



Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 02:47 am BST

PDB ID : 28LU / pdb_000028lu
EMDB ID : EMD-56602
Title : Structure of the Chlamydomonas reinhardtii chlororibosome with factor pY
Authors : Waltz, F.; Kater, L.; Engel, B.D.
Deposited on : 2026-02-05
Resolution : 2.60 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:

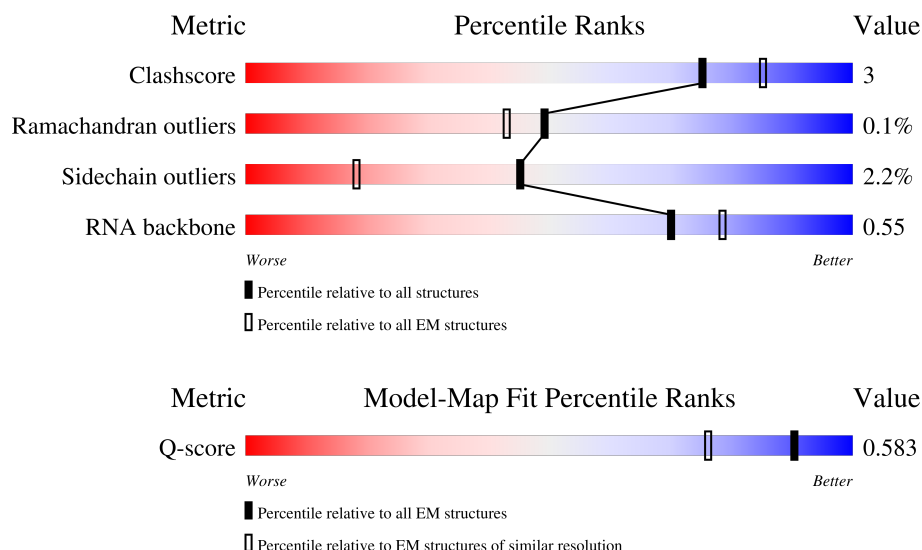
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.60 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.



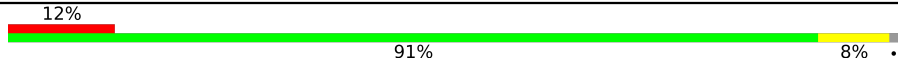
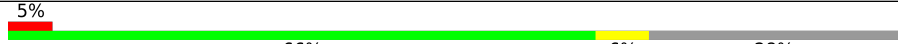
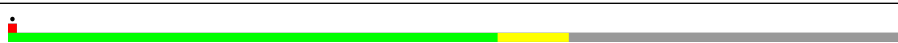
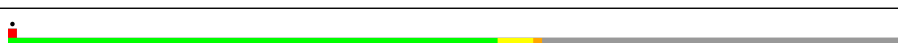
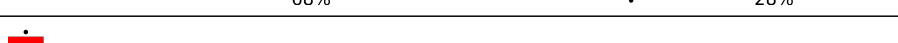
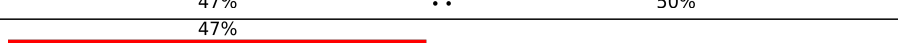
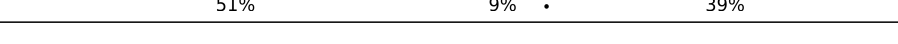
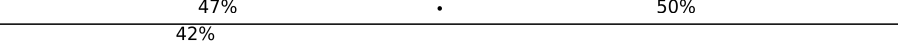
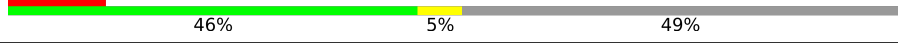
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	436	
2	d	257	
3	f	171	

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Mol	Chain	Length	Quality of chain
4	g	168	
5	h	141	
6	j	169	
7	k	130	
8	l	133	
9	m	164	
10	n	100	
11	o	141	
12	p	128	
13	q	105	
14	r	137	
15	s	92	
16	t	166	
17	u	184	
18	v	298	
19	x	120	
20	w	560	
21	2	1470	
22	b	910	
23	c	712	
24	e	673	
25	i	191	
26	y	286	
27	0	66	
28	3	121	

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Mol	Chain	Length	Quality of chain
29	5	47	
30	6	101	
31	7	124	
32	8	114	
33	9	37	
34	B	278	
35	C	259	
36	D	243	
37	E	179	
38	F	207	
39	G	200	
40	H	235	
41	I	176	
42	J	225	
43	K	122	
44	L	241	
45	M	136	
46	N	173	
47	O	145	
48	P	153	
49	Q	112	
50	R	179	
51	S	175	
52	T	111	
53	U	170	

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Mol	Chain	Length	Quality of chain
54	V	161	
55	W	195	
56	X	134	
57	Z	98	
58	Y	136	
59	1	2375	
60	4	272	

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 159560 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 Ribosomal protein S1 homologue.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	236	Total	C	N	O	S	0	0
			1868	1175	285	395	13		

- Molecule 2 is a protein called Small ribosomal subunit protein uS4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	d	256	Total	C	N	O	S	0	0
			2107	1356	403	341	7		

- Molecule 3 is a protein called bS6c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	f	103	Total	C	N	O	S	0	0
			850	543	148	156	3		

- Molecule 4 is a protein called Small ribosomal subunit protein uS7c.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	g	167	Total	C	N	O	S	0	0
			1334	846	253	229	6		

- Molecule 5 is a protein called Small ribosomal subunit protein uS8c.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	h	141	Total	C	N	O	S	0	0
			1113	698	206	203	6		

- Molecule 6 is a protein called Small ribosomal subunit protein uS10 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	j	122	Total	C	N	O	S	0	0
			957	597	173	178	9		

- Molecule 7 is a protein called Small ribosomal subunit protein uS11c.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	k	117	Total	C	N	O	S	0	0
			894	560	179	151	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS12c.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	l	121	Total	C	N	O	S	0	0
			941	591	190	157	3		

- Molecule 9 is a protein called uS13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	m	114	Total	C	N	O	S	0	0
			924	569	181	172	2		

- Molecule 10 is a protein called Small ribosomal subunit protein uS14c.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	n	99	Total	C	N	O	S	0	0
			814	513	163	132	6		

- Molecule 11 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	o	101	Total	C	N	O	S	0	0
			813	502	156	151	4		

- Molecule 12 is a protein called 30S ribosomal protein S16, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	p	80	Total	C	N	O	S	0	0
			666	433	120	112	1		

- Molecule 13 is a protein called Small ribosomal subunit protein uS17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	q	78	Total	C	N	O	S	0	0
			621	386	117	116	2		

- Molecule 14 is a protein called Small ribosomal subunit protein bS18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	r	81	Total	C	N	O	S	0	0
			664	434	123	106	1		

- Molecule 15 is a protein called Small ribosomal subunit protein uS19c.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	s	81	Total	C	N	O	S	0	0
			645	414	122	106	3		

- Molecule 16 is a protein called bS20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	t	119	Total	C	N	O	S	0	0
			935	592	172	167	4		

- Molecule 17 is a protein called bS21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	u	92	Total	C	N	O	S	0	0
			789	494	144	147	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
u	652	ARG	ASP	conflict	UNP A8HPN4

- Molecule 18 is a protein called 30S ribosomal protein 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	v	181	Total	C	N	O	S	0	0
			1430	907	245	276	2		

- Molecule 19 is a protein called cS26/PSRP8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	x	60	Total	C	N	O	S	0	0
			462	299	80	81	2		

- Molecule 20 is a protein called Plastid-specific ribosomal protein-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	w	365	Total	C	N	O	S	0	0
			2786	1749	429	598	10		

- Molecule 21 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	2	1470	Total	C	N	O	P	0	0
			31537	14077	5779	10211	1470		

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	?	-	C	deletion	GB 41179002
2	?	-	A	deletion	GB 41179002
2	372	A	-	insertion	GB 41179002
2	373	G	-	insertion	GB 41179002
2	871	G	-	insertion	GB 41179002
2	872	G	-	insertion	GB 41179002
2	912	2MG	A	conflict	GB 41179002
2	982	A	-	insertion	GB 41179002
2	983	C	-	insertion	GB 41179002
2	1200	C	-	insertion	GB 41179002
2	1218	A	C	conflict	GB 41179002

- Molecule 22 is a protein called Small ribosomal subunit protein uS2c.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	685	Total	C	N	O	S	0	0
			5545	3581	1010	934	20		

- Molecule 23 is a protein called Small ribosomal subunit protein uS3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	c	607	Total	C	N	O	S	0	0
			4939	3179	905	844	11		

- Molecule 24 is a protein called uS5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	536	Total	C	N	O	S	0	0
			3988	2477	658	838	15		

- Molecule 25 is a protein called Small ribosomal subunit protein uS9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	i	153	Total	C	N	O	S	0	0
			1189	750	219	217	3		

- Molecule 26 is a protein called Sigma 54 modulation/S30EA ribosomal protein C-terminal domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	146	Total	C	N	O	S	0	0
			1155	725	203	225	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	236	ALA	-	insertion	UNP A0A2K3DSW0

- Molecule 27 is a protein called cL38/PSRP6.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	0	47	Total	C	N	O	0	0
			369	233	76	60		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	17	SER	THR	conflict	UNP A0A835SZL0
0	37	ARG	ALA	conflict	UNP A0A835SZL0
0	38	ALA	SER	conflict	UNP A0A835SZL0
0	41	ASN	ARG	conflict	UNP A0A835SZL0
0	63	ALA	GLY	conflict	UNP A0A835SZL0

- Molecule 28 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	121	Total	C	N	O	P	0	0
			2571	1148	449	853	121		

- Molecule 29 is a RNA chain called 3S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5	47	Total	C	N	O	P	0	0
			1006	450	185	324	47		

- Molecule 30 is a protein called bL33c.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	58	Total	C	N	O	S	0	0
			473	293	91	86	3		

- Molecule 31 is a protein called bL34c.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	60	Total	C	N	O	S	0	0
			455	271	104	77	3		

- Molecule 32 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	68	Total	C	N	O	S	0	0
			520	322	104	91	3		

- Molecule 33 is a protein called Large ribosomal subunit protein bL36c.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	9	37	Total	C	N	O	S	0	0
			292	177	63	46	6		

- Molecule 34 is a protein called Large ribosomal subunit protein uL2c.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	B	276	Total	C	N	O	S	0	0
			2159	1347	431	377	4		

- Molecule 35 is a protein called Large ribosomal subunit protein uL3c.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	C	223	Total	C	N	O	S	0	0
			1681	1057	310	305	9		

- Molecule 36 is a protein called Large ribosomal subunit protein uL4c.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	D	216	Total	C	N	O	S	0	0
			1599	997	290	306	6		

- Molecule 37 is a protein called Large ribosomal subunit protein uL5c.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	E	178	Total	C	N	O	S	0	0
			1413	900	247	260	6		

- Molecule 38 is a protein called Plastid ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	F	177	Total	C	N	O	S	0	0
			1338	845	245	244	4		

- Molecule 39 is a protein called Large ribosomal subunit protein bL9c.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	G	54	Total	C	N	O	S	0	0
			418	272	72	73	1		

- Molecule 40 is a protein called uL10c.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	H	141	Total	C	N	O	S	0	0
			1114	711	189	209	5		

- Molecule 41 is a protein called Large ribosomal subunit protein uL11c.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	I	132	Total	C	N	O	S	0	0
			980	623	171	181	5		

- Molecule 42 is a protein called uL13c.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	J	173	Total	C	N	O	S	0	0
			1346	857	243	243	3		

- Molecule 43 is a protein called Large ribosomal subunit protein uL14c.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	K	122	Total	C	N	O	S	0	0
			942	588	180	169	5		

- Molecule 44 is a protein called uL15c.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	L	198	Total	C	N	O	S	0	0
			1484	921	282	276	5		

- Molecule 45 is a protein called Large ribosomal subunit protein uL16c.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	M	135	Total	C	N	O	S	0	0
			1080	689	211	173	7		

- Molecule 46 is a protein called Large ribosomal subunit protein bL17c.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	N	117	Total	C	N	O	S	0	0
			937	585	185	162	5		

- Molecule 47 is a protein called Large ribosomal subunit protein uL18c.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	O	118	Total	C	N	O	S	0	0
			902	557	173	168	4		

- Molecule 48 is a protein called bL19c.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	P	130	Total	C	N	O	S	0	0
			995	620	199	174	2		

- Molecule 49 is a protein called Large ribosomal subunit protein bL20c.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Q	111	Total	C	N	O	S	0	0
			943	592	193	152	6		

- Molecule 50 is a protein called bL21c.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	R	115	Total	C	N	O	S	0	0
			907	585	161	157	4		

- Molecule 51 is a protein called Large ribosomal subunit protein uL22c.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S	115	Total	C	N	O	S	0	0
			903	564	174	157	8		

- Molecule 52 is a protein called uL23c, Large ribosomal subunit protein uL23c.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	T	107	Total	C	N	O	S	0	0
			837	542	148	146	1		

- Molecule 53 is a protein called KOW domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	U	132	Total	C	N	O	S	0	0
			1020	650	189	178	3		

- Molecule 54 is a protein called bL27c.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	V	114	Total	C	N	O	S	0	0
			869	535	172	159	3		

- Molecule 55 is a protein called Large ribosomal subunit protein bL28c.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	W	138	Total	C	N	O	S	0	0
			1104	700	205	193	6		

- Molecule 56 is a protein called uL29c.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	X	106	Total	C	N	O	S	0	0
			843	518	169	153	3		

- Molecule 57 is a protein called bL32c.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	Z	41	Total	C	N	O	0	0
			323	213	57	53		

- Molecule 58 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	Y	65	Total	C	N	O	S	0	0
			521	331	90	98	2		

- Molecule 59 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	1	2375	Total	C	N	O	P	0	0
			50934	22751	9345	16463	2375		

- Molecule 60 is a RNA chain called 7S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
60	4	272	Total	C	N	O	P	0	0
			5856	2616	1106	1862	272		

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
61	2	47	Total	K	0
			47	47	
61	U	1	Total	K	0
			1	1	
61	1	86	Total	K	0
			86	86	
61	4	4	Total	K	0
			4	4	

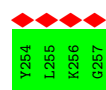
- Molecule 62 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
62	2	98	Total	Mg	0
			98	98	
62	3	5	Total	Mg	0
			5	5	
62	5	4	Total	Mg	0
			4	4	
62	D	1	Total	Mg	0
			1	1	
62	L	1	Total	Mg	0
			1	1	
62	N	1	Total	Mg	0
			1	1	

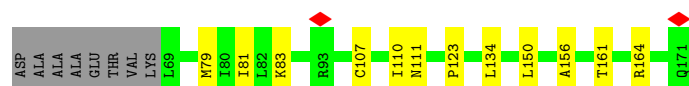
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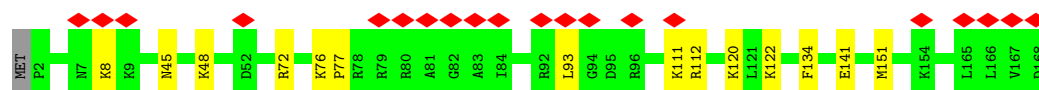
Mol	Chain	Residues	Atoms		AltConf
62	1	205	Total 205	Mg 205	0
62	4	7	Total 7	Mg 7	0



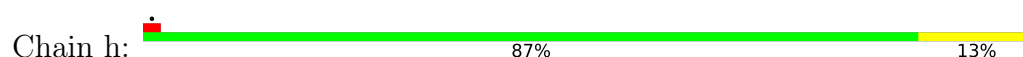
- Molecule 3: bS6c



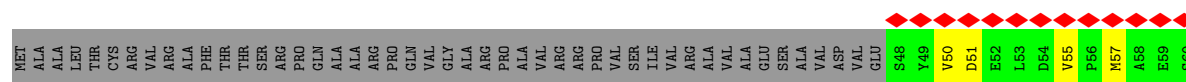
- Molecule 4: Small ribosomal subunit protein uS7c



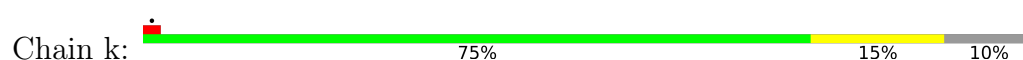
- Molecule 5: Small ribosomal subunit protein uS8c



- Molecule 6: Small ribosomal subunit protein uS10 domain-containing protein



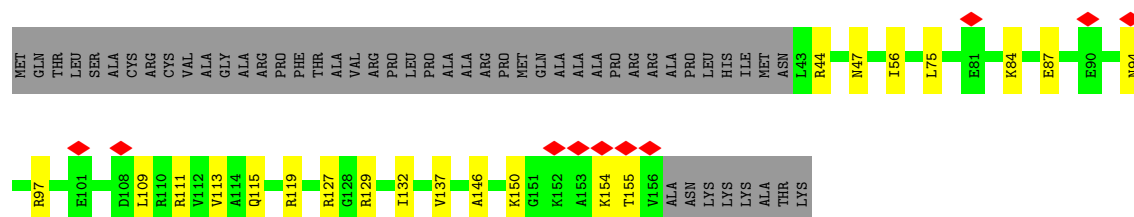
- Molecule 7: Small ribosomal subunit protein uS11c



- Molecule 8: Small ribosomal subunit protein uS12c

MET	P2	T3	I4	K17	V40	R50	Y66	K88	D89	L90	R110	R114	V119	K120	M121	G122	SER	LYS	THR	ALA	ALA	LYS	THR	ALA	GLY	LYS	LYS
-----	----	----	----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

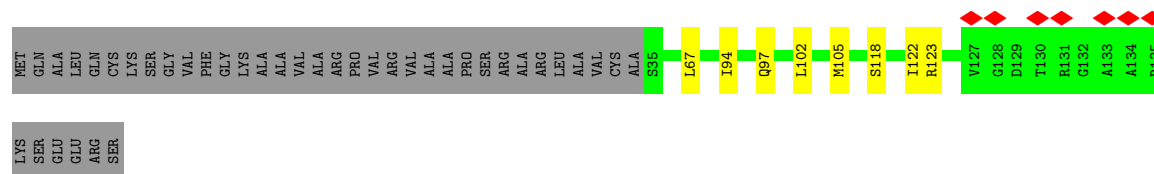
Chain m:



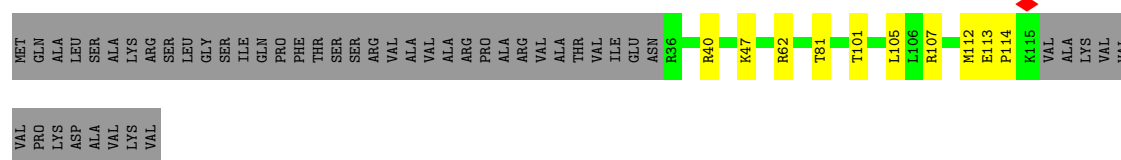
Chain n: 90% 9% .



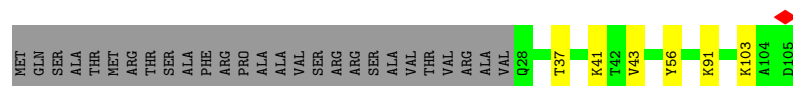
Chain o: 5% 66% 6% 28%



Chain p:

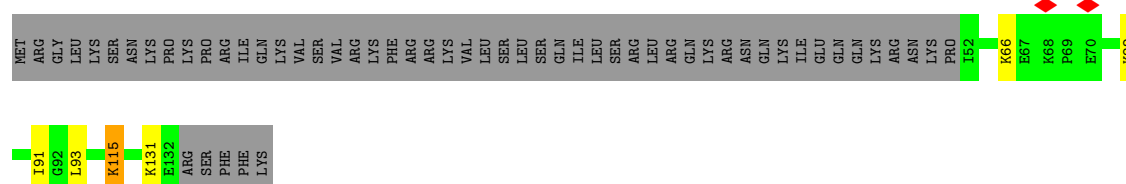


Chain q:



- Molecule 14: Small ribosomal subunit protein bS18c

Chain r:  55% 41%



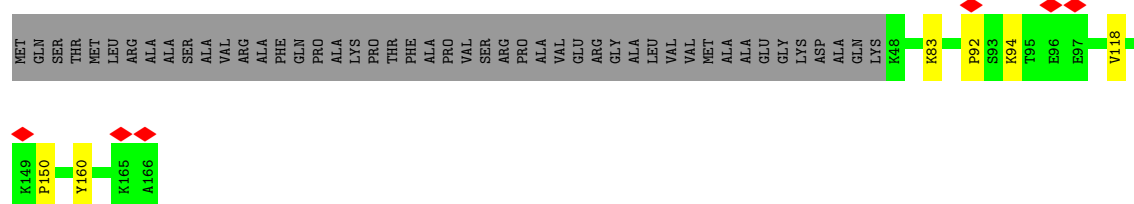
- Molecule 15: Small ribosomal subunit protein uS19c

Chain s:  70% 17% 12%



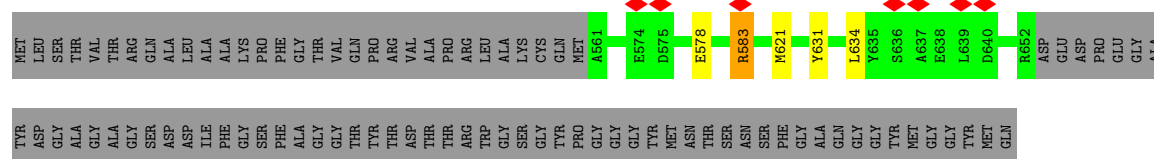
- Molecule 16: bS20c

Chain t:  68% 28%

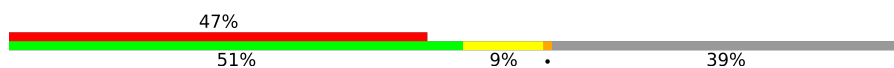


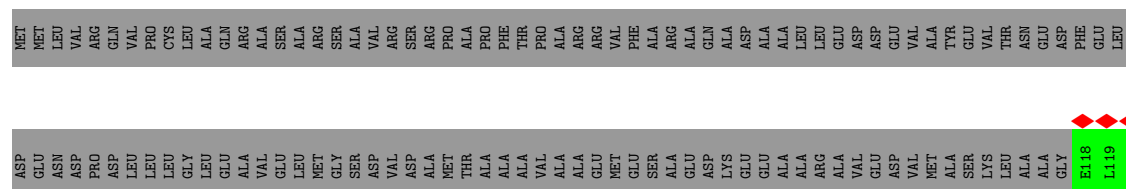
- Molecule 17: bS21c

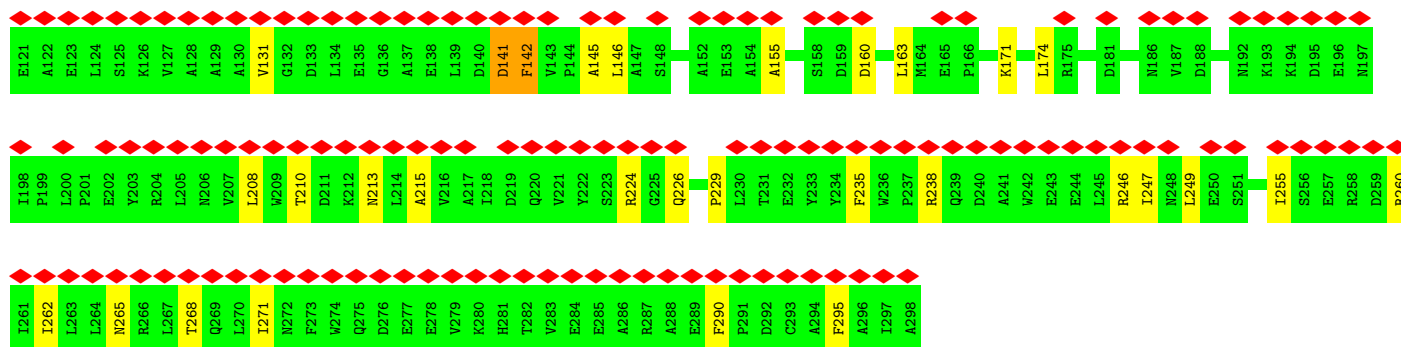
Chain u:  47% 50%



- Molecule 18: 30S ribosomal protein 3, chloroplastic

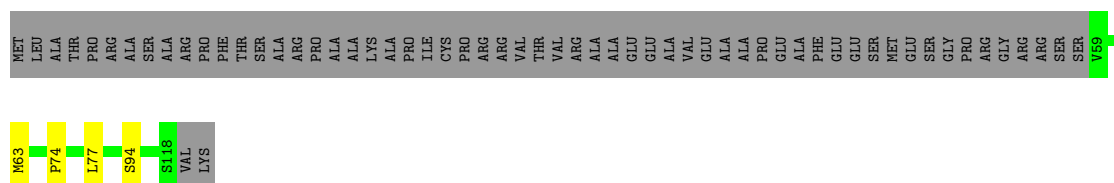
Chain v:  47% 51% 9% 39%





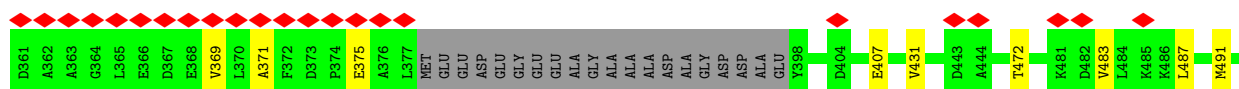
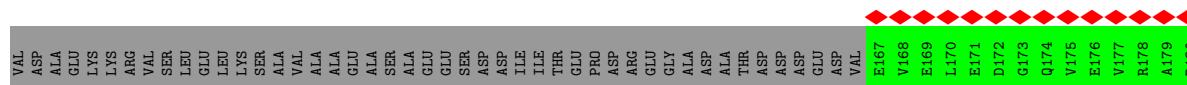
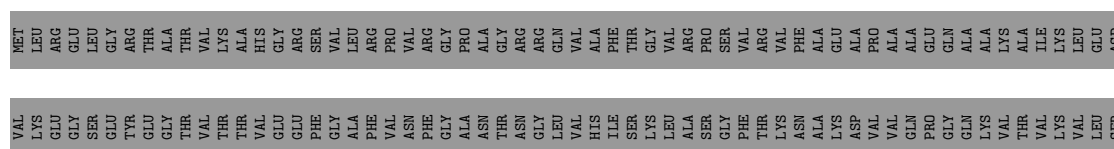
• Molecule 19: cS26/PSRP8

