Full wwPDB EM Validation Report (i)

May 19, 2024 – 09:27 AM EDT

PDB ID	:	7MSH
EMDB ID	:	EMD-23962
Title	:	Mtb 70SIC in complex with MtbEttA at Pre_R1 state
Authors	:	Cui, Z.; Zhang, J.
Deposited on	:	2021-05-11
Resolution	:	3.23 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

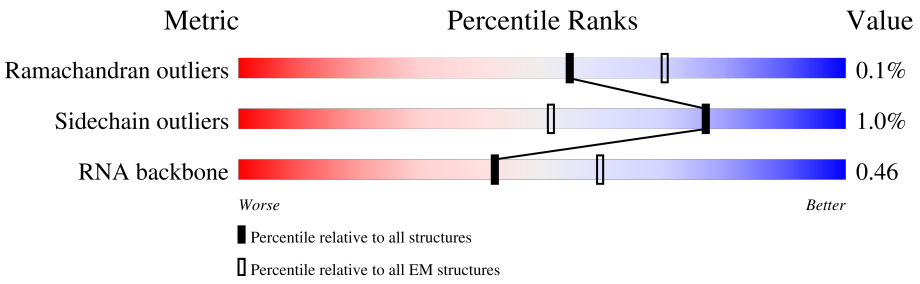
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.23 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	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	0	57	21% 95% 5%
2	1	55	87% 13%
3	2	47	94% 6%
4	3	64	97%
5	4	37	16% 97%
6	6	80	9% 56% 41%
7	7	24	25% 33% 67%
8	8	235	58% 96%

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Mol	Chain	Length	Quality of chain
9	A	3138	8%, 75%, 23%
10	B	115	77%, 23%
11	C	280	96%
12	D	217	98%
13	E	223	92%, 7%
14	F	187	10%, 94%, 5%
15	G	179	16%, 97%
16	H	152	30%, 69%
17	J	195	75%, 25%
18	K	122	99%
19	L	146	99%
20	M	138	51%, 96%
21	N	180	64%, 36%
22	O	122	96%
23	P	113	99%
24	Q	129	96%
25	R	104	94%
26	S	197	57%, 43%
27	T	100	93%, 5%
28	U	105	5%, 84%, 14%
29	V	215	64%, 81%, 18%
30	W	86	84%, 16%
31	X	64	94%
32	Y	77	88%, 12%
33	Z	65	88%, 9%

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Mol	Chain	Length	Quality of chain
34	a	1537	75% 23%
35	c	274	6% 75% 24%
36	d	201	6% 99%
37	e	220	76% 23%
38	f	96	6% 99%
39	g	156	99%
40	h	132	98%
41	i	151	8% 83% 16%
42	j	101	23% 98%
43	k	139	84% 16%
44	l	124	93% 6%
45	m	124	8% 93% 6%
46	n	61	95%
47	o	89	97%
48	p	162	69% 30%
49	q	135	68% 30%
50	r	84	73% 24%
51	s	93	13% 89% 11%
52	t	86	98%
53	x	558	12% 96%
54	y	77	69% 29%
55	z	26	12% 8% 77%

2 Entry composition (i)

There are 58 unique types of molecules in this entry. The entry contains 152103 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	54	429	266	94	69	0	0

- Molecule 2 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	48	400	245	84	67	4	0	0

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	44	374	222	97	54	1	0	0

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	3	62	494	298	112	84	0	0

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	37	299	182	66	47	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
4	1	VAL	MET	conflict	UNP P9WH89

- Molecule 6 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	47	356	220	62	69	5	0	0

- Molecule 7 is a protein called 50S ribosomal protein L37.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	7	8	69	41	20	8	0	0

- Molecule 8 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	8	230	1704	1068	310	323	3	0	0

- Molecule 9 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	A	3118	66958	29847	12340	21653	3118	0	0

- Molecule 10 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	B	115	2458	1097	456	790	115	0	0

- Molecule 11 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	272	2088	1277	437	369	5	0	0

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	D	213	1590	985	307	292	6	0	0

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	207	1552	958	303	289	2	0	0

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	F	178	1408	885	267	251	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	G	174	1330	836	249	244	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	H	47	350	220	64	65	1	0	0

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	J	146	1143	724	217	199	3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	K	122	941	590	180	169	2	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	1	VAL	MET	conflict	UNP A0A045HTP7

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	L	144	1075	666	217	190	2	0	0

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	M	134	1072	679	215	177	1	0	0

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	N	116	908	574	175	158	1	0	0

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
22	O	119	905	552	191	162	0	0

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	P	112	907	573	174	159	1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	Q	124	993	616	207	170	0	0

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
25	R	100	757	482	138	137	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	MET	-	insertion	UNP P9WHC3

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	S	113	860	533	178	149	0	0

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	T	95	741	469	138	134	0	0

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	U	90	699	430	138	129	2	0	0

- Molecule 29 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	V	177	1319	822	243	254	0	0

- Molecule 30 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
30	W	72	537	331	112	94	0	0

- Molecule 31 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	X	62	468	284	100	80	4	0	0

- Molecule 32 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	Y	68	560	343	109	107	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Z	59	476	293	101	82	0	0

- Molecule 34 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
34	a	1519	32620	14535	5961	10605	1519	0	0

- Molecule 35 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	c	207	1654	1030	322	298	4	0	0

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	d	200	1650	1036	316	296	2	0	0

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	e	169	1222	770	231	218	3	0	0

- Molecule 38 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	f	95	757	480	133	141	3	0	0

- Molecule 39 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	g	155	1230	768	241	219	2	0	0

- Molecule 40 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	h	131	1006	631	188	186	1	0	0

- Molecule 41 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	i	127	992	628	195	169	0	0

- Molecule 42 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	j	99	789	496	146	144	3	0	0

- Molecule 43 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
43	k	117	873	540	175	158	0	0

- Molecule 44 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	l	122	959	594	197	166	2	0	0

- Molecule 45 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	m	116	945	578	196	168	3	0	0

- Molecule 46 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	n	60	468	294	96	73	5	0	0

- Molecule 47 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
47	o	87	718	449	144	125	0	0

- Molecule 48 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	p	113	884	564	166	154	0	0

- Molecule 49 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	q	95	770	482	152	133	3	0	0

- Molecule 50 is a protein called 30S ribosomal protein S18 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	r	64	506	315	98	90	3	0	0

- Molecule 51 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	s	83	672	432	125	114	1	0	0

- Molecule 52 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
52	t	85	652	394	141	117	0	0

- Molecule 53 is a protein called Energy-dependent translational throttle protein EttA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	x	550	4297	2703	751	831	12	0	0

- Molecule 54 is a RNA chain called initiator tRNA (Met).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
54	y	75	1602	713	289	525	75	0	0

- Molecule 55 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	z	6	129	58	25	40	6	0	0

- Molecule 56 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
56	1	1	1	1	0
56	4	1	1	1	0
56	6	1	1	1	0
56	X	1	1	1	0
56	n	1	1	1	0
56	r	1	1	1	0

- Molecule 57 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	3	1	1	1	0
57	A	286	286	286	0
57	B	4	4	4	0
57	D	1	1	1	0

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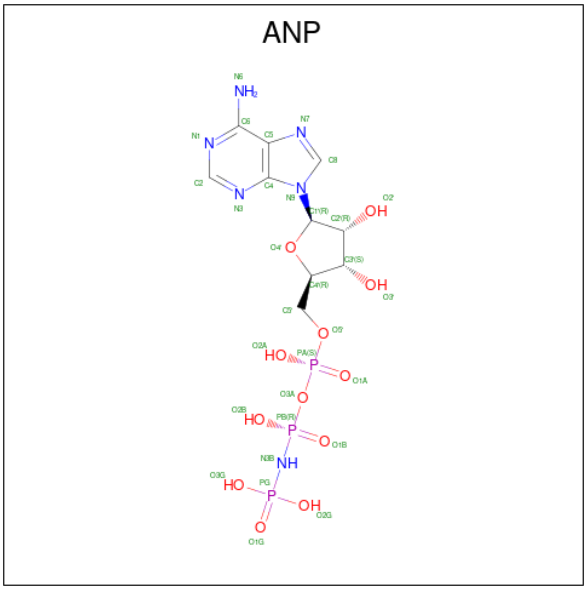
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
57	H	1	1	1	0
57	L	1	1	1	0
57	a	121	121	121	0
57	r	1	1	1	0
57	t	1	1	1	0
57	x	2	2	2	0
57	y	1	1	1	0

- Molecule 58 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



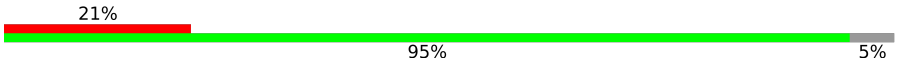
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
58	x	1	31	10	6	12	3	0
58	x	1	31	10	6	12	3	0

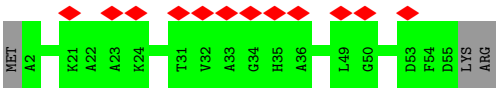
3 Residue-property plots (i)

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

- Molecule 1: 50S ribosomal protein L32

Chain 0:



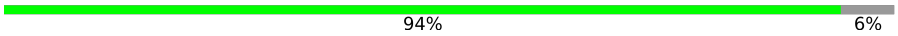


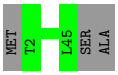
- Molecule 2: 50S ribosomal protein L33 2

Chain 1:

- Molecule 3: 50S ribosomal protein L34

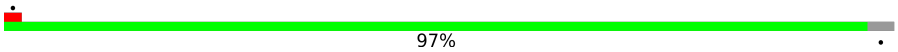
Chain 2:

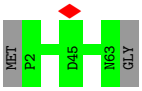




- Molecule 4: 50S ribosomal protein L35

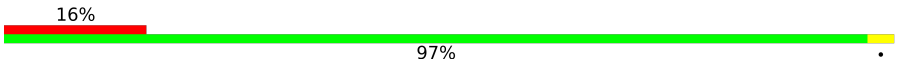
Chain 3:

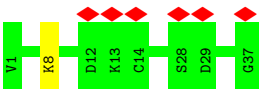




- Molecule 5: 50S ribosomal protein L36

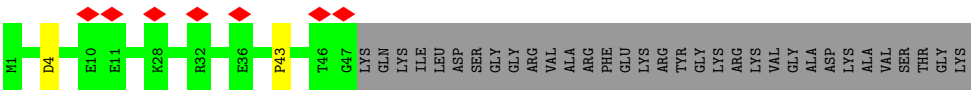
Chain 4:





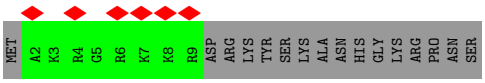
- Molecule 6: 50S ribosomal protein L31

Chain 6:



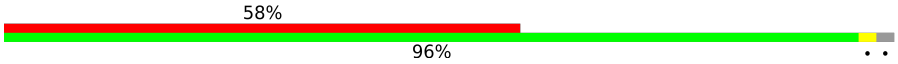
- Molecule 7: 50S ribosomal protein L37

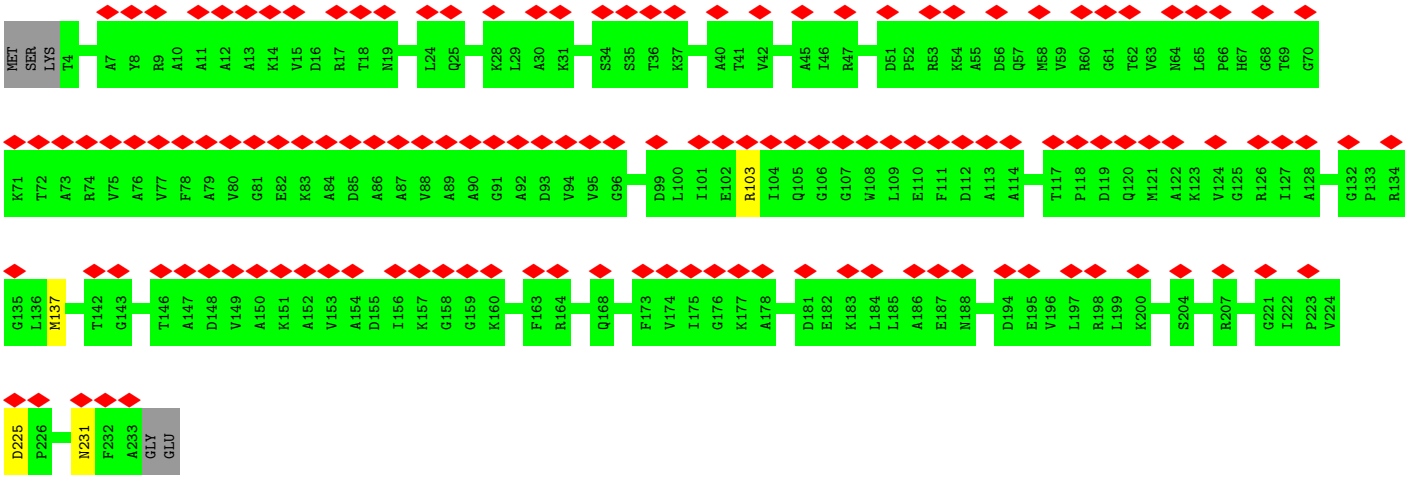
Chain 7:



- Molecule 8: 50S ribosomal protein L1

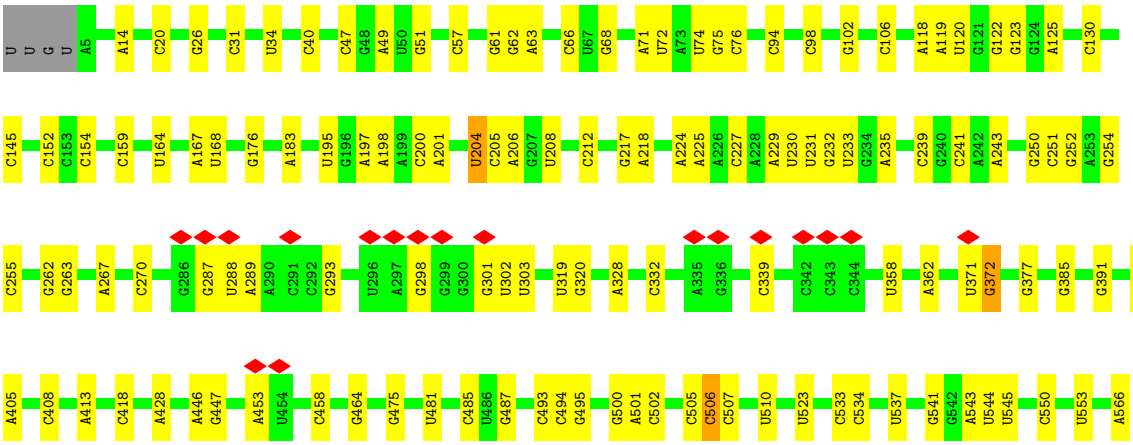
Chain 8:

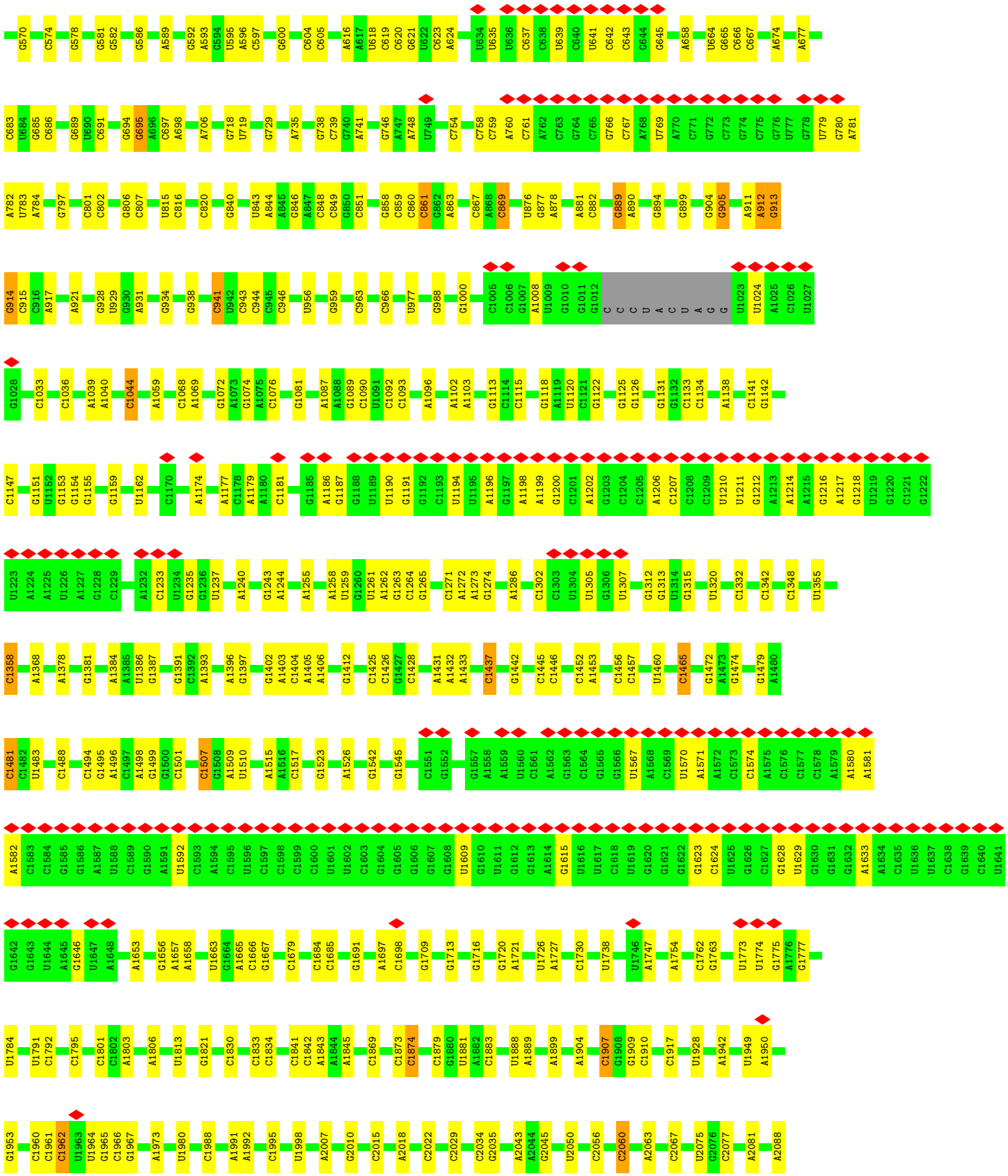




- Molecule 9: 23S rRNA

Chain A:

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C683 U684 G685 C686 G689 U690 C691 G694 G695 A696 C697 A698 A706 G718 U719 G729 A735 G738 C739 G740 A741 G746 A747 A748 U749 C754 C758 C759 A760 C761 A762 C763 G764 C765 G766 C767 A768 U769 A770 C771 G772 C773 G774 C775 G776 U777 G778 U779 G780 A781
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G914 C915 C916 A917 A921 G928 U929 G930 A931 G934 G938 C941 U942 C943 C944 C945 C946 U956 G959 C963 C966 U977 G988 G1000 C1005 C1006 G1007 A1008 U1009 G1010 G1011 G1012 C C C U A C U A G G U1023 U1024 A1025 C1026 U1027
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C1147 G1151 U1152 G1153 G1154 G1155 G1159 U1162 C1170 A1174 A1177 C1178 A1179 A1180 C1181 G1185 A1186 G1187 G1188 U1189 U1190 G1191 G1192 C1193 U1194 U1195 A1196 G1197 A1198 A1199 G1200 C1201 A1202 G1203 C1204 C1205 A1206 C1207 C1208 C1209 U1210 U1211 G1212 A1213 A1214 A1215 G1216 A1217 G1218 U1219 G1220 C1221 G1222
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C1358 A1368 A1378 G1381 A1384 A1385 U1386 G1387 G1391 C1392 A1393 A1396 G1397 G1402 A1403 C1404 A1405 A1406 G1412 C1425 C1426 G1427 C1428 A1431 A1432 A1433 C1437 G1442 C1445 C1446 C1452 A1453 C1456 C1457 U1460 C1465 G1472 A1473 G1474 G1479 A1480
C1481 C1482 U1483 C1488 C1494 G1495 A1496 C1497 A1498 G1499 G1500 C1501 C1507 G1508 A1509 U1510 A1515 A1516 C1517 G1523 A1526 G1542 G1545 C1551 G1552 G1557 A1558 A1559 U1560 C1561 A1562 G1563 C1564 G1565 G1566 U1567 A1568 C1569 U1570 A1571 A1572 C1573 C1574 A1575 C1576 C1577 C1578 A1579 A1580 A1581
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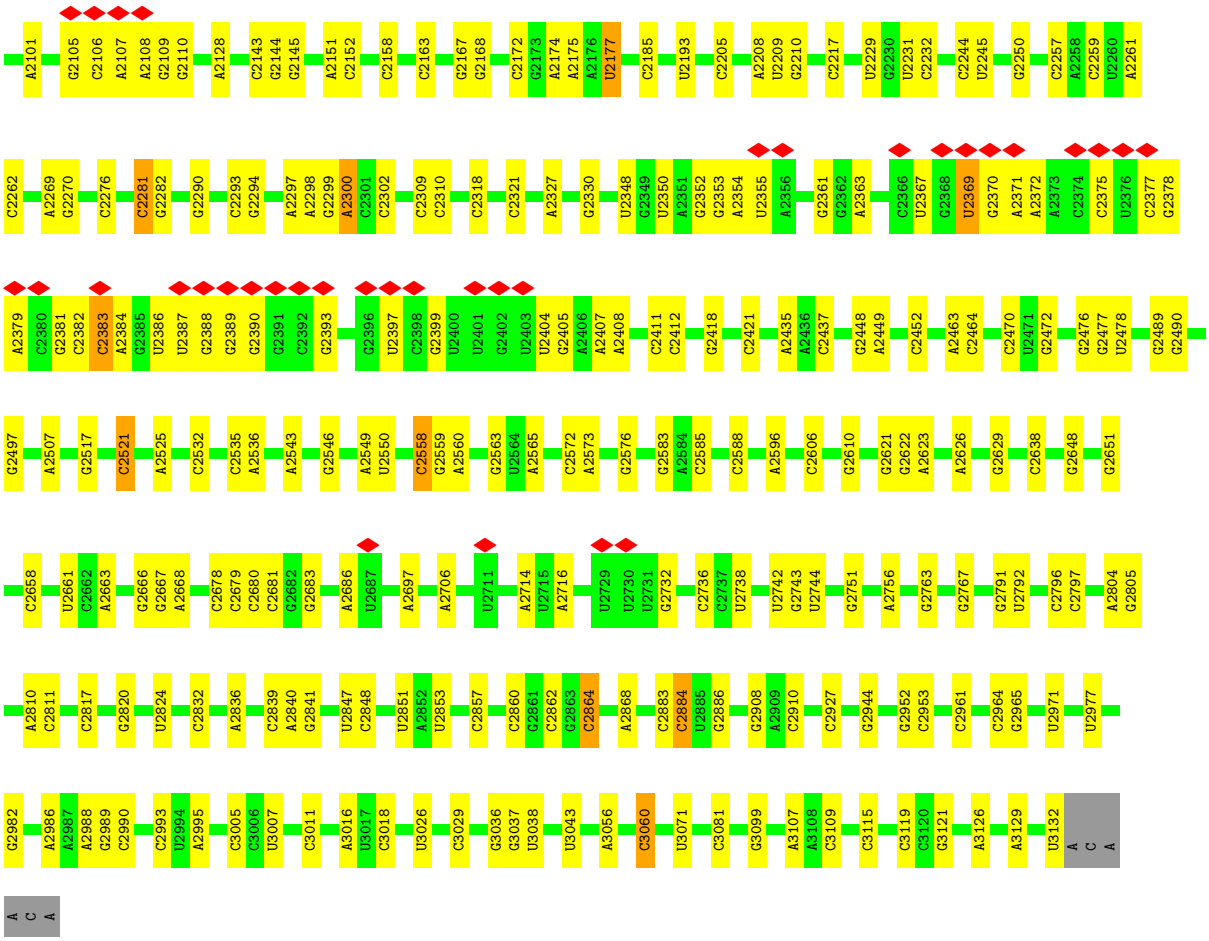
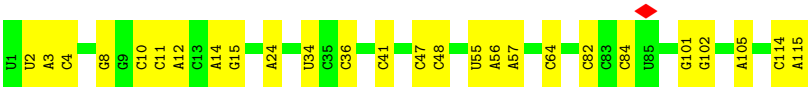


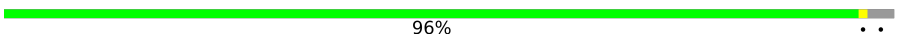
- Molecule 10: 5S rRNA

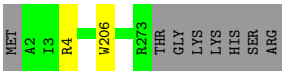
Chain B:



- Molecule 11: 50S ribosomal protein L2

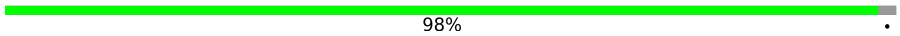
Chain C:

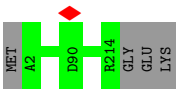




- Molecule 12: 50S ribosomal protein L3

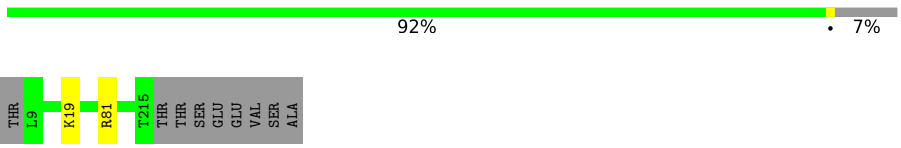
Chain D:





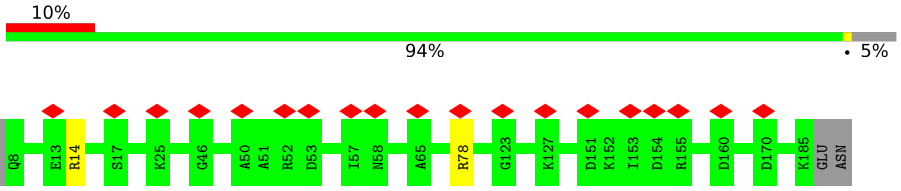
- Molecule 13: 50S ribosomal protein L4

Chain E:



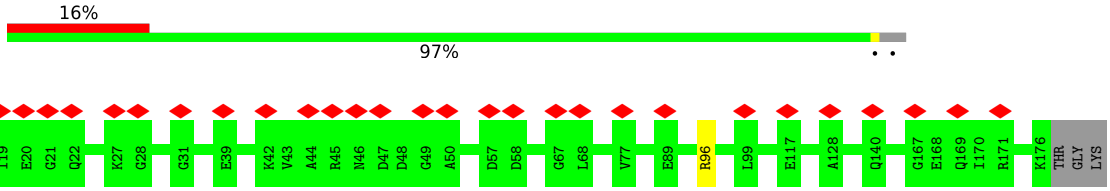
• Molecule 14: 50S ribosomal protein L5

Chain F:



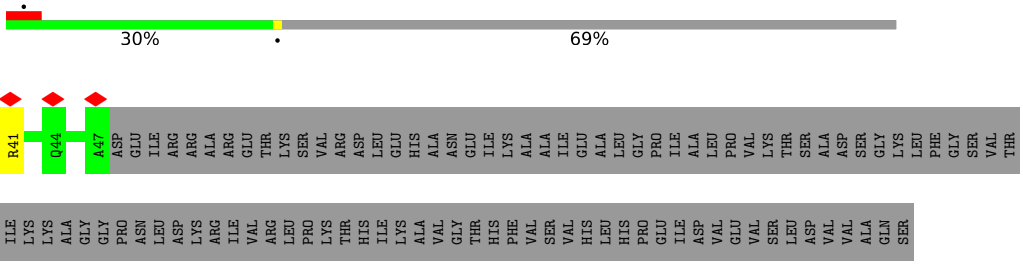
• Molecule 15: 50S ribosomal protein L6

Chain G:



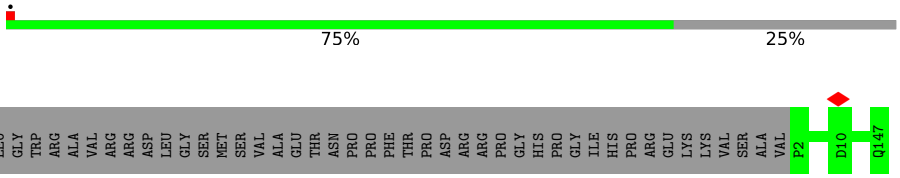
• Molecule 16: 50S ribosomal protein L9

Chain H:



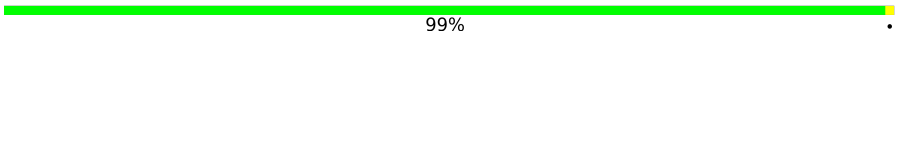
• Molecule 17: 50S ribosomal protein L13

Chain J:



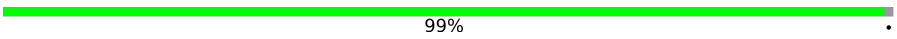
• Molecule 18: 50S ribosomal protein L14

Chain K:



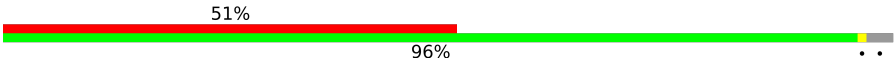
• Molecule 19: 50S ribosomal protein L15

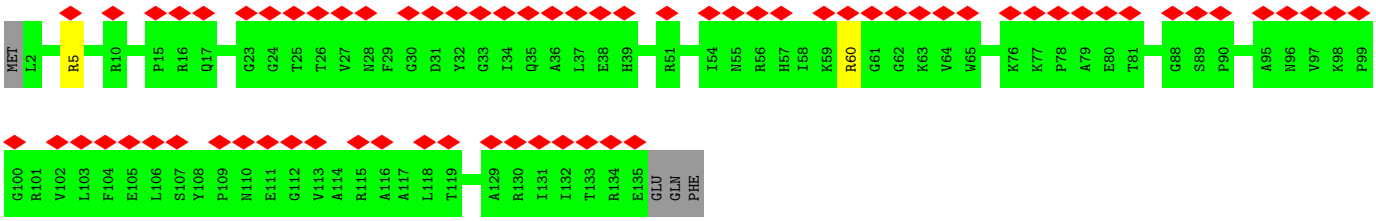
Chain L:



• Molecule 20: 50S ribosomal protein L16

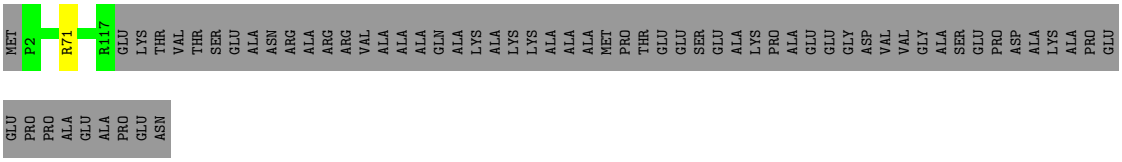
Chain M:





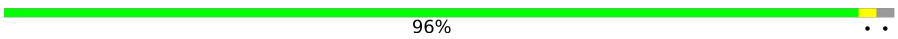
• Molecule 21: 50S ribosomal protein L17

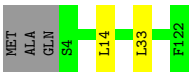
Chain N:



• Molecule 22: 50S ribosomal protein L18

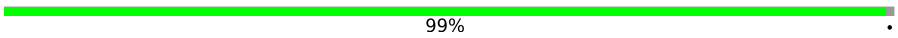
Chain O:





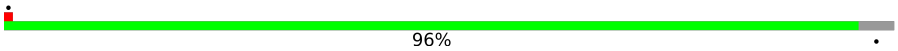
• Molecule 23: 50S ribosomal protein L19

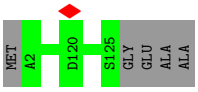
Chain P:



• Molecule 24: 50S ribosomal protein L20

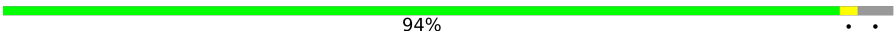
Chain Q:

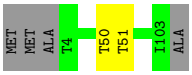




• Molecule 25: 50S ribosomal protein L21

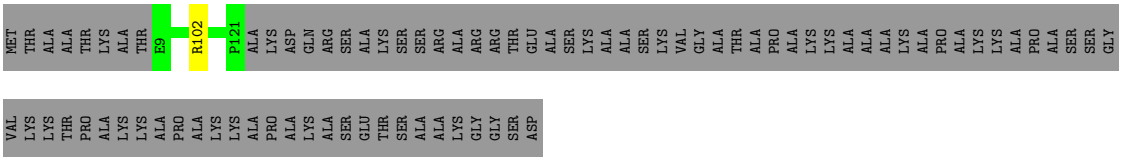
Chain R:





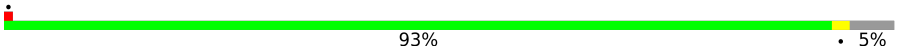
- Molecule 26: 50S ribosomal protein L22

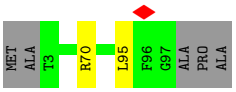
Chain S:



- Molecule 27: 50S ribosomal protein L23

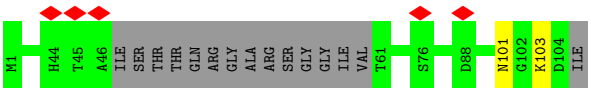
Chain T:





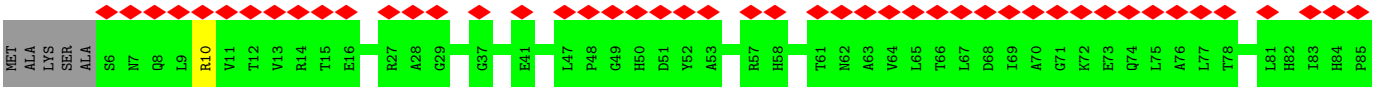
- Molecule 28: 50S ribosomal protein L24

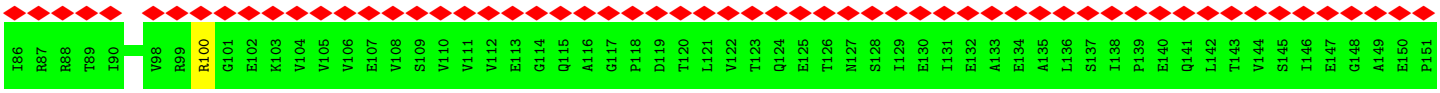
Chain U:

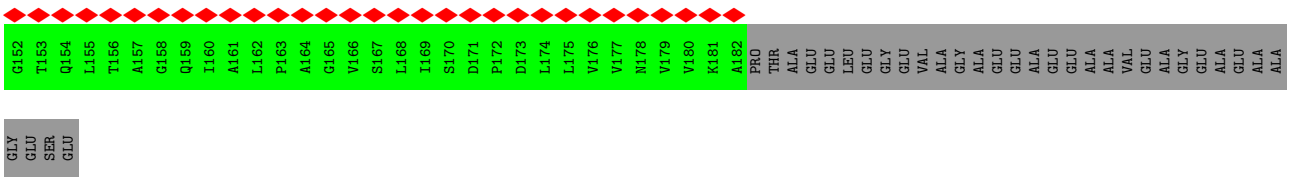


- Molecule 29: 50S ribosomal protein L25

Chain V:





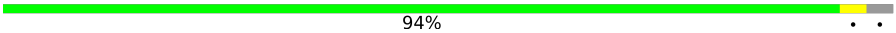


- Molecule 30: 50S ribosomal protein L27

Chain W:

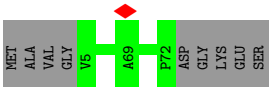
• Molecule 31: 50S ribosomal protein L28

Chain X:



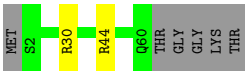
• Molecule 32: 50S ribosomal protein L29

Chain Y:



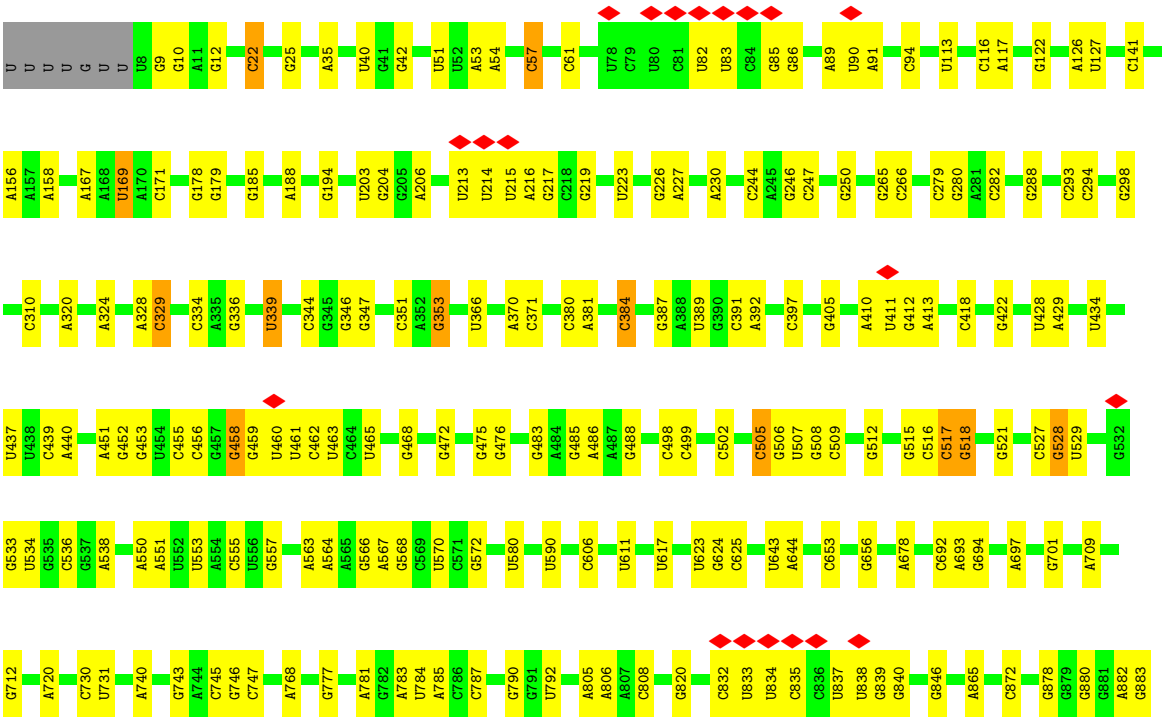
• Molecule 33: 50S ribosomal protein L30

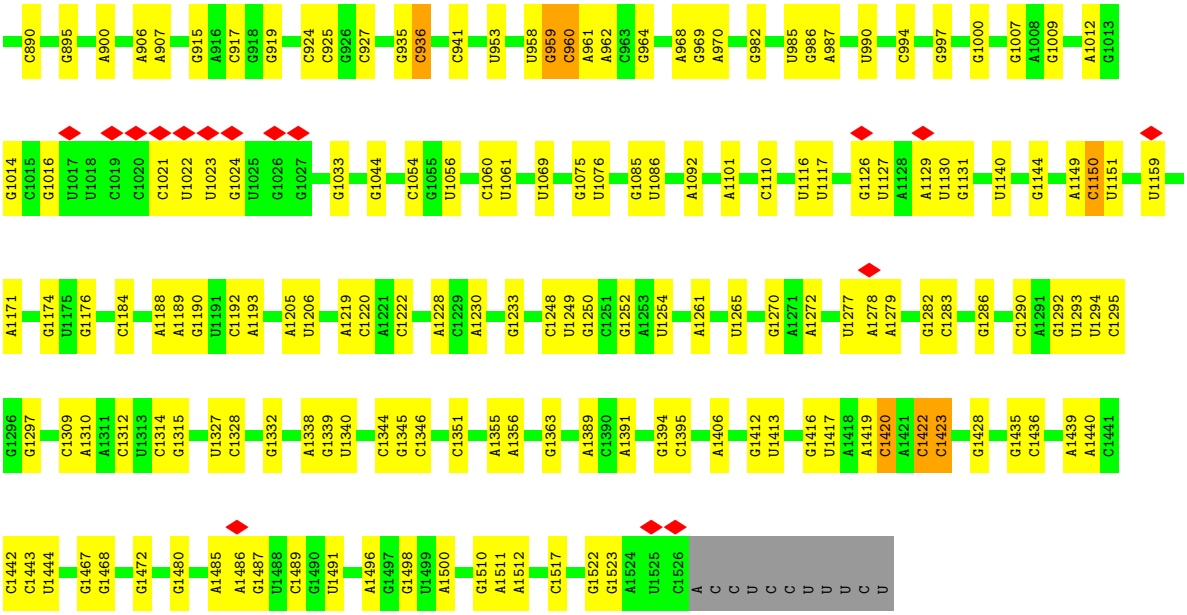
Chain Z:



• Molecule 34: 16S rRNA

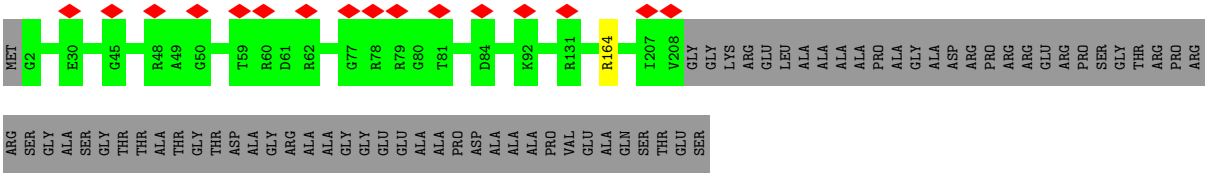
Chain a:





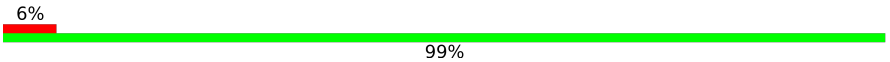
• Molecule 35: 30S ribosomal protein S3

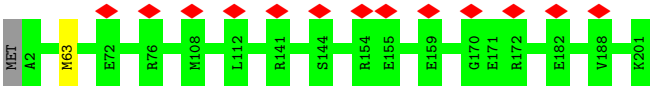
Chain c:



• Molecule 36: 30S ribosomal protein S4

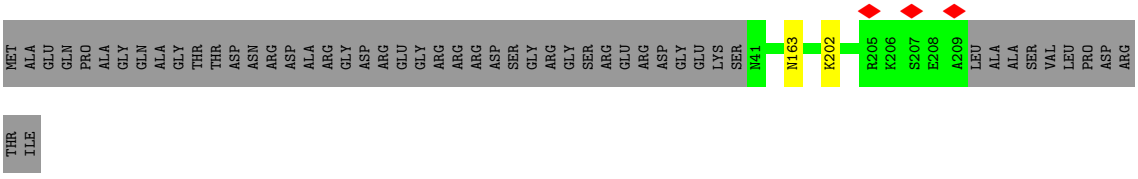
Chain d:





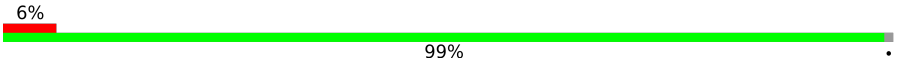
• Molecule 37: 30S ribosomal protein S5

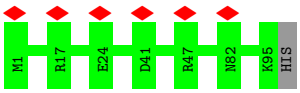
Chain e:



• Molecule 38: 30S ribosomal protein S6

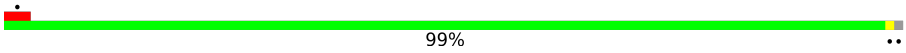
Chain f:

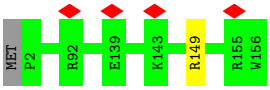




• Molecule 39: 30S ribosomal protein S7

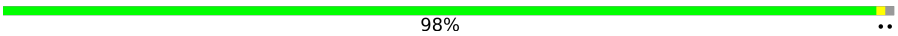
Chain g:

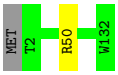




• Molecule 40: 30S ribosomal protein S8

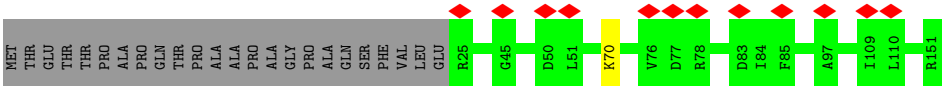
Chain h:





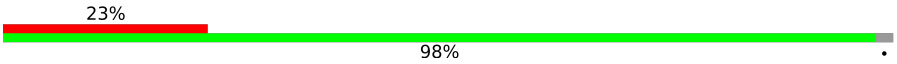
• Molecule 41: 30S ribosomal protein S9

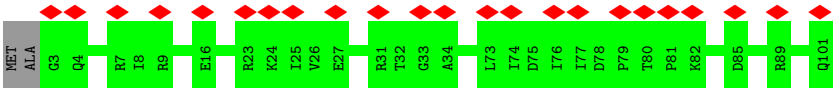
Chain i:



• Molecule 42: 30S ribosomal protein S10

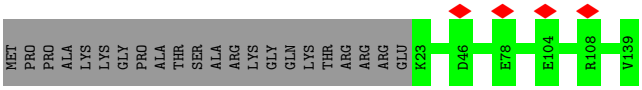
Chain j:





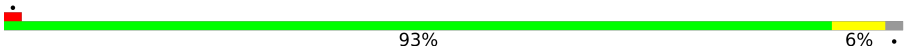
• Molecule 43: 30S ribosomal protein S11

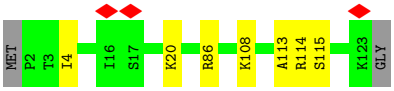
Chain k:



• Molecule 44: 30S ribosomal protein S12

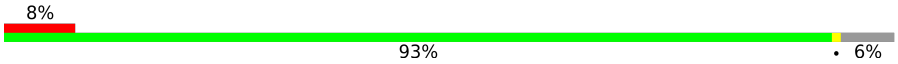
Chain l:

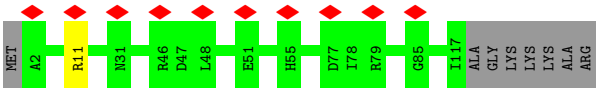




• Molecule 45: 30S ribosomal protein S13

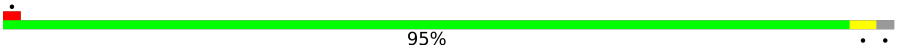
Chain m:

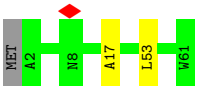




• Molecule 46: 30S ribosomal protein S14 type Z

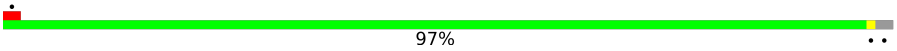
Chain n:

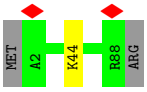




• Molecule 47: 30S ribosomal protein S15

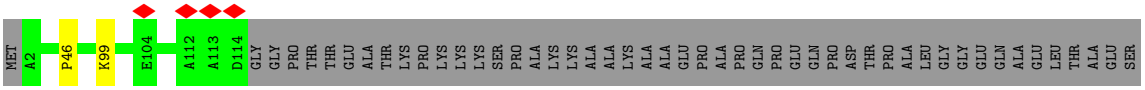
Chain o:





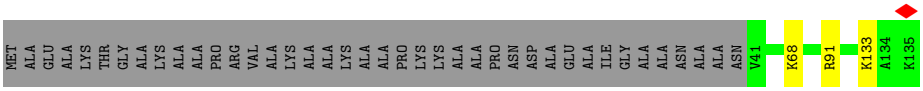
• Molecule 48: 30S ribosomal protein S16

Chain p:



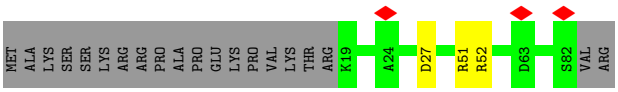
• Molecule 49: 30S ribosomal protein S17

Chain q:



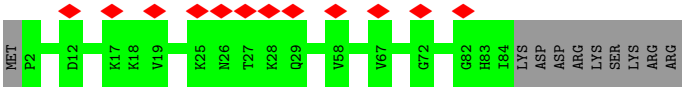
• Molecule 50: 30S ribosomal protein S18 1

Chain r:



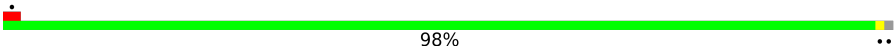
• Molecule 51: 30S ribosomal protein S19

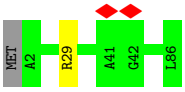
Chain s:



• Molecule 52: 30S ribosomal protein S20

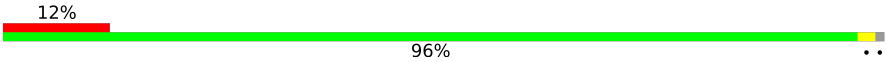
Chain t:

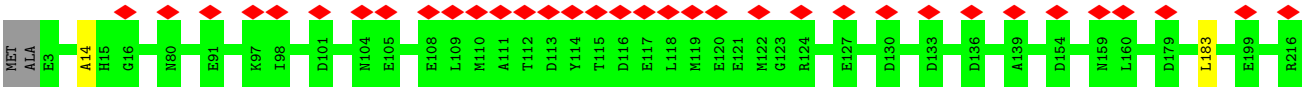


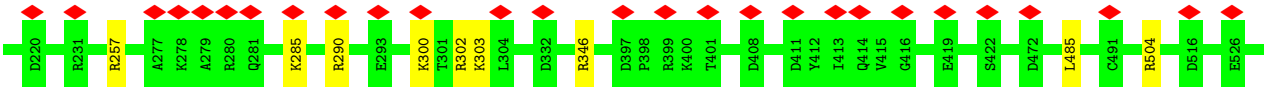


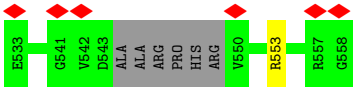
• Molecule 53: Energy-dependent translational throttle protein EttA

Chain x:



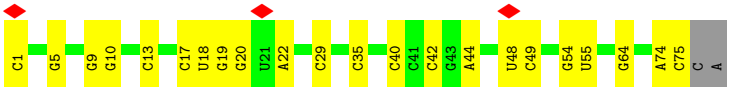






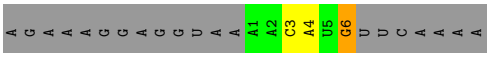
• Molecule 54: initiator tRNA (Met)

Chain y:



• Molecule 55: mRNA

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34158	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	48	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.506	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 4OC, MA6, ZN, OMG, ANP, MG, G7M, 5MC, 2MG, UR3, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.40	0/435	0.57	0/581
2	1	0.44	0/407	0.55	0/543
3	2	0.55	0/377	0.59	0/494
4	3	0.39	0/499	0.54	0/664
5	4	0.35	0/303	0.57	0/402
6	6	0.28	0/364	0.68	1/493 (0.2%)
7	7	0.23	0/68	0.42	0/84
8	8	0.27	0/1728	0.52	0/2339
9	A	1.00	5/74925 (0.0%)	1.07	258/116904 (0.2%)
10	B	0.69	0/2749	0.98	8/4284 (0.2%)
11	C	0.53	0/2129	0.64	0/2861
12	D	0.52	0/1613	0.61	0/2174
13	E	0.50	0/1575	0.61	0/2129
14	F	0.32	0/1429	0.54	0/1921
15	G	0.29	0/1351	0.56	0/1824
16	H	0.31	0/353	0.63	0/474
17	J	0.51	0/1170	0.56	0/1584
18	K	0.51	0/951	0.64	0/1278
19	L	0.50	0/1088	0.62	0/1453
20	M	0.29	0/1098	0.51	0/1481
21	N	0.50	0/925	0.60	0/1242
22	O	0.37	0/914	0.62	2/1228 (0.2%)
23	P	0.53	0/922	0.61	0/1236
24	Q	0.59	0/1006	0.61	0/1349
25	R	0.50	0/766	0.59	0/1030
26	S	0.52	0/874	0.57	0/1186
27	T	0.45	0/751	0.62	1/1012 (0.1%)
28	U	0.43	0/705	0.68	0/941
29	V	0.28	0/1336	0.60	0/1820
30	W	0.50	0/542	0.62	0/721
31	X	0.57	0/476	0.65	1/638 (0.2%)
32	Y	0.39	0/564	0.57	0/756

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Z	0.42	0/480	0.60	0/645
34	a	0.79	1/36331 (0.0%)	1.01	98/56686 (0.2%)
35	c	0.36	0/1678	0.55	0/2254
36	d	0.36	0/1683	0.55	0/2269
37	e	0.39	0/1238	0.57	0/1673
38	f	0.31	0/767	0.52	0/1036
39	g	0.33	0/1250	0.53	0/1686
40	h	0.39	0/1021	0.58	0/1379
41	i	0.33	0/1010	0.57	0/1356
42	j	0.36	0/803	0.65	0/1086
43	k	0.36	0/891	0.54	0/1204
44	l	0.42	0/970	0.67	0/1295
45	m	0.28	0/953	0.59	0/1274
46	n	0.43	0/477	0.62	1/634 (0.2%)
47	o	0.34	0/727	0.55	0/973
48	p	0.37	0/901	0.59	0/1217
49	q	0.36	0/782	0.66	0/1045
50	r	0.34	0/511	0.57	1/685 (0.1%)
51	s	0.30	0/690	0.59	0/928
52	t	0.31	0/654	0.50	0/867
53	x	0.33	0/4375	0.60	2/5921 (0.0%)
54	y	0.64	1/1789 (0.1%)	1.02	7/2786 (0.3%)
55	z	1.03	1/144 (0.7%)	1.20	1/222 (0.5%)
All	All	0.81	8/164518 (0.0%)	0.95	381/246247 (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
6	6	0	1
8	8	0	1
11	C	0	1
25	R	0	1
28	U	0	1
44	l	0	2
47	o	0	1
53	x	0	1
All	All	0	9

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	y	1	C	OP3-P	-10.67	1.48	1.61
9	A	912	A	N7-C5	-5.99	1.35	1.39
9	A	890	A	N9-C4	-5.81	1.34	1.37
9	A	917	A	N9-C4	-5.51	1.34	1.37
9	A	890	A	N3-C4	-5.33	1.31	1.34
55	z	6	G	N9-C8	-5.23	1.34	1.37
34	a	906	A	N9-C4	-5.11	1.34	1.37
9	A	2407	A	N9-C4	5.10	1.41	1.37

