Full wwPDB EM Validation Report (i)

Mar 10, 2025 – 04:51 PM JST

PDB ID	:	9J1M
EMDB ID	:	EMD-61076
Title	:	KU13-bond Mycobacterium tuberculosis 70S ribosome
Authors	:	Nishihara, D.; Fujino, M.; Tanaka, Y.; Yokoyama, T.
Deposited on	:	2024-08-05
Resolution	:	2.33 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:

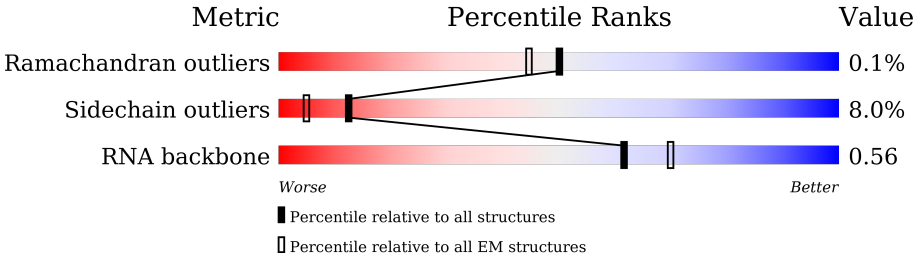
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 2.33 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	7%, 93%, • 5%
2	1	55	82%, 5%, 13%
3	2	47	89%, • 6%
4	3	64	91%, 6%, •
5	4	37	92%, 8%
6	7	24	83%, 8%, 8%
7	A	3138	6%, 80%, 13%, 7%
8	B	115	•, 83%, 16%, •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	C	280	94%
10	D	217	92% 6%
11	E	223	89% 7%
12	F	187	28% 84% 10% 5%
13	G	179	20% 89% 8%
14	H	152	12% 29% 69%
15	J	195	71% 25%
16	K	122	89% 11%
17	L	146	90% 8%
18	M	138	91% 6%
19	N	180	61% 36%
20	O	122	90% 7%
21	P	113	6% 92% 7%
22	Q	129	93%
23	R	104	89% 7%
24	S	197	55% 43%
25	T	100	7% 83% 12% 5%
26	U	105	10% 77% 9% 14%
27	V	215	28% 78% 18%
28	W	86	86% 10%
29	X	64	91% 6%
30	Y	77	6% 79% 9% 12%
31	Z	65	86% 5% 9%
32	a	1537	22% 82% 17%
33	c	274	57% 68% 7% 24%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	d	201	92% 93% 7%
35	e	220	14% 73% • 23%
36	f	96	24% 90% 9% •
37	g	156	78% 90% 9% ••
38	h	132	12% 91% 8% •
39	i	151	65% 76% 8% 16%
40	j	101	78% 91% 7% •
41	k	139	14% 80% • 16%
42	l	124	40% 91% 7% •
43	m	124	77% 87% 6% 6%
44	n	61	46% 92% 7% •
45	o	89	18% 89% 7% • •
46	p	162	36% 54% • 43%
47	q	135	36% 64% 5% • 30%
48	r	84	13% 68% 8% 24%
49	s	93	81% 83% 6% 11%
50	t	86	59% 86% 12% ••
51	x	66	9% 45% • 53%
52	u	3	67% 33%

2 Entry composition (i)

There are 55 unique types of molecules in this entry. The entry contains 139822 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 Large ribosomal subunit protein bL32.

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 Large ribosomal subunit protein bL33A.

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 Large ribosomal subunit protein bL34.

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 Large ribosomal subunit protein bL35.

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 Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	37	300	182	66	47	5	0	0

- Molecule 6 is a protein called 30S ribosomal protein THX.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	7	22	186	111	47	28	0	0

- Molecule 7 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	A	2904	62388	27811	11529	20144	2904	0	0

- Molecule 8 is a RNA chain called 5S rRNA.

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

- Molecule 9 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 14 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 15 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	K	122	942	590	180	169	3	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	L	144	1074	664	217	191	2	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 20 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 23 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 27 is a protein called Large ribosomal subunit protein bL25.

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

- Molecule 28 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
28	W	77	564	345	117	102	0	0

- Molecule 29 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL30.

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

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

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

- Molecule 33 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 35 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 36 is a protein called Small ribosomal subunit protein bS6.

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

- Molecule 37 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 38 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 39 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 40 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 41 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
41	k	117	872	538	175	159	0	0

- Molecule 42 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 43 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 44 is a protein called Small ribosomal subunit protein uS14B.

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

- Molecule 45 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 46 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
46	p	93	745	474	143	128	0	0

- Molecule 47 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 48 is a protein called Small ribosomal subunit protein bS18A.

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

- Molecule 49 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 50 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 51 is a protein called Mitochondrial domain of uncharacterised function (DUF1713).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	x	31	271	166	69	35	1	0	0

- Molecule 52 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
52	u	3	62	28	11	20	3	0	0

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
53	1	1	1	1	0
53	4	1	1	1	0
53	X	1	1	1	0
53	n	1	1	1	0
53	r	1	1	1	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

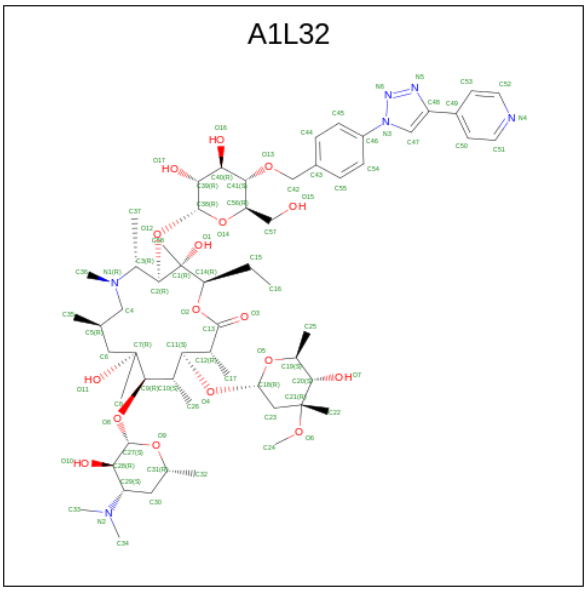
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	A	300	300	300	0
54	B	5	5	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
54	C	2	2	2	0
54	D	1	1	1	0
54	L	1	1	1	0
54	U	1	1	1	0
54	a	129	129	129	0
54	r	1	1	1	0
54	u	1	1	1	0

- Molecule 55 is (2 {R},3 {R},4 {R},5 {R},8 {R},10 {R},11 {R},12 {S},13 {S},14 {R})-11-[(2 {S},3 {R},4 {S},6 {R})-4-(dimethylamino)-6-methyl-3-oxidanyl-oxan-2-yl]oxy-2-ethyl-4-[(2 {R},3 {R},4 {R},5 {S},6 {R})-6-(hydroxymethyl)-3,4-bis(oxidanyl)-5-[[4-(4-pyridin-4-yl-1,2,3-triazol-1-yl)phenyl]methoxy]oxan-2-yl]oxy-13-[(2 {R},4 {R},5 {S},6 {S})-4-methoxy-4,6-dimethyl-5-oxidanyl-oxan-2-yl]oxy-3,5,6,8,10,12,14-heptamethyl-3,10-bis(oxidanyl)-1-oxa-6-azacyclopentadecan-15-one (three-letter code: A1L32) (formula: $C_{58}H_{92}N_6O_{17}$) (labeled as "Ligand of Interest" by depositor).



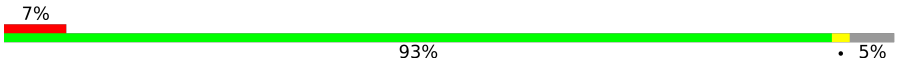
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
55	A	1	81	58	6	17	0

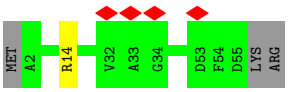
3 Residue-property plots (i)

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: Large ribosomal subunit protein bL32

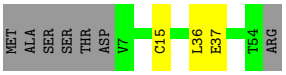
Chain 0:





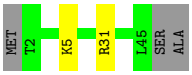
- Molecule 2: Large ribosomal subunit protein bL33A

Chain 1:



- Molecule 3: Large ribosomal subunit protein bL34

Chain 2:



- Molecule 4: Large ribosomal subunit protein bL35

Chain 3:

- Molecule 5: Large ribosomal subunit protein bL36

Chain 4:

- Molecule 6: 30S ribosomal protein THX

Chain 7: 83% 8% 8%

MET A2 N17 N23 SER

• Molecule 7: 23S rRNA

Chain A: 6% 80% 13% 7%

U U G U A5 U8 G9 U10 C11 G43 G51 A63 A71 U74 G75 C90 A91 A92 C93 C94 A118 A119 U120 G143 A165 U166 A167 G176 A183 A198 A201 G217 A218 A224 A225 A226 U230 U231 G232 G249 G250

G277 C278 U284 G285 G286 G287 U288 A289 A290 C291 C292 G293 G294 G295 U296 A297 G298 G299 G300 G301 U302 U303 G314 G315 U316 G322 A323 A326 U327 A328 U329 G330 U331 C332 U333 C334 A335 G336 C337 G338 C339 U340 A341 C342 C343 C344 G345 G346 C347 U348 G349 A350 G351 U358

A364 G365 U366 G367 U368 C369 G370 U371 G372 U394 U399 G400 C401 A413 G414 A428 A429 U445 A446 G447 U448 A449 U450 C451 A452 A453 U454 U455 C472 C473 C474 G475 U476 G477 G478 A479 A480 C494 G495 G500 U544 U545 G570 G592 A593 G594 U595 A596 C597

G600 A616 A617 U618 C619 C620 G621 U633 U U U C C U C U C C G G A G G A G650 G665 A674 G675 A676 A677 G689 G693 G694 A706 U717 G718 U719 G738 C739 G740 A741 U749 C757 C758 C759 A760 C763