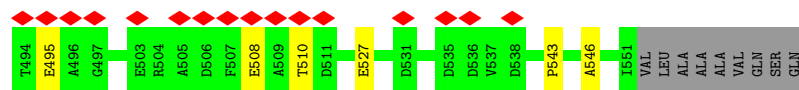
Chain x: 47% 50%



• Molecule 20: Plastid-specific ribosomal protein-7

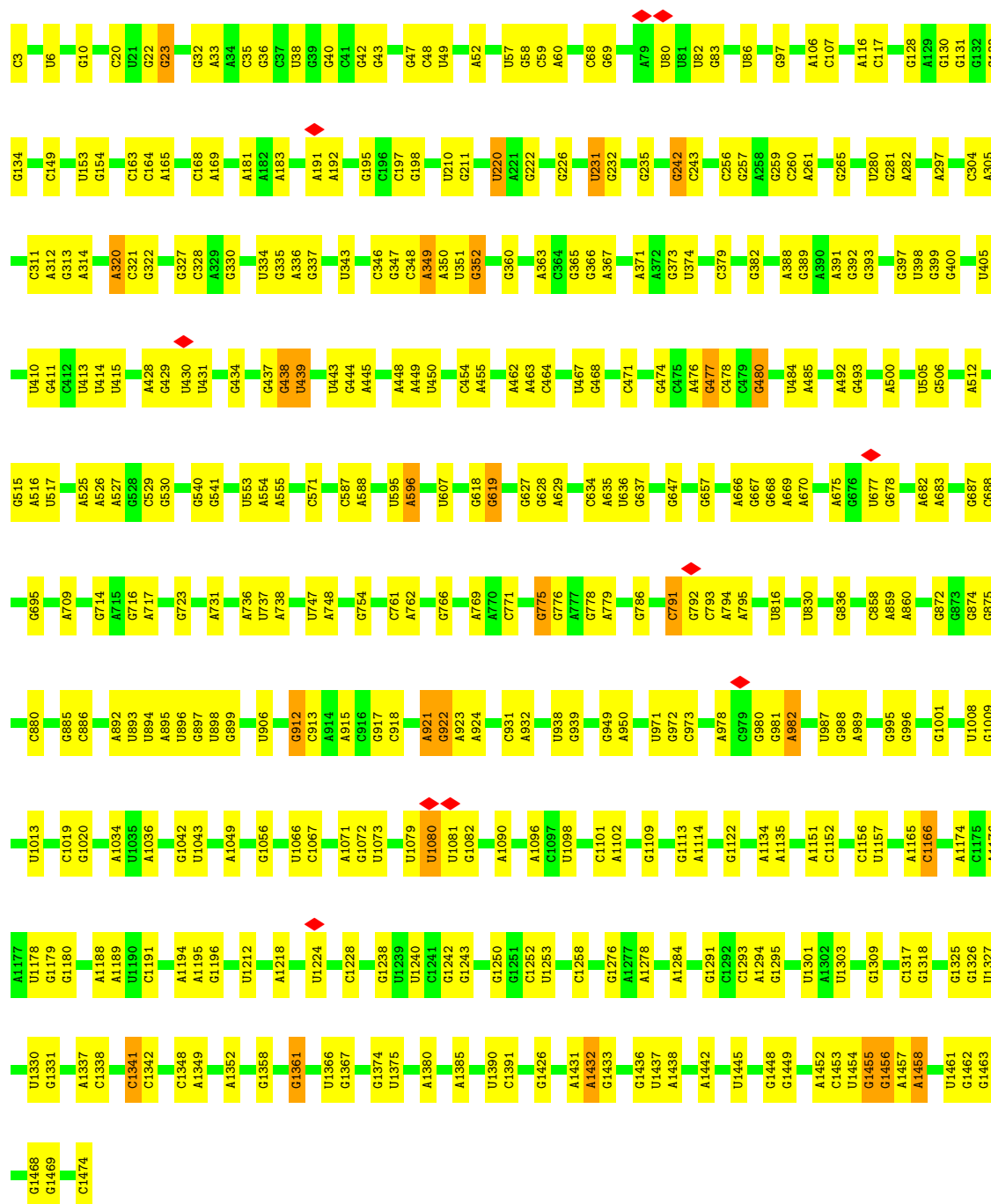
Chain w: 42% 57% 8% 35%





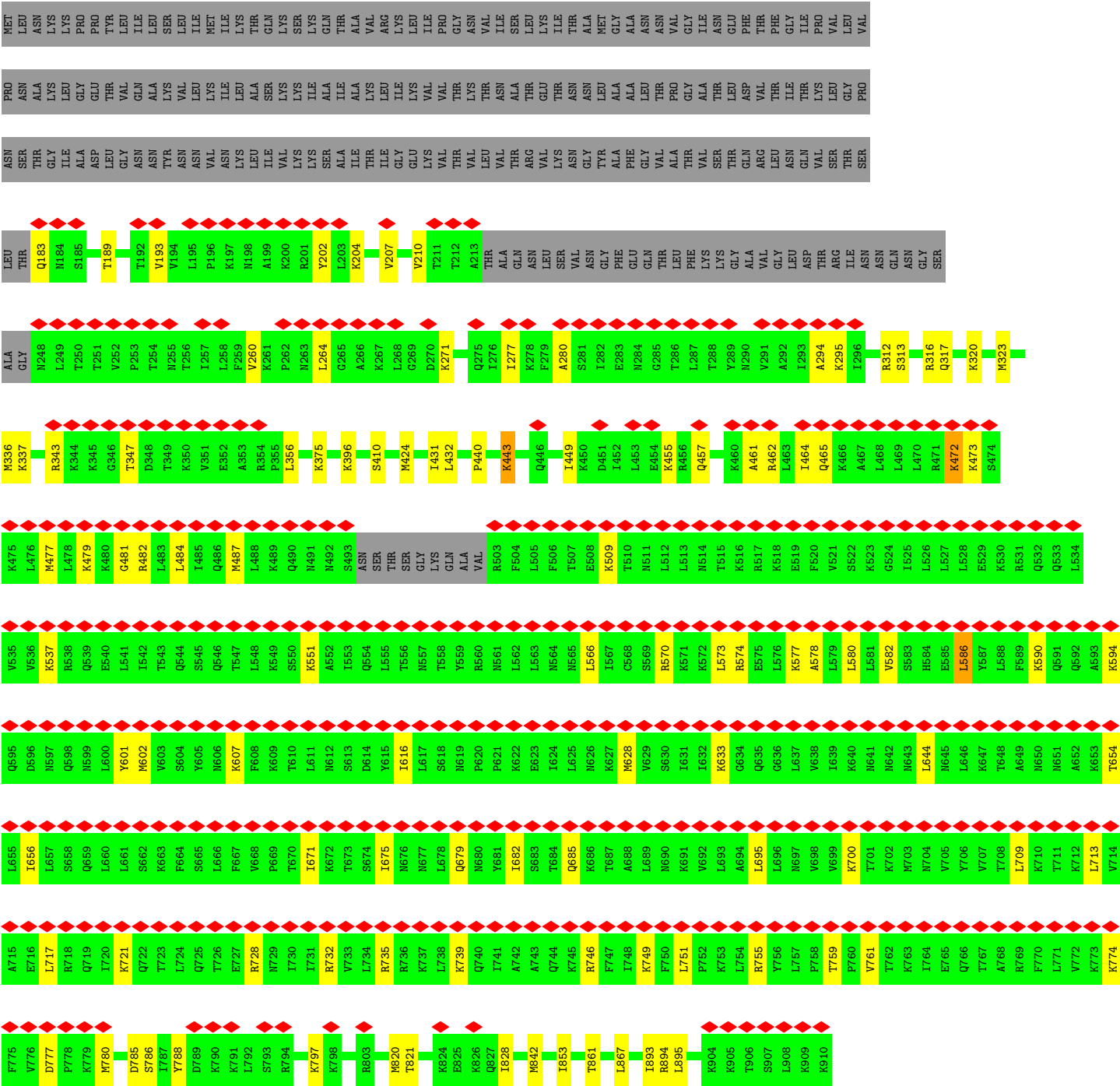
• Molecule 21: 16S rRNA

Chain 2: 73% 25%

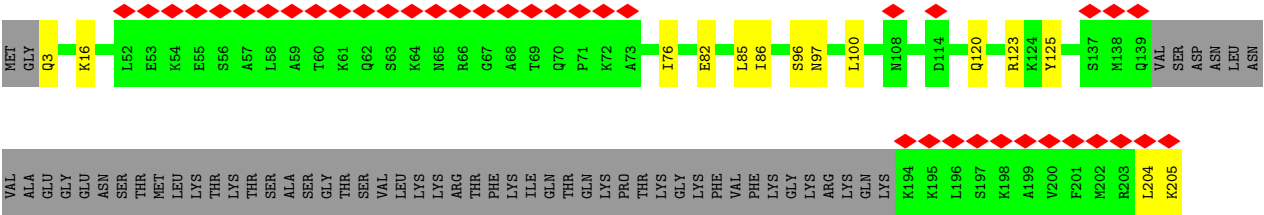
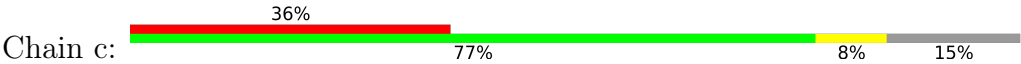


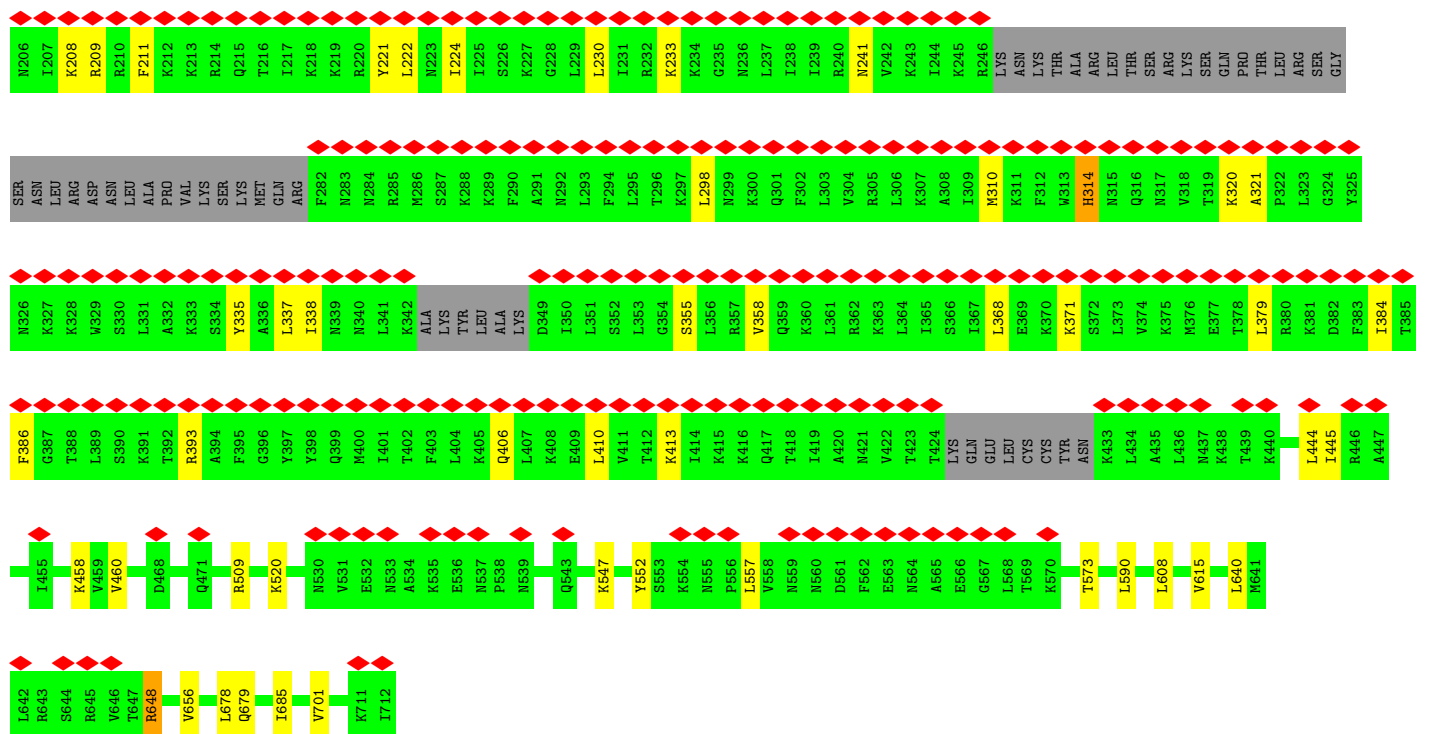
• Molecule 22: Small ribosomal subunit protein uS2c

Chain b: 44% 63% 12% 25%

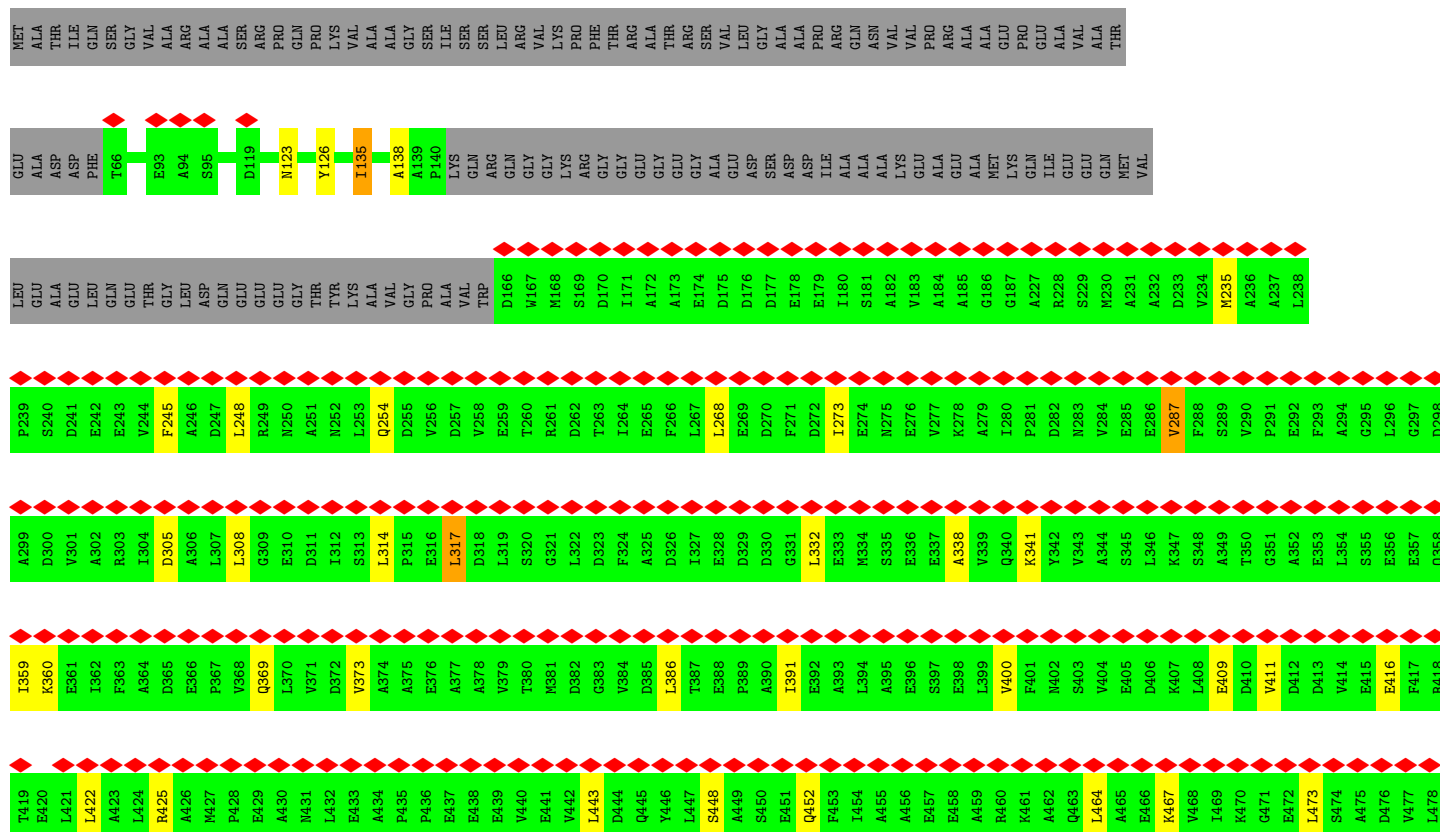
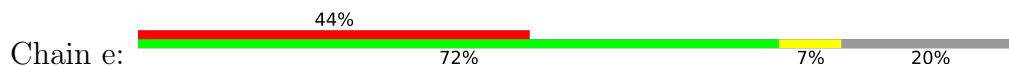


● Molecule 23: Small ribosomal subunit protein uS3c



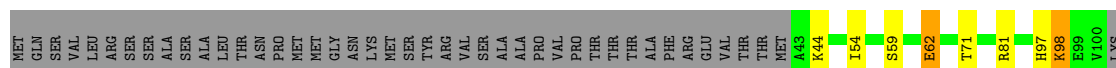


• Molecule 24: uS5c

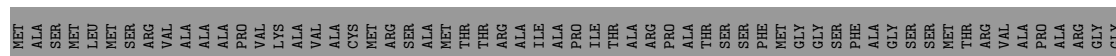




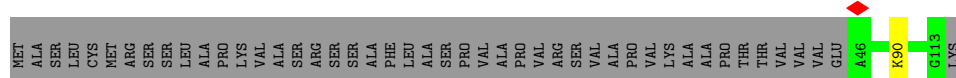
- Molecule 30: bL33c



- Molecule 31: bL34c



- Molecule 32: 50S ribosomal protein L35



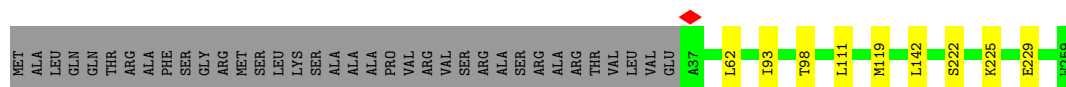
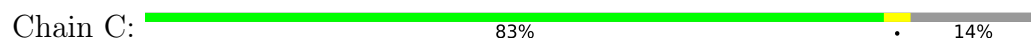
- Molecule 33: Large ribosomal subunit protein bL36c



- Molecule 34: Large ribosomal subunit protein uL2c



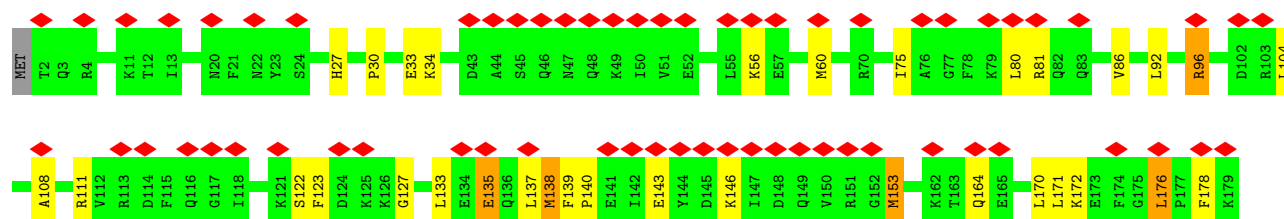
- Molecule 35: Large ribosomal subunit protein uL3c



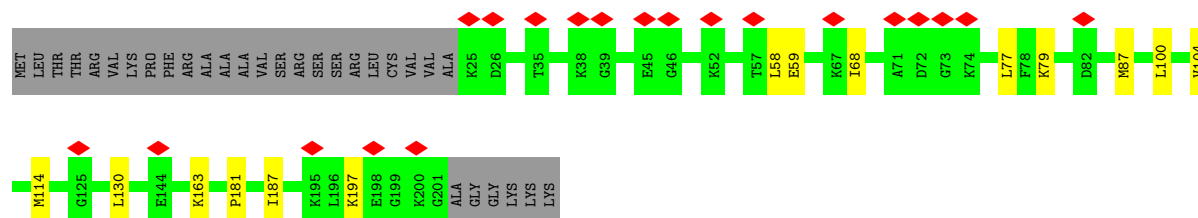
- Molecule 36: Large ribosomal subunit protein uL4c

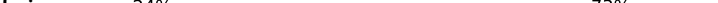
MET	GLN	THR	MET	ARG	VAL	ALA	PHE	ARG	PRO	PRO	ALA	ALA	THR	SER	ARG	SER	THR	VAL	THR	ARG	ALA	ALA	S23	L48	H60	V66	S106	K119	N128	E131	L140	M165	R189	V192	T203	F213	N217	Y235	A238	ALA	PRO	ALA	SER	ALA
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----

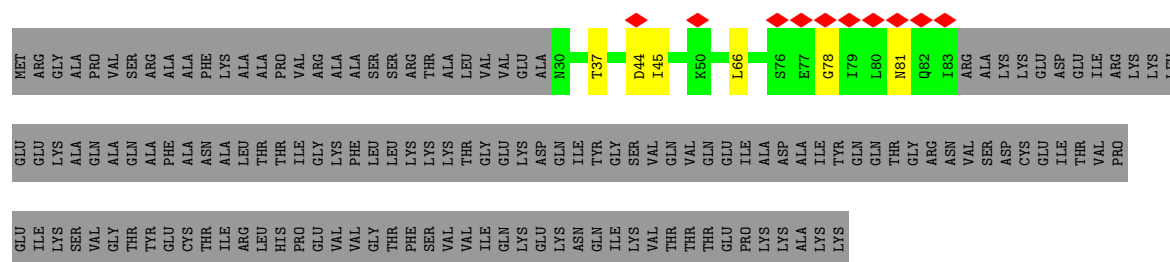
- Chain E:  35% 81% 16%

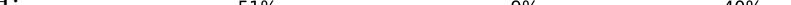


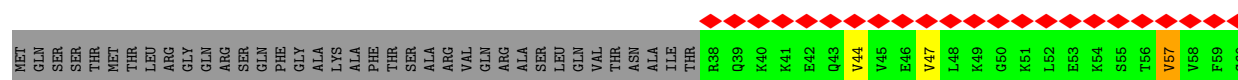
- Chain F:  10% 79% 7% 4%

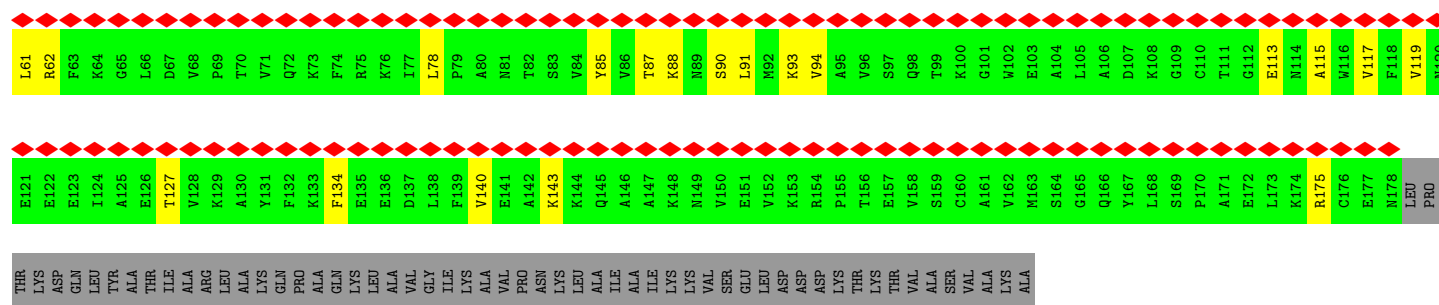


- Chain G:  5% 24% 73%

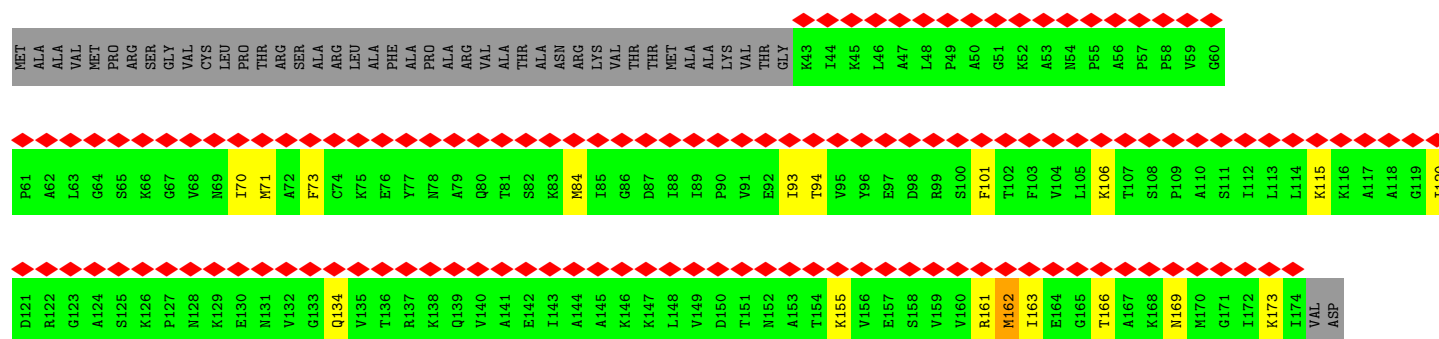
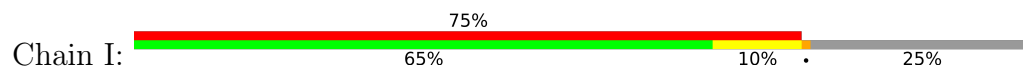


- Chain H: 

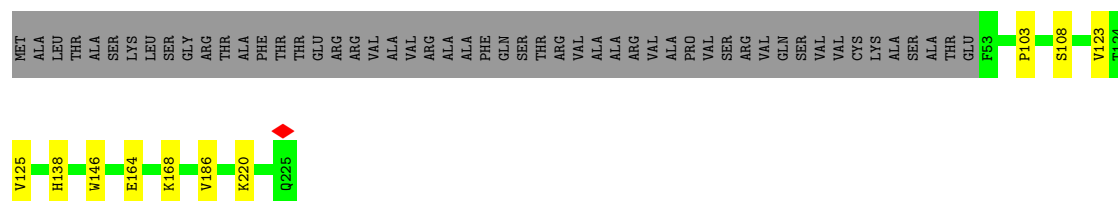




- Molecule 41: Large ribosomal subunit protein uL11c



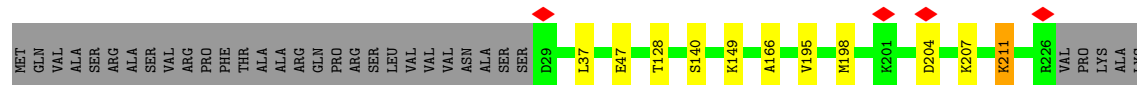
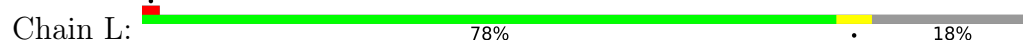
- Molecule 42: uL13c



- Molecule 43: Large ribosomal subunit protein uL14c



- Molecule 44: uL15c



PRO
ALA
ALA
ALA
ALA
GLY
LYS
LYS

- Molecule 45: Large ribosomal subunit protein uL16c

Chain M:  93% 5% ..

MET K5 I27 L34 E38 R56 R59 R60 M118 V127 L132 T135 VAL

- Molecule 46: Large ribosomal subunit protein bL17c

Chain N:  62% 6% 32%

MET ALA THR LEU GLN MET ALA ARG SER GLY VAL PHE THR SER ARG ALA SER ALA PRO ARG ALA VAL VAL ARG ALA VAL VAL PRO PRO VAL VAL ALA ARG PRO ARG SER SER THR GLN ALA THR SER SER PHE LEU GLY GLU ALA THR LEU VAL VAL ALA PRO SER SER GLY MET LYS TRP THR MET M57 L66

S79 E83 T93 V93 M123 L126 K129 V132 E156 V173

- Molecule 47: Large ribosomal subunit protein uL18c

Chain O:  6% 73% 8% 19%

MET GLN SER THR MET PHE LYS ALA THR LEU ALA PRO THR ARG PRO VAL ARG ARG ALA PHE THR THR PRO VAL VAL CYS LYS ALA A28 A32 E50 R51 P52 A55 E61 R64 D85 L86 K87 E88 S89 L90 E91 S92 G93 A94 G103 E108 V118 D121 A137

F145

- Molecule 48: bL19c

Chain P:  5% 80% 5% 15%

MET LEU ALA SER ARG SER ALA VAL ARG PRO PHE VAL ALA GLY ARG ARG PRO THR VAL ALA CYS SER A23 K24 M34 V54 G61 N62 G63 K64 T65 R66 V97 M101 R136 R144 D147 K152 GLN

- Molecule 49: Large ribosomal subunit protein bL20c

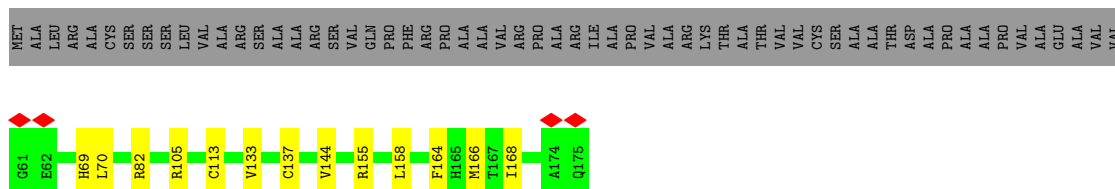
Chain Q:  92% 7% .