All (381) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2309	C	N3-C2-O2	-10.65	114.45	121.90
9	A	3060	C	C6-N1-C2	-10.64	116.04	120.30
9	A	1134	C	C6-N1-C2	-10.40	116.14	120.30
9	A	3060	C	N3-C2-O2	-10.05	114.87	121.90
9	A	1134	C	C5-C6-N1	9.93	125.96	121.00
9	A	946	C	N3-C2-O2	-9.79	115.04	121.90
9	A	2309	C	N1-C2-O2	9.55	124.63	118.90
9	A	3060	C	C2-N1-C1'	9.54	129.29	118.80
9	A	2309	C	C6-N1-C2	-9.51	116.50	120.30
9	A	2217	C	C6-N1-C2	-9.07	116.67	120.30
9	A	739	C	C2-N1-C1'	9.05	128.76	118.80
9	A	2310	C	C6-N1-C2	-8.89	116.74	120.30
9	A	946	C	N1-C2-O2	8.85	124.21	118.90
34	a	528	G	N3-C4-C5	-8.75	124.23	128.60
9	A	1134	C	C2-N1-C1'	8.59	128.25	118.80
9	A	882	C	N3-C2-O2	-8.54	115.92	121.90
9	A	3060	C	N1-C2-O2	8.29	123.87	118.90
34	a	528	G	N3-C4-N9	8.25	130.95	126.00
34	a	1498	G	N3-C4-C5	-8.22	124.49	128.60
34	a	1498	G	C8-N9-C4	-8.15	103.14	106.40
9	A	1426	C	C6-N1-C2	-8.08	117.07	120.30
34	a	384	C	N1-C2-O2	8.06	123.74	118.90
9	A	882	C	N1-C2-O2	8.06	123.73	118.90
9	A	1517	C	N1-C2-O2	8.00	123.70	118.90
9	A	946	C	C2-N1-C1'	7.97	127.57	118.80
34	a	1254	U	C2-N1-C1'	7.92	127.21	117.70
34	a	1295	C	N1-C2-O2	7.84	123.60	118.90
34	a	1498	G	C4-N9-C1'	7.79	136.63	126.50
9	A	946	C	C6-N1-C2	-7.77	117.19	120.30
34	a	625	C	C6-N1-C2	-7.75	117.20	120.30
9	A	1076	C	C6-N1-C2	-7.70	117.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2369	U	C2-N1-C1'	7.66	126.89	117.70
34	a	1295	C	N3-C2-O2	-7.64	116.55	121.90
9	A	2217	C	C2-N1-C1'	7.62	127.19	118.80
34	a	745	C	N1-C2-O2	7.56	123.43	118.90
34	a	1150	C	C2-N1-C1'	7.53	127.08	118.80
9	A	1332	C	C6-N1-C2	-7.53	117.29	120.30
9	A	3109	C	N1-C2-O2	7.52	123.41	118.90
34	a	528	G	C4-N9-C1'	7.50	136.24	126.50
9	A	2217	C	N3-C2-O2	-7.44	116.69	121.90
9	A	1684	C	C6-N1-C2	-7.37	117.35	120.30
34	a	384	C	N3-C2-O2	-7.34	116.76	121.90
9	A	2309	C	C2-N1-C1'	7.33	126.86	118.80
9	A	2559	G	C4-N9-C1'	7.29	135.98	126.50
10	B	82	C	C6-N1-C2	-7.29	117.38	120.30
34	a	745	C	C2-N1-C1'	7.26	126.78	118.80
34	a	1346	C	C6-N1-C2	-7.23	117.41	120.30
9	A	1093	C	C6-N1-C2	-7.17	117.43	120.30
34	a	505	C	C6-N1-C2	-7.16	117.44	120.30
9	A	2558	C	N1-C2-O2	7.12	123.17	118.90
9	A	550	C	C6-N1-C2	-7.12	117.45	120.30
9	A	1988	C	N1-C2-O2	7.11	123.16	118.90
9	A	861	C	N1-C2-O2	7.09	123.16	118.90
9	A	739	C	C6-N1-C1'	-7.02	112.37	120.80
9	A	2369	U	N3-C2-O2	-6.99	117.31	122.20
9	A	2860	C	C6-N1-C2	-6.97	117.51	120.30
9	A	3011	C	C6-N1-C2	-6.94	117.53	120.30
34	a	1254	U	N3-C2-O2	-6.92	117.36	122.20
34	a	528	G	C2-N3-C4	6.91	115.35	111.90
9	A	2369	U	N1-C2-O2	6.86	127.61	122.80
9	A	1076	C	C5-C6-N1	6.82	124.41	121.00
9	A	205	C	C6-N1-C2	-6.80	117.58	120.30
9	A	869	C	C6-N1-C2	-6.79	117.58	120.30
9	A	802	C	C6-N1-C2	-6.78	117.59	120.30
9	A	1068	C	C6-N1-C2	-6.74	117.61	120.30
9	A	3109	C	C6-N1-C2	-6.69	117.62	120.30
34	a	1498	G	N7-C8-N9	6.69	116.44	113.10
9	A	1134	C	N1-C2-O2	6.69	122.91	118.90
34	a	1150	C	N1-C2-O2	6.68	122.91	118.90
34	a	730	C	C6-N1-C2	-6.67	117.63	120.30
34	a	384	C	C6-N1-C2	-6.67	117.63	120.30
34	a	223	U	C2-N1-C1'	6.66	125.69	117.70
34	a	1254	U	N1-C2-O2	6.65	127.45	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1517	C	C2-N1-C1'	6.65	126.11	118.80
9	A	801	C	C6-N1-C2	-6.64	117.64	120.30
34	a	517	C	O4'-C1'-N1	6.63	113.51	108.20
9	A	1425	C	C6-N1-C2	-6.61	117.66	120.30
9	A	739	C	N3-C2-O2	-6.56	117.31	121.90
34	a	1422	C	C6-N1-C2	-6.55	117.68	120.30
9	A	600	G	O4'-C1'-N9	6.54	113.43	108.20
9	A	239	C	C6-N1-C2	-6.53	117.69	120.30
9	A	200	C	C6-N1-C2	-6.52	117.69	120.30
9	A	2281	C	C5-C6-N1	6.52	124.26	121.00
54	y	35	C	N1-C2-O2	6.51	122.80	118.90
34	a	1498	G	N3-C4-N9	6.50	129.90	126.00
9	A	408	C	C6-N1-C2	-6.47	117.71	120.30
9	A	1072	G	C4-N9-C1'	6.47	134.91	126.50
9	A	1517	C	N3-C2-O2	-6.46	117.38	121.90
9	A	941	C	C6-N1-C2	-6.44	117.72	120.30
9	A	2953	C	C6-N1-C2	-6.44	117.72	120.30
9	A	623	C	C6-N1-C2	-6.42	117.73	120.30
9	A	882	C	C2-N1-C1'	6.42	125.86	118.80
9	A	1358	C	C6-N1-C2	-6.42	117.73	120.30
9	A	2961	C	C6-N1-C2	-6.41	117.74	120.30
9	A	2857	C	C6-N1-C2	-6.40	117.74	120.30
9	A	20	C	C6-N1-C2	-6.39	117.74	120.30
9	A	3109	C	N3-C2-O2	-6.39	117.42	121.90
9	A	739	C	N1-C2-O2	6.39	122.73	118.90
34	a	1248	C	N1-C2-O2	6.39	122.73	118.90
9	A	2163	C	C6-N1-C2	-6.38	117.75	120.30
9	A	57	C	C6-N1-C2	-6.33	117.77	120.30
9	A	683	C	C6-N1-C2	-6.32	117.77	120.30
9	A	2077	C	C6-N1-C2	-6.30	117.78	120.30
34	a	1295	C	C6-N1-C2	-6.30	117.78	120.30
34	a	223	U	N3-C2-O2	-6.30	117.79	122.20
9	A	695	G	C4-N9-C1'	6.29	134.68	126.50
9	A	2067	C	C6-N1-C2	-6.28	117.79	120.30
9	A	2953	C	C5-C6-N1	6.28	124.14	121.00
9	A	2559	G	C8-N9-C1'	-6.28	118.84	127.00
34	a	625	C	C5-C6-N1	6.28	124.14	121.00
9	A	1685	C	C6-N1-C2	-6.24	117.80	120.30
9	A	963	C	C6-N1-C2	-6.24	117.80	120.30
9	A	697	C	C6-N1-C2	-6.22	117.81	120.30
9	A	2056	C	C6-N1-C2	-6.21	117.82	120.30
9	A	2217	C	N1-C2-O2	6.21	122.62	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	2029	C	C6-N1-C2	-6.19	117.82	120.30
9	A	605	C	C6-N1-C2	-6.19	117.82	120.30
9	A	418	C	C6-N1-C2	-6.19	117.82	120.30
9	A	2681	C	C6-N1-C2	-6.18	117.83	120.30
34	a	936	C	C2-N1-C1'	6.18	125.59	118.80
9	A	686	C	N3-C2-O2	-6.17	117.58	121.90
9	A	47	C	C6-N1-C2	-6.16	117.84	120.30
9	A	686	C	N1-C2-O2	6.14	122.59	118.90
9	A	912	A	C4-N9-C1'	6.14	137.34	126.30
9	A	550	C	C5-C6-N1	6.13	124.06	121.00
9	A	913	G	P-O3'-C3'	6.12	127.04	119.70
34	a	528	G	C8-N9-C1'	-6.10	119.07	127.00
9	A	820	C	C5-C6-N1	6.09	124.04	121.00
9	A	3109	C	C2-N1-C1'	6.08	125.49	118.80
54	y	35	C	C2-N1-C1'	6.08	125.48	118.80
9	A	1044	C	N1-C2-O2	6.07	122.55	118.90
10	B	82	C	C5-C6-N1	6.06	124.03	121.00
34	a	1054	C	C6-N1-C2	-6.06	117.88	120.30
34	a	590	U	C6-N1-C2	-6.06	117.36	121.00
34	a	936	C	N1-C2-O2	6.04	122.53	118.90
34	a	310	C	C6-N1-C2	-6.04	117.89	120.30
10	B	10	C	C6-N1-C2	-6.03	117.89	120.30
34	a	507	U	N3-C2-O2	-6.01	117.99	122.20
46	n	53	LEU	CA-CB-CG	6.01	129.12	115.30
9	A	882	C	C6-N1-C2	-6.01	117.90	120.30
9	A	20	C	C5-C6-N1	6.00	124.00	121.00
9	A	2559	G	N3-C4-N9	6.00	129.60	126.00
34	a	1346	C	C5-C6-N1	5.99	123.99	121.00
9	A	943	C	C6-N1-C2	-5.98	117.91	120.30
9	A	2075	U	C5-C6-N1	5.97	125.69	122.70
9	A	2864	C	C6-N1-C2	-5.96	117.92	120.30
9	A	869	C	N1-C2-O2	5.96	122.47	118.90
9	A	1332	C	C5-C6-N1	5.96	123.98	121.00
34	a	787	C	C6-N1-C2	-5.94	117.92	120.30
9	A	1457	C	N1-C2-O2	5.94	122.46	118.90
34	a	529	U	N1-C2-O2	5.93	126.95	122.80
9	A	534	C	C6-N1-C2	-5.92	117.93	120.30
34	a	223	U	N1-C2-O2	5.92	126.94	122.80
9	A	2383	C	C2-N1-C1'	5.92	125.31	118.80
9	A	507	C	C6-N1-C2	-5.91	117.94	120.30
9	A	905	G	C4-N9-C1'	5.90	134.17	126.50
9	A	1988	C	C5-C6-N1	5.90	123.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1072	G	C8-N9-C1'	-5.89	119.34	127.00
9	A	3011	C	C5-C6-N1	5.88	123.94	121.00
9	A	1437	C	C6-N1-C2	-5.87	117.95	120.30
9	A	2862	C	C6-N1-C2	-5.87	117.95	120.30
9	A	2407	A	C2-N3-C4	5.87	113.53	110.60
9	A	1834	C	C6-N1-C2	-5.86	117.96	120.30
34	a	730	C	N1-C2-O2	5.85	122.41	118.90
9	A	914	G	O5'-P-OP2	-5.85	100.44	105.70
34	a	936	C	C6-N1-C2	-5.85	117.96	120.30
9	A	2075	U	C6-N1-C2	-5.84	117.49	121.00
9	A	1397	G	N3-C4-N9	5.84	129.50	126.00
9	A	2559	G	N3-C4-C5	-5.82	125.69	128.60
9	A	2262	C	C6-N1-C2	-5.81	117.98	120.30
9	A	1457	C	C2-N1-C1'	5.80	125.18	118.80
9	A	145	C	C6-N1-C2	-5.80	117.98	120.30
9	A	912	A	N3-C4-N9	5.80	132.04	127.40
9	A	2310	C	C5-C6-N1	5.79	123.90	121.00
9	A	1488	C	C6-N1-C2	-5.79	117.98	120.30
54	y	40	C	C6-N1-C2	-5.79	117.98	120.30
9	A	2318	C	C6-N1-C2	-5.78	117.99	120.30
9	A	2383	C	N1-C2-O2	5.77	122.36	118.90
9	A	869	C	C5-C6-N1	5.77	123.89	121.00
9	A	2300	A	C2-N3-C4	5.77	113.48	110.60
9	A	1988	C	C2-N1-C1'	5.77	125.14	118.80
9	A	2558	C	C2-N1-C1'	5.77	125.14	118.80
9	A	458	C	N1-C2-O2	5.76	122.36	118.90
9	A	1481	C	N1-C2-O2	5.76	122.36	118.90
34	a	507	U	C2-N1-C1'	5.76	124.61	117.70
9	A	867	C	C6-N1-C2	-5.75	118.00	120.30
9	A	1953	G	N3-C2-N2	-5.75	115.87	119.90
9	A	2350	U	C2-N1-C1'	5.75	124.61	117.70
9	A	604	C	C6-N1-C2	-5.75	118.00	120.30
34	a	171	C	C6-N1-C2	-5.75	118.00	120.30
9	A	858	G	C4-N9-C1'	5.75	133.97	126.50
9	A	2185	C	C6-N1-C2	-5.73	118.01	120.30
10	B	82	C	N1-C2-O2	5.73	122.34	118.90
53	x	183	LEU	CA-CB-CG	5.73	128.48	115.30
9	A	2244	C	C5-C6-N1	5.72	123.86	121.00
9	A	506	C	C6-N1-C2	-5.71	118.02	120.30
9	A	2796	C	C6-N1-C2	-5.71	118.02	120.30
34	a	747	C	C6-N1-C2	-5.70	118.02	120.30
34	a	1517	C	C6-N1-C2	-5.69	118.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1465	C	C6-N1-C2	-5.68	118.03	120.30
34	a	293	C	C6-N1-C2	-5.67	118.03	120.30
9	A	1684	C	C5-C6-N1	5.66	123.83	121.00
34	a	745	C	C6-N1-C1'	-5.66	114.01	120.80
9	A	2452	C	C6-N1-C2	-5.65	118.04	120.30
9	A	1833	C	C5-C6-N1	5.65	123.82	121.00
10	B	48	C	C6-N1-C2	-5.64	118.04	120.30
9	A	912	A	C8-N9-C1'	-5.64	117.55	127.70
9	A	977	U	N3-C2-O2	-5.63	118.25	122.20
9	A	1093	C	C5-C6-N1	5.63	123.82	121.00
9	A	574	C	C6-N1-C2	-5.61	118.06	120.30
34	a	339	U	N3-C2-O2	-5.61	118.27	122.20
10	B	47	C	C6-N1-C2	-5.57	118.07	120.30
9	A	683	C	C5-C6-N1	5.56	123.78	121.00
9	A	2321	C	C6-N1-C2	-5.56	118.07	120.30
9	A	2558	C	N3-C2-O2	-5.55	118.02	121.90
9	A	2797	C	C6-N1-C2	-5.54	118.08	120.30
9	A	31	C	C6-N1-C2	-5.54	118.08	120.30
9	A	2350	U	N3-C2-O2	-5.54	118.32	122.20
9	A	372	G	C4-N9-C1'	5.54	133.69	126.50
9	A	905	G	C8-N9-C1'	-5.53	119.81	127.00
54	y	42	C	C6-N1-C2	-5.53	118.09	120.30
34	a	890	C	C6-N1-C2	-5.53	118.09	120.30
9	A	754	C	C6-N1-C2	-5.53	118.09	120.30
9	A	98	C	C6-N1-C2	-5.52	118.09	120.30
9	A	208	U	C2-N1-C1'	5.51	124.31	117.70
9	A	145	C	C5-C6-N1	5.51	123.75	121.00
9	A	1801	C	C6-N1-C2	-5.50	118.10	120.30
9	A	152	C	C6-N1-C2	-5.49	118.10	120.30
9	A	1960	C	C6-N1-C2	-5.49	118.10	120.30
9	A	2464	C	N1-C2-O2	5.49	122.19	118.90
9	A	2535	C	N1-C2-O2	5.48	122.19	118.90
9	A	1072	G	N3-C4-N9	5.48	129.29	126.00
9	A	1428	C	C6-N1-C2	-5.48	118.11	120.30
34	a	936	C	C5-C6-N1	5.47	123.74	121.00
9	A	212	C	C6-N1-C2	-5.47	118.11	120.30
34	a	206	A	O4'-C1'-N9	5.47	112.57	108.20
34	a	458	G	C4-N9-C1'	5.46	133.60	126.50
34	a	418	C	N1-C2-O2	5.46	122.17	118.90
22	O	14	LEU	CA-CB-CG	5.45	127.83	115.30
9	A	2232	C	N1-C2-O2	5.45	122.17	118.90
34	a	169	U	N1-C2-O2	5.44	126.61	122.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	1134	C	C2-N3-C4	5.44	122.62	119.90
34	a	57	C	N1-C2-O2	5.44	122.16	118.90
9	A	769	U	C2-N1-C1'	5.43	124.22	117.70
34	a	294	C	C6-N1-C2	-5.43	118.13	120.30
9	A	485	C	C6-N1-C2	-5.42	118.13	120.30
34	a	787	C	C5-C6-N1	5.42	123.71	121.00
9	A	2796	C	C5-C6-N1	5.42	123.71	121.00
9	A	533	C	C6-N1-C2	-5.42	118.13	120.30
9	A	623	C	C5-C6-N1	5.41	123.71	121.00
9	A	502	C	C6-N1-C2	-5.41	118.14	120.30
9	A	2352	G	C4-N9-C1'	5.41	133.53	126.50
9	A	1092	C	C6-N1-C2	-5.40	118.14	120.30
9	A	200	C	N3-C2-O2	-5.40	118.12	121.90
9	A	667	C	O5'-P-OP2	-5.40	100.84	105.70
9	A	941	C	C5-C6-N1	5.40	123.70	121.00
34	a	745	C	N3-C2-O2	-5.38	118.14	121.90
9	A	1445	C	C5-C6-N1	5.38	123.69	121.00
9	A	1962	C	N1-C2-O2	5.36	122.12	118.90
34	a	730	C	N3-C2-O2	-5.36	118.15	121.90
9	A	66	C	C6-N1-C2	-5.36	118.16	120.30
34	a	529	U	N3-C2-O2	-5.35	118.45	122.20
22	O	33	LEU	CA-CB-CG	5.35	127.60	115.30
34	a	1498	G	C8-N9-C1'	-5.35	120.05	127.00
9	A	2535	C	N3-C2-O2	-5.35	118.16	121.90
34	a	653	C	C6-N1-C2	-5.35	118.16	120.30
34	a	917	C	C6-N1-C2	-5.34	118.17	120.30
9	A	1044	C	N3-C2-O2	-5.33	118.17	121.90
9	A	1874	C	N1-C2-O2	5.33	122.10	118.90
9	A	1320	U	N1-C2-O2	5.33	126.53	122.80
9	A	1348	C	C6-N1-C2	-5.33	118.17	120.30
34	a	1150	C	C6-N1-C1'	-5.33	114.41	120.80
10	B	82	C	C2-N1-C1'	5.32	124.65	118.80
9	A	2352	G	N3-C4-N9	5.32	129.19	126.00
53	x	485	LEU	CA-CB-CG	5.31	127.52	115.30
9	A	869	C	N3-C2-O2	-5.31	118.18	121.90
50	r	27	ASP	CB-CG-OD1	5.31	123.08	118.30
9	A	270	C	C6-N1-C2	-5.30	118.18	120.30
34	a	384	C	C2-N1-C1'	5.30	124.62	118.80
9	A	807	C	C5-C6-N1	5.29	123.65	121.00
34	a	1498	G	C6-C5-N7	-5.29	127.22	130.40
9	A	2860	C	C5-C6-N1	5.29	123.64	121.00
34	a	1420	C	C6-N1-C2	-5.29	118.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	783	A	O4'-C1'-N9	5.29	112.43	108.20
9	A	1474	G	C4-N9-C1'	5.29	133.37	126.50
9	A	816	C	C5-C6-N1	5.28	123.64	121.00
9	A	204	U	N3-C2-O2	-5.27	118.51	122.20
34	a	1423	C	C6-N1-C2	-5.27	118.19	120.30
34	a	1222	C	C6-N1-C2	-5.26	118.19	120.30
9	A	1481	C	N3-C2-O2	-5.26	118.22	121.90
9	A	1834	C	C5-C6-N1	5.26	123.63	121.00
34	a	606	C	C6-N1-C2	-5.26	118.20	120.30
9	A	2680	C	C6-N1-C2	-5.25	118.20	120.30
9	A	1507	C	C2-N1-C1'	5.25	124.57	118.80
9	A	2884	C	N1-C2-O2	5.24	122.05	118.90
9	A	2060	C	C6-N1-C2	-5.24	118.20	120.30
9	A	807	C	C6-N1-C2	-5.24	118.21	120.30
9	A	2817	C	C6-N1-C2	-5.24	118.21	120.30
34	a	339	U	N1-C2-O2	5.24	126.47	122.80
9	A	1442	G	C4-N9-C1'	5.23	133.30	126.50
34	a	1150	C	N3-C2-O2	-5.23	118.24	121.90
9	A	1134	C	N3-C2-O2	-5.23	118.24	121.90
9	A	1457	C	C5-C6-N1	5.22	123.61	121.00
9	A	966	C	C6-N1-C2	-5.22	118.21	120.30
9	A	2521	C	N1-C2-O2	5.22	122.03	118.90
9	A	820	C	C6-N1-C2	-5.21	118.22	120.30
9	A	1446	C	C6-N1-C2	-5.21	118.22	120.30
34	a	418	C	C6-N1-C2	-5.21	118.22	120.30
34	a	507	U	N1-C2-O2	5.21	126.44	122.80
34	a	169	U	C2-N1-C1'	5.20	123.94	117.70
10	B	82	C	N3-C2-O2	-5.20	118.26	121.90
9	A	1907	C	C6-N1-C2	-5.19	118.22	120.30
34	a	293	C	C5-C6-N1	5.19	123.59	121.00
55	z	6	G	N7-C8-N9	5.18	115.69	113.10
9	A	816	C	C6-N1-C2	-5.18	118.23	120.30
34	a	113	U	C5-C6-N1	5.17	125.29	122.70
34	a	1184	C	N1-C2-O2	5.17	122.00	118.90
34	a	22	C	C6-N1-C2	-5.17	118.23	120.30
9	A	860	C	C6-N1-C2	-5.17	118.23	120.30
9	A	1501	C	C5-C6-N1	5.16	123.58	121.00
34	a	958	U	N3-C2-O2	-5.15	118.59	122.20
9	A	912	A	N9-C4-C5	-5.15	103.74	105.80
9	A	227	C	C6-N1-C2	-5.14	118.24	120.30
9	A	40	C	C6-N1-C2	-5.14	118.24	120.30
9	A	746	G	C8-N9-C4	-5.13	104.35	106.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	6	4	ASP	CB-CG-OD1	5.13	122.92	118.30
54	y	40	C	C5-C6-N1	5.12	123.56	121.00
9	A	3060	C	C6-N1-C1'	-5.12	114.66	120.80
9	A	905	G	C6-C5-N7	-5.11	127.33	130.40
27	T	95	LEU	CA-CB-CG	5.11	127.06	115.30
34	a	329	C	N1-C2-O2	5.11	121.97	118.90
9	A	1358	C	C5-C6-N1	5.11	123.56	121.00
9	A	1134	C	N3-C4-C5	-5.11	119.86	121.90
9	A	1507	C	N1-C2-O2	5.10	121.96	118.90
9	A	1115	C	C6-N1-C2	-5.10	118.26	120.30
34	a	1248	C	C2-N1-C1'	5.10	124.41	118.80
9	A	3005	C	C6-N1-C2	-5.10	118.26	120.30
9	A	154	C	C6-N1-C2	-5.09	118.26	120.30
9	A	2857	C	C5-C6-N1	5.09	123.55	121.00
9	A	2056	C	C5-C6-N1	5.09	123.55	121.00
34	a	353	G	C4-N9-C1'	5.09	133.12	126.50
9	A	2022	C	C6-N1-C2	-5.09	118.26	120.30
9	A	2350	U	N1-C2-O2	5.08	126.36	122.80
54	y	42	C	N3-C2-O2	-5.08	118.34	121.90
9	A	1320	U	N3-C2-O2	-5.08	118.64	122.20
34	a	1254	U	C6-N1-C1'	-5.08	114.09	121.20
9	A	1457	C	C6-N1-C2	-5.08	118.27	120.30
9	A	2276	C	C5-C6-N1	5.08	123.54	121.00
9	A	1833	C	C6-N1-C2	-5.07	118.27	120.30
34	a	1346	C	C6-N1-C1'	5.07	126.89	120.80
9	A	270	C	C5-C6-N1	5.07	123.53	121.00
34	a	1422	C	C5-C6-N1	5.07	123.53	121.00
9	A	2824	U	C2-N1-C1'	5.07	123.78	117.70
34	a	533	G	C8-N9-C4	-5.07	104.37	106.40
9	A	239	C	C5-C6-N1	5.06	123.53	121.00
9	A	3060	C	O4'-C1'-N1	5.06	112.25	108.20
9	A	2244	C	C6-N1-C2	-5.06	118.28	120.30
9	A	2658	C	C6-N1-C2	-5.06	118.28	120.30
34	a	527	C	C6-N1-C2	-5.06	118.28	120.30
9	A	106	C	C6-N1-C2	-5.05	118.28	120.30
9	A	861	C	N3-C2-O2	-5.05	118.36	121.90
9	A	3005	C	N3-C2-O2	-5.05	118.36	121.90
9	A	1879	C	C6-N1-C2	-5.05	118.28	120.30
34	a	1489	C	C6-N1-C2	-5.05	118.28	120.30
9	A	1494	C	C6-N1-C2	-5.05	118.28	120.30
54	y	29	C	N1-C2-O2	5.04	121.92	118.90
9	A	57	C	C5-C6-N1	5.04	123.52	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	A	3132	U	N1-C2-O2	5.04	126.33	122.80
9	A	915	C	C6-N1-C2	-5.03	118.29	120.30
9	A	2606	C	C6-N1-C2	-5.03	118.29	120.30
34	a	458	G	N3-C4-N9	5.03	129.02	126.00
9	A	401	C	C6-N1-C2	-5.03	118.29	120.30
9	A	849	C	C6-N1-C2	-5.03	118.29	120.30
9	A	666	C	C6-N1-C2	-5.02	118.29	120.30
9	A	889	G	N3-C4-C5	-5.02	126.09	128.60
9	A	2832	C	C6-N1-C2	-5.01	118.29	120.30
34	a	1283	C	C6-N1-C2	-5.01	118.29	120.30
34	a	1442	C	C6-N1-C2	-5.01	118.30	120.30
31	X	14	PHE	CB-CG-CD1	5.01	124.31	120.80
9	A	2407	A	N3-C4-N9	5.00	131.40	127.40
34	a	61	C	C6-N1-C2	-5.00	118.30	120.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	6	43	PRO	Peptide
8	8	225	ASP	Mainchain
11	C	206	TRP	Peptide
25	R	50	THR	Peptide
28	U	101	ASN	Peptide
44	l	113	ALA	Peptide
44	l	115	SER	Peptide
47	o	44	LYS	Peptide
53	x	14	ALA	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
2	1	46/55 (84%)	45 (98%)	1 (2%)	0	100	100
3	2	42/47 (89%)	42 (100%)	0	0	100	100
4	3	60/64 (94%)	57 (95%)	3 (5%)	0	100	100
5	4	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
6	6	45/80 (56%)	37 (82%)	8 (18%)	0	100	100
7	7	6/24 (25%)	6 (100%)	0	0	100	100
8	8	228/235 (97%)	211 (92%)	17 (8%)	0	100	100
11	C	270/280 (96%)	250 (93%)	20 (7%)	0	100	100
12	D	211/217 (97%)	187 (89%)	24 (11%)	0	100	100
13	E	205/223 (92%)	198 (97%)	7 (3%)	0	100	100
14	F	176/187 (94%)	157 (89%)	19 (11%)	0	100	100
15	G	172/179 (96%)	161 (94%)	11 (6%)	0	100	100
16	H	45/152 (30%)	36 (80%)	9 (20%)	0	100	100
17	J	144/195 (74%)	139 (96%)	5 (4%)	0	100	100
18	K	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
19	L	142/146 (97%)	128 (90%)	14 (10%)	0	100	100
20	M	132/138 (96%)	119 (90%)	13 (10%)	0	100	100
21	N	114/180 (63%)	109 (96%)	5 (4%)	0	100	100
22	O	117/122 (96%)	111 (95%)	6 (5%)	0	100	100
23	P	110/113 (97%)	98 (89%)	12 (11%)	0	100	100
24	Q	122/129 (95%)	119 (98%)	3 (2%)	0	100	100
25	R	98/104 (94%)	88 (90%)	9 (9%)	1 (1%)	15	50
26	S	111/197 (56%)	103 (93%)	8 (7%)	0	100	100
27	T	93/100 (93%)	85 (91%)	8 (9%)	0	100	100
28	U	86/105 (82%)	73 (85%)	13 (15%)	0	100	100
29	V	175/215 (81%)	159 (91%)	16 (9%)	0	100	100
30	W	70/86 (81%)	62 (89%)	8 (11%)	0	100	100
31	X	60/64 (94%)	54 (90%)	6 (10%)	0	100	100
32	Y	66/77 (86%)	63 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	Z	57/65 (88%)	55 (96%)	2 (4%)	0	100	100
35	c	205/274 (75%)	186 (91%)	19 (9%)	0	100	100
36	d	198/201 (98%)	178 (90%)	20 (10%)	0	100	100
37	e	167/220 (76%)	146 (87%)	21 (13%)	0	100	100
38	f	93/96 (97%)	85 (91%)	8 (9%)	0	100	100
39	g	153/156 (98%)	142 (93%)	11 (7%)	0	100	100
40	h	129/132 (98%)	120 (93%)	9 (7%)	0	100	100
41	i	125/151 (83%)	112 (90%)	13 (10%)	0	100	100
42	j	97/101 (96%)	85 (88%)	12 (12%)	0	100	100
43	k	115/139 (83%)	102 (89%)	13 (11%)	0	100	100
44	l	120/124 (97%)	90 (75%)	28 (23%)	2 (2%)	9	39
45	m	114/124 (92%)	99 (87%)	15 (13%)	0	100	100
46	n	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	9	39
47	o	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
48	p	111/162 (68%)	97 (87%)	13 (12%)	1 (1%)	17	52
49	q	93/135 (69%)	79 (85%)	14 (15%)	0	100	100
50	r	62/84 (74%)	59 (95%)	3 (5%)	0	100	100
51	s	81/93 (87%)	72 (89%)	9 (11%)	0	100	100
52	t	83/86 (96%)	81 (98%)	2 (2%)	0	100	100
53	x	546/558 (98%)	495 (91%)	51 (9%)	0	100	100
All	All	6045/6981 (87%)	5506 (91%)	534 (9%)	5 (0%)	54	83