G764 C765 G766 C767 A768 U769 A770 C771 G772 C773 G774 U777 G778 U779 G780 A781 A782 U783 U815 U843 G846 G852 G855 C859 U876 C882 G886 A893 G904 G905 A911 A912 G913 G914 G934 C941 C946 U956 U976 G988

G1011 G1012 C C C C U A C U A G G U1023 U1024 A1025 C1026 U1027 G1028 C1036 A1039 C1043 C1044 A1059 A1060 A1061 G1074 A1087 A1088 G1089 A1096 A1103 A1112 G1118 G1125 G1142 G1155 U1162 A1167 C1172 A1173 A1174 A1175 G1176 A1177

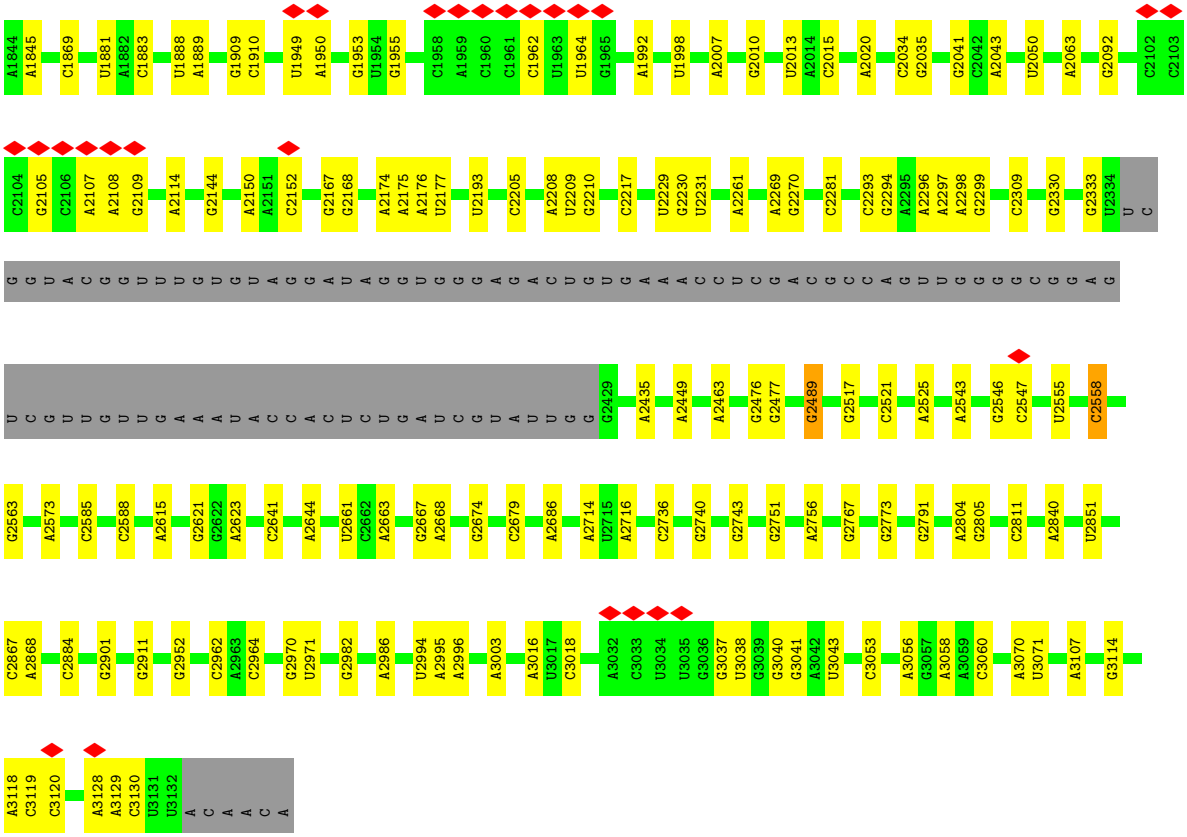
C1178 A1179 A1180 C1181 C1182 A1183 G1184 G1185 A1186 G1187 G1188 U1189 U1190 G1191 G1192 C1193 U1194 U1195 A1196 G1197 A1198 A1199 G1200 C1201 A1202 G1203 C1204 C1205 A1206 C1207 C1208 C1209 U1210 U1211 G1212 A1213 A1214 A1215 G1216 A1217 G1218 U1219 G1220 C1221 G1222 U1223 A1224 A1225 U1226 A1227 G1228 C1229 U1230 C1231 A1232 C1233 U1234 G1235 G1236 U1237

C1238 A1239 A1240 G1241 U1242 G1243 A1244 G1249 A1257 A1258 U1261 A1262 G1263 C1264 C1271 A1272 A1273 A1301 C1302 C1303 U1304 U1305 G1306 U1307 G1308 G1309 G1313 C1342 A1384 A1385 U1386 G1387 G1402 A1403 A1406 C1425 A1431 A1432 C1452 C1456 U1483 G1491 A1496

A1509 U1510 A1515 A1516 C1517 A1534 G1548 C C C G U G A C G A A U C A G C G G U A C U A A C C A C C C A A A C C G G A U C G A U C A C U C

C C C U U C G G G G G U G U G G G A G U U C U G G G C C G U G G G G A A C U U C G C U G G U A G U A G U C A A1653 G1656 A1657

A1665 C1666 G1675 C1689 A1690 G1691 U1692 G1693 A1697 C1698 A1699 U1714 G1720 A1721 G1722 A1727 C1730 U1734 C1743 A1744 C1745 U1746 A1747 A1748 A1754 G1755 C1770 G1771 G1772 U1773 U1774 G1775 A1776 G1777 C1802 A1803 A1806 G1821 C1830 G1831 G1832 C1833 C1842 A1843

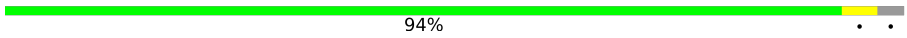


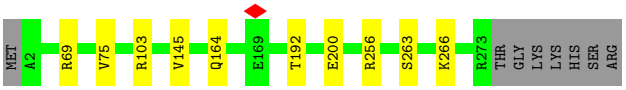
- Molecule 8: 5S rRNA

Chain B:

- Molecule 9: Large ribosomal subunit protein uL2

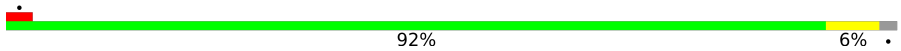
Chain C:

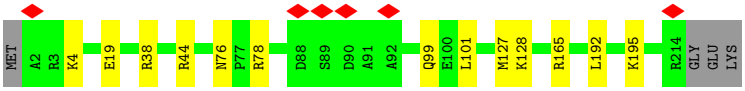




- Molecule 10: Large ribosomal subunit protein uL3

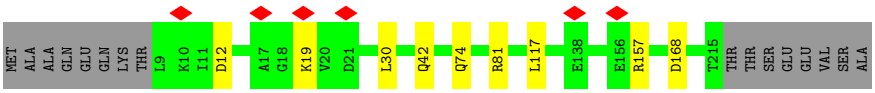
Chain D:





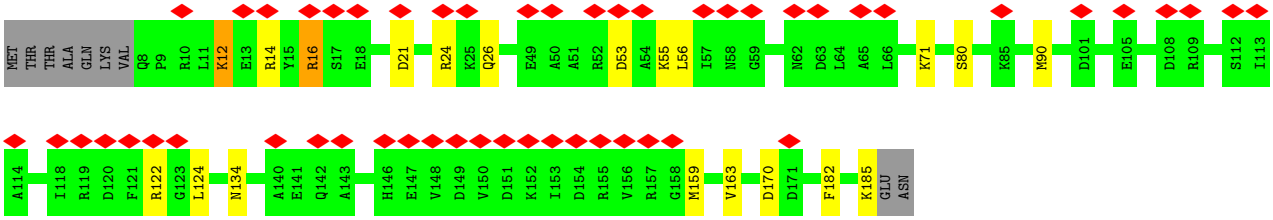
- Molecule 11: Large ribosomal subunit protein uL4

Chain E:



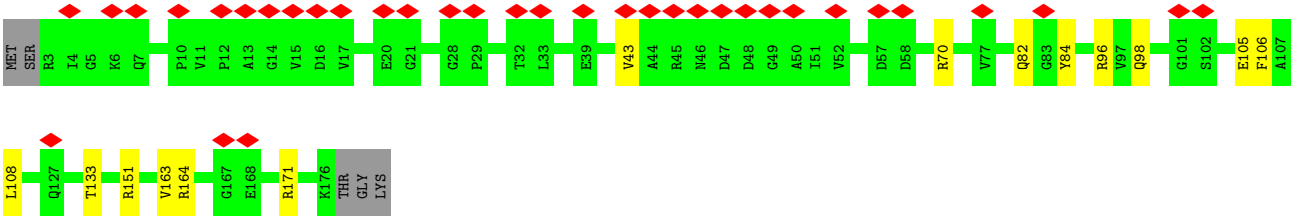
• Molecule 12: Large ribosomal subunit protein uL5

Chain F:



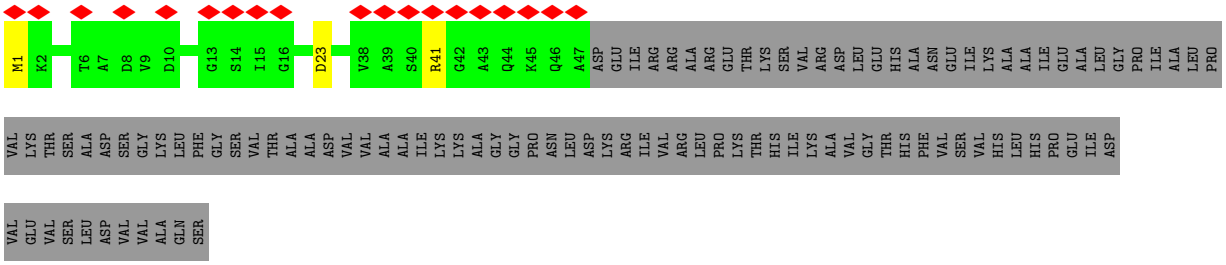
• Molecule 13: Large ribosomal subunit protein uL6

