg:14:HIS:HE1	83:gg:41:ILE:HG12	0.98	0.77
19:T:146:LYS:HD2	19:T:146:LYS:O	1.84	0.77
44:t:100:HIS:NE2	47:5:1978:C:OP1	2.18	0.77
50:9:583:A:C2'	50:9:584:A:H5'	2.13	0.76
19:T:80:VAL:HG21	19:T:85:LEU:HD12	1.67	0.76
47:5:1981:G:N1	45:ii:57:C:C4	2.53	0.76
56:FF:99:ILE:HG23	76:ZZ:67:LEU:HD21	1.67	0.76
47:5:1982:G:H2'	47:5:1983:A:H5''	1.67	0.76
44:t:16:ARG:HD2	47:5:1975:G:C2	2.21	0.75
83:gg:11:LEU:N	83:gg:11:LEU:HD12	2.02	0.75
21:V:6:ARG:HH21	21:V:6:ARG:CG	1.99	0.75
47:5:3914:U:C4	47:5:4378:A:N1	2.54	0.74
83:gg:11:LEU:O	83:gg:306:LEU:HD23	1.87	0.74
83:gg:14:HIS:CE1	83:gg:41:ILE:HB	2.21	0.74
43:s:6:ARG:CZ	47:5:1957:U:H3'	2.17	0.73
51:AA:185:MET:CE	72:VV:39:VAL:HG21	2.17	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:9:584:A:N6	50:9:585:C:C4	2.57	0.73
51:AA:189:ILE:CD1	51:AA:195:TRP:NE1	2.42	0.73
44:t:16:ARG:CD	47:5:1975:G:N2	2.52	0.73
25:Z:53:VAL:HG21	25:Z:62:ILE:HG23	1.71	0.73
47:5:3914:U:H3	47:5:4378:A:N6	1.86	0.73
6:F:153:ILE:HG22	6:F:186:MET:HE3	1.69	0.72
43:s:34:ASN:HB2	47:5:1969:G:OP1	1.89	0.72
50:9:1091:C:HO2'	73:WW:2:VAL:N	1.86	0.72
75:YY:34:THR:HG23	75:YY:69:THR:HG21	1.69	0.72
21:V:6:ARG:HG3	21:V:6:ARG:NH2	2.05	0.72
85:jj:142:THR:HG23	85:jj:435:VAL:HG13	1.72	0.71
50:9:561:A:O2'	60:JJ:134:HIS:NE2	2.24	0.71
85:jj:435:VAL:HG12	89:jj:503:7C4:C42	2.21	0.70
85:jj:367:HIS:O	85:jj:368:ILE:HG13	1.91	0.70
54:DD:70:THR:HG22	54:DD:86:LEU:HD13	1.72	0.70
9:I:191:ILE:HD11	9:I:212:LEU:HD11	1.73	0.69
14:O:27:VAL:HG12	14:O:98:ALA:HB1	1.73	0.69
43:s:6:ARG:HH21	47:5:1957:U:H3'	1.55	0.69
47:5:4579:U:H2'	47:5:4580:U:C6	2.28	0.69
47:5:1979:A:O2'	47:5:1980:U:OP1	2.11	0.68
47:5:2370:A:N1	47:5:2390:G:O2'	2.26	0.68
50:9:585:C:O2'	50:9:586:G:H5'	1.92	0.68
43:s:6:ARG:NH2	47:5:1957:U:P	2.66	0.68
47:5:2367:A:N6	47:5:2788:U:N3	2.42	0.68
53:CC:209:VAL:HG21	53:CC:233:LEU:HD13	1.76	0.68
45:ii:52:C:O3'	85:jj:357:TYR:HA	1.93	0.68
21:V:130:PRO:CG	85:jj:48:GLU:OE1	2.41	0.68
47:5:1962:A:N1	47:5:2026:A:O2'	2.25	0.68
47:5:1982:G:H2'	47:5:1983:A:C5'	2.24	0.67
45:ii:52:C:O2'	85:jj:357:TYR:HB2	1.94	0.67
47:5:3914:U:O4	47:5:4378:A:C2	2.47	0.67
50:9:1472:C:O3'	83:gg:15:ASN:ND2	2.26	0.67
50:9:464:A:C8	85:jj:37:ARG:NH2	2.63	0.67
50:9:566:U:O2	50:9:584:A:C2	2.47	0.67
1:A:180:LEU:HD11	41:p:26:VAL:HG21	1.76	0.67
11:L:116:ARG:NH1	11:L:155:MET:O	2.27	0.67
43:s:6:ARG:NH2	47:5:1957:U:C3'	2.53	0.67
54:DD:16:ILE:HD11	80:dd:36:LEU:HD23	1.77	0.66
65:OO:95:ILE:HD11	65:OO:126:ILE:HD12	1.77	0.66
50:9:980:A:H2'	50:9:981:A:C8	2.31	0.66
52:BB:38:MET:HE3	52:BB:185:VAL:HG11	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:1963:C:C5	47:5:1964:A:C2	2.84	0.66
63:MM:22:LEU:HD11	63:MM:89:VAL:HA	1.78	0.65
51:AA:60:LEU:HD13	51:AA:159:ILE:HD11	1.78	0.65
19:T:142:ARG:NH1	19:T:142:ARG:HB3	2.12	0.65
1:A:68:ARG:NH2	47:5:4084:G:N3	2.43	0.65
47:5:3914:U:N3	47:5:4378:A:N6	2.42	0.65
43:s:59:THR:HG21	47:5:1961:G:C8	2.32	0.65
37:l:2:SER:N	47:5:2406:G:N7	2.45	0.65
9:I:154:ARG:NH2	9:I:154:ARG:HG2	2.12	0.64
17:R:102:LEU:HD22	17:R:138:LEU:HD12	1.78	0.64
47:5:5047:C:O2'	47:5:5050:C:OP2	2.15	0.64
83:gg:87:LEU:HD21	83:gg:108:VAL:HG11	1.80	0.64
35:j:22:CYS:SG	87:j:101:ZN:ZN	1.84	0.64
85:jj:193:ILE:HD13	85:jj:228:LEU:HD12	1.79	0.64
44:t:16:ARG:CD	47:5:1975:G:C2	2.80	0.64
47:5:1982:G:C8	47:5:1983:A:C8	2.85	0.64
85:jj:362:ASP:OD1	85:jj:362:ASP:N	2.30	0.64
47:5:1986:U:C4	47:5:2013:A:N6	2.66	0.64
2:B:84:MET:HE1	2:B:183:ILE:HD11	1.80	0.63
19:T:144:ASN:ND2	19:T:144:ASN:H	1.94	0.63
9:I:97:ILE:HD13	9:I:126:VAL:HG11	1.80	0.63
44:t:32:ILE:HD13	44:t:42:VAL:HG11	1.80	0.63
47:5:4695:C:OP2	47:5:4695:C:H6	1.82	0.63
51:AA:189:ILE:HD11	51:AA:195:TRP:HE1	1.62	0.63
15:P:114:ILE:HD11	15:P:117:ILE:HB	1.81	0.63
40:o:4:VAL:O	40:o:94:GLY:N	2.31	0.63
53:CC:195:LEU:HD23	53:CC:224:THR:HG22	1.80	0.63
47:5:747:A:O2'	47:5:748:G:H3'	1.99	0.62
47:5:4606:G:H5''	85:jj:16:VAL:HG11	1.82	0.62
2:B:261:ARG:HB2	14:O:64:THR:HG21	1.82	0.62
18:S:95:ARG:NH2	47:5:1951:G:O2'	2.32	0.61
18:S:82:LEU:HD13	18:S:126:ILE:HD13	1.82	0.61
9:I:154:ARG:HH21	9:I:154:ARG:CG	2.12	0.61
1:A:68:ARG:CZ	47:5:4084:G:C2	2.84	0.61
18:S:34:ALA:HB1	18:S:39:VAL:HG23	1.82	0.61
14:O:54:TYR:CD1	14:O:145:VAL:HG21	2.35	0.61
4:D:68:ARG:HG3	4:D:73:MET:HE2	1.82	0.61
47:5:4476:C:O2'	47:5:4478:G:OP2	2.18	0.61
85:jj:361:LEU:HD11	85:jj:424:PHE:CD1	2.36	0.61
47:5:1962:A:N1	47:5:2026:A:C2'	2.63	0.61
50:9:945:U:H2'	50:9:946:U:C6	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:ARG:NE	47:5:4084:G:N1	2.48	0.60
45:ii:52:C:H4'	85:jj:357:TYR:HA	1.82	0.60
6:F:227:VAL:HA	18:S:39:VAL:HG12	1.83	0.60
50:9:501:C:H2'	50:9:501:C:O2	2.02	0.60
45:ii:57:C:O2	45:ii:57:C:C2'	2.43	0.60
47:5:4608:G:OP1	85:jj:69:ARG:NE	2.34	0.60
85:jj:249:PRO:CB	85:jj:365:THR:HG22	2.23	0.60
47:5:1963:C:C4	47:5:1964:A:C2	2.90	0.60
15:P:95:LEU:HD12	15:P:148:MET:HE1	1.83	0.59
47:5:1979:A:H2'	47:5:1980:U:O4'	2.03	0.59
47:5:1981:G:N1	45:ii:57:C:C5	2.70	0.59
61:KK:31:LYS:HA	61:KK:40:VAL:O	2.02	0.59
29:d:64:ILE:HG13	29:d:68:LEU:HD23	1.84	0.59
14:O:27:VAL:CG1	14:O:98:ALA:HB1	2.31	0.59
52:BB:69:VAL:HG11	52:BB:74:LEU:HD13	1.83	0.59
50:9:1611:G:OP2	69:SS:121:ARG:NH1	2.36	0.59
21:V:130:PRO:CB	85:jj:48:GLU:CD	2.76	0.59
44:t:16:ARG:CB	47:5:1975:G:N1	2.62	0.59
5:E:165:VAL:HG11	5:E:178:VAL:HG13	1.83	0.59
18:S:84:TYR:CE1	18:S:93:MET:HE3	2.38	0.59
34:i:69:ALA:O	34:i:73:ILE:HG13	2.02	0.59
12:M:24:LEU:HD11	12:M:86:TRP:CG	2.38	0.58
50:9:1473:G:P	83:gg:15:ASN:HD22	2.26	0.58
26:a:61:TYR:N	47:5:4354:U:O4	2.36	0.58
47:5:3896:C:O2	47:5:4564:A:N1	2.36	0.58
53:CC:251:LEU:HD23	72:VV:23:ILE:HG23	1.85	0.58
47:5:4942:C:H4'	47:5:4943:A:OP1	2.03	0.58
74:XX:51:VAL:HG13	74:XX:70:VAL:HG13	1.85	0.58
1:A:101:VAL:HB	1:A:165:VAL:HG12	1.84	0.58
21:V:5:GLY:O	21:V:6:ARG:C	2.47	0.58
47:5:1979:A:N3	47:5:1980:U:C2	2.72	0.58
47:5:1982:G:N7	47:5:1983:A:N7	2.52	0.58
19:T:80:VAL:CG2	19:T:85:LEU:HD12	2.34	0.57
50:9:1274:G:N7	61:KK:43:LEU:HD13	2.19	0.57
55:EE:31:PRO:HG2	55:EE:38:LEU:HD12	1.86	0.57
8:H:4:ILE:HD11	18:S:152:PHE:CD2	2.39	0.57
45:ii:66:G:H4'	85:jj:360:VAL:CG1	2.34	0.57
1:A:70:LYS:NZ	47:5:2503:G:N7	2.51	0.57
85:jj:423:ARG:NH1	89:jj:503:7C4:O16	2.37	0.57
61:KK:35:LEU:HD11	61:KK:38:LYS:HD3	1.87	0.57
77:aa:45:VAL:HG11	77:aa:53:ILE:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:EE:139:LEU:HD11	55:EE:154:ILE:HG21	1.87	0.57
51:AA:192:GLU:N	51:AA:192:GLU:OE2	2.37	0.57
23:X:146:ALA:O	23:X:149:VAL:HG12	2.05	0.57
47:5:3928:A:H2'	47:5:3929:G:O4'	2.05	0.57
2:B:14:LEU:HD23	2:B:17:LEU:HD23	1.85	0.57
31:f:48:ALA:HB2	31:f:71:TRP:CZ3	2.38	0.57
45:2:38:C:O2'	50:9:1058:A:OP1	2.22	0.57
77:aa:73:TYR:CE2	77:aa:83:VAL:HG21	2.40	0.57
83:gg:14:HIS:O	83:gg:305:ASN:HB3	2.04	0.57
85:jj:343:GLN:NE2	89:jj:503:7C4:C66	2.67	0.57
19:T:143:THR:HG23	19:T:143:THR:O	2.04	0.57
47:5:978:G:O2'	47:5:979:C:OP2	2.20	0.56
77:aa:44:ILE:HD12	77:aa:45:VAL:HG13	1.87	0.56
47:5:1979:A:C4	47:5:1980:U:C2	2.92	0.56
47:5:4723:A:H2'	47:5:4724:A:C8	2.40	0.56
44:t:139:VAL:O	47:5:1977:C:O2'	2.23	0.56
21:V:130:PRO:HB3	85:jj:48:GLU:CD	2.31	0.56
46:3:16:C:O2	46:3:16:C:O4'	2.24	0.56
6:F:131:MET:O	6:F:134:ILE:HG22	2.05	0.56
50:9:1298:G:O2'	50:9:1299:A:O5'	2.24	0.56
50:9:1535:U:H2'	50:9:1535:U:O2	2.05	0.56
33:h:50:VAL:O	33:h:53:SER:OG	2.19	0.56
1:A:48:ILE:HD11	1:A:82:ILE:HG22	1.86	0.56
7:G:151:LEU:HD13	7:G:271:LEU:HD12	1.88	0.56
15:P:32:THR:HG23	15:P:91:LEU:HD21	1.88	0.56
63:MM:35:ILE:HD13	63:MM:61:TYR:CE1	2.41	0.56
83:gg:79:LEU:HD22	83:gg:111:VAL:HG21	1.87	0.56
1:A:207:VAL:HG12	47:5:3919:C:C5'	2.36	0.55
26:a:72:THR:HG22	26:a:110:LYS:HB3	1.88	0.55
51:AA:8:LEU:CD2	51:AA:191:ARG:NH2	2.69	0.55
55:EE:87:MET:HE1	55:EE:236:ILE:HD13	1.88	0.55
56:FF:72:LEU:HD22	56:FF:112:LEU:HD11	1.87	0.55
21:V:3:LYS:HG3	21:V:128:LEU:CD1	2.24	0.55
30:e:31:ILE:HD11	47:5:2347:A:C4	2.41	0.55
50:9:1407:U:H2'	50:9:1408:U:C6	2.40	0.55
31:f:43:LEU:HD22	31:f:76:ARG:HA	1.88	0.55
50:9:464:A:C4	85:jj:37:ARG:CZ	2.89	0.55
56:FF:102:LEU:HD22	76:ZZ:110:THR:HG21	1.89	0.55
12:M:15:VAL:HG22	12:M:50:MET:HE1	1.89	0.55
47:5:3811:G:O2'	47:5:3814:U:OP2	2.22	0.55
85:jj:249:PRO:HB2	85:jj:365:THR:HG21	1.85	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
60:JJ:130:ILE:HG12	60:JJ:135:ILE:HD11	1.89	0.55
83:gg:11:LEU:HD12	83:gg:307:VAL:O	2.05	0.55
7:G:139:VAL:HG11	7:G:238:LYS:HG3	1.88	0.55
14:O:84:VAL:HG11	14:O:102:LEU:HD22	1.89	0.55
74:XX:4:CYS:SG	74:XX:9:THR:HG21	2.46	0.55
83:gg:15:ASN:O	83:gg:305:ASN:ND2	2.39	0.55
12:M:36:ALA:HB2	12:M:52:PHE:CZ	2.42	0.55
41:p:10:ILE:HG21	41:p:30:GLU:HB3	1.89	0.55
13:N:184:ILE:HG23	13:N:194:ARG:HH12	1.72	0.55
50:9:1139:C:O4'	50:9:1139:C:O2	2.25	0.55
85:jj:436:GLY:HA2	89:jj:503:7C4:C43	2.37	0.55
19:T:142:ARG:HB3	19:T:142:ARG:CZ	2.37	0.54
47:5:2045:G:O6	47:5:3870:C:O2'	2.20	0.54
47:5:2505:C:O2	47:5:2505:C:O4'	2.24	0.54
85:jj:361:LEU:CD1	85:jj:424:PHE:CD1	2.90	0.54
14:O:72:HIS:N	47:5:4586:G:OP1	2.39	0.54
15:P:95:LEU:CD1	15:P:148:MET:HE1	2.37	0.54
50:9:584:A:C6	50:9:585:C:N3	2.74	0.54
73:WW:52:ILE:HG22	73:WW:61:ILE:HG12	1.89	0.54
43:s:34:ASN:HB3	47:5:1968:G:O3'	2.05	0.54
14:O:23:VAL:HG13	14:O:33:VAL:HG11	1.90	0.54
19:T:147:GLU:CB	19:T:148:PRO:CD	2.80	0.54
57:GG:157:VAL:HB	57:GG:176:ILE:HD11	1.89	0.54
83:gg:11:LEU:CD1	83:gg:307:VAL:O	2.55	0.54
21:V:99:GLU:HB3	22:W:24:THR:HG23	1.90	0.54
3:C:40:VAL:HG21	3:C:123:ALA:HB2	1.90	0.54
47:5:4606:G:C5'	85:jj:16:VAL:HG11	2.37	0.54
50:9:681:U:H4'	74:XX:9:THR:HG22	1.88	0.54
52:BB:36:PRO:CG	52:BB:38:MET:HE2	2.38	0.54
61:KK:93:THR:HG23	61:KK:94:LEU:HD12	1.90	0.54
85:jj:142:THR:HG21	85:jj:425:ALA:HB2	1.89	0.54
15:P:41:ILE:HD12	15:P:150:LEU:HD13	1.90	0.54
31:f:28:LEU:HG	31:f:101:ILE:HD11	1.88	0.54
47:5:2367:A:C2	47:5:2788:U:O4	2.53	0.54
14:O:194:ASP:O	14:O:198:THR:HG23	2.08	0.54
15:P:36:ILE:HD12	15:P:48:LEU:HD11	1.90	0.54
73:WW:14:ILE:HD11	73:WW:41:MET:HE1	1.89	0.54
6:F:89:ALA:HB2	6:F:124:LEU:HD21	1.89	0.54
33:h:44:LEU:O	33:h:47:ILE:HG22	2.08	0.54
47:5:245:C:O4'	47:5:245:C:O2	2.25	0.54
40:o:81:ARG:NH2	47:5:4293:U:O2'	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:106:ILE:HG21	24:Y:109:LEU:HD23	1.89	0.53
29:d:88:LEU:HD12	29:d:106:VAL:HG22	1.90	0.53
77:aa:12:LYS:N	77:aa:33:ASP:OD2	2.42	0.53
1:A:234:LYS:HG2	1:A:238:ILE:HD12	1.89	0.53
2:B:168:MET:HE2	2:B:175:GLN:CG	2.39	0.53
16:Q:104:ARG:NH2	47:5:1353:G:N7	2.55	0.53
65:OO:44:VAL:HG11	65:OO:85:CYS:SG	2.48	0.53
45:ii:76:C:O2	45:ii:76:C:O4'	2.25	0.53
85:jj:149:ILE:HD12	85:jj:231:ALA:HB1	1.89	0.53
7:G:210:ILE:HG12	7:G:254:THR:HG22	1.91	0.53
47:5:1979:A:C6	47:5:1980:U:N3	2.77	0.53
50:9:1568:C:OP1	70:TT:96:SER:OG	2.21	0.53
55:EE:125:LYS:HA	55:EE:159:THR:HG22	1.91	0.53
15:P:36:ILE:HD11	15:P:44:ALA:HB1	1.91	0.53
29:d:33:ILE:HD11	29:d:41:ARG:HB3	1.91	0.53
31:f:39:THR:HG21	31:f:77:ALA:HB2	1.91	0.53
47:5:1483:C:O2	47:5:1483:C:O4'	2.24	0.53
54:DD:21:LEU:HD21	54:DD:48:ILE:HD11	1.90	0.53
6:F:88:LEU:HD22	6:F:89:ALA:N	2.23	0.53
45:2:16:C:O4'	45:2:16:C:O2	2.23	0.53
85:jj:435:VAL:CG1	89:jj:503:7C4:C42	2.86	0.53
19:T:85:LEU:HD13	47:5:4305:G:C2	2.44	0.53
24:Y:49:ILE:HD11	24:Y:55:VAL:HG21	1.90	0.53
42:r:16:PHE:CE2	42:r:43:LEU:HD11	2.44	0.53
47:5:1962:A:C2	47:5:2026:A:C4	2.89	0.53
68:RR:31:ASN:C	68:RR:31:ASN:HD22	2.17	0.53
45:ii:66:G:H5'	85:jj:360:VAL:HG11	1.90	0.53
1:A:90:CYS:HB2	1:A:101:VAL:HG13	1.91	0.53
4:D:208:MET:HE1	4:D:236:MET:HE1	1.91	0.53
14:O:35:VAL:HG21	14:O:80:PHE:CE2	2.44	0.53
29:d:36:VAL:HG11	29:d:44:ARG:HG2	1.90	0.53
47:5:1325:C:O2	47:5:1325:C:O5'	2.27	0.52
50:9:1364:U:O4'	50:9:1364:U:O2	2.27	0.52
55:EE:173:ILE:HD11	55:EE:235:TRP:CE3	2.44	0.52
21:V:3:LYS:HD3	21:V:129:TRP:CH2	2.45	0.52
26:a:12:ARG:NH2	47:5:1338:G:OP2	2.41	0.52
41:p:74:THR:O	41:p:78:THR:HG23	2.09	0.52
44:t:16:ARG:HB2	47:5:1975:G:C6	2.44	0.52
51:AA:122:LEU:HB3	51:AA:144:THR:HG23	1.92	0.52
1:A:82:ILE:HD11	1:A:99:GLY:CA	2.39	0.52
6:F:161:ILE:HB	6:F:166:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:t:100:HIS:HE2	47:5:1978:C:P	2.32	0.52
47:5:1979:A:C5	47:5:1980:U:N3	2.78	0.52
50:9:562:U:H2'	50:9:563:G:C8	2.44	0.52
50:9:1262:C:O2'	80:dd:12:ARG:NH1	2.43	0.52
50:9:1315:U:O2	50:9:1315:U:O4'	2.27	0.52
13:N:6:TYR:CZ	34:i:40:VAL:HG22	2.45	0.52
50:9:190:G:O2'	50:9:209:A:N6	2.43	0.52
20:U:23:LEU:HD11	20:U:83:LEU:HD21	1.91	0.52
47:5:1237:C:O2	47:5:1237:C:O4'	2.27	0.52
47:5:1982:G:P	47:5:1982:G:C3'	2.97	0.52
50:9:183:G:O2'	50:9:184:G:O5'	2.28	0.52
50:9:1298:G:O2'	50:9:1299:A:O4'	2.26	0.52
1:A:82:ILE:HD11	1:A:99:GLY:HA3	1.92	0.52
18:S:35:PRO:HD2	18:S:39:VAL:HG21	1.92	0.52
29:d:36:VAL:HG23	29:d:41:ARG:HG3	1.91	0.52
58:HH:95:ILE:HD11	58:HH:133:LEU:HG	1.91	0.52
24:Y:49:ILE:HD13	24:Y:80:ILE:HD13	1.92	0.52
3:C:95:MET:HE1	47:5:1521:C:H4'	1.91	0.51
11:L:47:ALA:HB3	11:L:48:PRO:HD3	1.91	0.51
44:t:16:ARG:HB2	47:5:1975:G:C2	2.45	0.51
47:5:224:U:O2	47:5:224:U:O4'	2.28	0.51
76:ZZ:73:VAL:HG12	76:ZZ:79:ILE:HD11	1.91	0.51
77:aa:50:VAL:HG23	77:aa:64:LEU:HD11	1.92	0.51
1:A:62:VAL:CG1	1:A:71:LYS:HG2	2.40	0.51
4:D:152:ARG:HG3	4:D:154:THR:HG23	1.91	0.51
21:V:26:ILE:HG22	21:V:101:ASN:HB3	1.93	0.51
47:5:4989:U:O2	47:5:4989:U:O4'	2.27	0.51
73:WW:75:ILE:HD11	73:WW:93:LEU:HD11	1.92	0.51
83:gg:11:LEU:HD12	83:gg:11:LEU:H	1.72	0.51
51:AA:159:ILE:HG23	51:AA:159:ILE:O	2.10	0.51
3:C:334:THR:HG21	6:F:50:TYR:OH	2.09	0.51
45:2:33:U:OP2	67:QQ:146:ARG:NH2	2.44	0.51
21:V:57:VAL:HG11	21:V:122:ALA:HB3	1.92	0.51
42:r:97:ILE:HG21	42:r:107:ARG:HA	1.92	0.51
50:9:1734:G:O2'	50:9:1800:A:N6	2.43	0.51
66:PP:37:TYR:OH	66:PP:45:LEU:HD11	2.10	0.51
83:gg:197:THR:HG21	83:gg:238:ALA:HA	1.92	0.51
7:G:225:ALA:HB3	34:i:43:MET:HE1	1.93	0.51
29:d:57:MET:HE1	29:d:88:LEU:O	2.10	0.51
35:j:22:CYS:HG	87:j:101:ZN:ZN	1.23	0.51
15:P:29:THR:HG21	15:P:146:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:5:747:A:H4'	47:5:748:G:OP1	2.11	0.51
47:5:1979:A:N1	47:5:1980:U:C2	2.76	0.51
47:5:3723:A:H2'	47:5:3724:A:C8	2.46	0.51
57:GG:63:MET:SD	57:GG:63:MET:N	2.84	0.51
14:O:54:TYR:OH	14:O:73:PHE:O	2.29	0.51
18:S:93:MET:HE1	18:S:117:HIS:NE2	2.26	0.51
48:7:11:A:O2'	48:7:13:A:OP2	2.29	0.51
2:B:219:VAL:HG21	2:B:333:LEU:HD23	1.92	0.51
61:KK:65:ARG:NH2	80:dd:20:SER:OG	2.44	0.51
73:WW:14:ILE:CD1	73:WW:41:MET:HE1	2.41	0.51
4:D:23:ARG:NH2	47:5:4280:A:OP2	2.44	0.50
47:5:62:A:N3	47:5:77:U:O2'	2.42	0.50
45:ii:66:G:H4'	85:jj:360:VAL:HG11	1.92	0.50
1:A:225:ILE:HD12	1:A:233:ARG:CZ	2.41	0.50
11:L:18:TRP:CE3	13:N:198:LEU:HD12	2.46	0.50
47:5:498:C:O2	47:5:498:C:O4'	2.30	0.50
55:EE:45:ILE:HD12	55:EE:80:ILE:HD12	1.92	0.50
18:S:53:LYS:NZ	48:7:74:A:O2'	2.45	0.50
47:5:3642:A:OP1	47:5:3644:U:OP1	2.30	0.50
47:5:4966:A:H2'	47:5:4967:A:C8	2.45	0.50
43:s:6:ARG:HH21	47:5:1957:U:C3'	2.21	0.50
44:t:98:ILE:HG23	44:t:98:ILE:O	2.11	0.50
47:5:4510:A:O2'	47:5:4511:A:O4'	2.30	0.50
50:9:1718:G:O2'	50:9:1815:A:N6	2.45	0.50
61:KK:38:LYS:N	61:KK:38:LYS:HD2	2.27	0.50
50:9:501:C:O2	50:9:501:C:C2'	2.59	0.50
50:9:584:A:C5	50:9:585:C:C5	2.99	0.50
53:CC:214:LEU:HD23	53:CC:219:ILE:HD12	1.93	0.50
64:NN:13:GLN:HE21	64:NN:13:GLN:N	2.09	0.50
4:D:64:ILE:HD13	4:D:109:LEU:HD22	1.94	0.50
5:E:119:TYR:CE1	42:r:108:MET:HE1	2.46	0.50
8:H:88:PHE:CE1	8:H:151:ILE:HD12	2.47	0.50
44:t:121:LEU:HD13	47:5:1973:G:OP1	2.11	0.50
56:FF:103:LEU:HD23	56:FF:178:ILE:HD13	1.93	0.50
1:A:208:GLU:HG2	47:5:1629:G:H1	1.76	0.50
5:E:165:VAL:HG13	5:E:180:GLY:N	2.27	0.50
9:I:184:MET:HE2	9:I:190:LEU:HG	1.94	0.50
11:L:169:ILE:HD13	26:a:142:GLY:HA2	1.94	0.50
61:KK:32:HIS:CD2	61:KK:45:VAL:HG21	2.46	0.50
73:WW:111:MET:HE3	73:WW:116:ALA:HA	1.93	0.50
85:jj:367:HIS:C	85:jj:368:ILE:HG13	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:N:135:ILE:CD1	13:N:151:ILE:HD13	2.42	0.50
47:5:3810:C:O4'	47:5:3810:C:O2	2.26	0.50
46:3:75:C:H2'	46:3:76:A:H4'	1.94	0.49
17:R:74:ARG:NH2	47:5:2891:U:OP2	2.45	0.49
15:P:127:ARG:NH2	47:5:2422:C:OP1	2.44	0.49
50:9:448:A:H5''	59:II:25:ARG:HA	1.93	0.49
55:EE:44:LEU:HD13	55:EE:72:ILE:HD11	1.94	0.49
76:ZZ:79:ILE:HB	76:ZZ:83:LEU:HD12	1.94	0.49
85:jj:10:ILE:HD12	85:jj:87:VAL:HG21	1.93	0.49
4:D:41:LYS:CG	19:T:93:ILE:HD11	2.43	0.49
23:X:80:PRO:HB2	23:X:155:ILE:HD13	1.95	0.49
51:AA:66:VAL:HG21	51:AA:185:MET:HB2	1.93	0.49
51:AA:185:MET:CE	72:VV:39:VAL:CG2	2.90	0.49
56:FF:88:MET:HE1	56:FF:92:ILE:HD11	1.93	0.49
1:A:77:ILE:HD13	1:A:128:ARG:HB2	1.95	0.49
41:p:61:MET:HE2	47:5:2652:G:N1	2.28	0.49
47:5:2088:A:O2'	47:5:2089:G:OP2	2.26	0.49
49:8:125:C:O2	49:8:125:C:O4'	2.31	0.49
50:9:93:U:H2'	50:9:94:G:O4'	2.12	0.49
50:9:526:A:O2'	60:JJ:125:HIS:HA	2.12	0.49
43:s:84:GLY:HA2	47:5:2021:G:O2'	2.13	0.49
56:FF:92:ILE:HD13	56:FF:169:ILE:HG21	1.94	0.49
4:D:163:LEU:HD11	4:D:173:ILE:HG21	1.94	0.49
29:d:46:LEU:CD2	29:d:72:VAL:HG11	2.43	0.49
50:9:964:A:N3	50:9:1054:G:O2'	2.41	0.49
7:G:139:VAL:HG11	7:G:238:LYS:CG	2.43	0.49
10:J:141:ILE:HD11	48:7:55:A:C2	2.48	0.49
44:t:123:ARG:HB2	47:5:1995:G:O2'	2.12	0.49
47:5:1979:A:O2'	47:5:1980:U:H5'	2.13	0.49
47:5:2268:A:H4'	47:5:2269:C:H5'	1.94	0.49
47:5:2763:U:O2	47:5:2763:U:O4'	2.31	0.49
50:9:1395:C:H2'	50:9:1396:A:O4'	2.13	0.49
21:V:82:ILE:HG12	21:V:121:VAL:HG13	1.93	0.49
26:a:21:ARG:HB2	47:5:1318:C:OP1	2.12	0.49
28:c:48:LEU:HD13	28:c:57:LYS:HG3	1.94	0.49
39:n:13:LEU:HD12	39:n:17:ARG:CZ	2.43	0.49
16:Q:67:ILE:HD12	16:Q:96:PRO:HD2	1.94	0.48
31:f:50:VAL:HG22	31:f:69:VAL:HG12	1.93	0.48
50:9:944:A:C5	50:9:945:U:C5	3.01	0.48
57:GG:5:ILE:HD12	57:GG:16:ILE:HD13	1.95	0.48
73:WW:26:LEU:HD11	73:WW:60:LYS:HB3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:77:THR:HG21	2:B:337:VAL:HG22	1.95	0.48
2:B:174:ARG:NH1	47:5:4985:U:O2	2.46	0.48
2:B:249:ARG:NH1	47:5:2837:U:OP1	2.46	0.48
43:s:112:ARG:HD3	47:5:1968:G:OP1	2.12	0.48
44:t:125:LEU:O	44:t:128:THR:OG1	2.25	0.48
50:9:1374:C:H2'	50:9:1375:G:O4'	2.13	0.48
50:9:1863:A:H1'	77:aa:79:ILE:HD13	1.93	0.48
83:gg:14:HIS:NE2	83:gg:41:ILE:CG1	2.66	0.48
9:I:191:ILE:CD1	9:I:212:LEU:HD11	2.40	0.48
59:II:113:TYR:CE1	59:II:121:LEU:HD23	2.48	0.48
60:JJ:146:SER:O	60:JJ:147:PHE:C	2.56	0.48
1:A:207:VAL:HG12	47:5:3919:C:H5''	1.95	0.48
29:d:22:THR:HG22	29:d:89:SER:CB	2.43	0.48
47:5:4608:G:OP1	85:jj:69:ARG:HD2	2.14	0.48
51:AA:134:LEU:CD2	51:AA:144:THR:HG21	2.42	0.48
51:AA:163:CYS:SG	51:AA:174:MET:HE2	2.54	0.48
1:A:207:VAL:HG11	47:5:1633:G:C6	2.49	0.48
6:F:89:ALA:CB	6:F:124:LEU:HD21	2.43	0.48
13:N:50:ARG:NH2	47:5:279:A:OP1	2.46	0.48
17:R:35:ALA:HA	17:R:40:GLN:HG2	1.95	0.48
22:W:3:VAL:HG21	22:W:12:LYS:CE	2.44	0.48
35:j:17:THR:CG2	35:j:29:LEU:HD21	2.43	0.48
51:AA:183:LEU:HD23	51:AA:186:ARG:NH1	2.29	0.48
12:M:119:ARG:NH1	14:O:202:LEU:HD21	2.27	0.48
44:t:77:ALA:CB	47:5:1974:U:OP1	2.62	0.48
47:5:1964:A:H4'	47:5:1964:A:OP1	2.13	0.48
50:9:1624:U:O2	50:9:1624:U:O4'	2.30	0.48
55:EE:126:VAL:HG23	55:EE:156:VAL:O	2.12	0.48
2:B:49:TYR:HH	2:B:179:HIS:HD1	1.62	0.48
47:5:4966:A:C2	47:5:5067:U:N3	2.81	0.48
65:OO:99:ALA:H	65:OO:133:THR:HG22	1.79	0.48
68:RR:16:ILE:HG22	68:RR:24:LEU:HD11	1.96	0.48
1:A:186:TYR:HB2	1:A:196:TRP:CZ3	2.49	0.48
13:N:135:ILE:HD13	13:N:151:ILE:HD13	1.94	0.48
18:S:80:ILE:HG22	18:S:82:LEU:HD22	1.95	0.48
36:k:35:LYS:NZ	47:5:2693:G:OP1	2.47	0.48
40:o:98:LYS:HE3	47:5:4233:A:H4'	1.95	0.48
43:s:59:THR:CG2	47:5:1961:G:C8	2.96	0.48
2:B:14:LEU:HD23	2:B:17:LEU:CD2	2.43	0.48
43:s:83:ARG:HA	47:5:2022:C:OP1	2.14	0.48
50:9:1149:A:C6	50:9:1151:G:C4	3.02	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:AA:181:GLU:O	51:AA:185:MET:CG	2.44	0.48
3:C:323:ARG:NH1	47:5:1279:A:O2'	2.46	0.48
44:t:78:SER:OG	47:5:1977:C:OP1	2.29	0.48
47:5:964:A:H2'	47:5:965:G:O4'	2.14	0.48
47:5:2094:C:O2	47:5:2094:C:O4'	2.32	0.48
50:9:488:U:OP2	85:jj:290:LYS:NZ	2.38	0.48
54:DD:105:LEU:HD23	54:DD:184:ILE:HG23	1.96	0.48
57:GG:32:MET:HE2	57:GG:63:MET:HG2	1.95	0.48
2:B:56:ILE:HG12	2:B:365:LEU:HD22	1.95	0.47
2:B:252:ALA:HB1	47:5:4524:G:N3	2.28	0.47
7:G:247:VAL:HG21	7:G:249:ARG:NH1	2.29	0.47
21:V:39:ILE:HG23	21:V:61:VAL:CG2	2.44	0.47
50:9:1589:A:N3	50:9:1653:U:O2'	2.43	0.47
35:j:17:THR:HG21	35:j:29:LEU:HD21	1.96	0.47
47:5:1981:G:H2'	47:5:1982:G:H5'	1.96	0.47
47:5:4723:A:C2	47:5:4724:A:C6	3.02	0.47
59:II:38:ILE:HD11	59:II:81:VAL:HG23	1.97	0.47
34:i:77:VAL:O	34:i:77:VAL:HG13	2.13	0.47
64:NN:13:GLN:N	64:NN:13:GLN:NE2	2.62	0.47
42:r:98:ARG:NH2	47:5:2262:G:OP2	2.48	0.47
68:RR:53:TYR:CE2	68:RR:57:LEU:HD11	2.49	0.47
83:gg:14:HIS:NE2	83:gg:41:ILE:CB	2.67	0.47
1:A:65:ASP:HB2	1:A:72:ARG:HG2	1.94	0.47
3:C:33:ARG:HD2	3:C:36:ILE:HD12	1.95	0.47
5:E:185:ASN:ND2	5:E:274:LEU:O	2.47	0.47
15:P:32:THR:HG21	15:P:87:SER:HB3	1.96	0.47
43:s:47:LEU:HB3	43:s:51:ALA:HB3	1.96	0.47
44:t:100:HIS:CE1	47:5:1978:C:OP1	2.67	0.47
50:9:914:U:O2	50:9:914:U:O4'	2.33	0.47
52:BB:212:VAL:HG23	52:BB:212:VAL:O	2.14	0.47
65:OO:129:ILE:HG21	77:aa:44:ILE:HD13	1.96	0.47
10:J:113:ILE:HD12	69:SS:14:ARG:HD2	1.95	0.47
15:P:54:LYS:HA	15:P:83:TRP:CD1	2.48	0.47
43:s:21:LEU:HD13	43:s:68:HIS:CD2	2.49	0.47
47:5:1872:G:O2'	47:5:4219:A:N3	2.43	0.47
47:5:1982:G:C2'	47:5:1983:A:C5'	2.92	0.47
47:5:2627:C:O4'	47:5:2627:C:O2	2.28	0.47
50:9:1444:U:H2'	50:9:1445:U:C6	2.49	0.47
3:C:334:THR:HG22	3:C:337:ARG:HH22	1.80	0.47
5:E:180:GLY:O	5:E:181:PRO:C	2.57	0.47
22:W:4:GLU:OE1	22:W:20:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:64:SER:HB2	33:h:69:LEU:HD13	1.95	0.47
23:X:127:LEU:HD11	23:X:135:LYS:HE3	1.96	0.47
24:Y:61:HIS:N	47:5:232:G:O6	2.46	0.47
46:3:35:U:O4'	50:9:1641:A:OP1	2.31	0.47
47:5:1982:G:N7	47:5:1983:A:C8	2.83	0.47
47:5:4724:A:C6	47:5:4725:C:C4	3.02	0.47
50:9:4:C:O2'	60:JJ:18:ARG:NH1	2.47	0.47
51:AA:33:GLN:HB3	51:AA:154:LEU:HD12	1.96	0.47
60:JJ:45:ARG:O	60:JJ:49:THR:HG23	2.15	0.47
1:A:126:LEU:HD13	1:A:150:LEU:HD21	1.96	0.47
1:A:158:ILE:HG23	1:A:162:ASN:HD21	1.80	0.47
4:D:61:ILE:HG23	4:D:79:TYR:CE2	2.50	0.47
4:D:146:LEU:HD11	4:D:159:VAL:HG11	1.96	0.47
44:t:16:ARG:HD2	47:5:1975:G:N3	2.29	0.47
66:PP:56:LEU:HD13	66:PP:78:THR:CG2	2.40	0.47
7:G:189:LEU:HD22	7:G:255:VAL:CG1	2.45	0.47
19:T:144:ASN:ND2	19:T:144:ASN:N	2.60	0.47
41:p:75:SER:O	41:p:78:THR:OG1	2.18	0.47
47:5:4305:G:N3	47:5:4305:G:H2'	2.30	0.47
47:5:4871:C:O4'	47:5:4871:C:O2	2.33	0.47
50:9:146:G:O2'	50:9:147:A:O5'	2.27	0.47
50:9:585:C:O2'	50:9:586:G:C5'	2.61	0.47
50:9:980:A:C2	50:9:981:A:C6	3.03	0.47
54:DD:162:ASP:N	54:DD:163:PRO:CD	2.77	0.47
57:GG:3:LEU:HD22	57:GG:111:LEU:HD11	1.97	0.47
11:L:106:SER:HB3	34:i:17:VAL:HG11	1.96	0.47
14:O:36:VAL:HG11	14:O:108:ILE:HD12	1.96	0.47
21:V:6:ARG:HH22	85:jj:50:GLY:C	2.23	0.47
47:5:222:C:H2'	47:5:223:G:O4'	2.15	0.47
47:5:4305:G:N3	47:5:4305:G:C2'	2.77	0.47
50:9:1700:C:C2	50:9:1834:A:N6	2.83	0.47
7:G:116:LEU:HD21	13:N:29:GLN:HG3	1.97	0.46
31:f:33:VAL:HG23	31:f:38:GLU:HB2	1.97	0.46
51:AA:94:THR:HG23	51:AA:182:VAL:HG21	1.97	0.46
83:gg:5:MET:HE1	83:gg:312:VAL:HG22	1.97	0.46
20:U:82:TYR:CZ	20:U:86:LEU:HD11	2.50	0.46
47:5:1381:U:O2	47:5:1381:U:O4'	2.31	0.46
79:cc:14:VAL:HG13	79:cc:30:VAL:HG13	1.97	0.46
8:H:41:ILE:HD11	8:H:69:THR:HB	1.98	0.46
9:I:154:ARG:NH2	9:I:154:ARG:CG	2.73	0.46
14:O:12:ARG:O	18:S:171:ARG:NH2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:3:VAL:HG21	22:W:12:LYS:HE3	1.97	0.46
47:5:4608:G:OP1	85:jj:69:ARG:CD	2.63	0.46
1:A:112:ILE:HG23	1:A:133:TYR:CD2	2.50	0.46
4:D:146:LEU:HD11	4:D:159:VAL:CG1	2.45	0.46
5:E:167:PHE:CE1	5:E:176:LEU:HD22	2.50	0.46
6:F:178:LEU:HD21	6:F:203:ALA:HA	1.96	0.46
11:L:58:ILE:HG23	11:L:70:VAL:CG1	2.46	0.46
32:g:15:THR:HG21	47:5:2514:G:H5''	1.98	0.46
47:5:3879:G:O2'	47:5:3881:G:OP2	2.30	0.46
58:HH:69:LEU:HD23	58:HH:96:ALA:HB2	1.98	0.46
69:SS:18:THR:HG21	69:SS:33:ILE:HA	1.96	0.46
79:cc:20:ARG:HD3	79:cc:28:THR:HG22	1.98	0.46
