Full wwPDB EM Validation Report ⓘ

Mar 25, 2024 – 03:59 pm GMT

PDB ID	:	8QBT
EMDB ID	:	EMD-18320
Title	:	E. coli ApdP-stalled ribosomal complex
Authors	:	Morici, M.; Wilson, D.N.
Deposited on	:	2023-08-25
Resolution	:	2.20 Å(reported)

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

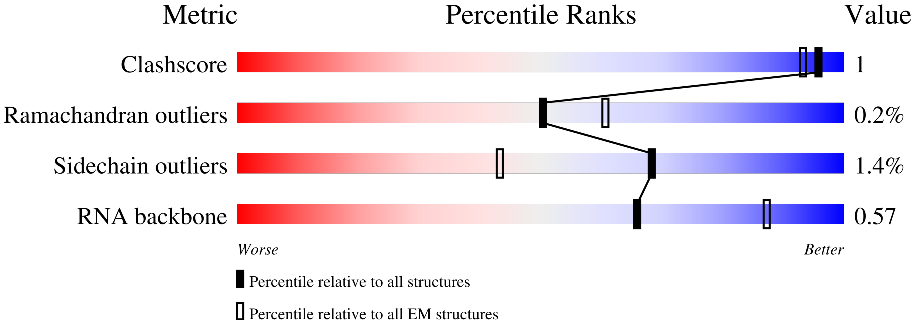
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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

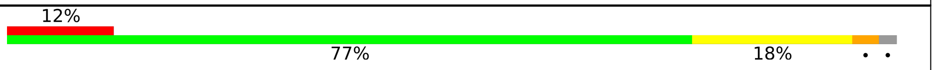
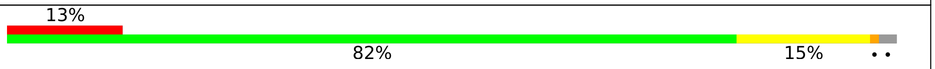
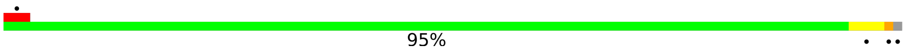
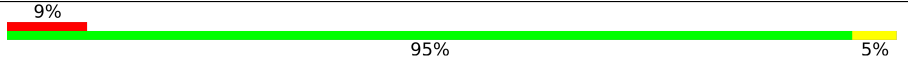
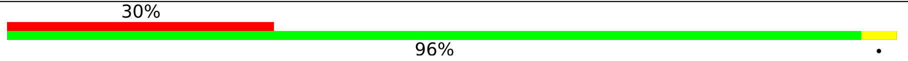
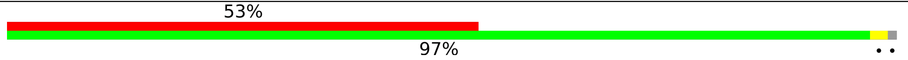
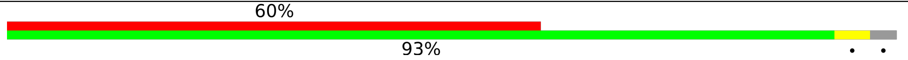
The reported resolution of this entry is 2.20 Å.

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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	2903	
2	B	120	
3	C	273	
4	D	209	
5	E	201	
6	F	179	
7	G	177	

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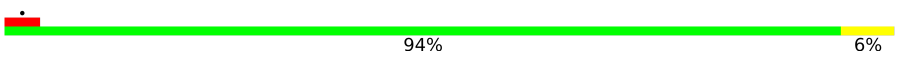
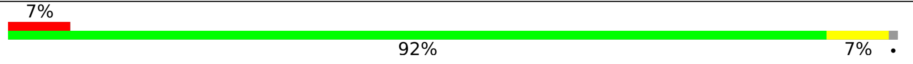
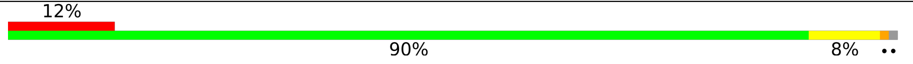
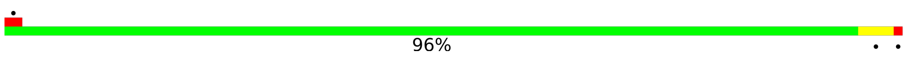
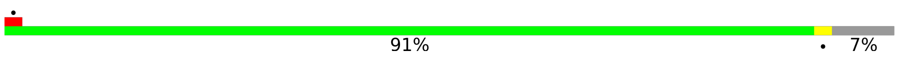
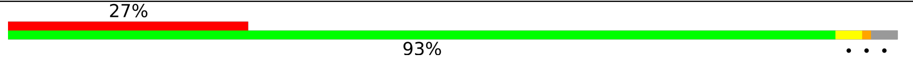
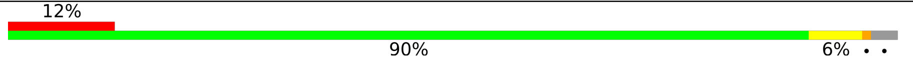
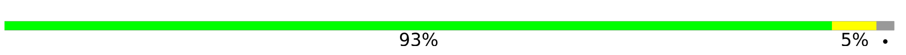
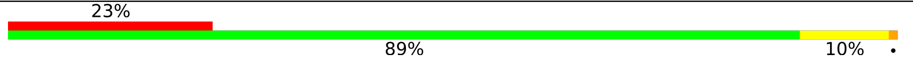
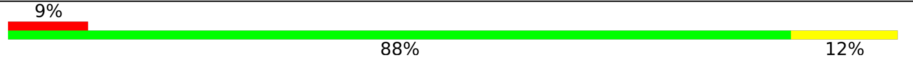
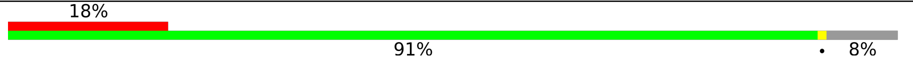
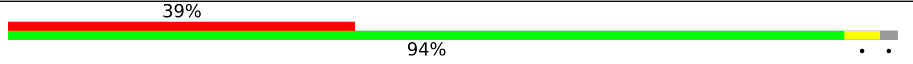
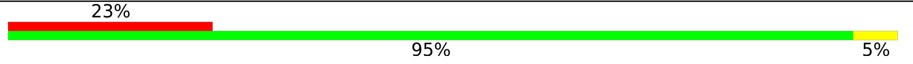
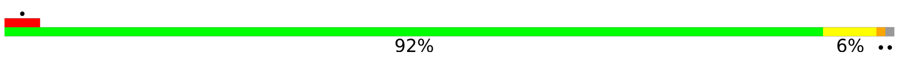
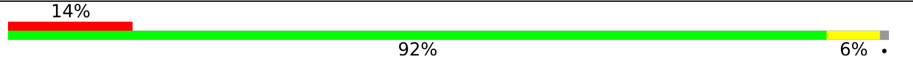
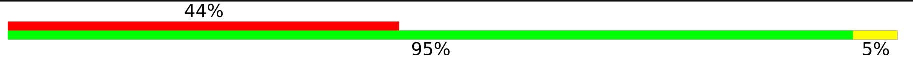
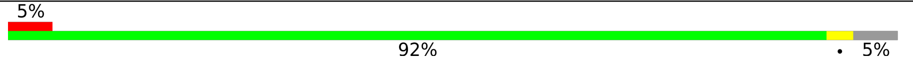
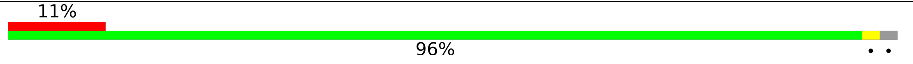
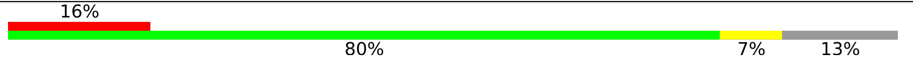
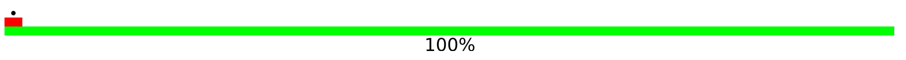
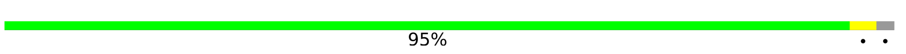
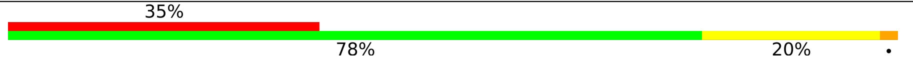
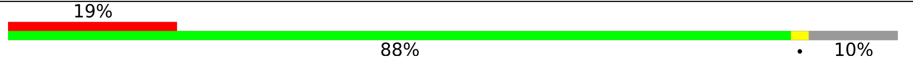
Mol	Chain	Length	Quality of chain
8	H	149	
9	J	142	
10	K	123	
11	L	144	
12	M	136	
13	N	127	
14	O	117	
15	P	115	
16	Q	118	
17	R	103	
18	S	110	
19	T	100	
20	U	104	
21	V	94	
22	W	85	
23	X	78	
24	Y	63	
25	Z	59	
26	a	57	
27	b	55	
28	c	46	
29	d	65	
30	i	1540	
31	j	241	
32	m	167	

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Mol	Chain	Length	Quality of chain
33	n	135	50% 72% • 26%
34	o	179	58% 83% • 16%
35	p	130	33% 98% • •
36	q	130	58% 86% 10% •
37	s	129	31% 88% • • 9%
38	t	124	64% 89% 6% • •
39	u	118	61% 92% • • 5%
40	v	101	45% 89% 6% 5%
41	w	89	38% 97% •
42	y	84	71% 94% • 5%
43	z	75	23% 72% • 27%
44	1	92	57% 78% • 20%
45	2	87	75% 89% • 10%
46	3	71	30% 51% 7% • 41%
47	4	10	20% 90% 10%
48	5	77	32% 75% 21% •
48	6	77	21% 83% 10% 6%
49	7	76	97% 62% 37% •
50	e	38	11% 97% •
51	f	6	17% 100%

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 141132 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 RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2841	60998	27210	11227	19720	2841	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2209	C	G	conflict	GB 991970073
A	2215	G	C	conflict	GB 991970073

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	118	2529	1126	464	821	118	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	271	2082	1288	423	364	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	209	1565	979	288	294	4	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	201	1552	974	283	290	5	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	177	Total 1410	C 899	N 249	O 256	S 6	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total 1285	C 811	N 235	O 237	S 2	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	47	Total 359	C 233	N 62	O 63	S 1	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	142	Total 1129	C 714	N 212	O 199	S 4	0	0

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	122	Total 938	C 587	N 180	O 165	S 6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	143	Total 1045	C 649	N 206	O 189	S 1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	136	Total 1074	C 686	N 205	O 177	S 6	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	118	Total 945	C 585	N 194	O 161	S 5	0	0

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	O	114	Total 875	C 542	N 175	O 158	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	112	Total 900	C 564	N 176	O 159	S 1	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	Q	116	Total 941	C 601	N 191	O 149	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	103	Total 816	C 516	N 153	O 145	S 2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	110	Total 857	C 532	N 166	O 156	S 3	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	92	Total 730	C 461	N 138	O 130	S 1	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	U	102	Total 779	C 492	N 146	O 141	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	94	Total 753	C 479	N 137	O 134	S 3	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	84	Total 628	C 388	N 126	O 113	S 1	0	0

- Molecule 23 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	77	Total 625	C 388	N 129	O 106	S 2	0	0

- Molecule 24 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	63	Total 509	C 313	N 99	O 95	S 2	0	0

- Molecule 25 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	56	Total 435	C 272	N 84	O 77	S 2	0	0

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	56	Total 444	C 269	N 94	O 80	S 1	0	0

- Molecule 27 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	b	48	395	254	72	69	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	c	46	377	228	90	57	2	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	d	64	504	323	105	74	2	0	0

- Molecule 30 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
30	i	1539	33015	14725	6052	10699	1539	0	0

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	j	215	1679	1067	299	307	6	0	0

- Molecule 32 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	m	150	1105	687	211	201	6	0	0

- Molecule 33 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	n	100	817	515	148	148	6	0	0

- Molecule 34 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	o	151	1181	735	227	215	4	0	0

- Molecule 35 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	p	129	979	616	173	184	6	0	0

- Molecule 36 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	q	125	1001	622	200	176	3	0	0

- Molecule 37 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	s	117	877	540	174	160	3	0	0

- Molecule 38 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	t	119	922	570	188	160	4	0	0

- Molecule 39 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	u	112	867	535	175	154	3	0	0

- Molecule 40 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	v	96	774	483	160	128	3	0	0

- Molecule 41 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	w	86	Total	C	N	O	S	0	0
			687	425	135	126	1		

- Molecule 42 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	y	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 43 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	z	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 44 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1	74	Total	C	N	O	S	0	0
			594	381	110	101	2		

- Molecule 45 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	2	78	Total	C	N	O	S	0	0
			612	376	126	107	3		

- Molecule 46 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	3	42	Total	C	N	O	S	0	0
			346	214	72	59	1		

- Molecule 47 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	4	10	Total	C	N	O	P	0	0
			214	95	40	69	10		

- Molecule 48 is a RNA chain called Pro-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
48	5	77	1644	733	295	540	76	0	0
48	6	77	1648	733	295	543	77	0	0

- Molecule 49 is a RNA chain called Ala-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
49	7	76	1618	722	289	532	75	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	e	38	302	185	65	48	4	0	0

- Molecule 51 is a protein called ApdP nascent chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	f	6	46	29	10	6	1	0	0

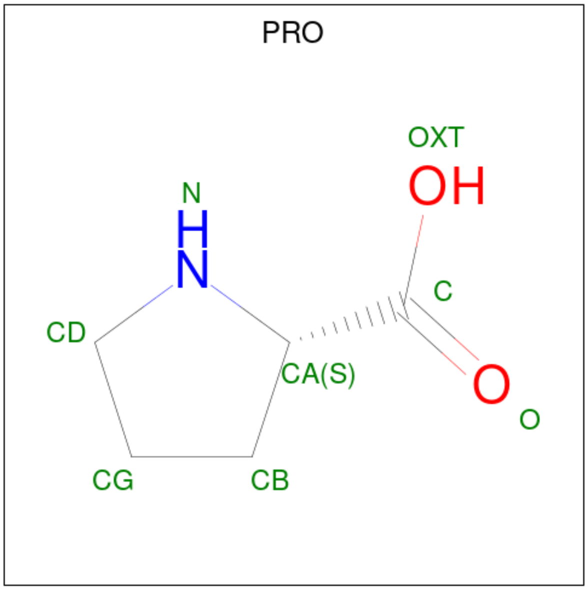
- Molecule 52 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
52	A	178	178	178	0
52	B	5	5	5	0
52	C	1	1	1	0
52	D	1	1	1	0
52	a	1	1	1	0
52	i	61	61	61	0
52	6	1	1	1	0

- Molecule 53 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
53	A	83	Total K 83 83	0
53	C	3	Total K 3 3	0
53	E	1	Total K 1 1	0
53	U	1	Total K 1 1	0
53	i	37	Total K 37 37	0
53	n	1	Total K 1 1	0
53	u	1	Total K 1 1	0

- Molecule 54 is PROLINE (three-letter code: PRO) (formula: $C_5H_9NO_2$).



Mol	Chain	Residues	Atoms	AltConf
54	5	1	Total C N O 7 5 1 1	0

- Molecule 55 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
55	e	1	Total Zn 1 1	0

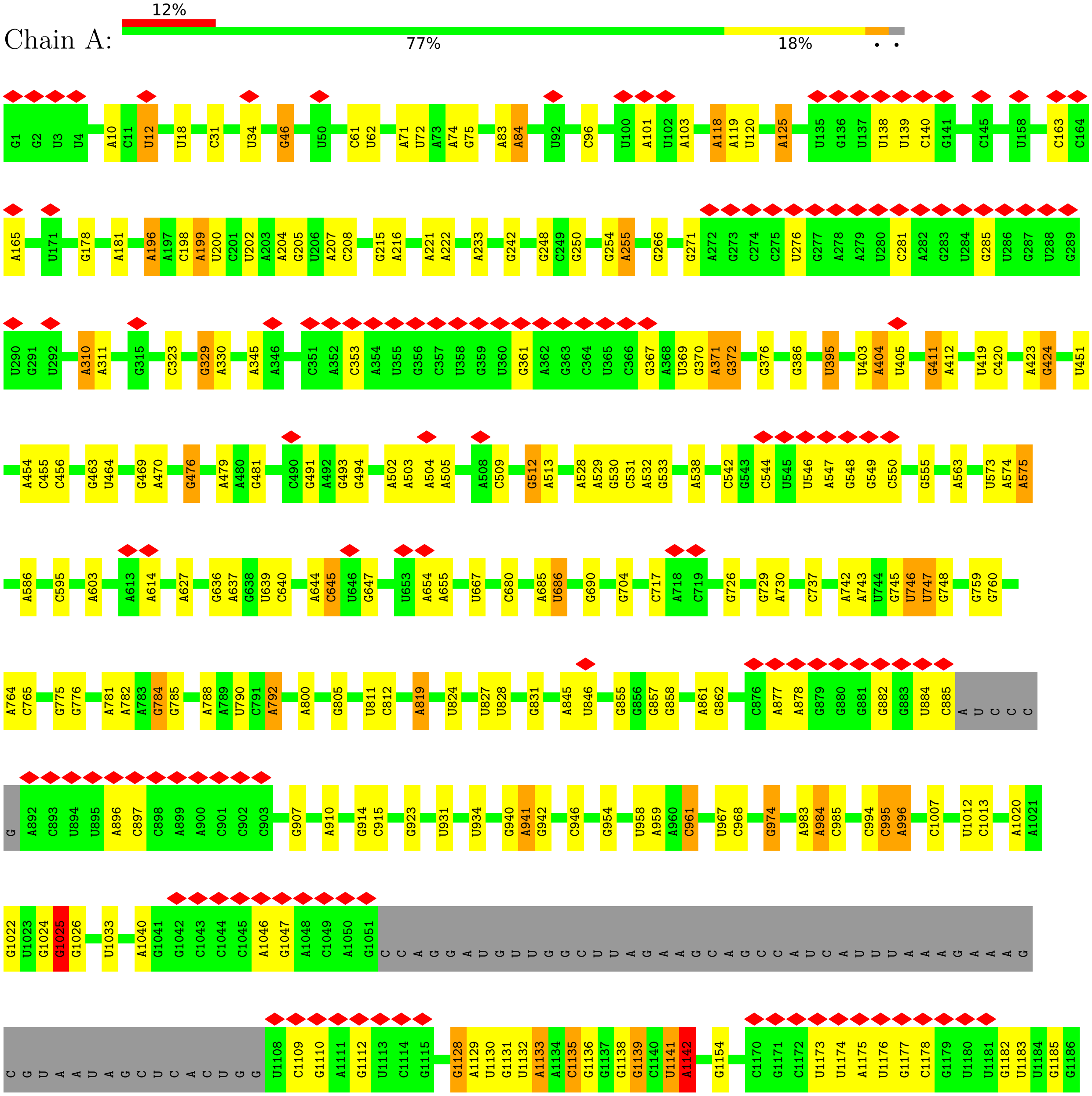
- Molecule 56 is water.

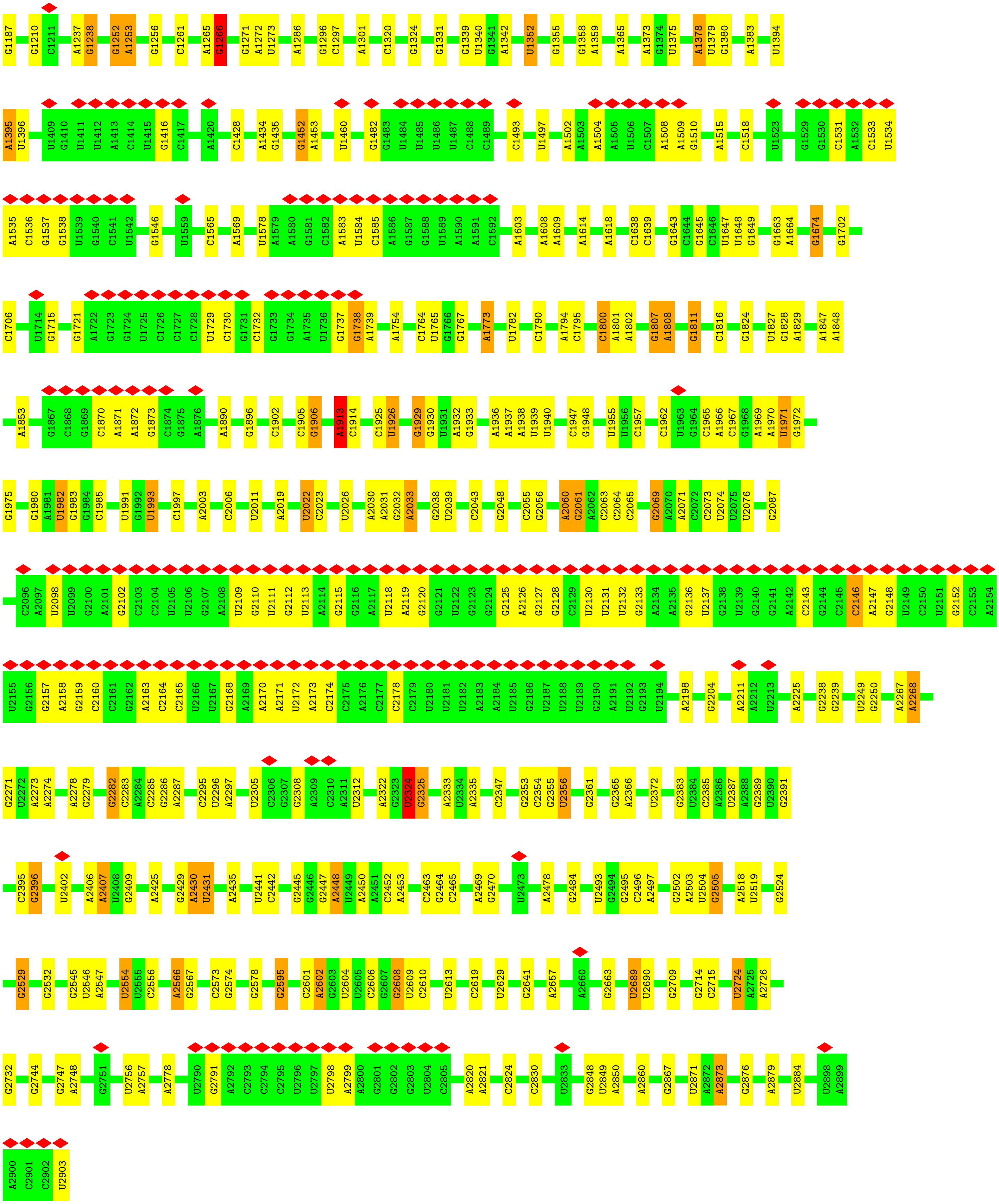
Mol	Chain	Residues	Atoms	AltConf
56	A	1006	Total O 1006 1006	0
56	B	10	Total O 10 10	0
56	C	14	Total O 14 14	0
56	D	2	Total O 2 2	0
56	E	3	Total O 3 3	0
56	L	4	Total O 4 4	0
56	N	3	Total O 3 3	0
56	T	1	Total O 1 1	0
56	a	4	Total O 4 4	0
56	d	4	Total O 4 4	0
56	i	176	Total O 176 176	0
56	s	1	Total O 1 1	0
56	4	3	Total O 3 3	0
56	5	3	Total O 3 3	0
56	6	2	Total O 2 2	0
56	f	3	Total O 3 3	0