MET T2 R6 L31 Q38 R44 M60 A68 L74 V94 F112

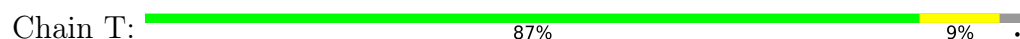
- Molecule 50: bL21c

Chain R:  55% 9% 36%

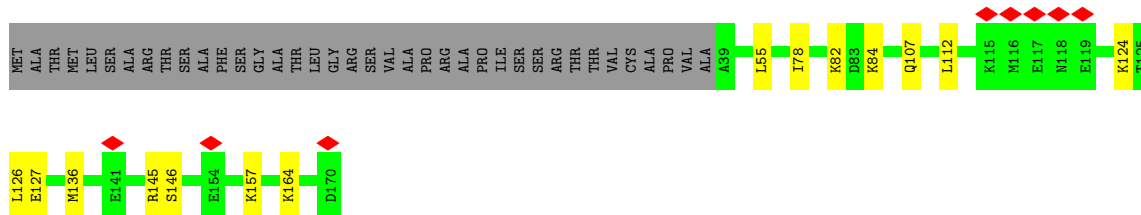
- Molecule 51: Large ribosomal subunit protein uL22c



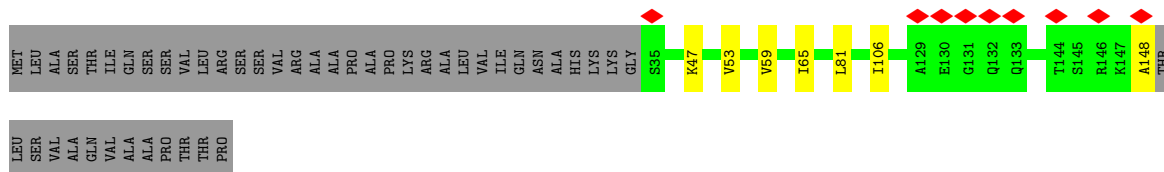
- Molecule 52: uL23c, Large ribosomal subunit protein uL23c



- Molecule 53: KOW domain-containing protein

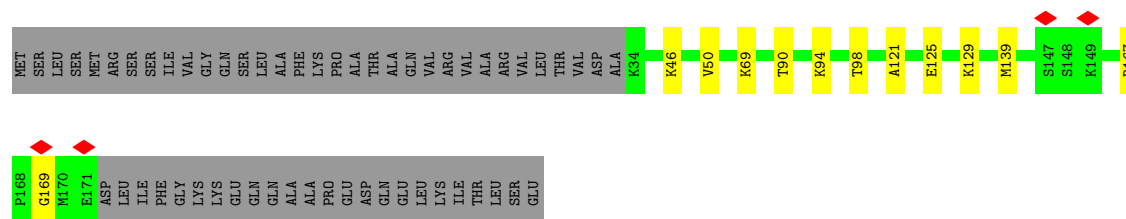


- Molecule 54: bL27c

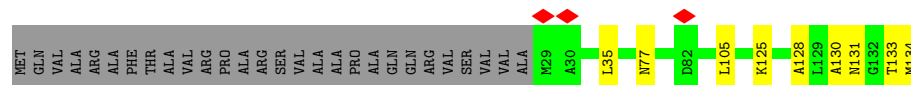


- Molecule 55: Large ribosomal subunit protein bL28c

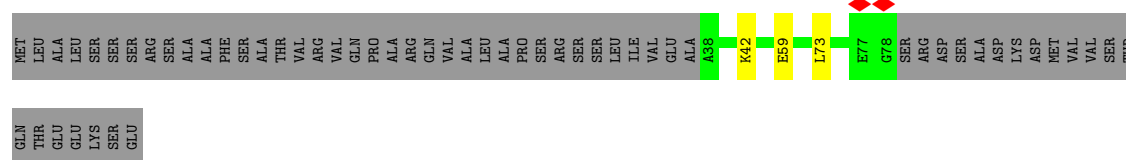




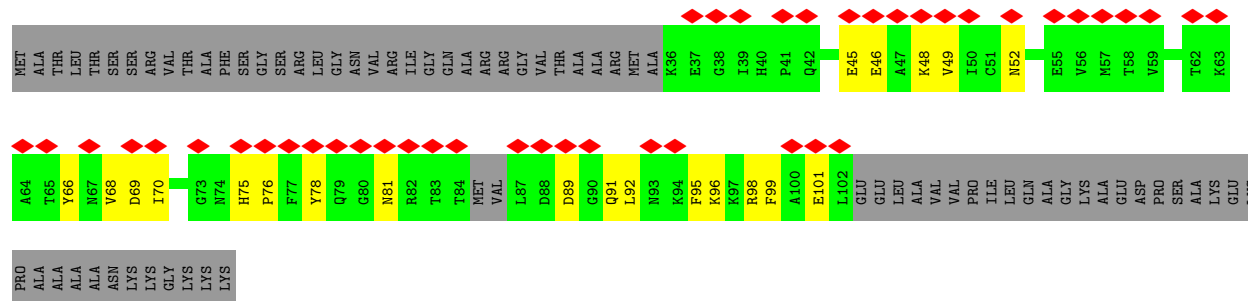
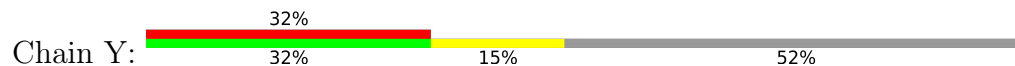
• Molecule 56: uL29c



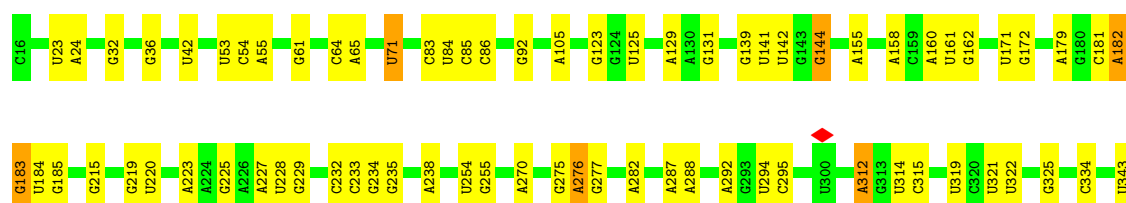
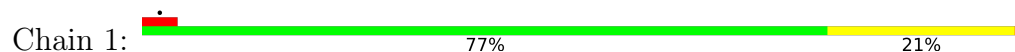
• Molecule 57: bL32c

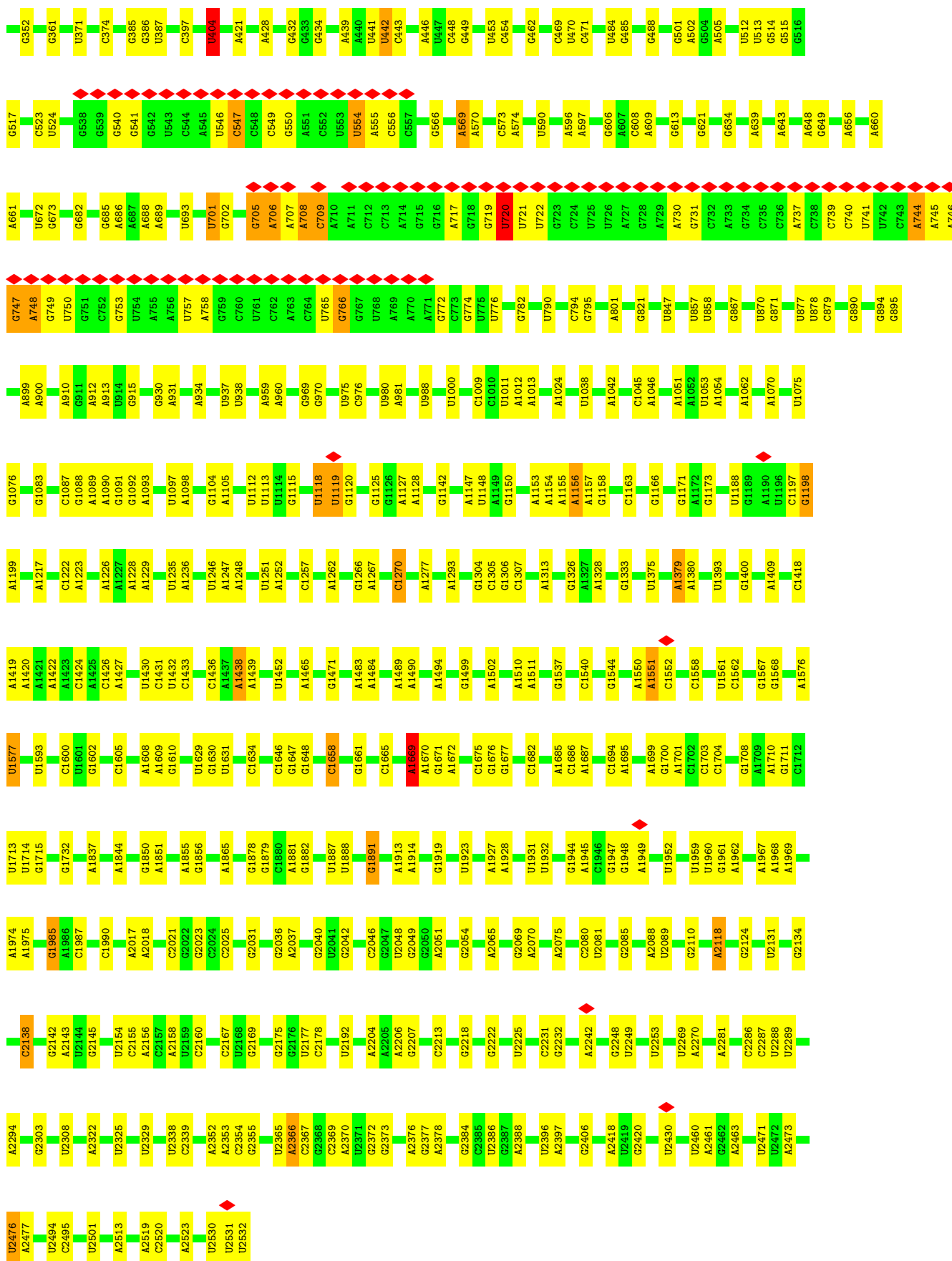


• Molecule 58: 50S ribosomal protein L31

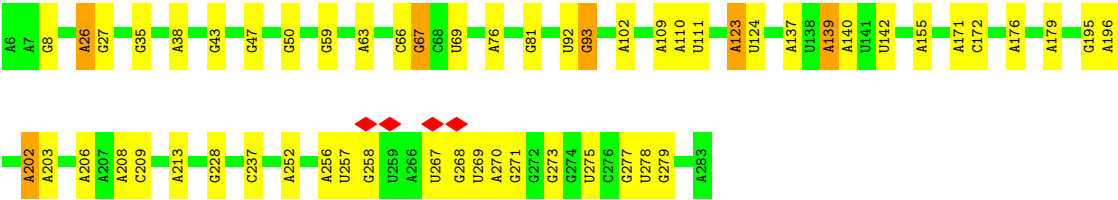
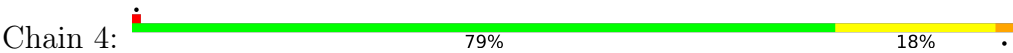


• Molecule 59: 23S rRNA





● Molecule 60: 7S rRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175058	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	75000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.538	Depositor
Minimum map value	-0.289	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.107	Depositor
Map size (Å)	544.3072, 544.3072, 544.3072	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0631, 1.0631, 1.0631	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MA6, G7M, 6MZ, OMC, 4OC, 2MA, OMG, H2U, UR3, OMU, 2MG, 5MC, K, 5MU

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	0.22	0/1899	0.59	0/2570
2	d	0.17	0/2144	0.40	0/2867
3	f	0.14	0/868	0.35	0/1172
4	g	0.19	0/1354	0.47	0/1820
5	h	0.14	0/1125	0.36	0/1505
6	j	0.16	0/974	0.48	0/1316
7	k	0.17	0/908	0.42	0/1210
8	l	0.15	0/955	0.36	0/1282
9	m	0.19	0/931	0.47	0/1246
10	n	0.13	0/827	0.32	0/1097
11	o	0.18	0/822	0.42	0/1098
12	p	0.15	0/682	0.39	0/917
13	q	0.15	0/626	0.35	0/836
14	r	0.17	0/676	0.40	0/907
15	s	0.17	0/661	0.44	0/887
16	t	0.18	0/948	0.40	0/1269
17	u	0.19	0/801	0.70	3/1070 (0.3%)
18	v	0.25	0/1463	0.69	3/1994 (0.2%)
19	x	0.14	0/472	0.37	0/637
20	w	0.18	0/2835	0.43	0/3845
21	2	0.15	2/35103 (0.0%)	0.31	0/54745
22	b	0.22	0/5616	0.53	3/7512 (0.0%)
23	c	0.16	0/5008	0.42	1/6698 (0.0%)
24	e	0.16	0/4029	0.44	1/5461 (0.0%)
25	i	0.20	0/1202	0.54	0/1605
26	y	0.28	1/1168 (0.1%)	0.50	0/1570
27	0	0.20	0/382	0.37	0/518
28	3	0.18	0/2871	0.36	0/4471
29	5	0.22	0/1126	0.38	0/1753
30	6	0.19	0/479	0.39	0/640
31	7	0.23	0/457	0.47	0/595
32	8	0.21	0/528	0.39	0/702

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	9	0.20	0/292	0.32	0/379
34	B	0.23	0/2200	0.42	0/2965
35	C	0.22	0/1711	0.41	0/2304
36	D	0.21	0/1619	0.40	0/2183
37	E	0.25	0/1433	0.63	2/1920 (0.1%)
38	F	0.17	0/1354	0.40	0/1821
39	G	0.20	0/424	0.46	0/570
40	H	0.19	0/1131	0.48	0/1520
41	I	2.27	3/992 (0.3%)	0.97	6/1336 (0.4%)
42	J	0.20	0/1375	0.40	0/1855
43	K	0.21	0/952	0.41	0/1280
44	L	0.21	0/1505	0.46	0/2009
45	M	0.19	0/1105	0.39	0/1482
46	N	0.22	0/951	0.43	0/1275
47	O	0.19	0/913	0.52	0/1222
48	P	0.18	0/1005	0.37	0/1351
49	Q	0.25	0/958	0.43	0/1272
50	R	0.21	0/927	0.39	0/1247
51	S	0.20	0/915	0.43	0/1221
52	T	0.22	0/772	0.44	0/1043
53	U	0.18	0/1036	0.35	0/1381
54	V	0.20	0/884	0.44	0/1187
55	W	0.19	0/1126	0.40	0/1507
56	X	0.20	0/853	0.36	0/1141
57	Z	0.21	0/328	0.39	0/436
58	Y	0.29	0/532	0.69	0/715
59	1	0.53	6/56765 (0.0%)	0.38	4/88499 (0.0%)
60	4	0.24	0/6566	0.37	0/10240
All	All	0.38	12/170564 (0.0%)	0.40	23/251176 (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
1	a	0	1
6	j	0	1
17	u	0	1
18	v	0	1
26	y	0	1
44	L	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
59	1	2	0
All	All	2	6

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	I	162	MET	CA-C	70.08	2.45	1.52
59	1	720	U	N3-C4	50.68	2.39	1.38
59	1	720	U	C2-N3	47.91	2.33	1.37
59	1	720	U	N1-C2	47.81	2.34	1.38
59	1	720	U	N1-C6	45.43	2.28	1.38
59	1	720	U	C4-C5	40.96	2.25	1.43
59	1	720	U	C5-C6	38.78	2.11	1.34
41	I	162	MET	CA-CB	6.73	1.64	1.53
26	y	206	PHE	CB-CG	6.38	1.65	1.50
41	I	162	MET	C-N	6.12	1.40	1.33
21	2	480	G7M	O3'-P	5.12	1.61	1.56
21	2	1437	UR3	O3'-P	5.02	1.61	1.56

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	I	162	MET	O-C-N	-18.55	97.64	122.49
41	I	162	MET	CB-CA-C	13.76	134.34	109.29
17	u	583	ARG	CB-CG-CD	11.32	137.34	111.30
41	I	162	MET	CA-C-O	9.23	129.30	119.14
41	I	162	MET	N-CA-C	8.91	124.46	113.50
17	u	583	ARG	CG-CD-NE	8.65	131.03	112.00
41	I	162	MET	N-CA-CB	-8.52	98.01	110.53
17	u	583	ARG	CA-CB-CG	8.29	130.67	114.10
59	1	312	A	O4'-C1'-N9	6.47	118.20	108.50
24	e	235	MET	CA-CB-CG	6.10	126.30	114.10
18	v	141	ASP	CA-C-N	5.73	132.48	121.54
18	v	141	ASP	C-N-CA	5.73	132.48	121.54
23	c	310	MET	CB-CG-SD	5.63	129.60	112.70
22	b	443	LYS	CA-CB-CG	5.55	125.21	114.10
41	I	71	MET	CB-CG-SD	5.51	129.22	112.70
59	1	1379	A	O4'-C1'-N9	5.49	116.73	108.50
59	1	1379	A	N9-C1'-C2'	5.46	120.19	112.00
22	b	472	LYS	CA-CB-CG	5.41	124.92	114.10
37	E	96	ARG	CB-CG-CD	5.30	123.49	111.30
22	b	472	LYS	CB-CG-CD	5.23	123.32	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	v	142	PHE	N-CA-C	5.14	121.75	110.80
37	E	135	GLU	CB-CG-CD	5.07	121.22	112.60
59	1	162	G	O4'-C1'-N9	5.04	115.76	108.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
59	1	312	A	C1'
59	1	1379	A	C1'