4:D:41:LYS:HG2	19:T:93:ILE:HD11	1.97	0.46
33:h:47:ILE:CG2	33:h:48:ARG:N	2.79	0.46
47:5:1979:A:C6	47:5:1980:U:C2	3.04	0.46
47:5:4266:G:O2'	47:5:4279:A:N6	2.48	0.46
4:D:16:TYR:O	48:7:11:A:N6	2.48	0.46
47:5:1667:A:N1	47:5:2281:U:OP2	2.48	0.46
47:5:1962:A:C2	47:5:2026:A:C1'	2.90	0.46
47:5:1986:U:C4	47:5:2013:A:C6	3.03	0.46
50:9:1228:A:H2'	50:9:1229:G:C8	2.50	0.46
50:9:1535:U:O2	50:9:1535:U:C2'	2.63	0.46
83:gg:81:GLY:CA	83:gg:87:LEU:HD23	2.46	0.46
3:C:54:VAL:HG21	3:C:101:MET:HE3	1.97	0.46
6:F:91:VAL:HG21	6:F:132:LEU:HD21	1.97	0.46
12:M:17:PHE:CE2	12:M:54:CYS:HA	2.51	0.46
50:9:1331:C:C5	45:ii:35:A:H1'	2.50	0.46
50:9:1336:C:H2'	50:9:1337:C:O4'	2.16	0.46
58:HH:66:VAL:HG22	58:HH:96:ALA:HB1	1.96	0.46
50:9:412:G:O2'	50:9:812:A:N6	2.47	0.46
58:HH:170:VAL:HG13	58:HH:187:PHE:HB2	1.98	0.46
11:L:18:TRP:CZ3	13:N:198:LEU:HD12	2.51	0.46
19:T:48:VAL:HG21	19:T:94:GLU:HG2	1.96	0.46
69:SS:15:VAL:HG22	69:SS:68:ILE:HD11	1.96	0.46
45:ii:24:C:H2'	45:ii:25:A:O4'	2.16	0.46
9:I:61:SER:HA	9:I:126:VAL:HG23	1.96	0.46
44:t:123:ARG:HD3	47:5:1996:C:H5''	1.98	0.46
47:5:4600:G:N7	85:jj:51:LYS:HD2	2.31	0.46
52:BB:79:VAL:HG21	52:BB:81:PHE:CZ	2.51	0.46
61:KK:3:MET:HE1	61:KK:48:ALA:HB2	1.98	0.46
21:V:16:ILE:HD12	21:V:16:ILE:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:s:10:LYS:HG2	43:s:60:MET:HE1	1.98	0.45
50:9:1395:C:O2'	50:9:1396:A:OP1	2.28	0.45
56:FF:99:ILE:CG2	76:ZZ:67:LEU:HD21	2.40	0.45
56:FF:144:LEU:HD23	79:cc:49:PRO:HG2	1.96	0.45
61:KK:49:MET:HE2	61:KK:49:MET:HA	1.97	0.45
71:UU:29:VAL:HG22	71:UU:85:HIS:CE1	2.51	0.45
9:I:91:LEU:HD12	9:I:135:ILE:HG23	1.98	0.45
47:5:1279:A:O2'	47:5:1281:G:N7	2.49	0.45
47:5:2042:A:N3	47:5:4462:C:O2'	2.44	0.45
50:9:464:A:C5	85:jj:37:ARG:CZ	2.99	0.45
2:B:10:ARG:C	2:B:10:ARG:CD	2.89	0.45
16:Q:70:MET:HE1	16:Q:137:VAL:HG21	1.98	0.45
33:h:47:ILE:HG23	33:h:48:ARG:N	2.32	0.45
50:9:380:G:OP2	59:II:56:ARG:NH2	2.49	0.45
50:9:566:U:C2	50:9:584:A:N1	2.84	0.45
54:DD:109:LEU:CD2	54:DD:115:VAL:HG22	2.47	0.45
73:WW:6:VAL:HG12	73:WW:34:ILE:HD11	1.97	0.45
74:XX:74:LEU:HD21	74:XX:81:ILE:HD12	1.97	0.45
50:9:1137:U:N3	50:9:1148:A:N6	2.63	0.45
7:G:189:LEU:HD22	7:G:255:VAL:HG12	1.99	0.45
18:S:127:MET:HE1	19:T:155:PRO:HA	1.98	0.45
73:WW:38:LEU:HD23	73:WW:41:MET:HE3	1.99	0.45
6:F:222:LYS:HE3	47:5:1907:A:H4'	1.98	0.45
14:O:85:ARG:HG3	14:O:99:LEU:HD11	1.99	0.45
19:T:142:ARG:NH1	19:T:142:ARG:CB	2.80	0.45
44:t:113:ALA:HA	44:t:132:ILE:CD1	2.47	0.45
44:t:147:HIS:N	44:t:148:PRO:CD	2.80	0.45
47:5:106:A:H2'	47:5:107:G:O4'	2.17	0.45
61:KK:43:LEU:C	61:KK:43:LEU:HD12	2.42	0.45
65:OO:56:VAL:HG13	65:OO:77:ALA:HB1	1.97	0.45
2:B:29:VAL:HG23	2:B:346:THR:HG21	1.98	0.45
33:h:60:VAL:O	33:h:64:THR:HG23	2.17	0.45
40:o:41:TYR:CD1	46:3:75:C:O2	2.69	0.45
47:5:4378:A:O2'	47:5:4379:A:H2'	2.16	0.45
50:9:581:U:O4'	75:YY:62:THR:HG21	2.17	0.45
56:FF:49:LEU:HD13	56:FF:50:PRO:HD2	1.98	0.45
60:JJ:46:VAL:HG11	60:JJ:106:LEU:CD1	2.47	0.45
5:E:124:VAL:HG21	47:5:702:U:H5'	1.99	0.45
47:5:4759:C:O2	47:5:4759:C:O4'	2.34	0.45
50:9:585:C:HO2'	50:9:586:G:H5'	1.82	0.45
56:FF:39:ILE:HG23	56:FF:68:ILE:HD13	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:QQ:32:ILE:HG21	67:QQ:39:LEU:HD11	1.99	0.45
80:dd:24:CYS:SG	80:dd:42:CYS:SG	3.09	0.45
83:gg:91:ASP:HB2	83:gg:98:THR:HG23	1.99	0.45
3:C:210:ILE:HG21	3:C:252:TRP:CZ3	2.51	0.45
39:n:13:LEU:HD11	50:9:1818:A:O2'	2.17	0.45
51:AA:122:LEU:HD13	51:AA:142:LEU:HD13	1.98	0.45
53:CC:106:VAL:HG22	53:CC:128:VAL:HG22	1.99	0.45
58:HH:133:LEU:HD21	58:HH:176:VAL:HG11	1.99	0.45
74:XX:128:VAL:HG11	74:XX:133:LEU:HD21	1.99	0.45
3:C:95:MET:HE1	47:5:1521:C:C4'	2.47	0.45
6:F:46:ARG:NH1	47:5:976:G:O3'	2.50	0.45
30:e:38:PRO:HD2	30:e:55:MET:HE3	1.98	0.45
47:5:119:G:H3'	47:5:120:A:C5'	2.47	0.45
50:9:955:A:H5''	65:OO:60:MET:HE3	1.99	0.45
51:AA:68:ILE:HG21	51:AA:74:VAL:HG23	1.98	0.45
54:DD:109:LEU:HD21	54:DD:115:VAL:HG22	1.99	0.45
63:MM:35:ILE:HD13	63:MM:61:TYR:CZ	2.52	0.45
74:XX:61:GLN:HB3	74:XX:62:PRO:CD	2.47	0.45
13:N:116:LEU:HD22	13:N:135:ILE:HD11	1.97	0.44
50:9:145:G:N7	57:GG:178:ARG:NH1	2.63	0.44
50:9:427:U:O2	50:9:427:U:O5'	2.35	0.44
52:BB:103:MET:HE1	52:BB:212:VAL:HG23	1.98	0.44
14:O:151:ALA:O	14:O:155:THR:HG23	2.17	0.44
44:t:121:LEU:CD1	47:5:1973:G:OP1	2.64	0.44
47:5:2862:G:H4'	47:5:3625:G:N7	2.32	0.44
47:5:4579:U:O2	47:5:4580:U:C2	2.71	0.44
67:QQ:51:LEU:HD22	67:QQ:84:ILE:HD11	1.99	0.44
79:cc:14:VAL:HG13	79:cc:30:VAL:CG1	2.48	0.44
79:cc:14:VAL:HG22	79:cc:30:VAL:HG11	1.98	0.44
3:C:327:LYS:O	6:F:46:ARG:NH2	2.50	0.44
30:e:103:VAL:O	30:e:108:ARG:NH2	2.50	0.44
47:5:1982:G:H3'	47:5:1982:G:OP2	2.17	0.44
50:9:572:U:OP1	75:YY:60:PHE:N	2.48	0.44
2:B:57:VAL:HG22	2:B:73:VAL:HG12	1.99	0.44
3:C:336:ARG:O	3:C:340:ILE:HG12	2.17	0.44
9:I:155:ALA:O	9:I:156:LYS:C	2.60	0.44
37:l:16:LYS:HG3	37:l:49:LEU:HD21	2.00	0.44
43:s:36:GLY:HA2	47:5:1969:G:O3'	2.17	0.44
47:5:27:C:O2'	47:5:60:A:N3	2.50	0.44
50:9:453:C:C2'	50:9:454:U:H5'	2.47	0.44
51:AA:124:VAL:HG13	51:AA:130:ASP:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:BB:36:PRO:HG2	52:BB:38:MET:HE2	1.99	0.44
83:gg:14:HIS:HE1	83:gg:41:ILE:CB	2.11	0.44
28:c:82:GLY:HA2	28:c:91:VAL:HG12	2.00	0.44
47:5:320:C:H2'	47:5:321:U:O4'	2.18	0.44
47:5:3724:A:N6	47:5:3725:G:C6	2.85	0.44
47:5:4423:U:O2	47:5:4423:U:O4'	2.35	0.44
51:AA:18:PHE:CE1	51:AA:177:MET:HE3	2.53	0.44
56:FF:39:ILE:HG23	56:FF:68:ILE:HG21	1.99	0.44
60:JJ:28:GLU:HG2	60:JJ:43:VAL:HG11	1.99	0.44
83:gg:81:GLY:HA2	83:gg:87:LEU:HD23	1.99	0.44
13:N:202:ARG:NH2	47:5:1372:A:OP1	2.50	0.44
47:5:113:A:H2'	47:5:114:G:O4'	2.18	0.44
47:5:1612:G:C2'	47:5:1612:G:N3	2.80	0.44
50:9:27:A:H2'	50:9:28:U:O4'	2.18	0.44
50:9:1616:U:H2'	50:9:1617:G:O4'	2.17	0.44
7:G:199:LEU:HD12	7:G:205:ALA:HB2	1.99	0.44
8:H:12:ILE:HG21	8:H:18:ILE:HD13	1.99	0.44
8:H:64:ARG:NH2	47:5:4693:C:OP1	2.51	0.44
16:Q:11:ARG:NH2	47:5:1690:C:OP2	2.51	0.44
23:X:65:ALA:HB2	33:h:69:LEU:HD11	1.99	0.44
47:5:4977:A:H2'	47:5:4978:G:O4'	2.18	0.44
50:9:459:C:H2'	50:9:460:A:O4'	2.18	0.44
50:9:507:G:OP1	75:YY:108:LYS:NZ	2.41	0.44
61:KK:35:LEU:HD13	61:KK:35:LEU:O	2.18	0.44
50:9:1401:A:C2	50:9:1402:A:C6	3.06	0.44
52:BB:44:ILE:HD11	52:BB:86:LEU:HD13	2.00	0.44
3:C:101:MET:HE2	47:5:2343:G:C4	2.53	0.44
3:C:188:ARG:NH2	47:5:2299:G:O6	2.51	0.44
8:H:92:MET:SD	8:H:161:ILE:HD11	2.58	0.44
25:Z:89:ILE:HD11	25:Z:117:LYS:HB3	2.00	0.44
47:5:82:U:H2'	47:5:83:C:O4'	2.17	0.44
47:5:1381:U:O2	47:5:1381:U:H5''	2.18	0.44
50:9:183:G:O2'	50:9:183:G:N3	2.50	0.44
51:AA:60:LEU:HD13	51:AA:159:ILE:CD1	2.47	0.44
58:HH:116:ARG:NH2	58:HH:121:THR:OG1	2.51	0.44
47:5:2517:A:N3	47:5:2539:C:O2'	2.51	0.43
1:A:196:TRP:O	1:A:198:ARG:N	2.51	0.43
5:E:165:VAL:CG1	5:E:178:VAL:HG13	2.47	0.43
6:F:97:ILE:HD11	16:Q:4:ASP:CG	2.43	0.43
7:G:119:GLN:HA	7:G:122:ILE:HD12	1.99	0.43
29:d:68:LEU:CD2	29:d:106:VAL:HG12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:g:11:LEU:HD22	32:g:18:ASN:HB2	2.00	0.43
47:5:4189:U:H2'	47:5:4190:U:O4'	2.18	0.43
50:9:183:G:N3	50:9:183:G:C2'	2.80	0.43
50:9:1401:A:H2'	50:9:1402:A:C8	2.53	0.43
73:WW:28:ARG:CZ	73:WW:28:ARG:HB3	2.48	0.43
7:G:223:LEU:CD1	7:G:254:THR:HG21	2.48	0.43
47:5:1236:C:O2'	47:5:1237:C:O5'	2.34	0.43
47:5:2439:G:C6	47:5:2440:U:C4	3.07	0.43
50:9:1303:C:O2	50:9:1303:C:O4'	2.36	0.43
50:9:1395:C:H2'	50:9:1396:A:N3	2.32	0.43
50:9:1661:A:C8	80:dd:14:PHE:CD1	3.06	0.43
55:EE:181:CYS:SG	55:EE:225:ILE:HG23	2.59	0.43
66:PP:53:GLN:HB3	66:PP:83:MET:HE3	2.00	0.43
77:aa:50:VAL:HG23	77:aa:64:LEU:CD1	2.48	0.43
14:O:54:TYR:HD1	14:O:145:VAL:HG21	1.82	0.43
14:O:85:ARG:CG	14:O:99:LEU:HD11	2.48	0.43
41:p:8:VAL:HG22	47:5:2876:G:OP1	2.19	0.43
50:9:433:A:H5''	59:II:22:HIS:HB3	2.00	0.43
50:9:1822:A:H2'	50:9:1823:A:O4'	2.18	0.43
57:GG:58:LYS:HA	57:GG:107:SER:HB2	2.00	0.43
79:cc:46:VAL:HG11	79:cc:50:VAL:CG2	2.48	0.43
6:F:75:ARG:NE	47:5:730:G:OP2	2.48	0.43
21:V:50:ASN:ND2	47:5:4457:U:OP1	2.52	0.43
25:Z:41:ALA:HB2	25:Z:77:TYR:CE1	2.54	0.43
44:t:82:ILE:HD11	47:5:1977:C:H4'	2.00	0.43
47:5:407:A:O2'	47:5:410:A:OP1	2.36	0.43
51:AA:63:ARG:HE	72:VV:78:ILE:HG23	1.83	0.43
56:FF:68:ILE:HD12	56:FF:112:LEU:HD22	1.99	0.43
71:UU:48:LEU:HD11	71:UU:91:LEU:HD22	2.00	0.43
74:XX:107:ARG:HB3	74:XX:110:HIS:HB3	2.00	0.43
85:jj:353:ILE:HG23	85:jj:357:TYR:CE1	2.54	0.43
1:A:117:GLU:HB2	1:A:162:ASN:HB2	2.00	0.43
2:B:91:GLY:CA	2:B:153:MET:HE3	2.49	0.43
3:C:67:TRP:CE3	3:C:73:VAL:HG21	2.54	0.43
21:V:60:MET:HE1	21:V:78:PRO:HB3	2.00	0.43
26:a:103:VAL:HG12	26:a:108:TYR:HB2	2.01	0.43
47:5:686:A:N3	47:5:686:A:H2'	2.34	0.43
47:5:1301:C:O2	47:5:1301:C:O4'	2.33	0.43
53:CC:84:PHE:HZ	53:CC:262:THR:HG23	1.82	0.43
54:DD:72:VAL:HG23	61:KK:20:VAL:HG21	1.99	0.43
2:B:56:ILE:CG1	2:B:365:LEU:HD22	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:128:LEU:HD11	10:J:130:PHE:CE1	2.53	0.43
11:L:28:GLN:HB3	11:L:29:PRO:HD3	2.01	0.43
44:t:16:ARG:CB	47:5:1975:G:C2	3.01	0.43
44:t:77:ALA:HB3	47:5:1974:U:OP1	2.18	0.43
50:9:428:U:C6	60:JJ:7:TRP:CH2	3.07	0.43
54:DD:109:LEU:HD12	54:DD:184:ILE:HD11	2.01	0.43
54:DD:227:LYS:HE3	83:gg:184:LEU:HD11	2.01	0.43
2:B:77:THR:C	2:B:78:ILE:HD12	2.43	0.43
43:s:58:ASN:CG	47:5:2021:G:OP1	2.61	0.43
47:5:294:G:O6	47:5:315:G:H1'	2.18	0.43
47:5:1990:A:H3'	47:5:1991:A:H5''	2.00	0.43
47:5:4525:C:H2'	47:5:4526:U:O4'	2.19	0.43
50:9:1551:U:O2	50:9:1551:U:O4'	2.36	0.43
57:GG:159:ARG:HB3	57:GG:173:ALA:HB2	2.00	0.43
2:B:86:VAL:HG13	2:B:162:VAL:HG22	2.01	0.43
6:F:178:LEU:HB3	6:F:183:ILE:HB	2.01	0.43
11:L:28:GLN:HB3	11:L:29:PRO:CD	2.49	0.43
13:N:65:ARG:HG3	13:N:129:PHE:CE1	2.54	0.43
17:R:10:LEU:HB3	17:R:41:ILE:CD1	2.49	0.43
47:5:2690:C:H2'	47:5:2691:U:O4'	2.19	0.43
47:5:3706:C:H2'	47:5:3707:U:O4'	2.19	0.43
50:9:1095:C:O2	50:9:1095:C:C2'	2.66	0.43
50:9:1255:G:OP1	50:9:1256:G:H1'	2.19	0.43
64:NN:13:GLN:HE21	64:NN:13:GLN:H	1.66	0.43
6:F:100:VAL:HG23	6:F:138:TYR:CZ	2.54	0.43
8:H:41:ILE:HG12	8:H:73:ILE:HD11	2.00	0.43
35:j:45:ARG:NH1	47:5:372:A:O3'	2.52	0.43
38:m:72:LYS:HD3	38:m:92:THR:HG21	2.01	0.43
50:9:1095:C:O2	50:9:1095:C:H2'	2.19	0.43
50:9:1298:G:O2'	50:9:1299:A:C8	2.69	0.43
50:9:1438:A:H2'	50:9:1439:A:C8	2.54	0.43
59:II:182:CYS:SG	59:II:183:GLY:N	2.92	0.43
7:G:207:LEU:HD23	7:G:208:VAL:N	2.34	0.42
25:Z:38:TYR:CD1	25:Z:76:ASN:OD1	2.72	0.42
47:5:1613:A:H3'	47:5:1614:C:H5'	2.00	0.42
47:5:2367:A:N6	47:5:2788:U:C4	2.84	0.42
52:BB:143:THR:HG21	52:BB:156:ALA:HB2	2.00	0.42
61:KK:11:ILE:HD12	61:KK:45:VAL:HG22	2.01	0.42
1:A:104:VAL:CG1	1:A:146:THR:HG21	2.48	0.42
2:B:299:ILE:N	2:B:299:ILE:HD12	2.34	0.42
5:E:261:LEU:N	5:E:262:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:199:LEU:CD1	7:G:205:ALA:HB2	2.49	0.42
9:I:81:GLY:CA	47:5:1990:A:OP1	2.67	0.42
10:J:155:HIS:HB2	48:7:55:A:H4'	2.01	0.42
13:N:115:VAL:HG22	13:N:134:LEU:CD2	2.49	0.42
20:U:70:ILE:HD12	20:U:70:ILE:N	2.34	0.42
33:h:62:ASN:ND2	49:8:60:G:O6	2.52	0.42
50:9:853:C:O2	50:9:853:C:O4'	2.35	0.42
51:AA:38:ILE:HD11	51:AA:150:THR:HG22	2.00	0.42
11:L:22:VAL:CG1	13:N:200:LEU:HD12	2.49	0.42
17:R:4:LEU:HD11	17:R:29:THR:HG23	2.00	0.42
47:5:4586:G:H8	47:5:4586:G:H5''	1.84	0.42
73:WW:56:HIS:O	73:WW:57:ARG:HG3	2.18	0.42
3:C:30:ALA:HB1	3:C:31:PRO:HD2	2.01	0.42
13:N:193:ARG:O	13:N:197:THR:HG23	2.20	0.42
47:5:976:G:N2	47:5:977:C:C2	2.87	0.42
50:9:933:G:H1'	50:9:1001:A:O4'	2.19	0.42
51:AA:104:THR:O	51:AA:107:THR:HG23	2.20	0.42
85:jj:343:GLN:CD	89:jj:503:7C4:C66	2.92	0.42
7:G:210:ILE:HG23	7:G:220:VAL:HG11	2.01	0.42
42:r:33:LYS:NZ	47:5:2265:G:OP2	2.52	0.42
50:9:1865:C:OP1	77:aa:87:ARG:NH2	2.53	0.42
63:MM:22:LEU:HD21	63:MM:89:VAL:HG23	2.01	0.42
85:jj:11:VAL:HG11	85:jj:106:THR:HG22	2.00	0.42
12:M:116:LYS:HE3	14:O:201:LEU:HD13	2.00	0.42
29:d:27:ILE:HD12	29:d:86:VAL:HG21	2.01	0.42
29:d:46:LEU:HD13	29:d:64:ILE:HD13	2.02	0.42
47:5:4530:U:H2'	47:5:4531:U:C6	2.54	0.42
50:9:384:U:O4	59:II:5:ARG:NH2	2.51	0.42
65:OO:119:LEU:HD11	65:OO:126:ILE:HD11	2.01	0.42
73:WW:37:PHE:CE2	73:WW:103:VAL:HG13	2.55	0.42
45:ii:52:C:C4'	85:jj:357:TYR:HA	2.48	0.42
85:jj:104:THR:OG1	85:jj:367:HIS:HE1	2.03	0.42
2:B:223:THR:HA	2:B:338:VAL:HG22	2.01	0.42
9:I:71:CYS:SG	9:I:154:ARG:HB3	2.60	0.42
14:O:152:VAL:O	14:O:155:THR:OG1	2.36	0.42
31:f:11:PHE:CE2	31:f:97:ILE:HD13	2.55	0.42
37:l:23:ILE:HG22	49:8:52:A:C2	2.55	0.42
47:5:1981:G:C6	45:ii:57:C:N3	2.85	0.42
47:5:3707:U:H2'	47:5:3708:C:C6	2.55	0.42
50:9:1199:A:H2'	50:9:1200:A:O4'	2.19	0.42
53:CC:176:LYS:O	53:CC:200:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
85:jj:24:THR:HG23	85:jj:89:ILE:HG21	2.00	0.42
85:jj:282:PRO:HG2	85:jj:324:ASN:HD22	1.84	0.42
1:A:179:ILE:O	47:5:3653:A:O3'	2.38	0.42
9:I:145:LYS:HE3	9:I:167:ILE:HD13	2.02	0.42
25:Z:41:ALA:HB2	25:Z:77:TYR:HE1	1.85	0.42
33:h:61:ILE:O	33:h:64:THR:OG1	2.30	0.42
42:r:86:ALA:HB1	42:r:118:LEU:HD23	2.01	0.42
47:5:481(A):C:O2	47:5:481(A):C:O4'	2.36	0.42
47:5:1982:G:C2'	47:5:1983:A:O5'	2.67	0.42
8:H:126:VAL:HG11	8:H:161:ILE:HG23	2.01	0.42
30:e:44:ARG:NH2	47:5:1312:A:O2'	2.53	0.42
42:r:60:VAL:HG22	42:r:117:ILE:HG21	2.02	0.42
50:9:92:A:O4'	55:EE:3:ARG:NH1	2.52	0.42
68:RR:31:ASN:C	68:RR:31:ASN:ND2	2.77	0.42
77:aa:45:VAL:CG2	77:aa:64:LEU:HD13	2.50	0.42
13:N:115:VAL:HA	13:N:134:LEU:HD23	2.01	0.42
26:a:12:ARG:NH1	47:5:2345:G:OP2	2.53	0.42
31:f:79:GLY:HA2	47:5:2066:C:O2'	2.20	0.42
47:5:1867:A:N3	47:5:4403:U:O2'	2.49	0.42
47:5:1962:A:H2	47:5:2026:A:C4	2.13	0.42
50:9:1628:C:H2'	50:9:1629:C:C6	2.54	0.42
75:YY:62:THR:HA	75:YY:69:THR:HG22	2.02	0.42
45:ii:54:G:O2'	85:jj:429:MET:CE	2.68	0.42
85:jj:361:LEU:HD12	85:jj:425:ALA:O	2.20	0.42
2:B:107:ALA:HB2	2:B:201:LEU:HG	2.02	0.41
14:O:18:ARG:NH2	47:5:2057:A:OP1	2.52	0.41
47:5:1982:G:O2'	47:5:1983:A:O5'	2.26	0.41
45:ii:52:C:O3'	85:jj:357:TYR:CA	2.64	0.41
1:A:196:TRP:O	1:A:197:PRO:C	2.63	0.41
7:G:136:PHE:HA	7:G:236:ILE:HD13	2.01	0.41
9:I:153:ARG:HA	9:I:165:ILE:HD11	2.02	0.41
20:U:23:LEU:HD11	20:U:83:LEU:CD2	2.49	0.41
22:W:3:VAL:O	22:W:3:VAL:HG23	2.20	0.41
44:t:98:ILE:HG22	47:5:1978:C:O3'	2.20	0.41
85:jj:100:LYS:HB2	85:jj:367:HIS:CD2	2.55	0.41
2:B:220:ILE:HG12	2:B:278:THR:HG23	2.01	0.41
3:C:340:ILE:HG21	5:E:52:LEU:HD12	2.03	0.41
5:E:153:LEU:HD13	5:E:197:VAL:HG11	2.02	0.41
8:H:26:ILE:C	8:H:26:ILE:HD12	2.44	0.41
20:U:33:ILE:HD12	20:U:96:LEU:HD22	2.02	0.41
50:9:1141:G:H2'	50:9:1142:G:O4'	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
67:QQ:51:LEU:HD22	67:QQ:84:ILE:CD1	2.49	0.41
73:WW:104:LEU:HB3	73:WW:125:ILE:HA	2.01	0.41
82:ff:130:VAL:HG11	82:ff:143:LYS:HZ1	1.85	0.41
10:J:103:GLY:O	10:J:134:LEU:HD12	2.21	0.41
11:L:58:ILE:HG23	11:L:70:VAL:HG11	2.01	0.41
16:Q:61:LEU:HD12	16:Q:82:VAL:HG22	2.02	0.41
34:i:90:LEU:O	34:i:93:VAL:HG22	2.21	0.41
47:5:4187:G:H2'	47:5:4188:U:O4'	2.21	0.41
50:9:1863:A:OP2	77:aa:4:LYS:NZ	2.45	0.41
51:AA:18:PHE:CD2	51:AA:51:LEU:HD22	2.55	0.41
62:LL:61:PRO:HA	62:LL:66:VAL:HG13	2.03	0.41
68:RR:119:VAL:HG13	68:RR:119:VAL:O	2.20	0.41
2:B:317:LEU:HD21	2:B:381:THR:HA	2.03	0.41
7:G:215:ASP:HB3	7:G:216:PRO:HD3	2.02	0.41
8:H:100:PRO:HG2	85:jj:159:GLU:HG2	2.01	0.41
9:I:36:LEU:HD12	9:I:87:ILE:HB	2.03	0.41
25:Z:100:VAL:HG13	25:Z:106:LEU:HB3	2.02	0.41
44:t:131:GLU:CD	47:5:1973:G:H1'	2.46	0.41
47:5:1546:C:N3	47:5:1612:G:O6	2.54	0.41
50:9:1599:U:O2	50:9:1599:U:O4'	2.38	0.41
53:CC:108:LYS:CB	53:CC:233:LEU:HD23	2.50	0.41
56:FF:35:LEU:HD22	56:FF:147:VAL:HG23	2.02	0.41
63:MM:19:GLN:HE22	63:MM:88:TRP:CG	2.39	0.41
83:gg:11:LEU:HB3	83:gg:43:TRP:CZ3	2.56	0.41
45:ii:66:G:C5'	85:jj:360:VAL:HG11	2.50	0.41
7:G:105:THR:HG22	23:X:41:ARG:HD3	2.02	0.41
15:P:79:THR:HG21	47:5:4569:U:O2	2.20	0.41
42:r:24:THR:OG1	47:5:2289:C:N4	2.54	0.41
46:3:75:C:O2	46:3:75:C:O4'	2.34	0.41
47:5:100:C:O2	47:5:100:C:O4'	2.36	0.41
47:5:2638:G:C2	47:5:2639:U:C4	3.08	0.41
47:5:4758:U:O2	47:5:4758:U:O4'	2.37	0.41
55:EE:44:LEU:HD21	55:EE:70:ILE:HG21	2.02	0.41
3:C:38:ASN:O	3:C:42:THR:HG23	2.20	0.41
13:N:9:GLU:CB	34:i:44:ILE:HD13	2.51	0.41
14:O:156:LEU:HD22	47:5:4910:A:C8	2.55	0.41
30:e:31:ILE:HD11	47:5:2347:A:C5	2.55	0.41
55:EE:150:PRO:HA	55:EE:169:ILE:HD11	2.02	0.41
65:OO:44:VAL:HG23	65:OO:81:VAL:HG11	2.03	0.41
65:OO:95:ILE:HD13	65:OO:116:LEU:HD21	2.02	0.41
4:D:244:HIS:O	4:D:248:ARG:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:98:ILE:HG21	47:5:4125:C:H4'	2.01	0.41
12:M:36:ALA:HB2	12:M:52:PHE:CE1	2.55	0.41
47:5:716:C:H2'	47:5:717:U:O4'	2.21	0.41
50:9:1566:G:N7	70:TT:101:ARG:NH2	2.69	0.41
51:AA:134:LEU:HD23	51:AA:144:THR:HG21	2.02	0.41
3:C:198:ASN:OD1	3:C:198:ASN:N	2.53	0.41
16:Q:85:THR:HG22	16:Q:104:ARG:HB2	2.03	0.41
21:V:57:VAL:HG23	21:V:84:GLN:CD	2.46	0.41
24:Y:79:VAL:HG21	24:Y:98:GLY:HA3	2.03	0.41
25:Z:14:LEU:HD21	32:g:92:LYS:HE3	2.02	0.41
44:t:85:LEU:HD21	44:t:104:ILE:HG13	2.02	0.41
44:t:128:THR:O	44:t:131:GLU:HG2	2.21	0.41
44:t:131:GLU:O	44:t:135:THR:HG23	2.20	0.41
47:5:1354:A:N1	47:5:1385:G:O2'	2.50	0.41
47:5:4729:A:O4'	47:5:4966:A:C8	2.74	0.41
50:9:441:C:H2'	50:9:442:C:C6	2.56	0.41
50:9:556:U:H2'	50:9:557:U:O4'	2.21	0.41
53:CC:130:ILE:HG22	53:CC:158:ALA:HB1	2.03	0.41
53:CC:177:PRO:HD3	72:VV:9:VAL:HG21	2.02	0.41
53:CC:196:ILE:HB	53:CC:223:TYR:HB2	2.02	0.41
54:DD:115:VAL:HG21	54:DD:142:LEU:HD23	2.03	0.41
56:FF:87:LEU:CD2	67:QQ:47:LEU:HD13	2.51	0.41
58:HH:66:VAL:N	58:HH:67:PRO:CD	2.83	0.41
61:KK:71:LEU:HD21	61:KK:79:LEU:HD12	2.03	0.41
3:C:130:ALA:HB3	3:C:246:VAL:HG12	2.03	0.41
6:F:115:GLN:CG	16:Q:3:VAL:HG22	2.50	0.41
47:5:1074:G:C2	47:5:1238:A:C2	3.09	0.41
49:8:15:G:C6	49:8:16:G:N1	2.89	0.41
50:9:1256:G:O6	71:UU:65:THR:HG22	2.21	0.41
45:ii:52:C:C3'	85:jj:357:TYR:HA	2.51	0.41
45:ii:54:G:OP1	85:jj:351:GLY:HA3	2.21	0.41
29:d:57:MET:O	29:d:59:THR:N	2.54	0.40
41:p:51:ALA:HB3	41:p:54:ILE:CG2	2.50	0.40
44:t:116:MET:HG3	44:t:132:ILE:HD11	2.03	0.40
47:5:2267:U:O2	47:5:2267:U:O4'	2.37	0.40
47:5:2396:A:N6	47:5:2814:C:O2	2.54	0.40
47:5:3871:A:H2'	47:5:3872:A:O4'	2.21	0.40
50:9:92:A:H2'	50:9:446:G:N2	2.36	0.40
50:9:584:A:H62	50:9:585:C:N4	2.17	0.40
50:9:1650:A:H5''	67:QQ:139:ALA:HB2	2.02	0.40
73:WW:42:MET:HE2	73:WW:49:GLU:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
76:ZZ:92:LEU:HD11	76:ZZ:99:LEU:HD12	2.02	0.40
85:jj:228:LEU:HD23	85:jj:232:LEU:HD13	2.03	0.40
6:F:131:MET:HA	6:F:134:ILE:HG22	2.03	0.40
22:W:9:SER:OG	22:W:36:CYS:SG	2.76	0.40
44:t:123:ARG:O	44:t:128:THR:HG23	2.21	0.40
47:5:4303:C:O2	47:5:4303:C:O4'	2.37	0.40
47:5:4579:U:H2'	47:5:4580:U:O4'	2.21	0.40
73:WW:7:LEU:HD13	73:WW:7:LEU:C	2.47	0.40
47:5:2750:G:H2'	47:5:2751:G:O4'	2.22	0.40
50:9:919:A:C2	50:9:1020:A:C4	3.10	0.40
52:BB:103:MET:SD	52:BB:188:LEU:HD22	2.61	0.40
54:DD:11:PHE:CZ	71:UU:84:ILE:HD11	2.57	0.40
68:RR:24:LEU:HD22	68:RR:54:VAL:HG11	2.02	0.40
75:YY:27:VAL:HG21	75:YY:40:ILE:HD11	2.03	0.40
2:B:168:MET:HE2	2:B:175:GLN:HG2	2.03	0.40
4:D:60:ILE:HD13	4:D:98:ALA:HB2	2.04	0.40
4:D:78:ALA:HB1	4:D:104:LEU:HD13	2.03	0.40
8:H:105:ILE:HG22	8:H:112:VAL:HG22	2.03	0.40
9:I:14:ASN:O	9:I:128:ARG:NH2	2.53	0.40
18:S:97:TYR:CZ	18:S:109:CYS:HA	2.56	0.40
29:d:88:LEU:CD1	29:d:106:VAL:HG22	2.52	0.40
47:5:1679:A:N1	47:5:4391:G:O2'	2.52	0.40
47:5:2367:A:C6	47:5:2788:U:C4	3.10	0.40
50:9:464:A:N7	85:jj:37:ARG:NH2	2.69	0.40
67:QQ:34:VAL:HG21	67:QQ:84:ILE:HD12	2.04	0.40
85:jj:60:LEU:HD22	85:jj:91:ASP:HB2	2.03	0.40
3:C:253:THR:O	3:C:254:GLU:C	2.64	0.40
16:Q:156:PRO:O	26:a:47:LYS:O	2.39	0.40
18:S:154:LEU:HD13	18:S:157:ARG:NH1	2.37	0.40
21:V:3:LYS:HD2	21:V:3:LYS:O	2.21	0.40
47:5:4459:U:H2'	47:5:4460:U:C6	2.56	0.40
50:9:823:U:O5'	50:9:823:U:O2	2.40	0.40
64:NN:33:VAL:HG21	64:NN:66:VAL:HG11	2.03	0.40
71:UU:102:THR:HG21	71:UU:114:VAL:HG21	2.04	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%)	225 (92%)	19 (8%)	2 (1%)	16	45
2	B	392/403 (97%)	364 (93%)	25 (6%)	3 (1%)	16	45
3	C	360/425 (85%)	337 (94%)	21 (6%)	2 (1%)	21	52
4	D	291/297 (98%)	275 (94%)	14 (5%)	2 (1%)	18	49
5	E	208/291 (72%)	189 (91%)	18 (9%)	1 (0%)	24	56
6	F	223/247 (90%)	211 (95%)	11 (5%)	1 (0%)	30	60
7	G	229/319 (72%)	217 (95%)	12 (5%)	0	100	100
8	H	188/192 (98%)	173 (92%)	15 (8%)	0	100	100
9	I	201/214 (94%)	185 (92%)	16 (8%)	0	100	100
10	J	168/178 (94%)	158 (94%)	10 (6%)	0	100	100
11	L	208/211 (99%)	198 (95%)	10 (5%)	0	100	100
12	M	136/218 (62%)	126 (93%)	10 (7%)	0	100	100
13	N	201/204 (98%)	190 (94%)	11 (6%)	0	100	100
14	O	197/203 (97%)	189 (96%)	8 (4%)	0	100	100
15	P	151/184 (82%)	145 (96%)	6 (4%)	0	100	100
16	Q	185/188 (98%)	175 (95%)	9 (5%)	1 (0%)	24	56
17	R	178/196 (91%)	172 (97%)	6 (3%)	0	100	100
18	S	174/176 (99%)	160 (92%)	12 (7%)	2 (1%)	11	40
19	T	157/160 (98%)	146 (93%)	10 (6%)	1 (1%)	21	52
20	U	97/128 (76%)	86 (89%)	11 (11%)	0	100	100
21	V	137/140 (98%)	125 (91%)	12 (9%)	0	100	100
22	W	102/157 (65%)	98 (96%)	3 (3%)	1 (1%)	12	41
23	X	116/156 (74%)	113 (97%)	3 (3%)	0	100	100
24	Y	132/145 (91%)	125 (95%)	7 (5%)	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%)	134 (92%)	11 (8%)	0	100	100
27	b	100/245 (41%)	93 (93%)	6 (6%)	1 (1%)	12	41
28	c	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
29	d	105/125 (84%)	94 (90%)	10 (10%)	1 (1%)	12	41
30	e	126/135 (93%)	118 (94%)	8 (6%)	0	100	100
31	f	107/110 (97%)	101 (94%)	4 (4%)	2 (2%)	6	29
32	g	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
33	h	120/123 (98%)	118 (98%)	1 (1%)	1 (1%)	16	45
34	i	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
35	j	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
36	k	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
37	l	48/51 (94%)	45 (94%)	3 (6%)	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%)	99 (97%)	3 (3%)	0	100	100
41	p	89/92 (97%)	80 (90%)	8 (9%)	1 (1%)	11	40
42	r	122/137 (89%)	110 (90%)	11 (9%)	1 (1%)	16	45
43	s	194/318 (61%)	171 (88%)	22 (11%)	1 (0%)	24	56
44	t	151/165 (92%)	134 (89%)	13 (9%)	4 (3%)	4	24
51	AA	215/295 (73%)	204 (95%)	10 (5%)	1 (0%)	24	56
52	BB	211/264 (80%)	199 (94%)	11 (5%)	1 (0%)	24	56
53	CC	219/293 (75%)	205 (94%)	13 (6%)	1 (0%)	24	56
54	DD	226/243 (93%)	214 (95%)	9 (4%)	3 (1%)	9	35
55	EE	260/263 (99%)	246 (95%)	14 (5%)	0	100	100
56	FF	181/204 (89%)	166 (92%)	11 (6%)	4 (2%)	5	27
57	GG	235/249 (94%)	224 (95%)	10 (4%)	1 (0%)	30	60
58	HH	181/194 (93%)	171 (94%)	10 (6%)	0	100	100
59	II	204/208 (98%)	192 (94%)	11 (5%)	1 (0%)	24	56
60	JJ	183/194 (94%)	177 (97%)	5 (3%)	1 (0%)	24	56
61	KK	94/165 (57%)	88 (94%)	5 (5%)	1 (1%)	11	40
62	LL	139/158 (88%)	129 (93%)	10 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
63	MM	115/132 (87%)	103 (90%)	12 (10%)	0	100	100
64	NN	147/151 (97%)	141 (96%)	6 (4%)	0	100	100
65	OO	134/168 (80%)	122 (91%)	10 (8%)	2 (2%)	8	33
66	PP	127/145 (88%)	117 (92%)	9 (7%)	1 (1%)	16	45
67	QQ	140/146 (96%)	130 (93%)	10 (7%)	0	100	100
68	RR	130/135 (96%)	118 (91%)	11 (8%)	1 (1%)	16	45
69	SS	142/152 (93%)	134 (94%)	8 (6%)	0	100	100
70	TT	139/145 (96%)	132 (95%)	7 (5%)	0	100	100
71	UU	98/119 (82%)	89 (91%)	9 (9%)	0	100	100
72	VV	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
73	WW	127/130 (98%)	120 (94%)	7 (6%)	0	100	100
74	XX	139/143 (97%)	129 (93%)	8 (6%)	2 (1%)	9	34
75	YY	122/130 (94%)	116 (95%)	5 (4%)	1 (1%)	16	45
76	ZZ	73/125 (58%)	71 (97%)	2 (3%)	0	100	100
77	aa	99/115 (86%)	90 (91%)	8 (8%)	1 (1%)	12	41
78	bb	81/84 (96%)	75 (93%)	5 (6%)	1 (1%)	10	37
79	cc	60/69 (87%)	59 (98%)	1 (2%)	0	100	100
80	dd	53/56 (95%)	49 (92%)	3 (6%)	1 (2%)	6	29
81	ee	55/133 (41%)	52 (94%)	3 (6%)	0	100	100
82	ff	66/156 (42%)	61 (92%)	5 (8%)	0	100	100
83	gg	311/317 (98%)	282 (91%)	28 (9%)	1 (0%)	36	66
85	jj	438/462 (95%)	419 (96%)	18 (4%)	1 (0%)	43	72
All	All	11976/13836 (87%)	11207 (94%)	713 (6%)	56 (0%)	26	56

