



Full wwPDB EM Validation Report ⓘ

Feb 10, 2025 – 11:57 PM EST

PDB ID : 5UQ8
EMDB ID : EMD-8597
Title : 70S ribosome complex with dnaX mRNA stem-loop and E-site tRNA ("out" conformation)
Authors : Zhang, Y.; Hong, S.; Skiniotis, G.; Dunham, C.M.
Deposited on : 2017-02-07
Resolution : 3.20 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:

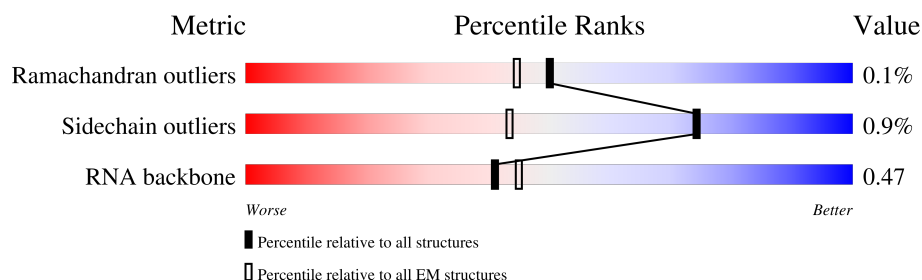
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	2915	
2	B	120	
3	D	275	
4	E	204	
5	F	203	
6	G	181	
7	H	173	
8	I	146	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	N	140	21% 99%
10	O	122	21% 99%
11	P	149	25% 100%
12	Q	141	23% 99%
13	R	118	12% 100%
14	S	110	31% 100%
15	T	131	24% 99%
16	U	116	12% 100%
17	V	101	33% 99%
18	W	112	21% 99%
19	X	95	24% 100%
20	Y	107	42% 98%
21	Z	187	72% 99%
22	0	77	16% 100%
23	1	97	29% 99%
24	2	70	34% 100%
25	3	59	25% 98%
26	4	69	71% 96%
27	5	59	14% 98%
28	6	53	25% 98%
29	7	48	17% 96%
30	8	64	14% 100%
31	9	37	30% 100%
32	a	1521	8% 77% 21%
33	b	231	62% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	c	206	<div> <div>35%</div> <div>100%</div> </div>
35	d	208	<div> <div>36%</div> <div>100%</div> </div>
36	e	148	<div> <div>17%</div> <div>99%</div> </div>
37	f	100	<div> <div>74%</div> <div>100%</div> </div>
38	g	155	<div> <div>44%</div> <div>99%</div> </div>
39	h	137	<div> <div>25%</div> <div>100%</div> </div>
40	i	126	<div> <div>49%</div> <div>98%</div> </div>
41	j	96	<div> <div>49%</div> <div>99%</div> </div>
42	k	114	<div> <div>35%</div> <div>100%</div> </div>
43	l	122	<div> <div>26%</div> <div>98%</div> </div>
44	m	114	<div> <div>54%</div> <div>99%</div> </div>
45	n	60	<div> <div>15%</div> <div>97%</div> </div>
46	o	88	<div> <div>35%</div> <div>99%</div> </div>
47	p	82	<div> <div>18%</div> <div>99%</div> </div>
48	q	99	<div> <div>26%</div> <div>100%</div> </div>
49	r	68	<div> <div>63%</div> <div>100%</div> </div>
50	s	83	<div> <div>52%</div> <div>100%</div> </div>
51	t	98	<div> <div>38%</div> <div>98%</div> </div>
52	u	23	<div> <div>30%</div> <div>100%</div> </div>
53	y	77	<div> <div>36%</div> <div>82%</div> <div>18%</div> </div>
54	C	226	<div> <div>100%</div> <div>100%</div> </div>
55	z	76	<div> <div>96%</div> <div>61%</div> <div>38%</div> </div>
56	x	55	<div> <div>95%</div> <div>56%</div> <div>42%</div> </div>

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 148590 atoms, of which 4 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2867	Total	C	N	O	P	0	0
			61758	27491	11552	19850	2865		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	P	0	0
			2573	1146	476	832	119		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	275	Total	C	N	O	S	0	0
			2136	1349	423	361	3		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	204	Total	C	N	O	S	0	0
			1559	985	298	270	6		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	203	Total	C	N	O	S	0	1
			1580	1007	297	274	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	181	Total	C	N	O	S	0	0
			1424	912	259	249	4		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	173	Total	C	N	O	S	0	0
			1324	842	247	234	1		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	146	Total	C	N	O	S	0	0
			1076	687	186	202	1		

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	140	Total	C	N	O	S	0	0
			1117	719	207	187	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	122	Total	C	N	O	S	0	0
			933	588	171	170	4		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	149	Total	C	N	O	S	0	0
			1135	706	230	196	3		

- Molecule 12 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0
			1122	715	212	188	7		

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	R	118	Total	C	N	O	S	0	0
			968	604	203	160	1		

- Molecule 14 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	S	110	Total	C	N	O		
			870	549	173	148	0	0

- Molecule 15 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	T	131	Total	C	N	O	S	
			1083	675	224	183	1	0

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	U	116	Total	C	N	O	S	
			959	608	201	149	1	0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	V	101	Total	C	N	O	S	
			771	495	140	135	1	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	W	112	Total	C	N	O	S	
			886	557	174	153	2	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	X	95	Total	C	N	O	S	
			750	488	135	126	1	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	Y	107	Total	C	N	O	S	
			810	519	153	132	6	0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Z	187	Total	C	N	O	S	0	0
			1459	932	257	268	2		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	0	77	Total	C	N	O	S	0	0
			608	375	129	103	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1	97	Total	C	N	O	S	0	0
			759	478	149	131	1		

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	2	70	Total	C	N	O	S	0	0
			592	368	119	103	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	3	59	Total	C	N	O	0	0
			464	296	90	78		

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	4	69	Total	C	N	O	S	0	0
			536	342	98	91	5		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	59	Total	C	N	O	S	0	0
			455	285	89	76	5		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	53	Total	C	N	O	S	0	0
			449	279	91	75	4		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	48	Total	C	N	O	S	0	0
			418	257	104	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	64	Total	C	N	O	S	0	0
			517	331	102	82	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	37	Total	C	N	O	S	0	0
			307	188	68	47	4		

- Molecule 32 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1513	Total	C	N	O	P	0	0
			32532	14488	6021	10510	1513		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1542	G	-	insertion	GB 55771382
a	1543	C	-	insertion	GB 55771382
a	1544	U	-	insertion	GB 55771382

- Molecule 33 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	231	Total	C	N	O	S	0	0
			1825	1167	326	327	5		

- Molecule 34 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	c	206	Total	C	N	O	S	0	0
			1542	968	300	273	1		

- Molecule 35 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	d	208	Total	C	N	O	S	0	0
			1668	1047	330	284	7		

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e	148	Total	C	N	O	S	0	0
			1133	716	214	199	4		

- Molecule 37 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	100	Total	C	N	O	S	0	0
			816	516	146	151	3		

- Molecule 38 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	g	155	Total	C	N	O	S	0	0
			1229	766	241	216	6		

- Molecule 39 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	137	Total	C	N	O	S	0	0
			1088	689	206	191	2		

- Molecule 40 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	i	126	Total	C	N	O		0	0
			966	613	186	167			

- Molecule 41 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	j	96	Total	C	N	O	0	0
			710	442	137	131		

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	k	114	Total	C	N	O	S	0	0
			833	519	156	155	3		

- Molecule 43 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	l	122	Total	C	N	O	S	0	0
			932	586	185	159	2		

- Molecule 44 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	m	114	Total	C	N	O	S	0	0
			895	550	186	157	2		

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	n	60	Total	C	N	O	S	0	0
			492	312	104	72	4		

- Molecule 46 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	o	88	Total	C	N	O	S	0	0
			728	456	144	126	2		

- Molecule 47 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	p	82	Total	C	N	O	S	0	0
			677	430	133	113	1		

- Molecule 48 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	q	99	Total	C	N	O	S	0	0
			823	528	151	142	2		

- Molecule 49 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	r	68	Total	C	N	O		0	0
			555	355	108	92			

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	83	Total	C	N	O	S	0	0
			645	410	118	115	2		

- Molecule 51 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	t	98	Total	C	N	O	S	0	0
			733	451	154	126	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
52	u	23	Total	C	N	O	0	0
			199	122	48	29		

- Molecule 53 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	77	Total	C	N	O	P	0	0
			1640	732	298	534	76		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
y	17B	C	U	conflict	GB 1126835761

- Molecule 54 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	C	225	Total	C	N	O	S	0	0
			1718	1085	315	316	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	MET	deletion	UNP Q5SLP7

- Molecule 55 is a RNA chain called E-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

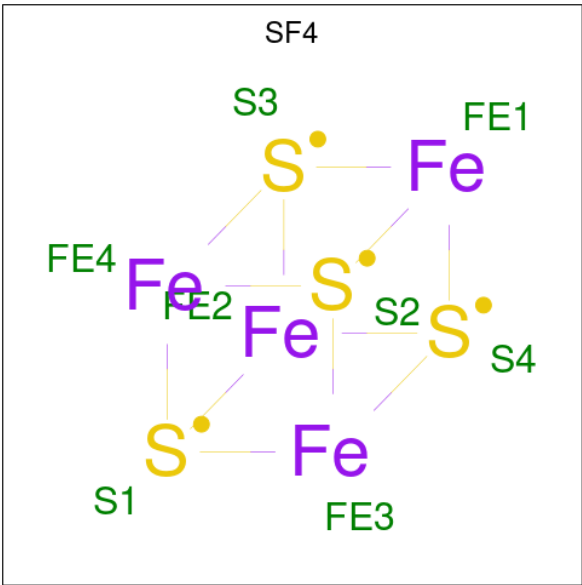
- Molecule 56 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	55	Total	C	H	N	O	P	
			1180	527	4	219	376	54	0

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	Y	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	
57	5	1	Total	Zn	0
			1	1	
57	6	1	Total	Zn	0
			1	1	
57	9	1	Total	Zn	0
			1	1	
57	n	1	Total	Zn	0
			1	1	

- Molecule 58 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).

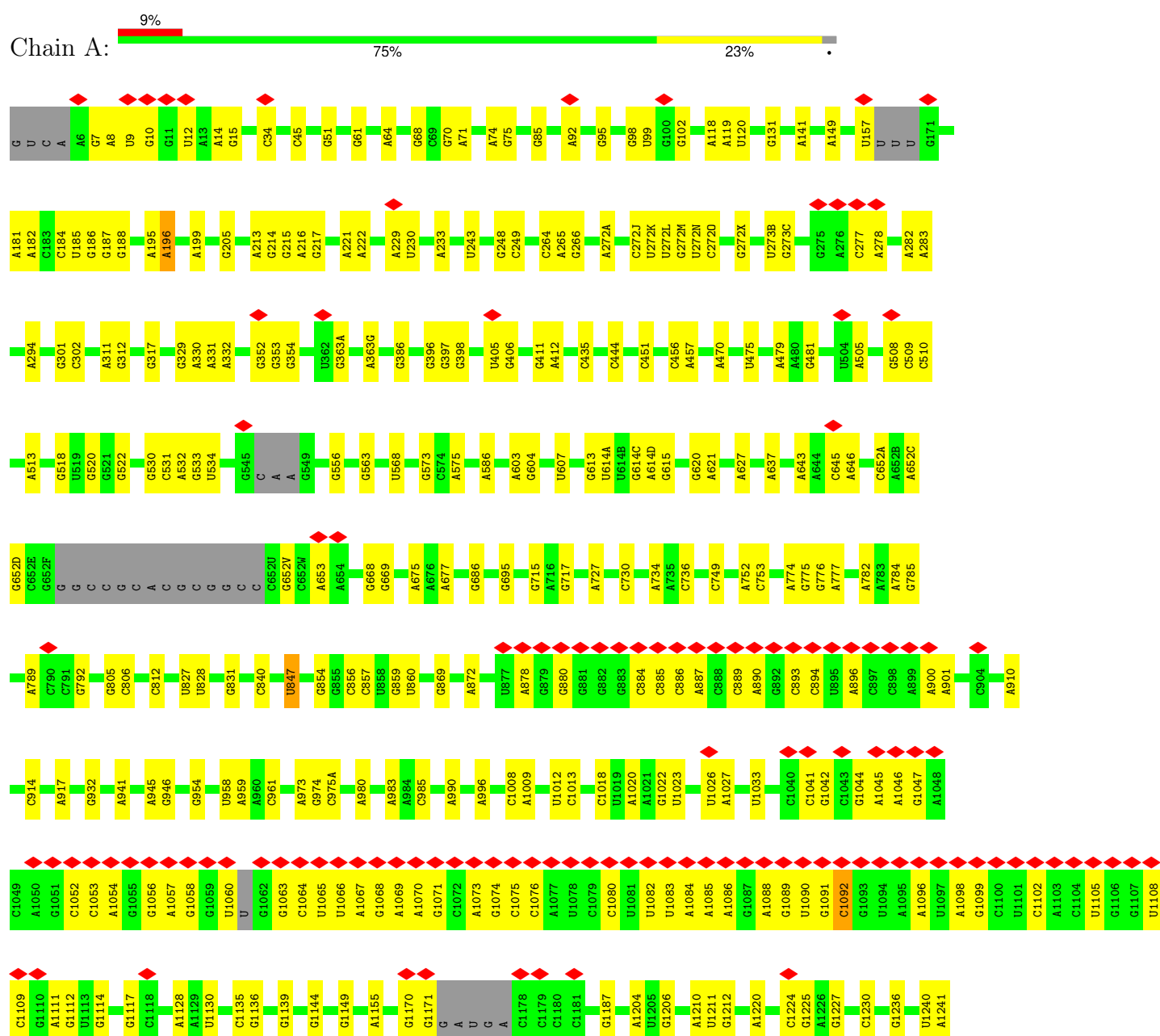


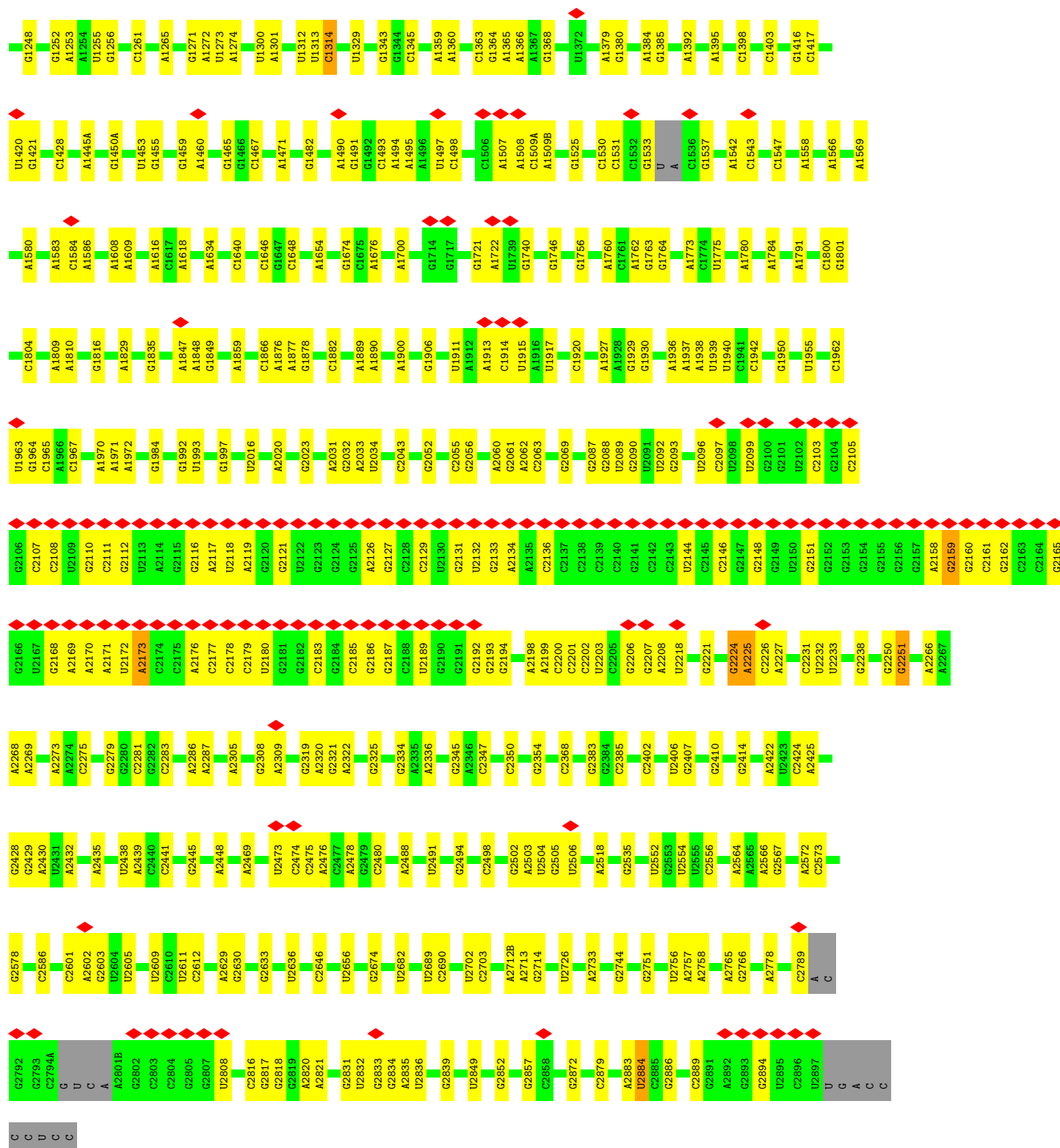
Mol	Chain	Residues	Atoms			AltConf
58	d	1	Total	Fe	S	0
			8	4	4	