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

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U1273
A1286
G1296
C1297
A1301
C1320
G1324
G1331
G1339
U1340
G1341
A1342
U1352
G1355
G1358
A1359
A1365
A1373
G1374
U1375
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U1379
G1380
A1383
U1394
A1395
U1396
U1409
G1410
U1411
U1412
A1413
C1414
U1415
G1416
C1417
A1420
C1428
A1434
G1435
G1452
A1453
U1460
G1482
G1483
U1484
U1485
U1486
U1487
C1488
C1489
C1493
U1497
A1502
A1503
A1504
A1505
U1506
C1507
A1508
A1509
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U1539
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U1542
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C2164
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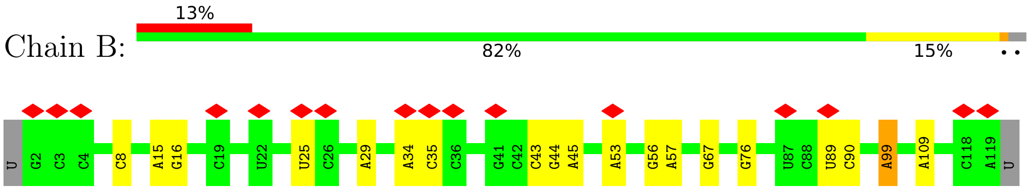
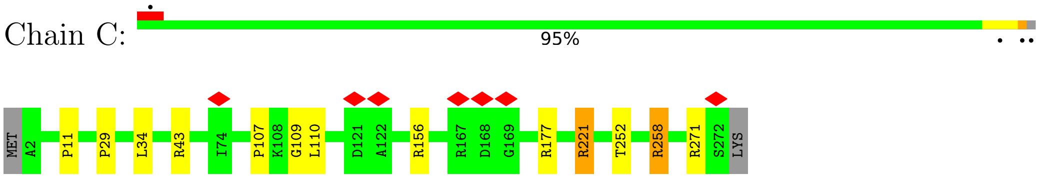
- Molecule 2: 5S rRNA

Chain B:



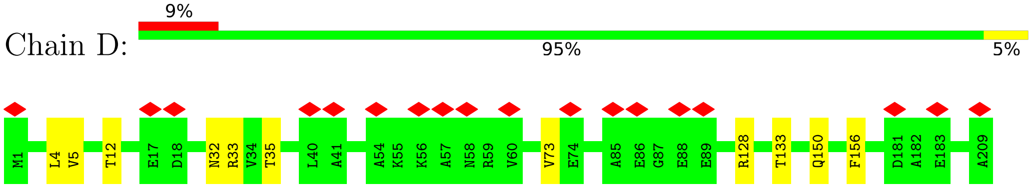
- Molecule 3: Large ribosomal subunit protein uL2

Chain C:



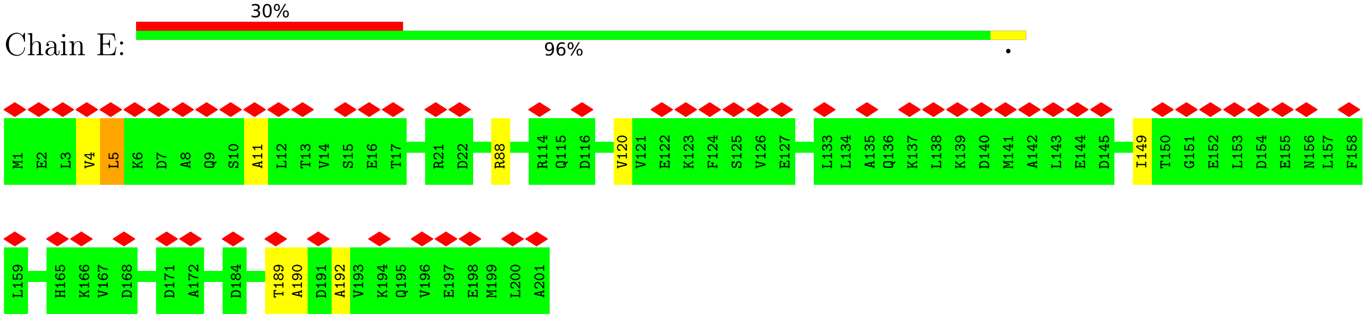
- Molecule 4: 50S ribosomal protein L3

Chain D:



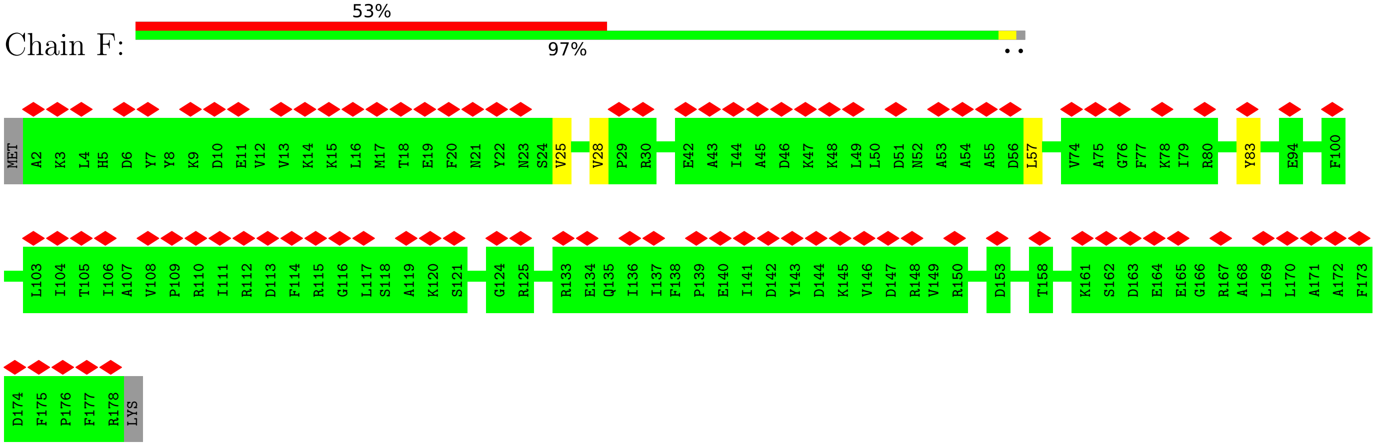
- Molecule 5: Large ribosomal subunit protein uL4

Chain E:

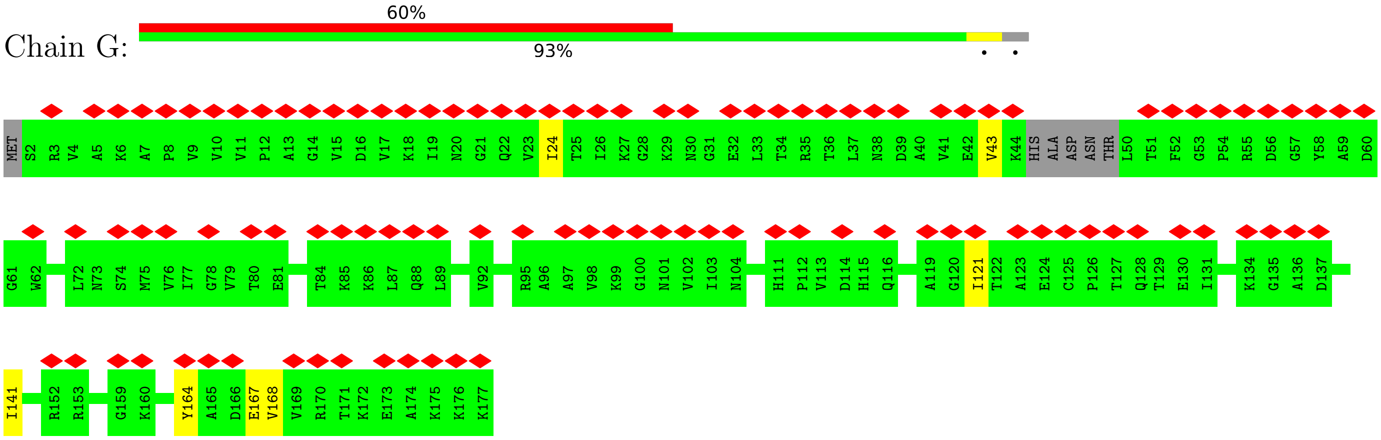


- Molecule 6: Large ribosomal subunit protein uL5

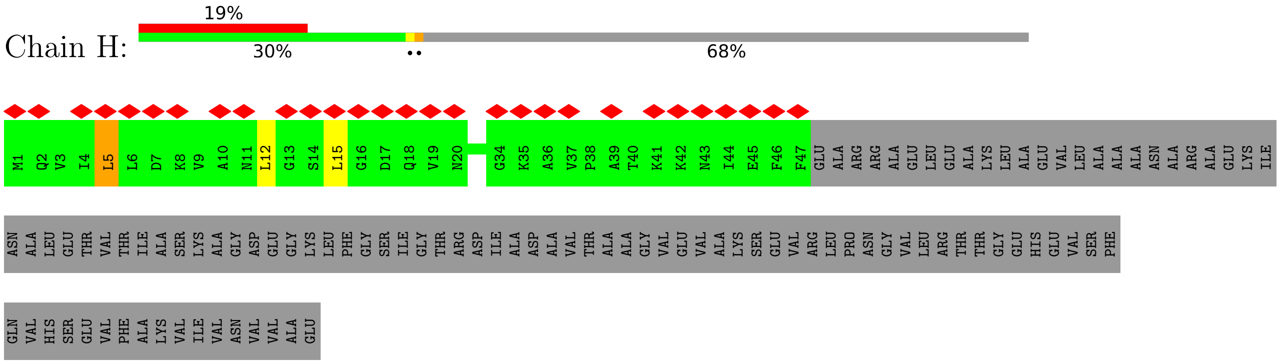
Chain F:



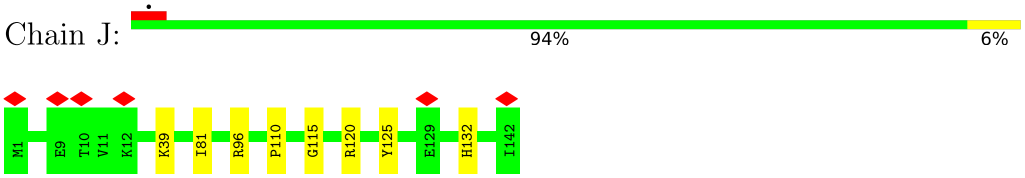
- Molecule 7: Large ribosomal subunit protein uL6



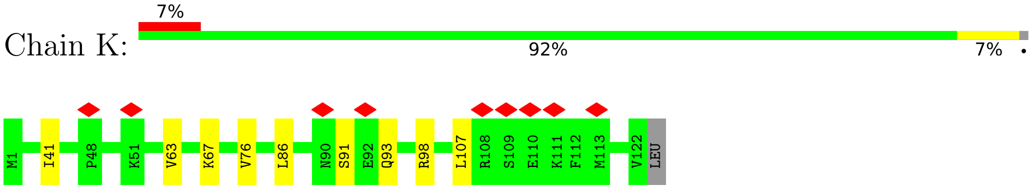
- Molecule 8: Large ribosomal subunit protein bL9



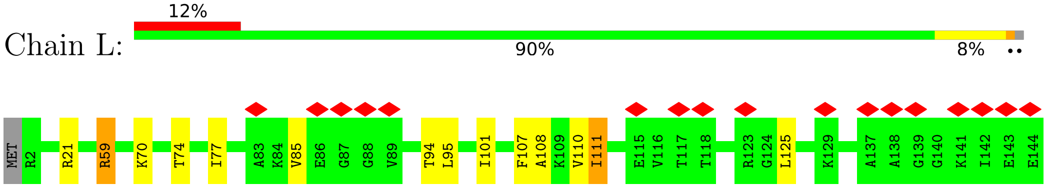
- Molecule 9: Large ribosomal subunit protein uL13



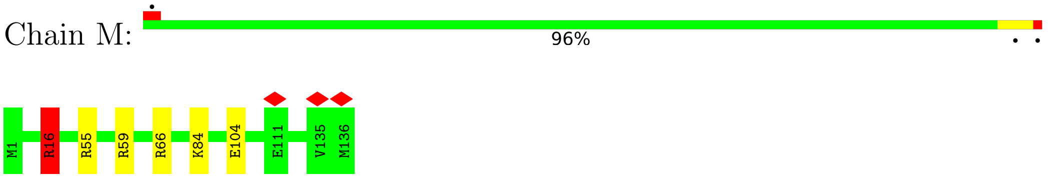
- Molecule 10: Large ribosomal subunit protein uL14



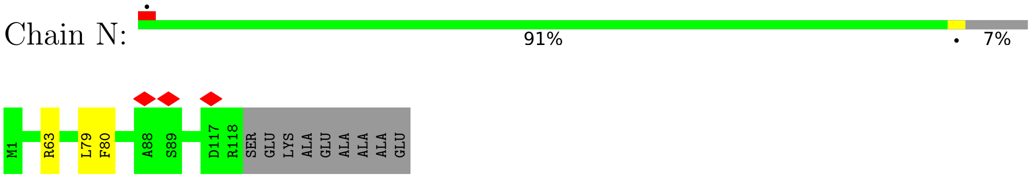
- Molecule 11: 50S ribosomal protein L15



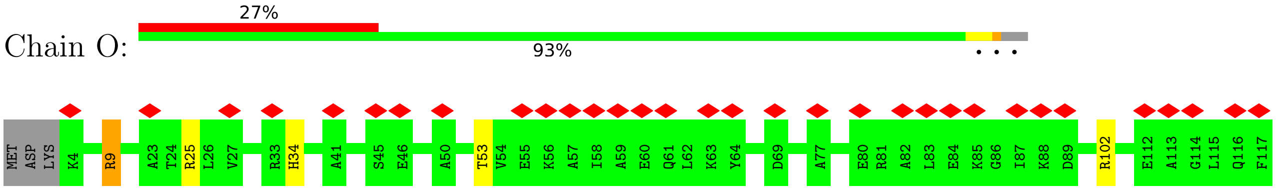
- Molecule 12: 50S ribosomal protein L16



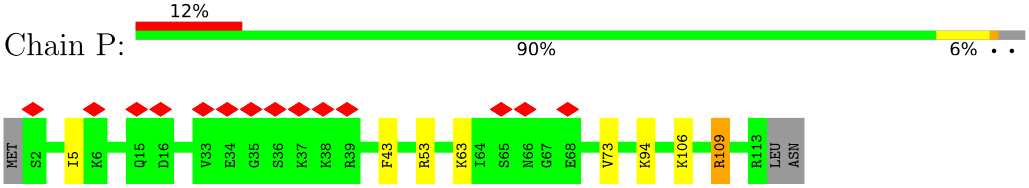
- Molecule 13: Large ribosomal subunit protein bL17



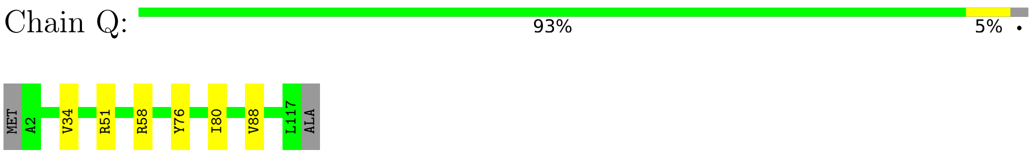
- Molecule 14: Large ribosomal subunit protein uL18



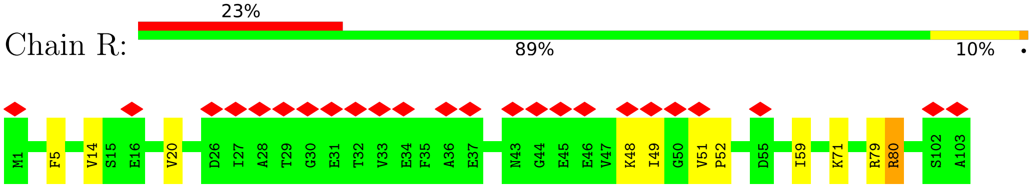
- Molecule 15: Large ribosomal subunit protein bL19



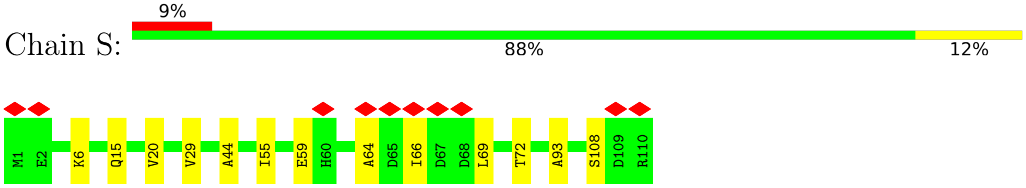
- Molecule 16: Large ribosomal subunit protein bL20



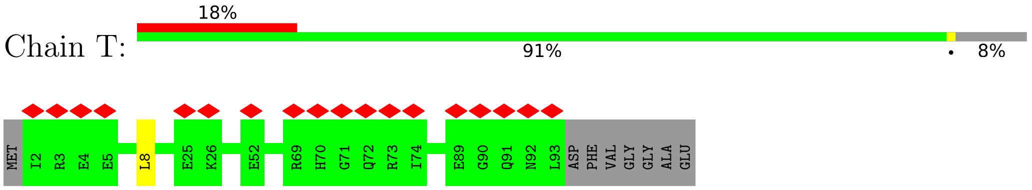
- Molecule 17: Large ribosomal subunit protein bL21



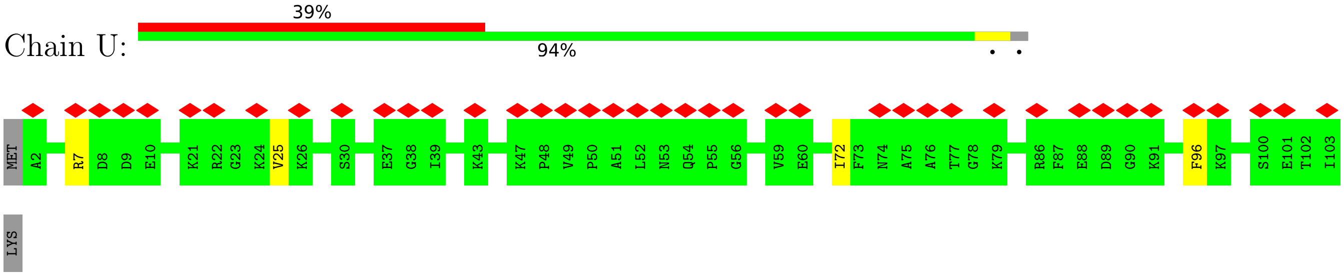
- Molecule 18: Large ribosomal subunit protein uL22



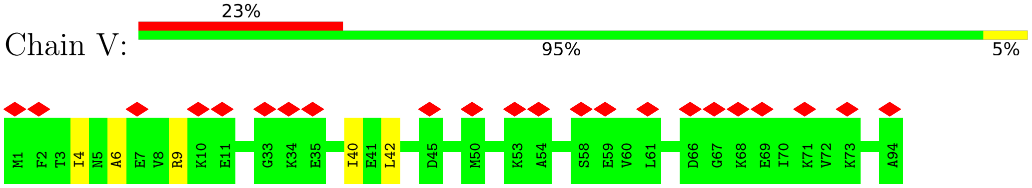
- Molecule 19: Large ribosomal subunit protein uL23



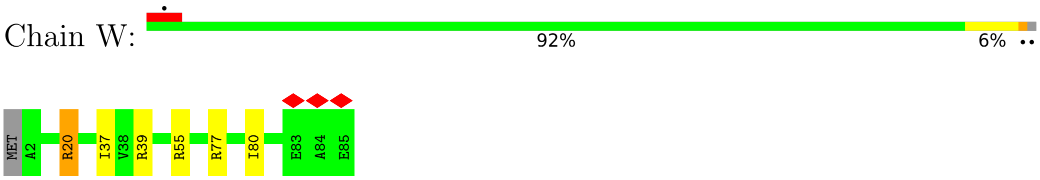
- Molecule 20: Large ribosomal subunit protein uL24



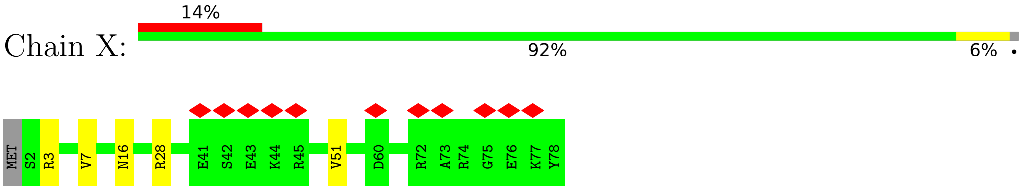
- Molecule 21: 50S ribosomal protein L25



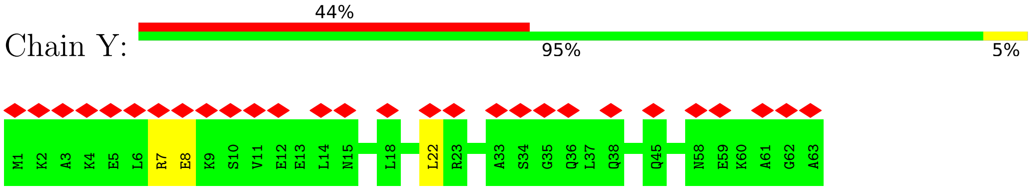
- Molecule 22: Large ribosomal subunit protein bL27



- Molecule 23: Large ribosomal subunit protein bL28

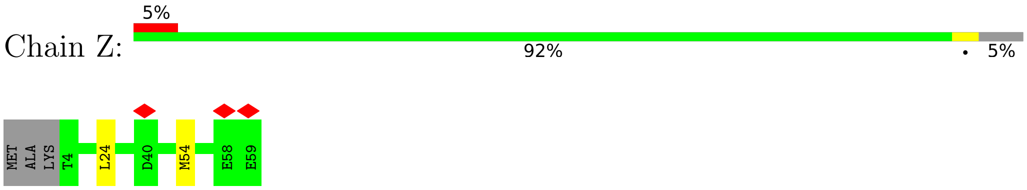


- Molecule 24: Large ribosomal subunit protein uL29



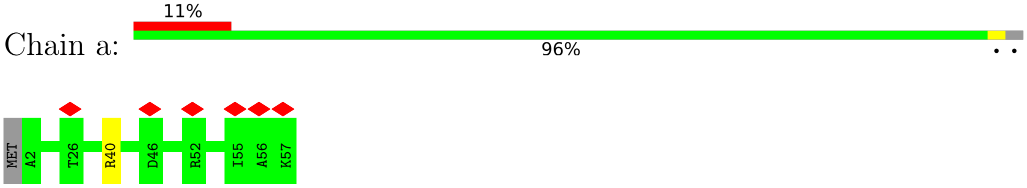
- Molecule 25: Large ribosomal subunit protein uL30

Chain Z:



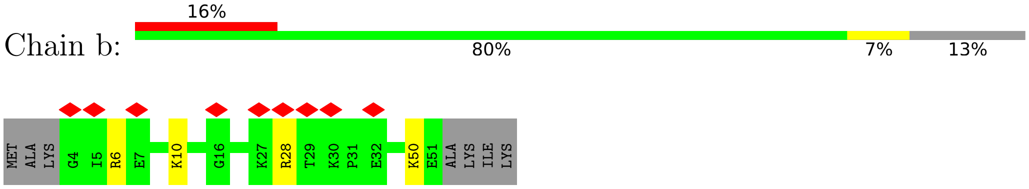
- Molecule 26: Large ribosomal subunit protein bL32

Chain a:



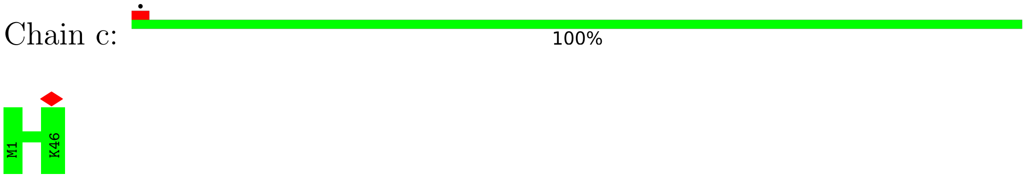
- Molecule 27: Large ribosomal subunit protein bL33

Chain b:



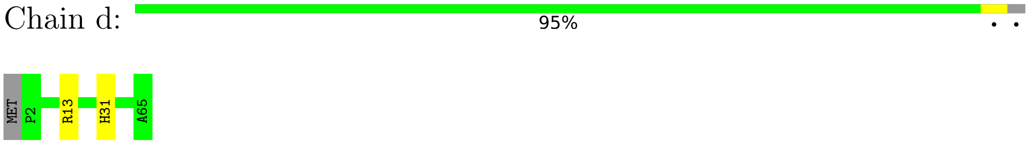
- Molecule 28: Large ribosomal subunit protein bL34

Chain c:



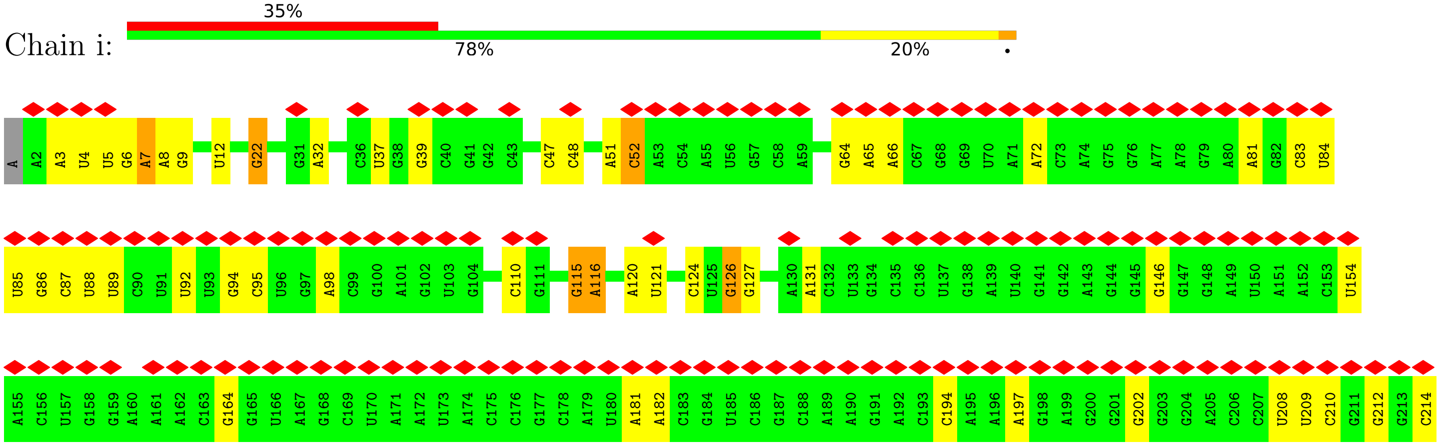
- Molecule 29: Large ribosomal subunit protein bL35

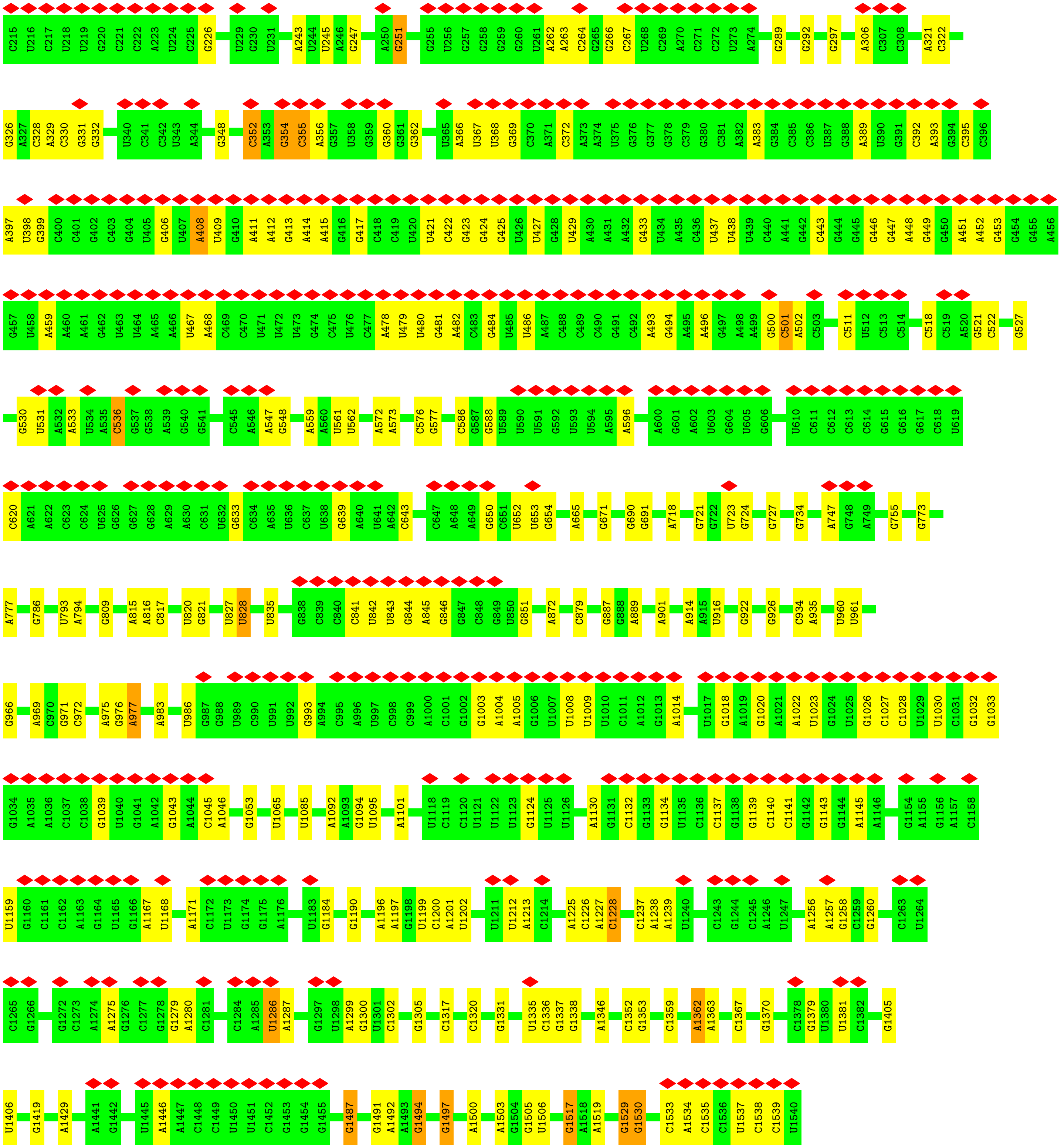
Chain d:



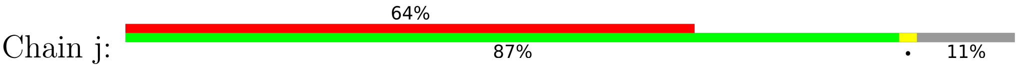
- Molecule 30: 16S rRNA

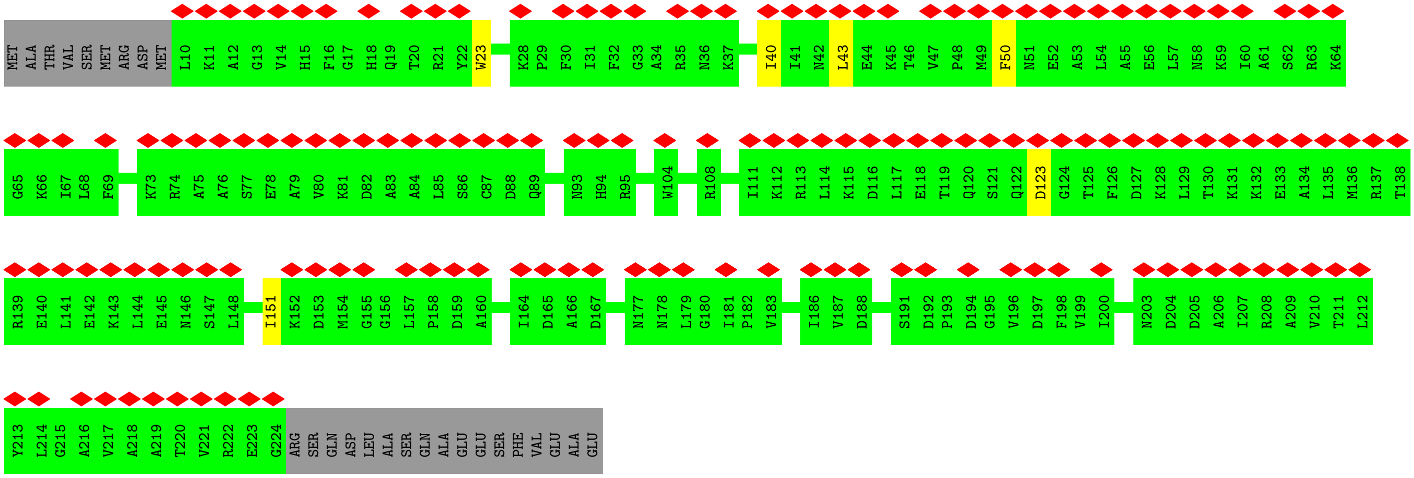
Chain i:



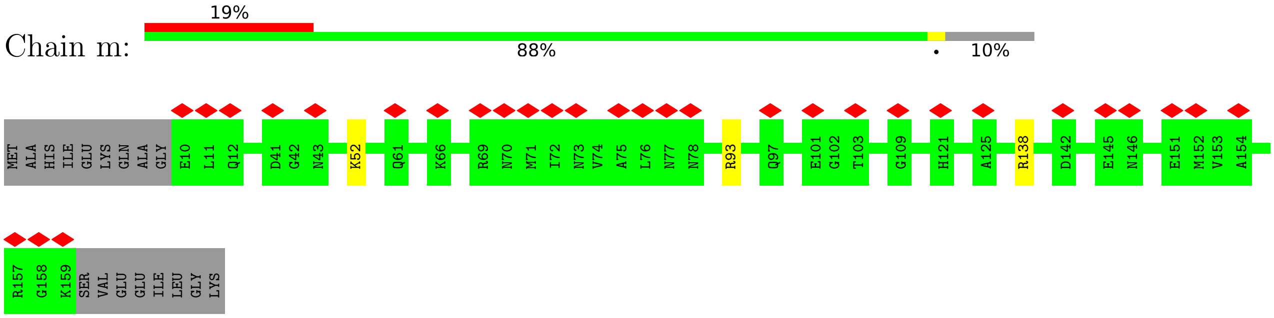


- Molecule 31: 30S ribosomal protein S2

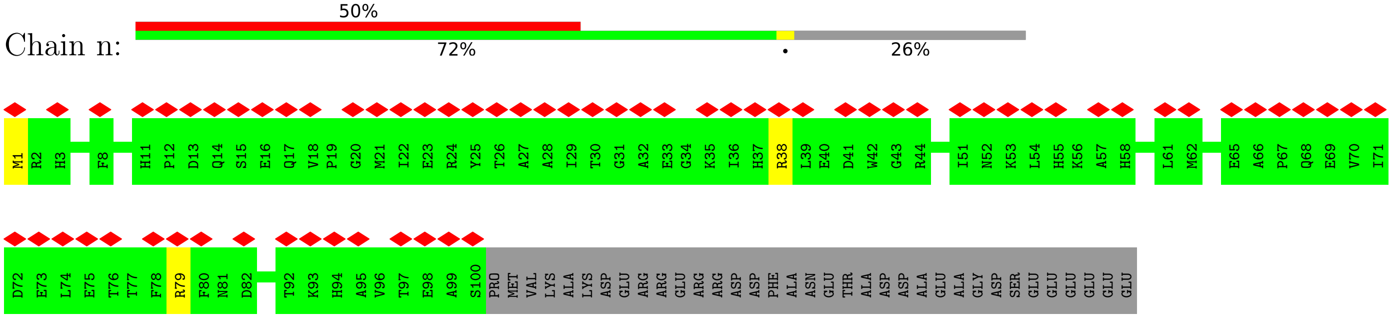




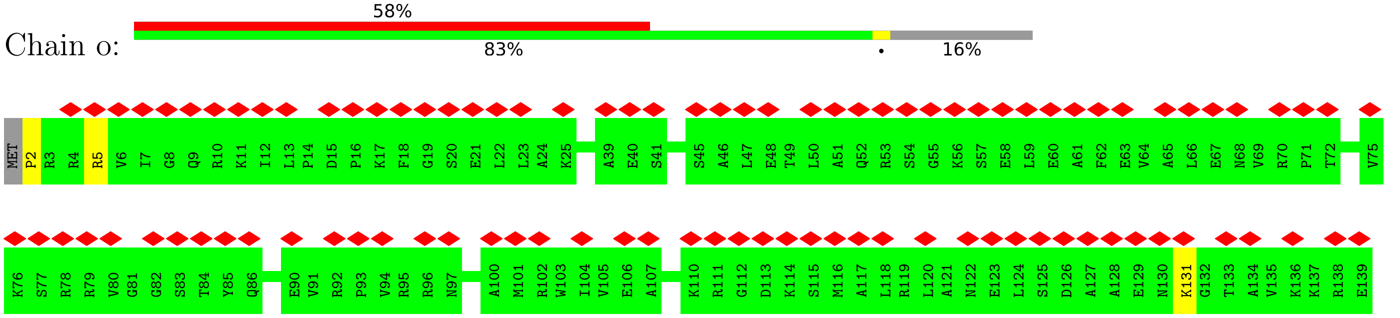
- Molecule 32: Small ribosomal subunit protein uS5

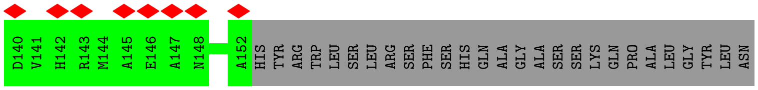


- Molecule 33: 30S ribosomal protein S6, fully modified isoform

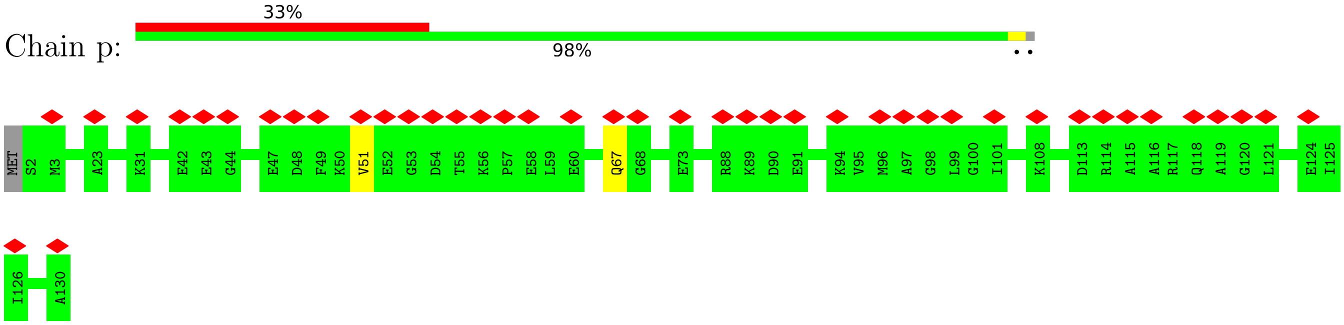


- Molecule 34: 30S ribosomal protein S7

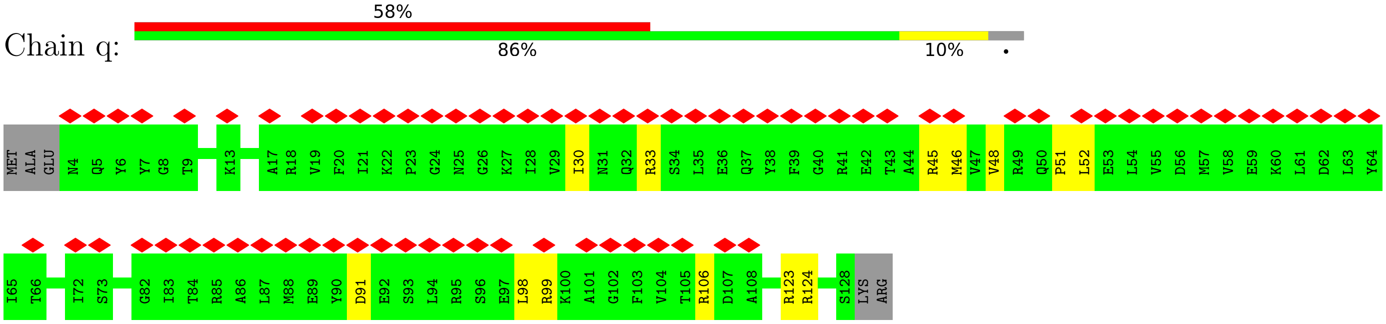




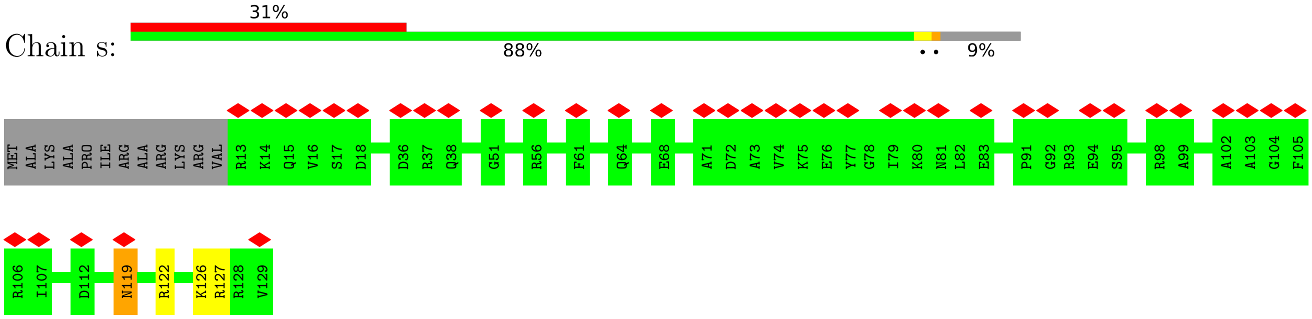
- Molecule 35: Small ribosomal subunit protein uS8



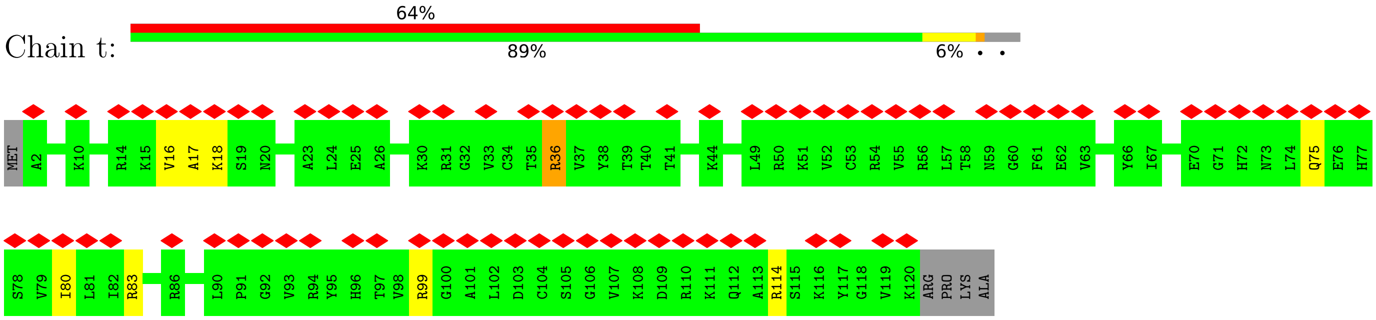
- Molecule 36: Small ribosomal subunit protein uS9



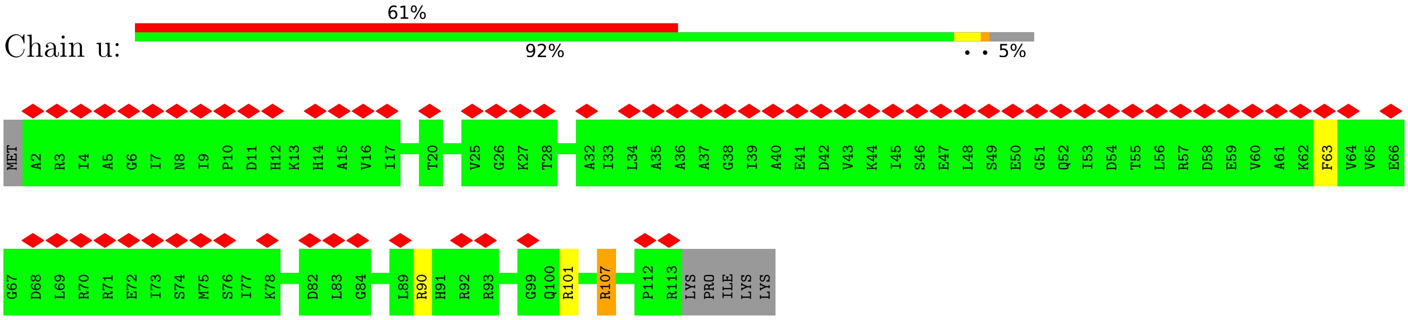
- Molecule 37: 30S ribosomal protein S11



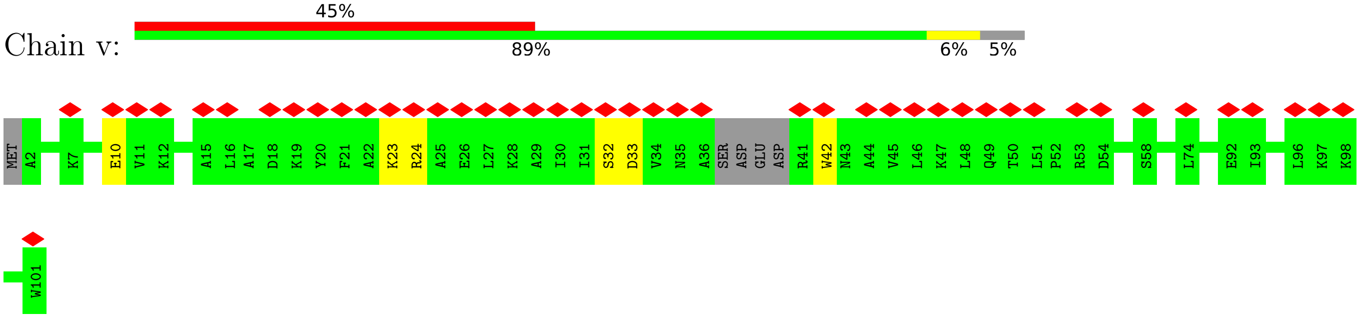
- Molecule 38: 30S ribosomal protein S12



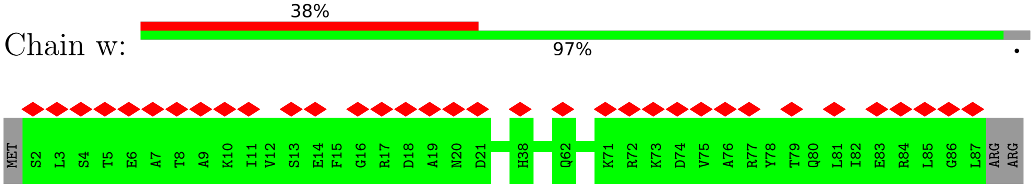
- Molecule 39: Small ribosomal subunit protein uS13



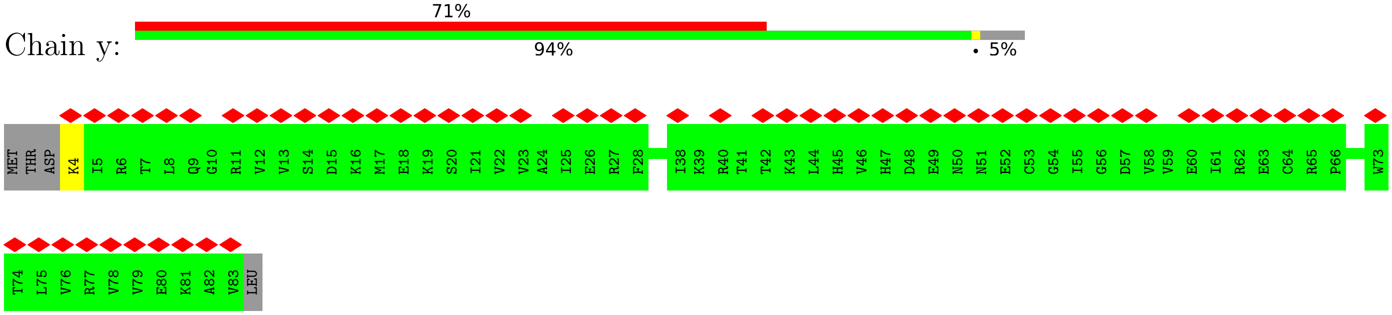
- Molecule 40: Small ribosomal subunit protein uS14



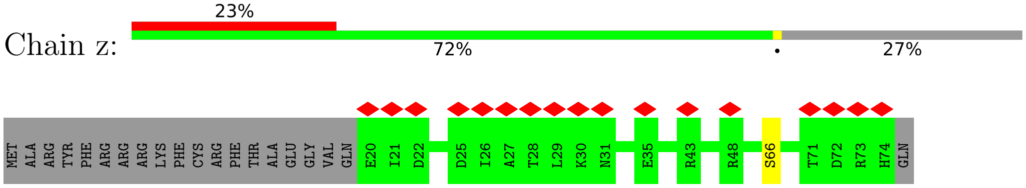
- Molecule 41: Small ribosomal subunit protein uS15