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
44	L	204	ASP	Peptide
1	a	291	VAL	Peptide
6	j	122	HIS	Peptide
17	u	583	ARG	Sidechain
18	v	141	ASP	Peptide
26	y	141	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	1868	0	1762	20	0
2	d	2107	0	2303	16	0
3	f	850	0	852	7	0
4	g	1334	0	1441	9	0
5	h	1113	0	1184	13	0
6	j	957	0	968	10	0
7	k	894	0	956	10	0
8	l	941	0	1029	7	0
9	m	924	0	971	32	0
10	n	814	0	877	7	0
11	o	813	0	828	4	0
12	p	666	0	697	7	0
13	q	621	0	658	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	r	664	0	743	6	0
15	s	645	0	677	24	0
16	t	935	0	1008	3	0
17	u	789	0	794	4	0
18	v	1430	0	1333	18	0
19	x	462	0	480	1	0
20	w	2786	0	2612	27	0
21	2	31537	0	15884	168	0
22	b	5545	0	6140	68	0
23	c	4939	0	5339	41	0
24	e	3988	0	3837	35	0
25	i	1189	0	1243	6	0
26	y	1155	0	1181	11	0
27	0	369	0	381	4	0
28	3	2571	0	1300	11	0
29	5	1006	0	508	1	0
30	6	473	0	498	3	0
31	7	455	0	500	0	0
32	8	520	0	543	0	0
33	9	292	0	332	3	0
34	B	2159	0	2239	7	0
35	C	1681	0	1736	4	0
36	D	1599	0	1659	9	0
37	E	1413	0	1479	17	0
38	F	1338	0	1434	7	0
39	G	418	0	456	2	0
40	H	1114	0	1149	11	0
41	I	980	0	1056	34	0
42	J	1346	0	1389	4	0
43	K	942	0	998	5	0
44	L	1484	0	1530	6	0
45	M	1080	0	1143	5	0
46	N	937	0	978	4	0
47	O	902	0	920	6	0
48	P	995	0	1057	5	0
49	Q	943	0	992	7	0
50	R	907	0	951	11	0
51	S	903	0	948	7	0
52	T	837	0	823	6	0
53	U	1020	0	1097	8	0
54	V	869	0	882	4	0
55	W	1104	0	1151	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	X	843	0	884	6	0
57	Z	323	0	367	2	0
58	Y	521	0	498	45	0
59	1	50934	0	25627	210	0
60	4	5856	0	2947	25	0
61	1	86	0	0	0	0
61	2	47	0	0	0	0
61	4	4	0	0	0	0
61	U	1	0	0	0	0
62	1	205	0	0	0	0
62	2	98	0	0	0	0
62	3	5	0	0	0	0
62	4	7	0	0	0	0
62	5	4	0	0	0	0
62	D	1	0	0	0	0
62	L	1	0	0	0	0
62	N	1	0	0	0	0
All	All	159560	0	116249	862	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 (862) 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)
59:1:1577:5MU:C5	59:1:1577:5MU:C4	1.82	1.62
59:1:404:5MU:C5	59:1:404:5MU:C4	1.82	1.61
59:1:720:U:C6	59:1:720:U:C5	2.11	1.37
59:1:720:U:C5	59:1:720:U:C4	2.25	1.24
41:I:162:MET:HA	59:1:720:U:C2	1.77	1.19
9:m:47:ASN:CG	58:Y:70:ILE:CD1	2.17	1.17
21:2:322:G:OP1	48:P:66:ARG:NH2	1.77	1.17
9:m:47:ASN:CG	58:Y:70:ILE:HD12	1.70	1.13
5:h:2:LYS:NZ	5:h:61:ASP:OD2	1.81	1.12
5:h:2:LYS:NZ	5:h:61:ASP:CG	2.06	1.11
15:s:42:PRO:HG3	58:Y:92:LEU:CD1	1.85	1.06
21:2:1432:A:C4	59:1:1551:A:C2	2.45	1.04
15:s:42:PRO:HG3	58:Y:92:LEU:HD12	1.41	1.02
59:1:720:U:C6	59:1:720:U:N1	2.28	1.01
21:2:791:C:H42	21:2:795:A:H61	1.12	0.98
9:m:47:ASN:OD1	58:Y:70:ILE:HD12	1.65	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:1:720:U:C2	59:1:720:U:N3	2.33	0.97
9:m:47:ASN:OD1	58:Y:70:ILE:CD1	2.13	0.96
41:I:162:MET:C	59:1:720:U:C2	2.43	0.96
21:2:1432:A:H2'	59:1:1551:A:H2	1.31	0.95
59:1:720:U:C2	59:1:720:U:N1	2.34	0.95
59:1:540:G:H1	59:1:554:U:H3	1.15	0.94
21:2:1352:A:H2	21:2:1426:G:H1	1.06	0.93
41:I:162:MET:HA	59:1:720:U:N1	1.84	0.93
21:2:47:G:H1	21:2:371:A:H2	1.04	0.93
9:m:47:ASN:CG	58:Y:70:ILE:HD11	1.93	0.91
5:h:2:LYS:NZ	5:h:61:ASP:OD1	2.03	0.90
10:n:38:LYS:HE3	58:Y:101:GLU:OE1	1.71	0.90
59:1:720:U:C4	59:1:720:U:N3	2.39	0.90
41:I:162:MET:C	41:I:162:MET:CA	2.45	0.90
60:4:252:A:H62	60:4:273:G:N2	1.68	0.90
5:h:2:LYS:HZ1	5:h:61:ASP:CG	1.76	0.86
41:I:162:MET:C	59:1:720:U:N3	2.33	0.86
9:m:97:ARG:HE	58:Y:69:ASP:CG	1.83	0.85
21:2:47:G:N1	21:2:371:A:C2	2.44	0.84
41:I:163:ILE:N	59:1:720:U:C4	2.45	0.84
21:2:1456:G:C8	59:1:1558:C:OP1	2.31	0.83
41:I:162:MET:HA	41:I:162:MET:C	2.01	0.83
41:I:162:MET:C	59:1:720:U:C4	2.56	0.83
21:2:1432:A:H2'	59:1:1551:A:C2	2.15	0.81
21:2:1433:G:O2'	59:1:1550:A:O2'	1.98	0.81
9:m:97:ARG:NE	58:Y:69:ASP:CG	2.39	0.80
15:s:42:PRO:HB3	58:Y:92:LEU:HD11	1.64	0.80
9:m:97:ARG:NE	58:Y:69:ASP:OD1	2.15	0.80
41:I:162:MET:C	59:1:720:U:C5	2.61	0.79
41:I:162:MET:CA	59:1:720:U:C2	2.63	0.79
41:I:162:MET:C	59:1:720:U:C6	2.60	0.79
60:4:258:G:H1	60:4:267:U:H3	1.29	0.77
21:2:791:C:N4	21:2:795:A:H61	1.80	0.77
21:2:220:U:O2	21:2:259:G:N1	2.16	0.77
15:s:65:GLN:HE22	58:Y:89:ASP:HB3	1.50	0.76
28:3:4:U:H3	28:3:120:G:H1	1.31	0.76
60:4:257:U:H3	60:4:268:G:H1	1.34	0.76
21:2:47:G:N1	21:2:371:A:H2	1.81	0.75
60:4:252:A:H62	60:4:273:G:H21	1.32	0.75
9:m:47:ASN:ND2	58:Y:70:ILE:HD12	2.02	0.74
9:m:47:ASN:CB	58:Y:70:ILE:HD11	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:s:42:PRO:HG3	58:Y:92:LEU:HD11	1.69	0.73
20:w:261:GLU:HB3	20:w:329:THR:HG23	1.71	0.73
41:I:162:MET:C	59:1:720:U:N1	2.46	0.73
41:I:162:MET:CA	59:1:720:U:C4	2.72	0.72
9:m:132:ILE:HG12	59:1:547:C:C2	2.25	0.72
21:2:1352:A:C2	21:2:1426:G:N1	2.48	0.71
21:2:1352:A:H2	21:2:1426:G:N1	1.85	0.71
18:v:155:ALA:HB1	22:b:264:LEU:HD11	1.73	0.71
10:n:38:LYS:HG2	58:Y:101:GLU:OE1	1.91	0.70
21:2:1432:A:N3	59:1:1551:A:C2	2.58	0.70
22:b:577:LYS:HZ1	24:e:386:LEU:HA	1.56	0.70
41:I:162:MET:O	59:1:720:U:N1	2.25	0.70
59:1:32:G:H22	59:1:42:U:H3	1.39	0.70
21:2:791:C:H42	21:2:795:A:N6	1.87	0.69
41:I:162:MET:CA	59:1:720:U:N3	2.56	0.69
15:s:42:PRO:CG	58:Y:92:LEU:HD11	2.21	0.69
15:s:42:PRO:CG	58:Y:92:LEU:CD1	2.68	0.69
60:4:252:A:N6	60:4:273:G:H21	1.90	0.69
15:s:40:ILE:HA	15:s:44:MET:HE3	1.75	0.68
59:1:219:G:H21	59:1:223:A:H8	1.40	0.68
15:s:42:PRO:CB	58:Y:92:LEU:HD11	2.23	0.68
41:I:93:ILE:HD11	41:I:101:PHE:HB2	1.74	0.68
59:1:753:G:H21	59:1:758:A:H62	1.40	0.68
15:s:25:LYS:HG3	15:s:27:LYS:HG2	1.76	0.67
59:1:220:U:H1'	59:1:1669:6MZ:H9C1	1.77	0.67
1:a:85:ASP:HA	1:a:88:GLN:HE21	1.60	0.67
30:6:81:ARG:HH21	30:6:98:LYS:HD2	1.60	0.67
21:2:618:G:H22	21:2:695:G:H1	1.44	0.66
21:2:1461:U:H2'	21:2:1462:G:H8	1.60	0.66
23:c:97:ASN:HB3	23:c:608:LEU:HD13	1.77	0.66
4:g:151:MET:HB3	7:k:62:PHE:HB3	1.76	0.66
20:w:290:ALA:HB2	23:c:320:LYS:HD2	1.78	0.66
56:X:35:LEU:HD22	60:4:69:U:H4'	1.78	0.65
15:s:41:VAL:HG12	58:Y:95:PHE:CZ	2.32	0.65
53:U:146:SER:HB3	53:U:164:LYS:HB2	1.77	0.65
53:U:136:MET:HE2	53:U:145:ARG:HG3	1.79	0.65
22:b:343:ARG:HG3	22:b:356:LEU:HG	1.79	0.64
1:a:130:MET:HE1	22:b:316:ARG:HE	1.62	0.64
24:e:422:LEU:HA	24:e:425:ARG:HE	1.62	0.64
41:I:162:MET:CA	59:1:720:U:N1	2.61	0.64
21:2:1352:A:N1	21:2:1426:G:O6	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:X:130:ALA:HB2	60:4:123:A:H62	1.62	0.64
59:1:238:A:H62	59:1:910:A:H2	1.45	0.63
9:m:84:LYS:HB2	9:m:87:GLU:HG3	1.80	0.63
22:b:455:LYS:HG3	22:b:780:MET:HE1	1.79	0.63
59:1:719:G:H2'	59:1:720:U:H3'	1.81	0.63
21:2:1361:G:O5'	43:K:48:PRO:HB3	1.98	0.62
59:1:540:G:H2'	59:1:541:G:H8	1.64	0.62
21:2:346:C:H42	21:2:367:A:H61	1.46	0.62
22:b:580:LEU:HB3	22:b:671:ILE:HG21	1.81	0.62
21:2:47:G:O6	21:2:371:A:N1	2.32	0.62
25:i:38:LEU:HD13	25:i:44:SER:HB2	1.82	0.62
22:b:509:LYS:HE3	24:e:287:VAL:HG11	1.82	0.61
23:c:460:VAL:HG13	23:c:557:LEU:HD22	1.82	0.61
37:E:171:LEU:HB3	37:E:176:LEU:HD22	1.81	0.61
15:s:67:VAL:O	58:Y:91:GLN:NE2	2.34	0.61
22:b:785:ASP:HA	22:b:788:TYR:HD2	1.64	0.61
59:1:1188:U:H3	59:1:1198:G:H1	1.49	0.61
21:2:628:G:H2'	21:2:629:A:H8	1.65	0.61
58:Y:92:LEU:HG	58:Y:96:LYS:HE2	1.81	0.61
23:c:678:LEU:HD23	23:c:685:ILE:HD13	1.82	0.60
8:l:50:ARG:HB3	8:l:66:TYR:HE1	1.66	0.60
16:t:92:PRO:HA	16:t:94:LYS:HE2	1.84	0.60
1:a:199:GLU:HG2	1:a:202:TYR:H	1.66	0.60
15:s:45:ILE:HD11	58:Y:92:LEU:HD13	1.83	0.60
20:w:354:GLU:HG2	23:c:208:LYS:HZ2	1.66	0.60
10:n:3:LYS:HG2	21:2:996:G:H5''	1.83	0.60
1:a:157:TYR:HB3	1:a:165:ILE:HD11	1.84	0.59
7:k:29:HIS:HA	7:k:59:SER:HB3	1.83	0.59
22:b:751:LEU:HD22	24:e:443:LEU:HD21	1.84	0.59
41:I:162:MET:CA	59:1:720:U:C5	2.86	0.59
6:j:72:LEU:HB2	6:j:145:LEU:HD11	1.84	0.59
25:i:96:VAL:HG11	25:i:110:ILE:HG12	1.83	0.59
6:j:104:GLY:HA3	21:2:1071:A:H4'	1.85	0.59
22:b:616:ILE:HG12	22:b:656:ILE:HB	1.85	0.58
59:1:705:G:H4'	59:1:706:A:H5''	1.86	0.58
21:2:365:G:H3'	21:2:366:G:H8	1.68	0.58
21:2:1008:U:H2'	21:2:1009:G:H8	1.68	0.58
22:b:537:LYS:HD3	24:e:308:LEU:HD13	1.85	0.58
41:I:163:ILE:N	59:1:720:U:N3	2.50	0.58
9:m:47:ASN:OD1	58:Y:70:ILE:HD11	1.95	0.58
24:e:501:LEU:HG	24:e:502:VAL:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:6:G:H1	28:3:118:U:H3	1.52	0.57
59:1:254:U:H3	59:1:312:A:H61	1.52	0.57
59:1:701:U:H3	59:1:774:G:H1	1.52	0.57
20:w:341:VAL:HG21	20:w:371:ALA:H	1.69	0.57
40:H:140:VAL:HG23	40:H:143:LYS:HE3	1.86	0.57
56:X:35:LEU:HD11	56:X:105:LEU:HB2	1.87	0.57
21:2:1432:A:C5	59:1:1551:A:N1	2.73	0.57
21:2:350:A:N6	21:2:366:G:H21	2.02	0.57
21:2:1432:A:C2'	59:1:1551:A:H2	2.13	0.57
59:1:740:C:H41	59:1:747:G:H5''	1.70	0.56
2:d:11:VAL:O	2:d:15:ILE:HB	2.05	0.56
21:2:1432:A:C4	59:1:1551:A:N1	2.73	0.56
44:L:140:SER:HB2	59:1:277:G:H5''	1.87	0.56
46:N:66:LEU:HD21	46:N:99:VAL:HG21	1.85	0.56
2:d:7:PRO:HB2	2:d:10:ARG:HG2	1.86	0.56
43:K:1:MET:HG3	43:K:67:LYS:HG2	1.88	0.56
21:2:668:G:H2'	21:2:669:A:C8	2.41	0.56
41:I:162:MET:CA	59:1:720:U:C6	2.89	0.56
59:1:1944:G:H22	59:1:1952:U:H3	1.53	0.56
22:b:424:MET:HA	22:b:431:ILE:HD12	1.86	0.56
41:I:162:MET:N	59:1:720:U:C4	2.73	0.56
38:F:58:LEU:HB3	38:F:100:LEU:HD22	1.88	0.56
43:K:17:ARG:HD2	43:K:47:LEU:HD12	1.88	0.56
59:1:514:G:H2'	59:1:515:G:C8	2.41	0.56
12:p:40:ARG:HB2	21:2:352:G:H5'	1.87	0.55
22:b:746:ARG:HA	22:b:749:LYS:HG3	1.86	0.55
48:P:54:VAL:HG21	48:P:101:MET:HE1	1.89	0.55
50:R:141:GLU:HB3	50:R:171:LYS:HB3	1.88	0.55
37:E:33:GLU:HG2	37:E:34:LYS:HG2	1.88	0.55
18:v:249:LEU:HB3	18:v:260:ARG:HH21	1.71	0.55
21:2:875:G:H1	21:2:1327:U:H3	1.55	0.55
36:D:66:VAL:HG22	59:1:270:A:H4'	1.87	0.55
54:V:148:ALA:HB2	59:1:501:G:H5''	1.89	0.55
58:Y:45:GLU:HG3	58:Y:46:GLU:HG2	1.88	0.55
9:m:119:ARG:HH21	58:Y:91:GLN:HG3	1.71	0.55
36:D:128:ASN:HB2	36:D:131:GLU:HB2	1.89	0.54
60:4:76:A:H62	60:4:93:G:H8	1.54	0.54
15:s:8:GLY:HA2	58:Y:99:PHE:HE1	1.72	0.54
59:1:737:A:H2	59:1:748:A:H8	1.55	0.54
13:q:41:LYS:HZ1	21:2:231:U:H5'	1.70	0.54
21:2:1432:A:C4	59:1:1551:A:H2	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:392:G:H2'	21:2:393:G:H8	1.71	0.54
21:2:921:A:H4'	21:2:922:G:H5''	1.89	0.54
22:b:570:ARG:HG2	22:b:574:ARG:HH21	1.73	0.54
59:1:1968:A:H2'	59:1:1969:A:C8	2.42	0.54
37:E:30:PRO:HB2	37:E:170:LEU:HD22	1.88	0.54
1:a:220:ARG:HH12	18:v:229:PRO:HB3	1.73	0.54
6:j:90:GLN:HG2	23:c:445:ILE:HD11	1.90	0.54
9:m:146:ALA:HB3	9:m:150:LYS:HE2	1.90	0.53
21:2:1294:A:H2'	21:2:1295:G:C8	2.42	0.53
25:i:181:LYS:HB2	25:i:184:LYS:HB3	1.90	0.53
37:E:123:PHE:HB3	37:E:164:GLN:HB2	1.89	0.53
21:2:365:G:H3'	21:2:366:G:C8	2.43	0.53
22:b:260:VAL:HG22	22:b:294:ALA:HB3	1.89	0.53
22:b:336:MET:HE2	22:b:861:THR:HA	1.91	0.53
51:S:113:CYS:HB3	51:S:168:ILE:HD12	1.89	0.53
18:v:290:PHE:HB2	18:v:295:PHE:HZ	1.72	0.53
5:h:11:ILE:HD11	5:h:36:LEU:HD23	1.91	0.53
10:n:53:ASN:HA	10:n:58:ARG:HD2	1.90	0.53
22:b:183:GLN:HG2	22:b:280:ALA:HA	1.89	0.53
46:N:123:MET:HG2	46:N:129:LYS:HG3	1.91	0.53
7:k:87:VAL:HG21	7:k:98:ILE:HD11	1.89	0.53
15:s:65:GLN:O	58:Y:91:GLN:HG3	2.08	0.53
15:s:65:GLN:OE1	58:Y:91:GLN:HB2	2.08	0.53
47:O:28:ALA:HB3	47:O:32:ALA:H	1.74	0.53
15:s:41:VAL:HG22	15:s:44:MET:HE2	1.91	0.52
42:J:138:HIS:CD2	42:J:146:TRP:HB3	2.44	0.52
51:S:164:PHE:HE2	51:S:166:MET:HE2	1.74	0.52
22:b:277:ILE:HD11	22:b:295:LYS:HG2	1.91	0.52
21:2:627:G:H2'	21:2:628:G:C8	2.45	0.52
35:C:62:LEU:HD22	43:K:72:GLU:HB3	1.91	0.52
40:H:57:VAL:HG22	40:H:119:VAL:HB	1.90	0.52
2:d:159:VAL:HG21	2:d:169:VAL:HG11	1.92	0.52
50:R:135:VAL:HG13	50:R:177:ILE:HG12	1.91	0.52
21:2:352:G:H1	21:2:363:A:H2	1.57	0.52
5:h:2:LYS:HG3	5:h:60:GLN:NE2	2.24	0.52
59:1:1676:G:H2'	59:1:1677:G:C8	2.45	0.52
60:4:252:A:N6	60:4:273:G:N2	2.45	0.52
1:a:110:VAL:HG11	22:b:375:LYS:HD3	1.91	0.52
36:D:165:MET:HE1	36:D:192:VAL:HG13	1.92	0.52
1:a:194:MET:HG2	1:a:211:ALA:HB3	1.91	0.52
15:s:8:GLY:HA2	58:Y:99:PHE:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:667:G:H2'	21:2:668:G:C8	2.45	0.52
41:I:162:MET:N	59:1:720:U:N3	2.58	0.52
20:w:225:ALA:HB3	20:w:228:GLU:HG3	1.92	0.51
21:2:1366:U:H2'	21:2:1367:G:H8	1.75	0.51
24:e:245:PHE:HA	24:e:248:LEU:HD12	1.91	0.51
24:e:618:LEU:HD13	24:e:626:VAL:HG11	1.91	0.51
9:m:132:ILE:HG12	59:1:547:C:N3	2.24	0.51
22:b:566:LEU:HD12	22:b:685:GLN:HE22	1.75	0.51
28:3:23:U:H2'	28:3:24:G:C8	2.45	0.51
36:D:48:LEU:HD22	36:D:235:TYR:HB2	1.93	0.51
47:O:55:ALA:HA	47:O:121:ASP:HB3	1.92	0.51
59:1:753:G:N2	59:1:758:A:H62	2.07	0.51
18:v:160:ASP:HA	18:v:163:LEU:HD12	1.92	0.51
23:c:221:TYR:HE1	23:c:386:PHE:HZ	1.59	0.51
10:n:17:VAL:HG11	10:n:59:LEU:HD11	1.93	0.51
18:v:249:LEU:HG	18:v:255:ILE:HD13	1.93	0.51
21:2:912:2MG:C5	26:y:141:ARG:HD3	2.45	0.51
43:K:122:LEU:HD13	48:P:97:VAL:HG11	1.92	0.51
59:1:540:G:N2	59:1:554:U:O2	2.38	0.51
21:2:778:G:H2'	21:2:779:A:H8	1.76	0.51
21:2:1352:A:N1	21:2:1426:G:C6	2.79	0.51
33:9:31:LYS:HE2	59:1:2118:A:H5'	1.92	0.51
37:E:80:LEU:HD21	37:E:86:VAL:HG11	1.93	0.51
37:E:92:LEU:HD22	37:E:96:ARG:HB3	1.93	0.51
59:1:1304:G:H5''	59:1:1305:C:H5'	1.92	0.51
21:2:894:U:H2'	21:2:895:A:H8	1.76	0.51
60:4:59:G:H1	60:4:66:C:H5	1.59	0.51
9:m:97:ARG:CD	58:Y:69:ASP:OD1	2.58	0.51
7:k:22:VAL:HG22	7:k:35:ILE:HG12	1.93	0.51
21:2:47:G:C6	21:2:371:A:N1	2.79	0.51
21:2:1293:C:H2'	21:2:1294:A:H8	1.76	0.51
21:2:1341:4OC:H2'	21:2:1342:C:O4'	2.10	0.51
6:j:107:MET:HE3	21:2:1090:A:H1'	1.93	0.50
21:2:60:A:H5''	21:2:363:A:H5''	1.94	0.50
45:M:27:ILE:HD11	45:M:132:LEU:HB3	1.93	0.50
1:a:281:LEU:HD11	1:a:293:SER:HB2	1.93	0.50
21:2:1433:G:HO2'	59:1:1550:A:HO2'	1.47	0.50
59:1:688:A:H2'	59:1:689:A:C8	2.46	0.50
12:p:81:THR:HG21	12:p:105:LEU:HD21	1.93	0.50
20:w:337:SER:HB2	20:w:369:VAL:HA	1.92	0.50
21:2:1432:A:C5	59:1:1551:A:C2	2.99	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:i:176:LYS:HB2	25:i:179:LEU:HD12	1.92	0.50
59:1:1931:U:H2'	59:1:1932:U:C6	2.46	0.50
21:2:723:G:H4'	21:2:1452:A:H4'	1.93	0.50
27:0:57:LEU:HD11	50:R:101:LEU:HD13	1.94	0.50
40:H:90:SER:HA	40:H:93:LYS:HD3	1.92	0.50
18:v:224:ARG:HH21	18:v:226:GLN:HB2	1.77	0.50
24:e:540:ILE:HG12	24:e:550:VAL:HG22	1.93	0.50
55:W:90:THR:HG22	55:W:94:LYS:HG3	1.93	0.50
15:s:42:PRO:HD2	58:Y:95:PHE:CE2	2.46	0.50
21:2:311:C:H2'	21:2:312:A:H8	1.77	0.50
49:Q:6:ARG:NH2	59:1:910:A:H2'	2.27	0.50
59:1:233:C:H2'	59:1:234:G:C8	2.47	0.50
2:d:177:TYR:HA	2:d:180:MET:HG2	1.92	0.50
59:1:71:U:H5'	60:4:202:A:H3'	1.94	0.50
1:a:213:GLU:HB3	18:v:229:PRO:HG2	1.92	0.50
21:2:164:C:H2'	21:2:165:A:H8	1.77	0.50
21:2:987:U:H2'	21:2:988:G:H8	1.77	0.50
23:c:76:ILE:HD13	23:c:96:SER:HB3	1.93	0.50
22:b:472:LYS:HG3	22:b:473:LYS:HG3	1.93	0.50
24:e:338:ALA:HA	24:e:341:LYS:HD3	1.93	0.50
11:o:123:ARG:NE	59:1:371:U:OP2	2.45	0.49
19:x:74:PRO:HD2	19:x:77:LEU:HD12	1.94	0.49
22:b:732:ARG:HA	22:b:735:ARG:HG2	1.94	0.49
22:b:797:LYS:H	22:b:797:LYS:HD2	1.77	0.49
1:a:235:VAL:HG11	1:a:243:MET:HE1	1.94	0.49
11:o:67:LEU:HD22	11:o:94:ILE:HG23	1.93	0.49
41:I:161:ARG:HG2	59:1:741:U:H5'	1.93	0.49
41:I:166:THR:HG22	59:1:748:A:H61	1.77	0.49
50:R:80:ILE:HD12	50:R:116:ALA:HB3	1.94	0.49
52:T:72:PRO:HB3	60:4:50:G:H5'	1.93	0.49
2:d:147:PRO:HD2	21:2:379:C:H5''	1.94	0.49
20:w:543:PRO:HG2	20:w:546:ALA:HB2	1.95	0.49
22:b:202:TYR:HB2	22:b:207:VAL:HG21	1.93	0.49
9:m:111:ARG:O	9:m:115:GLN:HG3	2.12	0.49
21:2:438:G:H1'	21:2:439:U:H5	1.76	0.49
59:1:1097:U:H2'	59:1:1098:A:H8	1.76	0.49
13:q:91:LYS:HB2	21:2:242:G:H3'	1.94	0.49
20:w:263:LYS:HB3	20:w:291:PHE:HB3	1.94	0.49
22:b:479:LYS:HA	22:b:482:ARG:HG2	1.95	0.49
23:c:120:GLN:HG3	23:c:123:ARG:HH21	1.77	0.49
37:E:172:LYS:HD3	37:E:178:PHE:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:Q:31:LEU:HD13	59:1:232:C:H4'	1.95	0.49
22:b:481:GLY:HA2	22:b:484:LEU:HD12	1.95	0.49
21:2:133:G:H2'	21:2:134:G:C8	2.48	0.49
24:e:585:PRO:HD2	24:e:650:LEU:HD22	1.95	0.49
45:M:34:LEU:HB2	45:M:118:MET:HG2	1.95	0.49
25:i:45:LEU:HA	25:i:48:VAL:HG12	1.94	0.49
59:1:1686:C:H2'	59:1:1687:A:H8	1.78	0.49
12:p:62:ARG:HG2	21:2:97:G:H5''	1.95	0.49
21:2:628:G:H2'	21:2:629:A:C8	2.45	0.49
15:s:11:VAL:HG11	15:s:16:LEU:HD13	1.94	0.49
21:2:931:C:H2'	21:2:932:A:H8	1.77	0.49
21:2:1179:G:H2'	21:2:1180:G:H8	1.77	0.49
23:c:509:ARG:HG3	23:c:590:LEU:HD21	1.95	0.49
38:F:68:ILE:HG13	38:F:77:LEU:HG	1.95	0.49
41:I:73:PHE:HE2	41:I:93:ILE:HD13	1.77	0.49
47:O:52:PRO:HG2	47:O:118:VAL:HG12	1.95	0.49
25:i:28:ILE:HB	25:i:95:ILE:HG22	1.95	0.48
40:H:61:LEU:HB3	40:H:115:ALA:HB3	1.95	0.48
21:2:931:C:H2'	21:2:932:A:C8	2.48	0.48
24:e:123:ASN:H	24:e:126:TYR:HB2	1.78	0.48
60:4:171:A:H2'	60:4:172:C:C6	2.48	0.48
2:d:164:ARG:HG2	21:2:413:U:H5'	1.95	0.48
4:g:45:ASN:HA	4:g:48:LYS:HE3	1.96	0.48
21:2:38:U:H3	21:2:373:G:H1	1.60	0.48
37:E:143:GLU:HB2	37:E:146:LYS:HD3	1.95	0.48
18:v:235:PHE:HD2	18:v:238:ARG:HD3	1.78	0.48
59:1:1686:C:H2'	59:1:1687:A:C8	2.48	0.48
28:3:54:U:H2'	28:3:55:G:H8	1.77	0.48
59:1:2322:A:H61	59:1:2369:C:H1'	1.79	0.48
3:f:79:MET:HE2	3:f:134:LEU:HD13	1.96	0.48
21:2:454:C:H2'	21:2:455:A:H8	1.78	0.48
5:h:116:SER:HB3	5:h:135:GLU:HB2	1.94	0.48
9:m:119:ARG:NH2	58:Y:91:GLN:HG3	2.27	0.48
18:v:246:ARG:HH22	18:v:247:ILE:HD13	1.79	0.48
20:w:227:MET:HE2	20:w:227:MET:HA	1.96	0.48
23:c:615:VAL:HG21	23:c:640:LEU:HD11	1.95	0.48
59:1:1118:U:H4'	59:1:1119:U:H5'	1.95	0.48
59:1:1855:A:H2'	59:1:1856:G:C8	2.48	0.48
9:m:155:THR:HA	21:2:1166:C:H4'	1.96	0.48
59:1:1489:A:H2'	59:1:1490:A:C8	2.49	0.48
21:2:874:G:H2'	21:2:875:G:C8	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:589:GLU:HG2	24:e:598:VAL:HG22	1.94	0.48
21:2:669:A:H2'	21:2:670:A:C8	2.49	0.47
59:1:701:U:H2'	59:1:702:G:H8	1.78	0.47
59:1:294:U:H2'	59:1:295:C:C6	2.49	0.47
60:4:67:G:H22	60:4:102:A:H2	1.62	0.47
20:w:259:LYS:HA	20:w:262:MET:HE2	1.96	0.47
21:2:454:C:H2'	21:2:455:A:C8	2.49	0.47
51:S:69:HIS:HB2	59:1:144:G:H4'	1.96	0.47
5:h:14:MET:HG3	5:h:31:ILE:HG21	1.96	0.47
20:w:289:PRO:HA	23:c:321:ALA:HB3	1.96	0.47
21:2:1019:C:H2'	21:2:1020:G:H8	1.79	0.47
56:X:131:ASN:HB3	56:X:133:THR:HG23	1.96	0.47
59:1:765:U:H2'	59:1:766:G:C8	2.49	0.47
59:1:1713:U:H2'	59:1:1714:U:C6	2.50	0.47
23:c:230:LEU:HD23	23:c:241:ASN:HB2	1.97	0.47
6:j:106:VAL:HB	6:j:139:LEU:HB3	1.97	0.47
7:k:86:LEU:HB3	7:k:114:LYS:HG3	1.97	0.47
16:t:83:LYS:HE2	16:t:83:LYS:HB2	1.74	0.47
20:w:227:MET:HE3	20:w:316:LEU:HD13	1.97	0.47
21:2:874:G:H2'	21:2:875:G:H8	1.78	0.47
47:O:61:GLU:HA	47:O:94:ALA:HB2	1.97	0.47
59:1:1246:U:H2'	59:1:1247:A:H8	1.79	0.47
59:1:1247:A:H2'	59:1:1248:A:C8	2.50	0.47
60:4:66:C:H5''	60:4:67:G:O4'	2.15	0.47
2:d:201:LEU:HD22	2:d:240:LEU:HD23	1.97	0.47
3:f:111:ASN:ND2	14:r:66:LYS:HE2	2.30	0.47
21:2:1454:U:H2'	21:2:1455:2MG:C8	2.50	0.47
33:9:30:ALA:HB1	59:1:2167:C:H5''	1.96	0.47
57:Z:42:LYS:HG3	59:1:1658:C:H5	1.80	0.47
23:c:298:LEU:HD21	23:c:384:ILE:HA	1.96	0.47
38:F:114:MET:HE3	38:F:187:ILE:HG12	1.97	0.47
59:1:1127:A:H2'	59:1:1128:A:C8	2.50	0.47
20:w:375:GLU:HG3	23:c:337:LEU:HD22	1.97	0.47
21:2:912:2MG:C4	26:y:141:ARG:HD3	2.51	0.47
23:c:393:ARG:HD2	23:c:393:ARG:HA	1.71	0.47
58:Y:48:LYS:HD2	58:Y:48:LYS:HA	1.73	0.47
9:m:94:ASN:ND2	58:Y:52:ASN:ND2	2.63	0.46
22:b:462:ARG:HA	22:b:465:GLN:HG2	1.97	0.46
59:1:184:U:H2'	59:1:185:G:C8	2.49	0.46
59:1:1045:C:H2'	59:1:1046:A:C8	2.50	0.46
59:1:1053:U:H4'	59:1:1262:A:H4'	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:1:1537:G:H21	59:1:1540:C:H41	1.63	0.46
21:2:553:U:H2'	21:2:554:A:H8	1.80	0.46
22:b:440:PRO:HA	22:b:443:LYS:HE3	1.97	0.46
22:b:820:MET:HE3	22:b:828:ILE:HD12	1.96	0.46
23:c:335:TYR:HA	23:c:338:ILE:HD12	1.98	0.46
20:w:407:GLU:HB3	23:c:458:LYS:HG2	1.97	0.46
59:1:1088:G:H2'	59:1:1089:A:C8	2.50	0.46
59:1:1710:A:H2'	59:1:1711:G:H8	1.79	0.46
60:4:206:A:H5'	60:4:237:C:H4'	1.97	0.46
20:w:296:ASP:HA	20:w:299:LEU:HB3	1.98	0.46
30:6:54:ILE:HB	30:6:97:HIS:HB3	1.96	0.46
4:g:112:ARG:HH21	4:g:120:LYS:HA	1.80	0.46
11:o:102:LEU:HD11	11:o:122:ILE:HD13	1.96	0.46
20:w:495:GLU:H	20:w:495:GLU:HG3	1.59	0.46
28:3:60:A:H2'	28:3:61:A:C8	2.51	0.46
59:1:1246:U:H2'	59:1:1247:A:C8	2.51	0.46
59:1:2287:C:H2'	59:1:2288:U:H6	1.80	0.46
9:m:129:ARG:HA	9:m:132:ILE:HD12	1.98	0.46
21:2:22:G:H2'	21:2:23:G:C8	2.51	0.46
21:2:1056:G:H5'	23:c:679:GLN:HG3	1.97	0.46
21:2:1294:A:H2'	21:2:1295:G:H8	1.79	0.46
59:1:314:U:H2'	59:1:315:C:C6	2.51	0.46
59:1:470:U:H2'	59:1:471:C:C6	2.51	0.46
3:f:81:ILE:HD12	3:f:164:ARG:HB3	1.97	0.46
21:2:153:U:H2'	21:2:154:G:H8	1.81	0.46
22:b:894:ARG:HH22	24:e:491:GLU:HG2	1.80	0.46
23:c:379:LEU:HD11	23:c:393:ARG:HB3	1.97	0.46
41:I:134:GLN:HG2	41:I:173:LYS:HE2	1.98	0.46
50:R:102:LYS:HE2	59:1:821:G:H5''	1.96	0.46
59:1:2155:C:H2'	59:1:2156:A:H8	1.80	0.46
59:1:228:U:H2'	59:1:229:G:C8	2.51	0.46
59:1:1913:A:H2'	59:1:1914:A:C8	2.51	0.46
7:k:107:LYS:HD3	7:k:107:LYS:HA	1.80	0.45
18:v:208:LEU:HB2	18:v:215:ALA:HB3	1.98	0.45
21:2:1366:U:H2'	21:2:1367:G:C8	2.51	0.45
34:B:169:LYS:HG2	34:B:174:VAL:HG22	1.97	0.45
46:N:126:LEU:HD12	46:N:132:VAL:HG22	1.98	0.45
59:1:1432:U:H2'	59:1:1433:C:C6	2.50	0.45
21:2:42:G:H2'	21:2:43:G:H8	1.82	0.45
22:b:709:LEU:HD21	24:e:308:LEU:HG	1.98	0.45
23:c:552:TYR:HB3	23:c:573:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:J:164:GLU:HG3	42:J:186:VAL:HG21	1.99	0.45
50:R:92:PRO:HD3	50:R:177:ILE:HD12	1.98	0.45
59:1:53:U:H4'	59:1:54:C:H5'	1.97	0.45
7:k:37:ASN:HD21	7:k:41:GLU:HB2	1.80	0.45
9:m:94:ASN:HD21	58:Y:52:ASN:ND2	2.14	0.45
18:v:265:ASN:HA	18:v:268:THR:HG22	1.98	0.45
21:2:1348:C:H2'	21:2:1349:A:H8	1.81	0.45
21:2:1455:2MG:HM21	21:2:1458:MA6:N7	2.31	0.45
22:b:432:LEU:HD23	22:b:821:THR:HG22	1.98	0.45
22:b:551:LYS:HG2	24:e:314:LEU:HD11	1.97	0.45
23:c:314:HIS:ND1	23:c:314:HIS:C	2.74	0.45
49:Q:6:ARG:HH22	59:1:910:A:H2'	1.81	0.45
52:T:-1:UNK:HA	52:T:44:LEU:HD21	1.98	0.45
20:w:277:LEU:O	20:w:281:TRP:HB2	2.17	0.45
21:2:131:G:H1	21:2:163:C:H5	1.64	0.45
22:b:312:ARG:O	22:b:316:ARG:HG2	2.15	0.45
23:c:656:VAL:HG12	23:c:701:VAL:HG22	1.97	0.45
34:B:43:LYS:HD3	34:B:57:GLY:HA2	1.97	0.45
11:o:67:LEU:HD11	11:o:97:GLN:HG2	1.99	0.45
59:1:1228:A:H2'	59:1:1229:A:C8	2.52	0.45
5:h:118:PRO:HA	21:2:596:A:N7	2.32	0.45
9:m:97:ARG:NE	58:Y:69:ASP:OD2	2.23	0.45
9:m:154:LYS:HB2	9:m:154:LYS:HE2	1.75	0.45
24:e:317:LEU:HD13	24:e:317:LEU:HA	1.81	0.45
36:D:189:ARG:HB2	36:D:192:VAL:HB	1.99	0.45
41:I:162:MET:CB	59:1:720:U:C6	2.99	0.45
59:1:569:A:H2'	59:1:570:A:C8	2.51	0.45
3:f:123:PRO:HD2	14:r:131:LYS:HD2	1.99	0.45
6:j:75:ARG:HD3	6:j:139:LEU:HD13	1.99	0.45
40:H:78:LEU:HD11	40:H:127:THR:HG23	1.97	0.45
59:1:1091:G:H2'	59:1:1092:G:C8	2.51	0.45
59:1:2377:G:H2'	59:1:2378:A:C8	2.52	0.45
60:4:139:A:H2'	60:4:140:A:C8	2.52	0.45
17:u:621:MET:HE3	17:u:621:MET:HB3	1.85	0.45
21:2:1066:U:H2'	21:2:1067:C:H6	1.82	0.45
28:3:82:U:H2'	28:3:83:U:C6	2.51	0.45
46:N:79:SER:O	46:N:83:GLU:HG2	2.16	0.45
59:1:123:G:H21	60:4:26:A:N6	2.15	0.45
59:1:442:U:H2'	59:1:443:C:C6	2.51	0.45
9:m:47:ASN:CB	58:Y:70:ILE:CD1	2.84	0.45
21:2:892:A:H2'	21:2:893:U:C6	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:578:ALA:O	22:b:582:VAL:HG23	2.16	0.45
23:c:648:ARG:H	23:c:648:ARG:HG2	1.58	0.45
35:C:93:ILE:HG21	35:C:142:LEU:HD11	1.98	0.45
59:1:161:U:H4'	59:1:894:G:H4'	1.99	0.45
1:a:81:LEU:HA	1:a:81:LEU:HD13	1.83	0.45
2:d:37:PHE:HD1	2:d:40:LYS:HD2	1.82	0.45
5:h:105:ARG:HH22	21:2:3:C:H41	1.64	0.45
21:2:1293:C:H2'	21:2:1294:A:C8	2.52	0.45
36:D:60:HIS:HB2	44:L:37:LEU:HB3	1.99	0.45
50:R:141:GLU:HG2	50:R:143:LEU:HD22	1.99	0.45
52:T:55:HIS:HB3	59:1:1000:U:H5'	1.98	0.45
59:1:969:G:H1'	59:1:1270:C:H5''	1.99	0.45
59:1:2231:C:H2'	59:1:2232:G:C8	2.52	0.45
12:p:47:LYS:HE2	12:p:47:LYS:HB3	1.61	0.44
18:v:210:THR:HG23	18:v:213:ASN:H	1.82	0.44
21:2:619:G:H1'	21:2:687:G:H5'	1.99	0.44
21:2:1179:G:H2'	21:2:1180:G:C8	2.52	0.44
22:b:457:GLN:HE21	22:b:461:ALA:HB2	1.82	0.44
37:E:133:LEU:HD13	37:E:138:MET:HE2	1.99	0.44
53:U:78:ILE:HG22	53:U:84:LYS:HA	1.98	0.44
59:1:765:U:H2'	59:1:766:G:H8	1.82	0.44
1:a:95:MET:HE2	1:a:95:MET:HB3	1.93	0.44
7:k:80:MET:HE3	7:k:83:ALA:HB2	2.00	0.44
8:l:110:ARG:HB3	8:l:119:VAL:HG21	1.99	0.44
21:2:351:U:H3	21:2:365:G:H1	1.64	0.44
21:2:1433:G:C2'	59:1:1550:A:O2'	2.65	0.44
22:b:580:LEU:HD22	22:b:675:ILE:HD11	1.99	0.44
59:1:1012:A:H2'	59:1:1013:A:C8	2.52	0.44
26:y:111:LEU:HD13	26:y:149:LEU:HD21	1.98	0.44
37:E:56:LYS:HD2	37:E:60:MET:HE1	1.99	0.44
37:E:127:GLY:HA2	37:E:164:GLN:HA	1.99	0.44
38:F:79:LYS:HB3	38:F:79:LYS:HE2	1.87	0.44
59:1:1537:G:H21	59:1:1540:C:N4	2.15	0.44
22:b:271:LYS:HE3	22:b:271:LYS:HB2	1.74	0.44
23:c:205:LYS:HE2	23:c:209:ARG:HE	1.81	0.44
42:J:103:PRO:HB3	49:Q:68:ALA:HB2	1.99	0.44
15:s:41:VAL:HB	15:s:43:PRO:HD2	1.99	0.44
21:2:347:G:H21	21:2:349:A:N6	2.15	0.44
21:2:553:U:H2'	21:2:554:A:C8	2.52	0.44
21:2:987:U:H2'	21:2:988:G:C8	2.53	0.44
22:b:477:MET:HE1	22:b:755:ARG:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:721:LYS:HG3	24:e:411:VAL:HG22	1.99	0.44
53:U:107:GLN:HG2	53:U:127:GLU:HG3	2.00	0.44
60:4:267:U:H2'	60:4:268:G:C8	2.53	0.44
60:4:267:U:H2'	60:4:268:G:H8	1.81	0.44
13:q:37:THR:HG22	13:q:43:VAL:HG12	2.00	0.44
21:2:896:U:H2'	21:2:897:G:H8	1.82	0.44
22:b:601:TYR:HE2	22:b:654:THR:HG23	1.82	0.44
50:R:82:GLU:HG2	50:R:87:GLN:HG2	2.00	0.44
54:V:65:ILE:HG21	54:V:106:ILE:HG21	1.99	0.44
59:1:453:U:H2'	59:1:454:C:C6	2.52	0.44
59:1:1887:U:H2'	59:1:1888:U:H6	1.83	0.44
1:a:158:VAL:HG13	1:a:166:ALA:HB3	1.98	0.44
3:f:83:LYS:HE2	3:f:161:THR:HA	2.00	0.44
13:q:103:LYS:HE3	13:q:103:LYS:HB2	1.64	0.44
21:2:350:A:H61	21:2:366:G:H21	1.64	0.44
22:b:628:MET:HE2	22:b:628:MET:HB2	1.78	0.44
41:I:162:MET:O	59:1:720:U:C2	2.71	0.44
59:1:275:G:H4'	59:1:276:A:H5'	2.00	0.44
59:1:744:A:H2'	59:1:745:A:C8	2.53	0.44
59:1:2287:C:H2'	59:1:2288:U:C6	2.53	0.44
21:2:896:U:H2'	21:2:897:G:C8	2.53	0.44
59:1:1646:C:H2'	59:1:1647:G:H8	1.83	0.44
5:h:8:ASN:HB2	21:2:540:G:H4'	1.99	0.44
21:2:42:G:H2'	21:2:43:G:C8	2.53	0.44
22:b:679:GLN:HA	22:b:682:ILE:HG12	2.00	0.44
30:6:62:GLU:H	30:6:62:GLU:HG2	1.65	0.44
41:I:106:LYS:HE3	41:I:106:LYS:HB2	1.75	0.44
50:R:95:TRP:HB3	50:R:173:MET:HE2	2.00	0.44
56:X:125:LYS:HG2	56:X:134:MET:HE1	1.99	0.44
59:1:64:C:H2'	59:1:65:A:C8	2.53	0.44
59:1:608:C:H2'	59:1:609:A:C8	2.53	0.44
59:1:1432:U:H2'	59:1:1433:C:H6	1.82	0.44
1:a:81:LEU:HG	18:v:171:LYS:HE3	1.99	0.43
51:S:105:ARG:HB2	59:1:1648:G:H5''	2.00	0.43
53:U:136:MET:HG2	53:U:145:ARG:HB2	2.00	0.43
59:1:1089:A:H2'	59:1:1090:A:C8	2.53	0.43
60:4:269:U:H2'	60:4:270:A:H8	1.82	0.43
21:2:492:A:H2'	21:2:493:G:C8	2.54	0.43
21:2:554:A:H2'	21:2:555:A:C8	2.53	0.43
22:b:551:LYS:HA	22:b:551:LYS:HD2	1.84	0.43
52:T:28:VAL:HB	52:T:32:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:505:U:H2'	21:2:506:G:H8	1.83	0.43
21:2:1156:C:H2'	21:2:1157:U:C6	2.52	0.43
21:2:1330:U:H2'	21:2:1331:G:C8	2.53	0.43
22:b:455:LYS:HE2	22:b:455:LYS:HB3	1.76	0.43
22:b:682:ILE:HA	22:b:685:GLN:HG3	2.00	0.43
41:I:162:MET:O	59:1:720:U:C6	2.70	0.43
44:L:47:GLU:HG3	59:1:319:U:H5''	1.99	0.43
51:S:70:LEU:HD12	51:S:70:LEU:HA	1.88	0.43
59:1:1438:A:H2'	59:1:1439:A:C8	2.54	0.43
1:a:88:GLN:NE2	18:v:174:LEU:HD11	2.34	0.43
1:a:127:VAL:HA	1:a:130:MET:HG3	2.00	0.43
21:2:636:U:H2'	21:2:637:G:H8	1.84	0.43
22:b:713:LEU:HD13	22:b:717:LEU:HD23	2.00	0.43
22:b:842:MET:HE1	22:b:867:LEU:HD13	2.00	0.43
23:c:520:LYS:HB2	23:c:520:LYS:HE2	1.90	0.43
24:e:448:SER:O	24:e:452:GLN:HG2	2.18	0.43
59:1:540:G:H2'	59:1:541:G:C8	2.49	0.43
59:1:2369:C:H2'	59:1:2370:A:C8	2.52	0.43
20:w:264:VAL:HG12	20:w:299:LEU:HD12	1.99	0.43
21:2:1101:C:H2'	21:2:1102:A:H8	1.83	0.43
58:Y:76:PRO:HA	58:Y:81:ASN:HB3	2.01	0.43
59:1:899:A:H2'	59:1:900:A:H8	1.82	0.43
59:1:1881:A:H2'	59:1:1882:G:C8	2.52	0.43
7:k:127:LYS:HE2	7:k:127:LYS:HB2	1.63	0.43
15:s:42:PRO:HA	15:s:45:ILE:HG13	2.01	0.43
20:w:337:SER:HA	23:c:211:PHE:HE2	1.83	0.43
27:0:29:ARG:HA	27:0:29:ARG:HD2	1.79	0.43
53:U:157:LYS:HB2	53:U:157:LYS:HE2	1.64	0.43
54:V:47:LYS:HD3	54:V:47:LYS:HA	1.80	0.43
59:1:125:U:H5''	59:1:160:A:H8	1.84	0.43
59:1:717:A:H62	59:1:746:A:H3'	1.84	0.43
21:2:311:C:H2'	21:2:312:A:C8	2.53	0.43
21:2:761:C:H2'	21:2:762:A:H8	1.84	0.43
21:2:1250:G:H5''	58:Y:98:ARG:HH12	1.58	0.43
22:b:410:SER:HB2	22:b:893:ILE:HG21	2.00	0.43
27:0:50:LEU:HD22	50:R:128:PRO:HG3	2.01	0.43
44:L:207:LYS:O	44:L:211:LYS:HE2	2.19	0.43
4:g:111:LYS:HD2	4:g:134:PHE:HE2	1.83	0.43
21:2:57:U:H2'	21:2:58:G:C8	2.54	0.43
24:e:490:LYS:HA	24:e:490:LYS:HD2	1.67	0.43
39:G:78:GLY:HA2	39:G:81:ASN:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:H:62:ARG:HH11	40:H:113:GLU:H	1.66	0.43
59:1:608:C:H2'	59:1:609:A:H8	1.83	0.43
59:1:1247:A:H2'	59:1:1248:A:H8	1.82	0.43
59:1:1710:A:H2'	59:1:1711:G:C8	2.52	0.43
1:a:191:ARG:HE	1:a:191:ARG:HB3	1.69	0.43
2:d:15:ILE:HG23	2:d:74:ARG:HG2	2.01	0.43
21:2:320:A:H5''	21:2:321:C:H5	1.83	0.43
21:2:347:G:N2	21:2:366:G:H22	2.17	0.43
21:2:737:U:H2'	21:2:738:A:H8	1.83	0.43
21:2:1174:A:H4'	21:2:1242:G:H4'	2.01	0.43
26:y:74:ILE:HD12	26:y:86:LYS:HE2	2.01	0.43
38:F:58:LEU:HD13	38:F:104:VAL:HG12	2.00	0.43
59:1:857:U:H2'	59:1:858:U:C6	2.54	0.43
14:r:91:ILE:HG13	17:u:631:TYR:HB2	1.99	0.43
21:2:334:U:H2'	21:2:335:G:H8	1.84	0.43
21:2:515:G:H5'	21:2:516:A:C5	2.54	0.43
21:2:554:A:H2'	21:2:555:A:H8	1.84	0.43
22:b:204:LYS:HE3	22:b:204:LYS:HB2	1.79	0.43
26:y:197:LYS:HA	26:y:197:LYS:HD2	1.92	0.43
28:3:60:A:H2'	28:3:61:A:H8	1.84	0.43
55:W:121:ALA:O	55:W:125:GLU:HG2	2.19	0.43
59:1:1046:A:H5'	59:1:1127:A:H1'	2.01	0.43
59:1:2288:U:H2'	59:1:2289:U:C6	2.54	0.43
60:4:270:A:H2'	60:4:271:G:C8	2.53	0.43
23:c:371:LYS:HA	23:c:371:LYS:HD3	1.73	0.42
26:y:196:LEU:O	26:y:200:LYS:HG2	2.19	0.42
44:L:195:VAL:HA	44:L:198:MET:HE2	2.01	0.42
59:1:1703:C:H2'	59:1:1704:C:C6	2.54	0.42
59:1:2231:C:H2'	59:1:2232:G:H8	1.83	0.42
60:4:270:A:H2'	60:4:271:G:H8	1.84	0.42
3:f:156:ALA:HB2	34:B:136:ASN:O	2.18	0.42
9:m:109:LEU:O	9:m:113:VAL:HG23	2.19	0.42
23:c:222:LEU:HD23	23:c:222:LEU:HA	1.89	0.42
37:E:139:PHE:HA	37:E:140:PRO:HD3	1.90	0.42
40:H:88:LYS:HB2	40:H:91:LEU:HG	2.00	0.42
59:1:470:U:H2'	59:1:471:C:H6	1.84	0.42
59:1:899:A:H2'	59:1:900:A:C8	2.54	0.42
59:1:1430:U:H2'	59:1:1431:C:H6	1.84	0.42
59:1:2476:U:H2'	59:1:2477:A:C8	2.54	0.42
21:2:392:G:H2'	21:2:393:G:C8	2.54	0.42
26:y:129:GLU:HB3	26:y:141:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L:149:LYS:HB2	44:L:166:ALA:HB3	2.01	0.42
58:Y:75:HIS:HB3	58:Y:78:TYR:HB2	2.01	0.42
14:r:93:LEU:HD12	17:u:634:LEU:HD21	2.02	0.42
21:2:280:U:H2'	21:2:281:G:C8	2.54	0.42
21:2:587:C:H2'	21:2:588:A:H8	1.84	0.42
21:2:1113:G:H2'	21:2:1114:A:H8	1.85	0.42
35:C:111:LEU:HD13	35:C:119:MET:H	1.84	0.42
35:C:225:LYS:HD3	48:P:34:MET:HE1	2.01	0.42
49:Q:38:GLN:HE22	59:1:182:A:H5'	1.84	0.42
59:1:1430:U:H2'	59:1:1431:C:C6	2.54	0.42
59:1:2036:G:H2'	59:1:2037:A:C8	2.55	0.42
8:l:40:VAL:HG23	8:l:90:LEU:HD22	2.00	0.42
24:e:248:LEU:HB3	24:e:268:LEU:HD21	2.00	0.42
33:9:9:LYS:HB3	33:9:9:LYS:HE3	1.74	0.42
49:Q:44:ARG:HD2	50:R:153:MET:HB3	2.00	0.42
49:Q:60:MET:HE2	49:Q:60:MET:HB3	1.78	0.42
59:1:1891:OMG:HM23	59:1:1891:OMG:H1'	1.67	0.42
1:a:143:LYS:HB3	1:a:143:LYS:HE3	1.76	0.42
6:j:76:MET:HG2	6:j:164:VAL:HG22	2.01	0.42
34:B:167:LEU:HD11	34:B:177:ARG:HB2	2.00	0.42
52:T:5:VAL:HG13	52:T:28:VAL:HG12	2.00	0.42
59:1:660:A:H2'	59:1:661:A:C8	2.54	0.42
59:1:1419:A:H5'	59:1:2248:G:H4'	2.02	0.42
59:1:2017:A:H2'	59:1:2018:A:C8	2.54	0.42
12:p:101:THR:HG23	21:2:428:A:H1'	2.02	0.42
21:2:1374:G:H2'	21:2:1375:U:C6	2.55	0.42
22:b:607:LYS:HB3	22:b:607:LYS:HE3	1.75	0.42
24:e:467:LYS:HE2	24:e:473:LEU:HG	2.00	0.42
36:D:119:LYS:HA	36:D:119:LYS:HD3	1.90	0.42
40:H:44:VAL:HA	40:H:47:VAL:HG22	2.00	0.42
45:M:38:GLU:HB2	45:M:127:VAL:HG23	2.00	0.42
59:1:287:A:H2'	59:1:288:A:C8	2.55	0.42
3:f:107:CYS:HB2	3:f:110:ILE:HD11	2.01	0.42
10:n:4:LYS:HD3	21:2:995:G:H5''	2.01	0.42
15:s:62:VAL:HA	15:s:66:MET:HE2	2.02	0.42
20:w:181:LEU:HD23	20:w:182:PRO:HD2	2.01	0.42
21:2:260:C:H2'	21:2:261:A:H8	1.84	0.42
21:2:1452:A:H2'	21:2:1453:C:C6	2.54	0.42
23:c:320:LYS:HE2	23:c:320:LYS:HB3	1.93	0.42
37:E:104:LEU:HA	37:E:108:ALA:HB3	2.01	0.42
41:I:162:MET:HB3	59:1:720:U:C6	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:O:85:ASP:HB2	47:O:86:LEU:HD22	2.01	0.42
8:l:114:ARG:HG2	8:l:119:VAL:HB	2.02	0.42
20:w:508:GLU:HB3	20:w:510:THR:HG23	2.02	0.42
21:2:1448:G:H2'	21:2:1449:G:H8	1.85	0.42
22:b:728:ARG:HH22	24:e:416:GLU:HG3	1.85	0.42
28:3:15:U:H4'	28:3:16:G:H5'	2.01	0.42
28:3:29:C:H2'	28:3:30:A:C8	2.55	0.42
42:J:168:LYS:HB3	42:J:168:LYS:HE2	1.69	0.42
59:1:254:U:H3	59:1:312:A:N6	2.17	0.42
59:1:701:U:H2'	59:1:702:G:C8	2.54	0.42
59:1:1156:A:H2'	59:1:1157:A:C8	2.54	0.42
59:1:2048:U:H2'	59:1:2049:G:C8	2.55	0.42
21:2:1252:C:H2'	21:2:1253:U:C6	2.54	0.42
26:y:141:ARG:HD2	26:y:141:ARG:HA	1.89	0.42
37:E:153:MET:HE3	37:E:153:MET:HB2	1.87	0.42
38:F:163:LYS:HE2	59:1:2386:U:H5''	2.01	0.42
59:1:2036:G:H2'	59:1:2037:A:H8	1.84	0.42
7:k:89:GLY:H	7:k:115:THR:HB	1.85	0.41
8:l:4:ILE:HD11	13:q:56:TYR:HB3	2.02	0.41
18:v:268:THR:HA	18:v:271:ILE:HG12	2.01	0.41
20:w:487:LEU:HD21	23:c:125:TYR:HD1	1.84	0.41
21:2:467:U:H2'	21:2:468:G:H8	1.85	0.41
21:2:988:G:H2'	21:2:989:A:H8	1.84	0.41
22:b:320:LYS:HE3	22:b:320:LYS:HB3	1.79	0.41
24:e:359:ILE:HD12	24:e:359:ILE:HA	1.90	0.41
41:I:115:LYS:HG2	41:I:120:ILE:HG13	2.02	0.41
59:1:937:U:H2'	59:1:938:U:C6	2.55	0.41
59:1:2372:G:H2'	59:1:2373:G:C8	2.55	0.41
59:1:2376:A:H2'	59:1:2377:G:C8	2.55	0.41
2:d:142:LYS:HB2	2:d:142:LYS:HE2	1.86	0.41
8:l:89:ASP:HB2	21:2:476:A:H61	1.85	0.41
18:v:145:ALA:HA	22:b:189:THR:HG22	2.03	0.41
21:2:82:U:H2'	21:2:83:G:C8	2.56	0.41
22:b:464:ILE:HD11	24:e:486:VAL:HG21	2.02	0.41
22:b:594:LYS:HB2	24:e:373:VAL:HG21	2.02	0.41
9:m:44:ARG:O	58:Y:69:ASP:OD2	2.38	0.41
15:s:11:VAL:HB	15:s:16:LEU:HD22	2.02	0.41
20:w:192:GLU:HB3	20:w:195:ASP:HB2	2.02	0.41
21:2:197:C:H2'	21:2:198:G:H8	1.85	0.41
21:2:443:U:H2'	21:2:444:G:H8	1.84	0.41
21:2:716:G:H2'	21:2:717:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:b:566:LEU:HD21	24:e:391:ILE:HG12	2.02	0.41
23:c:16:LYS:HE2	23:c:16:LYS:HB2	1.82	0.41
59:1:171:U:H2'	59:1:172:G:C8	2.55	0.41
59:1:1188:U:O2	59:1:1198:G:N2	2.41	0.41
59:1:2338:U:H2'	59:1:2339:C:C6	2.55	0.41
9:m:47:ASN:HB2	58:Y:70:ILE:HD11	1.96	0.41
21:2:313:G:H2'	21:2:314:A:C8	2.56	0.41
21:2:347:G:H1	21:2:366:G:H1	1.67	0.41
21:2:444:G:H2'	21:2:445:A:H8	1.85	0.41
21:2:736:A:H62	21:2:754:G:H21	1.67	0.41
24:e:360:LYS:HB3	24:e:360:LYS:HE3	1.75	0.41
40:H:140:VAL:HA	40:H:143:LYS:HG2	2.01	0.41
45:M:56:ARG:HA	45:M:59:ARG:HE	1.85	0.41
47:O:103:GLY:HA3	47:O:137:ALA:HB3	2.03	0.41
59:1:708:A:H5'	59:1:709:C:H5	1.85	0.41
21:2:477:G:H2'	21:2:478:C:C6	2.55	0.41
21:2:973:C:H42	21:2:982:A:H61	1.68	0.41
22:b:602:MET:SD	24:e:369:GLN:HG3	2.60	0.41
23:c:413:LYS:HE2	24:e:409:GLU:HA	2.02	0.41
26:y:142:VAL:HG11	26:y:160:ILE:HG13	2.01	0.41
38:F:181:PRO:HB2	38:F:197:LYS:HG3	2.01	0.41
59:1:83:C:H2'	59:1:84:U:C6	2.55	0.41
59:1:1499:G:H4'	59:1:2051:A:H4'	2.02	0.41
59:1:2177:U:H2'	59:1:2178:C:C6	2.56	0.41
2:d:17:LYS:HB3	2:d:17:LYS:HE2	1.75	0.41
9:m:129:ARG:HE	9:m:129:ARG:HB2	1.64	0.41
21:2:35:C:H2'	21:2:36:G:H8	1.86	0.41
21:2:210:U:H2'	21:2:211:G:H8	1.86	0.41
21:2:666:A:H2'	21:2:667:G:C8	2.55	0.41
21:2:775:G:H2'	21:2:776:G:H8	1.85	0.41
22:b:644:LEU:HB3	24:e:369:GLN:HB3	2.02	0.41
24:e:135:ILE:HD12	24:e:138:ALA:HB3	2.01	0.41
34:B:97:ARG:HG3	34:B:103:LYS:HD3	2.02	0.41
55:W:69:LYS:HE3	55:W:69:LYS:HB2	1.83	0.41
6:j:57:MET:HE1	23:c:547:LYS:HG3	2.03	0.41
9:m:127:ARG:HG2	9:m:137:VAL:HG13	2.02	0.41
18:v:247:ILE:HD12	18:v:247:ILE:HA	1.93	0.41
21:2:336:A:H2'	21:2:337:G:C8	2.56	0.41
21:2:682:A:H2'	21:2:683:A:C8	2.55	0.41
23:c:204:LEU:O	23:c:208:LYS:HG2	2.21	0.41
37:E:122:SER:HB3	59:1:1944:G:H5'	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:H:119:VAL:HG21	40:H:127:THR:HG21	2.01	0.41
55:W:46:LYS:HB3	55:W:46:LYS:HE2	1.89	0.41
56:X:128:ALA:HB1	56:X:134:MET:HB3	2.03	0.41
58:Y:49:VAL:HG12	58:Y:66:TYR:HB2	2.03	0.41
59:1:1646:C:H2'	59:1:1647:G:C8	2.56	0.41
2:d:96:ILE:HG22	2:d:98:GLU:H	1.86	0.41
4:g:122:LYS:HE2	4:g:122:LYS:HB3	1.87	0.41
23:c:314:HIS:C	23:c:314:HIS:HD1	2.29	0.41
23:c:355:SER:HA	23:c:358:VAL:HB	2.02	0.41
28:3:55:G:H21	37:E:27:HIS:CE1	2.39	0.41
39:G:45:ILE:HD13	39:G:66:LEU:HD22	2.03	0.41
54:V:53:VAL:HG21	54:V:59:VAL:HG23	2.02	0.41
59:1:182:A:H4'	59:1:183:G:C8	2.56	0.41
59:1:878:U:H2'	59:1:879:C:C6	2.56	0.41
59:1:975:U:H2'	59:1:976:C:C6	2.55	0.41
59:1:1092:G:H2'	59:1:1093:A:H8	1.86	0.41
59:1:1251:U:H2'	59:1:1252:A:C8	2.56	0.41
2:d:203:LEU:HD11	2:d:212:LEU:HD12	2.03	0.41
2:d:223:LYS:HE2	2:d:223:LYS:HB3	1.94	0.41
4:g:93:LEU:HD23	4:g:93:LEU:HA	1.90	0.41
4:g:111:LYS:HB2	4:g:111:LYS:HE3	1.84	0.41
12:p:107:ARG:HG3	12:p:112:MET:HE3	2.02	0.41
12:p:113:GLU:HA	12:p:114:PRO:HD3	1.97	0.41
14:r:82:LYS:HB2	14:r:82:LYS:HE2	1.93	0.41
20:w:244:LEU:HD13	20:w:313:ALA:HB2	2.03	0.41
21:2:153:U:H2'	21:2:154:G:C8	2.56	0.41
21:2:410:U:H2'	21:2:411:G:C8	2.55	0.41
21:2:898:U:H2'	21:2:899:G:H8	1.86	0.41
21:2:1462:G:H2'	21:2:1463:G:H8	1.85	0.41
22:b:590:LYS:HB2	22:b:590:LYS:HE3	1.86	0.41
23:c:86:ILE:HD13	23:c:86:ILE:HA	1.92	0.41
23:c:221:TYR:HA	23:c:224:ILE:HD12	2.03	0.41
23:c:233:LYS:HE3	23:c:233:LYS:HB3	1.90	0.41
23:c:406:GLN:O	23:c:410:LEU:HG	2.20	0.41
24:e:620:LEU:HD23	24:e:620:LEU:HA	1.87	0.41
27:0:34:LYS:HD3	27:0:39:ASP:HB3	2.03	0.41
28:3:82:U:H2'	28:3:83:U:H6	1.85	0.41
36:D:213:PHE:O	36:D:217:ASN:HB2	2.21	0.41
41:I:70:ILE:H	41:I:70:ILE:HG13	1.74	0.41
53:U:112:LEU:HD21	53:U:124:LYS:HE3	2.03	0.41
59:1:512:U:H2'	59:1:513:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
59:1:512:U:H2'	59:1:513:U:H6	1.86	0.41
59:1:2154:U:H2'	59:1:2155:C:C6	2.56	0.41
4:g:8:LYS:HB3	4:g:8:LYS:HE2	1.74	0.41
5:h:15:LEU:HD11	5:h:138:CYS:HB3	2.03	0.41
5:h:101:LYS:HB2	5:h:101:LYS:HE2	1.80	0.41
6:j:66:ALA:HB1	6:j:70:VAL:HG21	2.03	0.41
20:w:354:GLU:HA	20:w:357:LYS:HB2	2.03	0.41
21:2:334:U:H2'	21:2:335:G:C8	2.56	0.41
21:2:1188:A:H2'	21:2:1189:A:C8	2.56	0.41
22:b:739:LYS:HD3	22:b:739:LYS:HA	1.91	0.41
40:H:94:VAL:HG21	59:1:706:A:C4	2.56	0.41
51:S:155:ARG:NH1	59:1:404:5MU:H4'	2.36	0.41
59:1:321:U:H2'	59:1:322:U:C6	2.56	0.41
59:1:2494:U:H2'	59:1:2495:C:C6	2.56	0.41
2:d:180:MET:HA	2:d:183:TYR:CD2	2.56	0.40
16:t:150:PRO:HG2	16:t:160:TYR:HB2	2.04	0.40
21:2:647:G:C8	26:y:184:LYS:HD3	2.56	0.40
21:2:1080:U:H5'	21:2:1082:G:C5	2.56	0.40
22:b:774:LYS:HE2	22:b:774:LYS:HB3	1.79	0.40
37:E:135:GLU:HG2	37:E:137:LEU:H	1.86	0.40
55:W:129:LYS:HE3	55:W:129:LYS:HB2	1.87	0.40
59:1:485:G:H4'	59:1:488:G:N1	2.36	0.40
59:1:877:U:H5	59:1:890:G:H1	1.67	0.40
59:1:1053:U:H2'	59:1:1054:A:O4'	2.21	0.40
1:a:88:GLN:HG2	22:b:895:LEU:HD11	2.03	0.40
17:u:634:LEU:HD12	17:u:634:LEU:HA	1.93	0.40
22:b:695:LEU:HD21	24:e:317:LEU:HD11	2.04	0.40
34:B:226:VAL:HG11	59:1:1424:C:H5''	2.04	0.40
34:B:260:LEU:HD23	59:1:1433:C:H5''	2.04	0.40
59:1:71:U:OP1	60:4:202:A:H5''	2.21	0.40
59:1:232:C:H2'	59:1:233:C:C6	2.56	0.40
59:1:1967:A:H2'	59:1:1968:A:C8	2.56	0.40
2:d:195:LEU:HB3	2:d:203:LEU:HD12	2.03	0.40
4:g:76:LYS:HA	4:g:77:PRO:HD3	1.95	0.40
6:j:145:LEU:HD23	6:j:145:LEU:HA	1.96	0.40
8:l:88:LYS:HB2	8:l:88:LYS:HE2	1.74	0.40
10:n:22:THR:HG22	20:w:543:PRO:HD2	2.02	0.40
20:w:483:VAL:HG22	20:w:487:LEU:HD23	2.04	0.40
21:2:68:C:H2'	21:2:69:G:C8	2.56	0.40
21:2:634:C:H2'	21:2:635:A:H8	1.86	0.40
21:2:858:C:H2'	21:2:859:A:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:2:885:G:H2'	21:2:886:C:C6	2.56	0.40
22:b:396:LYS:H	22:b:396:LYS:HG3	1.72	0.40
24:e:254:GLN:H	24:e:254:GLN:HG3	1.66	0.40
45:M:5:LYS:HE2	45:M:5:LYS:HB2	1.93	0.40
55:W:167:ARG:HG3	55:W:169:GLY:H	1.86	0.40
1:a:243:MET:HB3	1:a:254:ILE:HB	2.04	0.40
14:r:115:LYS:HB3	14:r:115:LYS:HE2	1.90	0.40
22:b:582:VAL:O	22:b:586:LEU:HB2	2.21	0.40
41:I:155:LYS:HA	41:I:155:LYS:HD2	1.91	0.40
48:P:24:LYS:HE2	48:P:24:LYS:HB2	1.87	0.40
51:S:82:ARG:HH21	57:Z:59:GLU:HB2	1.87	0.40
53:U:55:LEU:HD12	60:4:81:G:H5''	2.02	0.40
59:1:23:U:H2'	59:1:24:A:H8	1.87	0.40
59:1:141:U:H2'	59:1:142:U:O4'	2.22	0.40
59:1:1561:U:H2'	59:1:1562:C:C6	2.57	0.40
59:1:1985:G:N3	59:1:2021:C:H2'	2.37	0.40
59:1:2365:U:H2'	59:1:2366:A:C8	2.56	0.40
9:m:56:ILE:HG23	9:m:75:LEU:HD11	2.04	0.40
21:2:1325:G:H2'	21:2:1326:G:H8	1.87	0.40
22:b:313:SER:O	22:b:317:GLN:HG2	2.22	0.40
22:b:337:LYS:HB2	22:b:337:LYS:HE2	1.88	0.40
26:y:184:LYS:HE2	26:y:184:LYS:HB2	1.90	0.40
29:5:14:A:H2'	29:5:35:A:H2	1.87	0.40
36:D:140:LEU:HD12	36:D:140:LEU:HA	1.97	0.40
52:T:2:LEU:HD23	52:T:2:LEU:HA	1.91	0.40
59:1:1426:C:H2'	59:1:1427:A:C5	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	234/436 (54%)	225 (96%)	8 (3%)	1 (0%)	30	51
2	d	254/257 (99%)	248 (98%)	6 (2%)	0	100	100
3	f	101/171 (59%)	99 (98%)	2 (2%)	0	100	100
4	g	165/168 (98%)	160 (97%)	5 (3%)	0	100	100
5	h	139/141 (99%)	134 (96%)	5 (4%)	0	100	100
6	j	120/169 (71%)	114 (95%)	3 (2%)	3 (2%)	4	8
7	k	115/130 (88%)	113 (98%)	2 (2%)	0	100	100
8	l	119/133 (90%)	113 (95%)	6 (5%)	0	100	100
9	m	112/164 (68%)	110 (98%)	2 (2%)	0	100	100
10	n	97/100 (97%)	97 (100%)	0	0	100	100
11	o	99/141 (70%)	96 (97%)	3 (3%)	0	100	100
12	p	78/128 (61%)	78 (100%)	0	0	100	100
13	q	76/105 (72%)	74 (97%)	2 (3%)	0	100	100
14	r	79/137 (58%)	76 (96%)	3 (4%)	0	100	100
15	s	79/92 (86%)	79 (100%)	0	0	100	100
16	t	117/166 (70%)	116 (99%)	1 (1%)	0	100	100
17	u	90/184 (49%)	87 (97%)	3 (3%)	0	100	100
18	v	179/298 (60%)	162 (90%)	14 (8%)	3 (2%)	7	15
19	x	58/120 (48%)	57 (98%)	1 (2%)	0	100	100
20	w	361/560 (64%)	351 (97%)	10 (3%)	0	100	100
22	b	679/910 (75%)	658 (97%)	20 (3%)	1 (0%)	48	70
23	c	597/712 (84%)	584 (98%)	13 (2%)	0	100	100
24	e	528/673 (78%)	505 (96%)	22 (4%)	1 (0%)	43	66
25	i	147/191 (77%)	132 (90%)	14 (10%)	1 (1%)	18	38
26	y	144/286 (50%)	142 (99%)	2 (1%)	0	100	100
27	0	45/66 (68%)	45 (100%)	0	0	100	100
30	6	56/101 (55%)	56 (100%)	0	0	100	100
31	7	58/124 (47%)	57 (98%)	1 (2%)	0	100	100
32	8	66/114 (58%)	64 (97%)	2 (3%)	0	100	100
33	9	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
34	B	274/278 (99%)	270 (98%)	4 (2%)	0	100	100
35	C	221/259 (85%)	217 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	D	214/243 (88%)	213 (100%)	1 (0%)	0	100	100
37	E	176/179 (98%)	169 (96%)	7 (4%)	0	100	100
38	F	175/207 (84%)	170 (97%)	5 (3%)	0	100	100
39	G	52/200 (26%)	52 (100%)	0	0	100	100
40	H	139/235 (59%)	135 (97%)	4 (3%)	0	100	100
41	I	130/176 (74%)	125 (96%)	5 (4%)	0	100	100
42	J	171/225 (76%)	165 (96%)	6 (4%)	0	100	100
43	K	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
44	L	196/241 (81%)	190 (97%)	6 (3%)	0	100	100
45	M	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
46	N	115/173 (66%)	112 (97%)	3 (3%)	0	100	100
47	O	116/145 (80%)	114 (98%)	2 (2%)	0	100	100
48	P	128/153 (84%)	123 (96%)	5 (4%)	0	100	100
49	Q	109/112 (97%)	109 (100%)	0	0	100	100
50	R	113/179 (63%)	112 (99%)	1 (1%)	0	100	100
51	S	113/175 (65%)	111 (98%)	2 (2%)	0	100	100
52	T	90/111 (81%)	88 (98%)	2 (2%)	0	100	100
53	U	130/170 (76%)	129 (99%)	1 (1%)	0	100	100
54	V	112/161 (70%)	109 (97%)	3 (3%)	0	100	100
55	W	136/195 (70%)	134 (98%)	2 (2%)	0	100	100
56	X	104/134 (78%)	104 (100%)	0	0	100	100
57	Z	39/98 (40%)	37 (95%)	2 (5%)	0	100	100
58	Y	61/136 (45%)	51 (84%)	10 (16%)	0	100	100
All	All	8394/11457 (73%)	8152 (97%)	232 (3%)	10 (0%)	49	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	j	123	VAL
1	a	71	VAL
6	j	50	VAL
6	j	51	ASP
18	v	142	PHE
18	v	146	LEU