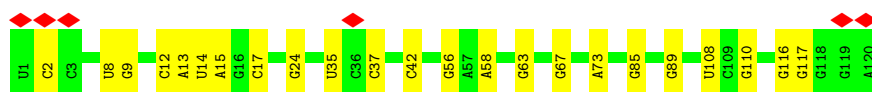
3 Residue-property plots

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

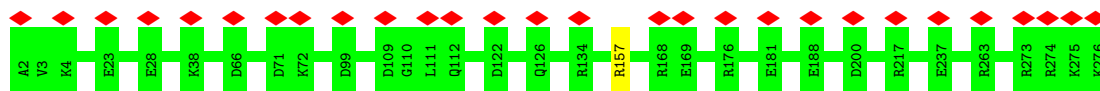
• Molecule 1: 23S rRNA



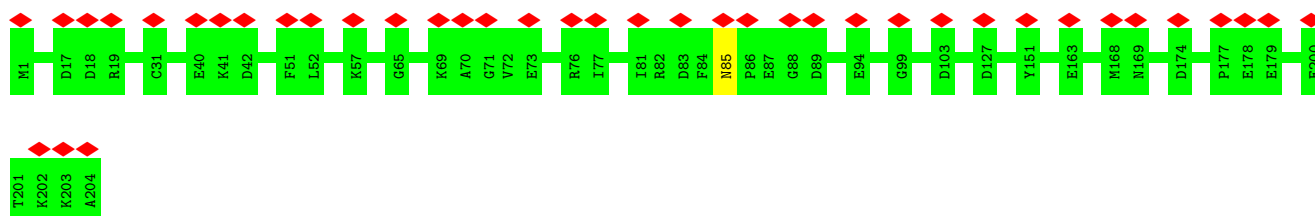




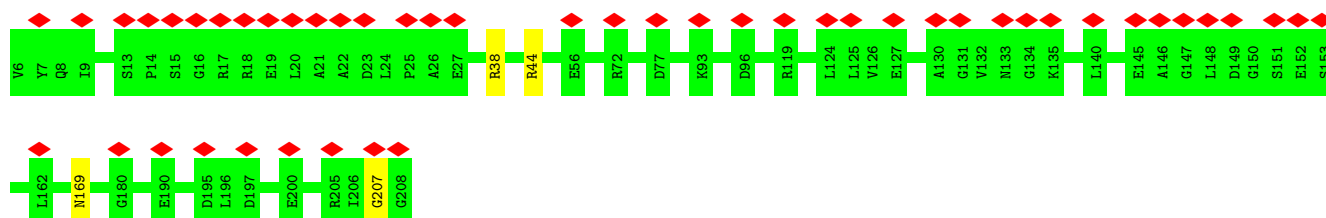
- Molecule 3: 50S ribosomal protein L2



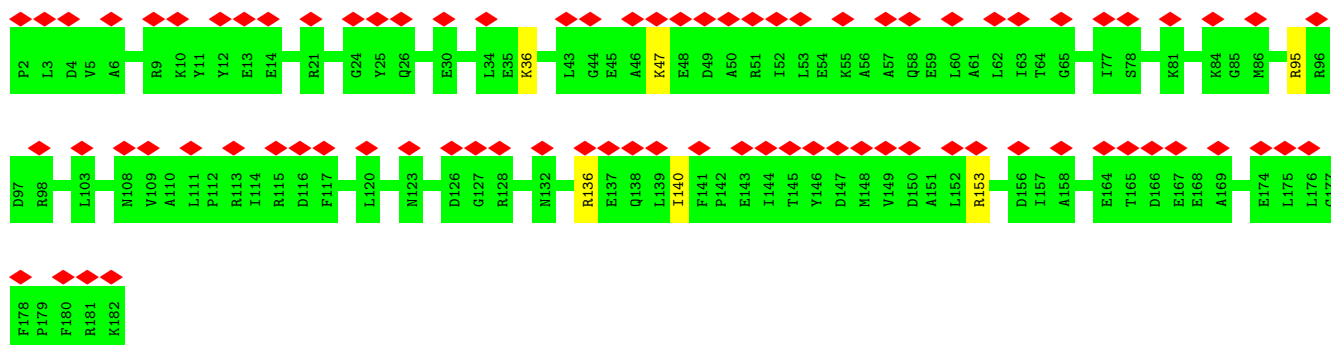
- Molecule 4: 50S ribosomal protein L3



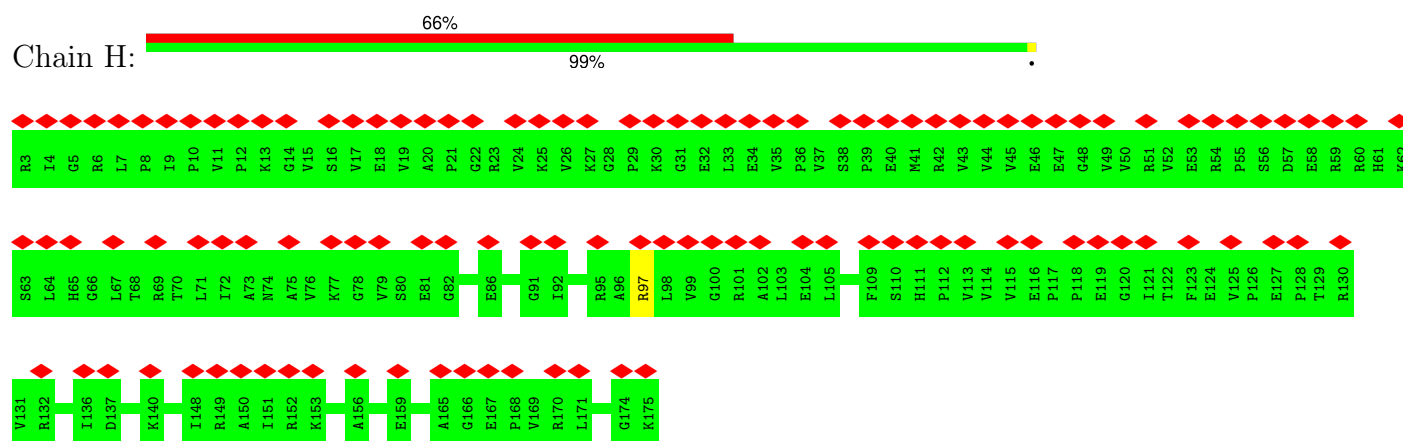
- Molecule 5: 50S ribosomal protein L4



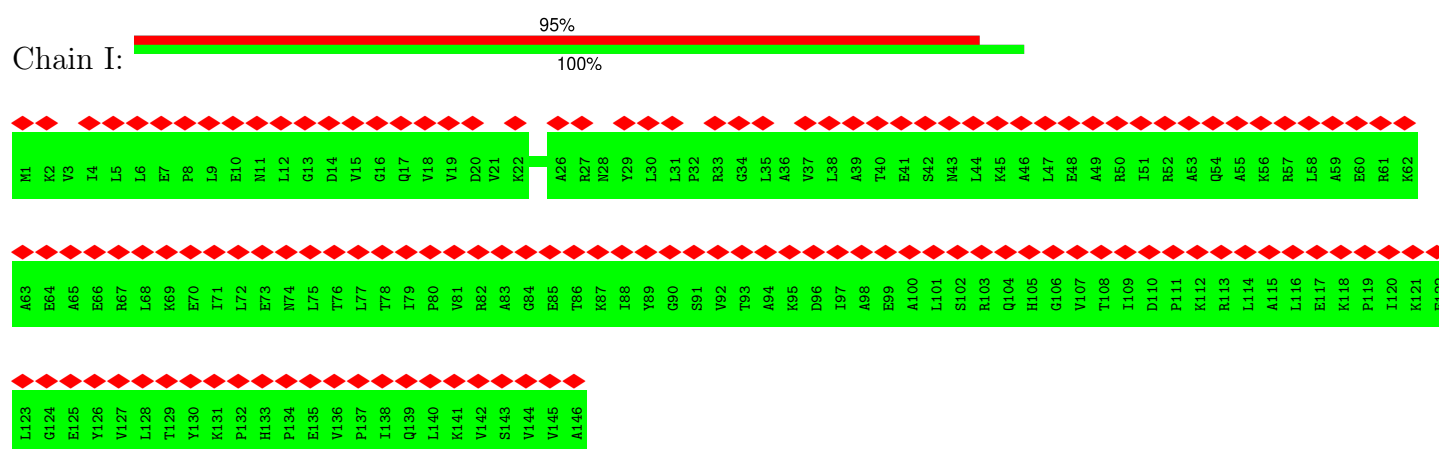
- Molecule 6: 50S ribosomal protein L5



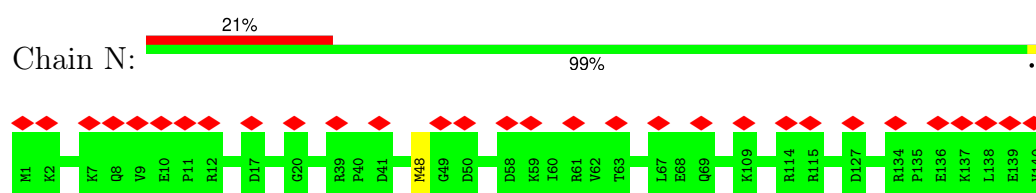
- Molecule 7: 50S ribosomal protein L6



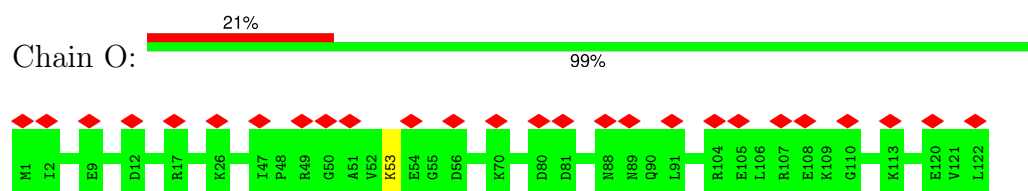
• Molecule 8: 50S ribosomal protein L9



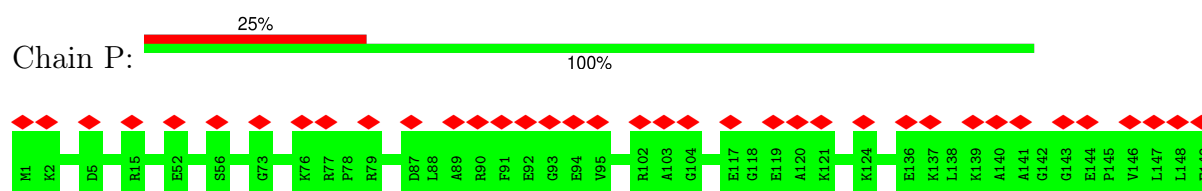
• Molecule 9: 50S ribosomal protein L13



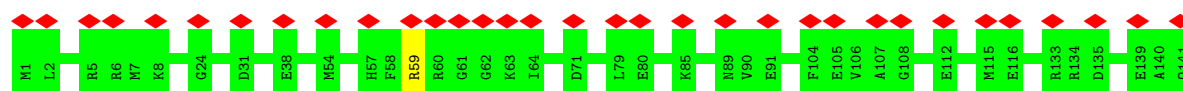
• Molecule 10: 50S ribosomal protein L14



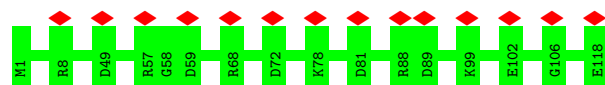
• Molecule 11: 50S ribosomal protein L15



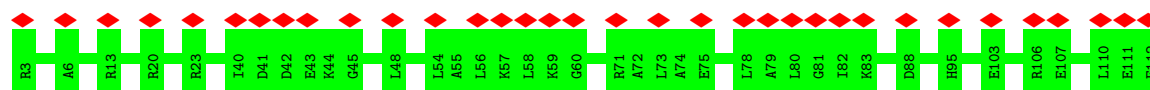
- Molecule 12: 50S ribosomal protein L16



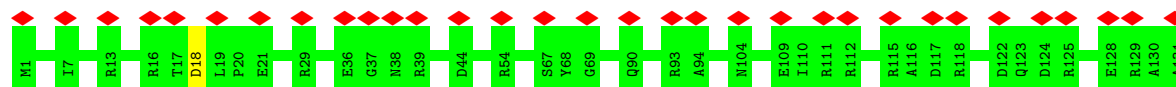
- Molecule 13: 50S ribosomal protein L17



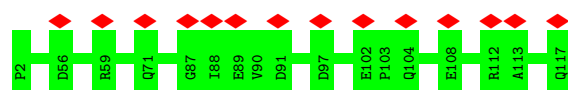
- Molecule 14: 50S ribosomal protein L18



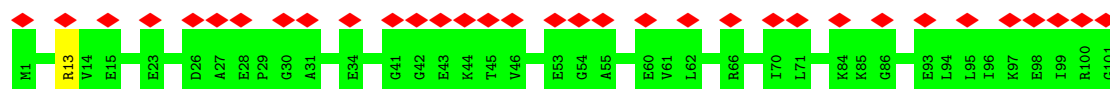
- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20

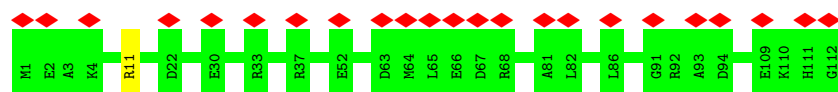


- Molecule 17: 50S ribosomal protein L21

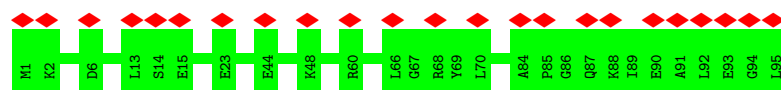


- Molecule 18: 50S ribosomal protein L22

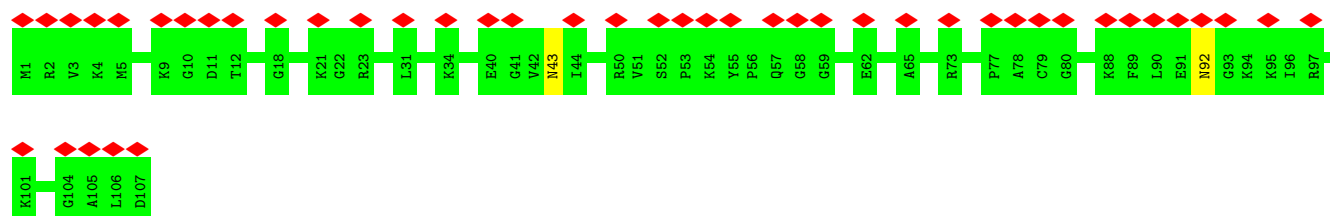
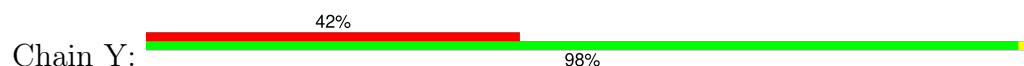




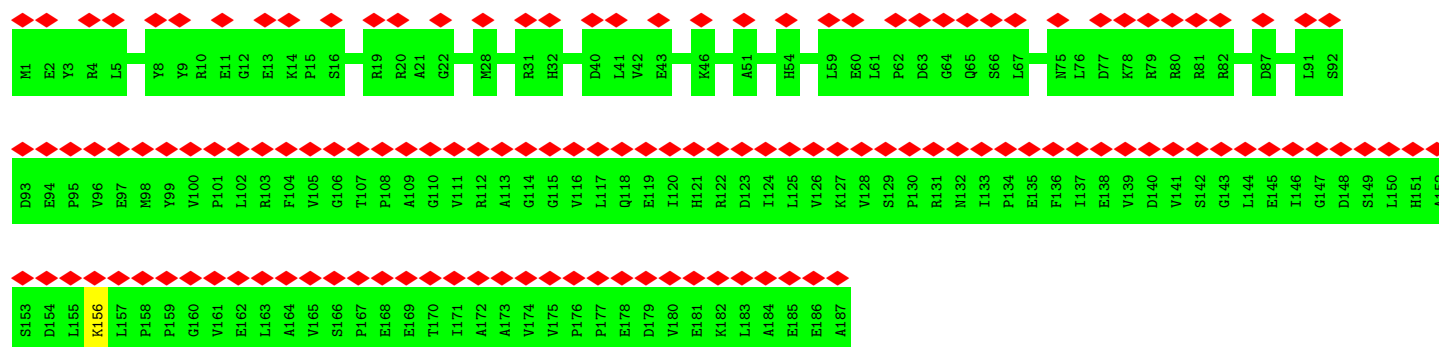
- Molecule 19: 50S ribosomal protein L23



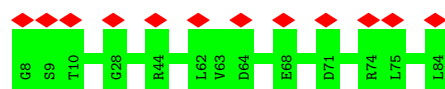
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25

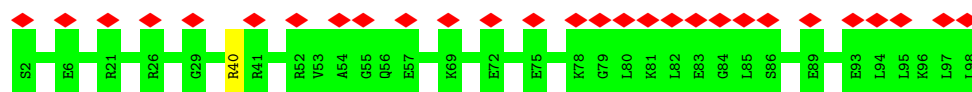


- Molecule 22: 50S ribosomal protein L27

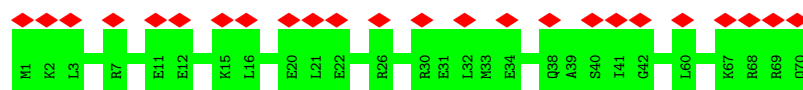


- Molecule 23: 50S ribosomal protein L28

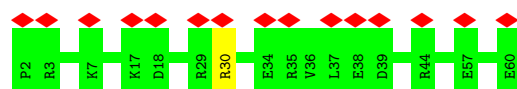




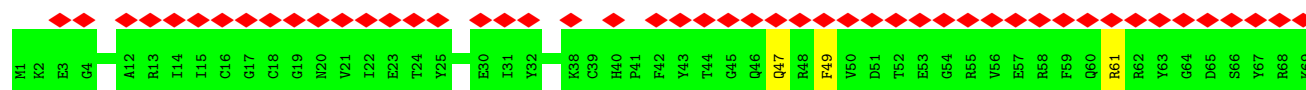
- Molecule 24: 50S ribosomal protein L29



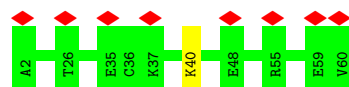
- Molecule 25: 50S ribosomal protein L30



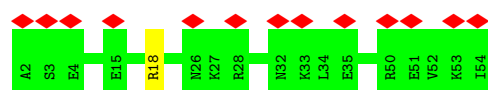
- Molecule 26: 50S ribosomal protein L31



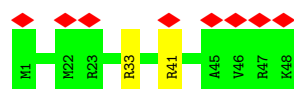
- Molecule 27: 50S ribosomal protein L32



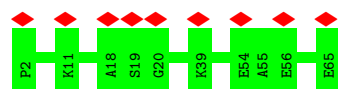
- Molecule 28: 50S ribosomal protein L33



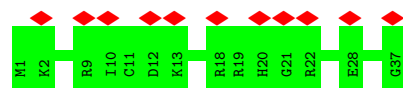
- Molecule 29: 50S ribosomal protein L34