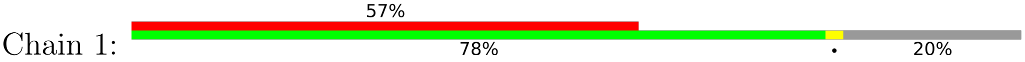
- Molecule 42: Small ribosomal subunit protein uS17

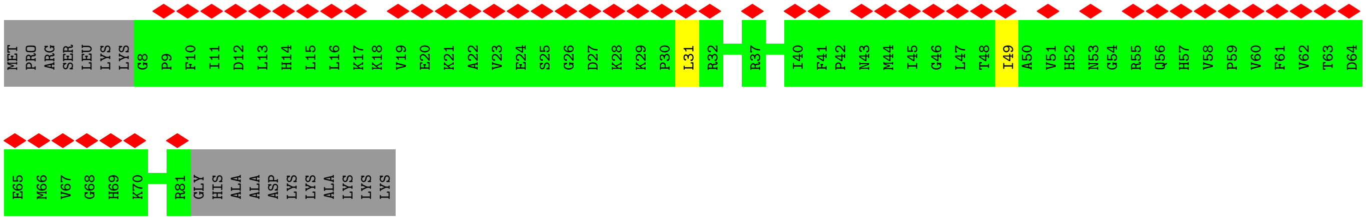


- Molecule 43: Small ribosomal subunit protein bS18



- Molecule 44: Small ribosomal subunit protein uS19



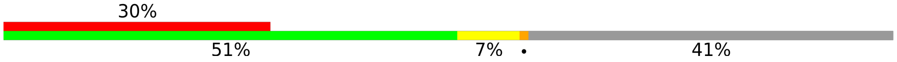


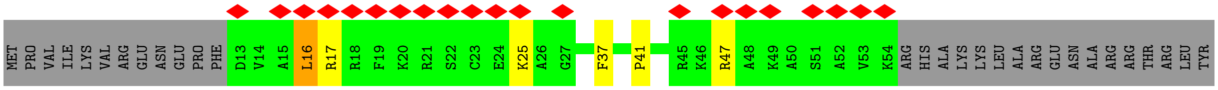
- Molecule 45: 30S ribosomal protein S20

Chain 2:

- Molecule 46: Small ribosomal subunit protein bS21

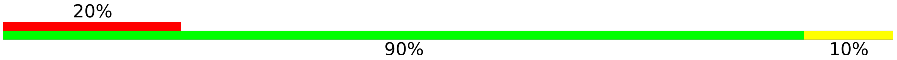
Chain 3:

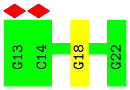




- Molecule 47: mRNA

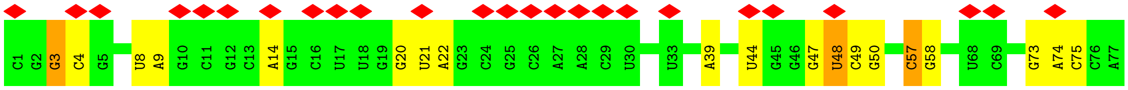
Chain 4:





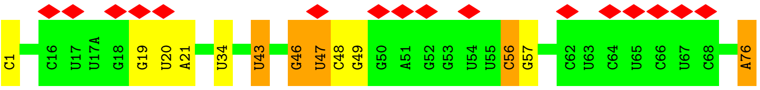
- Molecule 48: Pro-tRNA

Chain 5:



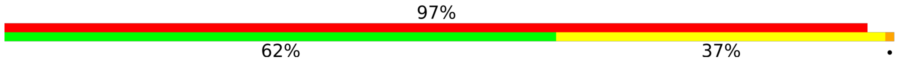
- Molecule 48: Pro-tRNA

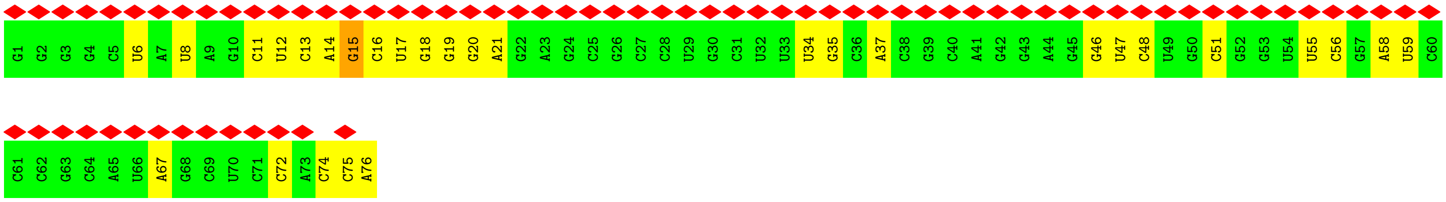
Chain 6:



- Molecule 49: Ala-tRNA

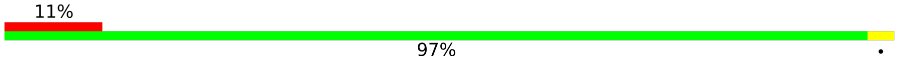
Chain 7:

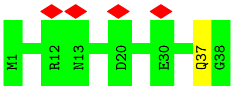




- Molecule 50: Large ribosomal subunit protein bL36A

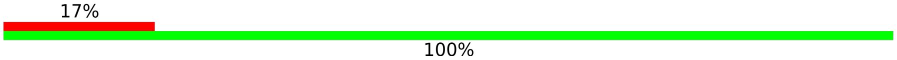
Chain e:

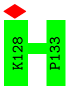




- Molecule 51: ApdP nascent chain

Chain f:





4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	205838	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 $(e^-/\text{Å}^2)$	75.6	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.418	Depositor
Minimum map value	-0.187	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	295.2, 295.2, 295.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82000005, 0.82000005, 0.82000005	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, MG, 2MA, PSU, K

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	0.61	1/68247 (0.0%)	1.29	302/106469 (0.3%)
2	B	0.51	0/2828	1.17	7/4410 (0.2%)
3	C	0.42	0/2121	0.87	4/2852 (0.1%)
4	D	0.41	0/1586	0.72	0/2134
5	E	0.38	0/1571	0.68	0/2113
6	F	0.29	0/1434	0.64	0/1926
7	G	0.31	0/1303	0.65	0/1759
8	H	0.31	0/364	0.66	0/490
9	J	0.35	0/1152	0.67	0/1551
10	K	0.36	0/947	0.81	0/1268
11	L	0.40	0/1054	0.76	0/1403
12	M	0.37	0/1093	0.76	1/1460 (0.1%)
13	N	0.38	0/958	0.77	0/1281
14	O	0.32	0/885	0.70	1/1187 (0.1%)
15	P	0.37	0/912	0.77	0/1220
16	Q	0.41	0/954	0.75	1/1271 (0.1%)
17	R	0.40	0/829	0.80	1/1107 (0.1%)
18	S	0.38	0/864	0.71	0/1156
19	T	0.32	0/736	0.67	0/984
20	U	0.30	0/787	0.71	0/1051
21	V	0.31	0/766	0.67	0/1025
22	W	0.41	0/636	0.76	0/841
23	X	0.38	0/635	0.79	1/848 (0.1%)
24	Y	0.29	0/510	0.63	0/677
25	Z	0.33	0/439	0.68	0/587
26	a	0.41	0/450	0.81	0/599
27	b	0.37	0/402	0.73	0/536
28	c	0.44	0/380	0.90	0/498
29	d	0.41	0/513	0.77	0/676
30	i	0.55	0/36966	1.20	85/57666 (0.1%)
31	j	0.30	0/1710	0.69	0/2306
32	m	0.33	0/1118	0.69	0/1504

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	n	0.29	0/835	0.67	0/1128
34	o	0.30	0/1195	0.70	1/1602 (0.1%)
35	p	0.29	0/989	0.65	0/1326
36	q	0.38	0/1013	0.76	0/1350
37	s	0.34	0/893	0.79	2/1205 (0.2%)
38	t	0.32	0/935	0.80	0/1256
39	u	0.31	0/875	0.74	0/1170
40	v	0.33	0/785	0.68	0/1043
41	w	0.31	0/695	0.58	0/931
42	y	0.28	0/657	0.71	0/881
43	z	0.30	0/462	0.65	0/621
44	1	0.32	0/609	0.67	0/822
45	2	0.30	0/616	0.69	0/814
46	3	0.40	0/349	0.86	0/461
47	4	0.61	0/238	1.16	0/369
48	5	0.56	0/1837	1.20	3/2864 (0.1%)
48	6	0.60	1/1841 (0.1%)	1.20	4/2868 (0.1%)
49	7	0.61	0/1807	1.10	1/2816 (0.0%)
50	e	0.36	0/303	0.91	0/397
51	f	0.39	0/46	0.81	0/60
All	All	0.54	2/152130 (0.0%)	1.15	414/228839 (0.2%)

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	6
3	C	0	6
4	D	0	2
5	E	0	1
9	J	0	1
11	L	0	1
12	M	0	2
13	N	0	1
14	O	0	1
15	P	0	1
16	Q	0	1
17	R	0	2
22	W	0	4
23	X	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
26	a	0	1
27	b	0	2
29	d	0	1
32	m	0	2
33	n	0	2
36	q	0	5
38	t	0	4
39	u	0	3
All	All	0	51

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	6	1	C	OP3-P	-7.30	1.52	1.61
1	A	2069	G	C8-N7	5.36	1.34	1.30