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Mol	Chain	Res	Type
22	b	347	THR
18	v	131	VAL
25	i	41	ASP
24	e	273	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	206/368 (56%)	202 (98%)	4 (2%)	50	75
2	d	233/234 (100%)	226 (97%)	7 (3%)	36	64
3	f	89/140 (64%)	88 (99%)	1 (1%)	65	84
4	g	146/147 (99%)	144 (99%)	2 (1%)	59	81
5	h	125/125 (100%)	122 (98%)	3 (2%)	43	70
6	j	107/143 (75%)	104 (97%)	3 (3%)	38	66
7	k	93/105 (89%)	91 (98%)	2 (2%)	45	72
8	l	103/111 (93%)	100 (97%)	3 (3%)	37	65
9	m	101/138 (73%)	101 (100%)	0	100	100
10	n	88/89 (99%)	87 (99%)	1 (1%)	65	84
11	o	86/115 (75%)	84 (98%)	2 (2%)	44	71
12	p	69/108 (64%)	69 (100%)	0	100	100
13	q	69/90 (77%)	69 (100%)	0	100	100
14	r	73/128 (57%)	72 (99%)	1 (1%)	59	81
15	s	71/80 (89%)	68 (96%)	3 (4%)	26	52
16	t	99/133 (74%)	98 (99%)	1 (1%)	68	86
17	u	85/149 (57%)	84 (99%)	1 (1%)	63	83
18	v	143/246 (58%)	142 (99%)	1 (1%)	76	89
19	x	50/95 (53%)	48 (96%)	2 (4%)	28	55
20	w	287/434 (66%)	279 (97%)	8 (3%)	38	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	b	620/807 (77%)	606 (98%)	14 (2%)	44	71
23	c	541/634 (85%)	533 (98%)	8 (2%)	57	80
24	e	411/527 (78%)	402 (98%)	9 (2%)	45	72
25	i	126/159 (79%)	120 (95%)	6 (5%)	23	47
26	y	124/238 (52%)	122 (98%)	2 (2%)	55	79
27	0	39/54 (72%)	38 (97%)	1 (3%)	40	68
30	6	53/90 (59%)	48 (91%)	5 (9%)	8	18
31	7	45/90 (50%)	43 (96%)	2 (4%)	25	50
32	8	55/92 (60%)	54 (98%)	1 (2%)	51	76
33	9	33/33 (100%)	33 (100%)	0	100	100
34	B	228/230 (99%)	223 (98%)	5 (2%)	45	72
35	C	176/204 (86%)	173 (98%)	3 (2%)	53	78
36	D	167/187 (89%)	165 (99%)	2 (1%)	63	83
37	E	156/157 (99%)	150 (96%)	6 (4%)	29	56
38	F	145/168 (86%)	142 (98%)	3 (2%)	47	73
39	G	46/167 (28%)	44 (96%)	2 (4%)	26	51
40	H	122/197 (62%)	116 (95%)	6 (5%)	22	47
41	I	106/138 (77%)	103 (97%)	3 (3%)	38	66
42	J	140/180 (78%)	136 (97%)	4 (3%)	37	65
43	K	101/101 (100%)	98 (97%)	3 (3%)	36	64
44	L	149/180 (83%)	147 (99%)	2 (1%)	61	82
45	M	110/111 (99%)	108 (98%)	2 (2%)	51	76
46	N	97/140 (69%)	95 (98%)	2 (2%)	47	73
47	O	93/116 (80%)	93 (100%)	0	100	100
48	P	104/122 (85%)	101 (97%)	3 (3%)	37	65
49	Q	100/101 (99%)	98 (98%)	2 (2%)	48	74
50	R	97/145 (67%)	95 (98%)	2 (2%)	47	73
51	S	94/136 (69%)	90 (96%)	4 (4%)	26	51
52	T	85/89 (96%)	83 (98%)	2 (2%)	43	70
53	U	109/137 (80%)	107 (98%)	2 (2%)	51	76
54	V	90/127 (71%)	89 (99%)	1 (1%)	65	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	W	116/164 (71%)	113 (97%)	3 (3%)	40	68
56	X	89/109 (82%)	88 (99%)	1 (1%)	65	84
57	Z	33/81 (41%)	32 (97%)	1 (3%)	36	64
58	Y	55/106 (52%)	54 (98%)	1 (2%)	51	76
All	All	7178/9495 (76%)	7020 (98%)	158 (2%)	45	72