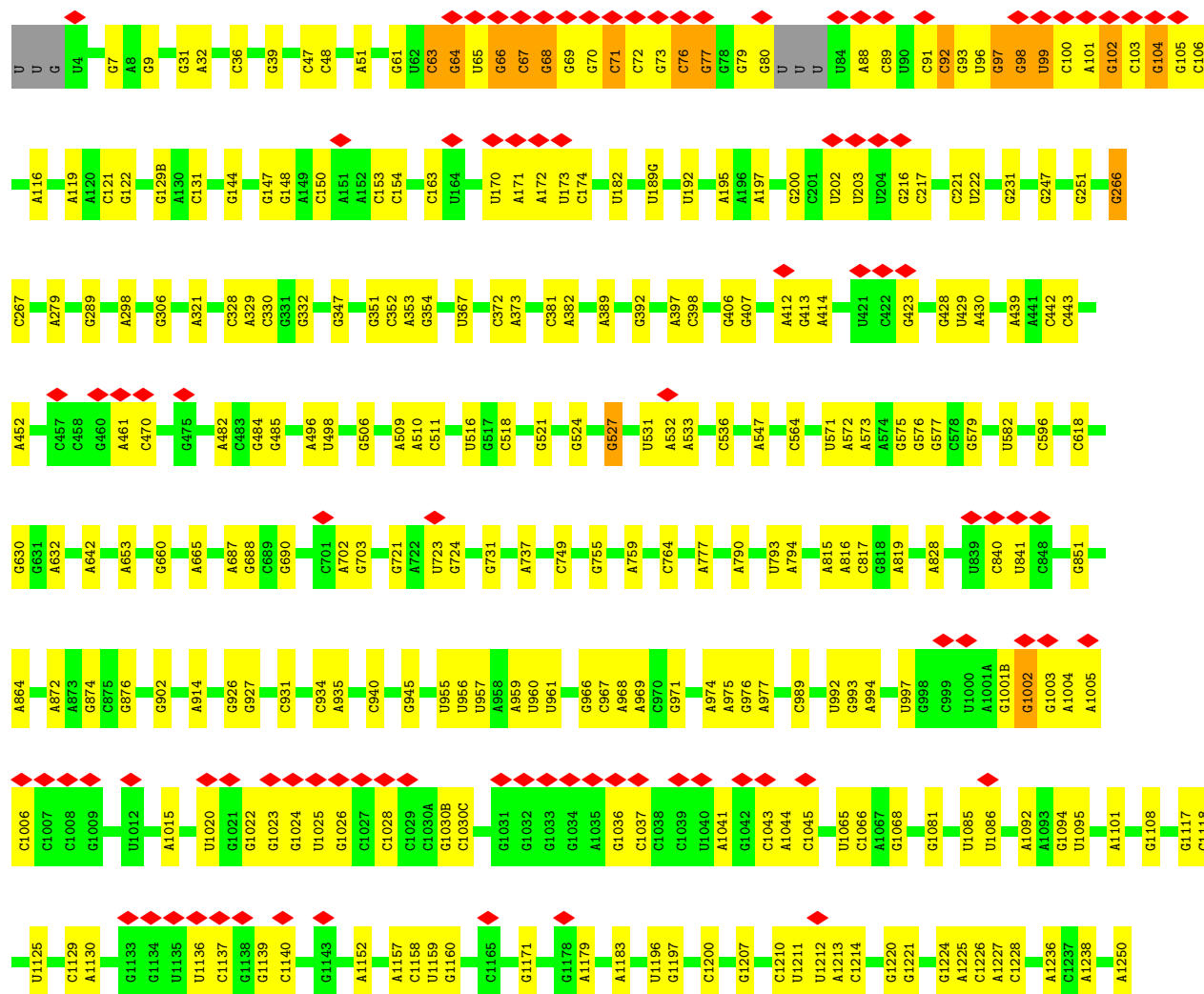
- Molecule 30: 50S ribosomal protein L35

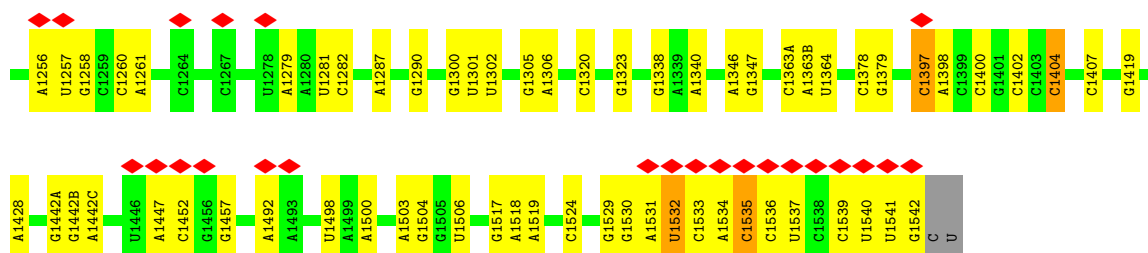


- Chain 9: 30% 100%

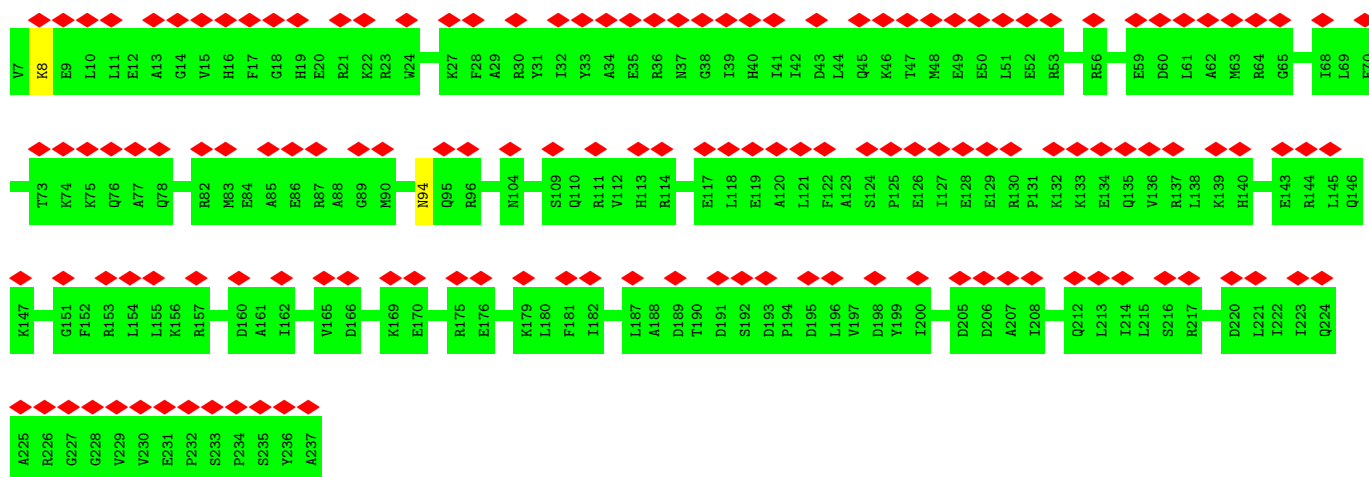


- Chain a:

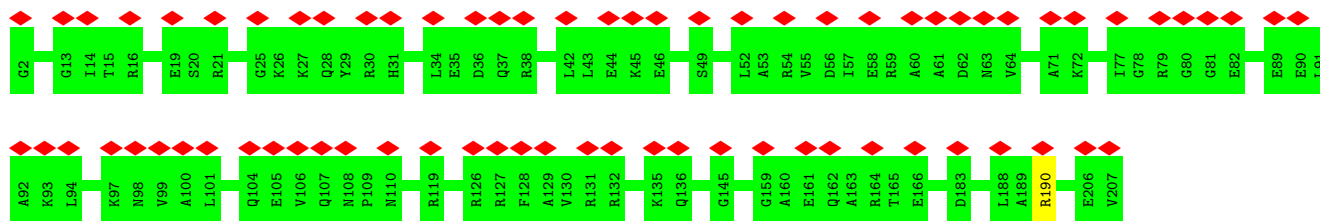




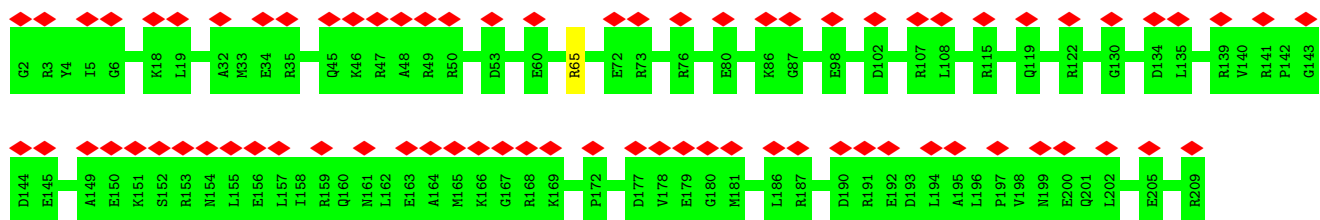
• Molecule 33: 30S ribosomal protein S2



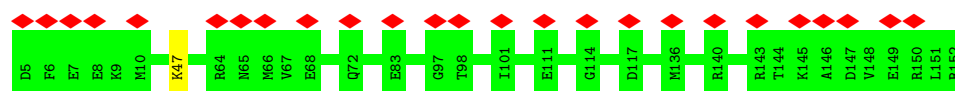
• Molecule 34: 30S ribosomal protein S3



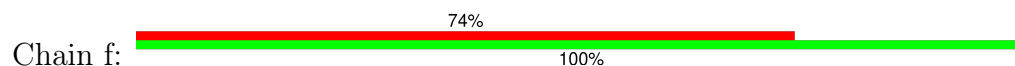
• Molecule 35: 30S ribosomal protein S4



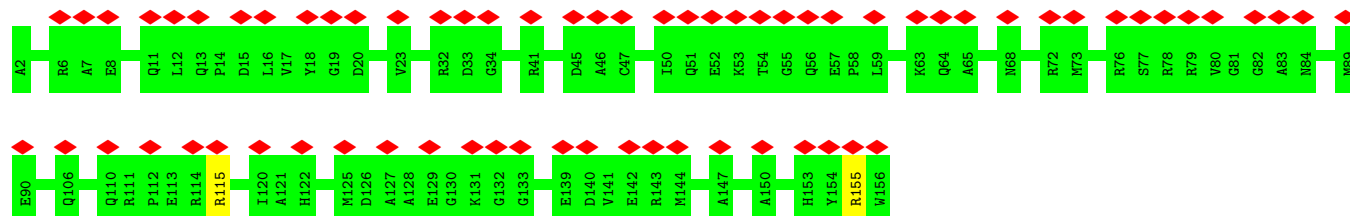
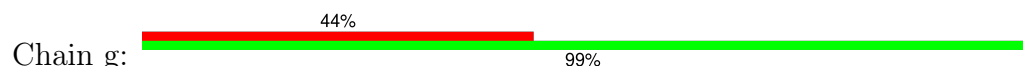
• Molecule 36: 30S ribosomal protein S5



• Molecule 37: 30S ribosomal protein S6



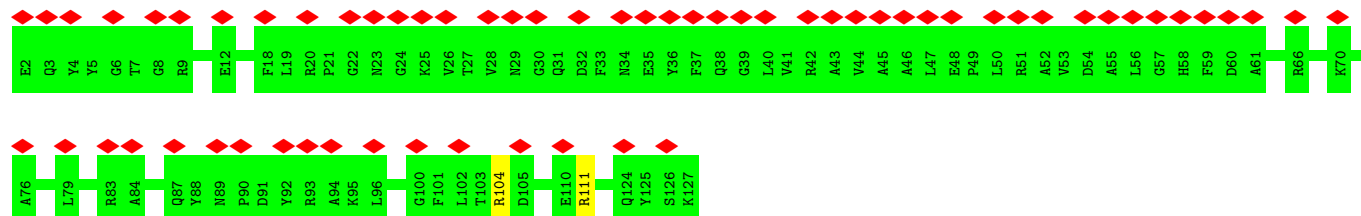
• Molecule 38: 30S ribosomal protein S7



• Molecule 39: 30S ribosomal protein S8

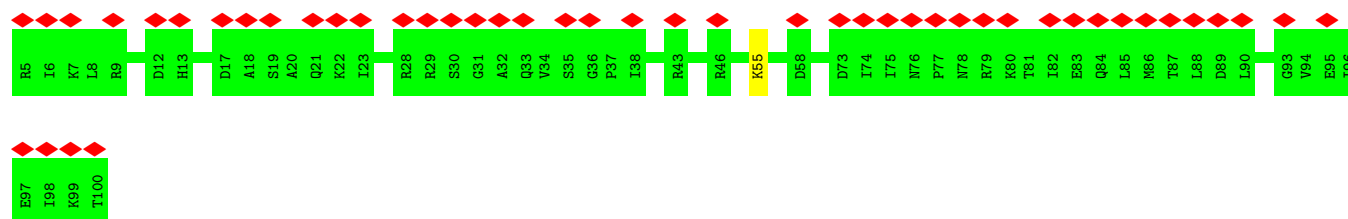


• Molecule 40: 30S ribosomal protein S9



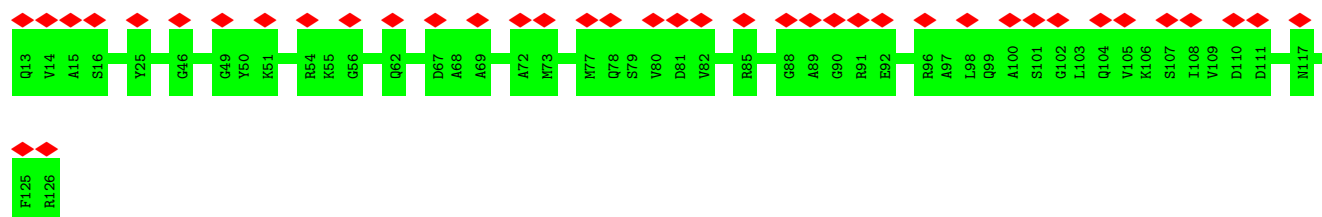
• Molecule 41: 30S ribosomal protein S10





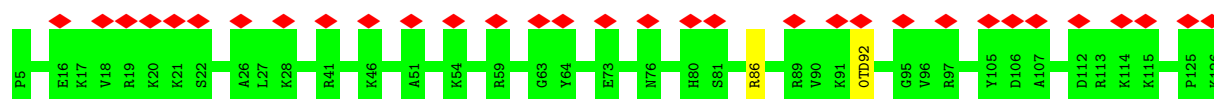
- Molecule 42: 30S ribosomal protein S11

Chain k: 35% 100%



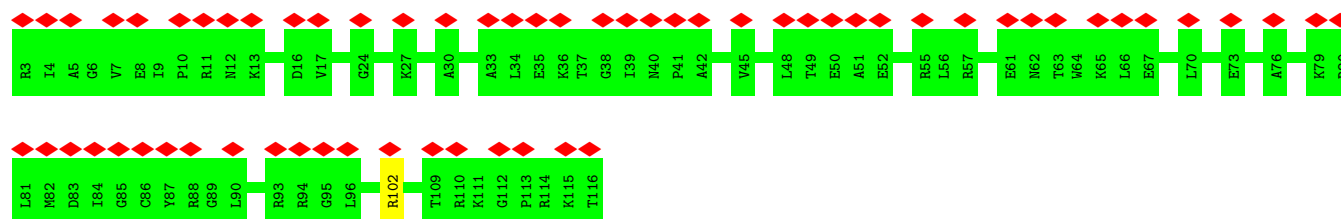
- Molecule 43: 30S ribosomal protein S12

Chain l: 26% 98%



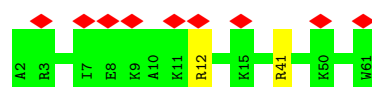
- Molecule 44: 30S ribosomal protein S13

Chain m: 54% 99%



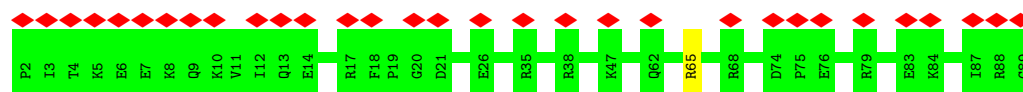
- Molecule 45: 30S ribosomal protein S14 type Z

Chain n: 15% 97%



- Molecule 46: 30S ribosomal protein S15

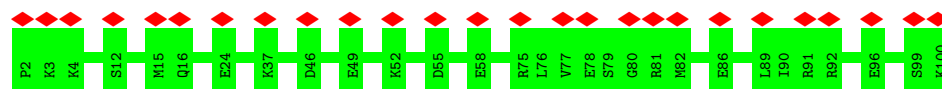
Chain o: 35% 99%



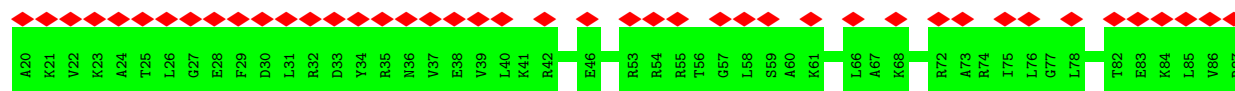
- Molecule 47: 30S ribosomal protein S16



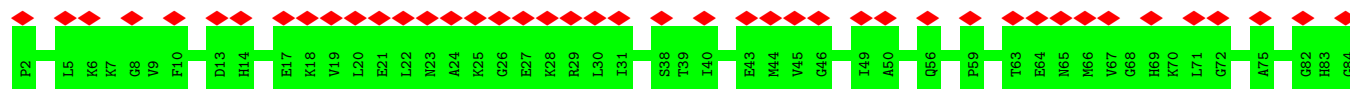
- Molecule 48: 30S ribosomal protein S17



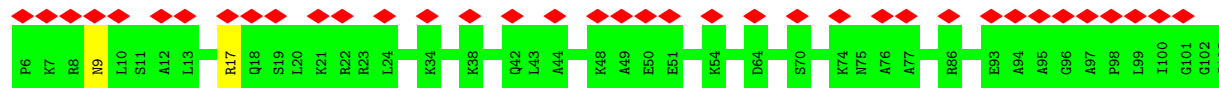
- Molecule 49: 30S ribosomal protein S18