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	R	51	THR
44	l	114	ARG
46	n	17	ALA
48	p	46	PRO
44	l	4	ILE

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	44/47 (94%)	44 (100%)	0	100	100
2	1	45/51 (88%)	45 (100%)	0	100	100
3	2	38/40 (95%)	38 (100%)	0	100	100
4	3	53/54 (98%)	53 (100%)	0	100	100
5	4	35/35 (100%)	34 (97%)	1 (3%)	42	71
6	6	41/66 (62%)	41 (100%)	0	100	100
7	7	6/20 (30%)	6 (100%)	0	100	100
8	8	175/179 (98%)	172 (98%)	3 (2%)	60	81
11	C	212/219 (97%)	211 (100%)	1 (0%)	88	94
12	D	163/166 (98%)	163 (100%)	0	100	100
13	E	159/172 (92%)	157 (99%)	2 (1%)	69	85
14	F	147/155 (95%)	145 (99%)	2 (1%)	67	84
15	G	143/147 (97%)	142 (99%)	1 (1%)	84	92
16	H	36/121 (30%)	35 (97%)	1 (3%)	43	72
17	J	120/161 (74%)	120 (100%)	0	100	100
18	K	101/101 (100%)	100 (99%)	1 (1%)	76	88
19	L	108/110 (98%)	108 (100%)	0	100	100
20	M	110/114 (96%)	108 (98%)	2 (2%)	59	80
21	N	94/139 (68%)	93 (99%)	1 (1%)	73	87
22	O	91/93 (98%)	91 (100%)	0	100	100
23	P	98/99 (99%)	98 (100%)	0	100	100
24	Q	97/99 (98%)	97 (100%)	0	100	100
25	R	81/83 (98%)	81 (100%)	0	100	100
26	S	87/140 (62%)	86 (99%)	1 (1%)	73	87
27	T	81/83 (98%)	80 (99%)	1 (1%)	71	86
28	U	77/88 (88%)	76 (99%)	1 (1%)	69	85
29	V	142/164 (87%)	140 (99%)	2 (1%)	67	84
30	W	52/62 (84%)	52 (100%)	0	100	100
31	X	51/52 (98%)	50 (98%)	1 (2%)	55	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	Y	60/66 (91%)	60 (100%)	0	100	100
33	Z	51/55 (93%)	49 (96%)	2 (4%)	32	65
35	c	170/210 (81%)	169 (99%)	1 (1%)	86	93
36	d	176/177 (99%)	175 (99%)	1 (1%)	86	93
37	e	121/159 (76%)	119 (98%)	2 (2%)	60	81
38	f	84/85 (99%)	84 (100%)	0	100	100
39	g	130/131 (99%)	129 (99%)	1 (1%)	81	91
40	h	107/108 (99%)	106 (99%)	1 (1%)	78	89
41	i	102/120 (85%)	101 (99%)	1 (1%)	76	88
42	j	89/90 (99%)	89 (100%)	0	100	100
43	k	90/107 (84%)	90 (100%)	0	100	100
44	l	104/105 (99%)	101 (97%)	3 (3%)	42	71
45	m	99/104 (95%)	98 (99%)	1 (1%)	76	88
46	n	46/47 (98%)	46 (100%)	0	100	100
47	o	77/79 (98%)	77 (100%)	0	100	100
48	p	90/125 (72%)	89 (99%)	1 (1%)	73	87
49	q	85/105 (81%)	82 (96%)	3 (4%)	36	67
50	r	54/72 (75%)	52 (96%)	2 (4%)	34	66
51	s	75/85 (88%)	75 (100%)	0	100	100
52	t	64/65 (98%)	63 (98%)	1 (2%)	62	82
53	x	455/460 (99%)	446 (98%)	9 (2%)	55	78
All	All	5016/5615 (89%)	4966 (99%)	50 (1%)	77	88

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	4	8	LYS
8	8	103	ARG
8	8	137	MET
8	8	231	ASN
11	C	4	ARG
13	E	19	LYS
13	E	81	ARG
14	F	14	ARG
14	F	78	ARG

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Mol	Chain	Res	Type
15	G	96	ARG
16	H	41	ARG
18	K	110	ARG
20	M	5	ARG
20	M	60	ARG
21	N	71	ARG
26	S	102	ARG
27	T	70	ARG
28	U	103	LYS
29	V	10	ARG
29	V	100	ARG
31	X	27	ARG
33	Z	30	ARG
33	Z	44	ARG
35	c	164	ARG
36	d	63	MET
37	e	163	ASN
37	e	202	LYS
39	g	149	ARG
40	h	50	ARG
41	i	70	LYS
44	l	20	LYS
44	l	86	ARG
44	l	108	LYS
45	m	11	ARG
48	p	99	LYS
49	q	68	LYS
49	q	91	ARG
49	q	133	LYS
50	r	51	ARG
50	r	52	ARG
52	t	29	ARG
53	x	257	ARG
53	x	285	LYS
53	x	290	ARG
53	x	300	LYS
53	x	302	ARG
53	x	303	LYS
53	x	346	ARG
53	x	504	ARG
53	x	553	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35)

such sidechains are listed below:

Mol	Chain	Res	Type
2	1	49	GLN
8	8	162	ASN
8	8	188	ASN
8	8	231	ASN
11	C	245	HIS
12	D	34	ASN
14	F	142	GLN
15	G	62	ASN
16	H	46	GLN
17	J	147	GLN
20	M	14	HIS
23	P	79	ASN
24	Q	11	HIS
24	Q	44	ASN
29	V	44	HIS
29	V	91	GLN
29	V	92	HIS
35	c	176	HIS
36	d	115	HIS
37	e	163	ASN
38	f	28	ASN
40	h	35	ASN
40	h	42	ASN
41	i	65	HIS
41	i	96	GLN
42	j	4	GLN
45	m	31	ASN
51	s	47	HIS
51	s	52	HIS
52	t	84	ASN
53	x	40	ASN
53	x	58	ASN
53	x	74	GLN
53	x	88	ASN
53	x	497	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	B	114/115 (99%)	22 (19%)	0
34	a	1515/1537 (98%)	331 (21%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	y	74/77 (96%)	17 (22%)	0
55	z	5/26 (19%)	3 (60%)	0
9	A	3116/3138 (99%)	621 (19%)	3 (0%)
All	All	4824/4893 (98%)	994 (20%)	3 (0%)

All (994) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	A	14	A
9	A	26	G
9	A	34	U
9	A	49	A
9	A	51	G
9	A	61	G
9	A	62	G
9	A	63	A
9	A	68	G
9	A	71	A
9	A	72	U
9	A	74	U
9	A	75	G
9	A	76	C
9	A	94	C
9	A	102	G
9	A	118	A
9	A	119	A
9	A	120	U
9	A	122	G
9	A	123	G
9	A	125	A
9	A	130	C
9	A	159	C
9	A	164	U
9	A	167	A
9	A	168	U
9	A	176	G
9	A	183	A
9	A	195	U
9	A	197	A
9	A	198	A
9	A	201	A
9	A	204	U

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Mol	Chain	Res	Type
9	A	206	A
9	A	217	G
9	A	218	A
9	A	224	A
9	A	225	A
9	A	229	A
9	A	230	U
9	A	231	U
9	A	232	G
9	A	233	U
9	A	235	A
9	A	241	C
9	A	243	A
9	A	250	G
9	A	251	C
9	A	252	G
9	A	254	G
9	A	255	C
9	A	262	G
9	A	263	G
9	A	267	A
9	A	287	G
9	A	288	U
9	A	289	A
9	A	293	G
9	A	298	G
9	A	301	G
9	A	302	U
9	A	303	U
9	A	319	U
9	A	320	G
9	A	328	A
9	A	332	C
9	A	339	C
9	A	358	U
9	A	362	A
9	A	371	U
9	A	372	G
9	A	377	G
9	A	385	G
9	A	391	G
9	A	394	U

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Mol	Chain	Res	Type
9	A	401	C
9	A	405	A
9	A	413	A
9	A	428	A
9	A	446	A
9	A	447	G
9	A	453	A
9	A	464	G
9	A	475	G
9	A	481	U
9	A	487	G
9	A	493	C
9	A	494	C
9	A	495	G
9	A	500	G
9	A	501	A
9	A	506	C
9	A	510	U
9	A	523	U
9	A	537	U
9	A	541	G
9	A	543	A
9	A	544	U
9	A	545	U
9	A	553	U
9	A	566	A
9	A	570	G
9	A	578	G
9	A	581	G
9	A	582	G
9	A	586	G
9	A	589	A
9	A	592	G
9	A	593	A
9	A	595	U
9	A	596	A
9	A	597	C
9	A	616	A
9	A	618	U
9	A	619	C
9	A	620	C
9	A	621	G

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Mol	Chain	Res	Type
9	A	624	A
9	A	635	U
9	A	637	C
9	A	639	U
9	A	641	U
9	A	642	C
9	A	643	C
9	A	645	G
9	A	658	A
9	A	664	U
9	A	665	G
9	A	674	A
9	A	677	A
9	A	685	G
9	A	689	G
9	A	691	C
9	A	694	G
9	A	695	G
9	A	698	A
9	A	706	A
9	A	718	G
9	A	719	U
9	A	729	G
9	A	735	A
9	A	738	G
9	A	741	A
9	A	748	A
9	A	758	C
9	A	759	C
9	A	760	A
9	A	761	C
9	A	766	G
9	A	767	C
9	A	779	U
9	A	780	G
9	A	781	A
9	A	782	A
9	A	783	U
9	A	784	A
9	A	797	G
9	A	806	G
9	A	815	U

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Mol	Chain	Res	Type
9	A	840	G
9	A	843	U
9	A	844	A
9	A	846	G
9	A	848	C
9	A	851	C
9	A	859	C
9	A	861	C
9	A	863	A
9	A	869	C
9	A	876	U
9	A	877	G
9	A	878	A
9	A	881	A
9	A	889	G
9	A	894	G
9	A	899	G
9	A	904	G
9	A	905	G
9	A	911	A
9	A	912	A
9	A	913	G
9	A	914	G
9	A	921	A
9	A	928	G
9	A	929	U
9	A	931	A
9	A	934	G
9	A	938	G
9	A	941	C
9	A	944	C
9	A	956	U
9	A	959	G
9	A	988	G
9	A	1000	G
9	A	1008	A
9	A	1024	U
9	A	1033	C
9	A	1036	C
9	A	1039	A
9	A	1040	A
9	A	1044	C

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Mol	Chain	Res	Type
9	A	1059	A
9	A	1069	A
9	A	1074	G
9	A	1081	G
9	A	1087	A
9	A	1089	G
9	A	1090	C
9	A	1096	A
9	A	1102	A
9	A	1103	A
9	A	1118	G
9	A	1120	U
9	A	1122	G
9	A	1125	G
9	A	1126	G
9	A	1131	G
9	A	1133	C
9	A	1138	A
9	A	1141	C
9	A	1142	G
9	A	1147	C
9	A	1151	G
9	A	1153	G
9	A	1154	G
9	A	1155	G
9	A	1159	G
9	A	1162	U
9	A	1174	A
9	A	1177	A
9	A	1179	A
9	A	1181	C
9	A	1186	A
9	A	1187	G
9	A	1190	U
9	A	1191	G
9	A	1194	U
9	A	1196	A
9	A	1198	A
9	A	1199	A
9	A	1200	G
9	A	1202	A
9	A	1206	A

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Mol	Chain	Res	Type
9	A	1207	C
9	A	1210	U
9	A	1211	U
9	A	1212	G
9	A	1214	A
9	A	1216	G
9	A	1217	A
9	A	1218	G
9	A	1233	C
9	A	1235	G
9	A	1237	U
9	A	1240	A
9	A	1243	G
9	A	1244	A
9	A	1255	A
9	A	1258	A
9	A	1259	U
9	A	1261	U
9	A	1262	A
9	A	1263	G
9	A	1264	C
9	A	1265	G
9	A	1271	C
9	A	1272	A
9	A	1273	A
9	A	1274	G
9	A	1286	A
9	A	1302	C
9	A	1305	U
9	A	1307	U
9	A	1312	G
9	A	1313	G
9	A	1315	G
9	A	1342	C
9	A	1355	U
9	A	1358	C
9	A	1368	A
9	A	1378	A
9	A	1381	G
9	A	1384	A
9	A	1386	U
9	A	1387	G

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Mol	Chain	Res	Type
9	A	1391	G
9	A	1393	A
9	A	1396	A
9	A	1402	G
9	A	1403	A
9	A	1404	C
9	A	1405	A
9	A	1406	A
9	A	1412	G
9	A	1431	A
9	A	1432	A
9	A	1433	A
9	A	1437	C
9	A	1452	C
9	A	1453	A
9	A	1456	C
9	A	1460	U
9	A	1465	C
9	A	1472	G
9	A	1479	G
9	A	1481	C
9	A	1483	U
9	A	1495	G
9	A	1496	A
9	A	1498	A
9	A	1499	G
9	A	1507	C
9	A	1509	A
9	A	1510	U
9	A	1515	A
9	A	1523	G
9	A	1526	A
9	A	1542	G
9	A	1545	G
9	A	1567	U
9	A	1570	U
9	A	1571	A
9	A	1574	C
9	A	1580	A
9	A	1581	A
9	A	1582	A
9	A	1592	U

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Mol	Chain	Res	Type
9	A	1609	U
9	A	1615	G
9	A	1623	G
9	A	1624	C
9	A	1628	G
9	A	1629	U
9	A	1633	A
9	A	1646	G
9	A	1653	A
9	A	1656	G
9	A	1657	A
9	A	1658	A
9	A	1663	U
9	A	1665	A
9	A	1666	C
9	A	1667	G
9	A	1679	C
9	A	1691	G
9	A	1697	A
9	A	1698	C
9	A	1709	G
9	A	1713	G
9	A	1716	G
9	A	1720	G
9	A	1721	A
9	A	1726	U
9	A	1727	A
9	A	1730	C
9	A	1738	U
9	A	1747	A
9	A	1754	A
9	A	1762	C
9	A	1763	G
9	A	1773	U
9	A	1774	U
9	A	1775	G
9	A	1777	G
9	A	1784	U
9	A	1791	U
9	A	1792	C
9	A	1795	C
9	A	1803	A

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Mol	Chain	Res	Type
9	A	1806	A
9	A	1813	U
9	A	1821	G
9	A	1830	C
9	A	1841	C
9	A	1842	C
9	A	1843	A
9	A	1845	A
9	A	1869	C
9	A	1873	C
9	A	1874	C
9	A	1881	U
9	A	1883	C
9	A	1888	U
9	A	1889	A
9	A	1899	A
9	A	1904	A
9	A	1907	C
9	A	1909	G
9	A	1910	C
9	A	1917	C
9	A	1928	U
9	A	1942	A
9	A	1949	U
9	A	1950	A
9	A	1961	C
9	A	1962	C
9	A	1964	U
9	A	1965	G
9	A	1966	C
9	A	1967	G
9	A	1973	A
9	A	1980	U
9	A	1991	A
9	A	1992	A
9	A	1995	C
9	A	1998	U
9	A	2007	A
9	A	2010	G
9	A	2015	C
9	A	2018	A
9	A	2034	C

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Mol	Chain	Res	Type
9	A	2035	G
9	A	2043	A
9	A	2045	G
9	A	2050	U
9	A	2060	C
9	A	2063	A
9	A	2081	A
9	A	2088	A
9	A	2101	A
9	A	2105	G
9	A	2106	C
9	A	2107	A
9	A	2108	A
9	A	2109	G
9	A	2110	G
9	A	2128	A
9	A	2143	C
9	A	2144	G
9	A	2145	G
9	A	2151	A
9	A	2152	C
9	A	2158	C
9	A	2167	G
9	A	2168	G
9	A	2172	C
9	A	2174	A
9	A	2175	A
9	A	2177	5MU
9	A	2193	U
9	A	2205	C
9	A	2208	A
9	A	2209	U
9	A	2210	G
9	A	2229	U
9	A	2231	U
9	A	2245	U
9	A	2250	G
9	A	2257	C
9	A	2259	C
9	A	2261	A
9	A	2269	A
9	A	2270	G