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	95	MET
1	a	158	VAL
1	a	170	VAL
1	a	180	THR
2	d	63	SER
2	d	72	LYS
2	d	100	THR
2	d	161	MET
2	d	165	SER
2	d	211	GLU
2	d	218	VAL
3	f	150	LEU
4	g	72	ARG
4	g	141	GLU
5	h	59	SER
5	h	65	ARG
5	h	121	LEU
6	j	55	VAL
6	j	123	VAL
6	j	152	MET
7	k	39	ARG
7	k	101	ILE
8	l	17	LYS
8	l	90	LEU
8	l	121	MET
10	n	6	MET
11	o	105	MET
11	o	118	SER
14	r	115	LYS
15	s	31	ILE
15	s	43	PRO
15	s	79	THR

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Mol	Chain	Res	Type
16	t	118	VAL
17	u	578	GLU
18	v	262	ILE
19	x	63	MET
19	x	94	SER
20	w	191	MET
20	w	201	SER
20	w	264	VAL
20	w	299	LEU
20	w	431	VAL
20	w	472	THR
20	w	491	MET
20	w	527	GLU
22	b	193	VAL
22	b	210	VAL
22	b	323	MET
22	b	449	ILE
22	b	487	MET
22	b	573	LEU
22	b	586	LEU
22	b	633	LYS
22	b	700	LYS
22	b	759	THR
22	b	761	VAL
22	b	777	ASP
22	b	786	SER
22	b	853	ILE
23	c	3	GLN
23	c	82	GLU
23	c	85	LEU
23	c	100	LEU
23	c	314	HIS
23	c	368	LEU
23	c	444	LEU
23	c	648	ARG
24	e	135	ILE
24	e	287	VAL
24	e	305	ASP
24	e	317	LEU
24	e	332	LEU
24	e	400	VAL
24	e	464	LEU

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Mol	Chain	Res	Type
24	e	588	VAL
24	e	627	LEU
25	i	18	VAL
25	i	42	PHE
25	i	81	MET
25	i	96	VAL
25	i	165	LEU
25	i	166	THR
26	y	112	SER
26	y	125	GLU
27	0	60	VAL
30	6	44	LYS
30	6	59	SER
30	6	62	GLU
30	6	71	THR
30	6	98	LYS
31	7	80	ARG
31	7	120	SER
32	8	90	LYS
34	B	121	ASP
34	B	186	VAL
34	B	203	TYR
34	B	205	LEU
34	B	221	THR
35	C	98	THR
35	C	222	SER
35	C	229	GLU
36	D	106	SER
36	D	203	THR
37	E	75	ILE
37	E	81	ARG
37	E	111	ARG
37	E	138	MET
37	E	153	MET
37	E	176	LEU
38	F	59	GLU
38	F	87	MET
38	F	130	LEU
39	G	37	THR
39	G	44	ASP
40	H	57	VAL
40	H	85	TYR

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Mol	Chain	Res	Type
40	H	87	THR
40	H	117	VAL
40	H	134	PHE
40	H	175	ARG
41	I	84	MET
41	I	94	THR
41	I	169	ASN
42	J	108	SER
42	J	123	VAL
42	J	125	VAL
42	J	220	LYS
43	K	54	ARG
43	K	90	GLU
43	K	113	LYS
44	L	128	THR
44	L	211	LYS
45	M	59	ARG
45	M	118	MET
46	N	93	THR
46	N	156	GLU
48	P	34	MET
48	P	64	LYS
48	P	136	ARG
49	Q	74	LEU
49	Q	94	VAL
50	R	82	GLU
50	R	110	LYS
51	S	133	VAL
51	S	137	CYS
51	S	144	VAL
51	S	158	LEU
52	T	1	MET
52	T	51	SER
53	U	82	LYS
53	U	126	LEU
54	V	81	LEU
55	W	50	VAL
55	W	98	THR
55	W	139	MET
56	X	77	ASN
57	Z	73	LEU
58	Y	68	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	88	GLN
1	a	225	GLN
2	d	46	GLN
2	d	217	ASN
3	f	171	GLN
5	h	60	GLN
6	j	90	GLN
7	k	23	HIS
7	k	29	HIS
7	k	92	GLN
9	m	89	ASN
9	m	94	ASN
10	n	30	GLN
10	n	49	GLN
10	n	89	GLN
11	o	81	ASN
11	o	97	GLN
20	w	430	GLN
20	w	442	ASN
22	b	598	GLN
22	b	606	ASN
22	b	875	ASN
22	b	880	ASN
23	c	215	GLN
23	c	462	ASN
23	c	679	GLN
24	e	553	GLN
26	y	99	ASN
26	y	126	GLN
26	y	148	ASN
27	0	21	HIS
27	0	26	HIS
34	B	149	GLN
34	B	155	GLN
34	B	189	ASN
35	C	89	ASN
37	E	7	ASN
37	E	46	GLN
37	E	48	GLN
38	F	60	GLN
38	F	176	GLN

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Mol	Chain	Res	Type
39	G	30	ASN
40	H	43	GLN
41	I	139	GLN
45	M	107	GLN
46	N	61	ASN
46	N	106	HIS
47	O	114	ASN
48	P	42	ASN
48	P	110	GLN
49	Q	38	GLN
49	Q	81	ASN
49	Q	108	GLN
50	R	165	HIS
51	S	124	ASN
52	T	12	GLN
52	T	55	HIS
53	U	77	GLN
54	V	74	ASN
54	V	127	GLN
55	W	45	ASN
55	W	48	ASN
56	X	98	GLN
58	Y	52	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
21	2	1468/1470 (99%)	202 (13%)	3 (0%)
28	3	120/121 (99%)	20 (16%)	1 (0%)
29	5	46/47 (97%)	3 (6%)	0
59	1	2362/2375 (99%)	331 (14%)	5 (0%)
60	4	270/272 (99%)	35 (12%)	1 (0%)
All	All	4266/4285 (99%)	591 (13%)	10 (0%)

All (591) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
21	2	6	U
21	2	10	G
21	2	20	C
21	2	23	G

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Mol	Chain	Res	Type
21	2	32	G
21	2	33	A
21	2	40	G
21	2	48	C
21	2	49	U
21	2	52	A
21	2	59	C
21	2	80	U
21	2	86	U
21	2	106	A
21	2	107	C
21	2	116	A
21	2	117	C
21	2	128	G
21	2	130	G
21	2	149	C
21	2	168	C
21	2	169	A
21	2	181	A
21	2	183	A
21	2	191	A
21	2	192	A
21	2	195	G
21	2	220	U
21	2	222	G
21	2	226	G
21	2	231	U
21	2	232	G
21	2	235	G
21	2	242	G
21	2	243	C
21	2	256	C
21	2	257	G
21	2	265	G
21	2	282	A
21	2	297	A
21	2	304	C
21	2	305	A
21	2	320	A
21	2	327	G
21	2	328	C
21	2	330	G

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Mol	Chain	Res	Type
21	2	343	U
21	2	348	C
21	2	349	A
21	2	352	G
21	2	360	G
21	2	374	U
21	2	382	G
21	2	388	A
21	2	389	G
21	2	391	A
21	2	397	G
21	2	398	U
21	2	399	G
21	2	400	G
21	2	405	U
21	2	414	U
21	2	415	U
21	2	429	G
21	2	430	U
21	2	431	U
21	2	434	G
21	2	437	G
21	2	438	G
21	2	439	U
21	2	448	A
21	2	449	A
21	2	450	U
21	2	462	A
21	2	463	A
21	2	464	C
21	2	471	C
21	2	474	G
21	2	477	G
21	2	480	G7M
21	2	484	U
21	2	485	A
21	2	500	A
21	2	512	A
21	2	517	U
21	2	525	A
21	2	526	A
21	2	527	A

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Mol	Chain	Res	Type
21	2	529	C
21	2	530	G
21	2	541	G
21	2	571	C
21	2	595	U
21	2	596	A
21	2	607	U
21	2	619	G
21	2	657	G
21	2	675	A
21	2	677	U
21	2	678	G
21	2	688	C
21	2	709	A
21	2	714	G
21	2	731	A
21	2	747	U
21	2	748	A
21	2	766	G
21	2	769	A
21	2	771	C
21	2	775	G
21	2	786	G
21	2	791	C
21	2	792	G
21	2	793	C
21	2	794	A
21	2	816	U
21	2	830	U
21	2	836	G
21	2	860	A
21	2	872	G
21	2	880	C
21	2	906	U
21	2	915	A
21	2	917	G
21	2	918	C
21	2	921	A
21	2	922	G
21	2	923	A
21	2	924	A
21	2	938	U

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Mol	Chain	Res	Type
21	2	939	G
21	2	949	G
21	2	950	A
21	2	971	U
21	2	972	G
21	2	978	A
21	2	980	G
21	2	981	G
21	2	982	A
21	2	1001	G
21	2	1013	U
21	2	1034	A
21	2	1036	A
21	2	1042	G
21	2	1043	U
21	2	1049	A
21	2	1072	G
21	2	1073	U
21	2	1079	U
21	2	1080	U
21	2	1081	U
21	2	1096	A
21	2	1098	U
21	2	1109	G
21	2	1122	G
21	2	1134	A
21	2	1135	A
21	2	1151	A
21	2	1152	C
21	2	1165	A
21	2	1166	C
21	2	1176	A
21	2	1178	U
21	2	1191	C
21	2	1194	A
21	2	1195	A
21	2	1196	G
21	2	1212	U
21	2	1218	A
21	2	1224	U
21	2	1228	C
21	2	1238	G

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Mol	Chain	Res	Type
21	2	1240	U
21	2	1243	G
21	2	1258	C
21	2	1276	G
21	2	1278	A
21	2	1284	A
21	2	1291	G
21	2	1301	U
21	2	1303	U
21	2	1309	G
21	2	1317	C
21	2	1318	G
21	2	1337	A
21	2	1338	C
21	2	1358	G
21	2	1361	G
21	2	1380	A
21	2	1385	A
21	2	1390	U
21	2	1391	C
21	2	1431	A
21	2	1432	A
21	2	1436	G
21	2	1438	A
21	2	1442	A
21	2	1445	U
21	2	1456	G
21	2	1468	G
21	2	1469	G
21	2	1474	C
28	3	14	U
28	3	16	G
28	3	19	C
28	3	25	G
28	3	33	C
28	3	35	A
28	3	36	A
28	3	37	U
28	3	42	C
28	3	54	U
28	3	57	G
28	3	66	G

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Mol	Chain	Res	Type
28	3	68	G
28	3	71	G
28	3	78	G
28	3	87	G
28	3	102	A
28	3	107	A
28	3	113	A
28	3	122	G
29	5	16	U
29	5	34	G
29	5	36	A
59	1	36	G
59	1	55	A
59	1	61	G
59	1	71	U
59	1	85	C
59	1	86	C
59	1	92	G
59	1	105	A
59	1	129	A
59	1	131	G
59	1	139	G
59	1	144	G
59	1	155	A
59	1	158	A
59	1	179	A
59	1	181	C
59	1	182	A
59	1	183	G
59	1	215	G
59	1	225	G
59	1	227	A
59	1	235	G
59	1	255	G
59	1	276	A
59	1	282	A
59	1	292	A
59	1	325	G
59	1	334	C
59	1	343	U
59	1	352	G
59	1	361	G

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Mol	Chain	Res	Type
59	1	374	C
59	1	385	G
59	1	386	G
59	1	387	U
59	1	397	C
59	1	404	5MU
59	1	421	A
59	1	428	A
59	1	432	G
59	1	434	G
59	1	439	A
59	1	441	U
59	1	442	U
59	1	446	A
59	1	448	C
59	1	449	G
59	1	462	G
59	1	469	C
59	1	484	U
59	1	502	A
59	1	505	A
59	1	517	G
59	1	523	C
59	1	524	U
59	1	546	U
59	1	547	C
59	1	549	C
59	1	550	G
59	1	554	U
59	1	555	A
59	1	556	C
59	1	566	G
59	1	569	A
59	1	573	C
59	1	574	A
59	1	590	U
59	1	596	A
59	1	597	A
59	1	606	G
59	1	613	G
59	1	621	G
59	1	634	G

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Mol	Chain	Res	Type
59	1	639	A
59	1	643	A
59	1	648	A
59	1	649	G
59	1	656	A
59	1	672	U
59	1	673	G
59	1	682	G
59	1	685	G
59	1	686	A
59	1	693	U
59	1	701	U
59	1	705	G
59	1	706	A
59	1	707	A
59	1	708	A
59	1	709	C
59	1	720	U
59	1	721	U
59	1	722	U
59	1	730	A
59	1	731	G
59	1	739	C
59	1	744	A
59	1	747	G
59	1	748	A
59	1	749	G
59	1	750	U
59	1	757	U
59	1	766	G
59	1	772	G
59	1	776	U
59	1	782	G
59	1	790	U
59	1	794	C
59	1	795	G
59	1	801	A
59	1	847	U
59	1	867	G
59	1	870	U
59	1	871	G
59	1	895	G

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Mol	Chain	Res	Type
59	1	912	A
59	1	913	A
59	1	915	G
59	1	930	G
59	1	931	A
59	1	934	A
59	1	959	A
59	1	960	A
59	1	970	G
59	1	980	U
59	1	981	A
59	1	988	U
59	1	1009	C
59	1	1011	U
59	1	1024	A
59	1	1038	U
59	1	1042	A
59	1	1051	A
59	1	1062	A
59	1	1070	A
59	1	1075	U
59	1	1076	G
59	1	1083	G
59	1	1087	C
59	1	1104	G
59	1	1105	A
59	1	1112	U
59	1	1113	U
59	1	1115	G
59	1	1118	U
59	1	1119	U
59	1	1120	G
59	1	1125	G
59	1	1142	G
59	1	1147	A
59	1	1148	U
59	1	1150	G
59	1	1153	A
59	1	1154	A
59	1	1155	A
59	1	1156	A
59	1	1158	G

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Mol	Chain	Res	Type
59	1	1163	C
59	1	1166	G
59	1	1171	G
59	1	1173	G
59	1	1197	C
59	1	1198	G
59	1	1199	A
59	1	1217	A
59	1	1222	C
59	1	1223	A
59	1	1226	A
59	1	1235	U
59	1	1236	A
59	1	1257	C
59	1	1266	G
59	1	1267	A
59	1	1270	C
59	1	1277	A
59	1	1293	A
59	1	1306	G
59	1	1307	C
59	1	1313	A
59	1	1326	G
59	1	1328	A
59	1	1333	G
59	1	1375	U
59	1	1379	A
59	1	1380	A
59	1	1393	U
59	1	1400	G
59	1	1409	A
59	1	1418	C
59	1	1420	A
59	1	1422	A
59	1	1436	C
59	1	1438	A
59	1	1452	U
59	1	1465	A
59	1	1483	A
59	1	1484	A
59	1	1494	A
59	1	1502	A

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Mol	Chain	Res	Type
59	1	1510	A
59	1	1511	A
59	1	1544	G
59	1	1551	A
59	1	1552	C
59	1	1567	G
59	1	1568	G
59	1	1576	A
59	1	1593	U
59	1	1602	G
59	1	1605	C
59	1	1608	A
59	1	1609	A
59	1	1610	G
59	1	1629	U
59	1	1630	G
59	1	1631	U
59	1	1634	C
59	1	1658	C
59	1	1661	G
59	1	1665	C
59	1	1669	6MZ
59	1	1670	A
59	1	1671	G
59	1	1672	A
59	1	1675	C
59	1	1682	C
59	1	1685	A
59	1	1694	C
59	1	1695	A
59	1	1699	A
59	1	1700	G
59	1	1701	A
59	1	1708	G
59	1	1715	G
59	1	1732	G
59	1	1837	A
59	1	1844	A
59	1	1850	G
59	1	1851	A
59	1	1865	A
59	1	1878	G

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Mol	Chain	Res	Type
59	1	1879	G
59	1	1919	G
59	1	1923	U
59	1	1927	A
59	1	1928	A
59	1	1945	A
59	1	1947	G
59	1	1948	G
59	1	1949	A
59	1	1959	U
59	1	1960	U
59	1	1961	G
59	1	1962	A
59	1	1974	A
59	1	1975	A
59	1	1985	G
59	1	1987	C
59	1	1990	C
59	1	2023	G
59	1	2025	C
59	1	2031	G
59	1	2040	G
59	1	2042	G
59	1	2046	C
59	1	2054	G
59	1	2065	A
59	1	2069	G
59	1	2070	A
59	1	2075	A
59	1	2080	C
59	1	2081	U
59	1	2088	A
59	1	2110	G
59	1	2118	A
59	1	2124	G
59	1	2131	U
59	1	2134	G
59	1	2138	OMC
59	1	2142	G
59	1	2145	G
59	1	2158	A
59	1	2160	C

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Mol	Chain	Res	Type
59	1	2169	G
59	1	2175	G
59	1	2204	A
59	1	2206	A
59	1	2207	G
59	1	2213	C
59	1	2218	G
59	1	2222	G
59	1	2225	U
59	1	2242	A
59	1	2249	U
59	1	2253	U
59	1	2269	U
59	1	2270	A
59	1	2281	A
59	1	2286	C
59	1	2294	A
59	1	2303	G
59	1	2308	U
59	1	2325	U
59	1	2329	U
59	1	2352	A
59	1	2353	A
59	1	2354	C
59	1	2355	G
59	1	2366	A
59	1	2367	C
59	1	2384	G
59	1	2388	A
59	1	2397	A
59	1	2406	G
59	1	2418	A
59	1	2420	G
59	1	2430	U
59	1	2460	U
59	1	2461	A
59	1	2463	A
59	1	2471	U
59	1	2473	A
59	1	2476	U
59	1	2501	U
59	1	2513	A