Chain G:



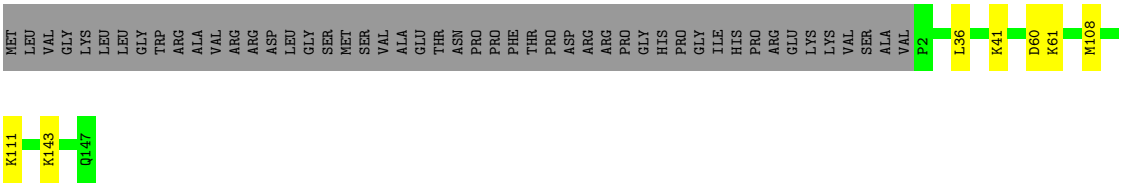
• Molecule 14: Large ribosomal subunit protein bL9

Chain H:



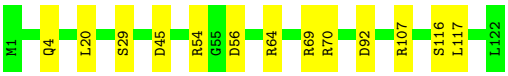
• Molecule 15: Large ribosomal subunit protein uL13

Chain J:



• Molecule 16: Large ribosomal subunit protein uL14

Chain K:

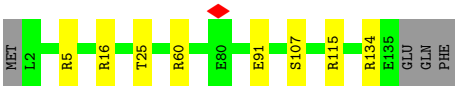


• Molecule 17: Large ribosomal subunit protein uL15

Chain L:

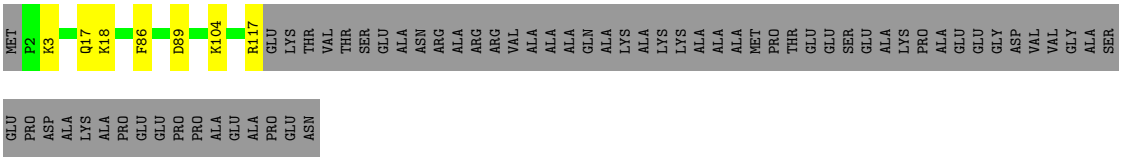
• Molecule 18: Large ribosomal subunit protein uL16

Chain M:



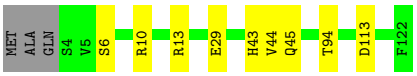
• Molecule 19: Large ribosomal subunit protein bL17

Chain N:



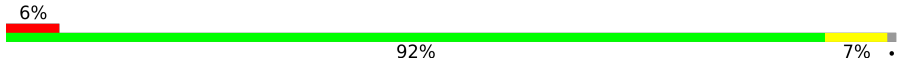
• Molecule 20: Large ribosomal subunit protein uL18

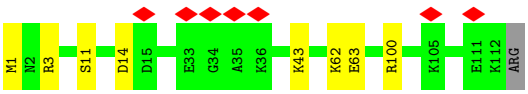
Chain O:



• Molecule 21: Large ribosomal subunit protein bL19

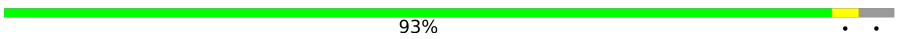
Chain P:





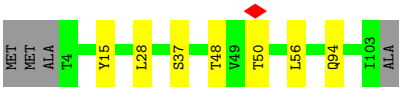
• Molecule 22: Large ribosomal subunit protein bL20

Chain Q:



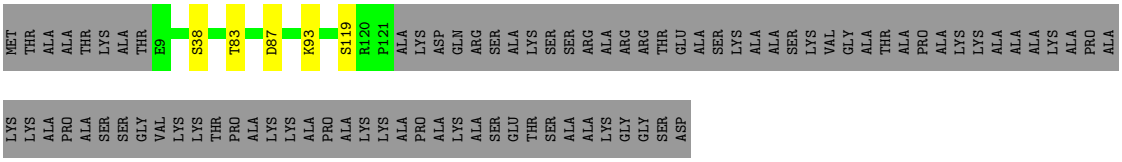
• Molecule 23: Large ribosomal subunit protein bL21

Chain R:



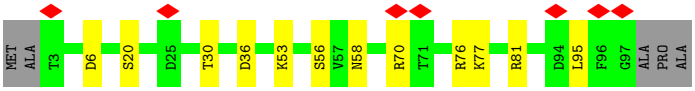
• Molecule 24: Large ribosomal subunit protein uL22

Chain S:



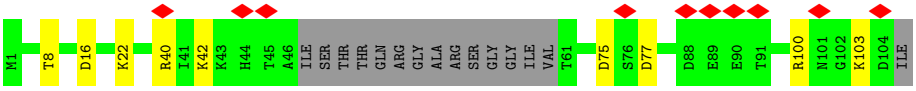
• Molecule 25: Large ribosomal subunit protein uL23

Chain T:



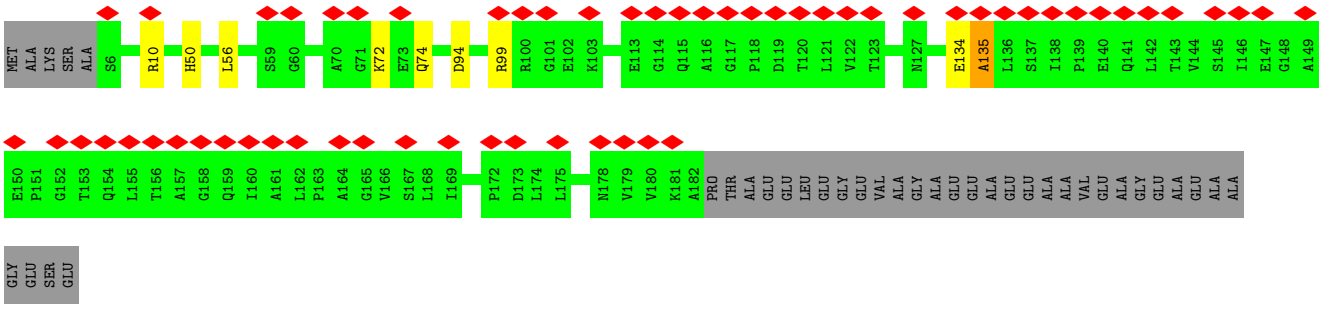
• Molecule 26: Large ribosomal subunit protein uL24

Chain U:



• Molecule 27: Large ribosomal subunit protein bL25

Chain V:



• Molecule 28: Large ribosomal subunit protein bL27

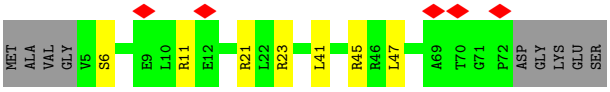
Chain W:

• Molecule 29: Large ribosomal subunit protein bL28

Chain X:

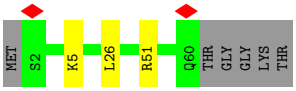
• Molecule 30: Large ribosomal subunit protein uL29

Chain Y:



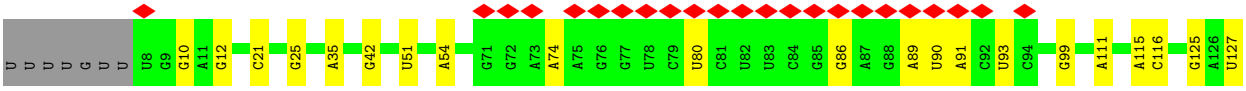
• Molecule 31: Large ribosomal subunit protein uL30

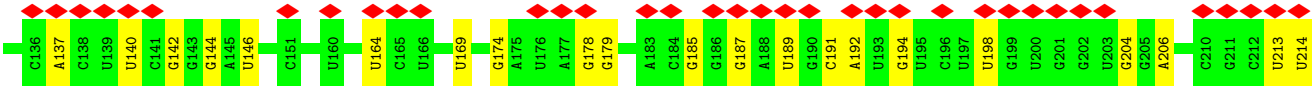
Chain Z:

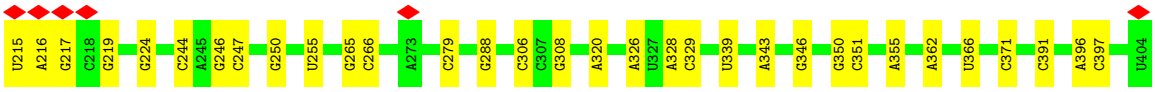


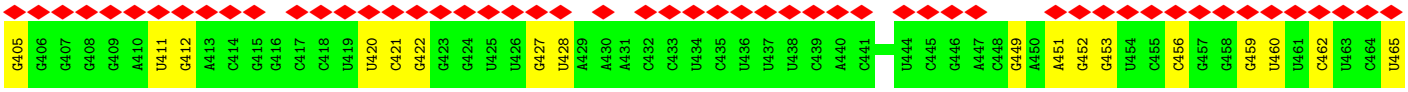
• Molecule 32: 16S rRNA

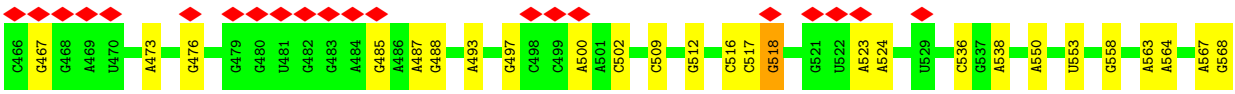
Chain a:

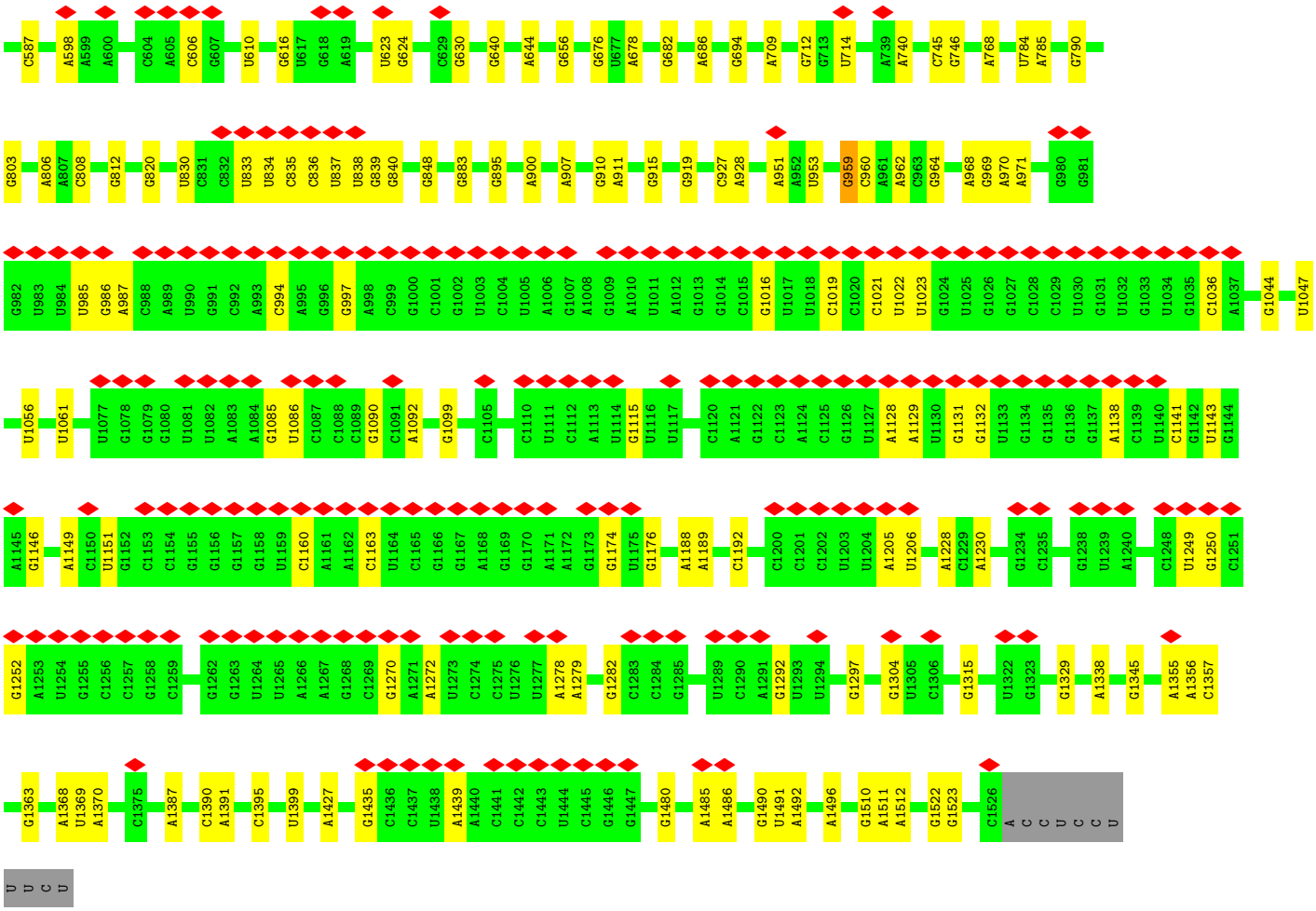






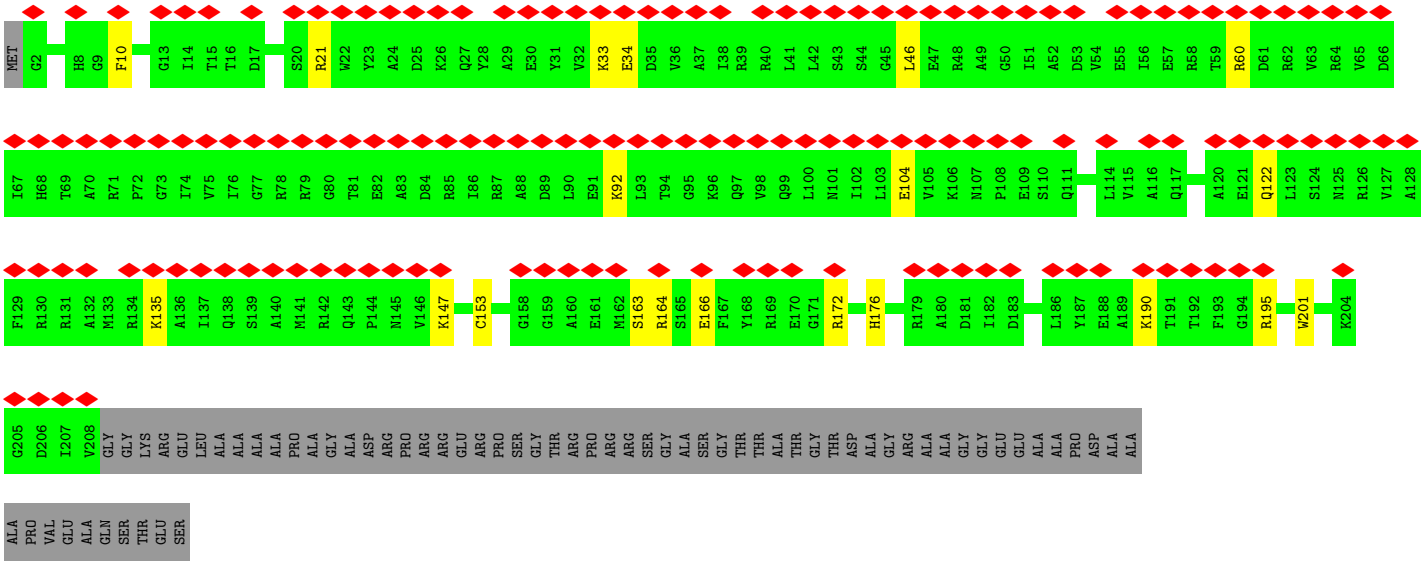






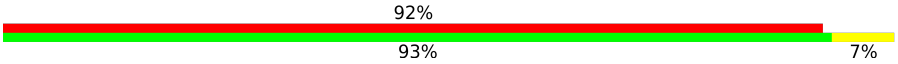
• Molecule 33: Small ribosomal subunit protein uS3

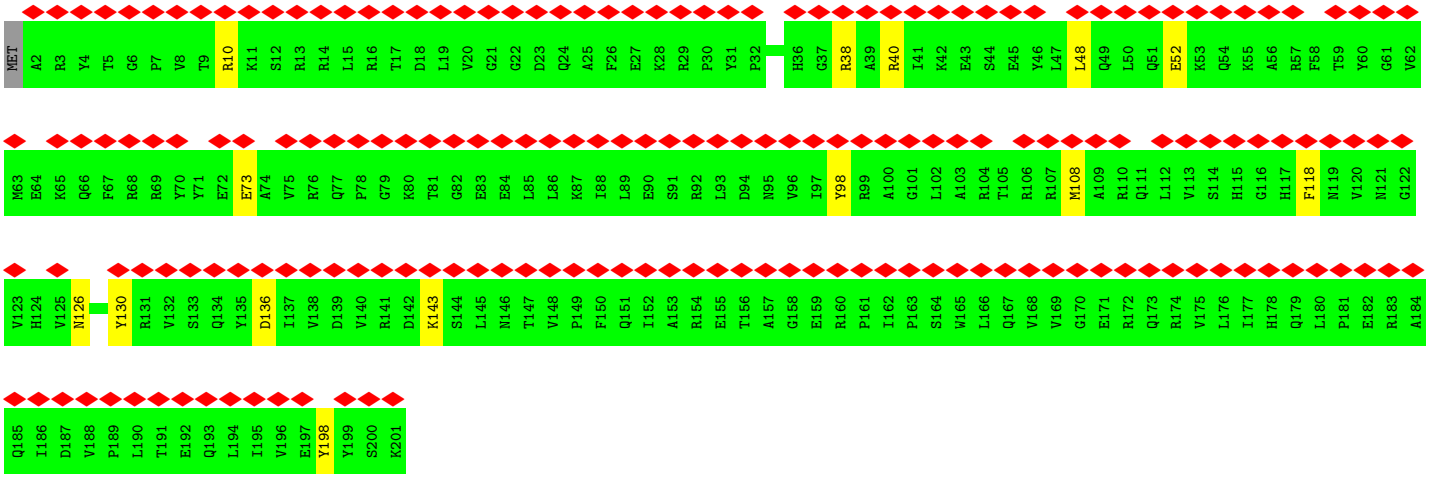
Chain c:



• Molecule 34: Small ribosomal subunit protein uS4

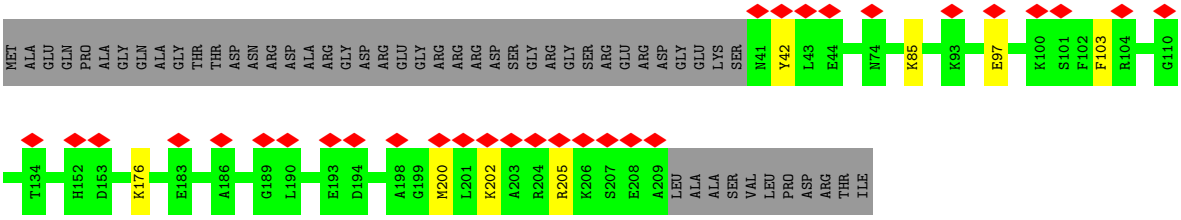
Chain d:





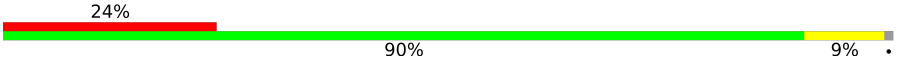
- Molecule 35: Small ribosomal subunit protein uS5

Chain e:



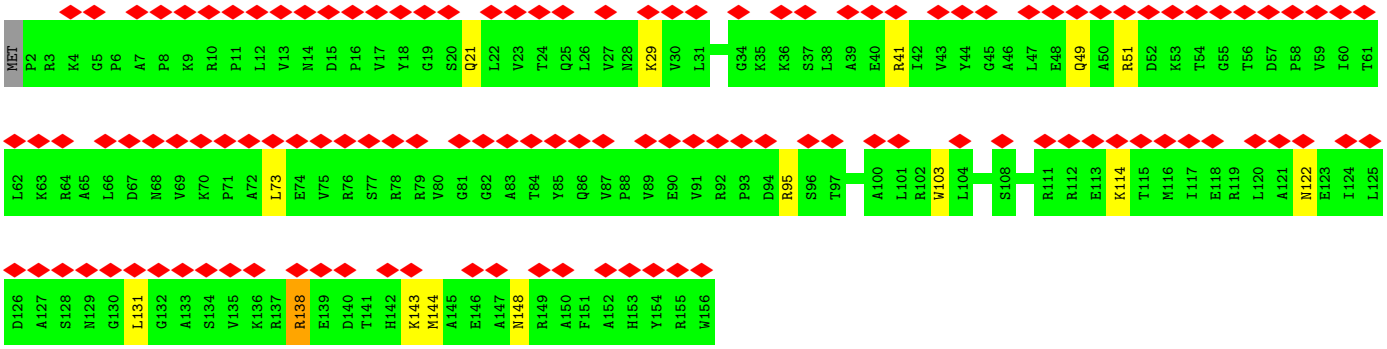
- Molecule 36: Small ribosomal subunit protein bS6

Chain f:



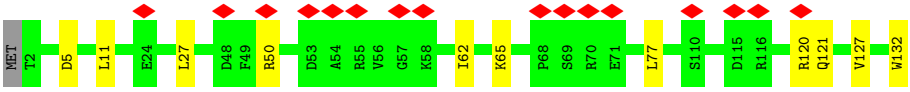
- Molecule 37: Small ribosomal subunit protein uS7

Chain g:



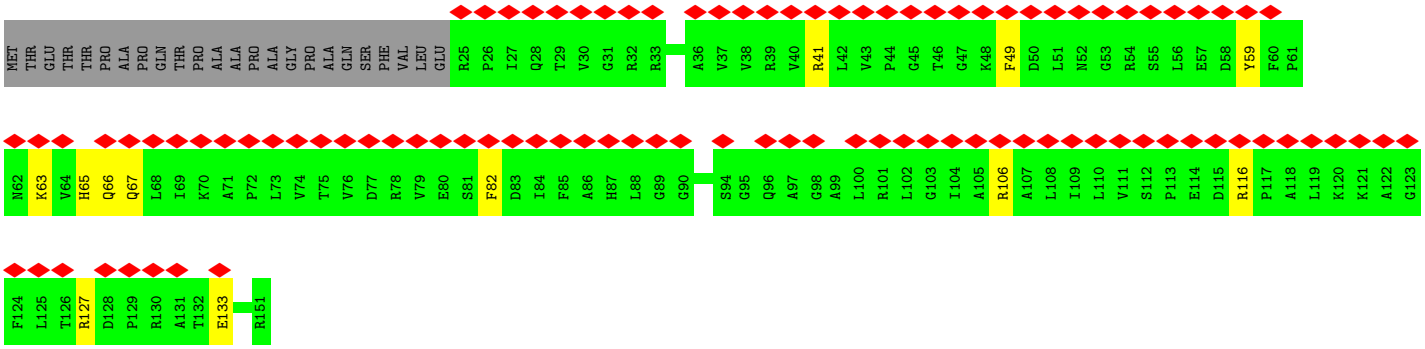
• Molecule 38: Small ribosomal subunit protein uS8

Chain h: 12% 91% 8%



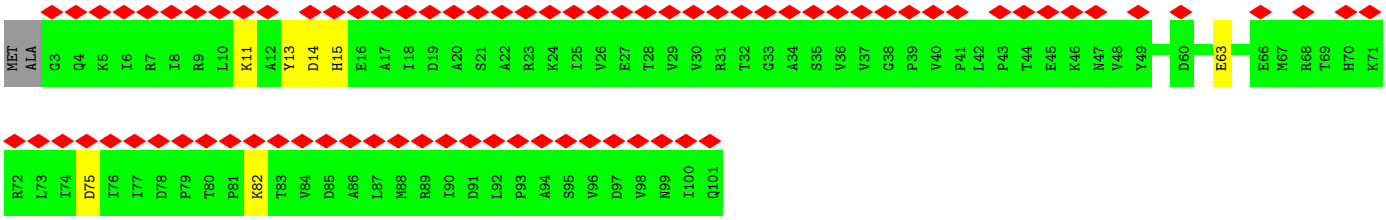
• Molecule 39: Small ribosomal subunit protein uS9

Chain i: 65% 76% 8% 16%



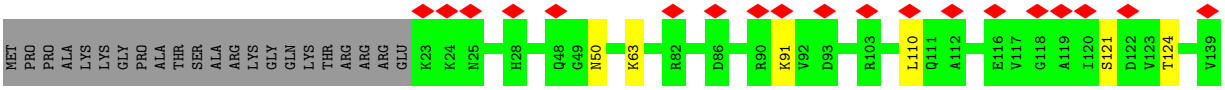
• Molecule 40: Small ribosomal subunit protein uS10

Chain j: 78% 91% 7%



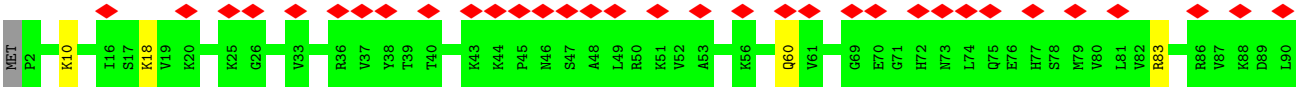
• Molecule 41: Small ribosomal subunit protein uS11

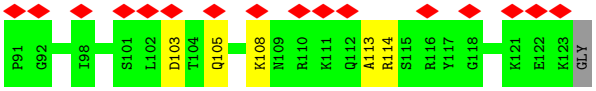
Chain k: 14% 80% 16%



• Molecule 42: Small ribosomal subunit protein uS12

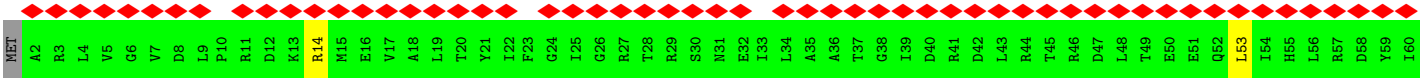
Chain l: 40% 91% 7%

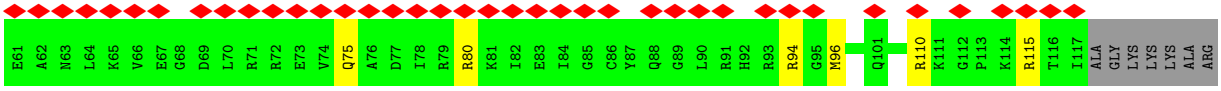




• Molecule 43: Small ribosomal subunit protein uS13

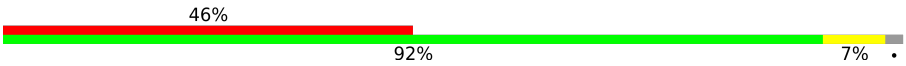
Chain m:

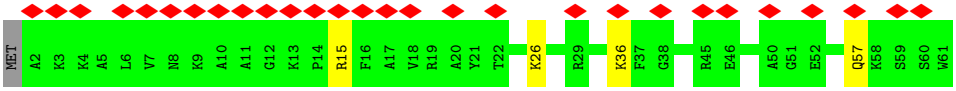




• Molecule 44: Small ribosomal subunit protein uS14B

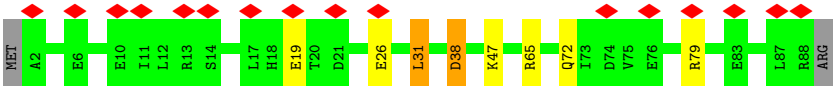
Chain n:





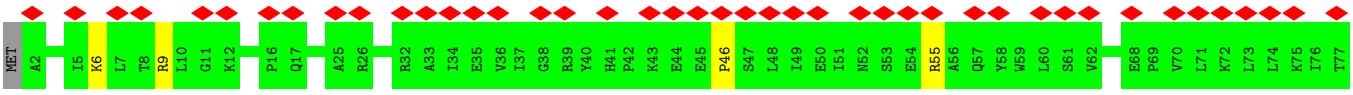
• Molecule 45: Small ribosomal subunit protein uS15

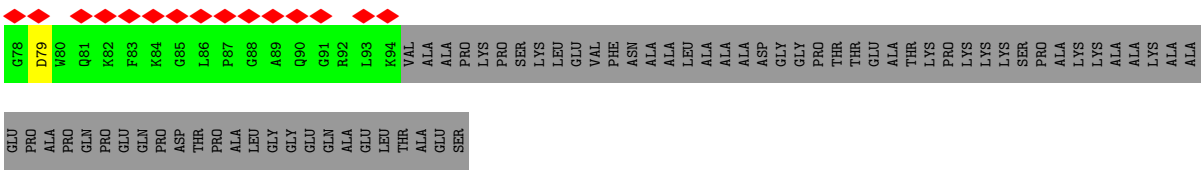
Chain o:



• Molecule 46: Small ribosomal subunit protein bS16

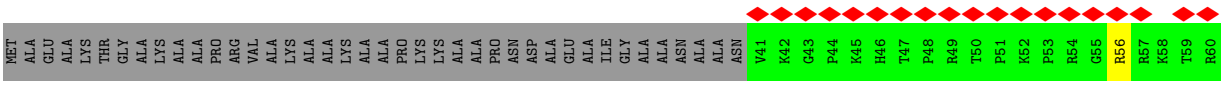
Chain p:

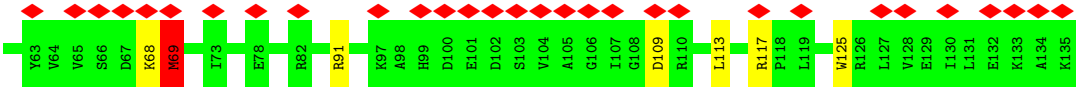




• Molecule 47: Small ribosomal subunit protein uS17

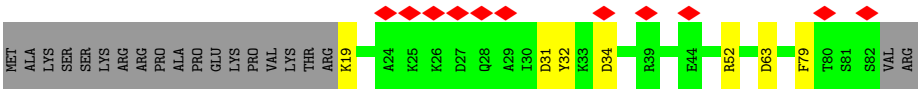
Chain q:





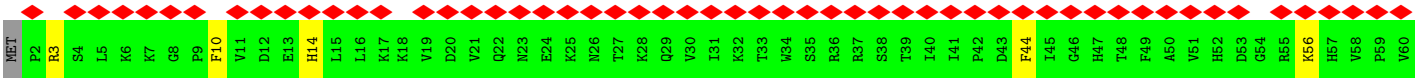
• Molecule 48: Small ribosomal subunit protein bS18A

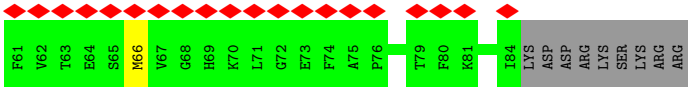
Chain r:



• Molecule 49: Small ribosomal subunit protein uS19

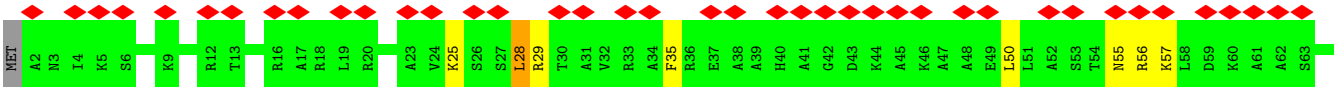
Chain s:

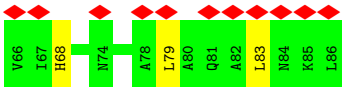




• Molecule 50: Small ribosomal subunit protein bS20

Chain t:





• Molecule 51: Mitochondrial domain of uncharacterised function (DUF1713)

Chain x:

• Molecule 52: tRNA

Chain u:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	205461	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	60000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.083	Depositor
Minimum map value	-0.022	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0085	Depositor
Map size (Å)	403.456, 403.456, 403.456	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.788, 0.788, 0.788	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: MA6, 5MC, G7M, ZN, 5MU, OMG, 2MG, UR3, MG, 4OC, A1L32

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	0.34	0/435	0.70	0/581
2	1	0.38	0/407	0.67	0/543
3	2	0.33	0/377	0.82	0/494
4	3	0.30	0/499	0.67	0/664
5	4	0.32	0/304	0.69	0/402
6	7	0.39	0/188	0.72	0/243
7	A	0.58	1/69786 (0.0%)	0.83	37/108882 (0.0%)
8	B	0.45	0/2749	0.85	1/4284 (0.0%)
9	C	0.37	0/2129	0.68	0/2861
10	D	0.39	0/1613	0.71	2/2174 (0.1%)
11	E	0.36	0/1575	0.67	1/2129 (0.0%)
12	F	0.60	4/1429 (0.3%)	0.89	4/1921 (0.2%)
13	G	0.33	0/1351	0.71	0/1824
14	H	0.29	0/353	0.74	1/474 (0.2%)
15	J	0.38	0/1170	0.62	1/1584 (0.1%)
16	K	0.42	0/952	0.75	2/1278 (0.2%)
17	L	0.38	0/1087	0.69	1/1452 (0.1%)
18	M	0.38	0/1098	0.66	0/1481
19	N	0.35	0/925	0.64	0/1242
20	O	0.34	0/914	0.78	0/1228
21	P	0.36	0/922	0.66	0/1236
22	Q	0.37	0/1006	0.68	0/1349
23	R	0.43	0/766	0.66	0/1030
24	S	0.36	0/874	0.67	0/1186
25	T	0.36	0/751	0.73	1/1012 (0.1%)
26	U	0.32	0/705	0.67	0/941
27	V	0.32	0/1336	0.66	1/1820 (0.1%)
28	W	0.37	0/569	0.65	0/757
29	X	0.35	0/476	0.65	0/638
30	Y	0.35	0/564	0.79	0/756
31	Z	0.32	0/480	0.75	1/645 (0.2%)
32	a	0.33	1/36331 (0.0%)	0.79	2/56686 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	c	0.35	0/1678	0.72	1/2254 (0.0%)
34	d	0.30	0/1683	0.63	0/2269
35	e	0.31	0/1238	0.64	0/1673
36	f	0.34	0/767	0.69	1/1036 (0.1%)
37	g	0.48	2/1250 (0.2%)	0.74	3/1686 (0.2%)
38	h	0.31	0/1021	0.68	1/1379 (0.1%)
39	i	0.28	0/1010	0.66	0/1356
40	j	0.26	0/803	0.64	0/1086
41	k	0.32	0/890	0.67	1/1204 (0.1%)
42	l	0.33	0/970	0.69	0/1295
43	m	0.30	0/953	0.74	1/1274 (0.1%)
44	n	0.31	0/477	0.69	0/634
45	o	0.29	0/727	0.77	2/973 (0.2%)
46	p	0.30	0/759	0.72	0/1022
47	q	0.32	0/782	0.79	1/1045 (0.1%)
48	r	0.31	0/511	0.72	1/685 (0.1%)
49	s	0.25	0/690	0.53	0/928
50	t	0.29	0/654	0.76	3/867 (0.3%)
51	x	0.25	0/271	0.70	0/348
52	u	0.29	0/68	0.80	0/103
All	All	0.47	8/151323 (0.0%)	0.79	70/226914 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
11	E	0	1
12	F	0	1
22	Q	0	1
23	R	0	1
27	V	0	1
33	c	0	1
39	i	0	1
42	l	0	1
47	q	0	1
All	All	0	9

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	16	ARG	CZ-NH2	-14.82	1.13	1.33
37	g	103	TRP	CE3-CZ3	-8.72	1.23	1.38
37	g	103	TRP	CZ2-CH2	-8.01	1.22	1.37
12	F	16	ARG	CZ-NH1	-7.11	1.23	1.33
32	a	840	G	C6-N1	6.08	1.43	1.39
12	F	12	LYS	CB-CG	5.80	1.68	1.52
7	A	616	A	N9-C4	-5.51	1.34	1.37
12	F	12	LYS	CA-CB	5.01	1.65	1.53

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	16	ARG	NE-CZ-NH1	19.38	129.99	120.30
12	F	16	ARG	NH1-CZ-NH2	-9.11	109.37	119.40
45	o	31	LEU	CA-CB-CG	7.66	132.91	115.30
7	A	3130	C	N3-C2-O2	-7.64	116.55	121.90
7	A	616	A	C2-N3-C4	-7.61	106.80	110.60
7	A	946	C	N3-C2-O2	-7.48	116.67	121.90
7	A	600	G	O4'-C1'-N9	7.42	114.14	108.20
37	g	138	ARG	NE-CZ-NH2	-7.33	116.64	120.30
50	t	79	LEU	CA-CB-CG	7.22	131.90	115.30
33	c	46	LEU	CA-CB-CG	6.95	131.29	115.30
8	B	6	G	N1-C6-O6	-6.91	115.75	119.90
16	K	117	LEU	CA-CB-CG	6.90	131.17	115.30
7	A	3130	C	N1-C2-O2	6.86	123.02	118.90
7	A	1955	G	N3-C4-N9	-6.84	121.90	126.00
7	A	1955	G	N3-C2-N2	-6.79	115.14	119.90
7	A	976	U	C2-N1-C1'	6.78	125.84	117.70
7	A	739	C	N3-C2-O2	-6.67	117.23	121.90
7	A	2558	C	N1-C2-O2	6.61	122.86	118.90
7	A	2309	C	N3-C2-O2	-6.53	117.33	121.90
7	A	739	C	C2-N1-C1'	6.45	125.89	118.80
7	A	2217	C	N3-C2-O2	-6.36	117.45	121.90
7	A	3060	C	N3-C2-O2	-6.35	117.45	121.90
7	A	882	C	N3-C2-O2	-6.18	117.57	121.90
12	F	12	LYS	CB-CA-C	6.12	122.65	110.40
7	A	570	G	O4'-C1'-N9	6.10	113.08	108.20
15	J	36	LEU	CA-CB-CG	6.09	129.30	115.30
7	A	1953	G	N3-C4-N9	-5.97	122.42	126.00
17	L	97	LEU	CA-CB-CG	5.97	129.02	115.30
38	h	11	LEU	CA-CB-CG	5.95	129.00	115.30
7	A	2217	C	C2-N1-C1'	5.92	125.32	118.80
7	A	2309	C	C2-N1-C1'	5.82	125.20	118.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	946	C	C2-N1-C1'	5.82	125.20	118.80
7	A	2558	C	N3-C2-O2	-5.80	117.84	121.90
7	A	3060	C	C2-N1-C1'	5.76	125.13	118.80
7	A	2555	U	C2-N3-C4	-5.68	123.59	127.00
43	m	53	LEU	CA-CB-CG	5.65	128.29	115.30
50	t	83	LEU	CA-CB-CG	5.63	128.25	115.30
7	A	882	C	C2-N1-C1'	5.60	124.96	118.80
41	k	110	LEU	CA-CB-CG	5.59	128.16	115.30
7	A	946	C	C6-N1-C2	-5.57	118.07	120.30
7	A	1953	G	N3-C2-N2	-5.55	116.01	119.90
31	Z	26	LEU	CA-CB-CG	5.52	128.00	115.30
32	a	745	C	C2-N1-C1'	5.51	124.86	118.80
7	A	2309	C	C6-N1-C2	-5.45	118.12	120.30
7	A	2174	A	C2-N3-C4	-5.44	107.88	110.60
7	A	2970	G	N3-C4-N9	-5.44	122.74	126.00
25	T	95	LEU	CA-CB-CG	5.43	127.79	115.30
50	t	28	LEU	CA-CB-CG	5.41	127.73	115.30
7	A	3060	C	C6-N1-C2	-5.40	118.14	120.30
7	A	2867	C	C2-N1-C1'	-5.40	112.86	118.80
11	E	30	LEU	CA-CB-CG	5.38	127.67	115.30
12	F	124	LEU	CA-CB-CG	5.37	127.65	115.30
45	o	38	ASP	CB-CG-OD1	5.32	123.09	118.30
37	g	73	LEU	CA-CB-CG	5.27	127.41	115.30
7	A	2555	U	N1-C2-N3	5.26	118.06	114.90
7	A	1517	C	C2-N1-C1'	5.26	124.58	118.80
7	A	2013	U	C5-C6-N1	-5.26	120.07	122.70
27	V	56	LEU	CA-CB-CG	5.22	127.30	115.30
7	A	616	A	N1-C2-N3	5.20	131.90	129.30
48	r	34	ASP	CB-CG-OD1	5.17	122.95	118.30
47	q	69	MET	CA-CB-CG	5.16	122.08	113.30
36	f	76	ASP	CB-CG-OD1	5.16	122.94	118.30
37	g	131	LEU	CA-CB-CG	5.14	127.12	115.30
16	K	20	LEU	CA-CB-CG	5.12	127.07	115.30
7	A	2558	C	C2-N1-C1'	5.11	124.42	118.80
14	H	23	ASP	CB-CG-OD1	5.08	122.87	118.30
32	a	306	C	N1-C2-O2	5.07	121.94	118.90
10	D	101	LEU	CA-CB-CG	5.06	126.93	115.30
10	D	127	MET	CB-CG-SD	-5.04	97.27	112.40
7	A	2555	U	N3-C2-O2	-5.02	118.68	122.20