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	t	120	SER
44	t	125	LEU
74	XX	62	PRO
74	XX	86	PRO
3	C	83	GLY
16	Q	14	ARG
33	h	89	ARG

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Mol	Chain	Res	Type
43	s	142	GLY
56	FF	77	MET
60	JJ	147	PHE
66	PP	80	LEU
2	B	17	LEU
5	E	69	ALA
25	Z	91	LEU
29	d	58	GLY
31	f	107	PRO
51	AA	159	ILE
56	FF	43	GLU
56	FF	80	GLY
75	YY	126	GLY
1	A	196	TRP
2	B	259	PRO
4	D	44	TYR
18	S	53	LYS
18	S	155	PRO
27	b	102	PRO
44	t	54	LYS
54	DD	93	THR
61	KK	41	PRO
65	OO	20	GLN
85	jj	259	ILE
1	A	14	SER
2	B	258	HIS
6	F	236	GLU
25	Z	90	PRO
31	f	106	TYR
42	r	33	LYS
54	DD	44	THR
57	GG	135	PRO
77	aa	47	ALA
80	dd	7	TYR
19	T	81	LYS
56	FF	21	GLY
78	bb	81	ARG
44	t	51	GLY
53	CC	171	GLY
65	OO	30	VAL
68	RR	119	VAL
83	gg	224	GLY