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Mol	Chain	Res	Type
59	1	2519	A
59	1	2520	C
59	1	2523	A
59	1	2530	U
59	1	2531	U
59	1	2532	U
60	4	8	G
60	4	26	A
60	4	27	G
60	4	35	G
60	4	38	A
60	4	43	G
60	4	47	G
60	4	63	A
60	4	67	G
60	4	92	U
60	4	93	G
60	4	109	A
60	4	110	A
60	4	111	U
60	4	123	A
60	4	124	U
60	4	137	A
60	4	139	A
60	4	142	U
60	4	155	A
60	4	176	A
60	4	179	A
60	4	195	G
60	4	196	A
60	4	202	A
60	4	203	A
60	4	208	A
60	4	209	C
60	4	213	A
60	4	228	G
60	4	256	A
60	4	275	U
60	4	277	G
60	4	278	U
60	4	279	G

All (10) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
21	2	191	A
21	2	595	U
21	2	980	G
28	3	15	U
59	1	484	U
59	1	1154	A
59	1	1379	A
59	1	1961	G
59	1	2396	U
60	4	277	G

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

19 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
21	MA6	2	1458	21	23,26,27	1.67	5 (21%)	34,38,41	3.46	12 (35%)
59	OMC	1	2138	62,59	19,22,23	2.85	8 (42%)	26,31,34	0.83	0
59	2MG	1	1471	59	23,26,27	2.86	7 (30%)	32,38,41	2.88	13 (40%)
21	2MG	2	1455	21	23,26,27	2.85	7 (30%)	32,38,41	2.93	11 (34%)
21	5MC	2	913	21	18,22,23	3.62	7 (38%)	26,32,35	0.99	2 (7%)
59	5MU	1	1577	61,59	19,22,23	7.65	9 (47%)	28,32,35	3.42	10 (35%)
59	6MZ	1	1669	59	22,25,26	4.32	13 (59%)	30,36,39	3.02	13 (43%)
21	UR3	2	1437	21	19,22,23	2.78	8 (42%)	26,32,35	1.33	2 (7%)
59	H2U	1	2089	59	18,21,22	0.52	0	21,30,33	0.92	1 (4%)
21	G7M	2	480	61,21	23,26,27	2.27	7 (30%)	35,39,42	2.99	10 (28%)
21	2MG	2	912	21	23,26,27	3.11	7 (30%)	32,38,41	3.18	13 (40%)
59	OMG	1	1891	61,59	23,26,27	2.39	7 (30%)	33,38,41	2.26	10 (30%)
21	MA6	2	1457	21	23,26,27	1.62	5 (21%)	34,38,41	3.38	11 (32%)
59	2MA	1	2143	61,59,62	22,25,26	4.07	7 (31%)	33,37,40	2.41	9 (27%)
59	5MC	1	1600	61,59	18,22,23	3.48	7 (38%)	26,32,35	0.99	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
59	OMU	1	2192	61,59	19,22,23	3.02	8 (42%)	26,31,34	1.74	5 (19%)
59	2MG	1	2085	59	23,26,27	2.72	7 (30%)	32,38,41	2.52	14 (43%)
59	5MU	1	404	59	19,22,23	7.68	8 (42%)	28,32,35	3.24	12 (42%)
21	4OC	2	1341	21	20,23,24	3.41	8 (40%)	26,32,35	0.87	1 (3%)

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
21	MA6	2	1458	21	-	2/11/29/30	0/3/3/3
59	OMC	1	2138	62,59	-	0/9/27/28	0/2/2/2
59	2MG	1	1471	59	-	0/9/27/28	0/3/3/3
21	2MG	2	1455	21	-	0/9/27/28	0/3/3/3
21	5MC	2	913	21	-	0/7/25/26	0/2/2/2
59	5MU	1	1577	61,59	-	0/7/25/26	0/2/2/2
59	6MZ	1	1669	59	-	2/9/27/28	0/3/3/3
21	UR3	2	1437	21	-	0/7/25/26	0/2/2/2
59	H2U	1	2089	59	-	0/7/38/39	0/2/2/2
21	G7M	2	480	61,21	-	3/7/25/26	0/3/3/3
21	2MG	2	912	21	-	0/9/27/28	0/3/3/3
59	OMG	1	1891	61,59	-	3/9/27/28	0/3/3/3
21	MA6	2	1457	21	-	0/11/29/30	0/3/3/3
59	2MA	1	2143	61,59,62	-	2/7/25/26	0/3/3/3
59	5MC	1	1600	61,59	-	0/7/25/26	0/2/2/2
59	OMU	1	2192	61,59	-	0/9/27/28	0/2/2/2
59	2MG	1	2085	59	-	1/9/27/28	0/3/3/3
59	5MU	1	404	59	-	1/7/25/26	0/2/2/2
21	4OC	2	1341	21	-	1/9/29/30	0/2/2/2

All (135) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1	1577	5MU	C4-C5	22.49	1.82	1.44
59	1	404	5MU	C4-C5	22.39	1.82	1.44
59	1	1577	5MU	C6-N1	15.73	1.64	1.38
59	1	404	5MU	C6-N1	15.62	1.64	1.38
59	1	1669	6MZ	C6-N6	13.74	1.49	1.34
59	1	2143	2MA	C4-N3	13.39	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1	404	5MU	C4-N3	-12.76	1.15	1.38
59	1	1577	5MU	C4-N3	-12.63	1.15	1.38
59	1	404	5MU	C6-C5	-11.99	1.14	1.34
59	1	1577	5MU	C6-C5	-11.62	1.15	1.34
21	2	913	5MC	C6-C5	8.79	1.49	1.34
21	2	912	2MG	C2-N3	8.41	1.48	1.31
59	1	1600	5MC	C6-C5	8.36	1.48	1.34
21	2	912	2MG	C2-N2	8.14	1.51	1.33
21	2	1455	2MG	C2-N3	7.62	1.46	1.31
59	1	2143	2MA	C2-N3	7.61	1.47	1.34
21	2	1341	4OC	C4-N3	7.55	1.46	1.32
59	1	1471	2MG	C2-N3	7.54	1.46	1.31
59	1	1669	6MZ	O4'-C1'	7.50	1.59	1.42
59	1	1471	2MG	C2-N2	7.42	1.49	1.33
21	2	1455	2MG	C2-N2	7.34	1.49	1.33
59	1	2085	2MG	C2-N2	7.14	1.49	1.33
21	2	1437	UR3	C2-N1	7.11	1.48	1.38
21	2	913	5MC	C4-N3	7.00	1.46	1.34
59	1	1600	5MC	C4-N3	6.90	1.45	1.34
59	1	2192	OMU	C2-N1	6.79	1.49	1.38
59	1	2192	OMU	C2-N3	6.77	1.50	1.38
21	2	1341	4OC	C2-N3	6.69	1.49	1.36
21	2	1341	4OC	C6-C5	6.57	1.50	1.35
59	1	2085	2MG	C2-N3	6.50	1.44	1.31
59	1	2143	2MA	C6-N1	6.47	1.44	1.35
59	1	1891	OMG	C4-N3	6.40	1.49	1.34
21	2	480	G7M	C4-N3	6.35	1.49	1.34
21	2	912	2MG	C4-N3	6.26	1.49	1.34
21	2	913	5MC	C2-N3	6.23	1.49	1.36
21	2	1437	UR3	C6-C5	6.20	1.49	1.35
59	1	1669	6MZ	C2'-C1'	-6.07	1.34	1.53
59	1	1600	5MC	C2-N3	6.00	1.48	1.36
21	2	1341	4OC	C4-N4	5.98	1.48	1.35
59	1	2138	OMC	C2-N3	5.91	1.48	1.36
59	1	1669	6MZ	O4'-C4'	-5.85	1.31	1.45
59	1	1471	2MG	C4-N3	5.80	1.48	1.34
59	1	2138	OMC	C6-C5	5.69	1.48	1.35
21	2	1455	2MG	C4-N3	5.58	1.47	1.34
59	1	2192	OMU	C6-C5	5.49	1.47	1.35
59	1	2143	2MA	C2-N1	5.44	1.43	1.34
59	1	1891	OMG	C2-N3	5.36	1.46	1.33
21	2	913	5MC	C6-N1	5.35	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1437	UR3	C2-N3	5.19	1.49	1.39
59	1	1600	5MC	C6-N1	5.12	1.46	1.38
59	1	2085	2MG	C4-N3	5.09	1.46	1.34
59	1	2143	2MA	C5-C6	5.07	1.55	1.41
59	1	404	5MU	C2-N3	5.03	1.46	1.38
59	1	1577	5MU	C2-N3	4.88	1.46	1.38
59	1	2138	OMC	C4-N3	4.85	1.44	1.34
21	2	1458	MA6	C6-N6	4.83	1.51	1.36
21	2	1457	MA6	C6-N6	4.81	1.51	1.36
21	2	912	2MG	C2-N1	4.59	1.44	1.36
59	1	2138	OMC	C4-N4	4.49	1.44	1.33
59	1	1891	OMG	C2-N2	4.42	1.44	1.34
21	2	1455	2MG	C2-N1	4.40	1.43	1.36
59	1	404	5MU	C2-N1	4.39	1.45	1.38
59	1	2085	2MG	C2-N1	4.33	1.43	1.36
59	1	2138	OMC	C2-N1	4.25	1.49	1.40
59	1	1471	2MG	C2-N1	4.20	1.43	1.36
21	2	913	5MC	C4-N4	4.20	1.45	1.34
21	2	480	G7M	C2-N2	4.19	1.44	1.34
59	1	2192	OMU	C4-N3	4.07	1.45	1.38
21	2	1341	4OC	C2-N1	4.03	1.48	1.40
59	1	1600	5MC	C4-N4	4.01	1.44	1.34
21	2	1341	4OC	C5-C4	3.99	1.49	1.40
59	1	1669	6MZ	C5-C4	-3.95	1.31	1.39
21	2	480	G7M	C2-N3	3.90	1.42	1.33
59	1	1669	6MZ	C5-N7	-3.75	1.31	1.39
21	2	480	G7M	C5-N7	-3.73	1.34	1.39
59	1	1577	5MU	C2-N1	3.69	1.44	1.38
21	2	913	5MC	C2-N1	3.62	1.47	1.40
59	1	1669	6MZ	C8-N9	-3.60	1.31	1.37
59	1	1669	6MZ	O3'-C3'	-3.60	1.34	1.43
59	1	2143	2MA	C6-N6	-3.59	1.25	1.34
59	1	1891	OMG	C5-N7	-3.36	1.32	1.39
59	1	1600	5MC	C2-N1	3.34	1.47	1.40
59	1	404	5MU	O4-C4	-3.34	1.17	1.23
59	1	1577	5MU	O4-C4	-3.33	1.17	1.23
21	2	1341	4OC	C6-N1	3.29	1.45	1.38
59	1	2192	OMU	C6-N1	3.19	1.45	1.38
59	1	2192	OMU	O4-C4	-3.16	1.18	1.24
59	1	2138	OMC	C6-N1	3.06	1.45	1.38
21	2	1437	UR3	C6-N1	3.01	1.45	1.38
59	1	2138	OMC	O2-C2	-3.01	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	2	1458	MA6	C5-N7	-2.98	1.33	1.39
21	2	480	G7M	C6-N1	2.95	1.44	1.38
59	1	1577	5MU	O2-C2	-2.93	1.17	1.23
59	1	404	5MU	O2-C2	-2.93	1.17	1.23
59	1	2085	2MG	C4-N9	-2.81	1.30	1.38
59	1	1669	6MZ	C9-N6	2.80	1.50	1.45
59	1	2192	OMU	O2-C2	-2.79	1.17	1.23
59	1	1891	OMG	O6-C6	-2.77	1.18	1.23
59	1	1600	5MC	O2-C2	-2.77	1.18	1.23
21	2	480	G7M	C5-C6	2.77	1.51	1.43
21	2	1455	2MG	C5-C6	2.69	1.54	1.44
21	2	1458	MA6	C5-C4	-2.66	1.34	1.39
59	1	1669	6MZ	C4-N9	-2.59	1.31	1.37
21	2	1458	MA6	C10-N6	2.59	1.51	1.45
21	2	913	5MC	O2-C2	-2.59	1.18	1.23
21	2	1457	MA6	C5-C4	-2.57	1.34	1.39
59	1	2143	2MA	C5-N7	-2.56	1.34	1.39
21	2	1457	MA6	C5-N7	-2.55	1.34	1.39
21	2	912	2MG	C6-N1	2.54	1.43	1.38
21	2	1457	MA6	C10-N6	2.50	1.51	1.45
21	2	1455	2MG	C6-N1	2.50	1.43	1.38
59	1	1891	OMG	C2-N1	2.48	1.43	1.37
59	1	1471	2MG	C5-C6	2.48	1.53	1.44
59	1	2085	2MG	C5-C6	2.47	1.53	1.44
21	2	480	G7M	C2-N1	2.47	1.43	1.37
59	1	2085	2MG	C6-N1	2.46	1.43	1.38
21	2	1341	4OC	O2-C2	-2.45	1.19	1.23
59	1	1669	6MZ	C6-N1	-2.45	1.31	1.35
21	2	912	2MG	C5-C6	2.43	1.53	1.44
59	1	1669	6MZ	O2'-C2'	2.43	1.48	1.43
21	2	912	2MG	C5-N7	-2.37	1.34	1.39
59	1	1891	OMG	C5-C6	2.34	1.53	1.44
59	1	1471	2MG	C6-N1	2.32	1.43	1.38
21	2	1458	MA6	C8-N9	-2.32	1.33	1.37
21	2	1437	UR3	C5-C4	2.30	1.49	1.43
59	1	2192	OMU	C5-C4	2.30	1.48	1.43
21	2	1437	UR3	O2-C2	-2.29	1.18	1.22
21	2	1457	MA6	C8-N9	-2.26	1.33	1.37
21	2	1437	UR3	O4-C4	-2.25	1.18	1.23
21	2	1437	UR3	C4-N3	2.23	1.45	1.40
59	1	1471	2MG	C5-N7	-2.19	1.34	1.39
59	1	1669	6MZ	C8-N7	2.14	1.35	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1	2138	OMC	C5-C4	2.14	1.47	1.42
59	1	1577	5MU	C5M-C5	2.06	1.55	1.50
21	2	1455	2MG	C5-N7	-2.04	1.35	1.39

All (151) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	1457	MA6	N1-C6-N6	-13.09	102.77	117.08
21	2	1458	MA6	N1-C6-N6	-13.02	102.85	117.08
59	1	1577	5MU	C5-C4-N3	10.78	124.51	115.31
59	1	404	5MU	C5-C4-N3	9.62	123.53	115.31
21	2	480	G7M	CN7-N7-C5	9.36	138.40	126.77
59	1	1577	5MU	C5-C6-N1	-8.66	114.43	123.34
59	1	404	5MU	C5-C6-N1	-8.33	114.77	123.34
59	1	2143	2MA	C5-C4-N3	-7.97	118.22	127.19
59	1	1471	2MG	C1'-N9-C8	-7.95	104.06	126.70
21	2	912	2MG	C2-N3-C4	7.80	121.71	112.04
21	2	912	2MG	C1'-N9-C4	7.78	149.62	126.50
59	1	1669	6MZ	C1'-N9-C8	-7.74	109.66	127.14
21	2	912	2MG	C1'-N9-C8	-7.71	104.74	126.70
59	1	1471	2MG	C1'-N9-C4	7.69	149.34	126.50
21	2	1455	2MG	C1'-N9-C8	-7.64	104.96	126.70
21	2	1455	2MG	C1'-N9-C4	7.57	149.00	126.50
59	1	1669	6MZ	N1-C2-N3	-7.46	116.93	128.60
59	1	1577	5MU	C4-N3-C2	-7.19	118.05	127.35
21	2	1458	MA6	C5-C6-N6	7.18	137.80	125.30
21	2	480	G7M	CN7-N7-C8	-7.18	113.77	124.84
21	2	1457	MA6	C5-C6-N6	7.11	137.69	125.30
21	2	912	2MG	C5-C4-N3	-6.61	117.73	128.46
59	1	2085	2MG	C1'-N9-C8	-6.58	107.97	126.70
59	1	1669	6MZ	C4-N9-C1'	6.57	142.25	126.59
21	2	480	G7M	C1'-N9-C4	6.45	145.66	126.50
59	1	1471	2MG	C2-N3-C4	6.34	119.90	112.04
21	2	1455	2MG	C2-N3-C4	6.26	119.81	112.04
59	1	404	5MU	C4-N3-C2	-6.21	119.31	127.35
59	1	2085	2MG	C1'-N9-C4	6.05	144.49	126.50
21	2	912	2MG	C2-N1-C6	-5.89	117.70	124.48
59	1	1891	OMG	C5-C4-N3	-5.89	118.91	128.46
21	2	480	G7M	C1'-N9-C8	-5.81	107.13	126.74
59	1	2085	2MG	C2-N3-C4	5.67	119.07	112.04
21	2	1457	MA6	N1-C2-N3	-5.58	119.88	128.60
59	1	2143	2MA	N3-C4-N9	5.49	134.61	126.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	1458	MA6	C5-C4-N3	-5.37	119.75	126.75
21	2	1458	MA6	N1-C2-N3	-5.37	120.21	128.60
21	2	1458	MA6	N9-C8-N7	-5.28	106.69	113.91
59	1	2192	OMU	C4-N3-C2	-5.20	119.72	126.58
59	1	1891	OMG	C1'-N9-C4	-5.06	111.46	126.50
21	2	1457	MA6	N9-C8-N7	-5.00	107.07	113.91
21	2	1455	2MG	C2-N1-C6	-4.99	118.73	124.48
21	2	1455	2MG	C5-C4-N3	-4.88	120.54	128.46
21	2	1437	UR3	C4-N3-C2	-4.88	119.97	124.56
21	2	1457	MA6	C5-C4-N3	-4.87	120.39	126.75
59	1	1669	6MZ	N9-C8-N7	-4.86	107.26	113.91
59	1	1471	2MG	C5-C4-N3	-4.79	120.68	128.46
59	1	1891	OMG	C1'-N9-C8	4.76	140.24	126.70
59	1	1577	5MU	N3-C2-N1	4.71	121.14	114.89
59	1	1471	2MG	C2-N1-C6	-4.56	119.23	124.48
21	2	1455	2MG	CM2-N2-C2	-4.44	114.05	123.86
21	2	480	G7M	C2-N3-C4	4.43	120.19	112.30
59	1	1891	OMG	C2-N3-C4	4.40	120.15	112.30
21	2	1458	MA6	C4-C5-C6	4.28	120.67	115.88
59	1	404	5MU	N3-C2-N1	4.09	120.32	114.89
59	1	1669	6MZ	C2-N3-C4	4.09	121.40	111.75
59	1	2192	OMU	N3-C2-N1	4.06	120.28	114.89
59	1	1577	5MU	O4-C4-C5	-4.06	120.20	124.90
59	1	404	5MU	C5M-C5-C6	-4.04	117.45	122.85
59	1	2143	2MA	N9-C8-N7	-4.00	108.44	113.91
21	2	1458	MA6	C5-N7-C8	4.00	109.19	103.51
59	1	1891	OMG	N9-C4-N3	3.97	133.91	125.94
21	2	480	G7M	C5-C6-N1	3.92	119.97	111.79
21	2	480	G7M	C5-C4-N3	-3.80	120.86	128.15
59	1	2085	2MG	C2-N1-C6	-3.73	120.18	124.48
21	2	1458	MA6	N3-C4-N9	3.73	133.23	127.08
21	2	1457	MA6	C2-N1-C6	3.68	120.45	111.75
59	1	404	5MU	C6-C5-C4	3.63	121.07	118.03
21	2	480	G7M	O6-C6-C5	-3.59	119.96	128.06
21	2	1457	MA6	C4-C5-C6	3.59	119.89	115.88
21	2	1458	MA6	C2-N1-C6	3.58	120.21	111.75
59	1	1577	5MU	C5M-C5-C6	-3.52	118.14	122.85
59	1	2143	2MA	C4-N9-C1'	-3.51	118.23	126.59
59	1	404	5MU	O4-C4-C5	-3.48	120.87	124.90
59	1	1669	6MZ	C5-C4-N3	-3.46	122.24	126.75
21	2	1457	MA6	C4-N9-C8	3.44	109.46	105.73
21	2	1457	MA6	C2-N3-C4	3.42	119.84	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	2	1458	MA6	C2-N3-C4	3.42	119.82	111.75
21	2	1457	MA6	N3-C4-N9	3.40	132.69	127.08
21	2	1457	MA6	C5-N7-C8	3.39	108.32	103.51
59	1	2192	OMU	C5-C4-N3	3.39	119.91	114.84
59	1	2143	2MA	N3-C2-N1	-3.33	119.59	125.72
59	1	1891	OMG	C2-N1-C6	-3.33	119.03	125.10
59	1	2085	2MG	N9-C8-N7	-3.30	107.18	113.39
21	2	912	2MG	N9-C4-N3	3.28	132.53	125.94
21	2	1458	MA6	C4-N9-C8	3.27	109.27	105.73
21	2	912	2MG	O6-C6-C5	-3.22	118.06	126.60
59	1	2143	2MA	C5-N7-C8	3.21	108.07	103.51
21	2	912	2MG	C5-C6-N1	3.20	121.32	113.19
59	1	1669	6MZ	C5-C4-N9	3.12	109.41	105.78
59	1	1600	5MC	C5-C6-N1	-3.09	120.16	123.34
59	1	1669	6MZ	C5-N7-C8	3.08	107.89	103.51
59	1	2192	OMU	O4-C4-C5	-3.06	119.78	125.16
59	1	2085	2MG	C5-C4-N3	-3.05	123.51	128.46
59	1	1577	5MU	C6-C5-C4	3.04	120.57	118.03
59	1	2143	2MA	C1'-N9-C8	3.04	133.99	127.14
21	2	913	5MC	C5-C6-N1	-3.03	120.22	123.34
59	1	1471	2MG	CM2-N2-C2	-3.00	117.24	123.86
59	1	1669	6MZ	C6-C5-N7	2.96	135.59	132.39
21	2	480	G7M	C2-N1-C6	-2.95	119.72	125.10
59	1	2089	H2U	C5-C4-N3	-2.95	113.33	116.65
59	1	2085	2MG	C6-C5-N7	2.88	135.60	130.25
59	1	1471	2MG	C5-C6-N1	2.79	120.29	113.19
59	1	2085	2MG	C5-C4-N9	2.79	110.70	105.63
59	1	404	5MU	C1'-N1-C6	-2.75	116.54	121.12
59	1	1891	OMG	N9-C8-N7	-2.75	108.22	113.39
21	2	1455	2MG	C5-C6-N1	2.70	120.03	113.19
59	1	404	5MU	C1'-N1-C2	2.69	122.44	117.57
59	1	1669	6MZ	C4-C5-N7	-2.69	107.34	110.62
59	1	1891	OMG	C5-C6-N1	2.69	120.02	113.19
59	1	1471	2MG	N9-C8-N7	-2.61	108.47	113.39
59	1	2085	2MG	N1-C2-N3	-2.58	119.96	123.95
21	2	1455	2MG	C5-C4-N9	2.58	110.31	105.63
59	1	2085	2MG	C4-C5-N7	-2.57	106.65	110.72
59	1	1577	5MU	O4-C4-N3	-2.52	115.29	120.12
59	1	1891	OMG	O6-C6-C5	-2.50	119.97	126.60
59	1	2085	2MG	C5-C6-N1	2.49	119.52	113.19
59	1	404	5MU	C5M-C5-C4	2.46	121.48	118.77
21	2	912	2MG	N1-C2-N3	-2.43	120.19	123.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1	2143	2MA	C6-C5-C4	2.43	120.44	117.18
21	2	912	2MG	N9-C8-N7	-2.42	108.84	113.39
59	1	1471	2MG	O6-C6-C5	-2.41	120.20	126.60
21	2	1455	2MG	C4-C5-N7	-2.40	106.92	110.72
21	2	1455	2MG	N9-C8-N7	-2.39	108.89	113.39
21	2	1455	2MG	O6-C6-C5	-2.36	120.34	126.60
59	1	404	5MU	O4-C4-N3	-2.35	115.61	120.12
21	2	480	G7M	N2-C2-N1	2.31	121.64	116.71
21	2	1458	MA6	C4-C5-N7	-2.30	107.82	110.62
59	1	2192	OMU	O2-C2-N1	-2.29	119.75	122.79
59	1	1577	5MU	C5M-C5-C4	2.29	121.28	118.77
59	1	1669	6MZ	C2-N1-C6	2.29	122.93	115.25
59	1	1471	2MG	N1-C2-N3	-2.26	120.45	123.95
21	2	912	2MG	C5-C4-N9	2.26	109.73	105.63
21	2	1341	4OC	C6-C5-C4	2.25	119.71	116.96
59	1	2085	2MG	CM2-N2-C2	-2.23	118.93	123.86
59	1	1471	2MG	C5-C4-N9	2.22	109.66	105.63
59	1	1577	5MU	O2-C2-N1	-2.22	119.84	122.79
21	2	912	2MG	C8-N7-C5	2.22	108.25	104.24
59	1	1891	OMG	C8-N7-C5	2.19	108.21	104.24
59	1	2085	2MG	O6-C6-C5	-2.19	120.78	126.60
59	1	1669	6MZ	C4-N9-C8	2.19	108.10	105.73
59	1	1471	2MG	C4-C5-N7	-2.11	107.38	110.72
21	2	1437	UR3	C1'-N1-C2	2.06	120.47	116.99
59	1	404	5MU	O2-C2-N3	-2.06	117.66	121.50
21	2	912	2MG	C4-C5-N7	-2.06	107.46	110.72
59	1	1669	6MZ	C9-N6-C6	-2.06	121.10	122.87
59	1	2085	2MG	C8-N7-C5	2.04	107.94	104.24
21	2	913	5MC	CM5-C5-C6	-2.04	120.12	122.85
59	1	2143	2MA	CM2-C2-N1	2.04	120.33	117.15
59	1	1600	5MC	CM5-C5-C6	-2.03	120.13	122.85
59	1	1471	2MG	C8-N7-C5	2.01	107.89	104.24

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1	1669	6MZ	C3'-C4'-C5'-O5'
59	1	1891	OMG	C1'-C2'-O2'-CM2
59	1	1669	6MZ	O4'-C4'-C5'-O5'
21	2	480	G7M	C3'-C4'-C5'-O5'
59	1	1891	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
21	2	1458	MA6	O4'-C4'-C5'-O5'
59	1	1891	OMG	C3'-C4'-C5'-O5'
21	2	480	G7M	C4'-C5'-O5'-P
59	1	2085	2MG	C3'-C4'-C5'-O5'
59	1	2143	2MA	O4'-C4'-C5'-O5'
21	2	480	G7M	O4'-C4'-C5'-O5'
21	2	1341	4OC	O4'-C4'-C5'-O5'
21	2	1458	MA6	C3'-C4'-C5'-O5'
59	1	404	5MU	C4'-C5'-O5'-P
59	1	2143	2MA	C4'-C5'-O5'-P

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	2	1458	MA6	1	0
21	2	1455	2MG	2	0
59	1	1577	5MU	1	0
59	1	1669	6MZ	1	0
21	2	912	2MG	2	0
59	1	1891	OMG	1	0
59	1	404	5MU	2	0
21	2	1341	4OC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 460 ligands modelled in this entry, 460 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
59	1	12
21	2	2
24	e	1
60	4	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	e	187:GLY	C	227:ALA	N	25.55
1	1	1190:A	O3'	1196:U	P	16.56
1	4	259:U	O3'	266:A	P	16.51
1	1	1506:C	O3'	1509:G	P	16.30
1	1	1738:G	O3'	1830:G	P	15.17
1	1	828:U	O3'	840:U	P	14.89
1	1	194:A	O3'	201:G	P	11.83
1	1	2430:U	O3'	2449:A	P	11.45
1	1	308:A	O3'	312:A	P	9.50
1	1	586:A	O3'	588:U	P	9.33
1	2	76:G	O3'	79:A	P	8.97
1	1	590:U	O3'	592:C	P	8.73
1	1	1242:U	O3'	1245:A	P	7.81
1	1	502:A	O3'	504:G	P	5.57
1	1	139:G	O3'	141:U	P	4.10
1	2	1472:C	O3'	1473:A	P	3.19

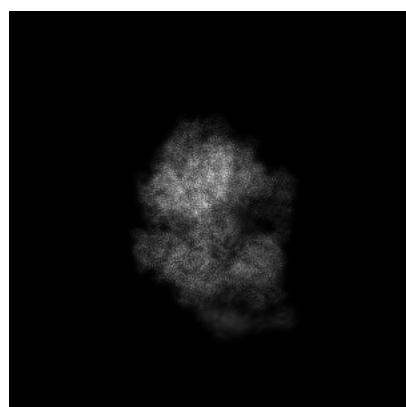
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56602. These allow visual inspection of the internal detail of the map and identification of artifacts.