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
11	E	157	ARG	Peptide
12	F	12	LYS	Mainchain
22	Q	6	ARG	Sidechain
23	R	50	THR	Peptide
27	V	135	ALA	Peptide
33	c	104	GLU	Peptide
39	i	66	GLN	Peptide
42	l	113	ALA	Peptide
47	q	69	MET	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%)	52 (100%)	0	0	100	100
2	1	46/55 (84%)	45 (98%)	1 (2%)	0	100	100
3	2	42/47 (89%)	41 (98%)	1 (2%)	0	100	100
4	3	60/64 (94%)	60 (100%)	0	0	100	100
5	4	35/37 (95%)	35 (100%)	0	0	100	100
6	7	20/24 (83%)	19 (95%)	1 (5%)	0	100	100
9	C	270/280 (96%)	254 (94%)	16 (6%)	0	100	100
10	D	211/217 (97%)	196 (93%)	15 (7%)	0	100	100
11	E	205/223 (92%)	201 (98%)	4 (2%)	0	100	100
12	F	176/187 (94%)	158 (90%)	18 (10%)	0	100	100
13	G	172/179 (96%)	159 (92%)	13 (8%)	0	100	100
14	H	45/152 (30%)	39 (87%)	6 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	J	144/195 (74%)	141 (98%)	3 (2%)	0	100	100
16	K	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
17	L	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
18	M	132/138 (96%)	122 (92%)	10 (8%)	0	100	100
19	N	114/180 (63%)	112 (98%)	2 (2%)	0	100	100
20	O	117/122 (96%)	113 (97%)	4 (3%)	0	100	100
21	P	110/113 (97%)	106 (96%)	4 (4%)	0	100	100
22	Q	122/129 (95%)	120 (98%)	2 (2%)	0	100	100
23	R	98/104 (94%)	92 (94%)	6 (6%)	0	100	100
24	S	111/197 (56%)	110 (99%)	1 (1%)	0	100	100
25	T	93/100 (93%)	90 (97%)	3 (3%)	0	100	100
26	U	86/105 (82%)	79 (92%)	7 (8%)	0	100	100
27	V	175/215 (81%)	153 (87%)	21 (12%)	1 (1%)	22	23
28	W	75/86 (87%)	71 (95%)	4 (5%)	0	100	100
29	X	60/64 (94%)	57 (95%)	3 (5%)	0	100	100
30	Y	66/77 (86%)	64 (97%)	2 (3%)	0	100	100
31	Z	57/65 (88%)	55 (96%)	2 (4%)	0	100	100
33	c	205/274 (75%)	187 (91%)	18 (9%)	0	100	100
34	d	198/201 (98%)	179 (90%)	19 (10%)	0	100	100
35	e	167/220 (76%)	155 (93%)	12 (7%)	0	100	100
36	f	93/96 (97%)	91 (98%)	2 (2%)	0	100	100
37	g	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
38	h	129/132 (98%)	120 (93%)	9 (7%)	0	100	100
39	i	125/151 (83%)	110 (88%)	15 (12%)	0	100	100
40	j	97/101 (96%)	88 (91%)	9 (9%)	0	100	100
41	k	115/139 (83%)	111 (96%)	4 (4%)	0	100	100
42	l	120/124 (97%)	96 (80%)	23 (19%)	1 (1%)	16	16
43	m	114/124 (92%)	104 (91%)	10 (9%)	0	100	100
44	n	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
45	o	85/89 (96%)	77 (91%)	7 (8%)	1 (1%)	11	9
46	p	91/162 (56%)	82 (90%)	8 (9%)	1 (1%)	12	10

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
47	q	93/135 (69%)	79 (85%)	14 (15%)	0	100	100
48	r	62/84 (74%)	60 (97%)	2 (3%)	0	100	100
49	s	81/93 (87%)	73 (90%)	8 (10%)	0	100	100
50	t	83/86 (96%)	80 (96%)	3 (4%)	0	100	100
51	x	29/66 (44%)	26 (90%)	3 (10%)	0	100	100
All	All	5254/6174 (85%)	4918 (94%)	332 (6%)	4 (0%)	50	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
42	l	114	ARG
27	V	135	ALA
45	o	19	GLU
46	p	46	PRO

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%)	43 (98%)	1 (2%)	45	56
2	1	45/51 (88%)	42 (93%)	3 (7%)	13	14
3	2	38/40 (95%)	36 (95%)	2 (5%)	19	23
4	3	53/54 (98%)	49 (92%)	4 (8%)	11	11
5	4	35/35 (100%)	32 (91%)	3 (9%)	8	8
6	7	18/20 (90%)	16 (89%)	2 (11%)	5	4
9	C	212/219 (97%)	202 (95%)	10 (5%)	22	28
10	D	163/166 (98%)	152 (93%)	11 (7%)	13	14
11	E	159/172 (92%)	152 (96%)	7 (4%)	24	30
12	F	147/155 (95%)	129 (88%)	18 (12%)	4	3
13	G	143/147 (97%)	129 (90%)	14 (10%)	6	5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	H	36/121 (30%)	34 (94%)	2 (6%)	17	20
15	J	120/161 (74%)	114 (95%)	6 (5%)	20	25
16	K	101/101 (100%)	90 (89%)	11 (11%)	5	4
17	L	108/110 (98%)	95 (88%)	13 (12%)	4	3
18	M	110/114 (96%)	102 (93%)	8 (7%)	11	12
19	N	94/139 (68%)	87 (93%)	7 (7%)	11	11
20	O	91/93 (98%)	82 (90%)	9 (10%)	6	5
21	P	98/99 (99%)	90 (92%)	8 (8%)	9	9
22	Q	97/99 (98%)	94 (97%)	3 (3%)	35	44
23	R	81/83 (98%)	75 (93%)	6 (7%)	11	11
24	S	87/140 (62%)	82 (94%)	5 (6%)	17	20
25	T	81/83 (98%)	70 (86%)	11 (14%)	3	2
26	U	77/88 (88%)	68 (88%)	9 (12%)	4	3
27	V	142/164 (87%)	135 (95%)	7 (5%)	21	26
28	W	55/62 (89%)	52 (94%)	3 (6%)	18	21
29	X	51/52 (98%)	47 (92%)	4 (8%)	10	10
30	Y	60/66 (91%)	53 (88%)	7 (12%)	4	3
31	Z	51/55 (93%)	49 (96%)	2 (4%)	27	35
33	c	170/210 (81%)	152 (89%)	18 (11%)	5	4
34	d	176/177 (99%)	162 (92%)	14 (8%)	10	10
35	e	121/159 (76%)	113 (93%)	8 (7%)	14	15
36	f	84/85 (99%)	76 (90%)	8 (10%)	7	6
37	g	130/131 (99%)	118 (91%)	12 (9%)	7	6
38	h	107/108 (99%)	97 (91%)	10 (9%)	7	6
39	i	102/120 (85%)	91 (89%)	11 (11%)	5	4
40	j	89/90 (99%)	82 (92%)	7 (8%)	10	10
41	k	90/107 (84%)	85 (94%)	5 (6%)	17	20
42	l	104/105 (99%)	97 (93%)	7 (7%)	13	14
43	m	99/104 (95%)	92 (93%)	7 (7%)	12	12
44	n	46/47 (98%)	42 (91%)	4 (9%)	8	7
45	o	77/79 (98%)	70 (91%)	7 (9%)	7	6

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	p	77/125 (62%)	73 (95%)	4 (5%)	19	24
47	q	85/105 (81%)	77 (91%)	8 (9%)	7	6
48	r	54/72 (75%)	48 (89%)	6 (11%)	5	4
49	s	75/85 (88%)	69 (92%)	6 (8%)	10	10
50	t	64/65 (98%)	55 (86%)	9 (14%)	3	2
51	x	29/62 (47%)	28 (97%)	1 (3%)	32	41
All	All	4376/4972 (88%)	4028 (92%)	348 (8%)	12	10