All (414) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2061	G	O5'-P-OP2	-28.61	76.37	110.70
1	A	575	A	O5'-P-OP1	-20.21	86.45	110.70
1	A	1139	G	O5'-P-OP2	-18.09	88.99	110.70
1	A	1395	A	O5'-P-OP1	-17.95	89.16	110.70
1	A	2250	G	O5'-P-OP2	-17.42	89.80	110.70
1	A	2430	A	O5'-P-OP2	-17.30	89.93	110.70
1	A	2554	U	O5'-P-OP1	-17.17	90.10	110.70
1	A	819	A	O5'-P-OP1	-15.46	91.79	105.70
1	A	1253	A	O5'-P-OP1	-15.29	91.94	105.70
1	A	255	A	O5'-P-OP1	-14.51	92.64	105.70
1	A	2296	U	O3'-P-O5'	-14.45	76.55	104.00
1	A	685	A	O3'-P-O5'	-13.42	78.50	104.00
30	i	1519	A	O5'-P-OP2	-13.05	93.96	105.70
30	i	1494	G	O5'-P-OP2	-12.39	94.55	105.70
1	A	2602	A	O5'-P-OP2	-11.67	95.20	105.70
1	A	2061	G	O5'-P-OP1	11.60	124.62	110.70
1	A	961	C	O5'-P-OP2	-10.99	95.81	105.70
1	A	995	C	O5'-P-OP1	10.97	123.87	110.70
1	A	512	G	O4'-C1'-N9	10.75	116.80	108.20
1	A	1266	G	O5'-P-OP1	-10.73	96.04	105.70
1	A	686	U	O5'-P-OP1	10.68	123.52	110.70
1	A	574	A	O5'-P-OP1	-10.65	96.12	105.70
30	i	110	C	O5'-P-OP2	10.48	123.27	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	115	G	P-O3'-C3'	10.37	132.15	119.70
1	A	2022	U	O5'-P-OP1	-10.31	96.42	105.70
1	A	994	C	O3'-P-O5'	-10.12	84.77	104.00
1	A	2505	G	O5'-P-OP2	-10.03	96.67	105.70
3	C	221	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	A	2361	G	O5'-P-OP2	-9.98	96.72	105.70
30	i	500	G	O3'-P-O5'	-9.97	85.05	104.00
1	A	1352	U	O5'-P-OP2	-9.97	96.73	105.70
30	i	501	C	O3'-P-O5'	-9.97	85.06	104.00
2	B	99	A	O5'-P-OP1	-9.89	96.80	105.70
1	A	1811	G	O5'-P-OP2	-9.78	96.90	105.70
1	A	574	A	O5'-P-OP2	9.77	122.42	110.70
1	A	2430	A	O5'-P-OP1	9.58	122.19	110.70
30	i	889	A	O3'-P-O5'	-9.56	85.84	104.00
1	A	2033	A	O5'-P-OP2	-9.52	97.13	105.70
1	A	83	A	O3'-P-O5'	-9.43	86.08	104.00
1	A	2022	U	O5'-P-OP2	9.29	121.85	110.70
1	A	2065	C	O5'-P-OP2	-9.29	97.34	105.70
1	A	1939	U	P-O3'-C3'	-9.24	108.61	119.70
1	A	470	A	O5'-P-OP1	9.22	121.77	110.70
1	A	941	A	O5'-P-OP1	-9.07	97.54	105.70
1	A	2431	U	O5'-P-OP1	-9.06	97.55	105.70
1	A	1395	A	O5'-P-OP2	9.01	121.51	110.70
1	A	743	A	O5'-P-OP2	-8.97	97.63	105.70
1	A	996	A	O5'-P-OP1	-8.96	97.64	105.70
1	A	1790	C	O5'-P-OP2	-8.87	97.71	105.70
1	A	1940	U	O5'-P-OP2	-8.83	97.75	105.70
1	A	2848	G	O4'-C1'-N9	8.66	115.13	108.20
1	A	1394	U	OP1-P-O3'	8.59	124.09	105.20
1	A	1375	U	C5-C4-O4	8.58	131.05	125.90
1	A	1905	C	O5'-P-OP2	-8.56	98.00	105.70
1	A	2546	U	O3'-P-O5'	-8.52	87.81	104.00
30	i	1487	G	O5'-P-OP2	-8.48	98.07	105.70
1	A	1565	C	O3'-P-O5'	-8.44	87.96	104.00
1	A	1807	G	O5'-P-OP2	-8.43	98.11	105.70
1	A	746	PSU	P-O3'-C3'	8.41	129.80	119.70
1	A	329	G	O5'-P-OP2	-8.28	98.25	105.70
30	i	972	C	O5'-P-OP2	-8.25	98.28	105.70
17	R	80	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	A	1373	A	O3'-P-O5'	-8.17	88.47	104.00
30	i	22	G	O5'-P-OP2	-8.17	98.35	105.70
30	i	1529	G	O3'-P-O5'	-8.12	88.57	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	A	O3'-P-O5'	-8.12	88.58	104.00
1	A	1237	A	O3'-P-O5'	-8.09	88.64	104.00
1	A	940	G	O3'-P-O5'	8.05	119.29	104.00
1	A	575	A	O5'-P-OP2	8.04	120.35	110.70
1	A	2465	C	O5'-P-OP2	-7.98	98.51	105.70
30	i	1491	G	O3'-P-O5'	-7.98	88.83	104.00
1	A	329	G	O3'-P-O5'	-7.97	88.86	104.00
1	A	2268	A	O5'-P-OP2	-7.95	98.55	105.70
1	A	1238	G	O5'-P-OP1	7.86	120.13	110.70
1	A	2071	A	O5'-P-OP2	-7.77	98.71	105.70
1	A	1985	C	O5'-P-OP2	-7.75	98.73	105.70
1	A	2724	U	O5'-P-OP2	-7.72	98.75	105.70
1	A	1639	C	O5'-P-OP1	-7.68	98.79	105.70
30	i	773	G	O5'-P-OP2	-7.65	98.81	105.70
1	A	2452	C	O5'-P-OP2	-7.65	98.81	105.70
3	C	258	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	A	1025	G	O3'-P-O5'	7.61	118.45	104.00
1	A	1643	G	O3'-P-O5'	-7.57	89.61	104.00
1	A	2463	C	O5'-P-OP2	-7.48	98.97	105.70
1	A	2445	G	C2-N3-C4	7.48	115.64	111.90
1	A	959	A	O5'-P-OP1	-7.47	98.98	105.70
1	A	395	U	O4'-C1'-N1	7.42	114.14	108.20
1	A	1518	C	O3'-P-O5'	-7.42	89.90	104.00
1	A	370	G	O3'-P-O5'	-7.39	89.95	104.00
1	A	205	G	O5'-P-OP1	7.38	119.56	110.70
1	A	2608	G	O5'-P-OP2	-7.37	99.07	105.70
1	A	424	G	O5'-P-OP1	7.32	119.48	110.70
1	A	1905	C	O3'-P-O5'	-7.30	90.12	104.00
1	A	476	G	O5'-P-OP2	-7.30	99.13	105.70
30	i	1517	G	O5'-P-OP2	-7.30	99.13	105.70
30	i	1406	U	O5'-P-OP2	-7.29	99.14	105.70
1	A	2442	C	O5'-P-OP2	-7.25	99.17	105.70
1	A	1847	A	O3'-P-O5'	-7.24	90.25	104.00
1	A	2602	A	O5'-P-OP1	7.23	119.37	110.70
1	A	196	A	O5'-P-OP1	-7.21	99.21	105.70
1	A	2048	G	O5'-P-OP2	-7.17	99.24	105.70
1	A	1702	G	O3'-P-O5'	-7.09	90.53	104.00
1	A	1936	A	O4'-C1'-N9	7.03	113.83	108.20
30	i	561	U	O3'-P-O5'	-7.02	90.65	104.00
1	A	204	A	O3'-P-O5'	-6.99	90.72	104.00
1	A	747	U	O3'-P-O5'	-6.99	90.73	104.00
1	A	2353	G	O3'-P-O5'	-6.96	90.77	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	958	U	OP1-P-O3’	6.93	120.44	105.20
1	A	2278	A	O3’-P-O5’	-6.90	90.90	104.00
48	5	57	C	C2’-C3’-O3’	6.89	124.72	113.70
2	B	29	A	O5’-P-OP2	-6.89	99.50	105.70
1	A	198	C	O5’-P-OP1	-6.88	99.51	105.70
1	A	704	G	O4’-C1’-N9	6.85	113.68	108.20
1	A	1828	G	C5-C6-O6	-6.83	124.50	128.60
1	A	2006	C	O5’-P-OP2	-6.81	99.57	105.70
30	i	1201	A	P-O3’-C3’	6.79	127.85	119.70
30	i	251	G	O4’-C1’-N9	-6.73	102.82	108.20
1	A	2249	U	OP2-P-O3’	6.72	119.98	105.20
1	A	2578	G	O5’-P-OP1	-6.70	99.67	105.70
2	B	15	A	O4’-C1’-N9	6.70	113.56	108.20
1	A	2824	C	O5’-P-OP2	-6.70	99.67	105.70
1	A	1355	G	C4-C5-N7	-6.68	108.13	110.80
30	i	326	G	C5-C6-O6	-6.67	124.60	128.60
1	A	2524	G	O3’-P-O5’	-6.66	91.36	104.00
1	A	2545	G	O5’-P-OP2	-6.65	99.71	105.70
1	A	745	G	C5-C6-O6	-6.64	124.61	128.60
30	i	292	G	O5’-P-OP2	-6.61	99.75	105.70
1	A	2076	U	O4’-C1’-N1	6.61	113.48	108.20
1	A	1355	G	C5-C6-O6	6.55	132.53	128.60
30	i	352	C	O3’-P-O5’	-6.53	91.60	104.00
30	i	1279	G	O3’-P-O5’	-6.49	91.66	104.00
1	A	974	G	C5-C6-O6	-6.49	124.71	128.60
30	i	586	C	O5’-P-OP2	-6.46	99.88	105.70
1	A	2556	C	O5’-P-OP2	-6.46	99.89	105.70
1	A	1971	U	O3’-P-O5’	-6.45	91.75	104.00
48	6	47	U	P-O3’-C3’	6.44	127.43	119.70
48	6	56	C	C2’-C3’-O3’	6.44	124.00	113.70
1	A	372	G	O5’-P-OP1	-6.43	99.91	105.70
1	A	781	A	O3’-P-O5’	-6.43	91.78	104.00
1	A	831	G	O5’-P-OP1	-6.40	99.94	105.70
1	A	760	G	O5’-P-OP2	-6.38	99.96	105.70
1	A	1252	G	O3’-P-O5’	6.37	116.11	104.00
1	A	2354	C	O3’-P-O5’	-6.36	91.91	104.00
1	A	2391	G	O4’-C1’-N9	6.36	113.29	108.20
1	A	974	G	N1-C6-O6	6.36	123.72	119.90
1	A	2850	A	O5’-P-OP1	6.36	118.33	110.70
1	A	984	A	O4’-C1’-N9	6.35	113.28	108.20
1	A	1913	A	C2’-C3’-O3’	6.32	123.82	113.70
30	i	1494	G	O5’-P-OP1	6.31	118.27	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	5	48	U	O3'-P-O5'	-6.28	92.07	104.00
1	A	1355	G	N9-C4-C5	6.28	107.91	105.40
30	i	828	U	O5'-P-OP2	-6.28	100.05	105.70
1	A	2606	C	O5'-P-OP2	-6.27	100.05	105.70
30	i	1497	G	O5'-P-OP2	-6.27	100.06	105.70
30	i	1199	U	O3'-P-O5'	-6.26	92.10	104.00
30	i	1500	A	O5'-P-OP2	-6.25	100.08	105.70
1	A	46	G	O5'-P-OP2	-6.23	100.09	105.70
1	A	2064	C	OP2-P-O3'	6.22	118.89	105.20
1	A	528	A	O5'-P-OP1	6.21	118.16	110.70
1	A	1185	G	O5'-P-OP2	-6.21	100.11	105.70
1	A	667	U	O3'-P-O5'	-6.21	92.20	104.00
1	A	455	C	O5'-P-OP2	-6.20	100.12	105.70
1	A	2715	C	O5'-P-OP2	-6.19	100.13	105.70
1	A	464	U	O5'-P-OP2	-6.18	100.14	105.70
1	A	742	A	OP2-P-O3'	6.18	118.80	105.20
1	A	1969	A	O3'-P-O5'	-6.17	92.28	104.00
1	A	2074	U	O5'-P-OP2	-6.15	100.16	105.70
30	i	1190	G	O3'-P-O5'	-6.14	92.33	104.00
1	A	1913	A	P-O3'-C3'	6.13	127.06	119.70
30	i	986	U	O3'-P-O5'	-6.13	92.36	104.00
1	A	759	G	O5'-P-OP2	-6.13	100.19	105.70
1	A	1355	G	C5-C6-N1	-6.12	108.44	111.50
30	i	297	G	O3'-P-O5'	-6.08	92.45	104.00
1	A	404	A	P-O3'-C3'	6.07	126.99	119.70
1	A	1802	A	O5'-P-OP1	-6.07	100.23	105.70
30	i	124	C	O5'-P-OP2	-6.07	100.23	105.70
1	A	1663	G	O5'-P-OP2	-6.07	100.24	105.70
30	i	809	G	O5'-P-OP2	-6.07	100.24	105.70
1	A	2267	A	O4'-C1'-N9	-6.07	103.35	108.20
1	A	1378	A	O4'-C1'-N9	6.05	113.04	108.20
1	A	2496	C	P-O5'-C5'	-6.05	111.22	120.90
1	A	1975	G	O5'-P-OP2	-6.04	100.26	105.70
1	A	1131	G	O3'-P-O5'	-6.04	92.52	104.00
1	A	1906	G	O3'-P-O5'	-6.03	92.54	104.00
30	i	1530	G	O4'-C1'-N9	6.02	113.01	108.20
1	A	2747	G	O3'-P-O5'	-6.01	92.58	104.00
1	A	310	A	O3'-P-O5'	-6.01	92.58	104.00
1	A	748	G	C1'-O4'-C4'	-6.01	105.09	109.90
1	A	1452	G	O3'-P-O5'	-6.00	92.60	104.00
30	i	115	G	C4'-C3'-O3'	6.00	125.00	113.00
1	A	995	C	O5'-P-OP2	-5.98	100.32	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1324	G	O4'-C1'-N9	5.98	112.98	108.20
1	A	857	G	OP2-P-O3'	5.97	118.33	105.20
30	i	115	G	O3'-P-O5'	5.96	115.33	104.00
1	A	1925	C	O3'-P-O5'	-5.93	92.74	104.00
1	A	2389	G	O5'-P-OP2	-5.92	100.37	105.70
1	A	1210	G	C5-N7-C8	-5.91	101.35	104.30
1	A	31	C	O5'-P-OP2	-5.91	100.38	105.70
1	A	1800	C	O5'-P-OP2	-5.90	100.39	105.70
30	i	1405	G	OP2-P-O3'	5.90	118.17	105.20
1	A	370	G	O4'-C1'-N9	-5.89	103.49	108.20
1	A	479	A	C3'-C2'-C1'	-5.88	96.79	101.50
1	A	1358	G	O3'-P-O5'	-5.88	92.83	104.00
2	B	8	C	O3'-P-O5'	-5.88	92.83	104.00
1	A	2033	A	O5'-P-OP1	5.86	117.73	110.70
1	A	1936	A	C1'-O4'-C4'	-5.85	105.22	109.90
1	A	923	G	O5'-P-OP2	-5.84	100.44	105.70
1	A	1948	G	O5'-P-OP2	-5.80	100.48	105.70
1	A	2689	U	C5-C6-N1	-5.80	119.80	122.70
1	A	2026	U	O3'-P-O5'	-5.80	92.98	104.00
1	A	1706	C	O4'-C1'-N1	5.80	112.84	108.20
1	A	2069	G	C5-N7-C8	-5.79	101.41	104.30
1	A	2060	A	O3'-P-O5'	5.78	114.99	104.00
1	A	2445	G	N1-C2-N2	5.78	121.40	116.20
1	A	2873	A	C1'-O4'-C4'	-5.77	105.28	109.90
1	A	784	G	P-O3'-C3'	5.76	126.61	119.70
1	A	1261	C	O5'-P-OP2	-5.76	100.52	105.70
1	A	1265	A	O3'-P-O5'	5.76	114.94	104.00
1	A	2011	U	O5'-P-OP2	-5.75	100.52	105.70
1	A	2409	G	O3'-P-O5'	-5.75	93.07	104.00
1	A	792	A	O5'-P-OP2	-5.74	100.54	105.70
30	i	52	C	OP2-P-O3'	5.73	117.81	105.20
1	A	1138	G	O3'-P-O5'	5.73	114.88	104.00
12	M	16	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	A	745	G	N3-C2-N2	-5.72	115.89	119.90
1	A	967	U	O3'-P-O5'	-5.72	93.12	104.00
30	i	1228	C	O5'-P-OP2	-5.72	100.55	105.70
1	A	242	G	C3'-C2'-C1'	-5.70	96.94	101.50
37	s	122	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	1971	U	O4'-C1'-N1	5.68	112.75	108.20
30	i	816	A	O3'-P-O5'	-5.68	93.22	104.00
1	A	2641	G	C4'-C3'-C2'	-5.67	96.92	102.60
30	i	1362	A	OP2-P-O3'	5.67	117.67	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	15	A	C3'-C2'-C1'	-5.67	96.97	101.50
30	i	1367	C	O3'-P-O5'	-5.66	93.24	104.00
1	A	1896	G	O3'-P-O5'	-5.66	93.25	104.00
1	A	1929	G	O5'-P-OP1	5.65	117.48	110.70
1	A	1025	G	O4'-C1'-N9	-5.65	103.68	108.20
1	A	1983	G	OP2-P-O3'	5.64	117.61	105.20
1	A	2448	A	O5'-P-OP1	-5.64	100.62	105.70
3	C	221	ARG	NE-CZ-NH1	5.59	123.10	120.30
1	A	2249	U	O5'-P-OP2	-5.59	100.67	105.70
1	A	1133	A	C1'-O4'-C4'	-5.59	105.43	109.90
30	i	727	G	O5'-P-OP2	-5.58	100.67	105.70
1	A	72	U	C3'-C2'-C1'	-5.58	97.04	101.50
23	X	28	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	A	62	U	O3'-P-O5'	-5.56	93.43	104.00
14	O	102	ARG	NE-CZ-NH2	5.56	123.08	120.30
1	A	371	A	O5'-P-OP2	5.56	117.37	110.70
1	A	595	C	O5'-P-OP2	-5.55	100.70	105.70
1	A	2529	G	O4'-C1'-N9	-5.55	103.76	108.20
30	i	835	U	O3'-P-O5'	-5.55	93.45	104.00
37	s	127	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	376	G	O3'-P-O5'	-5.54	93.47	104.00
1	A	2595	G	O5'-P-OP2	-5.54	100.71	105.70
1	A	1939	U	O4'-C1'-N1	5.54	112.63	108.20
1	A	538	A	O5'-P-OP2	-5.53	100.72	105.70
30	i	827	U	O3'-P-O5'	5.53	114.50	104.00
1	A	729	G	C1'-O4'-C4'	-5.52	105.48	109.90
16	Q	58	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	2830	C	O5'-P-OP2	-5.51	100.75	105.70
1	A	2296	U	OP1-P-O3'	5.49	117.29	105.20
1	A	1890	A	O5'-P-OP2	-5.49	100.76	105.70
1	A	1142	A	O4'-C1'-N9	5.49	112.59	108.20
1	A	1154	G	O3'-P-O5'	-5.48	93.58	104.00
1	A	1638	C	OP2-P-O3'	5.48	117.25	105.20
30	i	356	A	OP1-P-O3'	5.48	117.25	105.20
1	A	1737	G	O3'-P-O5'	-5.48	93.59	104.00
30	i	536	C	O5'-P-OP2	-5.47	100.78	105.70
30	i	116	A	C5-N7-C8	-5.46	101.17	103.90
1	A	529	A	O3'-P-O5'	-5.45	93.64	104.00
1	A	1339	G	O5'-P-OP2	-5.45	100.79	105.70
1	A	2073	C	O4'-C1'-N1	5.45	112.56	108.20
1	A	1808	A	O4'-C1'-N9	-5.45	103.84	108.20
30	i	652	U	O3'-P-O5'	-5.44	93.67	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	469	G	O3'-P-O5'	-5.43	93.67	104.00
30	i	879	C	OP2-P-O3'	5.43	117.16	105.20
30	i	1092	A	O3'-P-O5'	-5.43	93.67	104.00
1	A	1767	G	OP2-P-O3'	5.43	117.15	105.20
30	i	820	U	O5'-P-OP2	-5.43	100.82	105.70
1	A	2447	G	O5'-P-OP1	-5.42	100.82	105.70
1	A	2030	A	C5-C6-N6	5.41	128.03	123.70
1	A	2879	A	O3'-P-O5'	-5.41	93.72	104.00
1	A	18	U	O5'-P-OP2	-5.40	100.84	105.70
1	A	2356	U	O3'-P-O5'	-5.40	93.73	104.00
1	A	2484	G	C4'-C3'-C2'	-5.40	97.20	102.60
30	i	126	G	O3'-P-O5'	-5.40	93.74	104.00
1	A	513	A	O5'-P-OP2	-5.40	100.84	105.70
1	A	1546	G	OP1-P-O3'	5.39	117.06	105.20
30	i	7	A	C1'-O4'-C4'	-5.39	105.59	109.90
1	A	1024	G	C5-C6-O6	-5.37	125.38	128.60
30	i	263	A	O3'-P-O5'	-5.37	93.81	104.00
1	A	2493	U	O3'-P-O5'	-5.36	93.81	104.00
1	A	2279	G	O3'-P-O5'	-5.36	93.82	104.00
1	A	745	G	C6-N1-C2	-5.36	121.89	125.10
1	A	1502	A	O3'-P-O5'	-5.36	93.83	104.00
1	A	2003	A	O3'-P-O5'	-5.35	93.83	104.00
30	i	1239	A	O3'-P-O5'	-5.35	93.83	104.00
30	i	1237	C	OP1-P-O3'	5.35	116.97	105.20
30	i	354	G	OP2-P-O3'	5.35	116.96	105.20
1	A	2282	G	O4'-C1'-N9	5.33	112.47	108.20
1	A	1135	C	OP1-P-O3'	5.32	116.91	105.20
30	i	352	C	OP2-P-O3'	5.32	116.90	105.20
34	o	2	PRO	CA-N-CD	-5.32	104.05	111.50
1	A	242	G	O3'-P-O5'	-5.32	93.90	104.00
30	i	1331	G	O4'-C1'-N9	5.32	112.45	108.20
1	A	2876	G	O5'-P-OP2	-5.32	100.92	105.70
30	i	691	G	O5'-P-OP2	-5.31	100.92	105.70
30	i	671	G	O5'-P-OP2	-5.31	100.92	105.70
1	A	2519	U	O3'-P-O5'	-5.30	93.93	104.00
2	B	16	G	O3'-P-O5'	-5.30	93.94	104.00
1	A	1130	U	O4'-C1'-N1	5.29	112.43	108.20
30	i	916	U	O5'-P-OP2	-5.28	100.94	105.70
1	A	2285	C	O4'-C1'-N1	5.28	112.43	108.20
30	i	872	A	C1'-O4'-C4'	-5.28	105.68	109.90
1	A	512	G	C1'-O4'-C4'	-5.28	105.68	109.90
1	A	1957	C	OP2-P-O3'	5.27	116.80	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	355	C	O3'-P-O5'	-5.27	93.98	104.00
30	i	901	A	O3'-P-O5'	-5.27	93.98	104.00
1	A	542	C	O3'-P-O5'	-5.27	93.99	104.00
1	A	2464	G	C2-N3-C4	-5.26	109.27	111.90
1	A	1765	U	OP2-P-O3'	5.26	116.78	105.20
1	A	2871	U	O3'-P-O5'	-5.25	94.02	104.00
1	A	1962	C	N3-C4-N4	-5.25	114.33	118.00
1	A	737	C	O3'-P-O5'	-5.25	94.03	104.00
1	A	2604	U	O4'-C1'-N1	5.24	112.39	108.20
30	i	243	A	OP1-P-O3'	5.24	116.74	105.20
1	A	2286	G	C5-N7-C8	-5.24	101.68	104.30
1	A	1253	A	O4'-C1'-N9	-5.24	104.01	108.20
30	i	362	G	O3'-P-O5'	-5.24	94.05	104.00
1	A	2601	C	O3'-P-O5'	-5.23	94.06	104.00
1	A	690	G	O5'-P-OP2	-5.23	100.99	105.70
1	A	994	C	OP2-P-O3'	5.22	116.70	105.20
1	A	2619	C	OP2-P-O3'	5.22	116.69	105.20
1	A	2453	A	O4'-C1'-N9	5.22	112.38	108.20
48	6	43	U	O4'-C1'-N1	5.21	112.37	108.20
1	A	2146	C	P-O3'-C3'	5.21	125.95	119.70
30	i	522	C	O5'-P-OP1	-5.21	101.01	105.70
3	C	11	PRO	N-CA-C	-5.21	98.56	112.10
1	A	1359	A	O3'-P-O5'	-5.21	94.11	104.00
1	A	1926	U	P-O5'-C5'	-5.21	112.57	120.90
1	A	1962	C	C2-N1-C1'	-5.20	113.08	118.80
1	A	2860	A	O3'-P-O5'	-5.20	94.12	104.00
1	A	942	G	O5'-P-OP2	-5.20	101.02	105.70
1	A	1674	G	C3'-C2'-C1'	5.19	105.65	101.50
1	A	2365	G	O5'-P-OP2	-5.18	101.03	105.70
30	i	690	G	O5'-P-OP2	-5.18	101.03	105.70
49	7	15	G	P-O3'-C3'	5.18	125.92	119.70
1	A	2267	A	OP1-P-O3'	5.18	116.59	105.20
1	A	2732	G	O4'-C1'-N9	5.17	112.34	108.20
1	A	784	G	OP1-P-O3'	5.17	116.58	105.20
1	A	2464	G	N9-C4-C5	-5.17	103.33	105.40
1	A	2495	G	OP2-P-O3'	5.17	116.58	105.20
1	A	199	A	C1'-O4'-C4'	-5.16	105.77	109.90
1	A	1939	U	C1'-O4'-C4'	-5.16	105.77	109.90
1	A	1394	U	O4'-C1'-N1	-5.16	104.07	108.20
1	A	323	C	O4'-C1'-N1	5.16	112.32	108.20
1	A	1827	U	O5'-P-OP2	-5.15	101.06	105.70
1	A	205	G	C3'-C2'-C1'	-5.15	97.38	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	i	977	A	O3'-P-O5'	-5.15	94.22	104.00
1	A	2430	A	C1'-O4'-C4'	-5.15	105.78	109.90
30	i	264	C	OP1-P-O3'	5.14	116.52	105.20
1	A	419	U	O3'-P-O5'	-5.14	94.23	104.00
1	A	1966	A	P-O3'-C3'	-5.14	113.53	119.70
1	A	2610	C	OP1-P-O3'	5.13	116.50	105.20
1	A	2566	A	O4'-C1'-N9	5.13	112.31	108.20
1	A	454	A	O4'-C1'-N9	-5.13	104.10	108.20
1	A	1808	A	O5'-P-OP2	-5.13	101.08	105.70
1	A	329	G	O5'-P-OP1	5.12	116.85	110.70
1	A	800	A	O4'-C1'-N9	-5.12	104.11	108.20
1	A	1947	C	OP2-P-O3'	5.11	116.44	105.20
48	5	3	G	C2'-C3'-O3'	5.11	121.87	113.70
30	i	786	G	O3'-P-O5'	-5.11	94.30	104.00
1	A	824	U	O5'-P-OP2	-5.10	101.11	105.70
1	A	2387	U	O5'-P-OP2	-5.10	101.11	105.70
1	A	84	A	C3'-C2'-C1'	-5.10	97.42	101.50
1	A	1962	C	C5-C4-N4	5.10	123.77	120.20
30	i	110	C	P-O5'-C5'	-5.10	112.74	120.90
30	i	408	A	C3'-C2'-C1'	5.09	105.58	101.50
1	A	202	U	O4'-C1'-N1	5.09	112.27	108.20
1	A	1645	G	OP1-P-O3'	5.09	116.39	105.20
30	i	1359	C	OP2-P-O3'	5.09	116.39	105.20
1	A	555	G	O3'-P-O5'	-5.08	94.34	104.00
30	i	12	U	O3'-P-O5'	-5.08	94.34	104.00
30	i	262	A	O3'-P-O5'	-5.08	94.34	104.00
1	A	84	A	O5'-P-OP2	5.07	116.79	110.70
1	A	1128	G	C1'-O4'-C4'	-5.07	105.84	109.90
1	A	1773	A	O4'-C1'-N9	5.06	112.25	108.20
1	A	2324	U	O3'-P-O5'	5.05	113.60	104.00
1	A	2286	G	C3'-C2'-C1'	5.05	105.54	101.50
1	A	1396	U	OP1-P-O3'	5.05	116.31	105.20
1	A	680	C	C6-N1-C2	-5.04	118.28	120.30
30	i	1429	A	O3'-P-O5'	-5.04	94.42	104.00
1	A	1902	C	O5'-P-OP2	-5.04	101.16	105.70
30	i	1352	C	O3'-P-O5'	-5.04	94.42	104.00
30	i	194	C	O3'-P-O5'	-5.04	94.42	104.00
48	6	46	G	C3'-C2'-C1'	5.04	105.53	101.50
1	A	2497	A	OP1-P-O3'	5.03	116.27	105.20
1	A	198	C	N3-C4-C5	-5.02	119.89	121.90
2	B	43	C	O3'-P-O5'	5.02	113.54	104.00
1	A	726	G	O3'-P-O5'	-5.02	94.47	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	i	331	G	OP1-P-O3'	5.02	116.24	105.20
1	A	907	G	O3'-P-O5'	-5.02	94.47	104.00
1	A	125	A	O5'-P-OP2	-5.01	101.19	105.70
30	i	1286	U	O3'-P-O5'	-5.01	94.47	104.00
30	i	322	C	O3'-P-O5'	-5.01	94.47	104.00
30	i	643	C	O3'-P-O5'	-5.01	94.48	104.00
1	A	855	G	O3'-P-O5'	-5.01	94.48	104.00
1	A	1342	A	O5'-P-OP2	-5.01	101.19	105.70
1	A	2366	A	O5'-P-OP2	-5.01	101.19	105.70
1	A	255	A	O4'-C1'-N9	5.01	112.21	108.20
1	A	1297	C	OP2-P-O3'	5.01	116.21	105.20
1	A	254	G	O3'-P-O5'	5.00	113.51	104.00
1	A	2447	G	C3'-C2'-C1'	-5.00	97.50	101.50

There are no chirality outliers.

All (51) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1025	G	Sidechain
1	A	250	G	Sidechain
1	A	2595	G	Sidechain
1	A	395	U	Sidechain
1	A	463	G	Sidechain
1	A	512	G	Sidechain
3	C	109	GLY	Peptide
3	C	156	ARG	Sidechain
3	C	177	ARG	Sidechain
3	C	221	ARG	Sidechain
3	C	258	ARG	Sidechain
3	C	271	ARG	Sidechain
4	D	128	ARG	Sidechain
4	D	33	ARG	Sidechain
5	E	88	ARG	Sidechain
9	J	120	ARG	Sidechain
11	L	59	ARG	Sidechain
12	M	16	ARG	Sidechain
12	M	55	ARG	Sidechain
13	N	63	ARG	Sidechain
14	O	9	ARG	Sidechain
15	P	109	ARG	Sidechain
16	Q	51	ARG	Sidechain
17	R	79	ARG	Sidechain

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Mol	Chain	Res	Type	Group
17	R	80	ARG	Sidechain
22	W	20	ARG	Sidechain
22	W	39	ARG	Sidechain
22	W	55	ARG	Sidechain
22	W	77	ARG	Sidechain
23	X	16	ASN	Peptide
23	X	3	ARG	Sidechain
26	a	40	ARG	Sidechain
27	b	50	LYS	Peptide
27	b	6	ARG	Sidechain
29	d	13	ARG	Sidechain
32	m	138	ARG	Sidechain
32	m	93	ARG	Sidechain
33	n	38	ARG	Sidechain
33	n	79	ARG	Sidechain
36	q	123	ARG	Sidechain
36	q	124	ARG	Sidechain
36	q	33	ARG	Sidechain
36	q	45	ARG	Sidechain
36	q	99	ARG	Sidechain
38	t	114	ARG	Sidechain
38	t	36	ARG	Sidechain
38	t	83	ARG	Sidechain
38	t	99	ARG	Sidechain
39	u	101	ARG	Sidechain
39	u	107	ARG	Sidechain
39	u	90	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	60998	0	30646	50	0
2	B	2529	0	1281	1	0
3	C	2082	0	2153	3	0
4	D	1565	0	1616	9	0
5	E	1552	0	1619	4	0
6	F	1410	0	1444	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	G	1285	0	1341	3	0
8	H	359	0	381	1	0
9	J	1129	0	1162	4	0
10	K	938	0	1012	5	0
11	L	1045	0	1117	13	0
12	M	1074	0	1157	2	0
13	N	945	0	989	1	0
14	O	875	0	906	2	0
15	P	900	0	945	5	0
16	Q	941	0	1014	3	0
17	R	816	0	839	5	0
18	S	857	0	922	8	0
19	T	730	0	795	1	0
20	U	779	0	830	2	0
21	V	753	0	780	3	0
22	W	628	0	642	3	0
23	X	625	0	652	1	0
24	Y	509	0	543	2	0
25	Z	435	0	470	1	0
26	a	444	0	458	0	0
27	b	395	0	422	0	0
28	c	377	0	418	0	0
29	d	504	0	572	0	0
30	i	33015	0	16604	0	0
31	j	1679	0	1705	0	0
32	m	1105	0	1148	0	0
33	n	817	0	808	0	0
34	o	1181	0	1238	0	0
35	p	979	0	1031	0	0
36	q	1001	0	1044	0	0
37	s	877	0	887	0	0
38	t	922	0	978	0	0
39	u	867	0	921	0	0
40	v	774	0	824	0	0
41	w	687	0	702	0	0
42	y	648	0	691	0	0
43	z	455	0	478	0	0
44	1	594	0	610	1	0
45	2	612	0	650	0	0
46	3	346	0	369	3	0
47	4	214	0	111	1	0
48	5	1644	0	832	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	6	1648	0	831	2	0
49	7	1618	0	823	0	0
50	e	302	0	340	0	0
51	f	46	0	53	0	0
52	6	1	0	0	0	0
52	A	178	0	0	0	0
52	B	5	0	0	0	0
52	C	1	0	0	0	0
52	D	1	0	0	0	0
52	a	1	0	0	0	0
52	i	61	0	0	0	0
53	A	83	0	0	0	0
53	C	3	0	0	0	0
53	E	1	0	0	0	0
53	U	1	0	0	0	0
53	i	37	0	0	0	0
53	n	1	0	0	0	0
53	u	1	0	0	0	0
54	5	7	0	7	1	0
55	e	1	0	0	0	0
56	4	3	0	0	0	0
56	5	3	0	0	0	0
56	6	2	0	0	0	0
56	A	1006	0	0	0	0
56	B	10	0	0	0	0
56	C	14	0	0	0	0
56	D	2	0	0	0	0
56	E	3	0	0	0	0
56	L	4	0	0	0	0
56	N	3	0	0	0	0
56	T	1	0	0	0	0
56	a	4	0	0	0	0
56	d	4	0	0	0	0
56	f	3	0	0	0	0
56	i	176	0	0	0	0
56	s	1	0	0	0	0
All	All	141132	0	90811	119	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 1.