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Mol	Chain	Res	Type
9	A	2281	C
9	A	2282	G
9	A	2290	G
9	A	2293	C
9	A	2294	G
9	A	2297	A
9	A	2298	A
9	A	2299	G
9	A	2300	A
9	A	2302	C
9	A	2327	A
9	A	2330	G
9	A	2348	U
9	A	2353	G
9	A	2354	A
9	A	2355	U
9	A	2361	G
9	A	2363	A
9	A	2367	U
9	A	2369	U
9	A	2370	G
9	A	2371	A
9	A	2372	A
9	A	2375	C
9	A	2377	C
9	A	2378	G
9	A	2379	A
9	A	2381	G
9	A	2382	C
9	A	2383	C
9	A	2384	A
9	A	2386	U
9	A	2387	U
9	A	2388	G
9	A	2389	G
9	A	2390	G
9	A	2393	G
9	A	2397	U
9	A	2399	G
9	A	2404	U
9	A	2405	G
9	A	2408	A

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Mol	Chain	Res	Type
9	A	2411	C
9	A	2412	C
9	A	2418	G
9	A	2421	C
9	A	2435	A
9	A	2437	C
9	A	2448	G
9	A	2449	A
9	A	2463	A
9	A	2470	C
9	A	2472	G
9	A	2476	G
9	A	2477	G
9	A	2478	U
9	A	2489	G
9	A	2490	G
9	A	2497	G
9	A	2507	A
9	A	2517	G
9	A	2521	C
9	A	2525	A
9	A	2532	C
9	A	2536	A
9	A	2543	A
9	A	2546	G
9	A	2549	A
9	A	2550	U
9	A	2558	C
9	A	2560	A
9	A	2563	G
9	A	2565	A
9	A	2572	C
9	A	2573	A
9	A	2576	G
9	A	2583	G
9	A	2585	C
9	A	2588	C
9	A	2596	A
9	A	2610	G
9	A	2621	G
9	A	2622	G
9	A	2623	A

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Mol	Chain	Res	Type
9	A	2626	A
9	A	2629	G
9	A	2638	C
9	A	2648	G
9	A	2651	G
9	A	2661	U
9	A	2663	A
9	A	2666	G
9	A	2667	G
9	A	2668	A
9	A	2678	C
9	A	2679	C
9	A	2683	G
9	A	2686	A
9	A	2697	A
9	A	2706	A
9	A	2714	A
9	A	2716	A
9	A	2732	G
9	A	2736	C
9	A	2738	U
9	A	2742	U
9	A	2743	G
9	A	2744	U
9	A	2751	G
9	A	2756	A
9	A	2763	G
9	A	2767	G
9	A	2792	U
9	A	2804	A
9	A	2805	G
9	A	2810	A
9	A	2811	C
9	A	2820	G
9	A	2836	A
9	A	2839	C
9	A	2840	A
9	A	2841	G
9	A	2847	U
9	A	2848	C
9	A	2851	U
9	A	2853	U

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Mol	Chain	Res	Type
9	A	2864	C
9	A	2868	A
9	A	2883	C
9	A	2884	C
9	A	2886	G
9	A	2908	G
9	A	2910	C
9	A	2927	C
9	A	2944	G
9	A	2952	G
9	A	2964	C
9	A	2965	G
9	A	2971	U
9	A	2977	U
9	A	2982	G
9	A	2986	A
9	A	2988	A
9	A	2989	G
9	A	2990	C
9	A	2993	C
9	A	2995	A
9	A	3007	U
9	A	3016	A
9	A	3018	C
9	A	3026	U
9	A	3029	C
9	A	3036	G
9	A	3037	G
9	A	3038	U
9	A	3043	U
9	A	3056	A
9	A	3060	C
9	A	3071	U
9	A	3081	C
9	A	3099	G
9	A	3107	A
9	A	3115	C
9	A	3119	C
9	A	3121	G
9	A	3126	A
9	A	3129	A
10	B	2	U

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Mol	Chain	Res	Type
10	B	3	A
10	B	4	C
10	B	8	G
10	B	11	C
10	B	12	A
10	B	14	A
10	B	15	G
10	B	24	A
10	B	34	U
10	B	36	C
10	B	41	C
10	B	55	U
10	B	56	A
10	B	57	A
10	B	64	C
10	B	84	C
10	B	101	G
10	B	102	G
10	B	105	A
10	B	114	C
10	B	115	A
34	a	9	G
34	a	10	G
34	a	12	G
34	a	22	C
34	a	25	G
34	a	35	A
34	a	40	U
34	a	42	G
34	a	51	U
34	a	53	A
34	a	54	A
34	a	57	C
34	a	82	U
34	a	83	U
34	a	85	G
34	a	86	G
34	a	89	A
34	a	90	U
34	a	91	A
34	a	94	C
34	a	116	C

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Mol	Chain	Res	Type
34	a	117	A
34	a	122	G
34	a	126	A
34	a	127	U
34	a	141	C
34	a	156	A
34	a	158	A
34	a	167	A
34	a	169	U
34	a	178	G
34	a	179	G
34	a	185	G
34	a	188	A
34	a	194	G
34	a	203	U
34	a	204	G
34	a	213	U
34	a	214	U
34	a	215	U
34	a	216	A
34	a	217	G
34	a	219	G
34	a	226	G
34	a	227	A
34	a	230	A
34	a	244	C
34	a	246	G
34	a	247	C
34	a	250	G
34	a	265	G
34	a	266	C
34	a	279	C
34	a	280	G
34	a	282	C
34	a	288	G
34	a	298	G
34	a	320	A
34	a	324	A
34	a	328	A
34	a	329	C
34	a	334	C
34	a	336	G

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Mol	Chain	Res	Type
34	a	339	U
34	a	344	C
34	a	346	G
34	a	347	G
34	a	351	C
34	a	353	G
34	a	366	U
34	a	370	A
34	a	371	C
34	a	380	C
34	a	381	A
34	a	384	C
34	a	387	G
34	a	389	U
34	a	391	C
34	a	392	A
34	a	397	C
34	a	405	G
34	a	410	A
34	a	411	U
34	a	412	G
34	a	413	A
34	a	422	G
34	a	428	U
34	a	429	A
34	a	434	U
34	a	437	U
34	a	439	C
34	a	440	A
34	a	451	A
34	a	452	G
34	a	453	G
34	a	455	C
34	a	456	C
34	a	458	G
34	a	459	G
34	a	460	U
34	a	461	U
34	a	462	C
34	a	463	U
34	a	465	U
34	a	468	G

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Mol	Chain	Res	Type
34	a	472	G
34	a	475	G
34	a	476	G
34	a	483	G
34	a	485	G
34	a	486	A
34	a	488	G
34	a	498	C
34	a	499	C
34	a	502	C
34	a	505	C
34	a	506	G
34	a	508	G
34	a	509	C
34	a	512	G
34	a	515	G
34	a	516	C
34	a	517	C
34	a	518	G7M
34	a	521	G
34	a	528	G
34	a	534	U
34	a	536	C
34	a	538	A
34	a	550	A
34	a	551	A
34	a	553	U
34	a	555	C
34	a	557	G
34	a	563	A
34	a	564	A
34	a	566	G
34	a	567	A
34	a	568	G
34	a	570	U
34	a	572	G
34	a	580	U
34	a	611	U
34	a	617	U
34	a	623	U
34	a	624	G
34	a	643	U

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Mol	Chain	Res	Type
34	a	644	A
34	a	656	G
34	a	678	A
34	a	692	C
34	a	693	A
34	a	694	G
34	a	697	A
34	a	701	G
34	a	709	A
34	a	712	G
34	a	720	A
34	a	731	U
34	a	740	A
34	a	743	G
34	a	746	G
34	a	768	A
34	a	777	G
34	a	781	A
34	a	784	U
34	a	785	A
34	a	790	G
34	a	792	U
34	a	805	A
34	a	806	A
34	a	808	C
34	a	820	G
34	a	832	C
34	a	833	U
34	a	834	U
34	a	835	C
34	a	837	U
34	a	838	U
34	a	839	G
34	a	840	G
34	a	846	G
34	a	865	A
34	a	872	C
34	a	878	G
34	a	880	G
34	a	882	A
34	a	883	G
34	a	895	G

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Mol	Chain	Res	Type
34	a	900	A
34	a	907	A
34	a	915	G
34	a	919	G
34	a	924	C
34	a	925	C
34	a	927	C
34	a	935	G
34	a	936	C
34	a	941	C
34	a	953	U
34	a	959	2MG
34	a	960	5MC
34	a	961	A
34	a	962	A
34	a	964	G
34	a	968	A
34	a	969	G
34	a	970	A
34	a	982	G
34	a	985	U
34	a	986	G
34	a	987	A
34	a	990	U
34	a	994	C
34	a	997	G
34	a	1000	G
34	a	1007	G
34	a	1009	G
34	a	1012	A
34	a	1014	G
34	a	1016	G
34	a	1021	C
34	a	1022	U
34	a	1023	U
34	a	1024	G
34	a	1033	G
34	a	1044	G
34	a	1056	U
34	a	1060	C
34	a	1061	U
34	a	1069	U

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Mol	Chain	Res	Type
34	a	1075	G
34	a	1076	U
34	a	1085	G
34	a	1086	U
34	a	1092	A
34	a	1101	A
34	a	1110	C
34	a	1116	U
34	a	1117	U
34	a	1126	G
34	a	1127	U
34	a	1129	A
34	a	1130	U
34	a	1131	G
34	a	1140	U
34	a	1144	G
34	a	1149	A
34	a	1150	C
34	a	1151	U
34	a	1159	U
34	a	1171	A
34	a	1174	G
34	a	1176	G
34	a	1188	A
34	a	1189	A
34	a	1190	G
34	a	1192	C
34	a	1193	A
34	a	1205	A
34	a	1206	U
34	a	1219	A
34	a	1220	C
34	a	1228	A
34	a	1230	A
34	a	1233	G
34	a	1249	U
34	a	1250	G
34	a	1252	G
34	a	1261	A
34	a	1265	U
34	a	1270	G
34	a	1272	A

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Mol	Chain	Res	Type
34	a	1277	U
34	a	1278	A
34	a	1279	A
34	a	1282	G
34	a	1286	G
34	a	1290	C
34	a	1292	G
34	a	1293	U
34	a	1294	U
34	a	1297	G
34	a	1309	C
34	a	1310	A
34	a	1312	C
34	a	1314	C
34	a	1315	G
34	a	1327	U
34	a	1328	C
34	a	1332	G
34	a	1338	A
34	a	1339	G
34	a	1340	U
34	a	1344	C
34	a	1345	G
34	a	1351	C
34	a	1355	A
34	a	1356	A
34	a	1363	G
34	a	1389	A
34	a	1391	A
34	a	1394	G
34	a	1406	A
34	a	1412	G
34	a	1413	U
34	a	1416	G
34	a	1417	U
34	a	1419	A
34	a	1420	C
34	a	1422	C
34	a	1423	C
34	a	1428	G
34	a	1435	G
34	a	1436	C

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Mol	Chain	Res	Type
34	a	1439	A
34	a	1440	A
34	a	1443	C
34	a	1444	U
34	a	1467	G
34	a	1468	G
34	a	1472	G
34	a	1480	G
34	a	1485	A
34	a	1486	A
34	a	1487	G
34	a	1496	A
34	a	1500	A
34	a	1510	G
34	a	1522	G
34	a	1523	G
54	y	5	G
54	y	9	G
54	y	10	G
54	y	13	C
54	y	17	C
54	y	18	U
54	y	19	G
54	y	20	G
54	y	22	A
54	y	44	A
54	y	48	U
54	y	49	C
54	y	54	G
54	y	55	U
54	y	64	G
54	y	74	A
54	y	75	C
55	z	3	C
55	z	4	A
55	z	6	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	A	505	C
9	A	913	G

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Mol	Chain	Res	Type
9	A	1113	G

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

9 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	$\#\|Z\| > 2$
34	5MC	a	960	34	18,22,23	3.46	7 (38%)	26,32,35	1.06	1 (3%)
34	G7M	a	518	34	20,26,27	3.86	9 (45%)	17,39,42	1.22	2 (11%)
34	2MG	a	959	34	18,26,27	2.34	7 (38%)	16,38,41	1.47	3 (18%)
34	MA6	a	1512	34	18,26,27	1.11	1 (5%)	19,38,41	3.51	2 (10%)
34	UR3	a	1491	34	19,22,23	2.55	5 (26%)	26,32,35	1.24	1 (3%)
34	MA6	a	1511	34	18,26,27	1.09	1 (5%)	19,38,41	3.35	2 (10%)
9	5MU	A	2177	9	19,22,23	4.49	7 (36%)	28,32,35	4.08	11 (39%)
9	OMG	A	2791	9	18,26,27	2.51	8 (44%)	19,38,41	1.46	4 (21%)
34	4OC	a	1395	34	20,23,24	2.89	8 (40%)	26,32,35	0.96	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
34	5MC	a	960	34	-	2/7/25/26	0/2/2/2
34	G7M	a	518	34	-	0/3/25/26	0/3/3/3
34	2MG	a	959	34	-	2/5/27/28	0/3/3/3
34	MA6	a	1512	34	-	2/7/29/30	0/3/3/3
34	UR3	a	1491	34	-	0/7/25/26	0/2/2/2
34	MA6	a	1511	34	-	0/7/29/30	0/3/3/3
9	5MU	A	2177	9	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	OMG	A	2791	9	-	2/5/27/28	0/3/3/3
34	4OC	a	1395	34	-	2/9/29/30	0/2/2/2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2177	5MU	C6-N1	9.93	1.55	1.38
34	a	518	G7M	C8-N9	9.64	1.50	1.33
34	a	518	G7M	C8-N7	9.56	1.50	1.33
9	A	2177	5MU	C2-N1	9.00	1.52	1.38
34	a	960	5MC	C6-C5	8.65	1.48	1.34
9	A	2177	5MU	C4-C5	8.64	1.59	1.44
9	A	2177	5MU	C4-N3	-8.35	1.23	1.38
34	a	1491	UR3	C6-C5	6.56	1.50	1.35
34	a	960	5MC	C4-N3	6.43	1.45	1.34
34	a	1395	4OC	C4-N3	6.28	1.43	1.32
34	a	960	5MC	C2-N3	5.98	1.48	1.36
9	A	2177	5MU	C6-C5	5.84	1.44	1.34
34	a	1395	4OC	C2-N3	5.79	1.48	1.36
9	A	2791	OMG	C2-N3	5.71	1.47	1.33
34	a	1395	4OC	C6-C5	5.67	1.48	1.35
34	a	518	G7M	C2-N3	5.44	1.46	1.33
34	a	1491	UR3	C2-N1	5.22	1.46	1.38
34	a	959	2MG	C2-N2	5.09	1.44	1.33
34	a	1491	UR3	C2-N3	4.88	1.48	1.39
9	A	2791	OMG	C4-N3	4.80	1.49	1.37
34	a	518	G7M	C2-N2	4.80	1.45	1.34
34	a	959	2MG	C4-N3	4.78	1.49	1.37
34	a	1395	4OC	C4-N4	4.44	1.45	1.35
34	a	960	5MC	C6-N1	4.23	1.45	1.38
34	a	960	5MC	C4-N4	4.20	1.45	1.34
34	a	518	G7M	C6-N1	4.08	1.43	1.37
34	a	960	5MC	C2-N1	3.97	1.48	1.40
9	A	2791	OMG	C2-N2	3.97	1.43	1.34
34	a	959	2MG	C2-N1	3.95	1.43	1.36
34	a	518	G7M	C4-N3	3.77	1.46	1.37
9	A	2791	OMG	C6-N1	3.72	1.43	1.37
34	a	1395	4OC	C6-N1	3.43	1.46	1.38
9	A	2177	5MU	O4-C4	-3.38	1.17	1.23
34	a	518	G7M	C2-N1	3.23	1.45	1.37
34	a	1395	4OC	C2-N1	3.21	1.46	1.40
34	a	959	2MG	C6-N1	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2177	5MU	O2-C2	-3.09	1.17	1.23
34	a	1395	4OC	O2-C2	-3.04	1.18	1.23
34	a	1395	4OC	C5-C4	2.95	1.47	1.40
34	a	1512	MA6	C5-C4	-2.93	1.33	1.40
34	a	1491	UR3	C6-N1	2.91	1.45	1.38
9	A	2791	OMG	C5-C6	2.90	1.53	1.47
34	a	959	2MG	C5-C4	-2.89	1.35	1.43
34	a	960	5MC	O2-C2	-2.84	1.18	1.23
34	a	1511	MA6	C5-C4	-2.81	1.33	1.40
34	a	959	2MG	C5-C6	2.78	1.53	1.47
9	A	2791	OMG	C5-C4	-2.61	1.36	1.43
34	a	518	G7M	O6-C6	-2.51	1.18	1.23
9	A	2791	OMG	O6-C6	-2.40	1.18	1.23
9	A	2791	OMG	C2-N1	2.37	1.43	1.37
34	a	1491	UR3	O2-C2	-2.33	1.18	1.22
34	a	518	G7M	C5-C6	2.33	1.51	1.45
34	a	959	2MG	O6-C6	-2.29	1.18	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1512	MA6	N1-C6-N6	-13.84	102.49	117.06
34	a	1511	MA6	N1-C6-N6	-13.11	103.25	117.06
9	A	2177	5MU	C5-C4-N3	12.38	125.88	115.31
9	A	2177	5MU	C5-C6-N1	-11.53	111.47	123.34
34	a	1512	MA6	N3-C2-N1	-6.02	119.27	128.68
9	A	2177	5MU	C4-N3-C2	-6.00	119.58	127.35
34	a	1511	MA6	N3-C2-N1	-5.78	119.64	128.68
9	A	2177	5MU	N3-C2-N1	5.60	122.32	114.89
9	A	2177	5MU	O4-C4-C5	-5.51	118.52	124.90
9	A	2177	5MU	O2-C2-N1	-4.74	116.49	122.79
34	a	1491	UR3	C4-N3-C2	-4.44	120.39	124.56
9	A	2177	5MU	C5M-C5-C6	-4.10	117.37	122.85
34	a	959	2MG	C5-C6-N1	3.77	120.61	113.95
9	A	2791	OMG	C5-C6-N1	3.44	120.03	113.95
9	A	2177	5MU	C5M-C5-C4	3.10	122.18	118.77
9	A	2791	OMG	C2-N1-C6	-2.94	119.67	125.10
9	A	2177	5MU	C6-C5-C4	2.90	120.45	118.03
34	a	960	5MC	C5-C6-N1	-2.79	120.47	123.34
34	a	518	G7M	C2-N1-C6	-2.77	120.00	125.10
9	A	2177	5MU	C1'-N1-C6	2.62	125.49	121.12
9	A	2791	OMG	C8-N7-C5	2.54	107.83	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	959	2MG	C8-N7-C5	2.53	107.81	102.99
34	a	959	2MG	O6-C6-C5	-2.39	119.71	124.37
34	a	518	G7M	O6-C6-N1	-2.39	117.83	120.65
9	A	2177	5MU	O4-C4-N3	-2.36	115.60	120.12
9	A	2791	OMG	O6-C6-C5	-2.35	119.79	124.37

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	2177	5MU	C3'-C4'-C5'-O5'
9	A	2177	5MU	O4'-C4'-C5'-O5'
34	a	960	5MC	C3'-C4'-C5'-O5'
34	a	1395	4OC	O4'-C4'-C5'-O5'
34	a	1512	MA6	O4'-C4'-C5'-O5'
34	a	1512	MA6	C3'-C4'-C5'-O5'
34	a	959	2MG	C3'-C4'-C5'-O5'
34	a	960	5MC	O4'-C4'-C5'-O5'
34	a	1395	4OC	C3'-C4'-C5'-O5'
34	a	959	2MG	O4'-C4'-C5'-O5'
9	A	2791	OMG	C3'-C4'-C5'-O5'
9	A	2791	OMG	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 428 ligands modelled in this entry, 426 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	ANP	x	602	57	29,33,33	1.06	3 (10%)	31,52,52	1.26	4 (12%)
58	ANP	x	601	57	29,33,33	1.04	4 (13%)	31,52,52	1.12	4 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	ANP	x	602	57	-	7/14/38/38	0/3/3/3
58	ANP	x	601	57	-	4/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	x	602	ANP	PB-O3A	-3.16	1.55	1.59
58	x	601	ANP	PB-O3A	-2.64	1.55	1.59
58	x	601	ANP	PG-N3B	2.23	1.69	1.63
58	x	601	ANP	PB-O1B	2.21	1.49	1.46
58	x	601	ANP	C8-N7	-2.10	1.31	1.34
58	x	602	ANP	PG-O1G	2.09	1.49	1.46
58	x	602	ANP	PG-N3B	2.08	1.68	1.63