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Mol	Chain	Res	Type
41	p	9	GLY
59	II	3	ILE
3	C	90	GLY
4	D	125	VAL
22	W	3	VAL
52	BB	93	GLY
54	DD	48	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	190/199 (96%)	174 (92%)	16 (8%)	10	35
2	B	342/348 (98%)	321 (94%)	21 (6%)	17	45
3	C	302/347 (87%)	282 (93%)	20 (7%)	15	43
4	D	247/250 (99%)	234 (95%)	13 (5%)	20	49
5	E	190/251 (76%)	179 (94%)	11 (6%)	18	47
6	F	196/215 (91%)	185 (94%)	11 (6%)	19	47
7	G	200/272 (74%)	189 (94%)	11 (6%)	19	47
8	H	169/171 (99%)	156 (92%)	13 (8%)	12	38
9	I	175/181 (97%)	164 (94%)	11 (6%)	16	44
10	J	143/149 (96%)	135 (94%)	8 (6%)	19	47
11	L	175/176 (99%)	170 (97%)	5 (3%)	37	62
12	M	117/161 (73%)	109 (93%)	8 (7%)	14	42
13	N	171/172 (99%)	165 (96%)	6 (4%)	32	59
14	O	171/173 (99%)	156 (91%)	15 (9%)	9	33
15	P	134/163 (82%)	127 (95%)	7 (5%)	21	49
16	Q	164/165 (99%)	151 (92%)	13 (8%)	11	37
17	R	159/175 (91%)	145 (91%)	14 (9%)	9	33
18	S	157/157 (100%)	146 (93%)	11 (7%)	14	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	T	139/140 (99%)	132 (95%)	7 (5%)	22	50
20	U	89/114 (78%)	88 (99%)	1 (1%)	65	74
21	V	106/107 (99%)	91 (86%)	15 (14%)	3	15
22	W	86/126 (68%)	84 (98%)	2 (2%)	44	66
23	X	106/134 (79%)	99 (93%)	7 (7%)	15	43
24	Y	124/135 (92%)	118 (95%)	6 (5%)	23	52
25	Z	117/118 (99%)	115 (98%)	2 (2%)	53	70
26	a	119/120 (99%)	116 (98%)	3 (2%)	42	64
27	b	84/184 (46%)	80 (95%)	4 (5%)	23	52
28	c	84/98 (86%)	80 (95%)	4 (5%)	23	52
29	d	98/110 (89%)	92 (94%)	6 (6%)	17	45
30	e	114/121 (94%)	104 (91%)	10 (9%)	9	33
31	f	88/89 (99%)	81 (92%)	7 (8%)	11	37
32	g	98/99 (99%)	91 (93%)	7 (7%)	13	40
33	h	109/110 (99%)	105 (96%)	4 (4%)	30	58
34	i	86/89 (97%)	82 (95%)	4 (5%)	23	52
35	j	73/80 (91%)	69 (94%)	4 (6%)	19	47
36	k	64/65 (98%)	62 (97%)	2 (3%)	35	61
37	l	47/48 (98%)	45 (96%)	2 (4%)	26	54
38	m	48/90 (53%)	44 (92%)	4 (8%)	10	35
39	n	24/24 (100%)	23 (96%)	1 (4%)	26	55
40	o	92/94 (98%)	88 (96%)	4 (4%)	26	54
41	p	74/75 (99%)	71 (96%)	3 (4%)	27	55
42	r	108/121 (89%)	98 (91%)	10 (9%)	8	31
43	s	164/258 (64%)	155 (94%)	9 (6%)	19	47
44	t	126/137 (92%)	122 (97%)	4 (3%)	34	60
51	AA	180/245 (74%)	162 (90%)	18 (10%)	7	27
52	BB	194/231 (84%)	173 (89%)	21 (11%)	6	24
53	CC	187/225 (83%)	173 (92%)	14 (8%)	12	38
54	DD	190/202 (94%)	178 (94%)	12 (6%)	16	44
55	EE	224/225 (100%)	205 (92%)	19 (8%)	10	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
56	FF	158/170 (93%)	147 (93%)	11 (7%)	14	41
57	GG	207/218 (95%)	191 (92%)	16 (8%)	12	38
58	HH	165/174 (95%)	156 (94%)	9 (6%)	19	47
59	II	178/180 (99%)	166 (93%)	12 (7%)	15	43
60	JJ	161/168 (96%)	146 (91%)	15 (9%)	8	31
61	KK	87/136 (64%)	76 (87%)	11 (13%)	4	19
62	LL	130/142 (92%)	115 (88%)	15 (12%)	5	21
63	MM	99/108 (92%)	86 (87%)	13 (13%)	4	17
64	NN	130/131 (99%)	116 (89%)	14 (11%)	6	24
65	OO	106/130 (82%)	100 (94%)	6 (6%)	18	47
66	PP	115/130 (88%)	106 (92%)	9 (8%)	11	37
67	QQ	117/121 (97%)	107 (92%)	10 (8%)	10	34
68	RR	119/121 (98%)	108 (91%)	11 (9%)	8	31
69	SS	125/132 (95%)	109 (87%)	16 (13%)	4	18
70	TT	111/115 (96%)	101 (91%)	10 (9%)	9	32
71	UU	92/107 (86%)	87 (95%)	5 (5%)	20	48
72	VV	67/67 (100%)	64 (96%)	3 (4%)	24	53
73	WW	112/113 (99%)	103 (92%)	9 (8%)	11	37
74	XX	113/115 (98%)	109 (96%)	4 (4%)	32	59
75	YY	107/112 (96%)	96 (90%)	11 (10%)	7	26
76	ZZ	66/103 (64%)	59 (89%)	7 (11%)	6	25
77	aa	88/98 (90%)	82 (93%)	6 (7%)	14	42
78	bb	75/76 (99%)	69 (92%)	6 (8%)	11	37
79	cc	55/62 (89%)	50 (91%)	5 (9%)	9	32
80	dd	48/49 (98%)	46 (96%)	2 (4%)	26	55
81	ee	47/106 (44%)	45 (96%)	2 (4%)	26	54
82	ff	61/140 (44%)	53 (87%)	8 (13%)	4	17
83	gg	272/275 (99%)	264 (97%)	8 (3%)	37	62
85	jj	365/378 (97%)	355 (97%)	10 (3%)	39	63
All	All	10420/11716 (89%)	9726 (93%)	694 (7%)	17	43

All (694) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ILE
1	A	64	ARG
1	A	71	LYS
1	A	102	LEU
1	A	109	GLU
1	A	128	ARG
1	A	158	ILE
1	A	163	ARG
1	A	175	ILE
1	A	200	ARG
1	A	207	VAL
1	A	221	LYS
1	A	233	ARG
1	A	235	VAL
1	A	242	ARG
1	A	243	THR
2	B	10	ARG
2	B	17	LEU
2	B	53	MET
2	B	56	ILE
2	B	60	VAL
2	B	66	LYS
2	B	74	GLU
2	B	90	VAL
2	B	135	LYS
2	B	173	LEU
2	B	204	GLN
2	B	248	LEU
2	B	262	VAL
2	B	279	GLU
2	B	294	LYS
2	B	314	ILE
2	B	333	LEU
2	B	351	LEU
2	B	356	LYS
2	B	366	LYS
2	B	383	GLU
3	C	20	LYS
3	C	29	LYS
3	C	89	GLN
3	C	95	MET
3	C	101	MET
3	C	124	ILE

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Mol	Chain	Res	Type
3	C	144	ILE
3	C	150	LEU
3	C	165	LYS
3	C	175	LYS
3	C	193	LYS
3	C	198	ASN
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	322	LEU
3	C	333	LYS
4	D	37	VAL
4	D	45	ASN
4	D	50	ARG
4	D	56	THR
4	D	89	LYS
4	D	104	LEU
4	D	110	LEU
4	D	124	GLU
4	D	202	GLN
4	D	221	LYS
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	143	LEU
5	E	144	ARG
5	E	169	LYS
5	E	178	VAL
5	E	189	LEU
5	E	197	VAL
5	E	213	LYS
5	E	291	PHE
6	F	38	GLN
6	F	46	ARG
6	F	65	ARG
6	F	67	GLU

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Mol	Chain	Res	Type
6	F	88	LEU
6	F	134	ILE
6	F	151	GLU
6	F	198	LYS
6	F	211	LYS
6	F	231	ASP
6	F	245	ARG
7	G	148	LEU
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	229	LYS
7	G	230	MET
7	G	293	ASN
7	G	312	LYS
8	H	1	MET
8	H	20	LEU
8	H	52	LYS
8	H	59	LYS
8	H	66	GLU
8	H	74	CYS
8	H	82	LYS
8	H	105	ILE
8	H	106	GLN
8	H	128	MET
8	H	129	ARG
8	H	141	LYS
8	H	173	ARG
9	I	36	LEU
9	I	39	LYS
9	I	97	ILE
9	I	116	ARG
9	I	146	GLU
9	I	153	ARG
9	I	154	ARG
9	I	163	GLN
9	I	164	LYS
9	I	208	LYS
9	I	212	LEU

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Mol	Chain	Res	Type
10	J	16	ARG
10	J	28	GLU
10	J	33	LEU
10	J	81	GLU
10	J	96	LYS
10	J	113	ILE
10	J	128	LEU
10	J	175	LEU
11	L	46	ILE
11	L	59	VAL
11	L	63	THR
11	L	162	LYS
11	L	186	ARG
12	M	2	VAL
12	M	8	GLU
12	M	32	ASP
12	M	37	LEU
12	M	57	LEU
12	M	62	LEU
12	M	96	GLU
12	M	105	THR
13	N	9	GLU
13	N	44	ARG
13	N	64	ILE
13	N	72	LYS
13	N	89	VAL
13	N	199	GLN
14	O	27	VAL
14	O	36	VAL
14	O	37	ARG
14	O	67	SER
14	O	82	ARG
14	O	128	ARG
14	O	129	LEU
14	O	130	LYS
14	O	140	ARG
14	O	145	VAL
14	O	157	GLU
14	O	165	LYS
14	O	175	MET
14	O	179	LYS
14	O	202	LEU

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Mol	Chain	Res	Type
15	P	36	ILE
15	P	57	CYS
15	P	69	ARG
15	P	86	LYS
15	P	91	LEU
15	P	128	ARG
15	P	147	GLU
16	Q	3	VAL
16	Q	22	ASP
16	Q	31	LEU
16	Q	38	ARG
16	Q	61	LEU
16	Q	63	LEU
16	Q	91	ARG
16	Q	95	VAL
16	Q	115	LYS
16	Q	126	LEU
16	Q	140	SER
16	Q	143	ARG
16	Q	172	ARG
17	R	6	LEU
17	R	10	LEU
17	R	36	ASN
17	R	40	GLN
17	R	50	ILE
17	R	82	LYS
17	R	89	MET
17	R	98	ARG
17	R	99	MET
17	R	103	ARG
17	R	113	LYS
17	R	138	LEU
17	R	148	ASP
17	R	178	GLN
18	S	7	LEU
18	S	9	GLU
18	S	13	VAL
18	S	24	THR
18	S	67	VAL
18	S	70	LYS
18	S	82	LEU
18	S	95	ARG

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Mol	Chain	Res	Type
18	S	149	LYS
18	S	159	LEU
18	S	174	THR
19	T	5	LYS
19	T	33	ILE
19	T	60	LYS
19	T	96	ILE
19	T	144	ASN
19	T	152	GLU
19	T	159	MET
20	U	33	ILE
21	V	2	SER
21	V	3	LYS
21	V	6	ARG
21	V	15	ARG
21	V	18	LEU
21	V	35	LYS
21	V	46	LYS
21	V	51	ARG
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
22	W	41	LEU
22	W	91	MET
23	X	39	LYS
23	X	52	LEU
23	X	53	ARG
23	X	59	LYS
23	X	63	LYS
23	X	95	THR
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	11	VAL

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Mol	Chain	Res	Type
25	Z	33	THR
26	a	4	ARG
26	a	59	ARG
26	a	122	VAL
27	b	9	THR
27	b	22	LYS
27	b	40	LEU
27	b	101	HIS
28	c	28	VAL
28	c	37	MET
28	c	50	ASN
28	c	78	ASN
29	d	23	ARG
29	d	26	THR
29	d	44	ARG
29	d	48	GLU
29	d	78	ARG
29	d	98	SER
30	e	9	LYS
30	e	11	LYS
30	e	21	ILE
30	e	22	ARG
30	e	64	LYS
30	e	78	LEU
30	e	86	GLU
30	e	106	LYS
30	e	113	GLU
30	e	128	ARG
31	f	5	LEU
31	f	7	CYS
31	f	23	GLU
31	f	33	VAL
31	f	52	LYS
31	f	80	ASN
31	f	101	ILE
32	g	15	THR
32	g	43	LYS
32	g	53	LEU
32	g	54	ARG
32	g	60	ARG
32	g	66	ARG
32	g	114	GLN

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Mol	Chain	Res	Type
33	h	14	LYS
33	h	28	LEU
33	h	67	GLU
33	h	89	ARG
34	i	33	LEU
34	i	34	THR
34	i	77	VAL
34	i	86	LYS
35	j	3	LYS
35	j	11	ARG
35	j	58	THR
35	j	63	ARG
36	k	69	LEU
36	k	70	LYS
37	l	11	ARG
37	l	16	LYS
38	m	59	LEU
38	m	71	ARG
38	m	92	THR
38	m	93	ASN
39	n	13	LEU
40	o	17	LYS
40	o	28	LYS
40	o	36	GLN
40	o	61	LYS
41	p	8	VAL
41	p	30	GLU
41	p	84	ARG
42	r	8	MET
42	r	10	VAL
42	r	18	ILE
42	r	32	LEU
42	r	39	ARG
42	r	67	ARG
42	r	80	THR
42	r	90	LEU
42	r	103	HIS
42	r	118	LEU
43	s	38	LYS
43	s	61	MET
43	s	68	HIS
43	s	95	LEU

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Mol	Chain	Res	Type
43	s	105	ASN
43	s	146	LYS
43	s	149	ARG
43	s	187	LEU
43	s	191	GLN
44	t	37	LEU
44	t	72	GLU
44	t	98	ILE
44	t	133	LEU
51	AA	5	LEU
51	AA	12	GLU
51	AA	15	VAL
51	AA	50	ASN
51	AA	56	GLU
51	AA	58	LEU
51	AA	59	LEU
51	AA	60	LEU
51	AA	109	THR
51	AA	132	GLN
51	AA	136	GLU
51	AA	163	CYS
51	AA	171	VAL
51	AA	178	LEU
51	AA	189	ILE
51	AA	192	GLU
51	AA	198	MET
51	AA	200	ASP
52	BB	29	ASP
52	BB	50	THR
52	BB	63	LYS
52	BB	71	LEU
52	BB	73	ASP
52	BB	82	ARG
52	BB	88	THR
52	BB	92	GLN
52	BB	105	LEU
52	BB	107	ARG
52	BB	125	VAL
52	BB	126	ASP
52	BB	129	THR
52	BB	157	GLN
52	BB	175	GLU