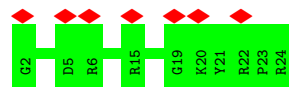
- Molecule 50: 30S ribosomal protein S19



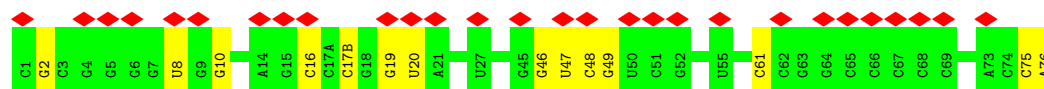
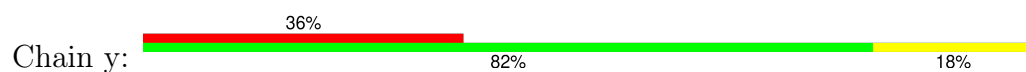
- Molecule 51: 30S ribosomal protein S20



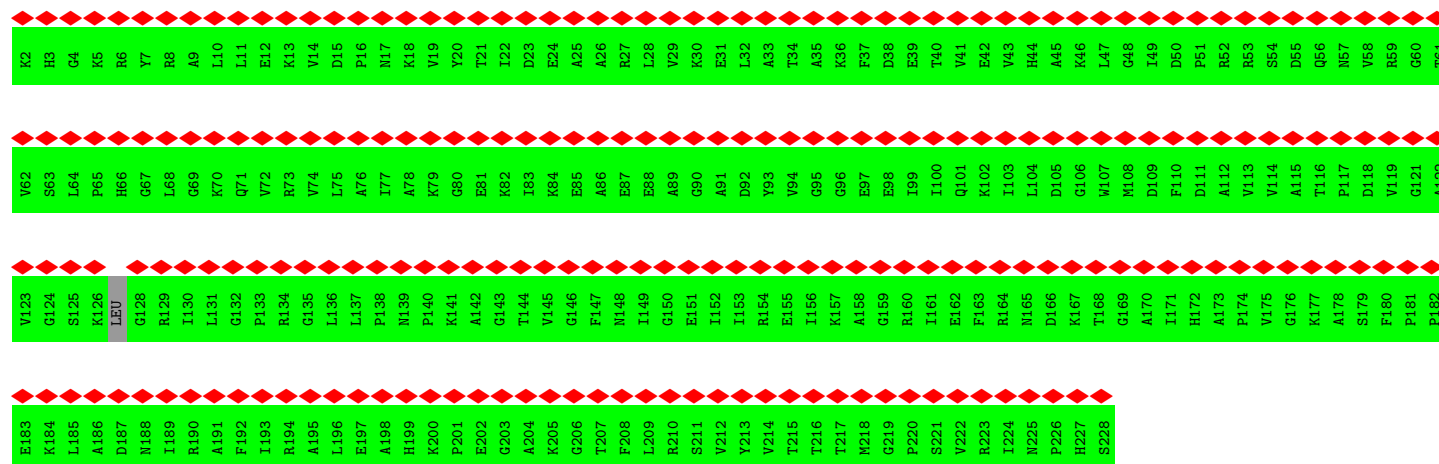
- Molecule 52: 30S ribosomal protein Thx



- Molecule 53: P-site tRNA fMet



• Molecule 54: 50S ribosomal protein L1



• Molecule 55: E-site tRNA Phe



• Molecule 56: messenger RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	36361	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.150	Depositor
Minimum map value	-0.080	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	384.0, 384.0, 384.0	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 7MG, UR3, 2MU, M2G, OMG, 0TD, 5MU, 4OC, MA6, 5MC, 2MA, 2MG, SF4, PSU

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	0.85	0/68899	0.93	27/107536 (0.0%)
2	B	0.73	0/2878	0.91	0/4490
3	D	0.44	0/2186	0.52	0/2944
4	E	0.42	0/1592	0.53	0/2149
5	F	0.41	0/1615	0.48	0/2188
6	G	0.36	0/1449	0.50	1/1957 (0.1%)
7	H	0.36	0/1347	0.47	0/1817
8	I	0.28	0/1091	0.46	0/1490
9	N	0.43	0/1144	0.47	0/1543
10	O	0.43	0/943	0.51	0/1269
11	P	0.39	0/1152	0.51	0/1533
12	Q	0.44	0/1143	0.48	0/1527
13	R	0.37	0/982	0.52	0/1312
14	S	0.38	0/880	0.45	0/1172
15	T	0.41	0/1097	0.53	1/1468 (0.1%)
16	U	0.40	0/977	0.44	0/1301
17	V	0.39	0/782	0.51	0/1049
18	W	0.42	0/897	0.47	0/1205
19	X	0.41	0/764	0.47	0/1025
20	Y	0.36	0/823	0.47	0/1100
21	Z	0.34	0/1491	0.48	0/2029
22	0	0.44	0/616	0.52	0/821
23	1	0.42	0/766	0.50	0/1018
24	2	0.33	0/594	0.42	0/785
25	3	0.39	0/469	0.48	0/630
26	4	0.37	0/549	0.53	0/741
27	5	0.40	0/469	0.47	0/635
28	6	0.43	0/456	0.52	0/608
29	7	0.40	0/426	0.49	0/561
30	8	0.38	0/525	0.49	0/691
31	9	0.41	0/310	0.46	0/407
32	a	1.57	10/36109 (0.0%)	0.99	70/56341 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.34	0/1860	0.44	0/2518
34	c	0.38	0/1566	0.47	0/2119
35	d	0.38	0/1698	0.44	0/2277
36	e	0.41	0/1149	0.51	0/1548
37	f	0.36	0/829	0.46	0/1123
38	g	0.35	0/1248	0.43	0/1676
39	h	0.41	0/1108	0.49	0/1494
40	i	0.38	0/985	0.46	0/1329
41	j	0.35	0/723	0.48	0/984
42	k	0.36	0/848	0.47	0/1149
43	l	0.40	0/937	0.53	0/1260
44	m	0.35	0/905	0.48	0/1217
45	n	0.42	0/501	0.47	0/664
46	o	0.34	0/739	0.46	0/985
47	p	0.40	0/693	0.47	0/935
48	q	0.43	0/836	0.49	0/1117
49	r	0.33	0/560	0.47	0/746
50	s	0.35	0/660	0.47	0/893
51	t	0.32	0/736	0.49	0/976
52	u	0.38	0/203	0.45	0/266
53	y	0.64	0/1832	0.93	1/2855 (0.0%)
54	C	0.27	0/1748	0.48	0/2354
55	z	0.43	0/1809	0.94	2/2819 (0.1%)
56	x	0.37	0/1315	1.00	3/2046 (0.1%)
All	All	0.96	10/160909 (0.0%)	0.85	105/240692 (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
6	G	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	71	C	N1-C6	131.97	2.16	1.37
32	a	71	C	N3-C4	115.18	2.14	1.33
32	a	71	C	C2-N3	103.78	2.18	1.35
32	a	71	C	C4-C5	94.47	2.18	1.43
32	a	71	C	C5-C6	93.90	2.09	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	71	C	N1-C2	82.58	2.22	1.40
32	a	64	G	C3'-O3'	16.79	1.65	1.42
32	a	102	G	C6-O6	-6.54	1.18	1.24
32	a	104	G	C8-N7	-5.16	1.27	1.30
32	a	104	G	N9-C4	5.01	1.42	1.38

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	x	46	G	C5-N7-C8	17.30	112.95	104.30
56	x	46	G	C4-C5-N7	13.07	116.03	110.80
1	A	2224	G	OP1-P-O3'	-12.77	77.11	105.20
32	a	71	C	C2-N3-C4	12.35	126.08	119.90
32	a	71	C	C6-N1-C2	12.00	125.10	120.30
32	a	104	G	N3-C4-N9	11.89	133.14	126.00
32	a	71	C	N1-C2-N3	-11.66	111.04	119.20
32	a	68	G	C5-N7-C8	11.52	110.06	104.30
32	a	102	G	C5-C6-N1	11.22	117.11	111.50
1	A	2883	A	OP2-P-O3'	-10.78	81.48	105.20
32	a	65	U	O5'-P-OP2	-10.60	96.16	105.70
1	A	2883	A	OP1-P-O3'	-10.33	82.47	105.20
32	a	68	G	N7-C8-N9	-10.27	107.97	113.10
32	a	71	C	N3-C4-C5	-10.08	117.87	121.90
32	a	67	C	N3-C4-C5	10.00	125.90	121.90
32	a	71	C	N1-C2-O2	9.88	124.83	118.90
32	a	104	G	N3-C4-C5	-9.76	123.72	128.60
32	a	76	C	C6-N1-C2	-9.44	116.52	120.30
1	A	2224	G	OP2-P-O3'	-9.04	85.30	105.20
32	a	104	G	C6-C5-N7	-7.93	125.64	130.40
32	a	68	G	C4-C5-N7	-7.59	107.76	110.80
32	a	63	C	N3-C4-C5	7.57	124.93	121.90
1	A	1092	C	C6-N1-C2	-7.45	117.32	120.30
1	A	2225	A	OP1-P-OP2	7.43	130.75	119.60
32	a	92	C	C6-N1-C1'	-7.35	111.98	120.80
32	a	153	C	N1-C2-O2	7.22	123.23	118.90
32	a	65	U	OP1-P-OP2	-7.12	108.92	119.60
32	a	104	G	C5-C6-O6	-7.08	124.35	128.60
15	T	18	ASP	C-N-CA	-7.00	104.19	121.70
1	A	2884	U	OP1-P-OP2	6.94	130.01	119.60
32	a	71	C	C4-C5-C6	6.94	120.87	117.40
32	a	65	U	O5'-P-OP1	-6.77	99.61	105.70
32	a	92	C	N3-C4-C5	6.73	124.59	121.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	104	G	C4-C5-C6	6.72	122.83	118.80
32	a	99	U	C2-N1-C1'	6.67	125.71	117.70
32	a	92	C	C2-N1-C1'	6.64	126.10	118.80
32	a	1397	C	N1-C2-O2	6.63	122.88	118.90
32	a	71	C	C6-N1-C1'	-6.59	112.89	120.80
32	a	153	C	C2-N1-C1'	6.58	126.04	118.80
32	a	67	C	N3-C4-N4	-6.58	113.40	118.00
1	A	1313	U	C2-N1-C1'	6.54	125.55	117.70
32	a	104	G	N1-C6-O6	6.51	123.81	119.90
32	a	68	G	C8-N9-C4	6.49	109.00	106.40
32	a	66	G	C6-C5-N7	6.40	134.24	130.40
32	a	68	G	O4'-C1'-N9	-6.40	103.08	108.20
1	A	2159	G	N3-C4-N9	-6.39	122.16	126.00
32	a	102	G	C8-N9-C4	6.38	108.95	106.40
32	a	266	G	P-O3'-C3'	6.37	127.34	119.70
1	A	847	U	C2-N1-C1'	6.33	125.30	117.70
32	a	102	G	N1-C6-O6	-6.31	116.11	119.90
1	A	1092	C	N3-C2-O2	-6.25	117.52	121.90
1	A	1092	C	C5-C6-N1	6.23	124.11	121.00
32	a	104	G	C4-N9-C1'	6.22	134.59	126.50
32	a	104	G	C8-N9-C1'	-6.17	118.98	127.00
32	a	1397	C	C2-N1-C1'	6.13	125.54	118.80
32	a	102	G	N9-C4-C5	-6.13	102.95	105.40
32	a	77	G	N3-C4-N9	6.07	129.64	126.00
32	a	76	C	C2-N1-C1'	6.04	125.44	118.80
32	a	102	G	C4-C5-N7	6.01	113.21	110.80
32	a	68	G	P-O3'-C3'	5.98	126.87	119.70
32	a	77	G	C5-C6-O6	-5.96	125.02	128.60
32	a	97	G	O4'-C1'-N9	5.92	112.94	108.20
32	a	97	G	N1-C2-N2	5.91	121.52	116.20
55	z	40	C	N3-C2-O2	-5.88	117.78	121.90
32	a	1535	C	C2-N1-C1'	5.83	125.21	118.80
32	a	1002	G	N3-C4-C5	5.81	131.50	128.60
32	a	104	G	N3-C2-N2	5.78	123.95	119.90
56	x	46	G	C6-C5-N7	-5.78	126.93	130.40
6	G	140	ILE	C-N-CA	-5.75	107.32	121.70
53	y	19	G	O4'-C1'-N9	-5.74	103.61	108.20
32	a	102	G	C4-C5-C6	-5.68	115.39	118.80
32	a	99	U	P-O3'-C3'	5.67	126.50	119.70
32	a	104	G	N9-C4-C5	-5.66	103.14	105.40
1	A	614(A)	U	N1-C2-O2	5.63	126.74	122.80
1	A	614(A)	U	N3-C2-O2	-5.59	118.29	122.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	1002	G	N3-C4-N9	-5.56	122.66	126.00
32	a	98	G	P-O3'-C3'	5.56	126.37	119.70
1	A	1092	C	N1-C2-O2	5.54	122.22	118.90
32	a	66	G	C4-C5-N7	-5.54	108.58	110.80
32	a	77	G	C6-C5-N7	-5.53	127.08	130.40
1	A	2159	G	N3-C4-C5	5.50	131.35	128.60
1	A	1775	U	C5-C4-O4	-5.45	122.63	125.90
1	A	2159	G	C4-N9-C1'	-5.43	119.44	126.50
55	z	39	U	C2-N1-C1'	5.42	124.20	117.70
32	a	76	C	N3-C2-O2	-5.42	118.11	121.90
1	A	1099	G	N3-C4-C5	5.42	131.31	128.60
1	A	1314	C	C2-N1-C1'	5.41	124.75	118.80
32	a	1532	U	OP2-P-O3'	5.40	117.07	105.20
32	a	67	C	C2-N3-C4	-5.39	117.20	119.90
1	A	1099	G	C5-C6-O6	5.39	131.83	128.60
32	a	91	C	N3-C4-N4	-5.39	114.23	118.00
32	a	153	C	O5'-P-OP1	-5.38	100.86	105.70
32	a	266	G	OP2-P-O3'	5.35	116.97	105.20
32	a	65	U	O4'-C1'-N1	-5.29	103.97	108.20
32	a	1397	C	N3-C2-O2	-5.27	118.21	121.90
32	a	63	C	C5-C4-N4	-5.25	116.52	120.20
1	A	1099	G	N3-C4-N9	-5.24	122.86	126.00
32	a	764	C	C6-N1-C2	5.23	122.39	120.30
1	A	1313	U	C6-N1-C1'	-5.15	113.99	121.20
32	a	64	G	N1-C2-N2	-5.10	111.61	116.20
32	a	153	C	C6-N1-C1'	-5.10	114.68	120.80
1	A	196	A	O4'-C1'-N9	5.04	112.23	108.20
1	A	2159	G	C8-N9-C1'	5.04	133.56	127.00
1	A	2173	A	O5'-P-OP1	-5.03	101.17	105.70
1	A	1224	C	O4'-C1'-N1	-5.02	104.18	108.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	G	95	ARG	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	273/275 (99%)	245 (90%)	28 (10%)	0	100	100
4	E	202/204 (99%)	188 (93%)	14 (7%)	0	100	100
5	F	201/203 (99%)	193 (96%)	7 (4%)	1 (0%)	25	60
6	G	179/181 (99%)	160 (89%)	19 (11%)	0	100	100
7	H	166/173 (96%)	152 (92%)	14 (8%)	0	100	100
8	I	144/146 (99%)	135 (94%)	9 (6%)	0	100	100
9	N	138/140 (99%)	127 (92%)	11 (8%)	0	100	100
10	O	120/122 (98%)	112 (93%)	8 (7%)	0	100	100
11	P	147/149 (99%)	135 (92%)	12 (8%)	0	100	100
12	Q	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
13	R	116/118 (98%)	112 (97%)	4 (3%)	0	100	100
14	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
15	T	129/131 (98%)	118 (92%)	11 (8%)	0	100	100
16	U	114/116 (98%)	112 (98%)	2 (2%)	0	100	100
17	V	99/101 (98%)	88 (89%)	11 (11%)	0	100	100
18	W	110/112 (98%)	97 (88%)	13 (12%)	0	100	100
19	X	93/95 (98%)	85 (91%)	8 (9%)	0	100	100
20	Y	105/107 (98%)	97 (92%)	8 (8%)	0	100	100
21	Z	185/187 (99%)	161 (87%)	24 (13%)	0	100	100
22	0	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
23	1	95/97 (98%)	90 (95%)	5 (5%)	0	100	100
24	2	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
25	3	57/59 (97%)	56 (98%)	1 (2%)	0	100	100
26	4	67/69 (97%)	55 (82%)	10 (15%)	2 (3%)	3	23
27	5	57/59 (97%)	53 (93%)	4 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	6	51/53 (96%)	46 (90%)	5 (10%)	0	100	100
29	7	46/48 (96%)	46 (100%)	0	0	100	100
30	8	62/64 (97%)	56 (90%)	6 (10%)	0	100	100
31	9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
33	b	229/231 (99%)	209 (91%)	20 (9%)	0	100	100
34	c	204/206 (99%)	185 (91%)	19 (9%)	0	100	100
35	d	206/208 (99%)	201 (98%)	5 (2%)	0	100	100
36	e	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
37	f	98/100 (98%)	85 (87%)	13 (13%)	0	100	100
38	g	153/155 (99%)	145 (95%)	8 (5%)	0	100	100
39	h	135/137 (98%)	123 (91%)	12 (9%)	0	100	100
40	i	124/126 (98%)	112 (90%)	12 (10%)	0	100	100
41	j	94/96 (98%)	82 (87%)	11 (12%)	1 (1%)	12	44
42	k	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	l	119/122 (98%)	107 (90%)	12 (10%)	0	100	100
44	m	112/114 (98%)	104 (93%)	8 (7%)	0	100	100
45	n	58/60 (97%)	57 (98%)	1 (2%)	0	100	100
46	o	86/88 (98%)	82 (95%)	4 (5%)	0	100	100
47	p	80/82 (98%)	73 (91%)	7 (9%)	0	100	100
48	q	97/99 (98%)	90 (93%)	7 (7%)	0	100	100
49	r	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
50	s	81/83 (98%)	75 (93%)	6 (7%)	0	100	100
51	t	96/98 (98%)	84 (88%)	12 (12%)	0	100	100
52	u	21/23 (91%)	21 (100%)	0	0	100	100
54	C	221/226 (98%)	199 (90%)	22 (10%)	0	100	100
All	All	5919/6028 (98%)	5464 (92%)	451 (8%)	4 (0%)	50	80