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	x	602	ANP	PB-O3A-PA	-4.39	117.15	132.62
58	x	601	ANP	PB-O3A-PA	-3.46	120.44	132.62
58	x	602	ANP	O1B-PB-N3B	-2.58	107.98	111.77
58	x	602	ANP	C5-C6-N6	2.45	124.08	120.35
58	x	601	ANP	O2G-PG-O1G	-2.43	107.36	113.45
58	x	601	ANP	C5-C6-N6	2.37	123.95	120.35
58	x	602	ANP	O1G-PG-N3B	-2.18	108.56	111.77
58	x	601	ANP	O3A-PB-N3B	2.00	112.14	106.59

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	x	601	ANP	PB-N3B-PG-O1G

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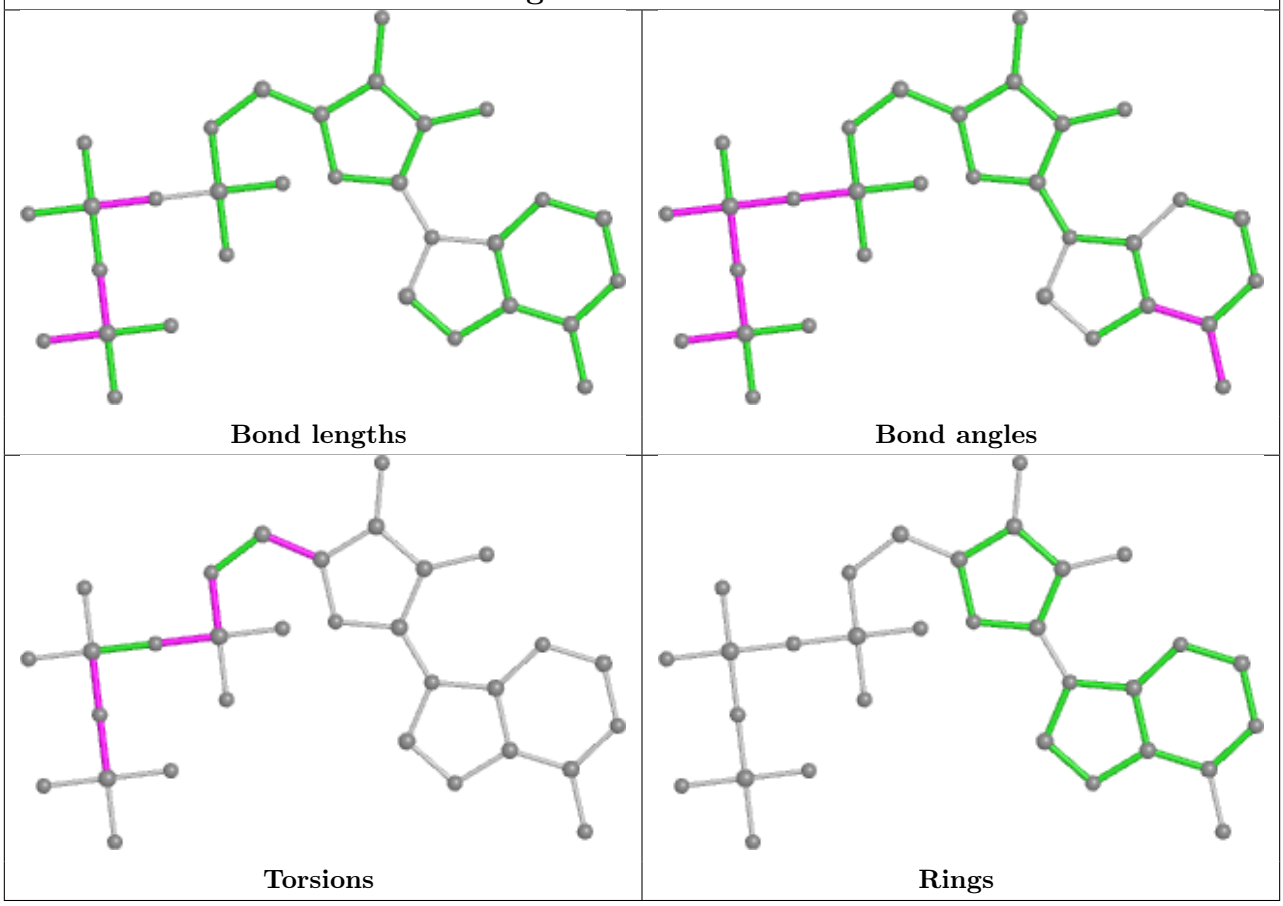
Mol	Chain	Res	Type	Atoms
58	x	601	ANP	PG-N3B-PB-O1B
58	x	602	ANP	PB-N3B-PG-O1G
58	x	602	ANP	PG-N3B-PB-O3A
58	x	601	ANP	O4'-C4'-C5'-O5'
58	x	602	ANP	O4'-C4'-C5'-O5'
58	x	601	ANP	C3'-C4'-C5'-O5'
58	x	602	ANP	C3'-C4'-C5'-O5'
58	x	602	ANP	PB-O3A-PA-O5'
58	x	602	ANP	PB-O3A-PA-O1A
58	x	602	ANP	C5'-O5'-PA-O1A

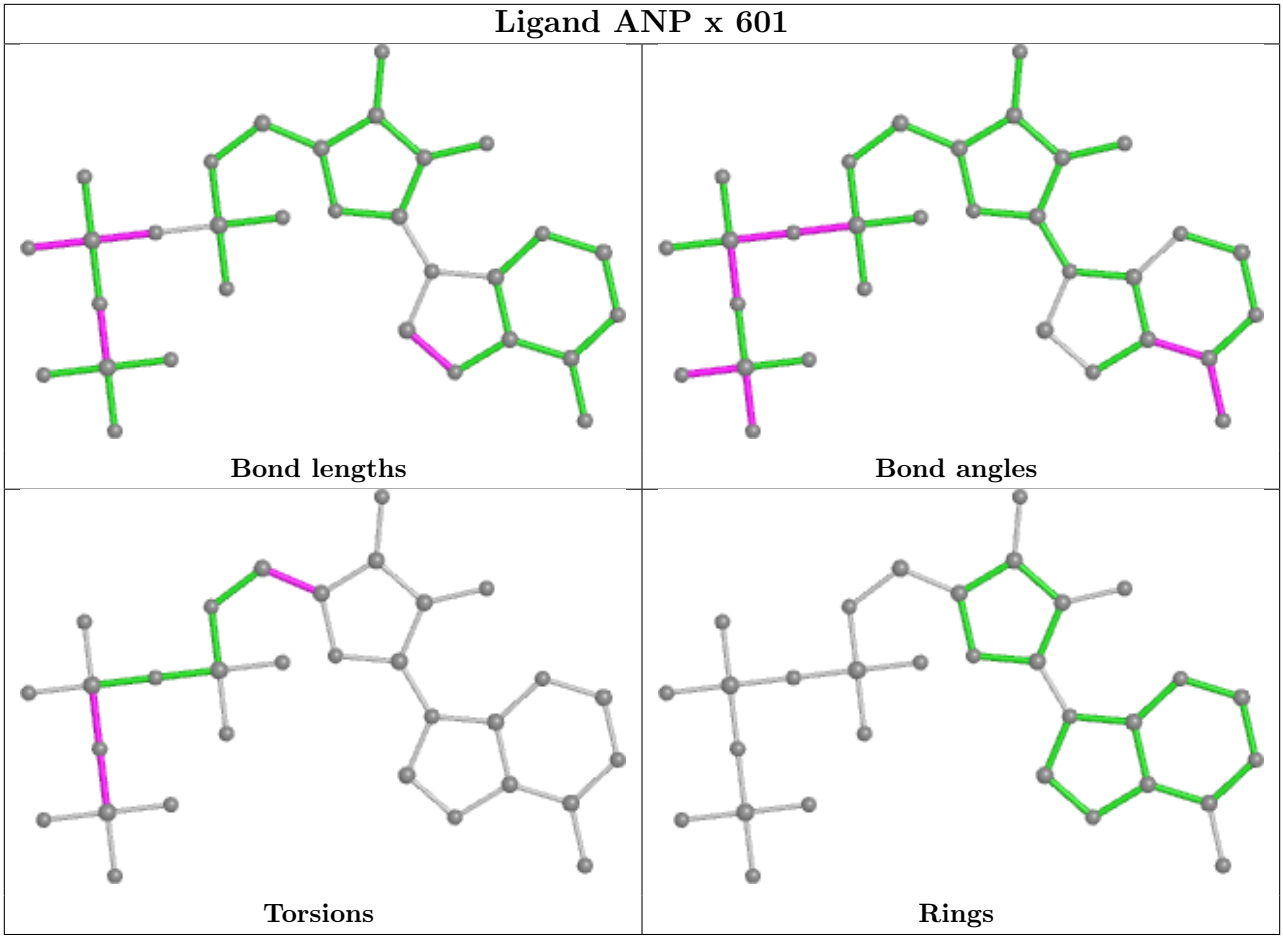
There are no ring outliers.

No monomer is involved in short contacts.

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

Ligand ANP x 602





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

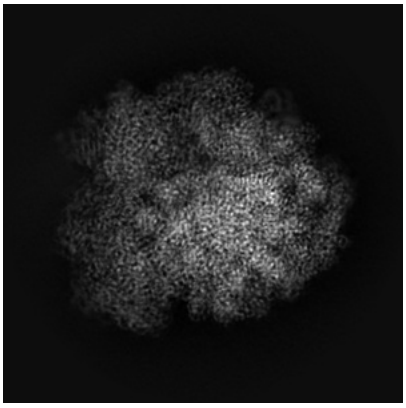
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-23962. These allow visual inspection of the internal detail of the map and identification of artifacts.

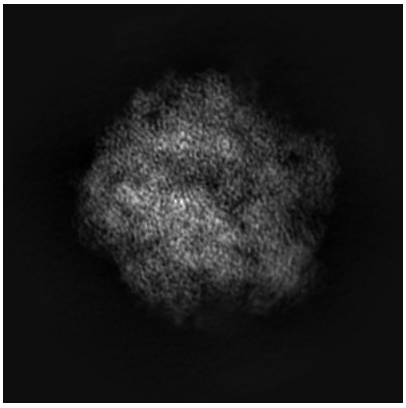
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

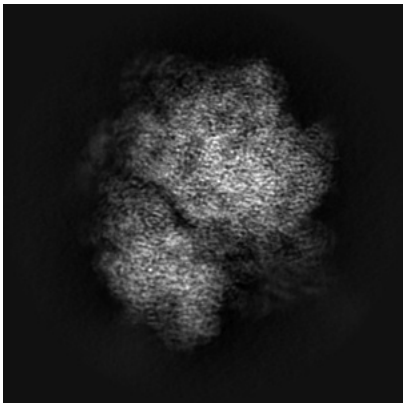
6.1.1 Primary map



X



Y

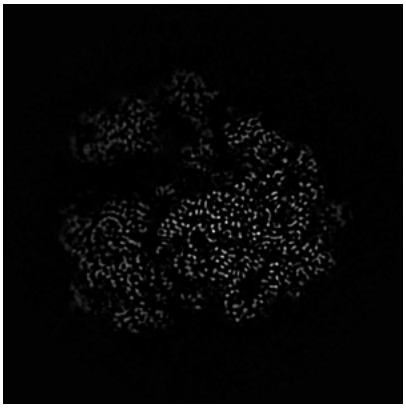


Z

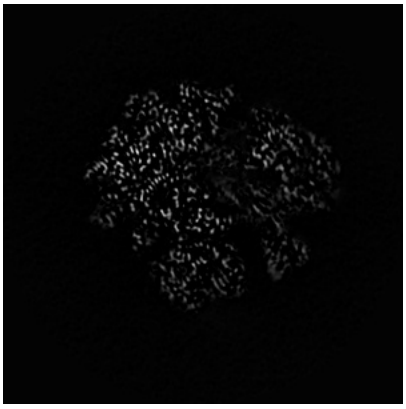
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

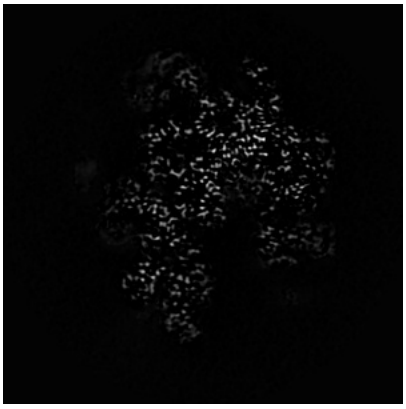
6.2.1 Primary map



X Index: 160



Y Index: 160

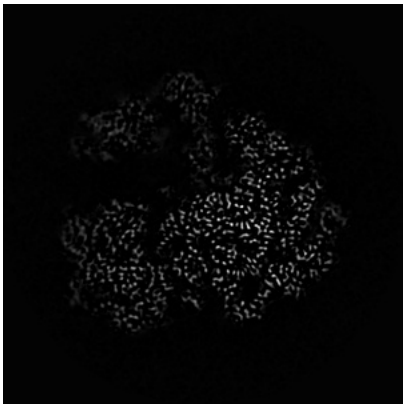


Z Index: 160

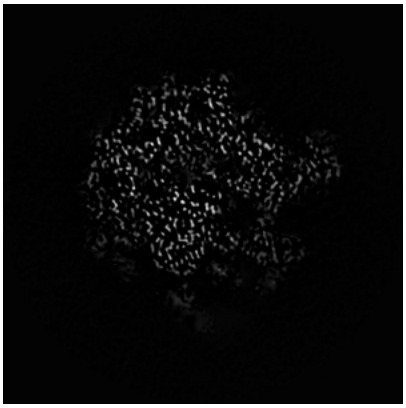
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 162



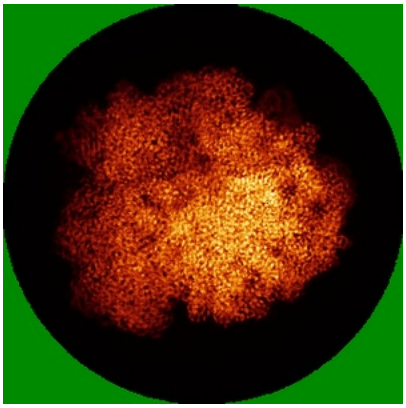
Y Index: 183

Z Index: 143

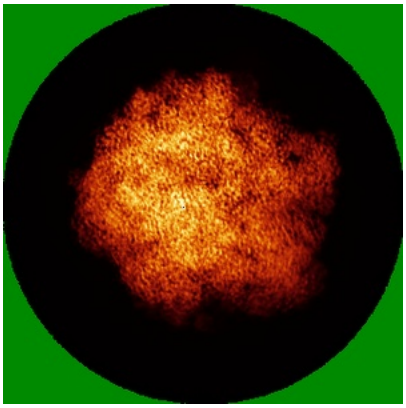
The images above show the largest variance slices of the map in three orthogonal directions.

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

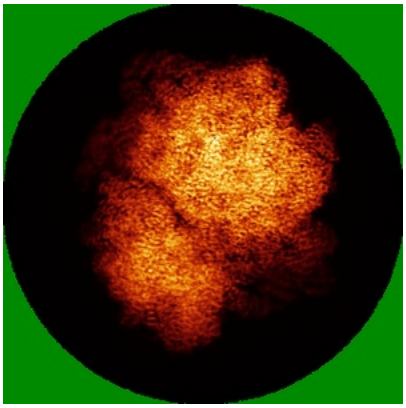
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X

Y

Z

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

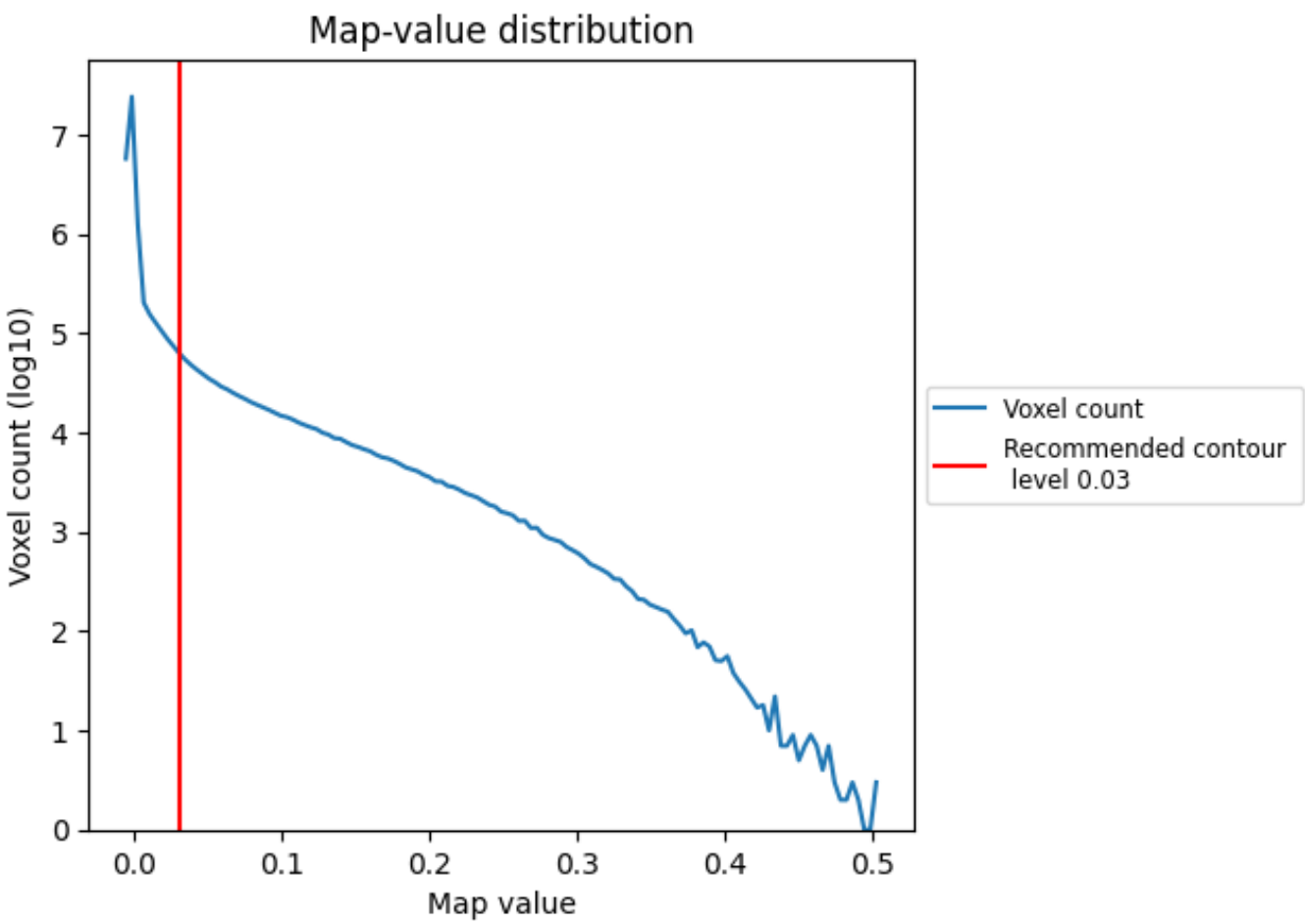
6.6 Mask visualisation (i)