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Mol	Chain	Res	Type
52	BB	181	LEU
52	BB	207	LEU
52	BB	209	ASP
52	BB	213	ARG
52	BB	225	LEU
52	BB	231	LEU
53	CC	78	LEU
53	CC	106	VAL
53	CC	114	LYS
53	CC	117	ARG
53	CC	121	ARG
53	CC	137	VAL
53	CC	146	GLU
53	CC	160	LEU
53	CC	167	ARG
53	CC	192	LEU
53	CC	196	ILE
53	CC	247	THR
53	CC	252	THR
53	CC	255	LEU
54	DD	28	GLU
54	DD	51	LEU
54	DD	65	ARG
54	DD	72	VAL
54	DD	123	LEU
54	DD	127	MET
54	DD	137	VAL
54	DD	142	LEU
54	DD	168	VAL
54	DD	216	GLU
54	DD	218	LEU
54	DD	223	ILE
55	EE	6	LYS
55	EE	21	ASP
55	EE	23	LEU
55	EE	42	LEU
55	EE	49	ARG
55	EE	50	ASN
55	EE	51	ARG
55	EE	65	CYS
55	EE	67	GLN
55	EE	77	ARG

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Mol	Chain	Res	Type
55	EE	81	THR
55	EE	123	LEU
55	EE	133	THR
55	EE	196	THR
55	EE	205	PHE
55	EE	222	LEU
55	EE	232	ASN
55	EE	238	LEU
55	EE	246	LEU
56	FF	19	LEU
56	FF	49	LEU
56	FF	55	ARG
56	FF	71	ARG
56	FF	88	MET
56	FF	89	THR
56	FF	124	ASP
56	FF	140	ASP
56	FF	169	ILE
56	FF	173	LEU
56	FF	199	VAL
57	GG	15	LEU
57	GG	41	LEU
57	GG	63	MET
57	GG	67	VAL
57	GG	121	ILE
57	GG	129	VAL
57	GG	135	PRO
57	GG	144	LEU
57	GG	170	ARG
57	GG	171	THR
57	GG	178	ARG
57	GG	183	ARG
57	GG	190	ARG
57	GG	201	LYS
57	GG	208	GLU
57	GG	216	ARG
58	HH	8	ILE
58	HH	36	LEU
58	HH	50	GLU
58	HH	76	GLN
58	HH	82	GLU
58	HH	100	ILE

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Mol	Chain	Res	Type
58	HH	121	THR
58	HH	145	ARG
58	HH	149	ASP
59	II	26	LYS
59	II	73	THR
59	II	74	ARG
59	II	100	CYS
59	II	121	LEU
59	II	130	THR
59	II	145	ILE
59	II	161	LEU
59	II	165	GLN
59	II	168	GLN
59	II	178	ARG
59	II	190	LEU
60	JJ	18	ARG
60	JJ	28	GLU
60	JJ	29	LEU
60	JJ	38	ARG
60	JJ	40	LYS
60	JJ	45	ARG
60	JJ	50	LEU
60	JJ	89	GLU
60	JJ	94	LEU
60	JJ	103	GLU
60	JJ	108	ARG
60	JJ	109	ARG
60	JJ	110	LEU
60	JJ	116	LYS
60	JJ	133	ARG
61	KK	1	MET
61	KK	2	LEU
61	KK	6	LYS
61	KK	21	MET
61	KK	29	MET
61	KK	40	VAL
61	KK	43	LEU
61	KK	50	GLN
61	KK	60	GLU
61	KK	89	ILE
61	KK	96	ARG
62	LL	16	ILE

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Mol	Chain	Res	Type
62	LL	20	LYS
62	LL	23	VAL
62	LL	32	LYS
62	LL	39	ASN
62	LL	40	ILE
62	LL	42	LEU
62	LL	49	GLU
62	LL	56	ILE
62	LL	69	ARG
62	LL	78	THR
62	LL	85	THR
62	LL	121	GLN
62	LL	126	VAL
62	LL	134	LEU
63	MM	19	GLN
63	MM	22	LEU
63	MM	24	THR
63	MM	31	LEU
63	MM	33	ARG
63	MM	40	LYS
63	MM	42	LEU
63	MM	49	LEU
63	MM	55	ASN
63	MM	85	LEU
63	MM	99	LYS
63	MM	101	ARG
63	MM	110	VAL
64	NN	9	LYS
64	NN	13	GLN
64	NN	27	LYS
64	NN	45	LEU
64	NN	49	GLN
64	NN	53	ILE
64	NN	55	ARG
64	NN	60	VAL
64	NN	70	LYS
64	NN	78	LYS
64	NN	80	LEU
64	NN	86	GLU
64	NN	107	LYS
64	NN	132	LYS
65	OO	51	GLU

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Mol	Chain	Res	Type
65	OO	56	VAL
65	OO	119	LEU
65	OO	131	ASP
65	OO	146	ARG
65	OO	151	LEU
66	PP	13	ARG
66	PP	14	LYS
66	PP	15	PHE
66	PP	27	ASP
66	PP	37	TYR
66	PP	76	VAL
66	PP	83	MET
66	PP	101	THR
66	PP	108	LYS
67	QQ	7	LEU
67	QQ	26	LYS
67	QQ	31	LEU
67	QQ	41	MET
67	QQ	46	THR
67	QQ	50	LYS
67	QQ	53	GLU
67	QQ	60	LYS
67	QQ	138	ARG
67	QQ	140	ARG
68	RR	5	ARG
68	RR	7	LYS
68	RR	31	ASN
68	RR	44	LYS
68	RR	62	GLN
68	RR	78	ARG
68	RR	88	VAL
68	RR	93	GLN
68	RR	98	VAL
68	RR	99	ASP
68	RR	105	MET
69	SS	8	LYS
69	SS	12	ILE
69	SS	36	VAL
69	SS	45	LEU
69	SS	46	ARG
69	SS	52	LEU
69	SS	59	LEU

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Mol	Chain	Res	Type
69	SS	60	THR
69	SS	63	GLU
69	SS	67	VAL
69	SS	86	ARG
69	SS	98	VAL
69	SS	99	LEU
69	SS	110	ASP
69	SS	132	ARG
69	SS	145	THR
70	TT	5	THR
70	TT	28	LEU
70	TT	39	LEU
70	TT	62	ARG
70	TT	102	ARG
70	TT	108	GLU
70	TT	110	LEU
70	TT	112	MET
70	TT	124	THR
70	TT	142	LYS
71	UU	56	MET
71	UU	76	THR
71	UU	88	LEU
71	UU	105	SER
71	UU	106	ILE
72	VV	32	ILE
72	VV	34	MET
72	VV	66	ASP
73	WW	23	ARG
73	WW	36	ARG
73	WW	51	GLU
73	WW	83	LEU
73	WW	85	ASP
73	WW	90	GLN
73	WW	103	VAL
73	WW	104	LEU
73	WW	106	THR
74	XX	7	LEU
74	XX	29	LYS
74	XX	67	ARG
74	XX	115	ILE
75	YY	8	ARG
75	YY	16	ARG

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Mol	Chain	Res	Type
75	YY	17	LEU
75	YY	32	LYS
75	YY	40	ILE
75	YY	46	LYS
75	YY	47	MET
75	YY	74	MET
75	YY	80	ASP
75	YY	88	LYS
75	YY	115	LYS
76	ZZ	52	LYS
76	ZZ	64	ASN
76	ZZ	69	THR
76	ZZ	89	GLN
76	ZZ	92	LEU
76	ZZ	99	LEU
76	ZZ	106	GLN
77	aa	12	LYS
77	aa	21	ILE
77	aa	41	ILE
77	aa	44	ILE
77	aa	55	GLU
77	aa	67	LEU
78	bb	25	VAL
78	bb	29	ASN
78	bb	42	LYS
78	bb	64	CYS
78	bb	72	ARG
78	bb	81	ARG
79	cc	27	CYS
79	cc	31	ARG
79	cc	38	THR
79	cc	40	ARG
79	cc	68	LEU
80	dd	32	ARG
80	dd	38	MET
81	ee	99	LYS
81	ee	124	LYS
82	ff	83	LYS
82	ff	86	THR
82	ff	94	LYS
82	ff	99	LYS
82	ff	110	GLU

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Mol	Chain	Res	Type
82	ff	113	LYS
82	ff	138	ARG
82	ff	140	TYR
83	gg	11	LEU
83	gg	17	TRP
83	gg	20	GLN
83	gg	119	GLN
83	gg	198	VAL
83	gg	207	CYS
83	gg	289	LEU
83	gg	305	ASN
85	jj	30	LYS
85	jj	34	ILE
85	jj	75	ILE
85	jj	102	MET
85	jj	148	LEU
85	jj	232	LEU
85	jj	313	LYS
85	jj	362	ASP
85	jj	392	LYS
85	jj	394	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
2	B	175	GLN
2	B	203	GLN
2	B	271	GLN
3	C	119	GLN
3	C	187	GLN
3	C	310	HIS
3	C	329	ASN
4	D	9	ASN
5	E	185	ASN
5	E	259	GLN
7	G	135	GLN
7	G	161	GLN
7	G	194	ASN
7	G	206	GLN
7	G	261	ASN
7	G	293	ASN

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Mol	Chain	Res	Type
8	H	98	HIS
8	H	162	GLN
9	I	51	HIS
9	I	59	GLN
9	I	73	ASN
9	I	86	HIS
9	I	95	HIS
10	J	71	HIS
11	L	27	ASN
11	L	28	GLN
11	L	87	HIS
14	O	50	ASN
14	O	63	ASN
15	P	34	GLN
15	P	40	HIS
15	P	56	GLN
15	P	137	ASN
15	P	145	HIS
16	Q	8	ASN
16	Q	57	ASN
16	Q	188	ASN
17	R	34	ASN
17	R	75	HIS
17	R	158	GLN
18	S	37	HIS
19	T	69	GLN
19	T	144	ASN
21	V	135	ASN
22	W	79	GLN
23	X	57	GLN
24	Y	56	GLN
26	a	67	GLN
26	a	85	GLN
27	b	60	ASN
29	d	30	HIS
30	e	57	ASN
30	e	92	ASN
31	f	24	HIS
32	g	14	ASN
33	h	107	GLN
33	h	108	GLN
38	m	78	HIS

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Mol	Chain	Res	Type
38	m	94	ASN
42	r	121	GLN
43	s	34	ASN
43	s	179	ASN
44	t	65	GLN
44	t	95	GLN
44	t	115	GLN
51	AA	81	ASN
51	AA	111	GLN
51	AA	113	GLN
52	BB	208	HIS
53	CC	115	GLN
54	DD	145	GLN
54	DD	226	GLN
55	EE	98	ASN
56	FF	29	GLN
56	FF	83	ASN
56	FF	137	GLN
58	HH	114	GLN
58	HH	168	HIS
59	II	64	ASN
59	II	146	GLN
60	JJ	132	GLN
60	JJ	143	ASN
60	JJ	156	HIS
61	KK	32	HIS
61	KK	42	ASN
61	KK	84	HIS
63	MM	19	GLN
63	MM	55	ASN
64	NN	49	GLN
64	NN	62	GLN
64	NN	69	ASN
65	OO	20	GLN
66	PP	54	HIS
67	QQ	24	HIS
69	SS	135	HIS
72	VV	35	ASN
72	VV	47	ASN
73	WW	15	ASN
75	YY	85	ASN
76	ZZ	89	GLN

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Mol	Chain	Res	Type
77	aa	7	ASN
77	aa	86	ASN
78	bb	26	GLN
78	bb	51	GLN
78	bb	65	GLN
81	ee	88	GLN
82	ff	91	ASN
83	gg	14	HIS
83	gg	159	ASN
83	gg	196	ASN
83	gg	222	ASN
83	gg	305	ASN
85	jj	9	ASN
85	jj	367	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	2	73/76 (96%)	14 (19%)	1 (1%)
45	ii	74/76 (97%)	20 (27%)	0
46	3	72/75 (96%)	28 (38%)	2 (2%)
47	5	3518/3543 (99%)	885 (25%)	171 (4%)
48	7	118/120 (98%)	12 (10%)	1 (0%)
49	8	150/156 (96%)	34 (22%)	7 (4%)
50	9	1681/1869 (89%)	426 (25%)	65 (3%)
84	hh	9/10 (90%)	1 (11%)	0
All	All	5695/5925 (96%)	1420 (24%)	247 (4%)

All (1420) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	2	9	A
45	2	13	U
45	2	16	C
45	2	19	G
45	2	21	A
45	2	34	A
45	2	43	A
45	2	46	G
45	2	47	U
45	2	49	C

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Mol	Chain	Res	Type
45	2	61	C
45	2	64	G
45	2	72	C
45	2	75	C
46	3	7	A
46	3	13	C
46	3	14	A
46	3	16	C
46	3	21	A
46	3	25	C
46	3	28	C
46	3	29	A
46	3	34	U
46	3	35	U
46	3	36	U
46	3	40	C
46	3	42	G
46	3	47	U
46	3	49	C
46	3	51	G
46	3	58	A
46	3	60	U
46	3	61	C
46	3	63	C
46	3	65	G
46	3	69	G
46	3	70	G
46	3	71	G
46	3	72	C
46	3	74	C
46	3	75	C
46	3	76	A
47	5	6	C
47	5	12	A
47	5	13	U
47	5	15	A
47	5	25	A
47	5	30	C
47	5	35	U
47	5	39	A
47	5	40	G
47	5	42	A

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Mol	Chain	Res	Type
47	5	43	U
47	5	44	A
47	5	48	G
47	5	49	U
47	5	56	A
47	5	58	G
47	5	59	A
47	5	64	A
47	5	65	A
47	5	73	A
47	5	75	G
47	5	91	G
47	5	93	G
47	5	107	G
47	5	108	A
47	5	109	G
47	5	116	G
47	5	118	C
47	5	119	G
47	5	120	A
47	5	126	C
47	5	134	G
47	5	135	G
47	5	136	C
47	5	143	C
47	5	144	G
47	5	159	C
47	5	160	G
47	5	172	C
47	5	173	C
47	5	177	G
47	5	179	G
47	5	197	A
47	5	200	U
47	5	201	C
47	5	205	C
47	5	209	U
47	5	216	C
47	5	217	C
47	5	218	A
47	5	220	C
47	5	221	C

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Mol	Chain	Res	Type
47	5	224	U
47	5	226	G
47	5	227	A
47	5	233	U
47	5	234	G
47	5	246	G
47	5	253	G
47	5	255	C
47	5	262	G
47	5	263	G
47	5	265	C
47	5	266	C
47	5	275	C
47	5	276	C
47	5	278	G
47	5	279	A
47	5	280	G
47	5	297	U
47	5	306	A
47	5	309	C
47	5	310	G
47	5	315	G
47	5	316	U
47	5	322	C
47	5	334	A
47	5	340	C
47	5	350	C
47	5	354	U
47	5	357	U
47	5	363	A
47	5	365	U
47	5	379	G
47	5	386	A
47	5	387	G
47	5	399	G
47	5	407	A
47	5	408	A
47	5	409	G
47	5	410	A
47	5	412	G
47	5	413	G
47	5	431	G

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Mol	Chain	Res	Type
47	5	432	U
47	5	446	C
47	5	449	C
47	5	450	G
47	5	452	A
47	5	453	G
47	5	454	U
47	5	455	C
47	5	457	G
47	5	464	G
47	5	466	A
47	5	467	U
47	5	468	U
47	5	469	C
47	5	481	G
47	5	481(A)	C
47	5	482	G
47	5	483	G
47	5	484	U
47	5	485	C
47	5	486	C
47	5	492	U
47	5	493	G
47	5	495	C
47	5	497	G
47	5	498	C
47	5	499	G
47	5	505	G
47	5	510	U
47	5	649	A
47	5	654	C
47	5	658	C
47	5	667	A
47	5	668	C
47	5	669	C
47	5	670	G
47	5	672	C
47	5	683	C
47	5	684	G
47	5	685	C
47	5	687	U
47	5	696	C

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Mol	Chain	Res	Type
47	5	697	G
47	5	704	C
47	5	705	G
47	5	708	G
47	5	719	C
47	5	722	G
47	5	729	G
47	5	730	G
47	5	731	G
47	5	734	G
47	5	738	C
47	5	738(A)	C
47	5	739	G
47	5	744	G
47	5	747	A
47	5	748	G
47	5	749	G
47	5	752	G
47	5	756	G
47	5	758	G
47	5	911	U
47	5	913	U
47	5	914	U
47	5	917	A
47	5	918	G
47	5	922(B)	C
47	5	923	C
47	5	924	C
47	5	925	C
47	5	926	G
47	5	929	A
47	5	931	C
47	5	932	A
47	5	933	G
47	5	934	C
47	5	935	A
47	5	935(A)	G
47	5	936	C
47	5	937	U
47	5	939	G
47	5	941	C
47	5	944	A

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Mol	Chain	Res	Type
47	5	945	U
47	5	955	G
47	5	956	A
47	5	959	G
47	5	960	A
47	5	961	G
47	5	962	C
47	5	963	G
47	5	964	A
47	5	965	G
47	5	966	A
47	5	967	C
47	5	968	C
47	5	969	C
47	5	972	C
47	5	973	G
47	5	979	C
47	5	983	C
47	5	990	C
47	5	1072	C
47	5	1073	G
47	5	1075	G
47	5	1076	C
47	5	1078	A
47	5	1079	C
47	5	1082	C
47	5	1177	U
47	5	1179	U
47	5	1180	C
47	5	1184	A
47	5	1185	G
47	5	1195	G
47	5	1209	U
47	5	1210	C
47	5	1211	G
47	5	1212	G
47	5	1214	C
47	5	1215	C
47	5	1234	G
47	5	1235	G
47	5	1236	C
47	5	1237	C

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Mol	Chain	Res	Type
47	5	1238	A
47	5	1239	C
47	5	1272	C
47	5	1273	G
47	5	1274	A
47	5	1275	G
47	5	1276	C
47	5	1280	C
47	5	1284	G
47	5	1285	U
47	5	1287	G
47	5	1288	G
47	5	1291	G
47	5	1292	C
47	5	1293	G
47	5	1295	U
47	5	1296	G
47	5	1301	C
47	5	1303	A
47	5	1304	C
47	5	1326	A
47	5	1328	G
47	5	1329	G
47	5	1330	A
47	5	1337	A
47	5	1354	A
47	5	1359	G
47	5	1364	U
47	5	1370	G
47	5	1371	A
47	5	1377	G
47	5	1378	C
47	5	1379	C
47	5	1380	G
47	5	1381	U
47	5	1387	A
47	5	1394	G
47	5	1397	A
47	5	1398	A
47	5	1401	C
47	5	1403	G
47	5	1416	G

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Mol	Chain	Res	Type
47	5	1419	G
47	5	1420	A
47	5	1421	G
47	5	1436	C
47	5	1437	C
47	5	1438	U
47	5	1440	U
47	5	1441	C
47	5	1442	C
47	5	1445	U
47	5	1446	C
47	5	1453	G
47	5	1455	G
47	5	1456	C
47	5	1457	G
47	5	1458	C
47	5	1475	G
47	5	1477	C
47	5	1478	C
47	5	1481	C
47	5	1482	G
47	5	1483	C
47	5	1484	G
47	5	1485	C
47	5	1486	C
47	5	1489	G
47	5	1497	A
47	5	1498	G
47	5	1502	G
47	5	1516	G
47	5	1518	A
47	5	1523	A
47	5	1534	A
47	5	1535	C
47	5	1547	A
47	5	1554	A
47	5	1563	A
47	5	1564	A
47	5	1566	C
47	5	1578	U
47	5	1591	U
47	5	1592	G

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Mol	Chain	Res	Type
47	5	1596	U
47	5	1602	U
47	5	1612	G
47	5	1613	A
47	5	1624	G
47	5	1625	G
47	5	1626	G
47	5	1631	A
47	5	1633	G
47	5	1634	A
47	5	1640	C
47	5	1654	G
47	5	1661	C
47	5	1676	C
47	5	1677	U
47	5	1726	U
47	5	1729	A
47	5	1733	G
47	5	1734	G
47	5	1741	G
47	5	1742	A
47	5	1750	G
47	5	1753	G
47	5	1755	C
47	5	1756	U
47	5	1757	U
47	5	1761	G
47	5	1763	C
47	5	1764	G
47	5	1768	C
47	5	1772	C
47	5	1773	U
47	5	1776	A
47	5	1781	U
47	5	1787	A
47	5	1797	G
47	5	1799	G
47	5	1803	G
47	5	1804	A
47	5	1805	A
47	5	1819	G
47	5	1821	G

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Mol	Chain	Res	Type
47	5	1822	U
47	5	1828	C
47	5	1833	G
47	5	1834	U
47	5	1835	G
47	5	1836	G
47	5	1837	A
47	5	1842	G
47	5	1855	G
47	5	1867	A
47	5	1869	G
47	5	1897	A
47	5	1910	G
47	5	1918	U
47	5	1919	G
47	5	1920	C
47	5	1921	C
47	5	1922	G
47	5	1923	A
47	5	1931	C
47	5	1933	G
47	5	1935	C
47	5	1936	C
47	5	1941	A
47	5	1948	G
47	5	1951	G
47	5	1952	G
47	5	1957	U
47	5	1959	U
47	5	1961	G
47	5	1962	A
47	5	1964	A
47	5	1965	G
47	5	1976	G
47	5	1977	C
47	5	1979	A
47	5	1980	U
47	5	1982	G
47	5	1983	A
47	5	1984	A
47	5	1986	U
47	5	1987	C

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Mol	Chain	Res	Type
47	5	1988	G
47	5	1991	A
47	5	1993	C
47	5	1997	U
47	5	2001	G
47	5	2002	A
47	5	2003	G
47	5	2004	U
47	5	2007	G
47	5	2008	U
47	5	2009	A
47	5	2010	A
47	5	2011	C
47	5	2016	C
47	5	2024	G
47	5	2025	A
47	5	2026	A
47	5	2033	A
47	5	2040	A
47	5	2047	A
47	5	2048	U
47	5	2052	G
47	5	2055	G
47	5	2056	G
47	5	2058	G
47	5	2062	C
47	5	2064	G
47	5	2069	A
47	5	2070	U
47	5	2084	U
47	5	2085	G
47	5	2089	G
47	5	2090	U
47	5	2092	G
47	5	2093	G
47	5	2094	C
47	5	2095	A
47	5	2097	A
47	5	2098	G
47	5	2100	G
47	5	2101	A
47	5	2102	G

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Mol	Chain	Res	Type
47	5	2104	A
47	5	2105	A
47	5	2106	G
47	5	2107	A
47	5	2108	G
47	5	2110	G
47	5	2259	G
47	5	2260	C
47	5	2262	G
47	5	2266	C
47	5	2267	U
47	5	2268	A
47	5	2269	C
47	5	2270	G
47	5	2274	C
47	5	2275	G
47	5	2279	A
47	5	2289	C
47	5	2299	G
47	5	2300	A
47	5	2301	G
47	5	2313	A
47	5	2314	G
47	5	2316	G
47	5	2325	C
47	5	2331	G
47	5	2332	A
47	5	2333	G
47	5	2348	G
47	5	2351	C
47	5	2364	G
47	5	2370	A
47	5	2371	U
47	5	2374	A
47	5	2395	A
47	5	2396	A
47	5	2397	G
47	5	2399	G
47	5	2402	G
47	5	2416	G
47	5	2417	A
47	5	2422	C

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Mol	Chain	Res	Type
47	5	2424	G
47	5	2425	U
47	5	2428	A
47	5	2429	A
47	5	2433	G
47	5	2441	C
47	5	2447	U
47	5	2450	G
47	5	2467	U
47	5	2468	U
47	5	2469	C
47	5	2470	C
47	5	2471	G
47	5	2475	G
47	5	2479	G
47	5	2483	G
47	5	2485	U
47	5	2488	C
47	5	2489	C
47	5	2490	U
47	5	2491	C
47	5	2493	G
47	5	2495	U
47	5	2503	G
47	5	2504	C
47	5	2505	C
47	5	2506	G
47	5	2512	A
47	5	2513	A
47	5	2530	U
47	5	2537	A
47	5	2546	G
47	5	2547	G
47	5	2553	A
47	5	2554	U
47	5	2555	G
47	5	2558	C
47	5	2564	G
47	5	2566	G
47	5	2571	C
47	5	2572	C
47	5	2575	U

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Mol	Chain	Res	Type
47	5	2583	C
47	5	2586	G
47	5	2587	A
47	5	2588	C
47	5	2601	A
47	5	2620	G
47	5	2627	C
47	5	2638	G
47	5	2640	G
47	5	2647	A
47	5	2661	U
47	5	2662	G
47	5	2663	G
47	5	2669	C
47	5	2670	C
47	5	2673	G
47	5	2676	A
47	5	2681	G
47	5	2686	G
47	5	2687	U
47	5	2688	G
47	5	2689	C
47	5	2695	A
47	5	2696	A
47	5	2707	U
47	5	2708	U
47	5	2709	C
47	5	2710	C
47	5	2711	G
47	5	2712	G
47	5	2714	G
47	5	2716	C
47	5	2719	C
47	5	2721	G
47	5	2725	A
47	5	2726	G
47	5	2740	U
47	5	2743	A
47	5	2744	A
47	5	2754	G
47	5	2760	G
47	5	2761	U

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Mol	Chain	Res	Type
47	5	2763	U
47	5	2764	A
47	5	2769	U
47	5	2772	C
47	5	2787	A
47	5	2788	U
47	5	2789	A
47	5	2790	U
47	5	2794	C
47	5	2795	A
47	5	2796	G
47	5	2798	A
47	5	2806	A
47	5	2807	A
47	5	2808	G
47	5	2814	C
47	5	2826	U
47	5	2827	G
47	5	2828	U
47	5	2829	U
47	5	2835	A
47	5	2838	G
47	5	2842	G
47	5	2845	A
47	5	2855	G
47	5	2857	A
47	5	2875	C
47	5	2884	G
47	5	2896	G
47	5	2897	G
47	5	3598	C
47	5	3599	A
47	5	3604	A
47	5	3605	C
47	5	3615	G
47	5	3617	G
47	5	3625	G
47	5	3626	G
47	5	3630	A
47	5	3635	A
47	5	3644	U
47	5	3653	A