All (119) 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)
46:3:37:PHE:O	46:3:41:PRO:HD2	1.76	0.84
48:5:8:U:H5	48:5:14:A:N7	1.86	0.73
18:S:59:GLU:HB3	18:S:66:ILE:HD11	1.78	0.65
1:A:1824:G:O2'	3:C:252:THR:HG21	1.97	0.64
54:5:101:PRO:N	48:6:76:A:HO2'	1.97	0.62
20:U:72:ILE:HD12	20:U:96:PHE:CE1	2.37	0.60
48:5:8:U:O5'	48:5:8:U:O2	2.20	0.59
11:L:77:ILE:HD13	11:L:108:ALA:HB1	1.85	0.58
5:E:4:VAL:HA	5:E:11:ALA:HA	1.86	0.58
16:Q:88:VAL:HG13	17:R:48:LYS:HE2	1.86	0.57
1:A:636:G:C6	11:L:111:ILE:HD11	2.40	0.56
1:A:2324:U:H3'	1:A:2325:G:H5"	1.86	0.56
1:A:1266:G:H5"	18:S:15:GLN:HE22	1.71	0.56
1:A:1993:U:H4'	4:D:133:THR:HG22	1.88	0.55
1:A:2032:G:O2'	4:D:150:GLN:NE2	2.39	0.55
21:V:6:ALA:HB1	21:V:40:ILE:HG23	1.88	0.54
18:S:72:THR:HG21	18:S:108:SER:HB3	1.89	0.54
3:C:29:PRO:HG2	3:C:34:LEU:HD11	1.89	0.54
20:U:7:ARG:O	20:U:25:VAL:O	2.26	0.54
44:1:31:LEU:HB2	44:1:49:ILE:HG22	1.89	0.53
8:H:5:LEU:HD11	8:H:12:LEU:HD23	1.90	0.53
1:A:811:U:H2'	11:L:21:ARG:HA	1.92	0.51
3:C:107:PRO:HD2	3:C:110:LEU:HD22	1.92	0.51
4:D:156:PHE:CE1	9:J:81:ILE:HD13	2.45	0.51
46:3:37:PHE:O	46:3:41:PRO:CD	2.52	0.51
1:A:1932:A:H2'	1:A:1933:G:O4'	2.11	0.51
17:R:51:VAL:HB	17:R:52:PRO:HD2	1.92	0.50
6:F:25:VAL:O	6:F:28:VAL:HG12	2.12	0.50
11:L:85:VAL:HB	11:L:94:THR:HG22	1.93	0.50
18:S:59:GLU:HA	18:S:64:ALA:HA	1.94	0.50
9:J:110:PRO:O	9:J:115:GLY:HA3	2.12	0.49
5:E:149:ILE:HG22	5:E:192:ALA:HB1	1.94	0.48
15:P:43:PHE:CE1	15:P:63:LYS:HE2	2.47	0.48
1:A:2273:A:H2'	1:A:2274:A:C8	2.46	0.48
11:L:77:ILE:CD1	11:L:108:ALA:HB1	2.42	0.48
11:L:95:LEU:HD11	11:L:125:LEU:HD21	1.95	0.48
1:A:954:G:OP2	12:M:16:ARG:NH2	2.38	0.48
17:R:48:LYS:HE3	17:R:49:ILE:O	2.14	0.47
18:S:55:ILE:HG23	18:S:66:ILE:HD12	1.96	0.47
5:E:5:LEU:HD23	5:E:120:VAL:HG12	1.96	0.47
4:D:4:LEU:HD22	4:D:32:ASN:HB2	1.97	0.47
11:L:110:VAL:O	11:L:111:ILE:O	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:125:TYR:OH	9:J:132:HIS:NE2	2.44	0.47
1:A:1296:G:OP1	1:A:2709:G:O2'	2.26	0.47
11:L:77:ILE:HD11	11:L:101:ILE:HG21	1.97	0.47
4:D:35:THR:HG22	4:D:73:VAL:HG21	1.96	0.46
7:G:164:TYR:HB2	7:G:167:GLU:HG3	1.97	0.46
48:5:8:U:C5	48:5:14:A:N7	2.75	0.46
11:L:70:LYS:O	11:L:74:THR:HG23	2.15	0.46
1:A:1853:A:N1	1:A:2087:G:H1'	2.30	0.46
1:A:2395:C:H2'	1:A:2396:G:O4'	2.16	0.46
11:L:77:ILE:N	11:L:77:ILE:HD12	2.30	0.46
1:A:494:G:H4'	18:S:6:LYS:HB2	1.98	0.46
1:A:1980:G:O2'	1:A:1982:U:OP2	2.33	0.46
13:N:79:LEU:O	13:N:80:PHE:HB2	2.16	0.46
1:A:493:G:H2'	1:A:494:G:O4'	2.16	0.46
21:V:4:ILE:CG2	21:V:42:LEU:HD22	2.46	0.46
1:A:1434:A:H2'	1:A:1435:G:C8	2.50	0.45
1:A:2532:G:O2'	1:A:2657:A:N1	2.49	0.45
7:G:24:ILE:HD11	7:G:43:VAL:HG11	1.97	0.45
10:K:91:SER:O	10:K:93:GLN:N	2.49	0.45
1:A:1378:A:O2'	1:A:1380:G:N7	2.50	0.45
5:E:189:THR:O	5:E:192:ALA:HB3	2.16	0.44
1:A:1434:A:H2'	1:A:1435:G:H8	1.81	0.44
1:A:118:A:N3	1:A:178:G:H1'	2.33	0.44
1:A:788:A:OP1	1:A:790:U:H5	2.01	0.44
1:A:1007:C:OP1	9:J:39:LYS:HD2	2.18	0.44
19:T:8:LEU:HD11	24:Y:22:LEU:HB2	2.00	0.44
1:A:476:G:H4'	1:A:502:A:N1	2.33	0.44
11:L:74:THR:HG22	11:L:107:PHE:HB2	1.99	0.44
1:A:636:G:C5	11:L:111:ILE:HD11	2.53	0.43
14:O:34:HIS:HA	14:O:53:THR:OG1	2.17	0.43
10:K:76:VAL:HG12	15:P:73:VAL:HB	2.00	0.43
1:A:1182:G:H2'	1:A:1183:U:O4'	2.19	0.43
1:A:2356:U:H4'	22:W:20:ARG:HG3	2.01	0.43
1:A:1721:G:N2	1:A:1738:G:O2'	2.52	0.43
25:Z:24:LEU:HD11	25:Z:54:MET:CE	2.49	0.43
16:Q:76:TYR:CZ	16:Q:80:ILE:HG13	2.54	0.43
1:A:411:G:P	1:A:2407:A:OP2	2.77	0.42
1:A:207:A:H2'	1:A:208:C:O4'	2.19	0.42
24:Y:7:ARG:O	24:Y:8:GLU:C	2.58	0.42
4:D:12:THR:CG2	15:P:5:ILE:HG23	2.49	0.42
1:A:644:A:H2'	1:A:645:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1664:A:N3	10:K:67:LYS:NZ	2.68	0.42
1:A:1340:U:C5	1:A:1603:A:C8	3.07	0.42
18:S:20:VAL:HG11	18:S:44:ALA:HA	2.01	0.42
1:A:639:U:H2'	1:A:640:C:C6	2.55	0.42
1:A:2019:A:H4'	16:Q:34:VAL:HG21	2.02	0.42
1:A:2038:G:H2'	1:A:2039:U:O4'	2.20	0.42
1:A:1141:U:H4'	1:A:1142:A:O4'	2.20	0.41
6:F:57:LEU:HD23	6:F:57:LEU:HA	1.94	0.41
10:K:63:VAL:HG12	10:K:107:LEU:HD11	2.01	0.41
46:3:16:LEU:H	46:3:16:LEU:HG	1.51	0.41
1:A:2063:C:O2	1:A:2450:A:N1	2.53	0.41
1:A:1020:A:N1	1:A:1141:U:O2'	2.43	0.41
1:A:1614:A:C2	18:S:93:ALA:HB2	2.55	0.41
7:G:121:ILE:HD12	7:G:141:ILE:CG2	2.50	0.41
10:K:41:ILE:HD11	10:K:86:LEU:HD22	2.02	0.41
1:A:861:A:H2'	1:A:862:G:O4'	2.20	0.41
17:R:5:PHE:HB3	17:R:59:ILE:HD12	2.01	0.41
1:A:1320:C:N3	1:A:1331:G:O6	2.54	0.41
1:A:1993:U:H4'	4:D:133:THR:CG2	2.50	0.41
15:P:106:LYS:O	15:P:109:ARG:HG2	2.21	0.41
23:X:7:VAL:HG23	23:X:51:VAL:HG12	2.02	0.41
1:A:1913:A:C6	48:5:39:A:H5'	2.56	0.41
4:D:5:VAL:HB	4:D:32:ASN:HD21	1.85	0.41
22:W:37:ILE:HG21	22:W:80:ILE:HG21	2.02	0.41
1:A:12:U:O2	1:A:12:U:H2'	2.21	0.41
4:D:5:VAL:H	4:D:32:ASN:ND2	2.18	0.41
17:R:14:VAL:HG21	17:R:20:VAL:HG21	2.03	0.41
47:4:18:G:H1	48:6:34:U:H3	1.69	0.41
1:A:2295:C:OP2	14:O:9:ARG:NH2	2.55	0.40
11:L:59:ARG:HG2	11:L:59:ARG:HH11	1.87	0.40
1:A:1794:A:H2'	1:A:1795:C:C6	2.57	0.40
1:A:1754:A:C8	15:P:94:LYS:CE	3.04	0.40
2:B:76:G:OP1	21:V:9:ARG:NH1	2.47	0.40
12:M:66:ARG:NH1	12:M:104:GLU:OE2	2.52	0.40
1:A:2271:G:H5'	22:W:20:ARG:HD2	2.03	0.40
1:A:2469:A:H2'	1:A:2470:G:O4'	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/273 (98%)	256 (95%)	13 (5%)	0	100	100
4	D	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
5	E	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	29	31
6	F	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
7	G	167/177 (94%)	158 (95%)	9 (5%)	0	100	100
8	H	45/149 (30%)	42 (93%)	2 (4%)	1 (2%)	6	4
9	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
10	K	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
11	L	141/144 (98%)	133 (94%)	7 (5%)	1 (1%)	22	22
12	M	134/136 (98%)	128 (96%)	6 (4%)	0	100	100
13	N	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
14	O	112/117 (96%)	107 (96%)	5 (4%)	0	100	100
15	P	110/115 (96%)	107 (97%)	3 (3%)	0	100	100
16	Q	114/118 (97%)	112 (98%)	2 (2%)	0	100	100
17	R	101/103 (98%)	93 (92%)	8 (8%)	0	100	100
18	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
19	T	90/100 (90%)	88 (98%)	2 (2%)	0	100	100
20	U	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
21	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
22	W	82/85 (96%)	80 (98%)	2 (2%)	0	100	100
23	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
24	Y	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
25	Z	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
26	a	54/57 (95%)	51 (94%)	3 (6%)	0	100	100
27	b	46/55 (84%)	46 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	c	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
29	d	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
31	j	213/241 (88%)	187 (88%)	25 (12%)	1 (0%)	29	31
32	m	148/167 (89%)	139 (94%)	9 (6%)	0	100	100
33	n	98/135 (73%)	88 (90%)	10 (10%)	0	100	100
34	o	149/179 (83%)	136 (91%)	13 (9%)	0	100	100
35	p	127/130 (98%)	121 (95%)	6 (5%)	0	100	100
36	q	123/130 (95%)	105 (85%)	16 (13%)	2 (2%)	9	7
37	s	115/129 (89%)	106 (92%)	8 (7%)	1 (1%)	17	16
38	t	117/124 (94%)	103 (88%)	13 (11%)	1 (1%)	17	16
39	u	110/118 (93%)	100 (91%)	10 (9%)	0	100	100
40	v	92/101 (91%)	87 (95%)	3 (3%)	2 (2%)	6	4
41	w	84/89 (94%)	82 (98%)	2 (2%)	0	100	100
42	y	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
43	z	53/75 (71%)	52 (98%)	1 (2%)	0	100	100
44	1	72/92 (78%)	71 (99%)	1 (1%)	0	100	100
45	2	74/87 (85%)	71 (96%)	3 (4%)	0	100	100
46	3	40/71 (56%)	39 (98%)	1 (2%)	0	100	100
50	e	36/38 (95%)	33 (92%)	2 (6%)	1 (3%)	5	2
51	f	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	4751/5225 (91%)	4480 (94%)	260 (6%)	11 (0%)	50	55

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	E	190	ALA
11	L	111	ILE
37	s	119	ASN
40	v	23	LYS
36	q	51	PRO
36	q	91	ASP
50	e	37	GLN
8	H	15	LEU
31	j	123	ASP
38	t	17	ALA

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Mol	Chain	Res	Type
40	v	32	SER

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	C	216/218 (99%)	215 (100%)	1 (0%)	88	94
4	D	164/164 (100%)	164 (100%)	0	100	100
5	E	165/165 (100%)	164 (99%)	1 (1%)	86	93
6	F	148/150 (99%)	147 (99%)	1 (1%)	84	91
7	G	133/138 (96%)	132 (99%)	1 (1%)	81	90
8	H	38/114 (33%)	37 (97%)	1 (3%)	46	58
9	J	116/116 (100%)	115 (99%)	1 (1%)	78	88
10	K	103/104 (99%)	102 (99%)	1 (1%)	76	86
11	L	102/103 (99%)	102 (100%)	0	100	100
12	M	109/109 (100%)	107 (98%)	2 (2%)	59	72
13	N	98/103 (95%)	98 (100%)	0	100	100
14	O	84/87 (97%)	83 (99%)	1 (1%)	71	83
15	P	97/100 (97%)	96 (99%)	1 (1%)	76	86
16	Q	89/90 (99%)	89 (100%)	0	100	100
17	R	84/84 (100%)	83 (99%)	1 (1%)	71	83
18	S	93/93 (100%)	91 (98%)	2 (2%)	52	65
19	T	79/84 (94%)	79 (100%)	0	100	100
20	U	83/85 (98%)	83 (100%)	0	100	100
21	V	78/78 (100%)	78 (100%)	0	100	100
22	W	61/63 (97%)	61 (100%)	0	100	100
23	X	67/68 (98%)	67 (100%)	0	100	100
24	Y	55/55 (100%)	55 (100%)	0	100	100
25	Z	47/49 (96%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	a	47/48 (98%)	47 (100%)	0	100	100
27	b	44/49 (90%)	42 (96%)	2 (4%)	27	34
28	c	38/38 (100%)	38 (100%)	0	100	100
29	d	51/52 (98%)	50 (98%)	1 (2%)	55	69
31	j	177/199 (89%)	172 (97%)	5 (3%)	43	56
32	m	113/126 (90%)	112 (99%)	1 (1%)	78	88
33	n	87/116 (75%)	86 (99%)	1 (1%)	73	85
34	o	124/147 (84%)	122 (98%)	2 (2%)	62	76
35	p	104/105 (99%)	102 (98%)	2 (2%)	57	71
36	q	103/107 (96%)	97 (94%)	6 (6%)	20	23
37	s	90/99 (91%)	88 (98%)	2 (2%)	52	65
38	t	100/104 (96%)	95 (95%)	5 (5%)	24	30
39	u	90/96 (94%)	88 (98%)	2 (2%)	52	65
40	v	79/84 (94%)	75 (95%)	4 (5%)	24	29
41	w	73/77 (95%)	73 (100%)	0	100	100
42	y	74/78 (95%)	73 (99%)	1 (1%)	67	80
43	z	48/65 (74%)	47 (98%)	1 (2%)	53	67
44	1	65/79 (82%)	65 (100%)	0	100	100
45	2	60/66 (91%)	59 (98%)	1 (2%)	60	74
46	3	35/61 (57%)	31 (89%)	4 (11%)	5	5
50	e	34/34 (100%)	34 (100%)	0	100	100
51	f	5/5 (100%)	5 (100%)	0	100	100
All	All	3950/4255 (93%)	3896 (99%)	54 (1%)	68	80

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	43	ARG
5	E	5	LEU
6	F	83	TYR
7	G	168	VAL
8	H	5	LEU
9	J	96	ARG
10	K	98	ARG

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Mol	Chain	Res	Type
12	M	59	ARG
12	M	84	LYS
14	O	25	ARG
15	P	53	ARG
17	R	71	LYS
18	S	29	VAL
18	S	69	LEU
27	b	10	LYS
27	b	28	ARG
29	d	31	HIS
31	j	23	TRP
31	j	40	ILE
31	j	43	LEU
31	j	50	PHE
31	j	151	ILE
32	m	52	LYS
33	n	1	MET
34	o	5	ARG
34	o	131	LYS
35	p	51	VAL
35	p	67	GLN
36	q	30	ILE
36	q	46	MET
36	q	48	VAL
36	q	52	LEU
36	q	98	LEU
36	q	106	ARG
37	s	119	ASN
37	s	126	LYS
38	t	16	VAL
38	t	18	LYS
38	t	36	ARG
38	t	75	GLN
38	t	80	ILE
39	u	63	PHE
39	u	107	ARG
40	v	10	GLU
40	v	24	ARG
40	v	33	ASP
40	v	42	TRP
42	y	4	LYS
43	z	66	SER

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Mol	Chain	Res	Type
45	2	54	MET
46	3	16	LEU
46	3	17	ARG
46	3	25	LYS
46	3	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	226	ASN
4	D	32	ASN
4	D	150	GLN
5	E	94	GLN
5	E	163	ASN
7	G	143	GLN
10	K	3	GLN
13	N	62	ASN
14	O	38	GLN
18	S	15	GLN
19	T	15	HIS
20	U	66	GLN
21	V	49	ASN
23	X	16	ASN
23	X	17	ASN
24	Y	15	ASN
26	a	5	GLN
28	c	13	ASN
31	j	19	GLN
31	j	89	GLN
31	j	103	ASN
31	j	146	ASN
32	m	12	GLN
32	m	89	HIS
34	o	28	ASN
34	o	148	ASN
38	t	5	ASN
38	t	75	GLN
40	v	43	ASN
41	w	37	ASN
45	2	48	GLN
45	2	52	ASN
50	e	35	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2837/2903 (97%)	345 (12%)	55 (1%)
2	B	117/120 (97%)	13 (11%)	1 (0%)
30	i	1538/1540 (99%)	280 (18%)	0
47	4	9/10 (90%)	0	0
48	5	76/77 (98%)	15 (19%)	4 (5%)
48	6	76/77 (98%)	11 (14%)	4 (5%)
49	7	75/76 (98%)	28 (37%)	3 (4%)
All	All	4728/4803 (98%)	692 (14%)	67 (1%)

All (692) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	34	U
1	A	46	G
1	A	61	C
1	A	71	A
1	A	74	A
1	A	75	G
1	A	84	A
1	A	96	C
1	A	101	A
1	A	103	A
1	A	118	A
1	A	119	A
1	A	120	U
1	A	138	U
1	A	139	U
1	A	163	C
1	A	165	A
1	A	181	A
1	A	196	A
1	A	199	A
1	A	200	U
1	A	215	G
1	A	216	A
1	A	221	A
1	A	222	A
1	A	233	A
1	A	248	G

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Mol	Chain	Res	Type
1	A	255	A
1	A	266	G
1	A	271	G
1	A	276	U
1	A	281	C
1	A	285	G
1	A	311	A
1	A	329	G
1	A	330	A
1	A	353	C
1	A	361	G
1	A	367	G
1	A	371	A
1	A	372	G
1	A	386	G
1	A	403	U
1	A	405	U
1	A	411	G
1	A	412	A
1	A	420	C
1	A	424	G
1	A	451	U
1	A	456	C
1	A	481	G
1	A	491	G
1	A	503	A
1	A	504	A
1	A	505	A
1	A	509	C
1	A	530	G
1	A	531	C
1	A	532	A
1	A	533	G
1	A	544	C
1	A	546	U
1	A	547	A
1	A	548	G
1	A	549	G
1	A	550	C
1	A	563	A
1	A	573	U
1	A	575	A

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Mol	Chain	Res	Type
1	A	586	A
1	A	603	A
1	A	614	A
1	A	627	A
1	A	637	A
1	A	645	C
1	A	647	G
1	A	654	A
1	A	655	A
1	A	686	U
1	A	717	C
1	A	730	A
1	A	747	U
1	A	764	A
1	A	765	C
1	A	775	G
1	A	776	G
1	A	782	A
1	A	784	G
1	A	785	G
1	A	792	A
1	A	805	G
1	A	812	C
1	A	819	A
1	A	827	U
1	A	828	U
1	A	845	A
1	A	846	U
1	A	858	G
1	A	877	A
1	A	878	A
1	A	882	G
1	A	884	U
1	A	885	C
1	A	896	A
1	A	897	C
1	A	910	A
1	A	914	G
1	A	915	C
1	A	931	U
1	A	934	U
1	A	941	A

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Mol	Chain	Res	Type
1	A	946	C
1	A	961	C
1	A	968	C
1	A	974	G
1	A	983	A
1	A	984	A
1	A	985	C
1	A	995	C
1	A	996	A
1	A	1012	U
1	A	1013	C
1	A	1022	G
1	A	1026	G
1	A	1033	U
1	A	1040	A
1	A	1046	A
1	A	1047	G
1	A	1109	C
1	A	1110	G
1	A	1112	G
1	A	1128	G
1	A	1129	A
1	A	1132	U
1	A	1133	A
1	A	1135	C
1	A	1136	G
1	A	1139	G
1	A	1142	A
1	A	1173	U
1	A	1174	U
1	A	1175	A
1	A	1176	U
1	A	1177	G
1	A	1178	C
1	A	1187	G
1	A	1238	G
1	A	1253	A
1	A	1256	G
1	A	1266	G
1	A	1271	G
1	A	1272	A
1	A	1273	U

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Mol	Chain	Res	Type
1	A	1301	A
1	A	1352	U
1	A	1365	A
1	A	1379	U
1	A	1383	A
1	A	1395	A
1	A	1416	G
1	A	1428	C
1	A	1452	G
1	A	1453	A
1	A	1460	U
1	A	1482	G
1	A	1493	C
1	A	1504	A
1	A	1508	A
1	A	1509	A
1	A	1510	G
1	A	1515	A
1	A	1531	C
1	A	1533	C
1	A	1534	U
1	A	1535	A
1	A	1536	C
1	A	1537	G
1	A	1538	G
1	A	1569	A
1	A	1578	U
1	A	1583	A
1	A	1584	U
1	A	1585	C
1	A	1608	A
1	A	1609	A
1	A	1647	U
1	A	1648	U
1	A	1649	G
1	A	1674	G
1	A	1715	G
1	A	1729	U
1	A	1730	C
1	A	1732	C
1	A	1738	G
1	A	1739	A

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Mol	Chain	Res	Type
1	A	1764	C
1	A	1773	A
1	A	1782	U
1	A	1800	C
1	A	1801	A
1	A	1807	G
1	A	1808	A
1	A	1811	G
1	A	1816	C
1	A	1829	A
1	A	1848	A
1	A	1870	C
1	A	1871	A
1	A	1873	G
1	A	1906	G
1	A	1914	C
1	A	1926	U
1	A	1929	G
1	A	1930	G
1	A	1937	A
1	A	1938	A
1	A	1955	U
1	A	1965	C
1	A	1967	C
1	A	1970	A
1	A	1971	U
1	A	1972	G
1	A	1982	U
1	A	1991	U
1	A	1993	U
1	A	1997	C
1	A	2022	U
1	A	2023	C
1	A	2031	A
1	A	2033	A
1	A	2043	C
1	A	2055	C
1	A	2056	G
1	A	2060	A
1	A	2061	G
1	A	2069	G
1	A	2098	U

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Mol	Chain	Res	Type
1	A	2102	G
1	A	2109	U
1	A	2110	G
1	A	2111	U
1	A	2112	G
1	A	2113	U
1	A	2115	G
1	A	2118	U
1	A	2119	A
1	A	2120	G
1	A	2125	G
1	A	2126	A
1	A	2127	G
1	A	2128	G
1	A	2130	U
1	A	2131	U
1	A	2132	U
1	A	2133	G
1	A	2136	G
1	A	2137	U
1	A	2143	C
1	A	2146	C
1	A	2147	A
1	A	2148	G
1	A	2152	G
1	A	2157	G
1	A	2158	A
1	A	2159	G
1	A	2160	C
1	A	2163	A
1	A	2164	C
1	A	2165	C
1	A	2168	G
1	A	2170	A
1	A	2171	A
1	A	2172	U
1	A	2173	A
1	A	2174	C
1	A	2178	C
1	A	2198	A
1	A	2204	G
1	A	2211	A

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Mol	Chain	Res	Type
1	A	2225	A
1	A	2238	G
1	A	2239	G
1	A	2268	A
1	A	2283	C
1	A	2287	A
1	A	2297	A
1	A	2305	U
1	A	2308	G
1	A	2312	U
1	A	2322	A
1	A	2325	G
1	A	2333	A
1	A	2335	A
1	A	2347	C
1	A	2355	G
1	A	2372	U
1	A	2383	G
1	A	2385	C
1	A	2396	G
1	A	2402	U
1	A	2406	A
1	A	2407	A
1	A	2425	A
1	A	2429	G
1	A	2430	A
1	A	2431	U
1	A	2435	A
1	A	2441	U
1	A	2448	A
1	A	2478	A
1	A	2502	G
1	A	2505	G
1	A	2518	A
1	A	2529	G
1	A	2547	A
1	A	2554	U
1	A	2566	A
1	A	2567	G
1	A	2573	C
1	A	2574	G
1	A	2602	A

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Mol	Chain	Res	Type
1	A	2608	G
1	A	2609	U
1	A	2613	U
1	A	2629	U
1	A	2663	G
1	A	2689	U
1	A	2690	U
1	A	2714	G
1	A	2724	U
1	A	2726	A
1	A	2744	G
1	A	2748	A
1	A	2757	A
1	A	2778	A
1	A	2791	G
1	A	2798	U
1	A	2799	A
1	A	2820	A
1	A	2821	A
1	A	2867	G
1	A	2884	U
1	A	2903	U
2	B	25	U
2	B	34	A
2	B	35	C
2	B	44	G
2	B	45	A
2	B	53	A
2	B	56	G
2	B	57	A
2	B	67	G
2	B	89	U
2	B	90	C
2	B	99	A
2	B	109	A
30	i	3	A
30	i	4	U
30	i	5	U
30	i	6	G
30	i	7	A
30	i	8	A
30	i	9	G

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Mol	Chain	Res	Type
30	i	22	G
30	i	32	A
30	i	37	U
30	i	39	G
30	i	47	C
30	i	48	C
30	i	51	A
30	i	52	C
30	i	64	G
30	i	65	A
30	i	66	A
30	i	72	A
30	i	81	A
30	i	83	C
30	i	84	U
30	i	85	U
30	i	86	G
30	i	87	C
30	i	88	U
30	i	89	U
30	i	92	U
30	i	94	G
30	i	95	C
30	i	98	A
30	i	115	G
30	i	116	A
30	i	120	A
30	i	121	U
30	i	126	G
30	i	127	G
30	i	131	A
30	i	146	G
30	i	154	U
30	i	164	G
30	i	181	A
30	i	182	A
30	i	197	A
30	i	202	G
30	i	208	U
30	i	209	U
30	i	210	C
30	i	212	G

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Mol	Chain	Res	Type
30	i	214	C
30	i	226	G
30	i	245	U
30	i	247	G
30	i	251	G
30	i	266	G
30	i	267	C
30	i	289	G
30	i	306	A
30	i	321	A
30	i	328	C
30	i	329	A
30	i	330	C
30	i	332	G
30	i	348	G
30	i	352	C
30	i	354	G
30	i	355	C
30	i	360	G
30	i	366	A
30	i	367	U
30	i	368	U
30	i	369	G
30	i	372	C
30	i	383	A
30	i	389	A
30	i	392	C
30	i	393	A
30	i	395	C
30	i	397	A
30	i	398	U
30	i	399	G
30	i	406	G
30	i	408	A
30	i	409	U
30	i	411	A
30	i	412	A
30	i	413	G
30	i	414	A
30	i	415	A
30	i	417	G
30	i	421	U