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

7 Map analysis (i)

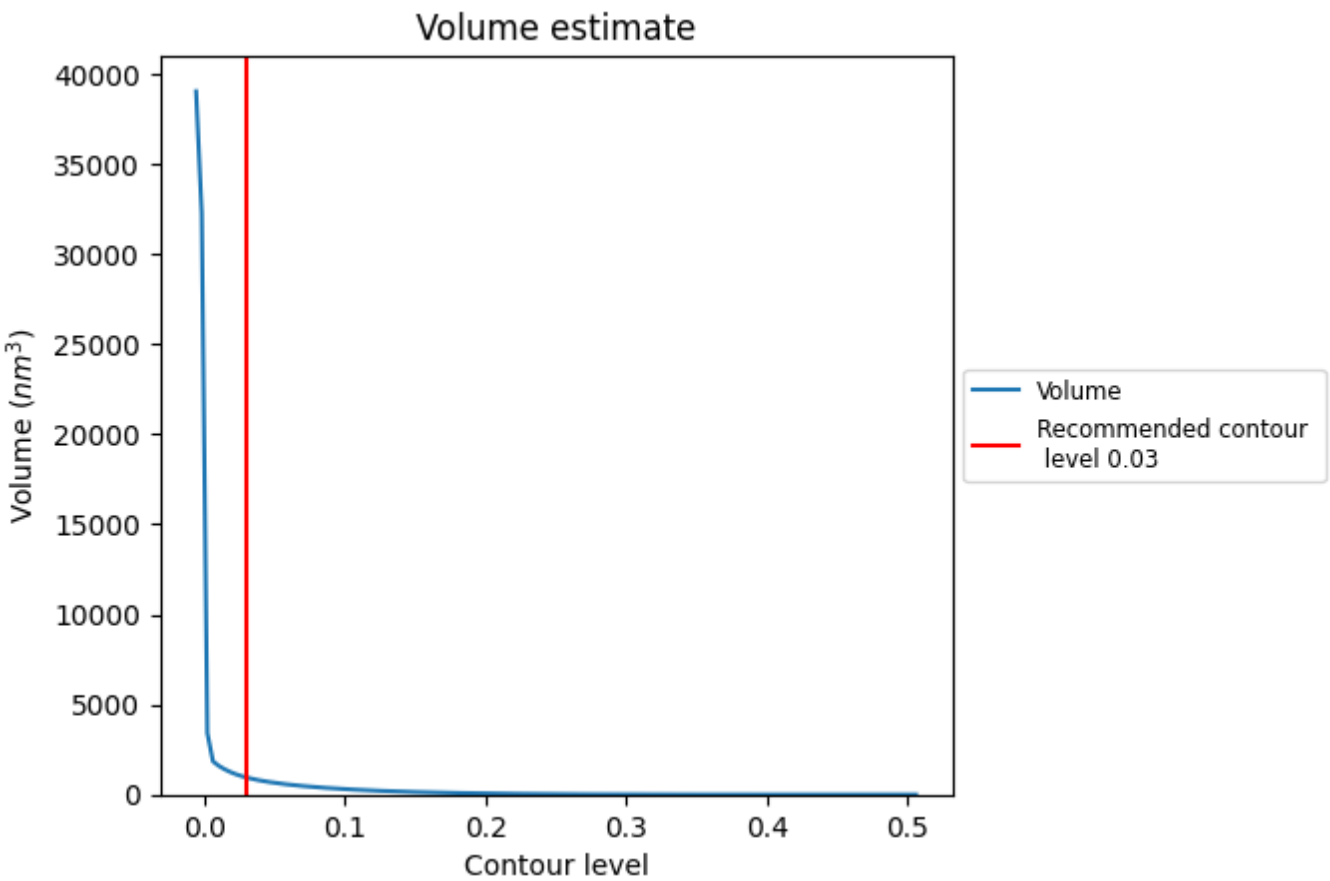
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

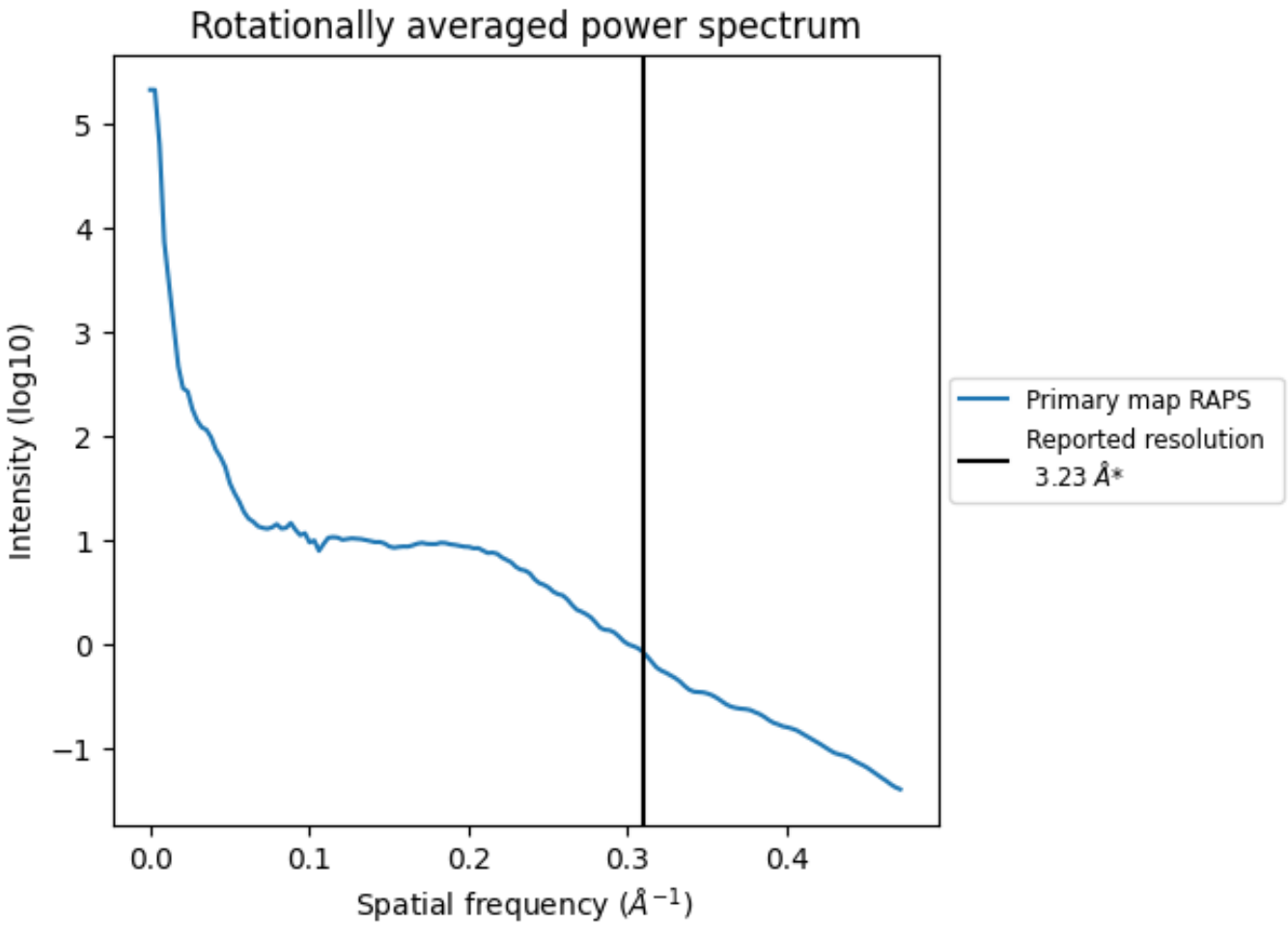
7.2 Volume estimate (i)



The volume at the recommended contour level is 948 nm^3; this corresponds to an approximate mass of 856 kDa.

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

7.3 Rotationally averaged power spectrum (i)

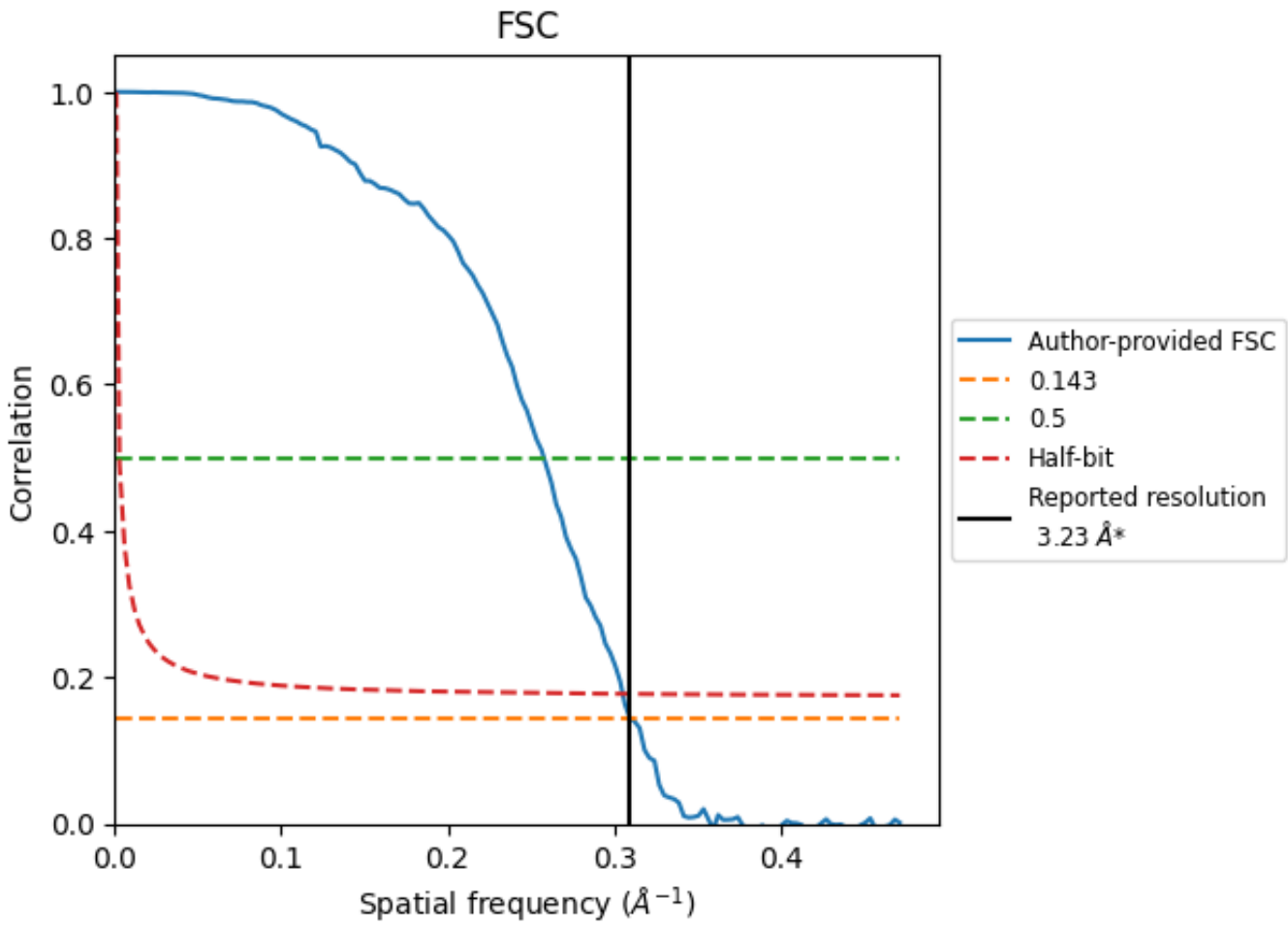


*Reported resolution corresponds to spatial frequency of 0.310 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.310 Å^{-1}

8.2 Resolution estimates (i)

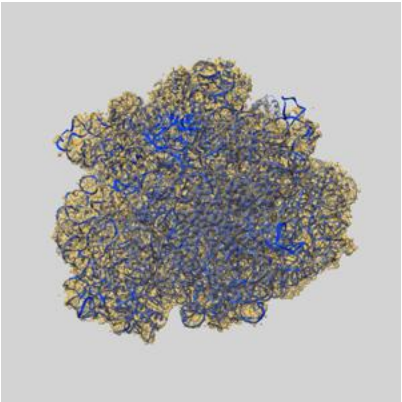
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.23	-	-
Author-provided FSC curve	3.22	3.88	3.28
Unmasked-calculated*	-	-	-

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

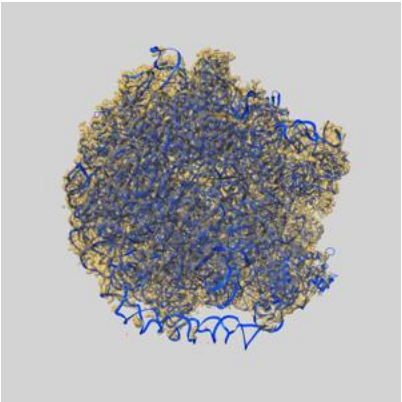
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-23962 and PDB model 7MSH. Per-residue inclusion information can be found in section 3 on page 15.

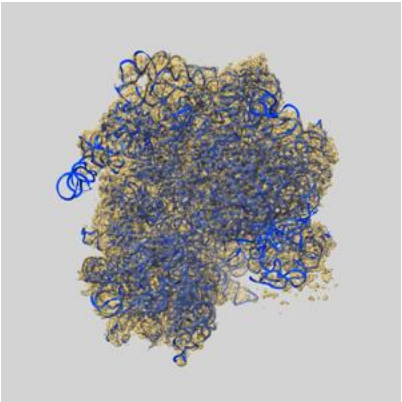
9.1 Map-model overlay (i)



X



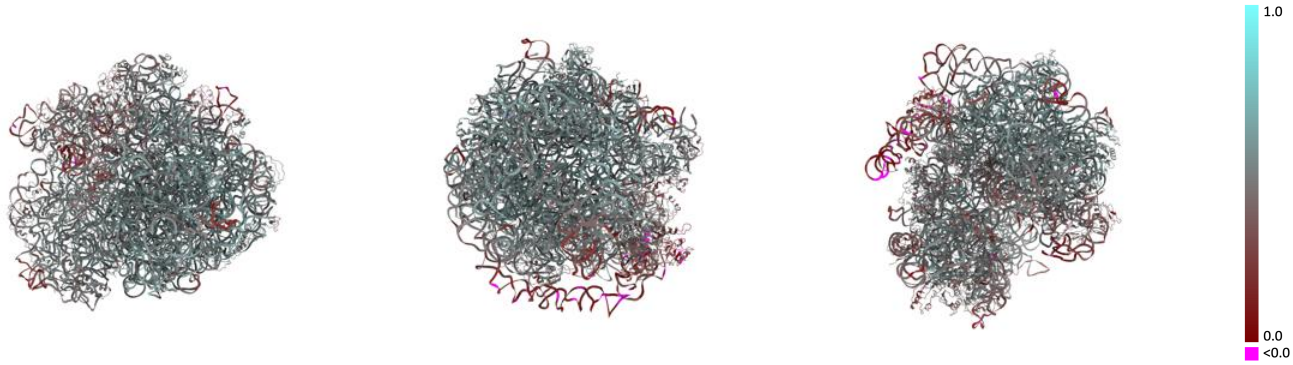
Y



Z

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

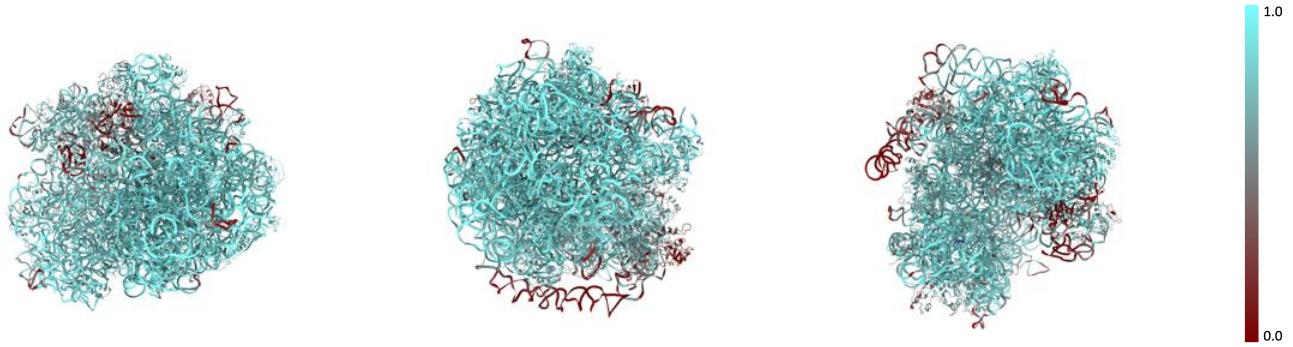
9.2 Q-score mapped to coordinate model (i)



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.

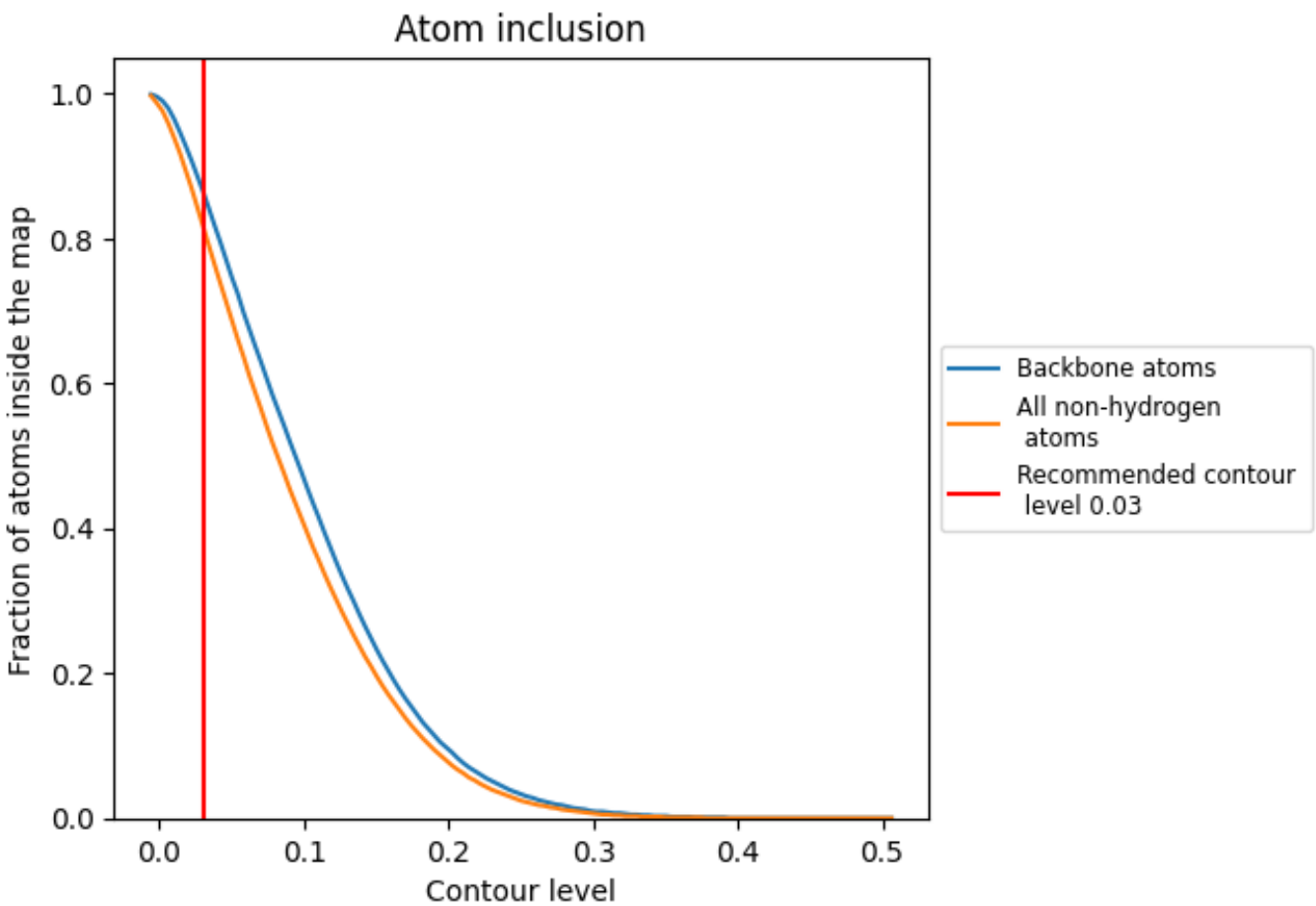
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 87% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.4870
0	0.6630	0.4850
1	0.8480	0.5230
2	0.9330	0.5900
3	0.8440	0.5530
4	0.6180	0.4350
6	0.6130	0.3560
7	0.3180	0.2690
8	0.3470	0.2530
A	0.8470	0.5010
B	0.8850	0.4990
C	0.8760	0.5540
D	0.8630	0.5380
E	0.8780	0.5340
F	0.6910	0.4000
G	0.6390	0.3960
H	0.6250	0.4150
J	0.8590	0.5310
K	0.8460	0.5260
L	0.8680	0.5430
M	0.3610	0.4100
N	0.8790	0.5490
O	0.8240	0.4990
P	0.8300	0.5180
Q	0.8700	0.5550
R	0.8640	0.5480
S	0.8740	0.5540
T	0.8420	0.5180
U	0.7930	0.4780
V	0.1740	0.3540
W	0.8860	0.5320
X	0.8960	0.5570
Y	0.8230	0.5190
Z	0.8460	0.5220
a	0.8710	0.4890

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	0.7340	0.4510
d	0.7270	0.4250
e	0.8010	0.5020
f	0.7140	0.4310
g	0.7550	0.4580
h	0.8030	0.4890
i	0.6960	0.4080
j	0.6150	0.3670
k	0.7800	0.4850
l	0.7920	0.4780
m	0.7000	0.3890
n	0.8200	0.4920
o	0.8000	0.4810
p	0.7540	0.4650
q	0.7870	0.4700
r	0.7600	0.4260
s	0.6690	0.3880
t	0.7560	0.4700
x	0.6740	0.4140
y	0.8070	0.4560
z	0.8370	0.4880