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Mol	Chain	Res	Type
47	5	3662	A
47	5	3673	C
47	5	3674	G
47	5	3682	A
47	5	3692	A
47	5	3696	C
47	5	3698	G
47	5	3711	A
47	5	3712	A
47	5	3722	G
47	5	3729	U
47	5	3740	G
47	5	3748	A
47	5	3750	G
47	5	3753	G
47	5	3756	A
47	5	3759	A
47	5	3760	A
47	5	3765	G
47	5	3766	A
47	5	3773	U
47	5	3774	A
47	5	3776	G
47	5	3777	G
47	5	3778	U
47	5	3783	A
47	5	3784	A
47	5	3785	A
47	5	3786	U
47	5	3798	U
47	5	3799	A
47	5	3809	G
47	5	3810	C
47	5	3811	G
47	5	3812	C
47	5	3814	U
47	5	3817	A
47	5	3819	G
47	5	3822	U
47	5	3831	U
47	5	3838	U
47	5	3839	G

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Mol	Chain	Res	Type
47	5	3840	U
47	5	3851	U
47	5	3859	G
47	5	3867	A
47	5	3871	A
47	5	3876	A
47	5	3877	A
47	5	3878	C
47	5	3879	G
47	5	3889	G
47	5	3897	G
47	5	3898	G
47	5	3901	A
47	5	3905	A
47	5	3906	A
47	5	3907	G
47	5	3908	A
47	5	3915	U
47	5	3916	G
47	5	3917	A
47	5	3927	U
47	5	3938	G
47	5	3939	G
47	5	3943	A
47	5	4067	U
47	5	4069	U
47	5	4071	U
47	5	4073	A
47	5	4076	G
47	5	4084	G
47	5	4085	A
47	5	4086	G
47	5	4088	C
47	5	4090	G
47	5	4099	G
47	5	4100	C
47	5	4116	C
47	5	4117	U
47	5	4118	U
47	5	4119	C
47	5	4120	U
47	5	4121	G

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Mol	Chain	Res	Type
47	5	4122	G
47	5	4125	C
47	5	4127	A
47	5	4138	C
47	5	4150	G
47	5	4158	C
47	5	4161	G
47	5	4162	C
47	5	4163	U
47	5	4166	G
47	5	4171	C
47	5	4183	G
47	5	4184	G
47	5	4191	G
47	5	4203	A
47	5	4213	A
47	5	4225	G
47	5	4229	U
47	5	4230	C
47	5	4232	U
47	5	4233	A
47	5	4237	C
47	5	4249	G
47	5	4251	A
47	5	4255	A
47	5	4257	A
47	5	4258	C
47	5	4268	A
47	5	4271	A
47	5	4273	A
47	5	4281	A
47	5	4291	G
47	5	4297	G
47	5	4304	A
47	5	4305	G
47	5	4306	U
47	5	4314	C
47	5	4317	A
47	5	4318	C
47	5	4319	C
47	5	4326	G
47	5	4329	G

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Mol	Chain	Res	Type
47	5	4330	G
47	5	4331	G
47	5	4332	C
47	5	4336	A
47	5	4349	C
47	5	4354	U
47	5	4355	G
47	5	4373	G
47	5	4377	G
47	5	4378	A
47	5	4379	A
47	5	4380	A
47	5	4387	C
47	5	4391	G
47	5	4393	G
47	5	4394	A
47	5	4395	U
47	5	4398	C
47	5	4401	G
47	5	4419	U
47	5	4421	C
47	5	4422	A
47	5	4437	U
47	5	4440	G
47	5	4444	C
47	5	4448	G
47	5	4449	A
47	5	4453	C
47	5	4464	A
47	5	4471	U
47	5	4475	G
47	5	4476	C
47	5	4482	U
47	5	4488	A
47	5	4495	G
47	5	4500	U
47	5	4510	A
47	5	4511	A
47	5	4512	U
47	5	4513	A
47	5	4515	G
47	5	4519	C

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Mol	Chain	Res	Type
47	5	4520	G
47	5	4524	G
47	5	4527	G
47	5	4528	G
47	5	4531	U
47	5	4535	A
47	5	4548	A
47	5	4549	G
47	5	4560	C
47	5	4567	G
47	5	4570	G
47	5	4573	G
47	5	4575	G
47	5	4584	A
47	5	4586	G
47	5	4590	A
47	5	4599	A
47	5	4606	G
47	5	4618	G
47	5	4627	U
47	5	4635	A
47	5	4636	U
47	5	4637	G
47	5	4656	A
47	5	4657	U
47	5	4661	G
47	5	4670	C
47	5	4672	A
47	5	4677	U
47	5	4678	G
47	5	4687	A
47	5	4694	G
47	5	4695	C
47	5	4700	A
47	5	4701	A
47	5	4709	U
47	5	4719	G
47	5	4720	C
47	5	4721	G
47	5	4728	U
47	5	4736	C
47	5	4737	G

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Mol	Chain	Res	Type
47	5	4745	G
47	5	4751	G
47	5	4752	U
47	5	4754	G
47	5	4756	C
47	5	4757	C
47	5	4759	C
47	5	4761	G
47	5	4765	G
47	5	4771	C
47	5	4772	C
47	5	4868	G
47	5	4870	G
47	5	4871	C
47	5	4872	G
47	5	4873	G
47	5	4874	A
47	5	4875	G
47	5	4876	A
47	5	4877	G
47	5	4882	U
47	5	4883	C
47	5	4885	U
47	5	4887	C
47	5	4891	G
47	5	4895	C
47	5	4897	G
47	5	4910	A
47	5	4912	G
47	5	4913	G
47	5	4914	G
47	5	4915	G
47	5	4919	G
47	5	4921	C
47	5	4922	C
47	5	4924	C
47	5	4925	U
47	5	4926	C
47	5	4928	C
47	5	4931	G
47	5	4935	C
47	5	4937	C

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Mol	Chain	Res	Type
47	5	4942	C
47	5	4943	A
47	5	4944	C
47	5	4947	U
47	5	4948	C
47	5	4949	G
47	5	4950	U
47	5	4951	G
47	5	4956	A
47	5	4957	C
47	5	4958	C
47	5	4964	C
47	5	4965	U
47	5	4966	A
47	5	4967	A
47	5	4976	U
47	5	4985	U
47	5	4988	U
47	5	4989	U
47	5	4990	C
47	5	4991	U
47	5	5014	A
47	5	5017	G
47	5	5018	C
47	5	5040	U
47	5	5041	G
47	5	5047	C
47	5	5050	C
47	5	5053	U
47	5	5054	C
47	5	5056	A
47	5	5058	A
47	5	5061	A
47	5	5062	G
47	5	5066	U
48	7	7	G
48	7	25	G
48	7	33	U
48	7	42	A
48	7	53	U
48	7	54	A
48	7	64	G

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Mol	Chain	Res	Type
48	7	97	G
48	7	100	A
48	7	109	U
48	7	110	G
48	7	111	C
49	8	2	G
49	8	3	A
49	8	32	C
49	8	34	U
49	8	35	C
49	8	49	G
49	8	51	U
49	8	52	A
49	8	59	A
49	8	62	A
49	8	63	U
49	8	75	G
49	8	79	G
49	8	86	U
49	8	87	G
49	8	94	G
49	8	95	A
49	8	103	A
49	8	104	A
49	8	105	C
49	8	107	C
49	8	109	C
49	8	110	U
49	8	111	U
49	8	112	G
49	8	114	G
49	8	121	G
49	8	123	U
49	8	124	U
49	8	125	C
49	8	126	C
49	8	127	U
49	8	137	A
49	8	143	G
50	9	2	A
50	9	3	C
50	9	4	C

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Mol	Chain	Res	Type
50	9	14	C
50	9	17	C
50	9	23	G
50	9	25	A
50	9	33	G
50	9	41	G
50	9	44	U
50	9	46	A
50	9	56	G
50	9	58	C
50	9	64	A
50	9	65	C
50	9	67	C
50	9	68	A
50	9	69	C
50	9	71	G
50	9	72	C
50	9	73	C
50	9	74	G
50	9	75	G
50	9	77	A
50	9	79	A
50	9	81	U
50	9	98	C
50	9	99	A
50	9	100	U
50	9	103	A
50	9	111	A
50	9	113	G
50	9	115	U
50	9	116	U
50	9	123	G
50	9	124	U
50	9	126	G
50	9	127	C
50	9	130	G
50	9	142	C
50	9	143	U
50	9	147	A
50	9	155	G
50	9	158	A
50	9	161	U

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Mol	Chain	Res	Type
50	9	162	C
50	9	163	U
50	9	177	G
50	9	180	G
50	9	181	A
50	9	182	C
50	9	183	G
50	9	184	G
50	9	188	C
50	9	189	U
50	9	192	C
50	9	206	G
50	9	213	G
50	9	215	G
50	9	292	A
50	9	293	C
50	9	294	U
50	9	302	A
50	9	307	G
50	9	308	G
50	9	309	G
50	9	312	G
50	9	314	U
50	9	317	C
50	9	318	A
50	9	319	C
50	9	322	C
50	9	330	G
50	9	335	G
50	9	347	G
50	9	351	G
50	9	362	C
50	9	364	A
50	9	368	U
50	9	369	C
50	9	370	G
50	9	372	U
50	9	377	G
50	9	381	C
50	9	382	C
50	9	383	G
50	9	384	U

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Mol	Chain	Res	Type
50	9	385	G
50	9	386	C
50	9	388	U
50	9	400	C
50	9	408	A
50	9	409	C
50	9	416	U
50	9	417	C
50	9	418	A
50	9	419	G
50	9	441	C
50	9	448	A
50	9	449	A
50	9	450	C
50	9	451	G
50	9	452	G
50	9	454	U
50	9	460	A
50	9	462	C
50	9	464	A
50	9	465	A
50	9	466	G
50	9	469	A
50	9	471	G
50	9	472	C
50	9	473	A
50	9	474	G
50	9	476	A
50	9	482	G
50	9	487	U
50	9	492	C
50	9	493	A
50	9	496	C
50	9	500	A
50	9	507	G
50	9	509	G
50	9	512	A
50	9	516	A
50	9	526	A
50	9	530	U
50	9	531	A
50	9	532	C

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Mol	Chain	Res	Type
50	9	533	A
50	9	544	G
50	9	546	G
50	9	548	C
50	9	549	C
50	9	550	C
50	9	551	U
50	9	554	A
50	9	555	A
50	9	556	U
50	9	557	U
50	9	559	G
50	9	562	U
50	9	563	G
50	9	564	A
50	9	568	C
50	9	571	U
50	9	572	U
50	9	574	A
50	9	576	A
50	9	583	A
50	9	585	C
50	9	587	A
50	9	588	G
50	9	590	A
50	9	591	U
50	9	597	G
50	9	604	A
50	9	606	G
50	9	607	U
50	9	608	C
50	9	609	U
50	9	614	C
50	9	617	G
50	9	620	G
50	9	621	C
50	9	627	U
50	9	628	A
50	9	629	A
50	9	632	C
50	9	637	U
50	9	643	A

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Mol	Chain	Res	Type
50	9	644	G
50	9	646	G
50	9	655	A
50	9	656	G
50	9	659	G
50	9	660	C
50	9	664	A
50	9	668	A
50	9	669	A
50	9	670	A
50	9	671	A
50	9	672	A
50	9	673	G
50	9	684	G
50	9	687	C
50	9	688	U
50	9	689	U
50	9	696	G
50	9	733	C
50	9	752	G
50	9	753	C
50	9	754	G
50	9	810	A
50	9	811	A
50	9	812	A
50	9	821	G
50	9	822	U
50	9	830	A
50	9	834	C
50	9	844	U
50	9	847	A
50	9	859	G
50	9	861	A
50	9	868	G
50	9	869	A
50	9	870	A
50	9	871	U
50	9	872	A
50	9	873	G
50	9	874	G
50	9	875	A
50	9	878	G

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Mol	Chain	Res	Type
50	9	885	U
50	9	887	U
50	9	888	U
50	9	889	U
50	9	890	U
50	9	907	G
50	9	909	G
50	9	912	C
50	9	913	A
50	9	914	U
50	9	920	A
50	9	921	G
50	9	922	A
50	9	930	C
50	9	933	G
50	9	934	G
50	9	943	U
50	9	971	G
50	9	985	G
50	9	990	A
50	9	992	A
50	9	999	G
50	9	1017	U
50	9	1023	A
50	9	1041	G
50	9	1053	C
50	9	1055	A
50	9	1060	A
50	9	1061	U
50	9	1062	A
50	9	1083	A
50	9	1085	C
50	9	1089	G
50	9	1100	A
50	9	1115	U
50	9	1116	C
50	9	1117	C
50	9	1118	C
50	9	1119	A
50	9	1121	G
50	9	1133	A
50	9	1137	U

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Mol	Chain	Res	Type
50	9	1138	C
50	9	1139	C
50	9	1140	G
50	9	1144	A
50	9	1148	A
50	9	1149	A
50	9	1153	C
50	9	1154	U
50	9	1165	G
50	9	1166	G
50	9	1168	G
50	9	1170	A
50	9	1195	A
50	9	1203	G
50	9	1207	G
50	9	1208	A
50	9	1215	C
50	9	1221	G
50	9	1224	G
50	9	1227	G
50	9	1235	G
50	9	1240	A
50	9	1242	U
50	9	1248	U
50	9	1250	A
50	9	1251	A
50	9	1253	A
50	9	1254	C
50	9	1256	G
50	9	1257	G
50	9	1259	A
50	9	1260	A
50	9	1269	G
50	9	1274	G
50	9	1275	G
50	9	1281	G
50	9	1284	A
50	9	1285	G
50	9	1286	G
50	9	1289	U
50	9	1293	A
50	9	1294	G

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Mol	Chain	Res	Type
50	9	1299	A
50	9	1300	U
50	9	1301	A
50	9	1302	G
50	9	1303	C
50	9	1304	U
50	9	1308	U
50	9	1309	C
50	9	1313	A
50	9	1314	U
50	9	1322	G
50	9	1324	G
50	9	1330	G
50	9	1331	C
50	9	1337	C
50	9	1342	U
50	9	1369	A
50	9	1371	U
50	9	1372	U
50	9	1375	G
50	9	1376	A
50	9	1378	A
50	9	1396	A
50	9	1397	U
50	9	1402	A
50	9	1406	G
50	9	1424	G
50	9	1428	G
50	9	1429	G
50	9	1439	A
50	9	1449	G
50	9	1454	A
50	9	1455	A
50	9	1458	G
50	9	1459	G
50	9	1462	U
50	9	1463	U
50	9	1466	G
50	9	1473	G
50	9	1475	G
50	9	1476	A
50	9	1477	U

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Mol	Chain	Res	Type
50	9	1478	U
50	9	1489	A
50	9	1490	G
50	9	1498	A
50	9	1509	U
50	9	1519	U
50	9	1520	G
50	9	1521	C
50	9	1522	A
50	9	1525	C
50	9	1531	A
50	9	1533	A
50	9	1534	C
50	9	1535	U
50	9	1536	G
50	9	1544	C
50	9	1548	G
50	9	1552	G
50	9	1553	C
50	9	1555	U
50	9	1556	A
50	9	1557	C
50	9	1558	C
50	9	1560	U
50	9	1570	G
50	9	1574	C
50	9	1575	G
50	9	1580	A
50	9	1581	C
50	9	1587	G
50	9	1588	A
50	9	1601	A
50	9	1602	U
50	9	1604	G
50	9	1612	G
50	9	1621	U
50	9	1622	U
50	9	1623	A
50	9	1637	A
50	9	1638	G
50	9	1639	G
50	9	1648	G

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Mol	Chain	Res	Type
50	9	1661	A
50	9	1664	A
50	9	1665	G
50	9	1671	G
50	9	1680	G
50	9	1683	C
50	9	1686	G
50	9	1689	C
50	9	1698	C
50	9	1699	A
50	9	1703	C
50	9	1715	A
50	9	1721	U
50	9	1722	G
50	9	1726	G
50	9	1730	U
50	9	1740	C
50	9	1747	C
50	9	1748	G
50	9	1750	C
50	9	1753	C
50	9	1757	G
50	9	1758	G
50	9	1760	G
50	9	1783	C
50	9	1785	C
50	9	1800	A
50	9	1819	A
50	9	1823	A
50	9	1824	A
50	9	1829	G
50	9	1835	A
50	9	1836	G
50	9	1838	U
50	9	1839	U
50	9	1849	G
50	9	1851	A
50	9	1852	C
50	9	1861	G
50	9	1862	G
50	9	1863	A
50	9	1865	C

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Mol	Chain	Res	Type
50	9	1866	A
50	9	1867	U
50	9	1869	A
84	hh	22	G
45	ii	7	G
45	ii	8	U
45	ii	10	G
45	ii	11	U
45	ii	13	U
45	ii	19	G
45	ii	20	U
45	ii	21	U
45	ii	22	A
45	ii	26	C
45	ii	31	G
45	ii	45	A
45	ii	49	C
45	ii	53	G
45	ii	60	A
45	ii	61	A
45	ii	62	C
45	ii	65	G
45	ii	76	C
45	ii	77	A

All (247) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	2	20(A)	U
46	3	7	A
46	3	74	C
47	5	12	A
47	5	20	U
47	5	47	A
47	5	48	G
47	5	64	A
47	5	119	G
47	5	125	C
47	5	134	G
47	5	143	C
47	5	159	C
47	5	200	U

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Mol	Chain	Res	Type
47	5	217	C
47	5	226	G
47	5	234	G
47	5	245	C
47	5	265	C
47	5	275	C
47	5	278	G
47	5	315	G
47	5	354	U
47	5	385	A
47	5	406	C
47	5	408	A
47	5	409	G
47	5	417	G
47	5	449	C
47	5	480	C
47	5	484	U
47	5	485	C
47	5	492	U
47	5	497	G
47	5	498	C
47	5	504	G
47	5	669	C
47	5	696	C
47	5	729	G
47	5	738(A)	C
47	5	747	A
47	5	915	A
47	5	916	C
47	5	930	G
47	5	933	G
47	5	935(A)	G
47	5	936	C
47	5	955	G
47	5	959	G
47	5	963	G
47	5	966	A
47	5	968	C
47	5	969	C
47	5	971(A)	G
47	5	1072	C
47	5	1209	U

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Mol	Chain	Res	Type
47	5	1211	G
47	5	1214	C
47	5	1236	C
47	5	1238	A
47	5	1287	G
47	5	1291	G
47	5	1295	U
47	5	1324	A
47	5	1329	G
47	5	1358	G
47	5	1359	G
47	5	1370	G
47	5	1378	C
47	5	1380	G
47	5	1420	A
47	5	1440	U
47	5	1445	U
47	5	1455	G
47	5	1477	C
47	5	1481	C
47	5	1484	G
47	5	1485	C
47	5	1611	C
47	5	1633	G
47	5	1654	G
47	5	1676	C
47	5	1733	G
47	5	1740	C
47	5	1804	A
47	5	1815	G
47	5	1818	G
47	5	1833	G
47	5	1834	U
47	5	1835	G
47	5	1919	G
47	5	1921	C
47	5	1935	C
47	5	1947	U
47	5	1979	A
47	5	1983	A
47	5	1984	A
47	5	1986	U

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Mol	Chain	Res	Type
47	5	2001	G
47	5	2025	A
47	5	2046	G
47	5	2054	U
47	5	2068	C
47	5	2088	A
47	5	2089	G
47	5	2094	C
47	5	2100	G
47	5	2265	G
47	5	2266	C
47	5	2278	G
47	5	2313	A
47	5	2370	A
47	5	2396	A
47	5	2398	U
47	5	2428	A
47	5	2467	U
47	5	2468	U
47	5	2474	G
47	5	2475	G
47	5	2490	U
47	5	2502	A
47	5	2529	A
47	5	2530	U
47	5	2546	G
47	5	2553	A
47	5	2587	A
47	5	2661	U
47	5	2695	A
47	5	2724	G
47	5	2754	G
47	5	2794	C
47	5	2806	A
47	5	2834	C
47	5	3603	G
47	5	3625	G
47	5	3673	C
47	5	3697	U
47	5	3710	G
47	5	3809	G
47	5	3876	A

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Mol	Chain	Res	Type
47	5	3878	C
47	5	3888	G
47	5	3904	G
47	5	4075	U
47	5	4076	G
47	5	4084	G
47	5	4116	C
47	5	4119	C
47	5	4120	U
47	5	4121	G
47	5	4124	G
47	5	4162	C
47	5	4170	A
47	5	4232	U
47	5	4254	G
47	5	4266	G
47	5	4272	G
47	5	4331	G
47	5	4378	A
47	5	4379	A
47	5	4395	U
47	5	4448	G
47	5	4463	U
47	5	4510	A
47	5	4527	G
47	5	4699	U
47	5	4719	G
47	5	4871	C
47	5	4884	G
47	5	4925	U
47	5	4936	G
47	5	4942	C
47	5	4947	U
47	5	4965	U
48	7	109	U
49	8	2	G
49	8	51	U
49	8	85	U
49	8	86	U
49	8	94	G
49	8	110	U
49	8	124	U

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Mol	Chain	Res	Type
50	9	2	A
50	9	3	C
50	9	24	C
50	9	25	A
50	9	43	U
50	9	72	C
50	9	98	C
50	9	110	U
50	9	126	G
50	9	142	C
50	9	160	U
50	9	182	C
50	9	293	C
50	9	369	C
50	9	370	G
50	9	448	A
50	9	464	A
50	9	465	A
50	9	500	A
50	9	516	A
50	9	532	C
50	9	550	C
50	9	553	U
50	9	555	A
50	9	561	A
50	9	563	G
50	9	584	A
50	9	620	G
50	9	627	U
50	9	655	A
50	9	670	A
50	9	688	U
50	9	752	G
50	9	861	A
50	9	869	A
50	9	870	A
50	9	872	A
50	9	912	C
50	9	1016	U
50	9	1137	U
50	9	1138	C
50	9	1165	G

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Mol	Chain	Res	Type
50	9	1253	A
50	9	1255	G
50	9	1284	A
50	9	1286	G
50	9	1313	A
50	9	1330	G
50	9	1395	C
50	9	1396	A
50	9	1441	U
50	9	1476	A
50	9	1489	A
50	9	1494	U
50	9	1534	C
50	9	1621	U
50	9	1636	G
50	9	1637	A
50	9	1647	A
50	9	1664	A
50	9	1679	A
50	9	1721	U
50	9	1835	A
50	9	1862	G
50	9	1868	U

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
85	SEP	jj	163	85	8,9,10	0.65	0	7,12,14	1.35	1 (14%)

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
85	SEP	jj	163	85	-	5/6/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
85	jj	163	SEP	OG-CB-CA	2.47	110.55	108.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
85	jj	163	SEP	N-CA-CB-OG
85	jj	163	SEP	CA-CB-OG-P
85	jj	163	SEP	CB-OG-P-O2P
85	jj	163	SEP	CB-OG-P-O3P
85	jj	163	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 286 ligands modelled in this entry, 284 are monoatomic - leaving 2 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
89	7C4	jj	503	-	81,82,82	1.00	4 (4%)	111,117,117	1.24	13 (11%)
88	GDP	jj	501	86	29,30,30	1.17	3 (10%)	45,47,47	1.82	8 (17%)

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
89	7C4	jj	503	-	-	7/120/140/140	0/3/4/4
88	GDP	jj	501	86	-	0/16/32/32	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
89	jj	503	7C4	C72-C71	-4.74	1.32	1.51
88	jj	501	GDP	C5-C4	3.23	1.47	1.38
89	jj	503	7C4	C54-C55	-2.45	1.50	1.53
89	jj	503	7C4	C53-C54	2.09	1.56	1.53
89	jj	503	7C4	C45-C47	2.05	1.55	1.52
88	jj	501	GDP	C5-N7	-2.02	1.35	1.39
88	jj	501	GDP	C6-N1	-2.00	1.35	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	jj	501	GDP	C5-C4-N3	-5.94	118.94	128.39
88	jj	501	GDP	C2-N3-C4	5.16	121.19	112.30
88	jj	501	GDP	N9-C4-N3	4.37	134.69	125.95
89	jj	503	7C4	O35-C79-C01	3.64	118.35	110.80
88	jj	501	GDP	C6-C5-N7	3.59	136.81	130.29
89	jj	503	7C4	C70-C69-N17	3.34	124.95	118.87
89	jj	503	7C4	C36-N05-C30	-3.07	107.19	112.01
89	jj	503	7C4	C30-C28-N02	2.76	123.90	118.87
89	jj	503	7C4	C73-N20-C70	-2.73	107.73	112.01
89	jj	503	7C4	C45-C44-N08	2.71	119.65	116.13
88	jj	501	GDP	C4-C5-N7	-2.71	106.37	110.67
89	jj	503	7C4	O37-C79-C01	-2.31	119.36	124.46
89	jj	503	7C4	C77-O35-C79	2.28	120.93	117.55
89	jj	503	7C4	O29-C69-C70	-2.27	115.53	120.28
89	jj	503	7C4	C71-C70-C69	2.22	115.19	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
88	jj	501	GDP	C3'-C2'-C1'	2.21	105.64	101.46
89	jj	503	7C4	C32-C30-C28	-2.18	106.55	110.83
88	jj	501	GDP	O6-C6-C5	-2.17	120.81	126.53
89	jj	503	7C4	C53-C54-C55	-2.05	110.19	113.00
89	jj	503	7C4	C71-C72-C73	2.02	110.53	104.90
88	jj	501	GDP	C5-C6-N1	2.02	118.39	113.25

There are no chirality outliers.