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
26	4	49	PHE
26	4	47	GLN
41	j	55	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	F	207	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	215/217 (99%)	214 (100%)	1 (0%)	86	93
4	E	164/165 (99%)	163 (99%)	1 (1%)	84	92
5	F	159/161 (99%)	156 (98%)	3 (2%)	52	76
6	G	142/155 (92%)	138 (97%)	4 (3%)	38	68
7	H	143/144 (99%)	142 (99%)	1 (1%)	81	92
8	I	108/122 (88%)	108 (100%)	0	100	100
9	N	118/119 (99%)	117 (99%)	1 (1%)	79	90
10	O	100/100 (100%)	99 (99%)	1 (1%)	73	87
11	P	115/116 (99%)	115 (100%)	0	100	100
12	Q	111/111 (100%)	110 (99%)	1 (1%)	75	89
13	R	101/101 (100%)	101 (100%)	0	100	100
14	S	85/87 (98%)	85 (100%)	0	100	100
15	T	113/115 (98%)	113 (100%)	0	100	100
16	U	93/93 (100%)	93 (100%)	0	100	100
17	V	80/82 (98%)	79 (99%)	1 (1%)	65	83
18	W	90/91 (99%)	89 (99%)	1 (1%)	70	86
19	X	77/77 (100%)	77 (100%)	0	100	100
20	Y	86/88 (98%)	84 (98%)	2 (2%)	45	72
21	Z	156/164 (95%)	155 (99%)	1 (1%)	84	92
22	0	61/62 (98%)	61 (100%)	0	100	100
23	1	81/82 (99%)	80 (99%)	1 (1%)	67	85
24	2	66/66 (100%)	66 (100%)	0	100	100
25	3	50/51 (98%)	49 (98%)	1 (2%)	50	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	4	54/62 (87%)	53 (98%)	1 (2%)	52	76
27	5	50/51 (98%)	49 (98%)	1 (2%)	50	75
28	6	50/51 (98%)	49 (98%)	1 (2%)	50	75
29	7	41/41 (100%)	39 (95%)	2 (5%)	21	54
30	8	54/54 (100%)	54 (100%)	0	100	100
31	9	34/34 (100%)	34 (100%)	0	100	100
33	b	187/199 (94%)	185 (99%)	2 (1%)	70	86
34	c	140/160 (88%)	139 (99%)	1 (1%)	81	92
35	d	172/180 (96%)	171 (99%)	1 (1%)	84	92
36	e	114/114 (100%)	113 (99%)	1 (1%)	75	89
37	f	85/90 (94%)	85 (100%)	0	100	100
38	g	119/126 (94%)	117 (98%)	2 (2%)	56	78
39	h	114/118 (97%)	114 (100%)	0	100	100
40	i	88/97 (91%)	86 (98%)	2 (2%)	45	72
41	j	68/86 (79%)	68 (100%)	0	100	100
42	k	83/86 (96%)	83 (100%)	0	100	100
43	l	96/102 (94%)	95 (99%)	1 (1%)	73	87
44	m	87/93 (94%)	86 (99%)	1 (1%)	70	86
45	n	49/49 (100%)	47 (96%)	2 (4%)	26	59
46	o	78/79 (99%)	77 (99%)	1 (1%)	65	83
47	p	68/71 (96%)	67 (98%)	1 (2%)	60	81
48	q	94/94 (100%)	94 (100%)	0	100	100
49	r	59/59 (100%)	59 (100%)	0	100	100
50	s	67/72 (93%)	67 (100%)	0	100	100
51	t	70/76 (92%)	68 (97%)	2 (3%)	37	67
52	u	18/18 (100%)	18 (100%)	0	100	100
54	C	177/178 (99%)	177 (100%)	0	100	100
All	All	4830/5009 (96%)	4788 (99%)	42 (1%)	74	89

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	157	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	E	85	ASN
5	F	38	ARG
5	F	44	ARG
5	F	169	ASN
6	G	36	LYS
6	G	47	LYS
6	G	136	ARG
6	G	153	ARG
7	H	97	ARG
9	N	48	MET
10	O	53	LYS
12	Q	59	ARG
17	V	13	ARG
18	W	11	ARG
20	Y	43	ASN
20	Y	92	ASN
21	Z	156	LYS
23	1	40	ARG
25	3	30	ARG
26	4	61	ARG
27	5	40	LYS
28	6	18	ARG
29	7	33	ARG
29	7	41	ARG
33	b	8	LYS
33	b	94	ASN
34	c	190	ARG
35	d	65	ARG
36	e	47	LYS
38	g	115	ARG
38	g	155	ARG
40	i	104	ARG
40	i	111	ARG
43	l	86	ARG
44	m	102	ARG
45	n	12	ARG
45	n	41	ARG
46	o	65	ARG
47	p	25	ARG
51	t	9	ASN
51	t	17	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61)

such sidechains are listed below:

Mol	Chain	Res	Type
3	D	87	ASN
3	D	96	HIS
3	D	116	GLN
3	D	253	GLN
4	E	85	ASN
4	E	137	HIS
4	E	159	HIS
7	H	74	ASN
8	I	54	GLN
8	I	105	HIS
9	N	69	GLN
10	O	3	GLN
11	P	9	ASN
11	P	27	HIS
12	Q	57	HIS
12	Q	141	GLN
15	T	43	GLN
15	T	58	ASN
16	U	117	GLN
19	X	82	GLN
20	Y	43	ASN
21	Z	34	ASN
21	Z	75	ASN
21	Z	151	HIS
23	1	56	GLN
24	2	65	ASN
28	6	29	ASN
33	b	40	HIS
33	b	94	ASN
33	b	113	HIS
33	b	135	GLN
33	b	140	HIS
33	b	212	GLN
34	c	6	HIS
34	c	108	ASN
34	c	176	HIS
35	d	119	GLN
35	d	125	HIS
36	e	20	GLN
36	e	78	HIS
37	f	32	ASN
37	f	73	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
38	g	28	ASN
38	g	56	GLN
38	g	68	ASN
38	g	86	GLN
38	g	109	ASN
41	j	69	ASN
43	l	80	HIS
44	m	77	ASN
44	m	106	ASN
46	o	28	GLN
46	o	53	HIS
47	p	16	HIS
47	p	65	GLN
48	q	26	GLN
50	s	69	HIS
50	s	83	HIS
51	t	9	ASN
54	C	101	GLN
54	C	188	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2853/2915 (97%)	634 (22%)	46 (1%)
2	B	119/120 (99%)	23 (19%)	0
32	a	1504/1521 (98%)	327 (21%)	0
53	y	76/77 (98%)	13 (17%)	0
55	z	75/76 (98%)	29 (38%)	0
56	x	54/55 (98%)	24 (44%)	0
All	All	4681/4764 (98%)	1050 (22%)	46 (0%)

All (1050) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	7	G
1	A	8	A
1	A	10	G
1	A	12	U
1	A	14	A
1	A	15	G
1	A	34	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	45	C
1	A	51	G
1	A	61	G
1	A	64	A
1	A	71	A
1	A	74	A
1	A	75	G
1	A	85	G
1	A	92	A
1	A	95	G
1	A	118	A
1	A	119	A
1	A	120	U
1	A	131	G
1	A	141	A
1	A	149	A
1	A	157	U
1	A	181	A
1	A	182	A
1	A	184	C
1	A	185	U
1	A	186	G
1	A	187	G
1	A	188	G
1	A	196	A
1	A	199	A
1	A	205	G
1	A	213	A
1	A	214	G
1	A	215	G
1	A	216	A
1	A	217	G
1	A	221	A
1	A	222	A
1	A	229	A
1	A	230	U
1	A	233	A
1	A	243	U
1	A	248	G
1	A	249	C
1	A	264	C
1	A	265	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	266	G
1	A	272(A)	A
1	A	272(J)	C
1	A	272(K)	U
1	A	272(L)	U
1	A	272(M)	G
1	A	272(N)	U
1	A	272(O)	C
1	A	272(X)	G
1	A	273(B)	U
1	A	273(C)	G
1	A	277	C
1	A	278	A
1	A	282	A
1	A	283	A
1	A	294	A
1	A	301	G
1	A	302	C
1	A	311	A
1	A	312	G
1	A	317	G
1	A	329	G
1	A	330	A
1	A	331	A
1	A	332	A
1	A	352	G
1	A	353	G
1	A	354	G
1	A	363(A)	G
1	A	363(G)	A
1	A	386	G
1	A	396	G
1	A	397	G
1	A	398	G
1	A	405	U
1	A	406	G
1	A	411	G
1	A	412	A
1	A	435	C
1	A	444	C
1	A	451	C
1	A	456	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	457	A
1	A	470	A
1	A	475	U
1	A	479	A
1	A	481	G
1	A	505	A
1	A	508	G
1	A	509	C
1	A	510	C
1	A	513	A
1	A	518	G
1	A	520	G
1	A	522	G
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	534	U
1	A	556	G
1	A	563	G
1	A	568	U
1	A	573	G
1	A	575	A
1	A	586	A
1	A	603	A
1	A	604	G
1	A	607	U
1	A	613	G
1	A	614(C)	G
1	A	614(D)	A
1	A	615	G
1	A	620	G
1	A	621	A
1	A	627	A
1	A	637	A
1	A	643	A
1	A	645	C
1	A	646	A
1	A	652(A)	C
1	A	652(C)	A
1	A	652(D)	G
1	A	652(V)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	653	A
1	A	668	G
1	A	669	G
1	A	675	A
1	A	677	A
1	A	686	G
1	A	695	G
1	A	715	G
1	A	717	G
1	A	727	A
1	A	730	C
1	A	734	A
1	A	736	C
1	A	749	C
1	A	752	A
1	A	753	C
1	A	774	A
1	A	775	G
1	A	776	G
1	A	777	A
1	A	782	A
1	A	784	A
1	A	785	G
1	A	789	A
1	A	792	G
1	A	805	G
1	A	806	C
1	A	812	C
1	A	827	U
1	A	828	U
1	A	831	G
1	A	847	U
1	A	854	G
1	A	857	C
1	A	859	G
1	A	860	U
1	A	869	G
1	A	872	A
1	A	878	A
1	A	880	G
1	A	884	C
1	A	885	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	886	C
1	A	887	A
1	A	889	C
1	A	890	A
1	A	893	C
1	A	894	C
1	A	896	A
1	A	900	A
1	A	901	A
1	A	910	A
1	A	914	C
1	A	917	A
1	A	932	G
1	A	941	A
1	A	945	A
1	A	946	G
1	A	958	U
1	A	959	A
1	A	961	C
1	A	973	A
1	A	974	G
1	A	975(A)	C
1	A	980	A
1	A	983	A
1	A	985	C
1	A	990	A
1	A	996	A
1	A	1008	C
1	A	1009	A
1	A	1012	U
1	A	1013	C
1	A	1018	C
1	A	1020	A
1	A	1022	G
1	A	1023	U
1	A	1026	U
1	A	1027	A
1	A	1033	U
1	A	1041	C
1	A	1042	G
1	A	1044	G
1	A	1045	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1046	A
1	A	1047	G
1	A	1052	C
1	A	1053	C
1	A	1054	A
1	A	1057	A
1	A	1058	G
1	A	1060	U
1	A	1063	G
1	A	1064	C
1	A	1065	U
1	A	1066	U
1	A	1067	A
1	A	1068	G
1	A	1069	A
1	A	1070	A
1	A	1071	G
1	A	1073	A
1	A	1074	G
1	A	1075	C
1	A	1076	C
1	A	1080	C
1	A	1082	U
1	A	1083	U
1	A	1084	A
1	A	1085	A
1	A	1086	A
1	A	1088	A
1	A	1089	G
1	A	1090	U
1	A	1091	G
1	A	1092	C
1	A	1096	A
1	A	1098	A
1	A	1102	C
1	A	1105	U
1	A	1108	U
1	A	1109	C
1	A	1111	A
1	A	1112	G
1	A	1114	G
1	A	1117	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1128	A
1	A	1130	U
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1144	G
1	A	1149	G
1	A	1155	A
1	A	1170	G
1	A	1171	G
1	A	1187	G
1	A	1204	A
1	A	1206	G
1	A	1211	U
1	A	1212	G
1	A	1220	A
1	A	1225	G
1	A	1227	G
1	A	1230	C
1	A	1236	G
1	A	1241	A
1	A	1248	G
1	A	1252	G
1	A	1253	A
1	A	1255	U
1	A	1256	G
1	A	1261	C
1	A	1265	A
1	A	1271	G
1	A	1272	A
1	A	1273	U
1	A	1274	A
1	A	1300	U
1	A	1301	A
1	A	1312	U
1	A	1314	C
1	A	1329	U
1	A	1343	G
1	A	1345	C
1	A	1359	A
1	A	1360	A
1	A	1363	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1364	G
1	A	1365	A
1	A	1366	A
1	A	1368	G
1	A	1380	G
1	A	1384	A
1	A	1385	G
1	A	1392	A
1	A	1395	A
1	A	1398	C
1	A	1403	C
1	A	1416	G
1	A	1417	C
1	A	1420	U
1	A	1421	G
1	A	1428	C
1	A	1445(A)	A
1	A	1450(A)	G
1	A	1453	U
1	A	1455	G
1	A	1459	G
1	A	1460	A
1	A	1465	G
1	A	1467	C
1	A	1471	A
1	A	1482	G
1	A	1490	A
1	A	1491	G
1	A	1493	C
1	A	1494	A
1	A	1495	A
1	A	1497	U
1	A	1498	C
1	A	1507	A
1	A	1508	A
1	A	1509(A)	C
1	A	1509(B)	A
1	A	1525	G
1	A	1530	C
1	A	1531	C
1	A	1533	G
1	A	1537	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1542	A
1	A	1543	C
1	A	1547	C
1	A	1558	A
1	A	1566	A
1	A	1569	A
1	A	1580	A
1	A	1583	A
1	A	1584	C
1	A	1586	A
1	A	1608	A
1	A	1609	A
1	A	1616	A
1	A	1618	A
1	A	1634	A
1	A	1640	C
1	A	1646	C
1	A	1648	C
1	A	1654	A
1	A	1674	G
1	A	1676	A
1	A	1700	A
1	A	1721	G
1	A	1722	A
1	A	1740	G
1	A	1746	G
1	A	1756	G
1	A	1760	A
1	A	1762	A
1	A	1763	G
1	A	1764	G
1	A	1773	A
1	A	1780	A
1	A	1784	A
1	A	1791	A
1	A	1800	C
1	A	1801	G
1	A	1804	C
1	A	1809	A
1	A	1810	A
1	A	1816	G
1	A	1829	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1835	G
1	A	1847	A
1	A	1848	A
1	A	1849	G
1	A	1859	A
1	A	1866	C
1	A	1876	A
1	A	1877	A
1	A	1878	G
1	A	1882	C
1	A	1890	A
1	A	1900	A
1	A	1906	G
1	A	1913	A
1	A	1914	C
1	A	1927	A
1	A	1929	G
1	A	1930	G
1	A	1936	A
1	A	1937	A
1	A	1938	A
1	A	1940	U
1	A	1950	G
1	A	1955	U
1	A	1963	U
1	A	1964	G
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	A
1	A	1972	A
1	A	1984	G
1	A	1993	U
1	A	1997	G
1	A	2016	U
1	A	2020	A
1	A	2023	G
1	A	2031	A
1	A	2032	G
1	A	2033	A
1	A	2034	U
1	A	2043	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2052	G
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2063	C
1	A	2069	G
1	A	2087	G
1	A	2088	G
1	A	2089	U
1	A	2090	G
1	A	2092	U
1	A	2093	G
1	A	2096	U
1	A	2097	C
1	A	2099	U
1	A	2103	C
1	A	2105	C
1	A	2107	C
1	A	2108	C
1	A	2110	G
1	A	2111	C
1	A	2112	G
1	A	2116	G
1	A	2117	A
1	A	2118	U
1	A	2119	A
1	A	2121	G
1	A	2126	A
1	A	2127	G
1	A	2129	C
1	A	2131	G
1	A	2132	U
1	A	2133	G
1	A	2134	A
1	A	2136	C
1	A	2144	U
1	A	2146	C
1	A	2148	G
1	A	2151	G
1	A	2158	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2159	G
1	A	2160	G
1	A	2161	C
1	A	2162	G
1	A	2165	G
1	A	2168	G
1	A	2169	A
1	A	2170	A
1	A	2172	U
1	A	2173	A
1	A	2176	A
1	A	2177	C
1	A	2178	C
1	A	2179	C
1	A	2180	U
1	A	2183	C
1	A	2185	C
1	A	2186	G
1	A	2187	G
1	A	2189	U
1	A	2192	G
1	A	2193	G
1	A	2194	G
1	A	2198	A
1	A	2199	A
1	A	2200	C
1	A	2201	C
1	A	2202	C
1	A	2203	U
1	A	2206	G
1	A	2207	G
1	A	2208	A
1	A	2218	U
1	A	2221	G
1	A	2224	G
1	A	2225	A
1	A	2226	C
1	A	2227	A
1	A	2231	C
1	A	2232	U
1	A	2233	U
1	A	2238	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2250	G
1	A	2251	OMG
1	A	2266	A
1	A	2268	A
1	A	2269	A
1	A	2273	A
1	A	2275	C
1	A	2279	G
1	A	2281	C
1	A	2283	C
1	A	2286	A
1	A	2287	A
1	A	2305	A
1	A	2308	G
1	A	2309	A
1	A	2319	G
1	A	2320	A
1	A	2321	G
1	A	2322	A
1	A	2325	G
1	A	2334	G
1	A	2336	A
1	A	2345	G
1	A	2347	C
1	A	2350	C
1	A	2354	G
1	A	2368	C
1	A	2383	G
1	A	2385	C
1	A	2402	C
1	A	2406	U
1	A	2407	G
1	A	2410	G
1	A	2414	G
1	A	2422	A
1	A	2424	C
1	A	2425	A
1	A	2428	G
1	A	2429	G
1	A	2430	A
1	A	2432	A
1	A	2435	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2439	A
1	A	2441	C
1	A	2445	G
1	A	2448	A
1	A	2469	A
1	A	2473	U
1	A	2474	C
1	A	2475	C
1	A	2476	A
1	A	2478	A
1	A	2480	C
1	A	2488	A
1	A	2491	U
1	A	2494	G
1	A	2498	C
1	A	2502	G
1	A	2504	U
1	A	2505	G
1	A	2506	U
1	A	2518	A
1	A	2535	G
1	A	2554	U
1	A	2556	C
1	A	2564	A
1	A	2566	A
1	A	2567	G
1	A	2572	A
1	A	2573	C
1	A	2578	G
1	A	2586	C
1	A	2602	A
1	A	2603	G
1	A	2609	U
1	A	2611	U
1	A	2612	C
1	A	2629	A
1	A	2630	G
1	A	2633	G
1	A	2636	U
1	A	2646	C
1	A	2656	U
1	A	2674	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2682	U
1	A	2689	U
1	A	2690	C
1	A	2702	U
1	A	2703	C
1	A	2712(B)	A
1	A	2713	A
1	A	2714	G
1	A	2726	U
1	A	2733	A
1	A	2744	G
1	A	2751	G
1	A	2757	A
1	A	2758	A
1	A	2765	A
1	A	2766	G
1	A	2778	A
1	A	2789	C
1	A	2808	U
1	A	2816	C
1	A	2817	G
1	A	2818	G
1	A	2820	A
1	A	2821	A
1	A	2831	G
1	A	2833	G
1	A	2834	G
1	A	2835	A
1	A	2836	U
1	A	2839	G
1	A	2849	U
1	A	2852	G
1	A	2857	G
1	A	2872	G
1	A	2879	C
1	A	2884	U
1	A	2886	G
1	A	2889	C
1	A	2894	G
2	B	2	C
2	B	8	U
2	B	9	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	12	C
2	B	13	A
2	B	14	U
2	B	15	A
2	B	17	C
2	B	24	G
2	B	35	U
2	B	37	C
2	B	42	C
2	B	56	G
2	B	58	A
2	B	63	G
2	B	67	G
2	B	73	A
2	B	85	G
2	B	89	G
2	B	108	U
2	B	110	G
2	B	116	G
2	B	117	G
32	a	7	G
32	a	9	G
32	a	31	G
32	a	32	A
32	a	36	C
32	a	39	G
32	a	47	C
32	a	48	C
32	a	51	A
32	a	61	G
32	a	63	C
32	a	64	G
32	a	66	G
32	a	67	C
32	a	68	G
32	a	69	G
32	a	70	G
32	a	71	C
32	a	72	C
32	a	73	G
32	a	76	C
32	a	77	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	79	G
32	a	80	G
32	a	88	A
32	a	89	C
32	a	92	C
32	a	93	G
32	a	96	U
32	a	97	G
32	a	98	G
32	a	99	U
32	a	100	C
32	a	101	A
32	a	102	G
32	a	103	C
32	a	104	G
32	a	105	G
32	a	106	C
32	a	116	A
32	a	119	A
32	a	121	C
32	a	122	G
32	a	129(B)	G
32	a	131	C
32	a	144	G
32	a	147	G
32	a	148	G
32	a	150	C
32	a	154	C
32	a	163	C
32	a	170	U
32	a	171	A
32	a	172	A
32	a	173	U
32	a	174	C
32	a	182	U
32	a	189(G)	U
32	a	192	U
32	a	195	A
32	a	197	A
32	a	200	G
32	a	202	U
32	a	203	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	216	G
32	a	217	C
32	a	221	C
32	a	222	U
32	a	231	G
32	a	247	G
32	a	251	G
32	a	266	G
32	a	267	C
32	a	279	A
32	a	289	G
32	a	298	A
32	a	306	G
32	a	321	A
32	a	328	C
32	a	329	A
32	a	330	C
32	a	332	G
32	a	347	G
32	a	351	G
32	a	352	C
32	a	353	A
32	a	354	G
32	a	367	U
32	a	372	C
32	a	373	A
32	a	381	C
32	a	382	A
32	a	389	A
32	a	392	G
32	a	397	A
32	a	398	C
32	a	406	G
32	a	407	G
32	a	412	A
32	a	413	G
32	a	414	A
32	a	423	G
32	a	428	G
32	a	429	U
32	a	430	A
32	a	439	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	442	C
32	a	443	C
32	a	452	A
32	a	461	A
32	a	470	C
32	a	482	A
32	a	484	G
32	a	485	G
32	a	496	A
32	a	498	U
32	a	506	G
32	a	509	A
32	a	510	A
32	a	511	C
32	a	518	C
32	a	521	G
32	a	524	G
32	a	527	7MG
32	a	531	U
32	a	532	A
32	a	533	A
32	a	536	C
32	a	547	A
32	a	564	C
32	a	571	U
32	a	572	A
32	a	573	A
32	a	575	G
32	a	576	G
32	a	577	G
32	a	579	G
32	a	582	U
32	a	596	C
32	a	618	C
32	a	630	G
32	a	632	A
32	a	642	A
32	a	653	A
32	a	660	G
32	a	665	A
32	a	687	A
32	a	688	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	690	G
32	a	702	A
32	a	703	G
32	a	721	G
32	a	723	U
32	a	724	G
32	a	731	G
32	a	737	A
32	a	749	C
32	a	755	G
32	a	759	A
32	a	777	A
32	a	790	A
32	a	793	U
32	a	794	A
32	a	815	A
32	a	816	A
32	a	817	C
32	a	819	A
32	a	828	A
32	a	840	C
32	a	841	U
32	a	851	G
32	a	864	A
32	a	872	A
32	a	874	G
32	a	876	G
32	a	902	G
32	a	914	A
32	a	926	G
32	a	927	G
32	a	931	C
32	a	934	C
32	a	935	A
32	a	940	C
32	a	945	G
32	a	955	U
32	a	956	U
32	a	957	U
32	a	959	A
32	a	960	U
32	a	961	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	968	A
32	a	969	A
32	a	971	G
32	a	974	A
32	a	975	A
32	a	976	G
32	a	977	A
32	a	989	C
32	a	992	U
32	a	993	G
32	a	994	A
32	a	997	U
32	a	1001(B)	G
32	a	1002	G
32	a	1003	G
32	a	1004	A
32	a	1005	A
32	a	1006	C
32	a	1015	A
32	a	1020	U
32	a	1022	G
32	a	1023	G
32	a	1024	G
32	a	1025	U
32	a	1026	G
32	a	1028	C
32	a	1030(B)	G
32	a	1030(C)	C
32	a	1036	G
32	a	1037	C
32	a	1041	A
32	a	1043	C
32	a	1044	A
32	a	1045	C
32	a	1065	U
32	a	1066	C
32	a	1068	G
32	a	1081	G
32	a	1085	U
32	a	1086	U
32	a	1092	A
32	a	1094	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1095	U
32	a	1101	A
32	a	1108	G
32	a	1117	G
32	a	1118	C
32	a	1125	U
32	a	1129	C
32	a	1130	A
32	a	1136	U
32	a	1137	C
32	a	1139	G
32	a	1140	C
32	a	1152	A
32	a	1157	A
32	a	1158	C
32	a	1159	U
32	a	1160	G
32	a	1171	G
32	a	1179	A
32	a	1183	A
32	a	1196	U
32	a	1197	G
32	a	1200	C
32	a	1210	C
32	a	1211	U
32	a	1212	U
32	a	1213	A
32	a	1214	C
32	a	1220	G
32	a	1221	G
32	a	1224	G
32	a	1225	A
32	a	1226	C
32	a	1227	A
32	a	1228	C
32	a	1236	A
32	a	1238	A
32	a	1250	A
32	a	1256	A
32	a	1257	U
32	a	1258	G
32	a	1260	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1261	A
32	a	1279	A
32	a	1281	U
32	a	1282	C
32	a	1287	A
32	a	1290	G
32	a	1300	G
32	a	1301	U
32	a	1302	U
32	a	1305	G
32	a	1306	A
32	a	1320	C
32	a	1323	G
32	a	1338	G
32	a	1340	A
32	a	1346	A
32	a	1347	G
32	a	1363(A)	C
32	a	1363(B)	A
32	a	1364	U
32	a	1378	C
32	a	1379	G
32	a	1397	C
32	a	1398	A
32	a	1404	5MC
32	a	1419	G
32	a	1428	A
32	a	1442(A)	G
32	a	1442(B)	G
32	a	1442(C)	A
32	a	1447	A
32	a	1452	C
32	a	1457	G
32	a	1492	A
32	a	1500	A
32	a	1503	A
32	a	1504	G
32	a	1506	U
32	a	1517	G
32	a	1524	C
32	a	1529	G
32	a	1530	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1531	A
32	a	1532	U
32	a	1533	C
32	a	1534	A
32	a	1535	C
32	a	1536	C
32	a	1537	U
32	a	1539	C
32	a	1540	U
32	a	1541	U
32	a	1542	G
53	y	2	G
53	y	8	U
53	y	10	G
53	y	16	C
53	y	17(B)	C
53	y	20	U
53	y	46	G
53	y	47	U
53	y	48	C
53	y	49	G
53	y	61	C
53	y	75	C
53	y	76	A
55	z	16	U
55	z	17	C
55	z	19	G
55	z	21	A
55	z	22	G
55	z	23	A
55	z	24	G
55	z	27	G
55	z	28	G
55	z	29	G
55	z	39	U
55	z	41	C
55	z	42	C
55	z	43	C
55	z	46	G
55	z	47	U
55	z	48	C
55	z	49	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
55	z	54	U
55	z	55	U
55	z	56	C
55	z	57	G
55	z	58	A
55	z	59	U
55	z	61	C
55	z	70	G
55	z	71	G
55	z	74	C
55	z	76	A
56	x	2	A
56	x	3	A
56	x	6	A
56	x	7	A
56	x	8	A
56	x	9	U
56	x	10	A
56	x	11	A
56	x	12	A
56	x	17	U
56	x	18	U
56	x	19	U
56	x	21	G
56	x	22	U
56	x	23	G
56	x	26	C
56	x	28	G
56	x	30	C
56	x	31	A
56	x	38	A
56	x	41	C
56	x	42	G
56	x	45	C
56	x	46	G