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Mol	Chain	Res	Type
30	i	422	C
30	i	423	G
30	i	424	G
30	i	425	G
30	i	427	U
30	i	429	U
30	i	433	G
30	i	437	U
30	i	438	U
30	i	443	C
30	i	446	G
30	i	447	G
30	i	448	A
30	i	449	G
30	i	451	A
30	i	452	A
30	i	453	G
30	i	459	A
30	i	467	U
30	i	468	A
30	i	478	A
30	i	479	U
30	i	480	U
30	i	481	G
30	i	482	A
30	i	484	G
30	i	486	U
30	i	493	A
30	i	494	G
30	i	496	A
30	i	501	C
30	i	502	A
30	i	511	C
30	i	518	C
30	i	521	G
30	i	527	G
30	i	530	G
30	i	531	U
30	i	533	A
30	i	536	C
30	i	547	A
30	i	548	G

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Mol	Chain	Res	Type
30	i	559	A
30	i	562	U
30	i	572	A
30	i	573	A
30	i	576	C
30	i	577	G
30	i	588	G
30	i	596	A
30	i	620	C
30	i	633	G
30	i	639	G
30	i	650	G
30	i	653	U
30	i	654	G
30	i	665	A
30	i	718	A
30	i	721	G
30	i	723	U
30	i	724	G
30	i	734	G
30	i	747	A
30	i	755	G
30	i	777	A
30	i	793	U
30	i	794	A
30	i	815	A
30	i	817	C
30	i	821	G
30	i	828	U
30	i	841	C
30	i	842	U
30	i	843	U
30	i	844	G
30	i	845	A
30	i	846	G
30	i	851	G
30	i	887	G
30	i	914	A
30	i	922	G
30	i	926	G
30	i	934	C
30	i	935	A

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Mol	Chain	Res	Type
30	i	960	U
30	i	961	U
30	i	966	G
30	i	969	A
30	i	971	G
30	i	975	A
30	i	976	G
30	i	977	A
30	i	983	A
30	i	993	G
30	i	1003	G
30	i	1004	A
30	i	1005	A
30	i	1008	U
30	i	1009	U
30	i	1014	A
30	i	1018	G
30	i	1020	G
30	i	1022	A
30	i	1023	U
30	i	1026	G
30	i	1027	C
30	i	1028	C
30	i	1030	U
30	i	1032	G
30	i	1033	G
30	i	1039	G
30	i	1043	G
30	i	1045	C
30	i	1046	A
30	i	1053	G
30	i	1065	U
30	i	1085	U
30	i	1094	G
30	i	1095	U
30	i	1101	A
30	i	1124	G
30	i	1130	A
30	i	1132	C
30	i	1134	G
30	i	1137	C
30	i	1139	G

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Mol	Chain	Res	Type
30	i	1140	C
30	i	1141	C
30	i	1143	G
30	i	1145	A
30	i	1159	U
30	i	1167	A
30	i	1168	U
30	i	1171	A
30	i	1184	G
30	i	1196	A
30	i	1197	A
30	i	1200	C
30	i	1202	U
30	i	1212	U
30	i	1213	A
30	i	1225	A
30	i	1226	C
30	i	1227	A
30	i	1228	C
30	i	1238	A
30	i	1256	A
30	i	1257	A
30	i	1258	G
30	i	1260	G
30	i	1275	A
30	i	1280	A
30	i	1286	U
30	i	1287	A
30	i	1299	A
30	i	1300	G
30	i	1302	C
30	i	1305	G
30	i	1317	C
30	i	1320	C
30	i	1335	U
30	i	1336	C
30	i	1337	G
30	i	1338	G
30	i	1346	A
30	i	1353	G
30	i	1362	A
30	i	1363	A

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Mol	Chain	Res	Type
30	i	1370	G
30	i	1379	G
30	i	1381	U
30	i	1419	G
30	i	1446	A
30	i	1487	G
30	i	1492	A
30	i	1494	G
30	i	1497	G
30	i	1503	A
30	i	1505	G
30	i	1506	U
30	i	1517	G
30	i	1529	G
30	i	1530	G
30	i	1533	C
30	i	1534	A
30	i	1535	C
30	i	1537	U
30	i	1538	C
30	i	1539	C
48	5	4	C
48	5	9	A
48	5	20	G
48	5	21	U
48	5	22	A
48	5	44	U
48	5	47	G
48	5	48	U
48	5	49	C
48	5	50	G
48	5	57	C
48	5	58	G
48	5	73	G
48	5	74	A
48	5	75	C
48	6	19	G
48	6	20	U
48	6	21	A
48	6	43	U
48	6	46	G
48	6	47	U

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Mol	Chain	Res	Type
48	6	48	C
48	6	49	G
48	6	56	C
48	6	57	G
48	6	76	A
49	7	6	U
49	7	8	U
49	7	11	C
49	7	12	U
49	7	13	C
49	7	14	A
49	7	16	C
49	7	17	U
49	7	18	G
49	7	19	G
49	7	20	G
49	7	21	A
49	7	34	U
49	7	35	G
49	7	37	A
49	7	46	G
49	7	47	U
49	7	48	C
49	7	51	C
49	7	55	U
49	7	56	C
49	7	58	A
49	7	59	U
49	7	67	A
49	7	72	C
49	7	74	C
49	7	75	C
49	7	76	A

All (67) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	125	A
1	A	140	C
1	A	199	A
1	A	221	A
1	A	271	G

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Mol	Chain	Res	Type
1	A	310	A
1	A	345	A
1	A	369	U
1	A	404	A
1	A	503	A
1	A	548	G
1	A	549	G
1	A	614	A
1	A	746	PSU
1	A	764	A
1	A	776	G
1	A	784	G
1	A	805	G
1	A	827	U
1	A	984	A
1	A	995	C
1	A	1025	G
1	A	1128	G
1	A	1133	A
1	A	1135	C
1	A	1141	U
1	A	1175	A
1	A	1252	G
1	A	1266	G
1	A	1286	A
1	A	1497	U
1	A	1583	A
1	A	1608	A
1	A	1618	A
1	A	1647	U
1	A	1738	G
1	A	1808	A
1	A	1872	A
1	A	1913	A
1	A	2022	U
1	A	2109	U
1	A	2146	C
1	A	2158	A
1	A	2170	A
1	A	2225	A
1	A	2282	G
1	A	2287	A

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Mol	Chain	Res	Type
1	A	2324	U
1	A	2335	A
1	A	2518	A
1	A	2602	A
1	A	2756	U
1	A	2798	U
1	A	2849	U
1	A	2873	A
2	B	34	A
48	5	3	G
48	5	20	G
48	5	47	G
48	5	57	C
48	6	19	G
48	6	46	G
48	6	47	U
48	6	56	C
49	7	15	G
49	7	74	C
49	7	75	C

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

3 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	$\#\|Z\| > 2$
1	PSU	A	2504	1,53	18,21,22	1.04	1 (5%)	22,30,33	1.00	1 (4%)
1	2MA	A	2503	1,52,53	17,25,26	1.00	1 (5%)	17,37,40	0.87	1 (5%)
1	PSU	A	746	1,52	18,21,22	0.96	1 (5%)	22,30,33	1.59	4 (18%)

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
1	PSU	A	2504	1,53	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	1,52,53	-	1/3/25/26	0/3/3/3
1	PSU	A	746	1,52	-	1/7/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2504	PSU	C6-C5	3.55	1.39	1.35
1	A	746	PSU	C6-C5	3.35	1.39	1.35
1	A	2503	2MA	C5-C4	-2.63	1.36	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	746	PSU	O3'-C3'-C4'	4.47	123.98	111.05
1	A	746	PSU	C3'-C2'-C1'	3.42	105.62	101.64
1	A	2503	2MA	CM2-C2-N1	2.58	121.97	116.23
1	A	746	PSU	C6-C5-C4	-2.42	116.50	118.20
1	A	2504	PSU	C5-C6-N1	-2.06	119.02	122.11
1	A	746	PSU	O2'-C2'-C3'	2.02	118.35	111.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	O4'-C1'-C5-C6
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 377 ligands modelled in this entry, 376 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	$\#\|Z\| > 2$
54	PRO	5	101	48	5,7,8	0.54	0	7,8,10	0.99	0

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
54	PRO	5	101	48	-	0/0/9/11	0/1/1/1

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	5	101	PRO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

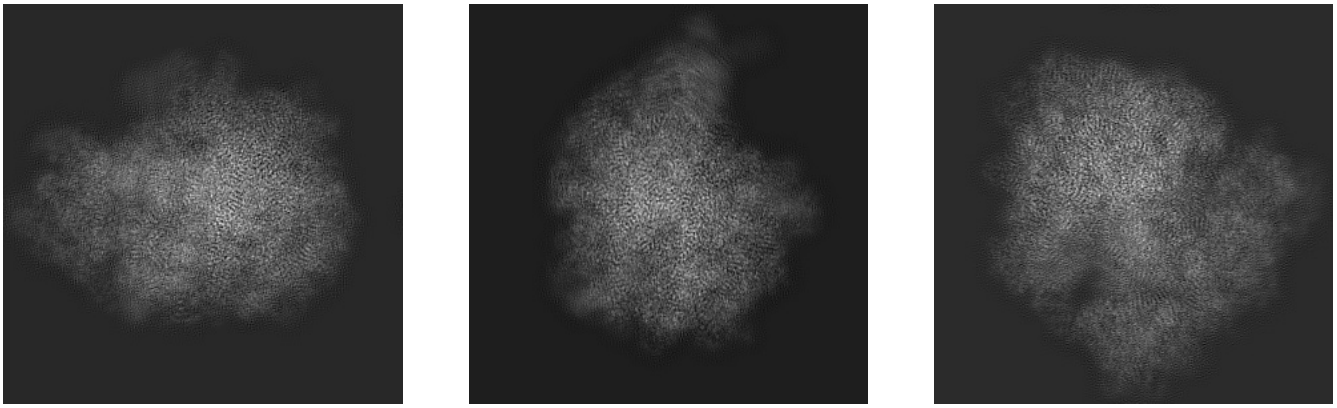
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-18320. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

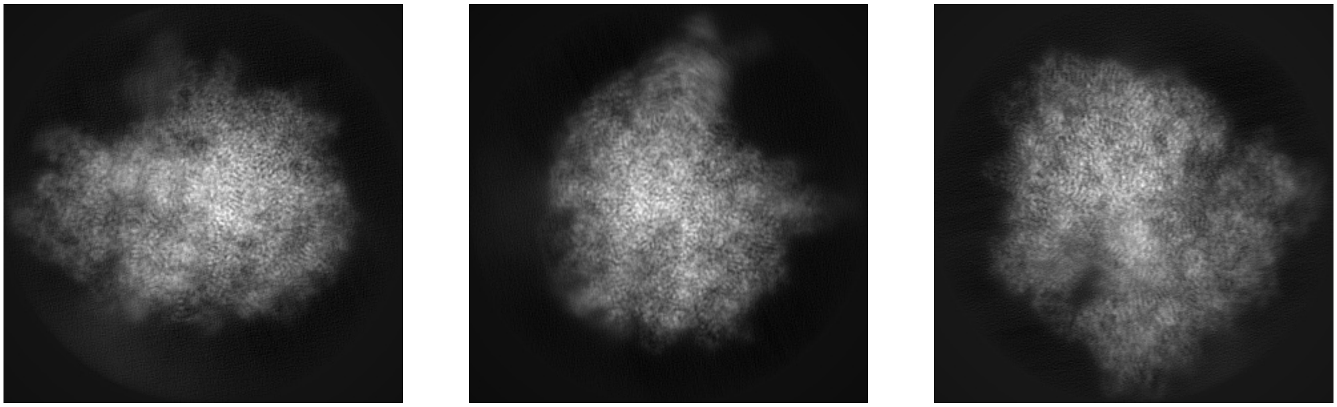
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

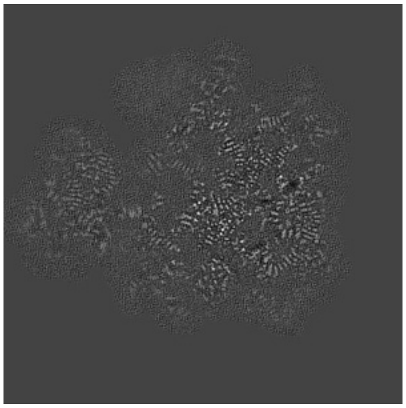


X Y Z

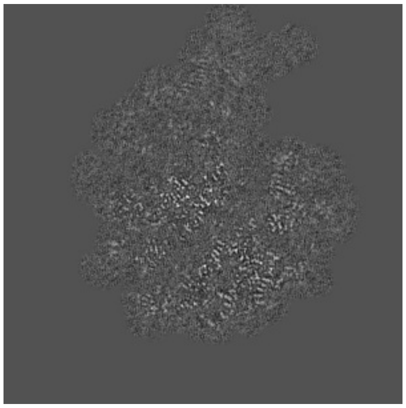
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

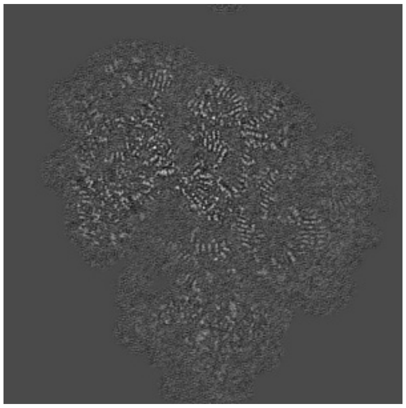
6.2.1 Primary map



X Index: 180

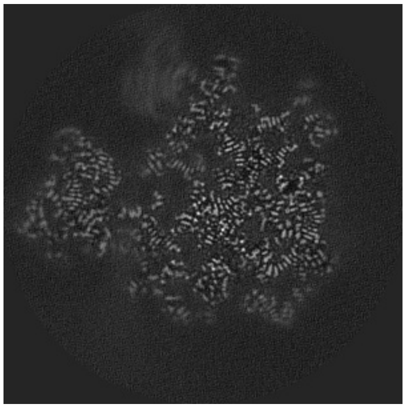


Y Index: 180

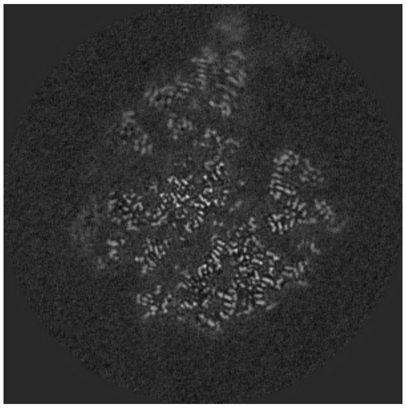


Z Index: 180

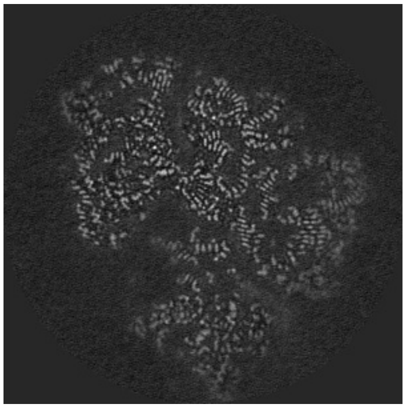
6.2.2 Raw map



X Index: 180



Y Index: 180

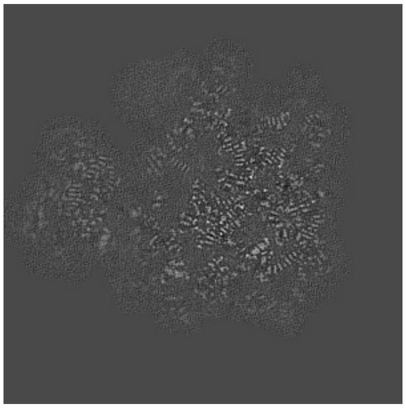


Z Index: 180

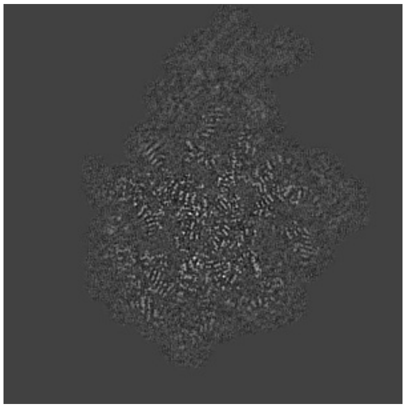
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

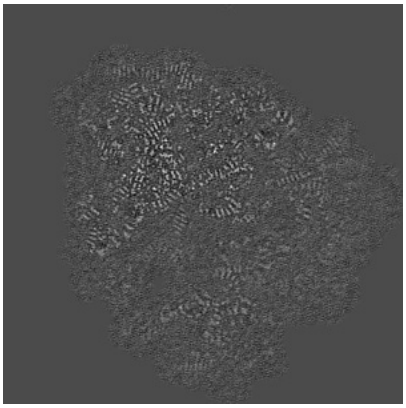
6.3.1 Primary map



X Index: 181

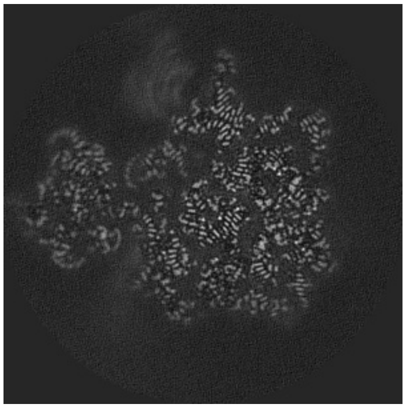


Y Index: 203

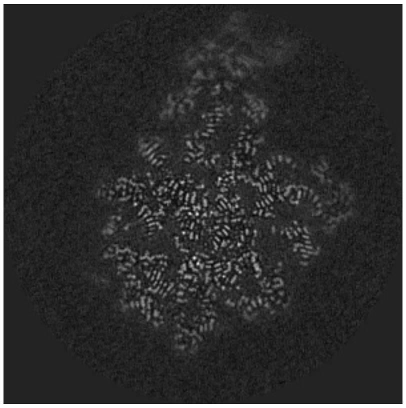


Z Index: 193

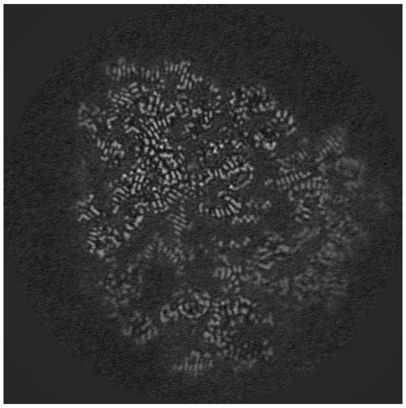
6.3.2 Raw map



X Index: 186



Y Index: 203

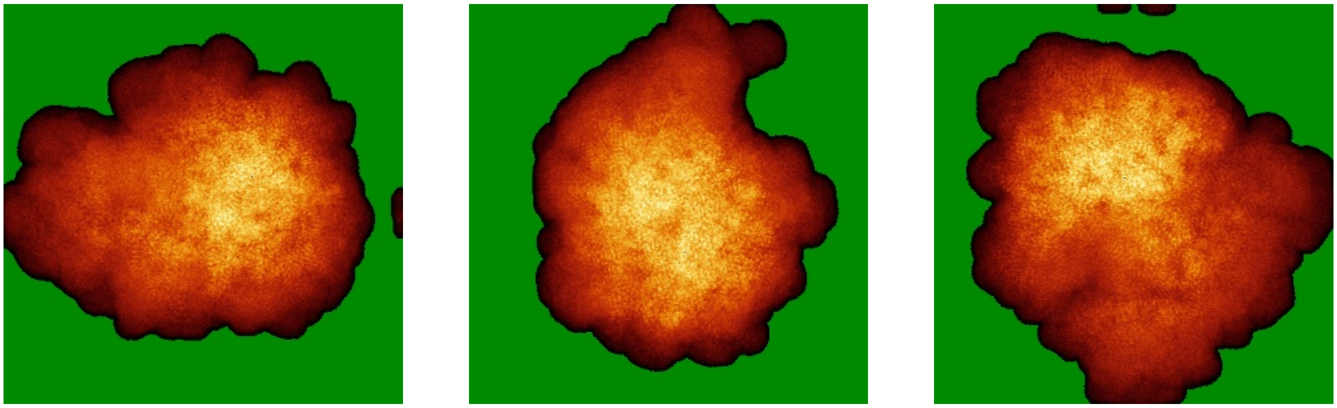


Z Index: 193

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

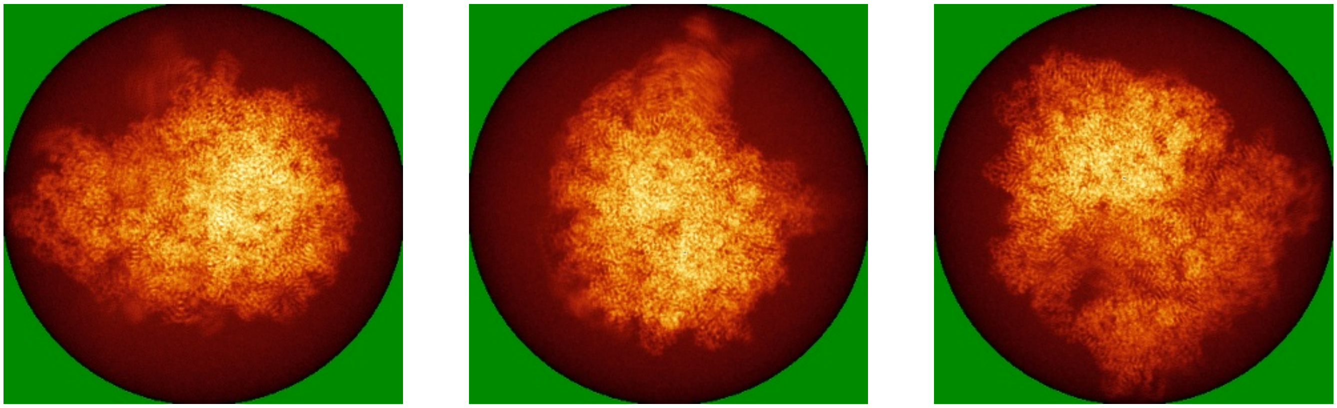
6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map



X Y Z

6.4.2 Raw map



X Y Z

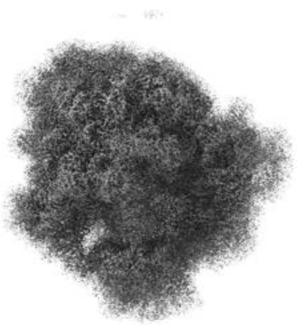
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map

X

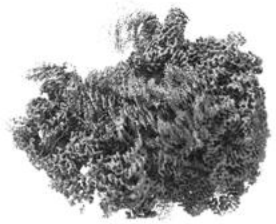
Y



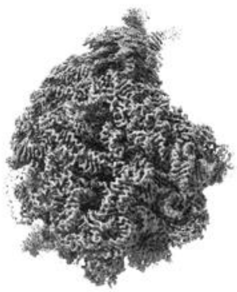
Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

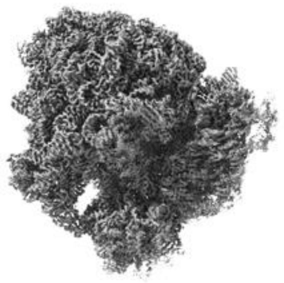
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