All (7) torsion outliers are listed below:

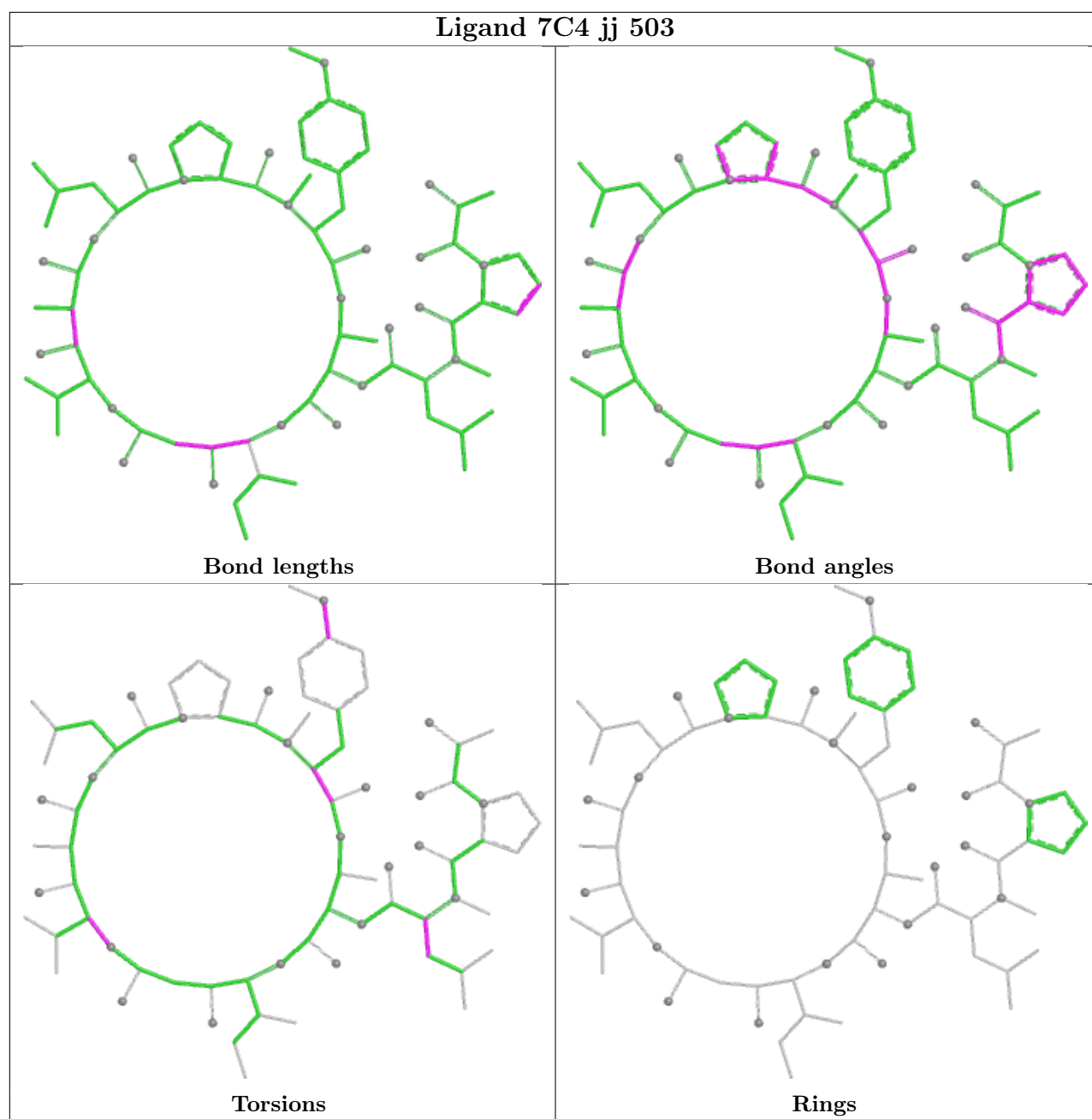
Mol	Chain	Res	Type	Atoms
89	jj	503	7C4	C47-C48-O18-C52
89	jj	503	7C4	C62-C63-C64-C65
89	jj	503	7C4	C22-C14-O03-C19
89	jj	503	7C4	C13-C14-O03-C19
89	jj	503	7C4	N17-C63-C64-C65
89	jj	503	7C4	C49-C48-O18-C52
89	jj	503	7C4	N02-C01-C79-O35

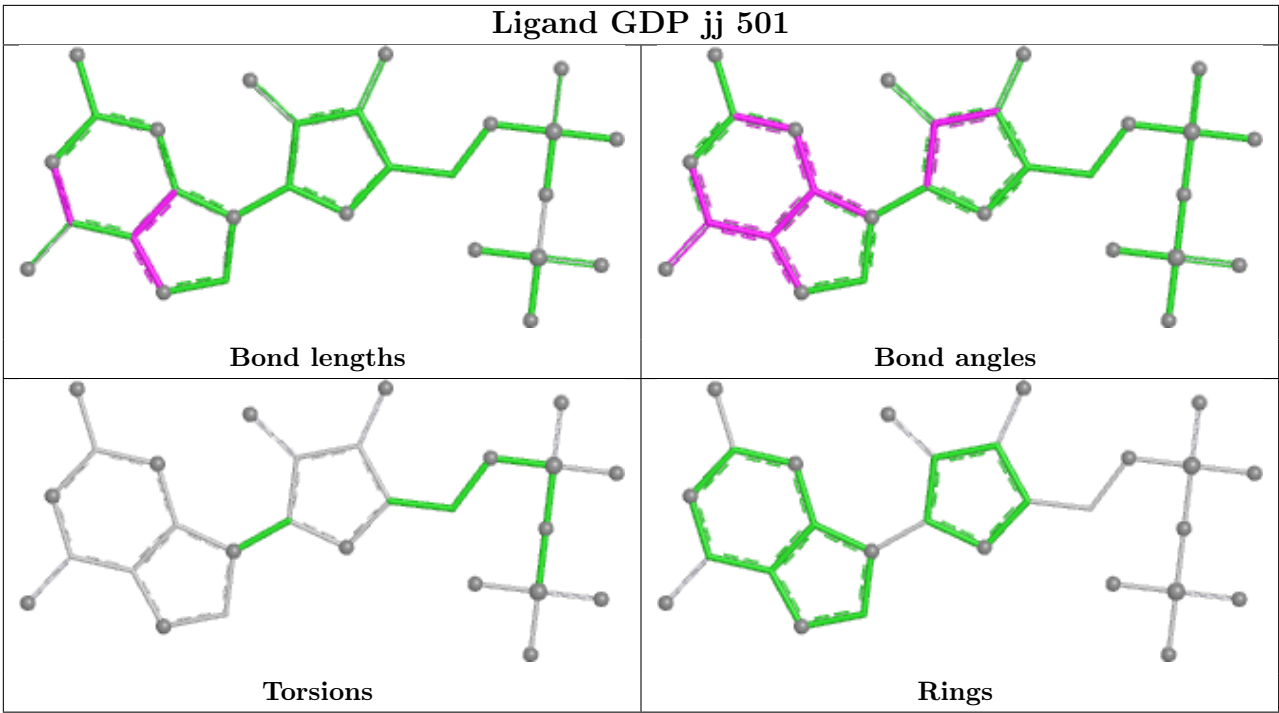
There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
89	jj	503	7C4	6	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
47	5	31
50	9	7
45	2	3
46	3	2
45	ii	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	41.26
1	5	1252:C	O3'	1271:G	P	36.28
1	5	1219:G	O3'	1233:G	P	22.71
1	5	3948:C	O3'	4065:G	P	19.70
1	5	1406(C):G	O3'	1411:C	P	18.70
1	5	990:C	O3'	1064:G	P	18.38
1	5	523:C	O3'	638:G	P	18.03

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	5	4138:C	O3'	4146:G	P	18.01
1	5	4101:C	O3'	4107:G	P	17.45
1	5	4777:C	O3'	4859:C	P	16.68
1	5	760:G	O3'	904:C	P	15.18
1	5	5022:U	O3'	5028:G	P	14.74
1	5	182:G	O3'	189:G	P	14.42
1	5	1364:U	O3'	1368:A	P	14.31
1	5	1696:C	O3'	1720:C	P	14.19
1	5	2901:G	O3'	3597:G	P	13.49
1	5	4729:A	O3'	4735:G	P	9.67
1	5	512:U	O3'	515:C	P	9.60
1	5	1180:C	O3'	1183:C	P	8.81
1	5	500:G	O3'	504:G	P	6.82
1	5	1100:U	O3'	1168:G	P	5.92
1	2	20:U	O3'	20(A):U	P	5.90
1	3	19:G	O3'	20:U	P	5.80
1	9	689:U	O3'	690:G	P	5.56
1	ii	16:C	O3'	18:G	P	5.55
1	3	16:C	O3'	18:U	P	5.33
1	5	1239:C	O3'	1244:G	P	5.32
1	9	322:C	O3'	323:C	P	5.23
1	5	4740:G	O3'	4743:G	P	4.91
1	2	19:G	O3'	20:U	P	4.72
1	9	798:G	O3'	799:U	P	4.67
1	2	16:C	O3'	18:G	P	4.42
1	9	304:C	O3'	305:U	P	4.35
1	5	170:C	O3'	171:U	P	3.94
1	5	1957:U	O3'	1958:A	P	3.81
1	9	902:G	O3'	903:A	P	3.38
1	5	1438:U	O3'	1440:U	P	3.34
1	5	4899:G	O3'	4902:C	P	3.34
1	9	886:A	O3'	887:U	P	3.33
1	5	5020:G	O3'	5021:C	P	3.30
1	9	903:A	O3'	904:A	P	3.30
1	5	267:G	O3'	268:G	P	3.19
1	5	751:G	O3'	752:G	P	3.03
1	5	2025:A	O3'	2026:A	P	1.24

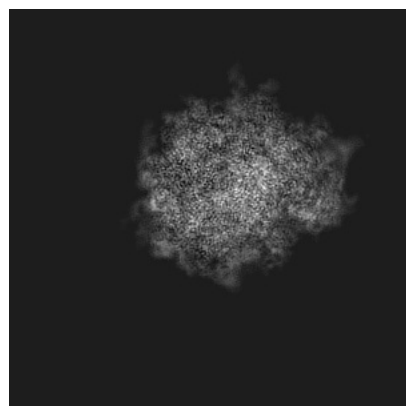
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4130. These allow visual inspection of the internal detail of the map and identification of artifacts.

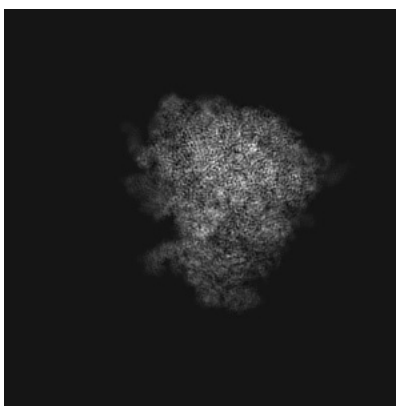
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

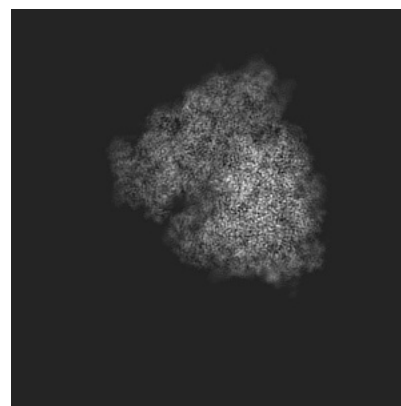
6.1.1 Primary map



X

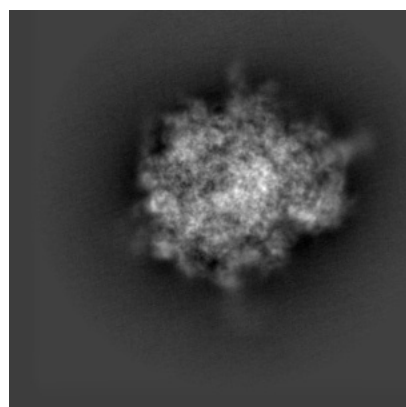


Y

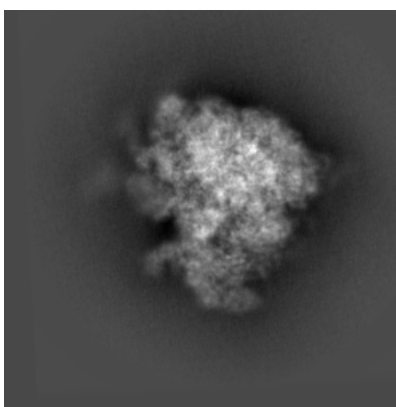


Z

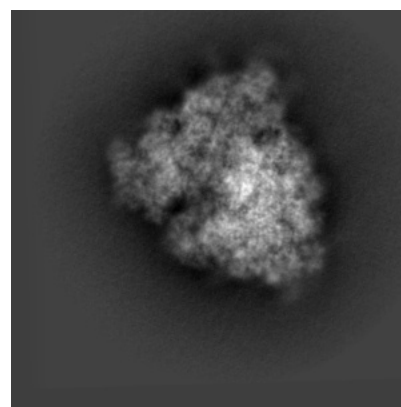
6.1.2 Raw map



X



Y

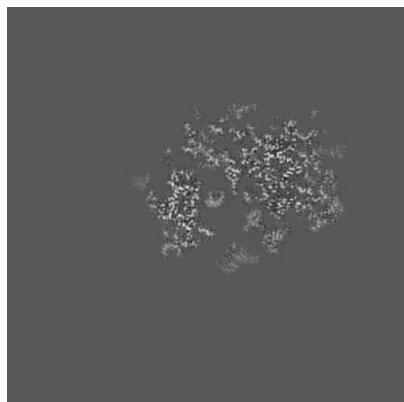


Z

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

6.2 Central slices [i](#)

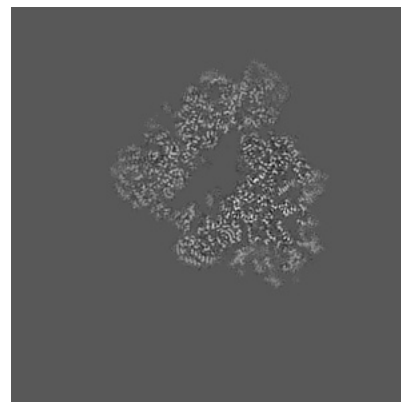
6.2.1 Primary map



X Index: 240

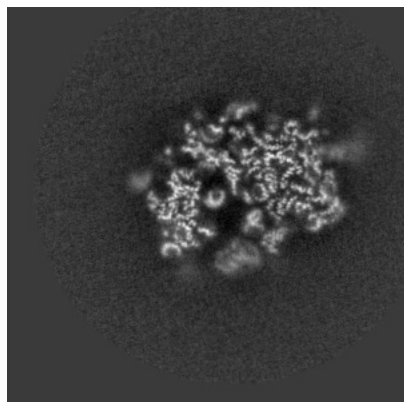


Y Index: 240

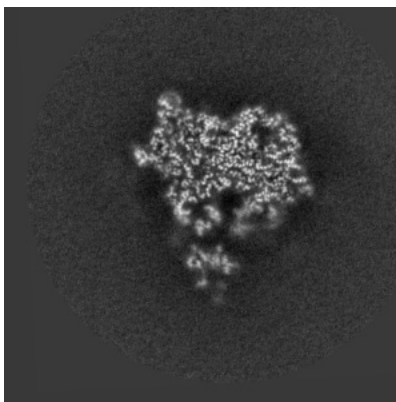


Z Index: 240

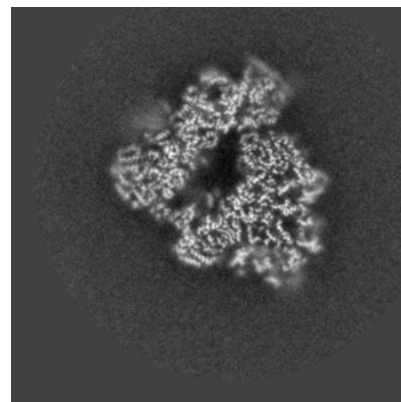
6.2.2 Raw map



X Index: 240



Y Index: 240

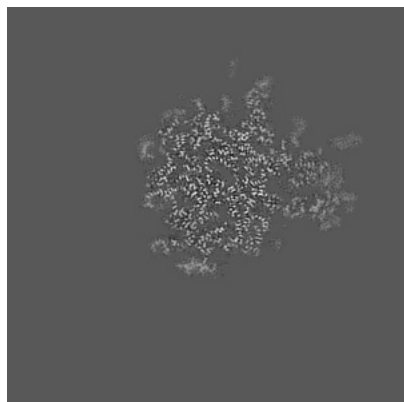


Z Index: 240

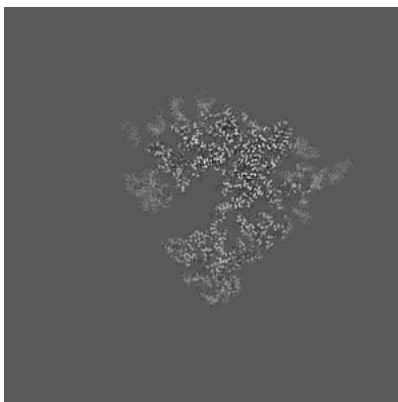
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

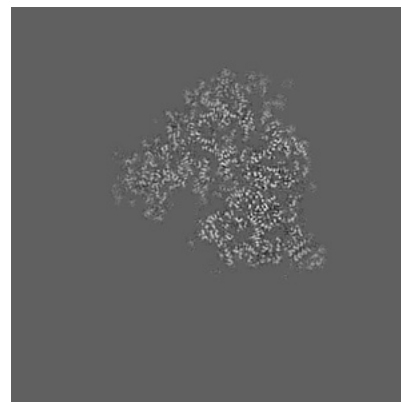
6.3.1 Primary map



X Index: 294

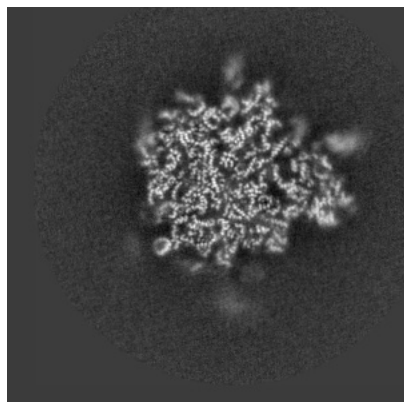


Y Index: 272

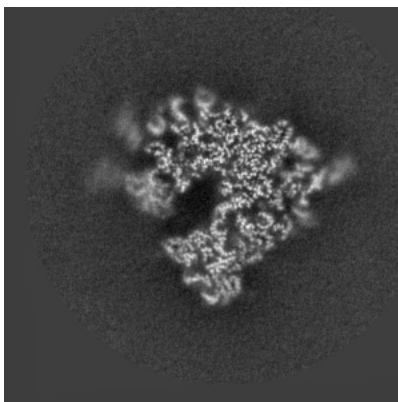


Z Index: 261

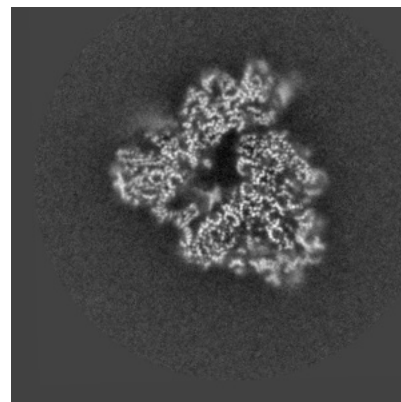
6.3.2 Raw map



X Index: 287



Y Index: 272

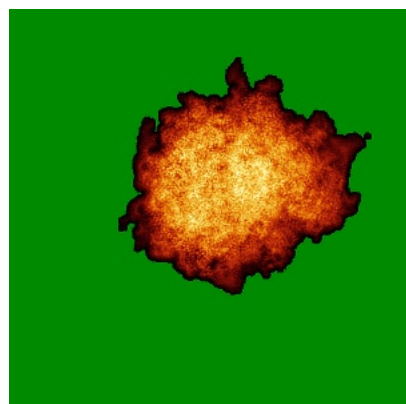


Z Index: 244

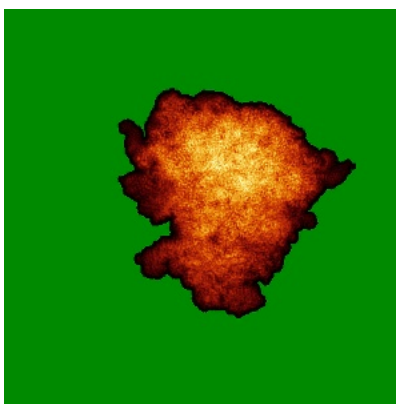
The images above show the largest variance slices of the map in three orthogonal directions.

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

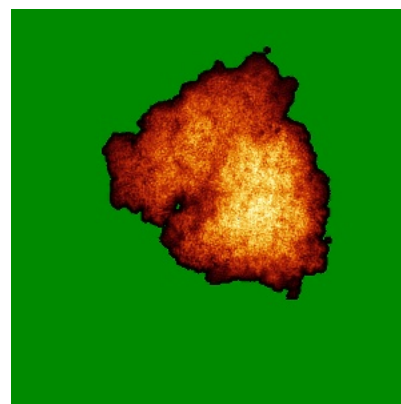
6.4.1 Primary map



X

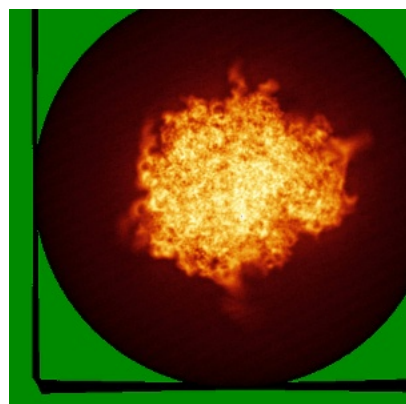


Y

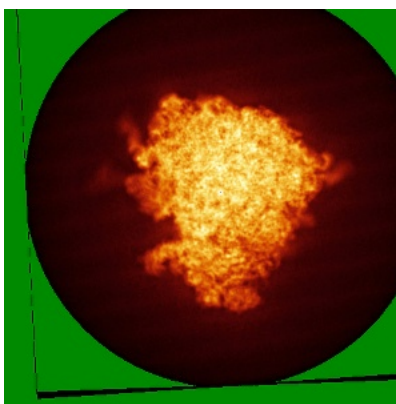


Z

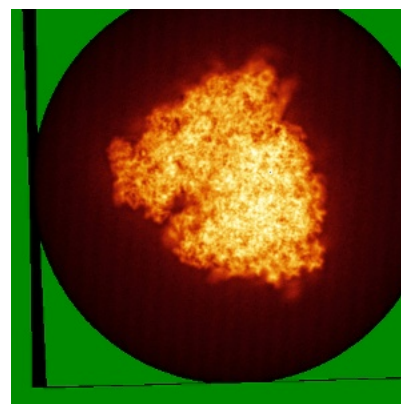
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.08. 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.