All (46) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	68	G
1	A	70	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	98	G
1	A	99	U
1	A	102	G
1	A	195	A
1	A	214	G
1	A	215	G
1	A	266	G
1	A	272(M)	G
1	A	277	C
1	A	532	A
1	A	752	A
1	A	784	A
1	A	840	C
1	A	856	C
1	A	900	A
1	A	954	G
1	A	959	A
1	A	1053	C
1	A	1056	G
1	A	1057	A
1	A	1065	U
1	A	1067	A
1	A	1210	A
1	A	1240	U
1	A	1379	A
1	A	1491	G
1	A	1493	C
1	A	1889	A
1	A	1992	G
1	A	2126	A
1	A	2133	G
1	A	2171	A
1	A	2172	U
1	A	2201	C
1	A	2321	G
1	A	2438	U
1	A	2601	C
1	A	2602	A
1	A	2689	U
1	A	2756	U
1	A	2816	C
1	A	2817	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	2832	U

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

24 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
32	5MC	a	1407	32	19,22,23	1.47	3 (15%)	26,32,35	1.26	2 (7%)
32	MA6	a	1519	32	19,26,27	0.87	0	18,38,41	2.28	7 (38%)
32	5MC	a	1400	32	19,22,23	1.44	3 (15%)	26,32,35	1.20	2 (7%)
32	5MC	a	967	32	19,22,23	1.44	3 (15%)	26,32,35	1.14	2 (7%)
32	7MG	a	527	32	23,26,27	1.35	4 (17%)	27,39,42	2.71	7 (25%)
32	PSU	a	516	32	18,21,22	1.45	5 (27%)	21,30,33	2.19	5 (23%)
1	PSU	A	2605	1	18,21,22	1.45	4 (22%)	21,30,33	2.25	4 (19%)
32	MA6	a	1518	32	19,26,27	0.80	0	18,38,41	2.22	7 (38%)
32	UR3	a	1498	32	19,22,23	0.94	2 (10%)	26,32,35	1.76	3 (11%)
1	PSU	A	1911	1	18,21,22	1.40	3 (16%)	21,30,33	2.19	4 (19%)
1	5MC	A	1942	1	19,22,23	1.41	3 (15%)	26,32,35	1.17	2 (7%)
32	5MC	a	1404	32	19,22,23	1.51	3 (15%)	26,32,35	1.25	3 (11%)
43	0TD	l	92	43	8,9,10	2.21	1 (12%)	6,11,13	1.20	0
32	2MG	a	1207	32	18,26,27	0.96	1 (5%)	16,38,41	1.60	5 (31%)
1	2MU	A	2552	1	19,22,24	1.37	4 (21%)	25,31,36	2.22	6 (24%)
32	M2G	a	966	32	20,27,28	1.25	3 (15%)	19,40,43	1.17	2 (10%)
32	4OC	a	1402	32	20,23,24	0.77	1 (5%)	25,32,35	0.93	0
1	5MU	A	1915	1	19,22,23	1.42	5 (26%)	27,32,35	2.44	9 (33%)
1	5MC	A	1962	1	19,22,23	1.42	3 (15%)	26,32,35	1.25	2 (7%)
1	PSU	A	1917	1	18,21,22	1.39	3 (16%)	21,30,33	2.11	5 (23%)
1	2MA	A	2503	1	17,25,26	1.07	1 (5%)	16,37,40	1.33	3 (18%)
1	OMG	A	2251	1,53	19,26,27	0.97	1 (5%)	21,38,41	1.06	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	4OC	A	1920	1	19,22,24	0.81	1 (5%)	25,31,35	0.85	0
1	5MU	A	1939	1	19,22,23	1.37	3 (15%)	27,32,35	2.35	6 (22%)

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
32	5MC	a	1407	32	-	0/7/25/26	0/2/2/2
32	MA6	a	1519	32	-	3/7/29/30	0/3/3/3
32	5MC	a	1400	32	-	2/7/25/26	0/2/2/2
32	5MC	a	967	32	-	0/7/25/26	0/2/2/2
32	7MG	a	527	32	-	3/7/37/38	0/3/3/3
32	PSU	a	516	32	-	0/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
32	MA6	a	1518	32	-	0/7/29/30	0/3/3/3
32	UR3	a	1498	32	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	5MC	A	1942	1	-	0/7/25/26	0/2/2/2
32	5MC	a	1404	32	-	1/7/25/26	0/2/2/2
43	0TD	l	92	43	-	4/7/12/14	-
32	2MG	a	1207	32	-	0/5/27/28	0/3/3/3
1	2MU	A	2552	1	-	0/9/27/28	0/2/2/2
32	M2G	a	966	32	-	0/7/29/30	0/3/3/3
32	4OC	a	1402	32	-	0/9/29/30	0/2/2/2
1	5MU	A	1915	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	1	-	1/3/25/26	0/3/3/3
1	OMG	A	2251	1,53	-	2/5/27/28	0/3/3/3
1	4OC	A	1920	1	-	0/9/27/30	0/2/2/2
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	1404	5MC	C5-C4	5.05	1.47	1.44
32	a	1407	5MC	C5-C4	5.03	1.47	1.44
43	l	92	0TD	CB-CA	-4.99	1.53	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1942	5MC	C5-C4	4.86	1.47	1.44
32	a	967	5MC	C5-C4	4.86	1.47	1.44
1	A	1962	5MC	C5-C4	4.80	1.47	1.44
32	a	1400	5MC	C5-C4	4.79	1.47	1.44
32	a	527	7MG	C4-N9	-3.65	1.33	1.37
1	A	2605	PSU	C4-N3	-3.33	1.32	1.38
32	a	966	M2G	C2-N3	3.30	1.35	1.30
1	A	1911	PSU	C4-N3	-3.21	1.32	1.38
1	A	2552	2MU	C4-N3	-3.14	1.33	1.38
1	A	1939	5MU	C4-N3	-3.10	1.33	1.38
1	A	1939	5MU	C6-N1	-3.08	1.32	1.38
1	A	1917	PSU	C4-N3	-3.02	1.33	1.38
32	a	516	PSU	C4-N3	-2.99	1.33	1.38
32	a	527	7MG	C5-C4	2.95	1.46	1.37
32	a	966	M2G	C6-N1	-2.92	1.33	1.37
32	a	1407	5MC	C6-N1	-2.91	1.33	1.38
1	A	2251	OMG	C6-N1	-2.89	1.33	1.37
1	A	1915	5MU	C4-N3	-2.89	1.33	1.38
32	a	1404	5MC	C6-N1	-2.87	1.33	1.38
1	A	1962	5MC	C6-N1	-2.84	1.33	1.38
32	a	967	5MC	C6-N1	-2.74	1.33	1.38
32	a	1207	2MG	C6-N1	-2.73	1.33	1.37
32	a	527	7MG	C6-N1	-2.68	1.33	1.38
32	a	1400	5MC	C6-N1	-2.66	1.33	1.38
1	A	1942	5MC	C6-N1	-2.65	1.33	1.38
1	A	2552	2MU	C2-N3	-2.64	1.33	1.38
1	A	1939	5MU	C2-N3	-2.60	1.33	1.38
1	A	1915	5MU	C2-N1	2.59	1.42	1.38
32	a	516	PSU	C6-C5	2.56	1.38	1.35
1	A	1917	PSU	C6-C5	2.56	1.38	1.35
32	a	1400	5MC	C6-C5	2.55	1.38	1.34
1	A	2605	PSU	C2-N3	-2.54	1.33	1.37
1	A	1915	5MU	C6-N1	-2.53	1.33	1.38
32	a	1404	5MC	C6-C5	2.51	1.38	1.34
1	A	2605	PSU	C6-C5	2.49	1.38	1.35
1	A	1915	5MU	C2-N3	-2.40	1.33	1.38
1	A	2503	2MA	C6-N1	-2.39	1.33	1.37
1	A	1911	PSU	C6-C5	2.37	1.37	1.35
32	a	967	5MC	C6-C5	2.34	1.38	1.34
1	A	1911	PSU	C2-N3	-2.28	1.33	1.37
1	A	1962	5MC	C6-C5	2.25	1.38	1.34
32	a	516	PSU	O4'-C1'	-2.22	1.40	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	516	PSU	C2-N3	-2.18	1.33	1.37
32	a	1498	UR3	C5-C4	-2.16	1.38	1.43
32	a	1407	5MC	C6-C5	2.16	1.38	1.34
32	a	1498	UR3	C6-N1	-2.15	1.33	1.38
32	a	527	7MG	C5-N7	-2.15	1.32	1.35
1	A	2552	2MU	C6-N1	-2.15	1.33	1.38
1	A	1942	5MC	C6-C5	2.14	1.38	1.34
1	A	1917	PSU	C2-N3	-2.14	1.33	1.37
32	a	966	M2G	C2-N2	2.13	1.39	1.35
1	A	1915	5MU	C6-C5	2.10	1.38	1.34
1	A	2605	PSU	C2-N1	-2.08	1.34	1.36
32	a	516	PSU	C2-N1	-2.05	1.34	1.36
32	a	1402	4OC	C6-N1	-2.02	1.33	1.38
1	A	1920	4OC	C6-N1	-2.02	1.33	1.38
1	A	2552	2MU	C5-C4	2.00	1.48	1.43