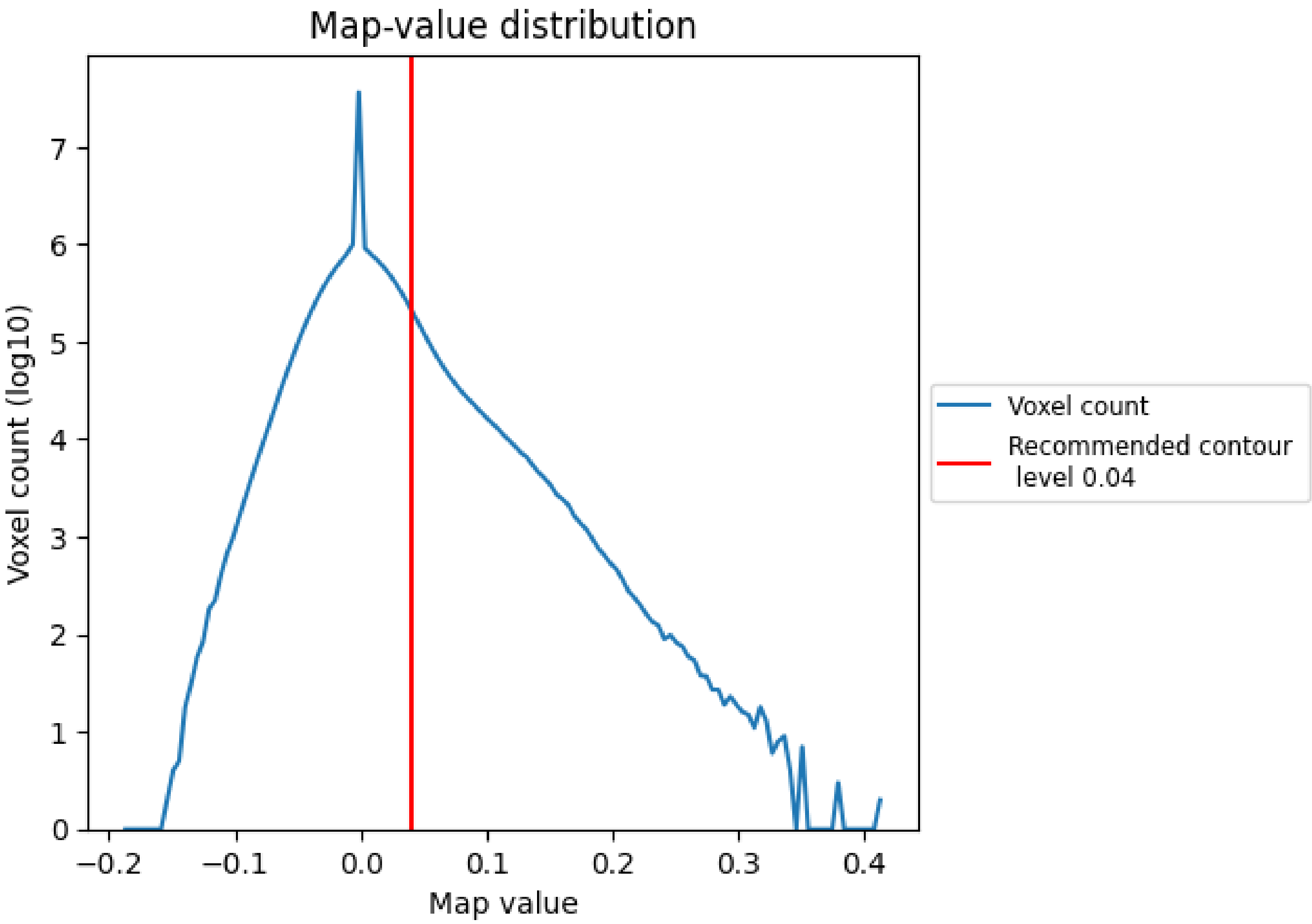
6.6 Mask visualisation

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

7 Map analysis ⓘ

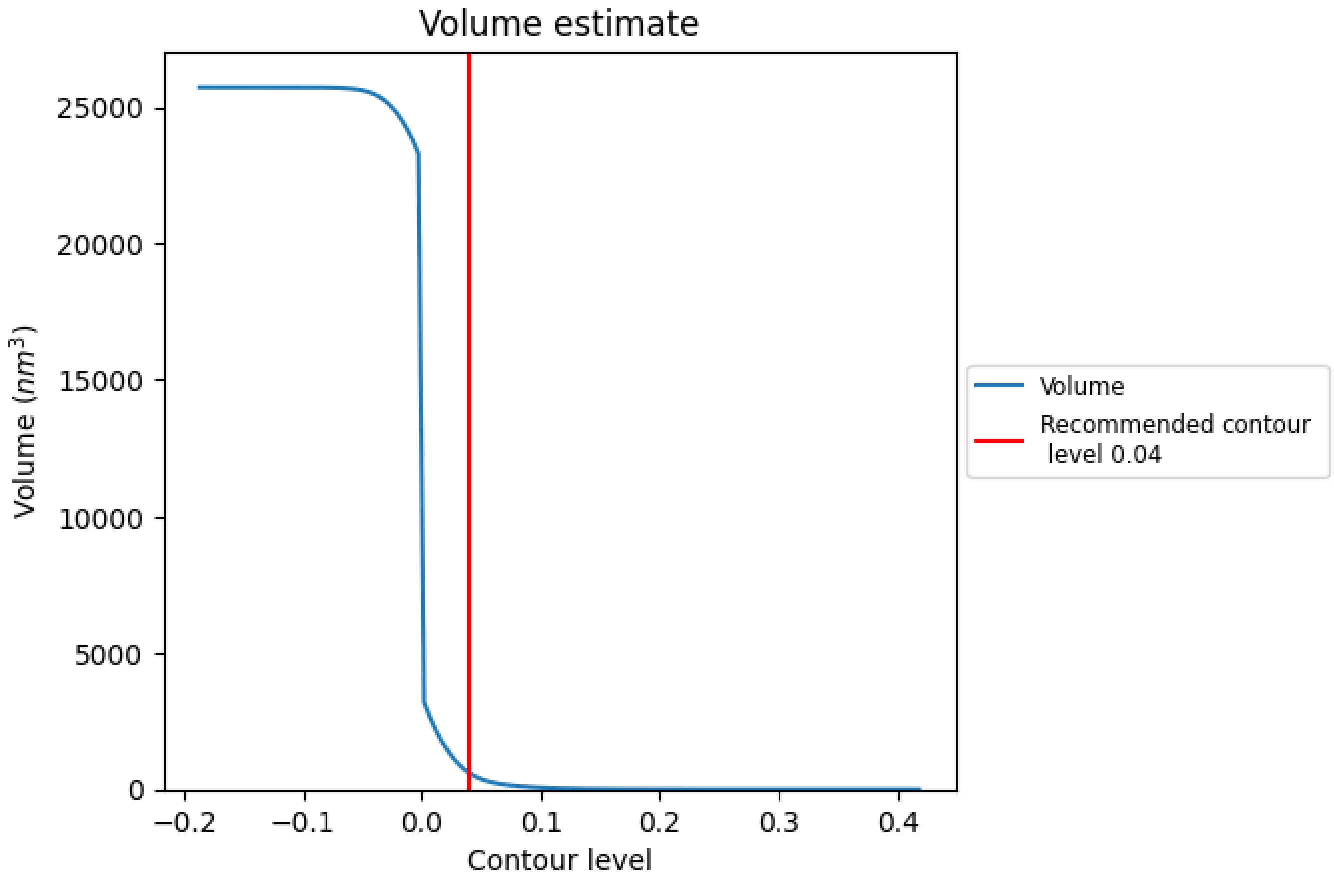
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

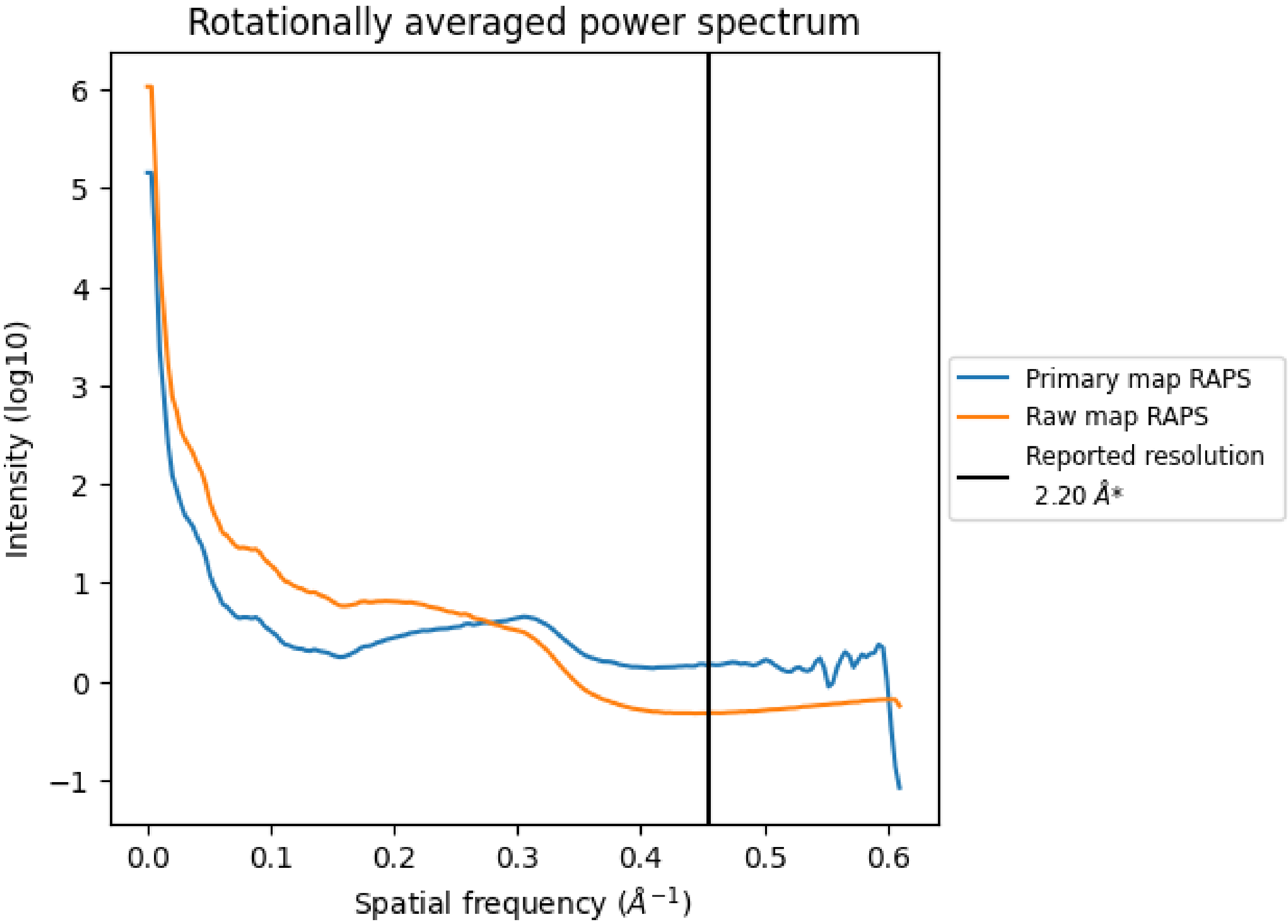
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 598 nm^3; this corresponds to an approximate mass of 540 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 ⓘ

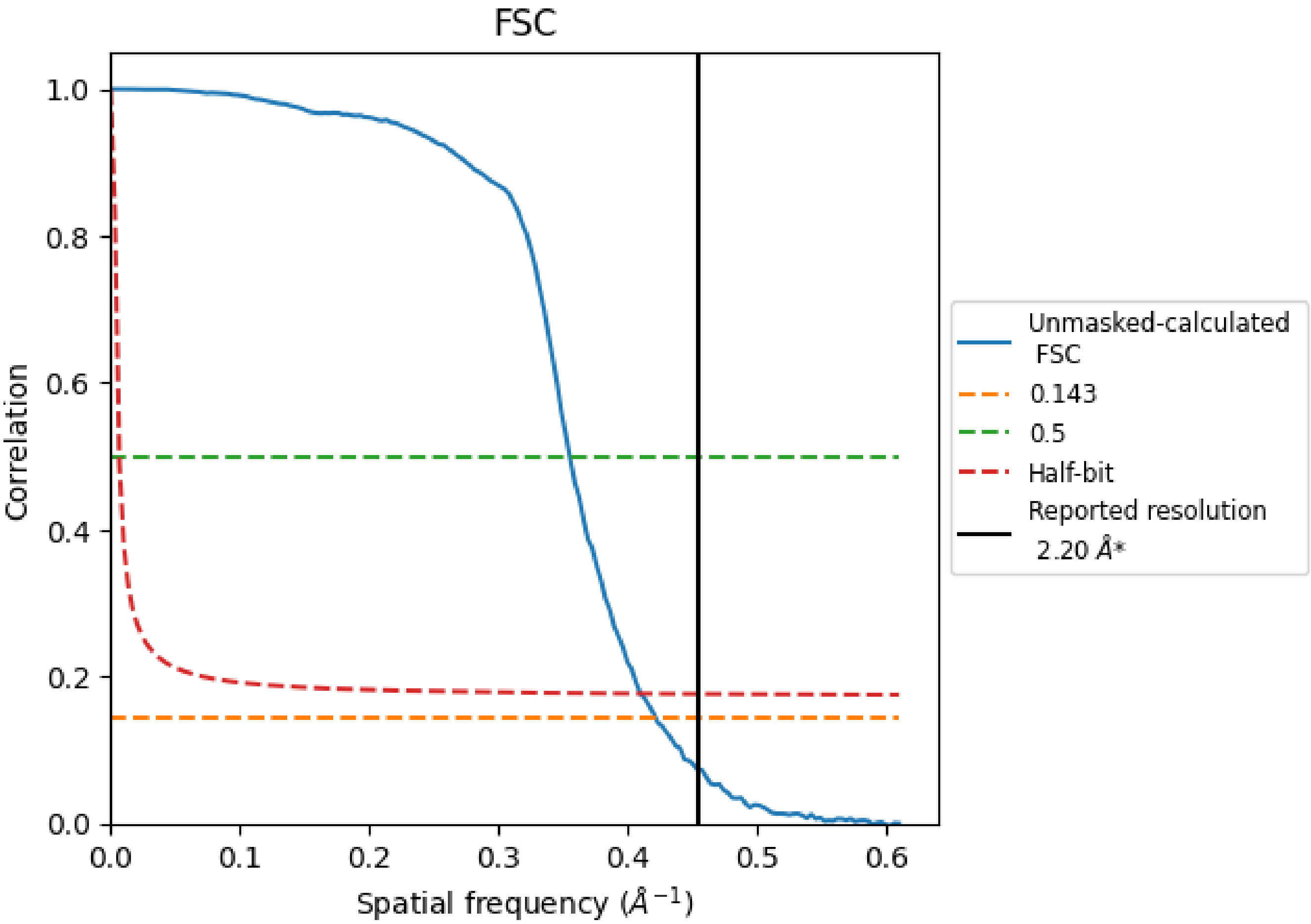


*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8 Fourier-Shell correlation ⓘ

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

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.455 Å^{-1}

8.2 Resolution estimates ⓘ

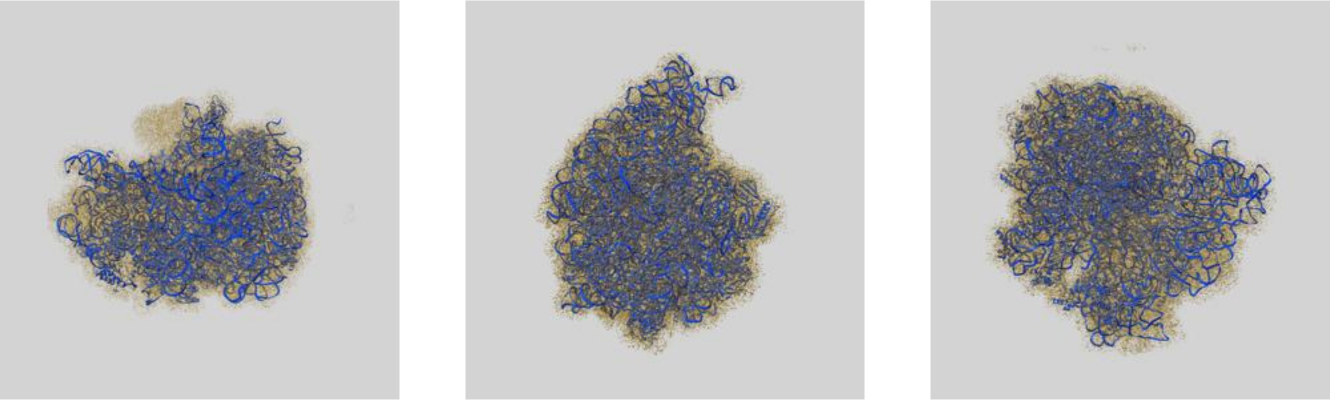
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	2.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.37	2.82	2.44

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-18320 and PDB model 8QBT. Per-residue inclusion information can be found in section 3 on page 15.

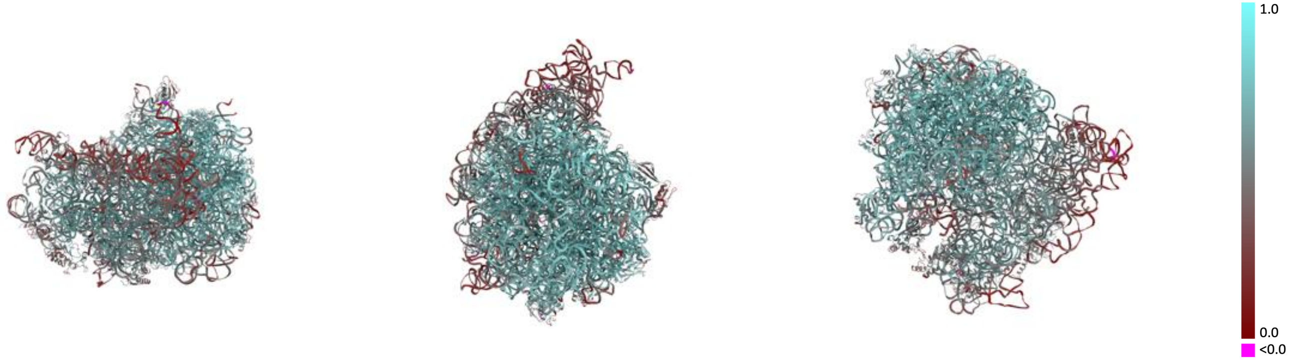
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.04 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.

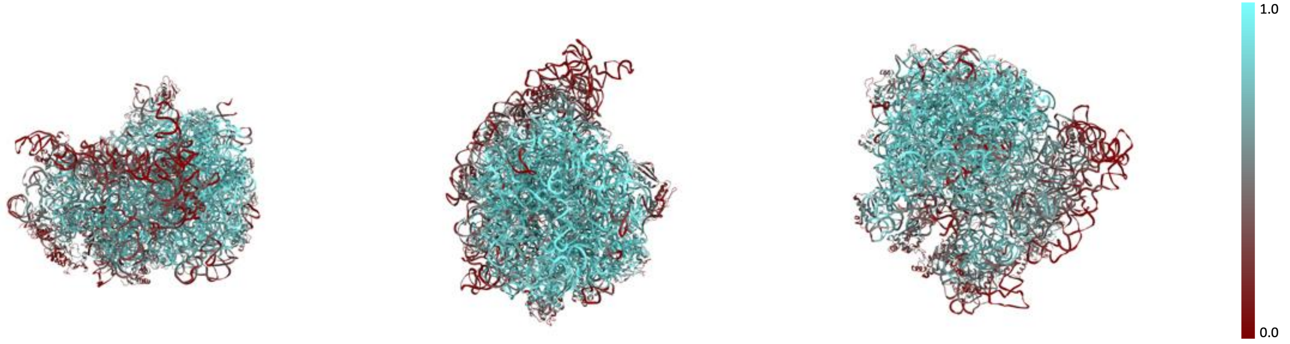
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

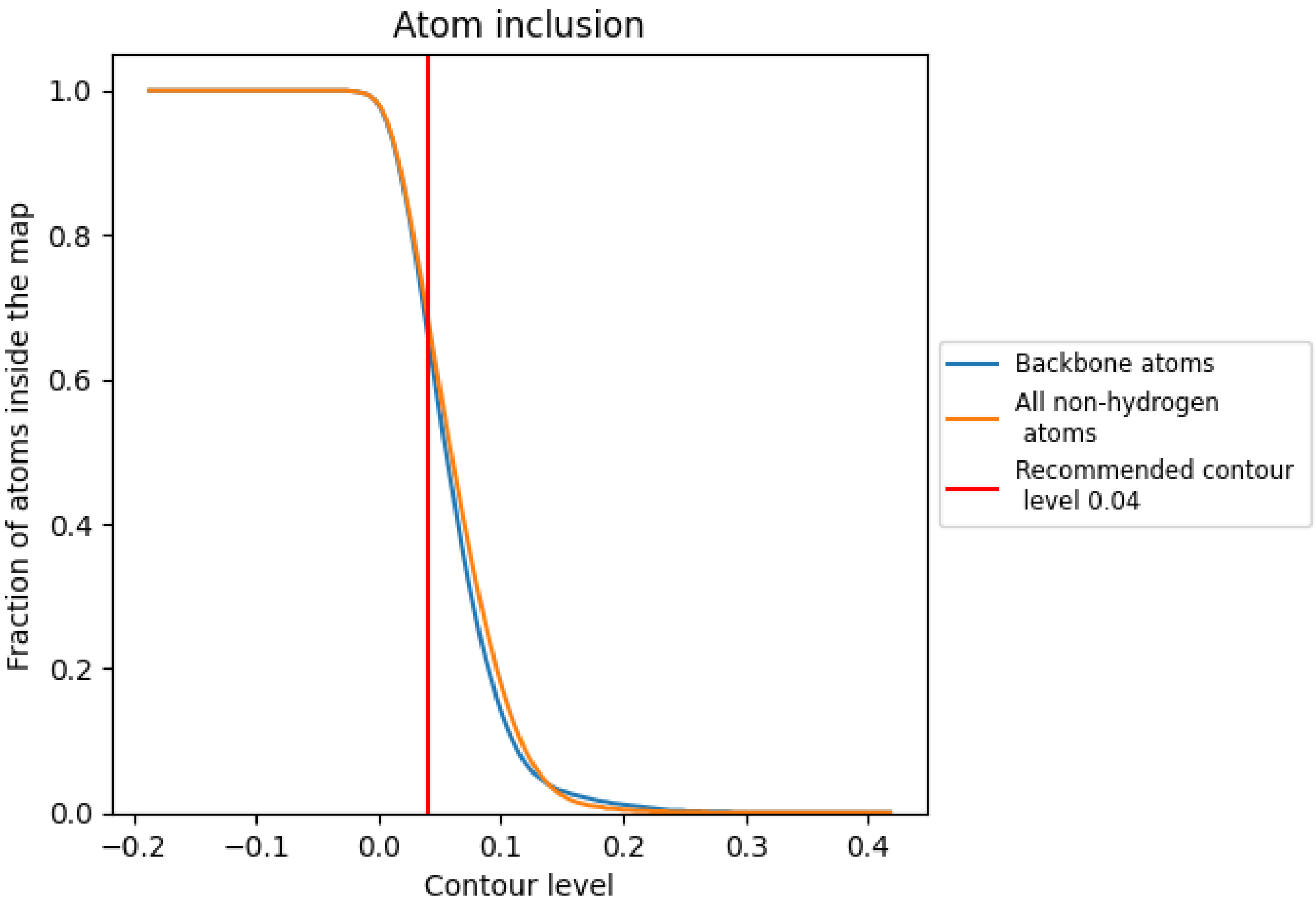
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.04).

9.4 Atom inclusion ⓘ



At the recommended contour level, 66% of all backbone atoms, 69% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	■ 0.6900	■ 0.6110
1	■ 0.3210	■ 0.4400
2	■ 0.2410	■ 0.3730
3	■ 0.4100	■ 0.4420
4	■ 0.7430	■ 0.6350
5	■ 0.5490	■ 0.5330
6	■ 0.5790	■ 0.5210
7	■ 0.0730	■ 0.1520
A	■ 0.8270	■ 0.6810
B	■ 0.6890	■ 0.6090
C	■ 0.8880	■ 0.7330
D	■ 0.8340	■ 0.7140
E	■ 0.6360	■ 0.6240
F	■ 0.3950	■ 0.4820
G	■ 0.3430	■ 0.4640
H	■ 0.3930	■ 0.5070
J	■ 0.8660	■ 0.7160
K	■ 0.8260	■ 0.7020
L	■ 0.7680	■ 0.6730
M	■ 0.8630	■ 0.7190
N	■ 0.9080	■ 0.7440
O	■ 0.5780	■ 0.5850
P	■ 0.7850	■ 0.6680
Q	■ 0.9020	■ 0.7520
R	■ 0.6860	■ 0.6300
S	■ 0.8230	■ 0.7030
T	■ 0.6790	■ 0.5940
U	■ 0.4820	■ 0.5260
V	■ 0.6170	■ 0.6020
W	■ 0.8780	■ 0.7130
X	■ 0.7820	■ 0.6830
Y	■ 0.4750	■ 0.5090
Z	■ 0.8270	■ 0.6930
a	■ 0.7920	■ 0.6930
b	■ 0.7360	■ 0.6220

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Chain	Atom inclusion	Q-score
c	0.9240	0.7480
d	0.9310	0.7560
e	0.7950	0.6670
f	0.8410	0.7340
i	0.5730	0.5310
j	0.2810	0.4470
m	0.6180	0.5950
n	0.3330	0.4650
o	0.3080	0.4380
p	0.5320	0.5740
q	0.3500	0.4600
s	0.5600	0.5680
t	0.3390	0.4610
u	0.3740	0.4670
v	0.4290	0.5130
w	0.5440	0.5520
y	0.2560	0.3830
z	0.6170	0.5680