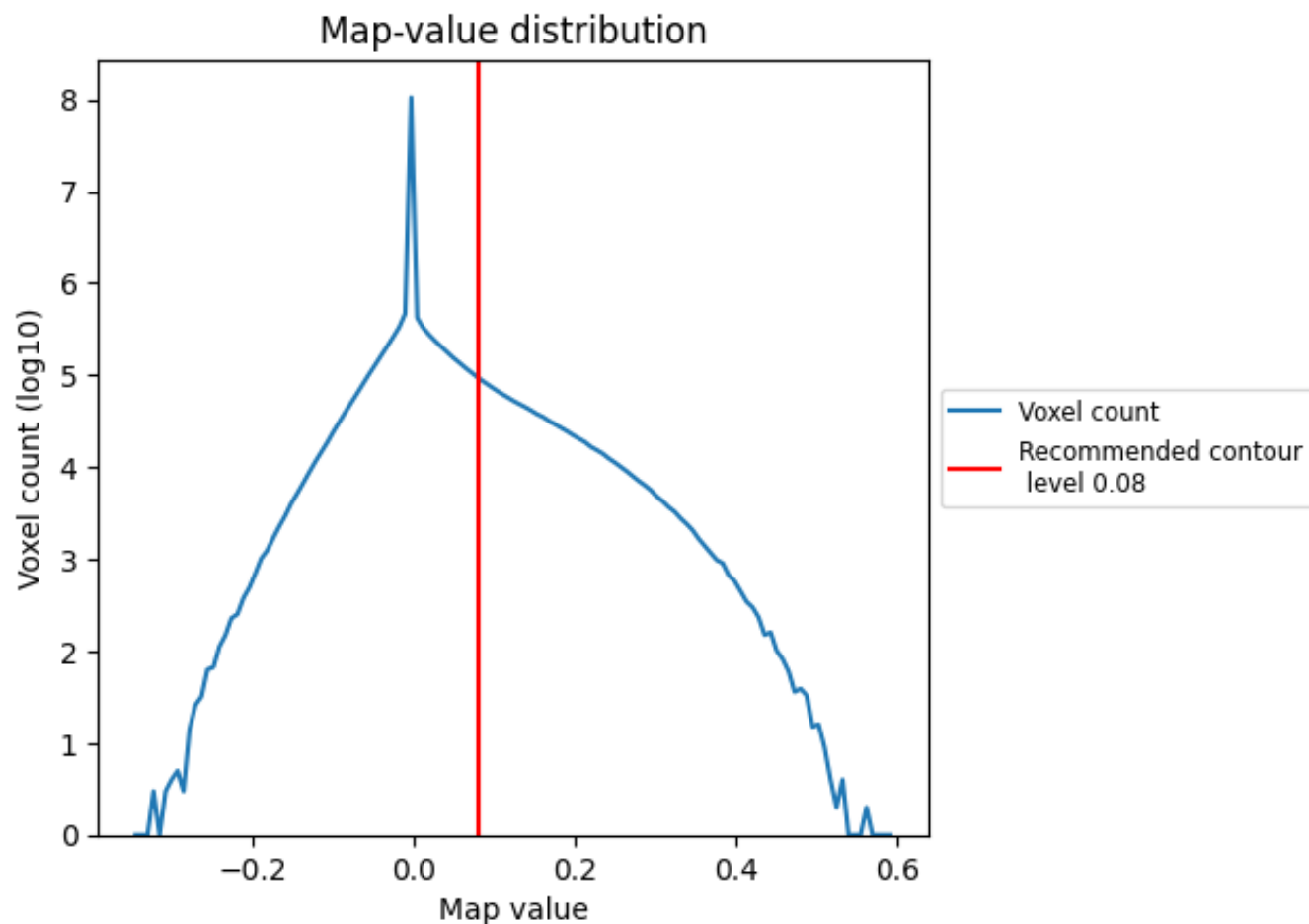
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

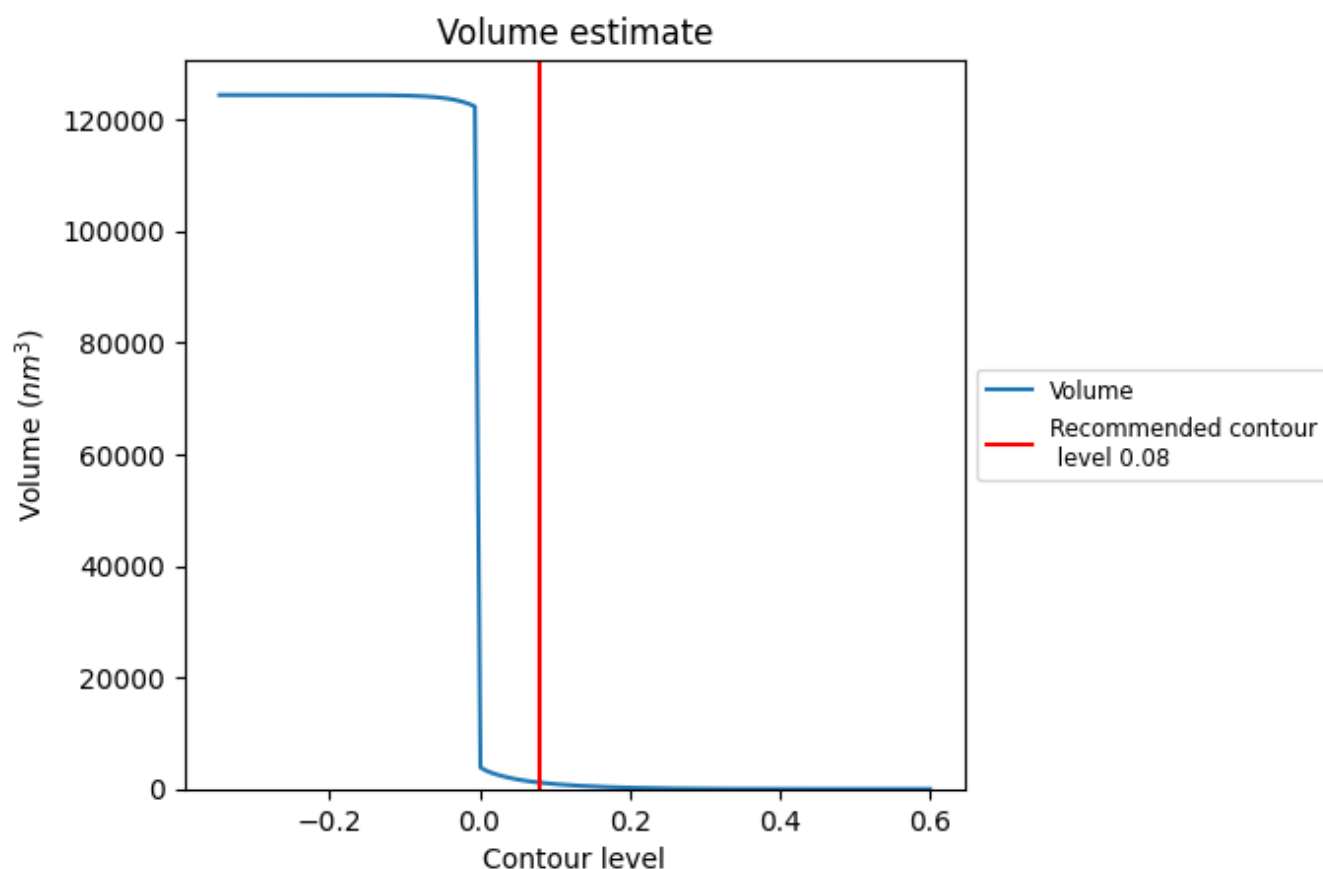
This section contains the results of statistical analysis of the map.

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.

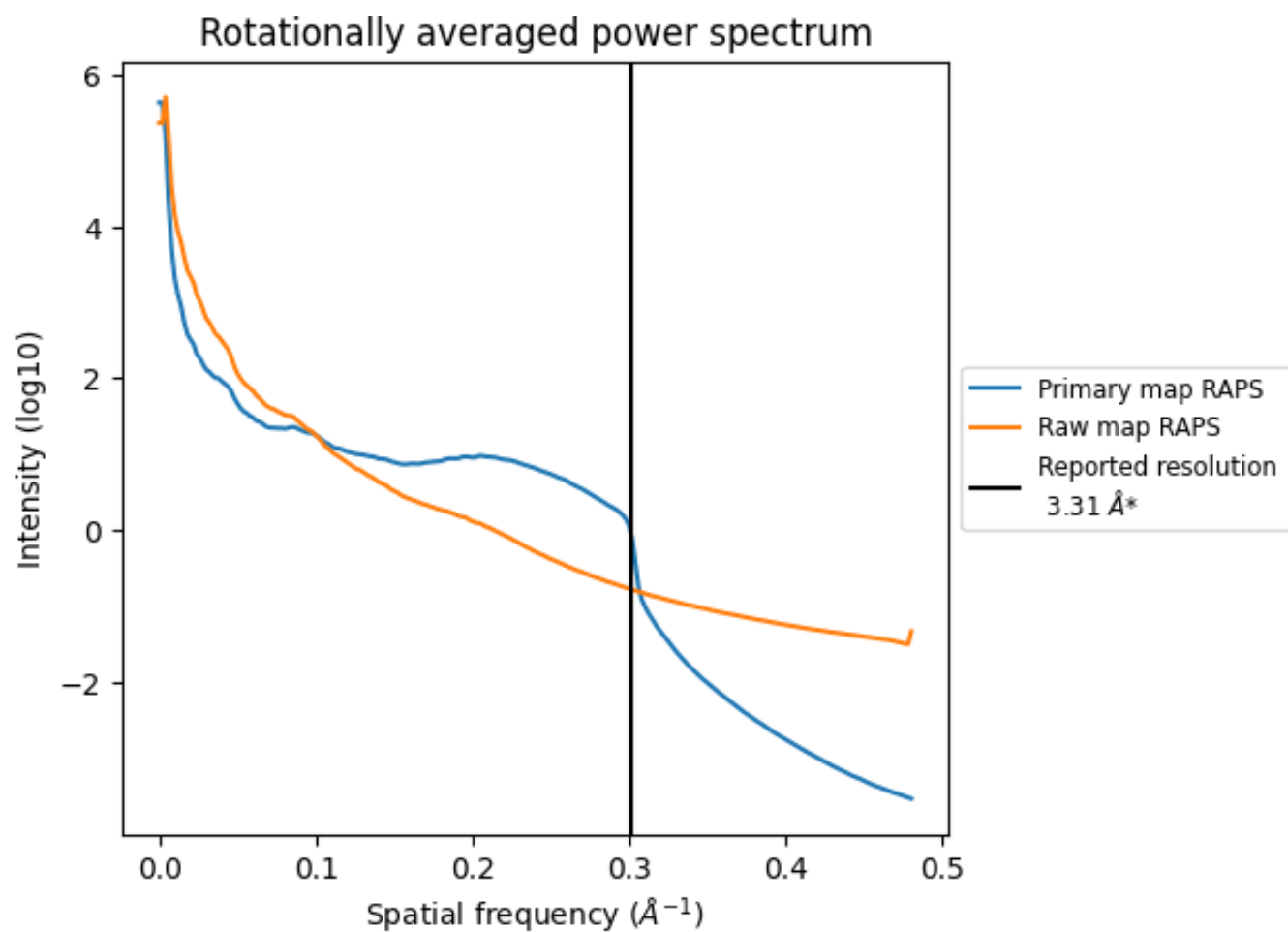
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1143 nm³; this corresponds to an approximate mass of 1033 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

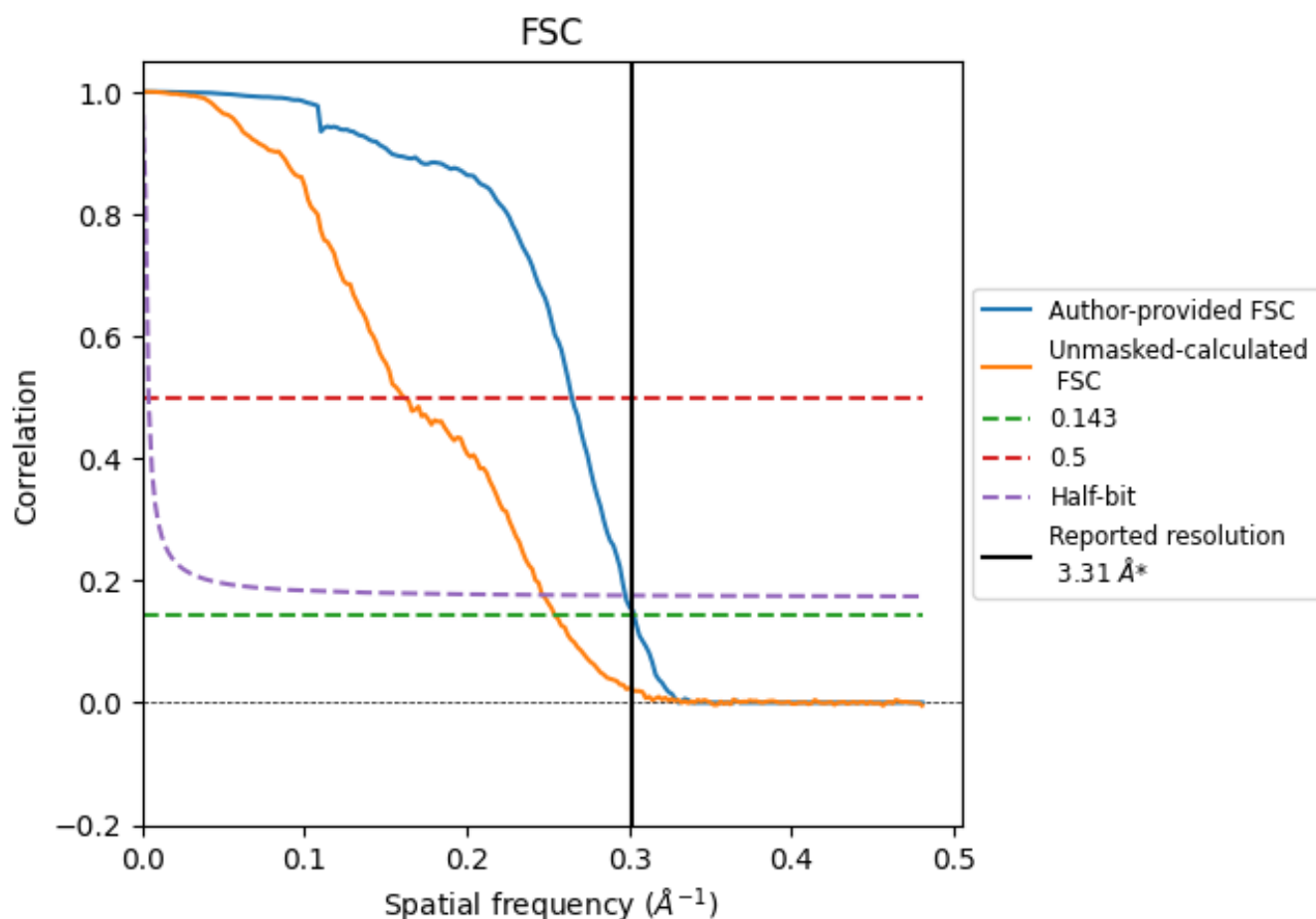


*Reported resolution corresponds to spatial frequency of 0.302 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.302 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

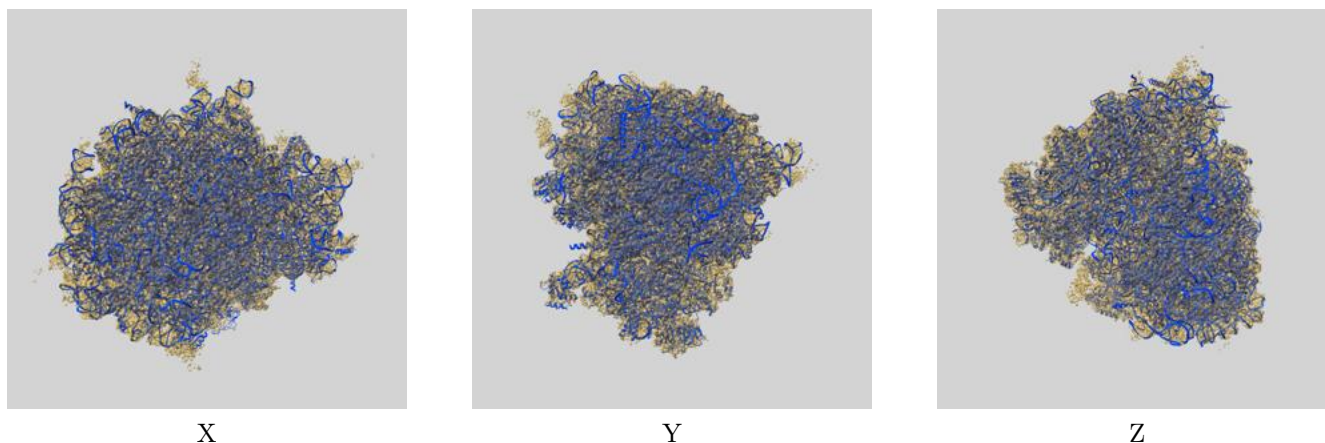
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.31	-	-
Author-provided FSC curve	3.30	3.78	3.36
Unmasked-calculated*	3.93	6.20	4.05

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.93 differs from the reported value 3.31 by more than 10 %

9 Map-model fit [i](#)

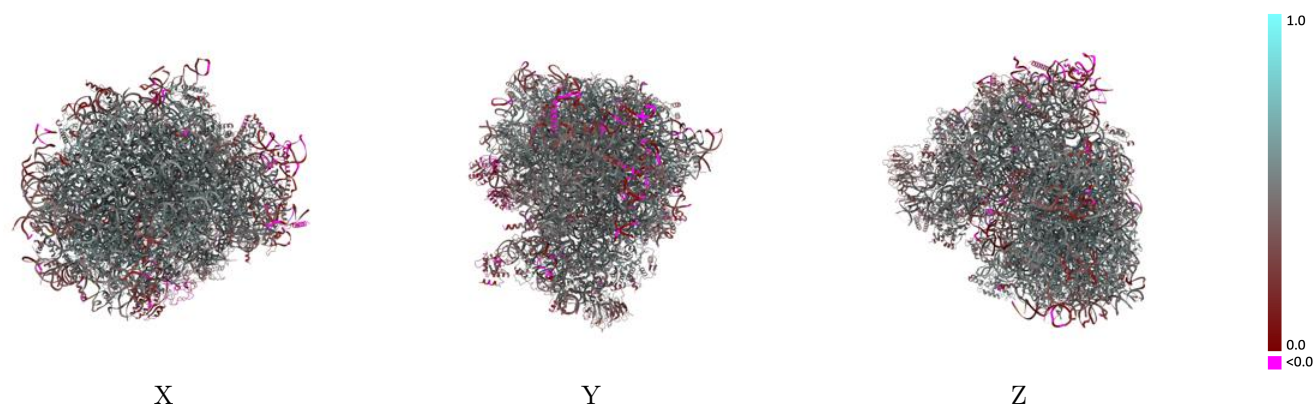
This section contains information regarding the fit between EMDB map EMD-4130 and PDB model 5LZS. Per-residue inclusion information can be found in [section 3](#) on [page 23](#).

9.1 Map-model overlay [i](#)



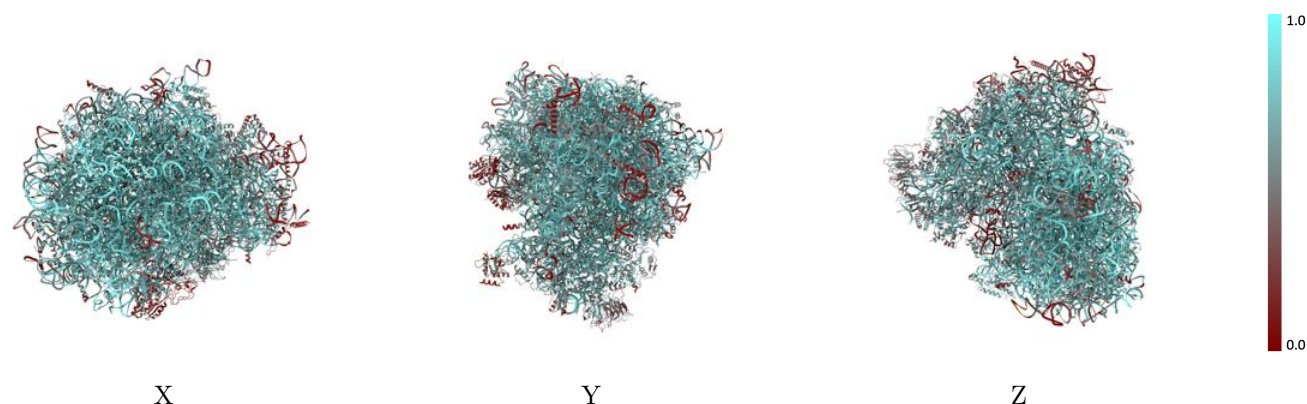
The images above show the 3D surface view of the map at the recommended contour level 0.08 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



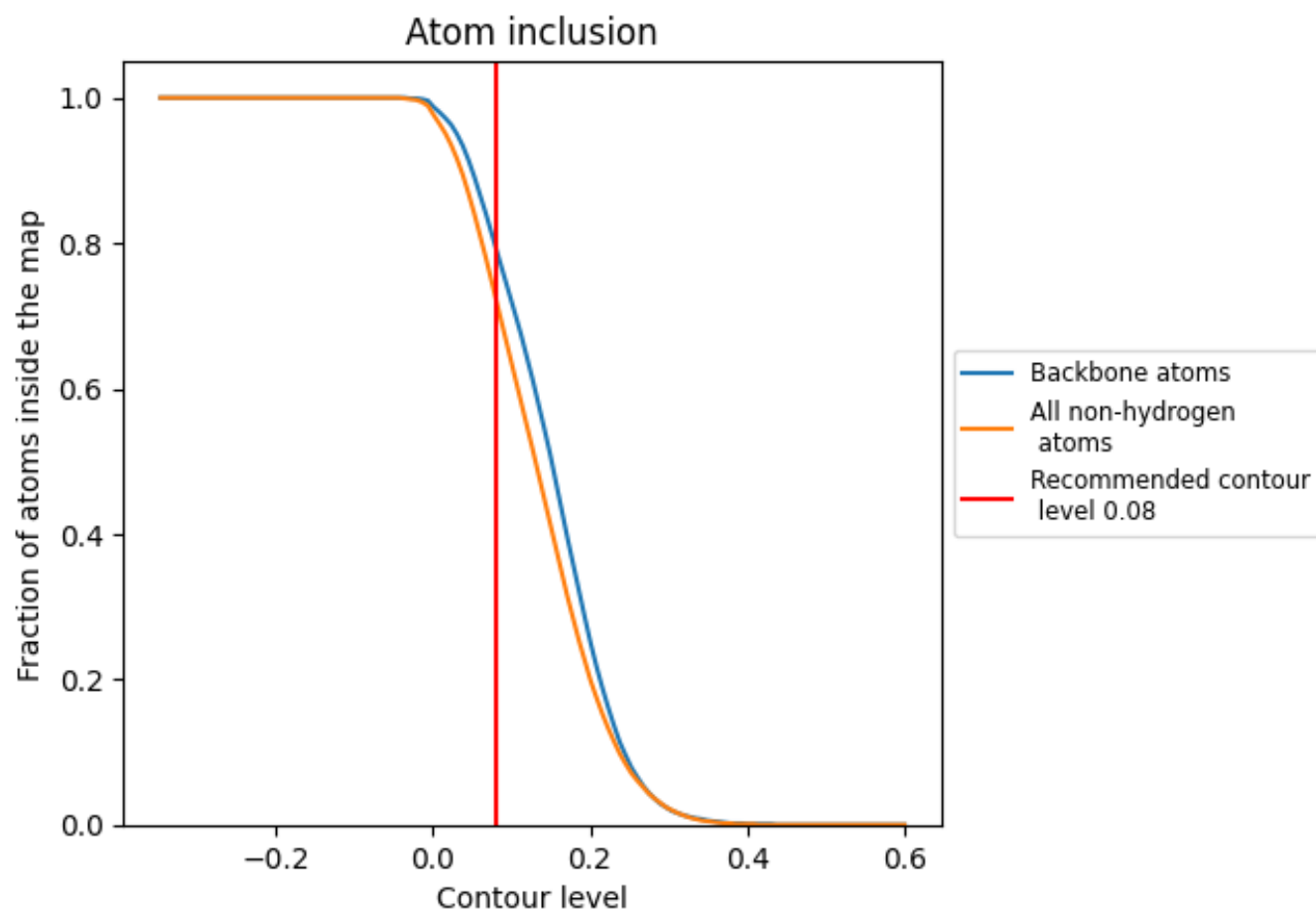
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7250	 0.4620
2	 0.6650	 0.4180
3	 0.1690	 0.1890
5	 0.8060	 0.4770
7	 0.9050	 0.5270
8	 0.8400	 0.4910
9	 0.7780	 0.4560
A	 0.7570	 0.5370
AA	 0.6610	 0.4730
B	 0.7540	 0.5190
BB	 0.6360	 0.4670
C	 0.7520	 0.5160
CC	 0.6530	 0.4790
D	 0.7080	 0.4770
DD	 0.5390	 0.4150
E	 0.7100	 0.4840
EE	 0.6040	 0.4370
F	 0.7510	 0.5180
FF	 0.6050	 0.4390
G	 0.6280	 0.4380
GG	 0.5250	 0.3680
H	 0.7000	 0.4960
HH	 0.5240	 0.3910
I	 0.7310	 0.5040
II	 0.5800	 0.4110
J	 0.6230	 0.4380
JJ	 0.6060	 0.4230
KK	 0.6080	 0.4340
L	 0.7030	 0.4780
LL	 0.6280	 0.4650
M	 0.7230	 0.5010
MM	 0.2690	 0.1980
N	 0.7970	 0.5450
NN	 0.6860	 0.4910
O	 0.7550	 0.5130



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Chain	Atom inclusion	Q-score
OO	 0.6430	 0.4810
P	 0.7610	 0.5240
PP	 0.5780	 0.4070
Q	 0.7480	 0.5230
QQ	 0.6260	 0.4460
R	 0.6730	 0.4610
RR	 0.5670	 0.4160
S	 0.7760	 0.5310
SS	 0.5620	 0.3940
T	 0.7110	 0.5010
TT	 0.6030	 0.4250
U	 0.6260	 0.4140
UU	 0.5180	 0.3980
V	 0.7030	 0.5220
VV	 0.6090	 0.4710
W	 0.4840	 0.3220
WW	 0.6980	 0.5020
X	 0.7030	 0.4890
XX	 0.6770	 0.5040
Y	 0.7200	 0.4950
YY	 0.5880	 0.4210
Z	 0.7180	 0.4870
ZZ	 0.5090	 0.3720
a	 0.7750	 0.5320
aa	 0.6510	 0.4840
b	 0.5940	 0.4180
bb	 0.5820	 0.4360
c	 0.6800	 0.4860
cc	 0.5490	 0.4180
d	 0.6930	 0.4860
dd	 0.7380	 0.5010
e	 0.7630	 0.5350
ee	 0.5070	 0.3870
f	 0.8080	 0.5430
ff	 0.3200	 0.2000
g	 0.7070	 0.5040
gg	 0.4700	 0.3590
h	 0.6860	 0.4900
hh	 0.7670	 0.4640
i	 0.6590	 0.4560
ii	 0.6790	 0.4100
j	 0.8040	 0.5440

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Chain	Atom inclusion	Q-score
jj	 0.6000	 0.4490
k	 0.5890	 0.4140
l	 0.7310	 0.4960
m	 0.7430	 0.4970
n	 0.6830	 0.4480
o	 0.7010	 0.5140
p	 0.6810	 0.4840
r	 0.7450	 0.5140
s	 0.1380	 0.1250
t	 0.0590	 0.0740