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	527	7MG	N9-C4-N3	9.30	139.09	125.46
32	a	1498	UR3	C4-N3-C2	-7.06	118.90	124.58
1	A	2605	PSU	N1-C2-N3	6.90	122.45	115.17
32	a	516	PSU	N1-C2-N3	6.80	122.34	115.17
1	A	1911	PSU	N1-C2-N3	6.68	122.21	115.17
1	A	1917	PSU	N1-C2-N3	6.52	122.05	115.17
32	a	527	7MG	N9-C8-N7	-5.88	95.05	103.37
1	A	1939	5MU	C4-N3-C2	-5.69	119.88	127.34
32	a	527	7MG	C5-C4-N3	-5.44	117.92	128.13
1	A	2552	2MU	C4-N3-C2	-5.30	120.03	126.61
1	A	1915	5MU	C4-N3-C2	-5.16	120.57	127.34
1	A	1939	5MU	O4-C4-C5	-5.08	119.11	124.92
1	A	1939	5MU	C5-C4-N3	5.06	119.72	115.32
1	A	2552	2MU	N3-C2-N1	5.04	121.45	114.89
1	A	1915	5MU	C5-C4-N3	5.00	119.67	115.32
1	A	2605	PSU	C4-N3-C2	-4.85	119.69	126.37
1	A	2552	2MU	C2'-C1'-N1	-4.85	105.04	114.24
32	a	1518	MA6	C2-N1-C6	4.82	121.57	116.84
1	A	1911	PSU	C4-N3-C2	-4.75	119.83	126.37
1	A	1939	5MU	N3-C2-N1	4.72	121.04	114.89
1	A	1939	5MU	C5-C6-N1	-4.67	118.24	123.31
1	A	1915	5MU	N3-C2-N1	4.61	120.89	114.89
32	a	1519	MA6	C2-N1-C6	4.57	121.32	116.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1915	5MU	C1'-N1-C6	-4.54	113.68	121.15
32	a	1407	5MC	C5-C6-N1	-4.42	118.51	123.31
1	A	1915	5MU	C1'-N1-C2	4.41	125.51	117.59
32	a	1519	MA6	C10-N6-C6	-4.40	107.27	119.40
32	a	516	PSU	C4-N3-C2	-4.39	120.33	126.37
1	A	1917	PSU	C4-N3-C2	-4.37	120.35	126.37
32	a	1518	MA6	C9-N6-C6	-4.29	107.56	119.40
1	A	1962	5MC	C5-C6-N1	-4.27	118.67	123.31
32	a	1404	5MC	C5-C6-N1	-4.26	118.69	123.31
32	a	527	7MG	C2-N3-C4	4.24	119.59	112.30
1	A	1915	5MU	O4-C4-C5	-4.13	120.19	124.92
1	A	1942	5MC	C5-C6-N1	-4.05	118.92	123.31
32	a	1519	MA6	C9-N6-C6	-3.91	108.61	119.40
32	a	1400	5MC	C5-C6-N1	-3.85	119.13	123.31
32	a	967	5MC	C5-C6-N1	-3.83	119.15	123.31
32	a	1519	MA6	N3-C2-N1	-3.82	123.49	128.67
32	a	516	PSU	O2-C2-N1	-3.79	118.88	122.79
32	a	1518	MA6	N3-C2-N1	-3.62	123.77	128.67
1	A	1917	PSU	O2-C2-N1	-3.54	119.13	122.79
1	A	1911	PSU	O2-C2-N1	-3.51	119.17	122.79
1	A	2552	2MU	C5-C4-N3	3.46	119.65	114.80
1	A	2605	PSU	O2-C2-N1	-3.46	119.22	122.79
32	a	1498	UR3	C5-C4-N3	3.45	119.59	115.04
32	a	1518	MA6	N1-C6-N6	3.45	120.82	116.83
1	A	2503	2MA	C4-N3-C2	-3.42	120.68	123.30
1	A	2552	2MU	O2-C2-N1	-3.37	118.41	122.80
1	A	1915	5MU	C5-C6-N1	-3.36	119.67	123.31
32	a	1518	MA6	C10-N6-C6	-3.35	110.16	119.40
1	A	1939	5MU	O2-C2-N1	-3.19	118.64	122.80
32	a	1207	2MG	N2-C2-N3	-2.94	116.77	120.51
32	a	1207	2MG	N1-C2-N2	2.83	119.45	116.56
32	a	1207	2MG	C8-N7-C5	2.80	107.31	102.55
1	A	2552	2MU	O4-C4-C5	-2.80	120.34	125.16
32	a	1519	MA6	N1-C6-N6	2.78	120.04	116.83
1	A	1911	PSU	C5-C6-N1	-2.77	118.30	122.14
32	a	1207	2MG	CM2-N2-C2	-2.76	117.71	123.65
1	A	2605	PSU	C5-C6-N1	-2.76	118.31	122.14
32	a	1400	5MC	C5-C4-N3	-2.70	118.98	121.75
32	a	527	7MG	C5-C6-N1	2.69	115.67	110.94
1	A	2503	2MA	C8-N7-C5	2.66	107.08	102.55
1	A	2251	OMG	C8-N7-C5	2.63	107.02	102.55
1	A	1915	5MU	O2-C2-N3	-2.62	116.65	121.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	966	M2G	C8-N7-C5	2.62	107.02	102.55
32	a	527	7MG	C5-C4-N9	-2.62	102.98	106.33
32	a	1519	MA6	C4-C5-N7	-2.54	106.65	109.34
32	a	1404	5MC	C5-C4-N3	-2.53	119.16	121.75
32	a	1519	MA6	C10-N6-C9	-2.41	108.45	116.18
1	A	1962	5MC	C5-C4-N3	-2.41	119.29	121.75
1	A	1917	PSU	C5-C6-N1	-2.37	118.84	122.14
32	a	967	5MC	C5-C4-N3	-2.34	119.35	121.75
32	a	516	PSU	O4'-C1'-C2'	2.34	108.39	105.15
1	A	2503	2MA	C5-C6-N1	2.28	118.38	114.12
32	a	516	PSU	C5-C6-N1	-2.25	119.02	122.14
1	A	1915	5MU	C5M-C5-C4	2.24	121.17	118.78
1	A	1917	PSU	O4'-C1'-C2'	2.18	108.17	105.15
1	A	2251	OMG	C5-C6-N1	2.16	118.18	114.07
32	a	1404	5MC	O2-C2-N3	-2.13	118.98	122.33
32	a	1518	MA6	C4-C5-N7	-2.11	107.11	109.34
32	a	1407	5MC	C5-C4-N3	-2.11	119.60	121.75
32	a	527	7MG	O6-C6-C5	-2.10	122.46	127.62
32	a	1518	MA6	C10-N6-C9	-2.10	109.44	116.18
32	a	1207	2MG	C5-C6-N1	2.10	118.07	114.07
32	a	966	M2G	C5-C6-N1	2.06	117.99	114.07
1	A	1942	5MC	C5-C4-N3	-2.05	119.65	121.75
32	a	1498	UR3	C3U-N3-C2	2.00	120.82	117.33

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1915	5MU	O4'-C1'-N1-C2
1	A	1915	5MU	O4'-C1'-N1-C6
32	a	527	7MG	C3'-C4'-C5'-O5'
32	a	1519	MA6	O4'-C4'-C5'-O5'
43	l	92	0TD	O-C-CA-CB
43	l	92	0TD	CA-CB-SB-CSB
32	a	527	7MG	O4'-C4'-C5'-O5'
32	a	1519	MA6	C3'-C4'-C5'-O5'
1	A	2251	OMG	O4'-C4'-C5'-O5'
1	A	2251	OMG	C3'-C4'-C5'-O5'
32	a	1400	5MC	O4'-C4'-C5'-O5'
32	a	527	7MG	C4'-C5'-O5'-P
43	l	92	0TD	CG-CB-SB-CSB
43	l	92	0TD	SB-CB-CG-OD1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
32	a	1519	MA6	C4'-C5'-O5'-P
32	a	1400	5MC	C3'-C4'-C5'-O5'
32	a	1404	5MC	C4'-C5'-O5'-P
1	A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	SF4	d	301	35	0,12,12	-	-	-		

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
58	SF4	d	301	35	-	-	0/6/5/5

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
32	a	4
7	H	3
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1000:U	O3'	1001(A):A	P	4.17
1	a	1029:C	O3'	1030(A):C	P	4.08
1	A	2103:C	O3'	2104:G	P	3.60
1	A	2180:U	O3'	2181:G	P	3.49
1	H	3:ARG	C	4:ILE	N	3.23
1	a	1030(E):A	O3'	1031:G	P	3.19
1	H	119:GLU	C	120:GLY	N	3.16
1	H	137:ASP	C	138:LYS	N	3.09
1	a	64:G	O3'	65:U	P	2.22

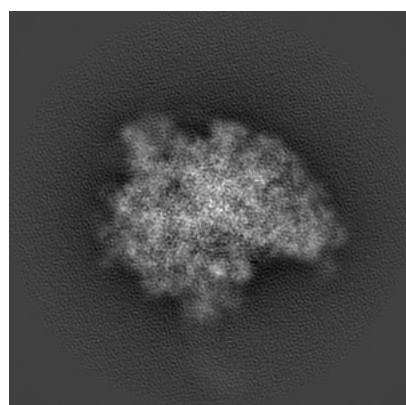
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8597. These allow visual inspection of the internal detail of the map and identification of artifacts.

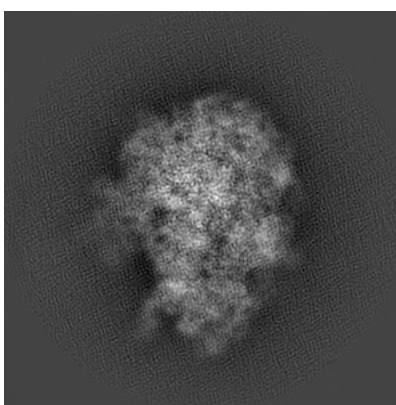
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

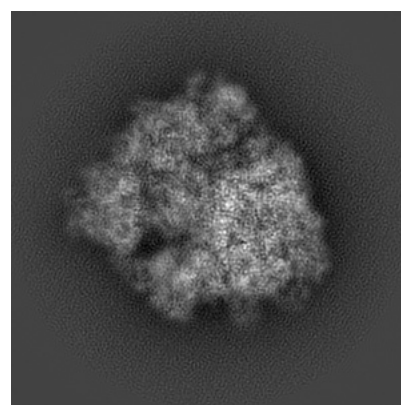
6.1.1 Primary map



X



Y

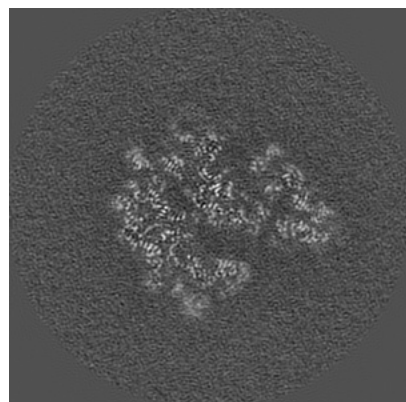


Z

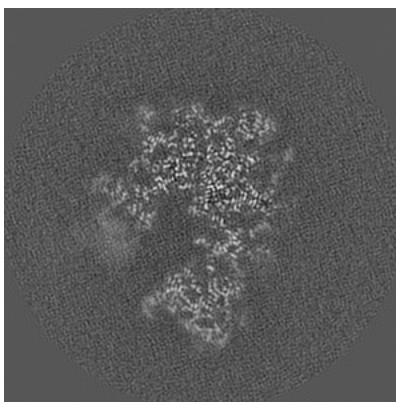
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

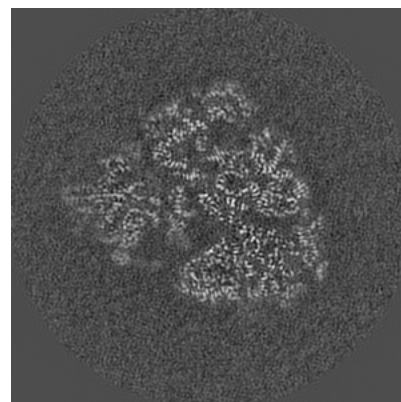
6.2.1 Primary map



X Index: 192



Y Index: 192

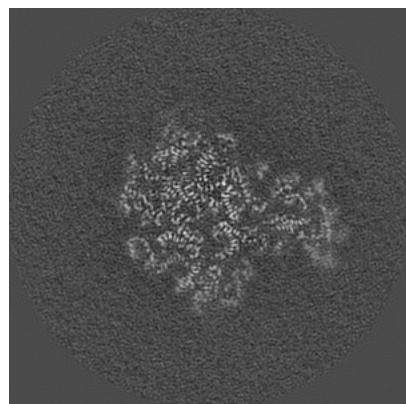


Z Index: 192

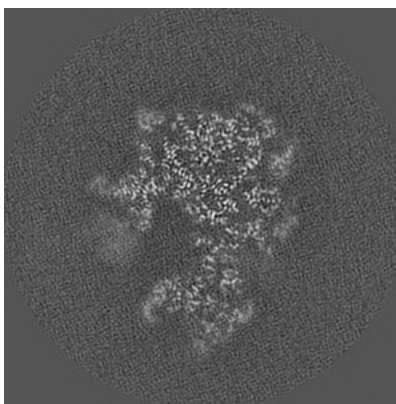
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

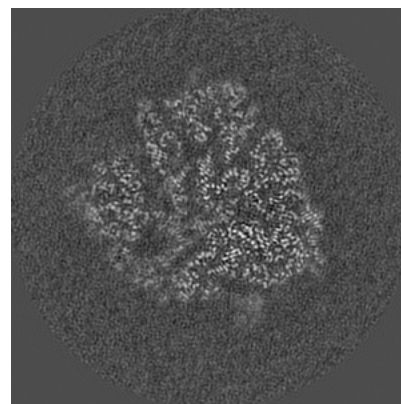
6.3.1 Primary map



X Index: 203



Y Index: 197

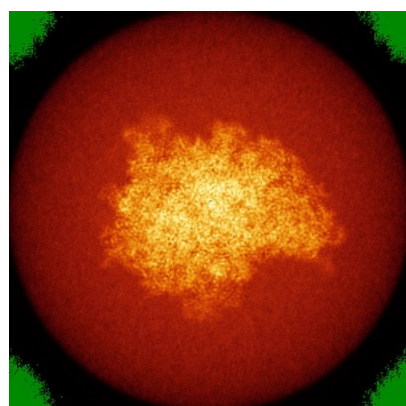


Z Index: 184

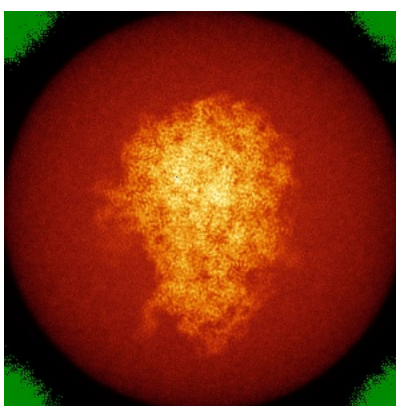
The images above show the largest variance slices of the map in three orthogonal directions.

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

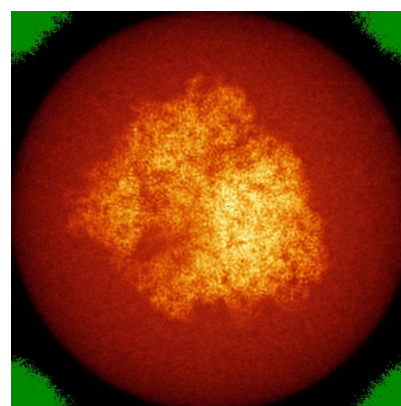
6.4.1 Primary map



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



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

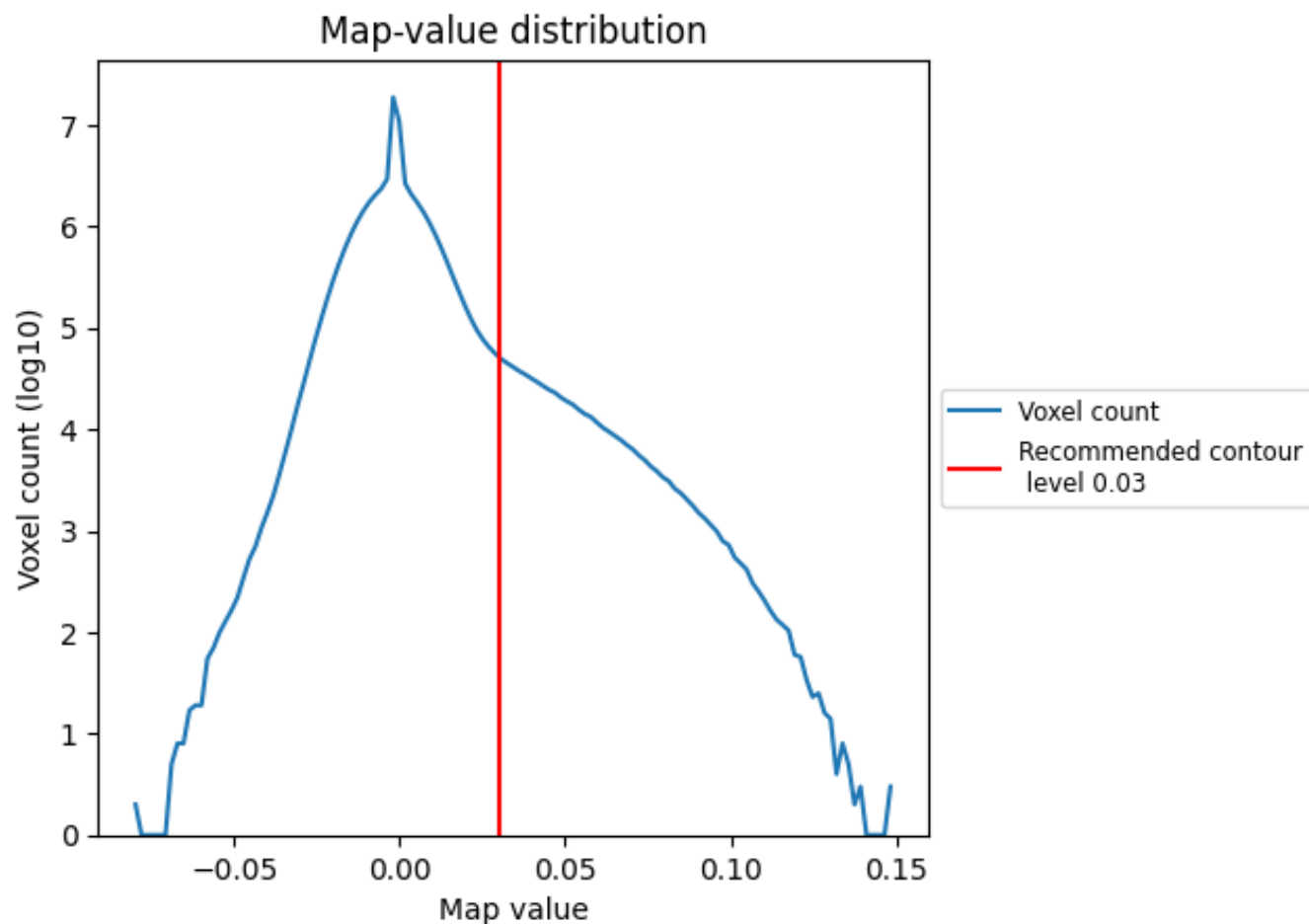
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