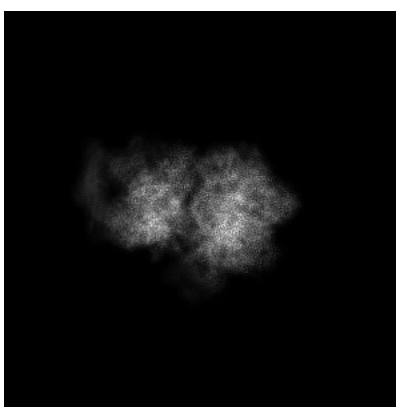
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

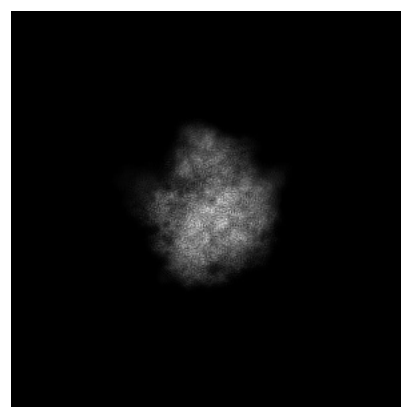
6.1.1 Primary map



X



Y

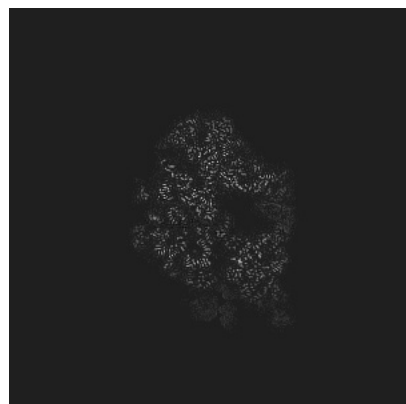


Z

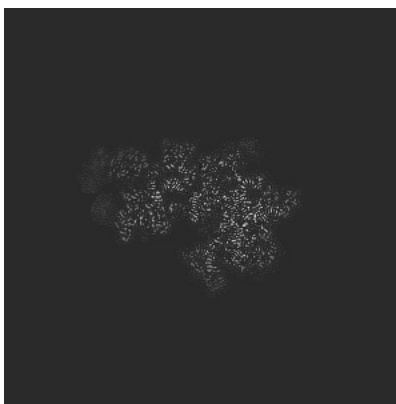
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

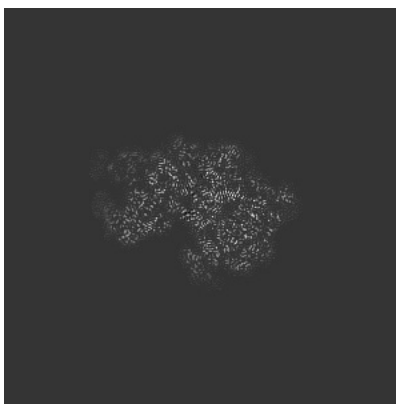
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

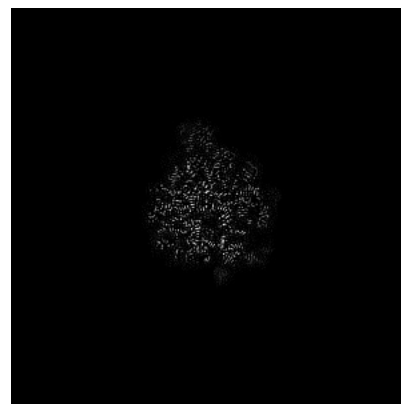
6.3.1 Primary map



X Index: 251



Y Index: 244

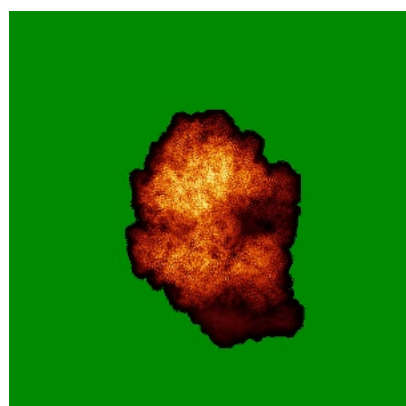


Z Index: 299

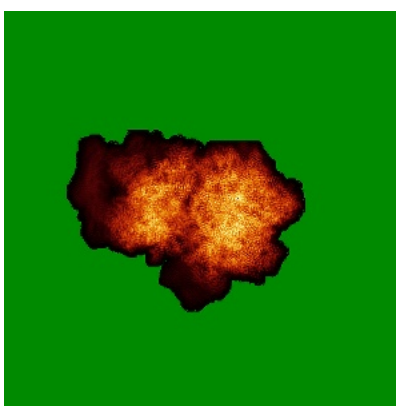
The images above show the largest variance slices of the map in three orthogonal directions.

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

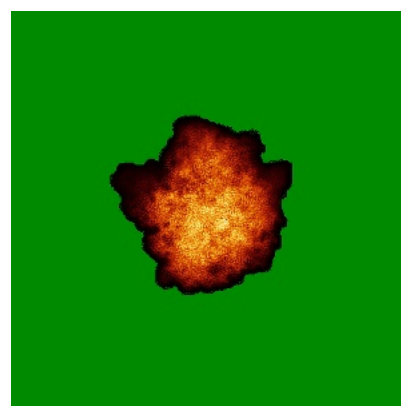
6.4.1 Primary map



X



Y

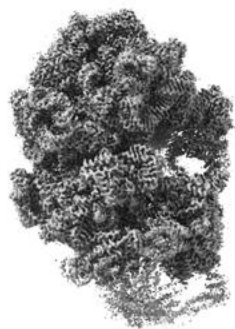


Z

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

6.5 Orthogonal surface views [i](#)

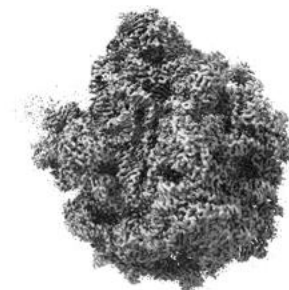
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.107. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

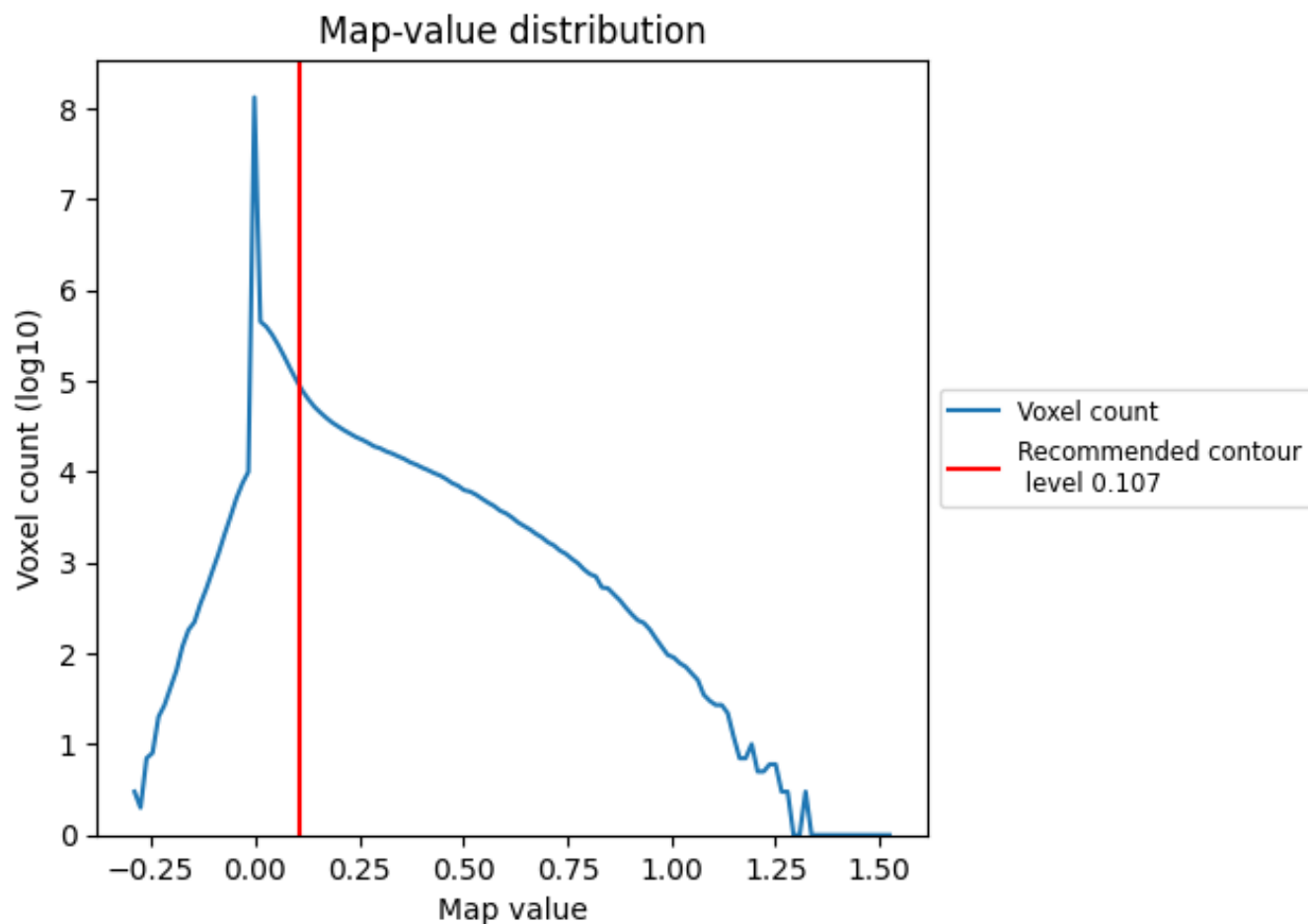
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

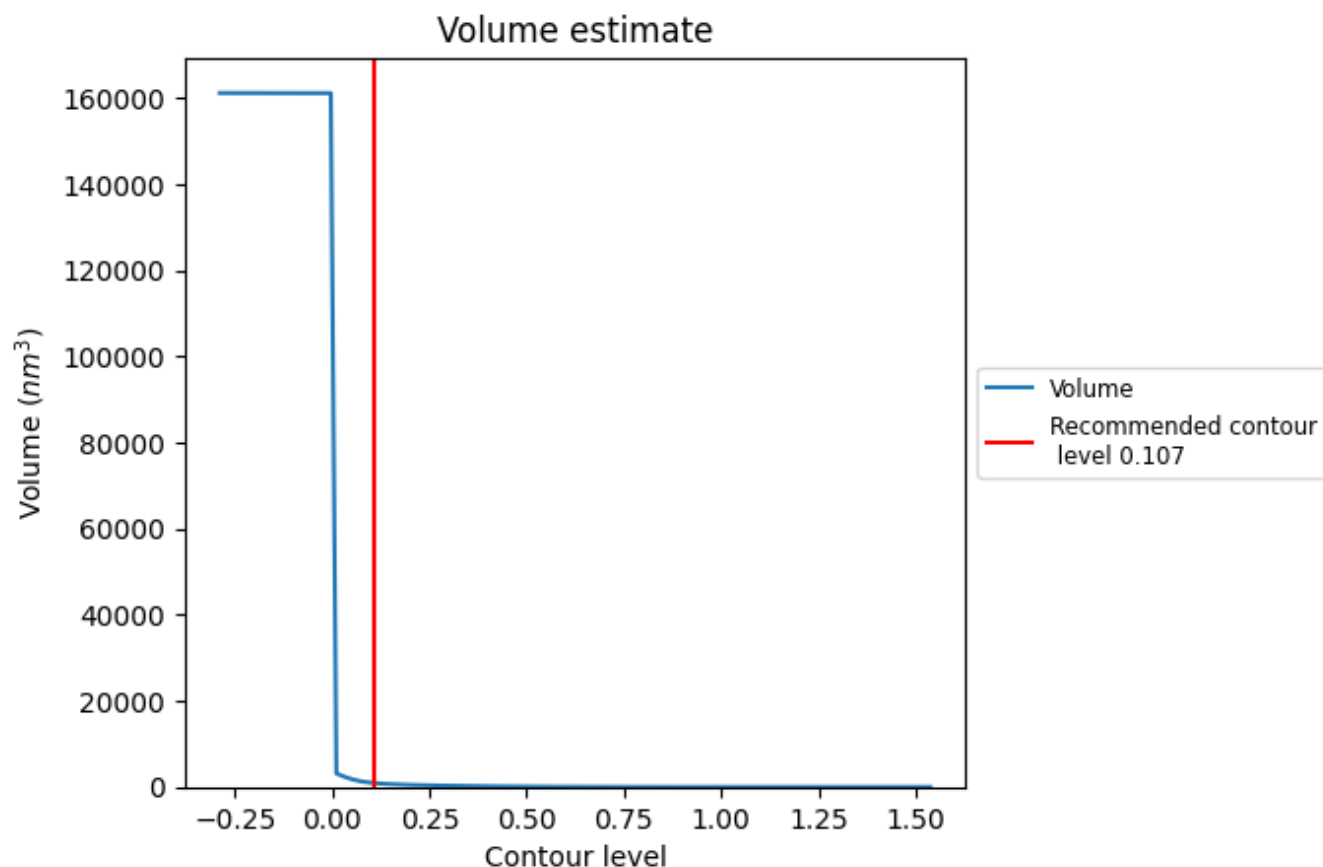
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

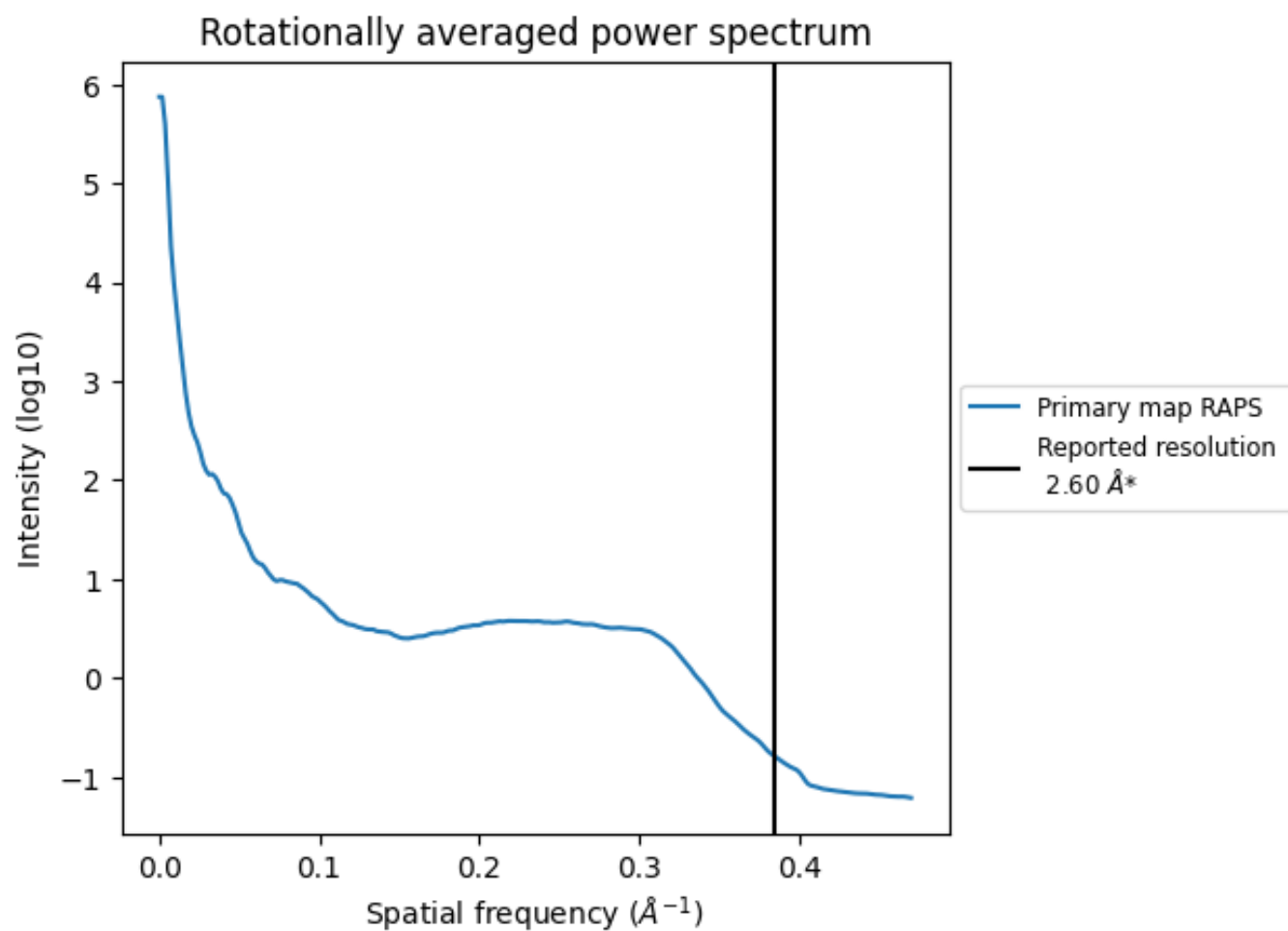
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 915 nm³; this corresponds to an approximate mass of 826 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 0.385 Å⁻¹

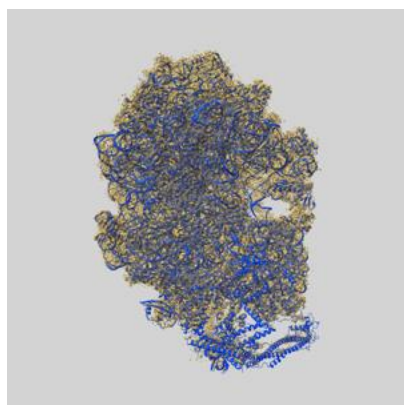
8 Fourier-Shell correlation ⓘ

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

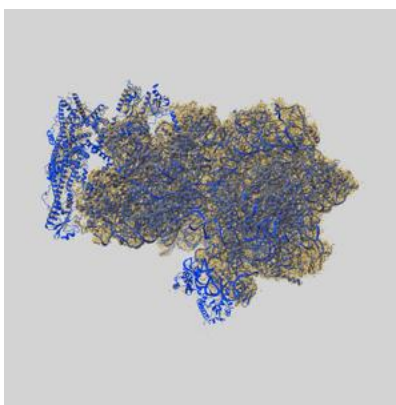
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56602 and PDB model 28LU. Per-residue inclusion information can be found in section [3](#) on page [17](#).

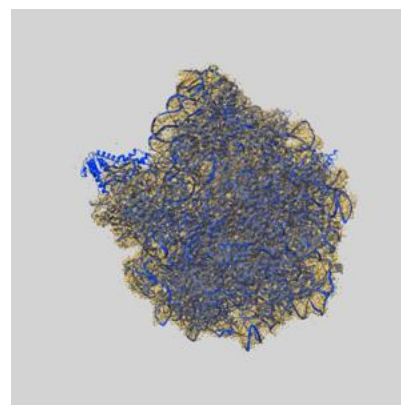
9.1 Map-model overlay [i](#)



X



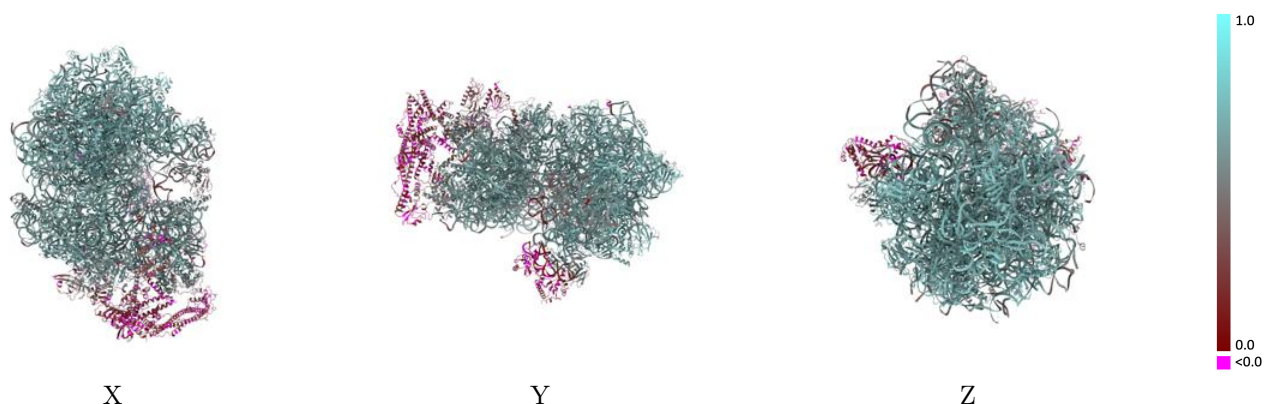
Y



Z

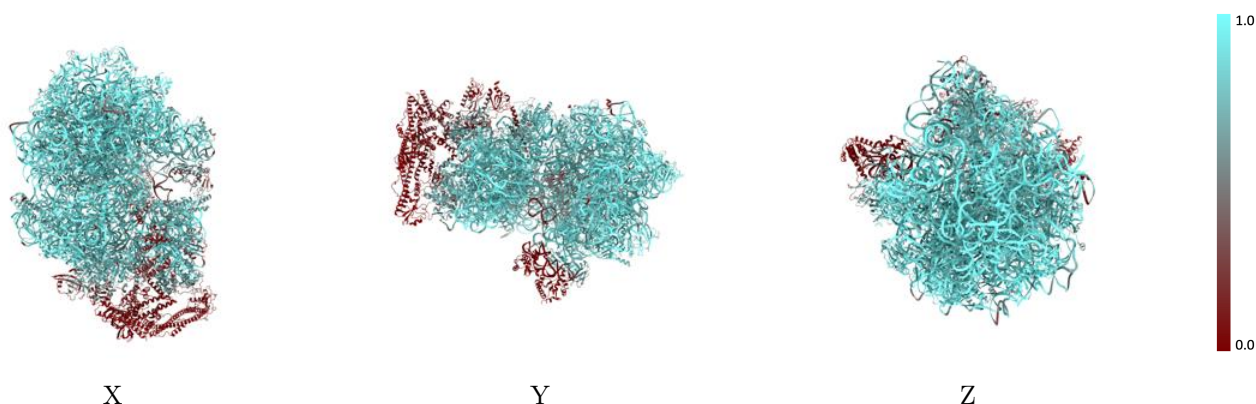
The images above show the 3D surface view of the map at the recommended contour level 0.107 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



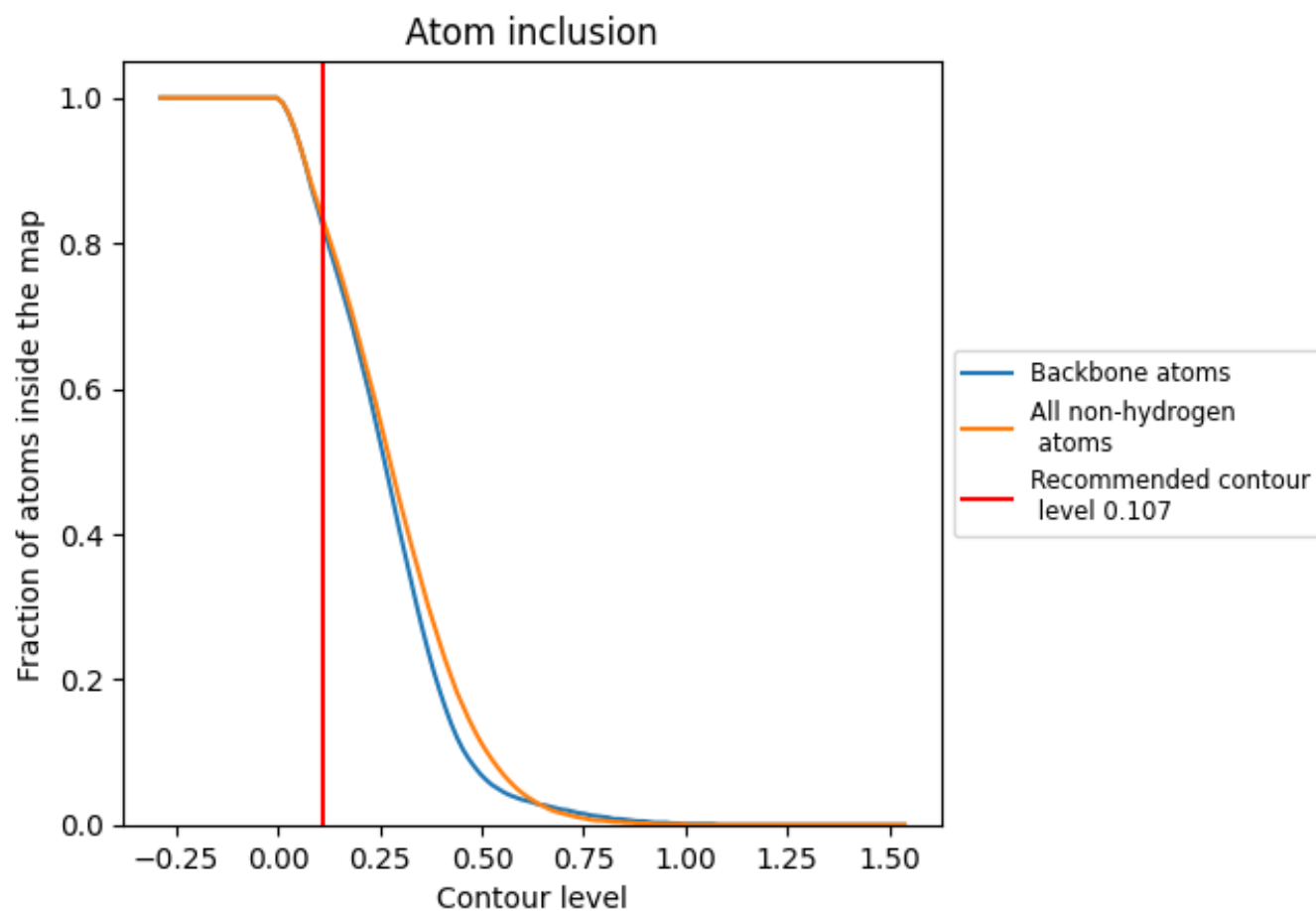
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.107).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 84% 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 (0.107) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8360	 0.5830
0	 0.9050	 0.6620
1	 0.9410	 0.6390
2	 0.9670	 0.6200
3	 0.8380	 0.5420
4	 0.9630	 0.6490
5	 0.9830	 0.6630
6	 0.9210	 0.6630
7	 0.9660	 0.6860
8	 0.9690	 0.6800
9	 0.9610	 0.6730
B	 0.9610	 0.6880
C	 0.9520	 0.6800
D	 0.9430	 0.6770
E	 0.4940	 0.4600
F	 0.7450	 0.5770
G	 0.7320	 0.5630
H	 0.0100	 0.1190
I	 0.0060	 0.0740
J	 0.9350	 0.6700
K	 0.9430	 0.6770
L	 0.8970	 0.6530
M	 0.9370	 0.6750
N	 0.9650	 0.6800
O	 0.7800	 0.5850
P	 0.8820	 0.6400
Q	 0.9860	 0.6900
R	 0.9380	 0.6740
S	 0.9260	 0.6710
T	 0.9540	 0.6670
U	 0.8860	 0.6510
V	 0.8510	 0.6120
W	 0.9110	 0.6570
X	 0.8910	 0.6490
Y	 0.3120	 0.3680



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Chain	Atom inclusion	Q-score
Z	 0.9370	 0.6630
a	 0.3650	 0.3400
b	 0.3670	 0.3470
c	 0.5000	 0.3990
d	 0.6720	 0.4920
e	 0.4100	 0.3370
f	 0.8350	 0.6060
g	 0.6950	 0.5370
h	 0.9100	 0.6370
i	 0.5910	 0.4800
j	 0.7850	 0.5760
k	 0.8600	 0.6120
l	 0.9330	 0.6460
m	 0.7700	 0.5620
n	 0.9330	 0.6330
o	 0.8630	 0.6030
p	 0.9350	 0.6380
q	 0.8740	 0.6210
r	 0.8940	 0.6230
s	 0.8650	 0.6080
t	 0.8260	 0.5770
u	 0.7740	 0.5800
v	 0.2530	 0.3050
w	 0.2890	 0.2770
x	 0.8960	 0.6180
y	 0.6690	 0.5580