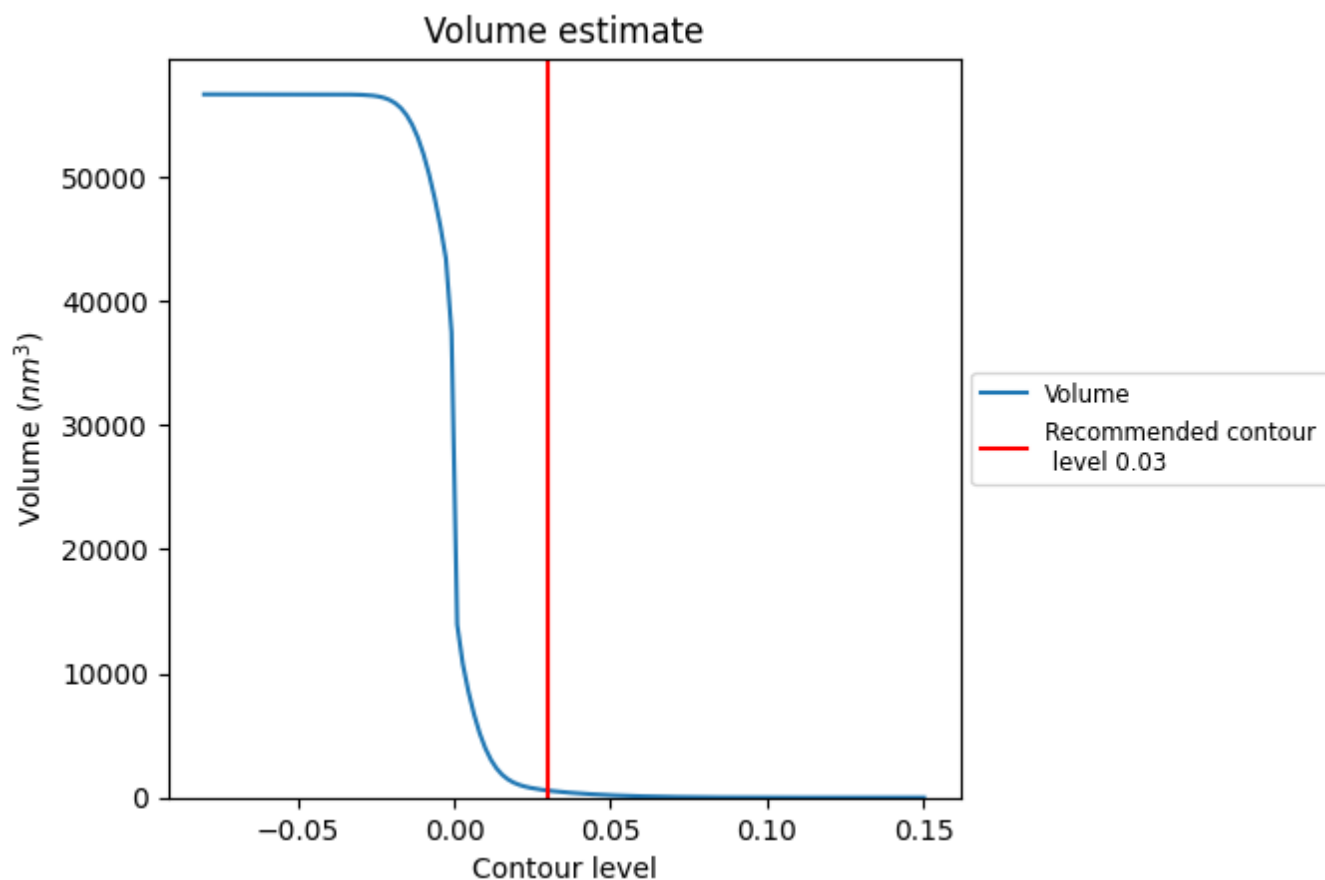
This section contains the results of statistical analysis of the map.

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.

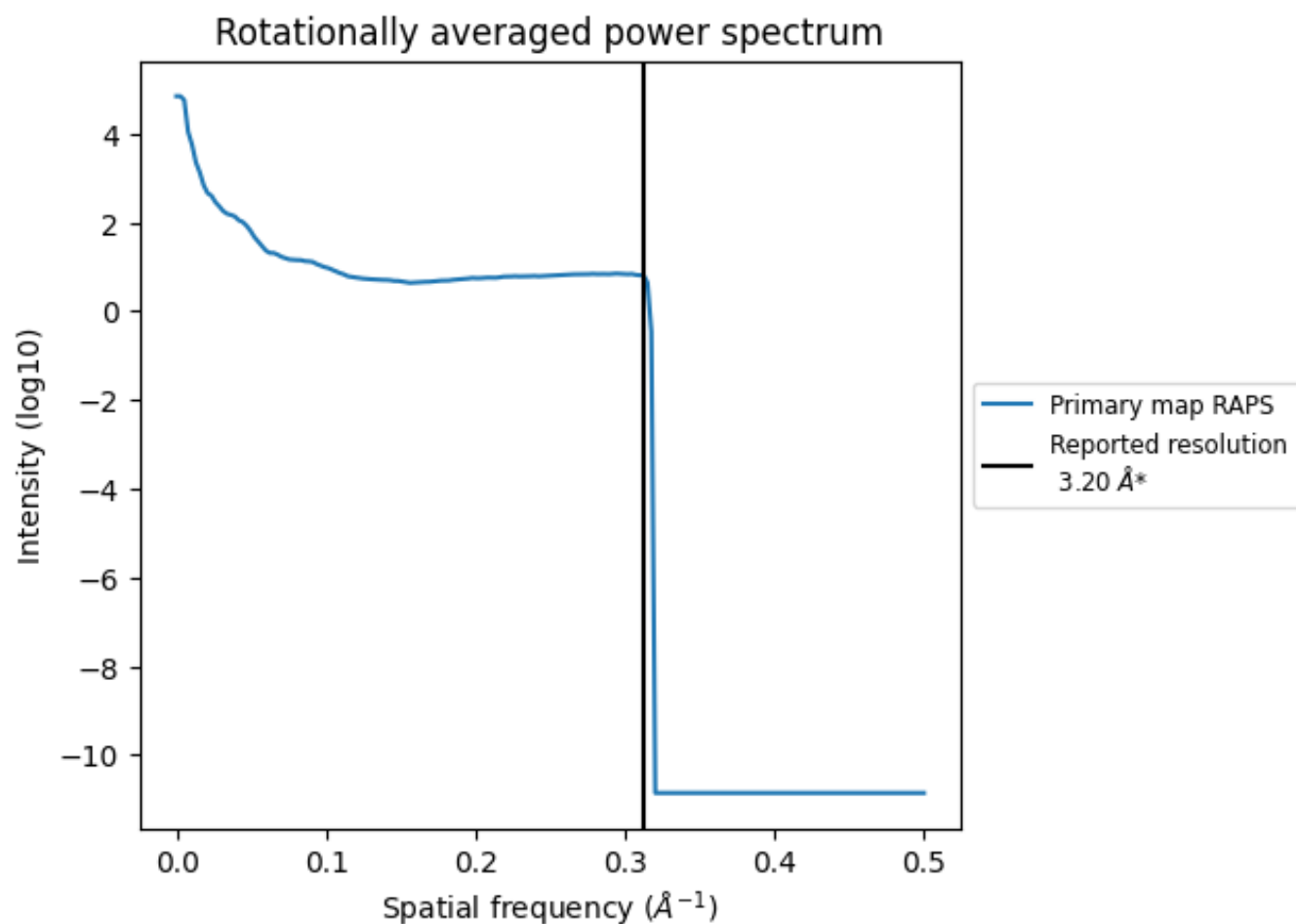
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 568 nm³; this corresponds to an approximate mass of 513 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 0.312 Å⁻¹

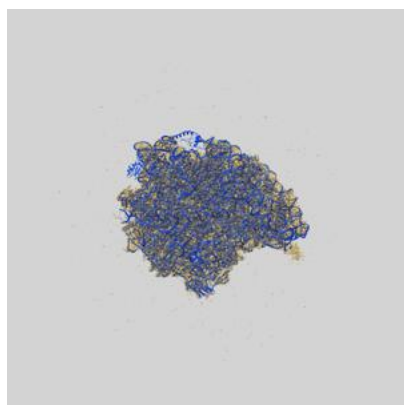
8 Fourier-Shell correlation

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

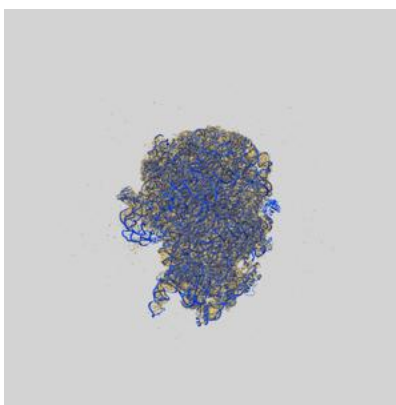
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8597 and PDB model 5UQ8. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

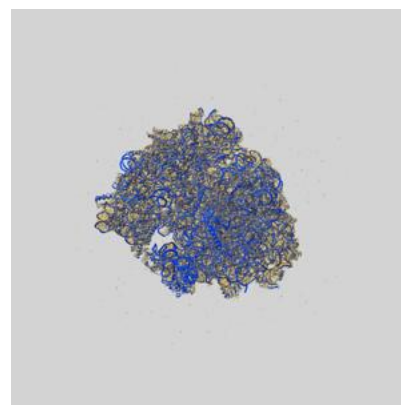
9.1 Map-model overlay [i](#)



X



Y



Z

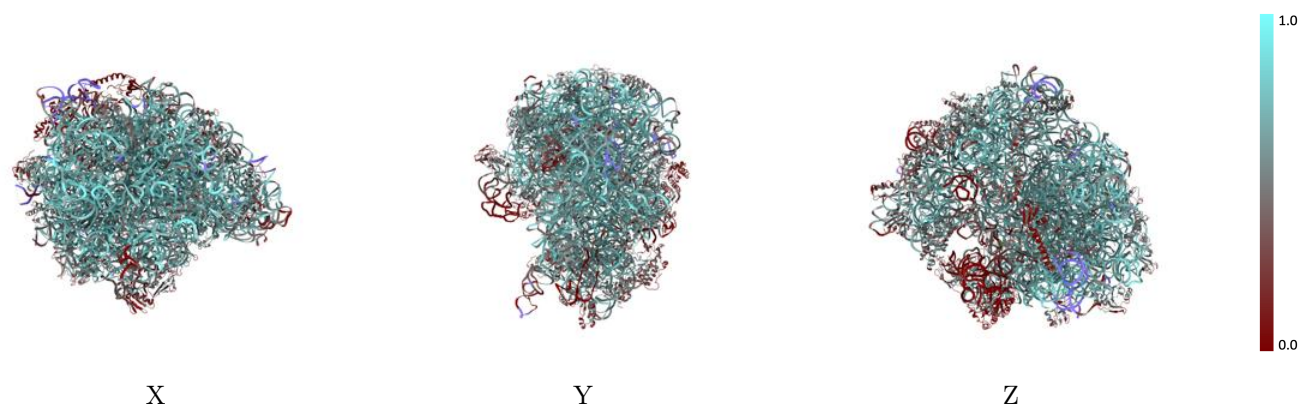
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



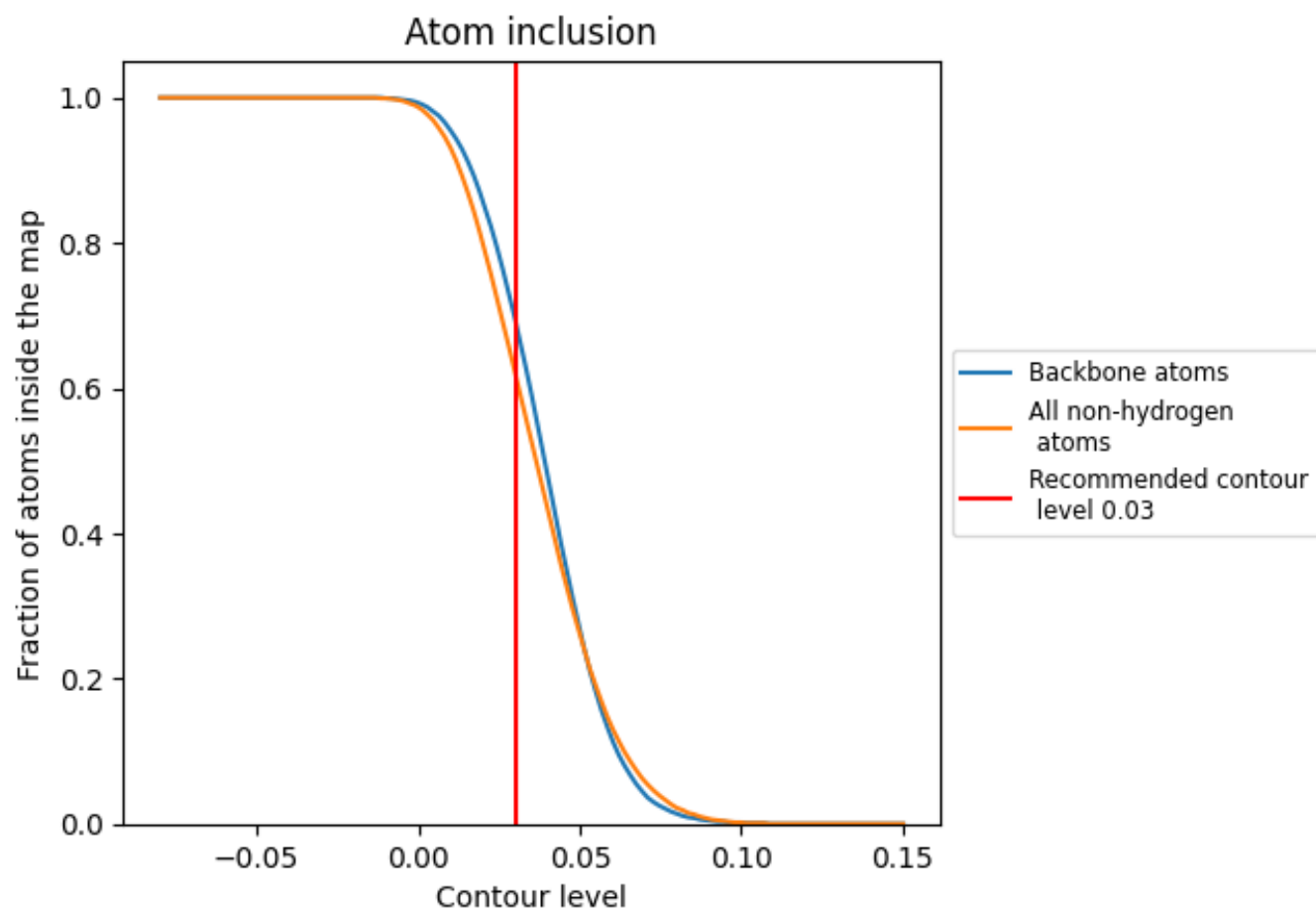
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 62% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6210	 0.4460
0	 0.6220	 0.5150
1	 0.4800	 0.4560
2	 0.4580	 0.4020
3	 0.5340	 0.4700
4	 0.2580	 0.2770
5	 0.6240	 0.4980
6	 0.6010	 0.4790
7	 0.6310	 0.5220
8	 0.5980	 0.5070
9	 0.5630	 0.4940
A	 0.7190	 0.4760
B	 0.6900	 0.4450
C	 0.0040	 0.1160
D	 0.6390	 0.5080
E	 0.5950	 0.4920
F	 0.5630	 0.4650
G	 0.4270	 0.3970
H	 0.3290	 0.3420
I	 0.0860	 0.2550
N	 0.5440	 0.4750
O	 0.5470	 0.4920
P	 0.5390	 0.4670
Q	 0.5380	 0.4550
R	 0.6130	 0.4880
S	 0.5100	 0.4270
T	 0.5540	 0.4570
U	 0.6370	 0.4910
V	 0.5000	 0.4490
W	 0.5840	 0.4930
X	 0.5290	 0.4570
Y	 0.4260	 0.4240
Z	 0.2590	 0.3350
a	 0.6970	 0.4530
b	 0.3650	 0.3780



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	 0.4980	 0.4410
d	 0.4770	 0.4090
e	 0.5410	 0.4680
f	 0.3390	 0.3510
g	 0.4250	 0.3840
h	 0.5610	 0.4710
i	 0.4220	 0.3910
j	 0.4030	 0.3890
k	 0.4760	 0.4330
l	 0.5440	 0.4880
m	 0.4260	 0.3980
n	 0.5790	 0.4760
o	 0.4890	 0.4180
p	 0.5700	 0.4630
q	 0.5150	 0.4750
r	 0.3600	 0.3650
s	 0.4030	 0.3860
t	 0.4630	 0.3910
u	 0.4890	 0.4420
x	 0.0590	 0.1030
y	 0.4630	 0.4070
z	 0.0920	 0.1510