All (348) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	14	ARG
2	1	15	CYS
2	1	36	LEU
2	1	37	GLU
3	2	5	LYS
3	2	31	ARG
4	3	31	HIS
4	3	38	SER
4	3	53	ASN
4	3	60	SER
5	4	22	ARG
5	4	27	CYS
5	4	35	ARG
6	7	17	ASN
6	7	23	ASN
9	C	69	ARG
9	C	75	VAL
9	C	103	ARG
9	C	145	VAL
9	C	164	GLN
9	C	192	THR
9	C	200	GLU
9	C	256	ARG
9	C	263	SER
9	C	266	LYS
10	D	4	LYS
10	D	19	GLU
10	D	38	ARG
10	D	44	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	D	76	ASN
10	D	78	ARG
10	D	99	GLN
10	D	128	LYS
10	D	165	ARG
10	D	192	LEU
10	D	195	LYS
11	E	12	ASP
11	E	19	LYS
11	E	42	GLN
11	E	74	GLN
11	E	81	ARG
11	E	117	LEU
11	E	168	ASP
12	F	14	ARG
12	F	16	ARG
12	F	21	ASP
12	F	24	ARG
12	F	26	GLN
12	F	53	ASP
12	F	55	LYS
12	F	56	LEU
12	F	71	LYS
12	F	80	SER
12	F	90	MET
12	F	122	ARG
12	F	134	ASN
12	F	159	MET
12	F	163	VAL
12	F	170	ASP
12	F	182	PHE
12	F	185	LYS
13	G	43	VAL
13	G	70	ARG
13	G	82	GLN
13	G	84	TYR
13	G	96	ARG
13	G	98	GLN
13	G	105	GLU
13	G	106	PHE
13	G	108	LEU
13	G	133	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	G	151	ARG
13	G	163	VAL
13	G	164	ARG
13	G	171	ARG
14	H	1	MET
14	H	41	ARG
15	J	41	LYS
15	J	60	ASP
15	J	61	LYS
15	J	108	MET
15	J	111	LYS
15	J	143	LYS
16	K	4	GLN
16	K	29	SER
16	K	45	ASP
16	K	54	ARG
16	K	56	ASP
16	K	64	ARG
16	K	69	ARG
16	K	70	ARG
16	K	92	ASP
16	K	107	ARG
16	K	116	SER
17	L	14	SER
17	L	15	LYS
17	L	16	THR
17	L	21	VAL
17	L	62	LYS
17	L	81	ASP
17	L	97	LEU
17	L	109	VAL
17	L	116	LYS
17	L	120	LYS
17	L	124	SER
17	L	131	SER
17	L	144	THR
18	M	5	ARG
18	M	16	ARG
18	M	25	THR
18	M	60	ARG
18	M	91	GLU
18	M	107	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	M	115	ARG
18	M	134	ARG
19	N	3	LYS
19	N	17	GLN
19	N	18	LYS
19	N	86	PHE
19	N	89	ASP
19	N	104	LYS
19	N	117	ARG
20	O	6	SER
20	O	10	ARG
20	O	13	ARG
20	O	29	GLU
20	O	43	HIS
20	O	44	VAL
20	O	45	GLN
20	O	94	THR
20	O	113	ASP
21	P	1	MET
21	P	3	ARG
21	P	11	SER
21	P	14	ASP
21	P	43	LYS
21	P	62	LYS
21	P	63	GLU
21	P	100	ARG
22	Q	19	LYS
22	Q	25	ARG
22	Q	121	VAL
23	R	15	TYR
23	R	28	LEU
23	R	37	SER
23	R	48	THR
23	R	56	LEU
23	R	94	GLN
24	S	38	SER
24	S	83	THR
24	S	87	ASP
24	S	93	LYS
24	S	119	SER
25	T	6	ASP
25	T	20	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	T	30	THR
25	T	36	ASP
25	T	53	LYS
25	T	56	SER
25	T	58	ASN
25	T	70	ARG
25	T	76	ARG
25	T	77	LYS
25	T	81	ARG
26	U	8	THR
26	U	16	ASP
26	U	22	LYS
26	U	40	ARG
26	U	42	LYS
26	U	75	ASP
26	U	77	ASP
26	U	100	ARG
26	U	103	LYS
27	V	10	ARG
27	V	50	HIS
27	V	72	LYS
27	V	74	GLN
27	V	94	ASP
27	V	99	ARG
27	V	134	GLU
28	W	36	ILE
28	W	38	VAL
28	W	39	ARG
29	X	24	ARG
29	X	27	ARG
29	X	41	ARG
29	X	50	ASN
30	Y	6	SER
30	Y	11	ARG
30	Y	21	ARG
30	Y	23	ARG
30	Y	41	LEU
30	Y	45	ARG
30	Y	47	LEU
31	Z	5	LYS
31	Z	51	ARG
33	c	10	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
33	c	21	ARG
33	c	33	LYS
33	c	34	GLU
33	c	60	ARG
33	c	92	LYS
33	c	122	GLN
33	c	135	LYS
33	c	147	LYS
33	c	153	CYS
33	c	163	SER
33	c	164	ARG
33	c	166	GLU
33	c	172	ARG
33	c	176	HIS
33	c	190	LYS
33	c	195	ARG
33	c	201	TRP
34	d	10	ARG
34	d	38	ARG
34	d	40	ARG
34	d	48	LEU
34	d	52	GLU
34	d	73	GLU
34	d	98	TYR
34	d	108	MET
34	d	118	PHE
34	d	126	ASN
34	d	130	TYR
34	d	136	ASP
34	d	143	LYS
34	d	198	TYR
35	e	42	TYR
35	e	85	LYS
35	e	97	GLU
35	e	103	PHE
35	e	176	LYS
35	e	200	MET
35	e	202	LYS
35	e	205	ARG
36	f	14	LEU
36	f	26	PHE
36	f	33	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
36	f	36	LYS
36	f	77	ARG
36	f	79	LEU
36	f	80	SER
36	f	91	MET
37	g	21	GLN
37	g	29	LYS
37	g	41	ARG
37	g	49	GLN
37	g	51	ARG
37	g	95	ARG
37	g	114	LYS
37	g	122	ASN
37	g	138	ARG
37	g	143	LYS
37	g	144	MET
37	g	148	ASN
38	h	5	ASP
38	h	27	LEU
38	h	50	ARG
38	h	62	ILE
38	h	65	LYS
38	h	77	LEU
38	h	120	ARG
38	h	121	GLN
38	h	127	VAL
38	h	132	TRP
39	i	41	ARG
39	i	49	PHE
39	i	59	TYR
39	i	63	LYS
39	i	65	HIS
39	i	67	GLN
39	i	82	PHE
39	i	106	ARG
39	i	116	ARG
39	i	127	ARG
39	i	133	GLU
40	j	11	LYS
40	j	13	TYR
40	j	14	ASP
40	j	15	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
40	j	63	GLU
40	j	75	ASP
40	j	82	LYS
41	k	50	ASN
41	k	63	LYS
41	k	91	LYS
41	k	121	SER
41	k	124	THR
42	l	10	LYS
42	l	18	LYS
42	l	60	GLN
42	l	83	ARG
42	l	103	ASP
42	l	105	GLN
42	l	108	LYS
43	m	14	ARG
43	m	75	GLN
43	m	80	ARG
43	m	94	ARG
43	m	96	MET
43	m	110	ARG
43	m	115	ARG
44	n	15	ARG
44	n	26	LYS
44	n	36	LYS
44	n	57	GLN
45	o	26	GLU
45	o	31	LEU
45	o	38	ASP
45	o	47	LYS
45	o	65	ARG
45	o	72	GLN
45	o	79	ARG
46	p	6	LYS
46	p	9	ARG
46	p	55	ARG
46	p	79	ASP
47	q	56	ARG
47	q	68	LYS
47	q	69	MET
47	q	91	ARG
47	q	109	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
47	q	113	LEU
47	q	117	ARG
47	q	125	TRP
48	r	19	LYS
48	r	31	ASP
48	r	32	TYR
48	r	52	ARG
48	r	63	ASP
48	r	79	PHE
49	s	3	ARG
49	s	10	PHE
49	s	14	HIS
49	s	44	PHE
49	s	56	LYS
49	s	66	MET
50	t	25	LYS
50	t	28	LEU
50	t	29	ARG
50	t	35	PHE
50	t	50	LEU
50	t	55	ASN
50	t	56	ARG
50	t	57	LYS
50	t	68	HIS
51	x	6	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	1	20	HIS
2	1	22	ASN
2	1	44	ASN
10	D	34	ASN
11	E	190	ASN
21	P	28	HIS
21	P	82	HIS
23	R	14	GLN
34	d	49	GLN
34	d	115	HIS
36	f	55	HIS
38	h	18	ASN
39	i	65	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	i	66	GLN
40	j	56	HIS
42	l	60	GLN
47	q	83	HIS
47	q	99	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1515/1537 (98%)	254 (16%)	0
52	u	2/3 (66%)	1 (50%)	0
7	A	2899/3138 (92%)	377 (13%)	4 (0%)
8	B	114/115 (99%)	19 (16%)	0
All	All	4530/4793 (94%)	651 (14%)	4 (0%)

All (651) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	8	U
7	A	9	G
7	A	10	U
7	A	11	C
7	A	43	G
7	A	51	G
7	A	63	A
7	A	71	A
7	A	74	U
7	A	75	G
7	A	90	C
7	A	92	A
7	A	94	C
7	A	118	A
7	A	119	A
7	A	120	U
7	A	143	G
7	A	165	A
7	A	167	A
7	A	176	G
7	A	183	A
7	A	198	A
7	A	201	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	217	G
7	A	218	A
7	A	224	A
7	A	226	A
7	A	230	U
7	A	231	U
7	A	232	G
7	A	249	G
7	A	250	G
7	A	277	G
7	A	278	C
7	A	287	G
7	A	289	A
7	A	293	G
7	A	297	A
7	A	303	U
7	A	314	G
7	A	315	G
7	A	316	U
7	A	322	G
7	A	323	A
7	A	328	A
7	A	331	U
7	A	332	C
7	A	339	C
7	A	358	U
7	A	364	A
7	A	371	U
7	A	372	G
7	A	394	U
7	A	399	U
7	A	401	C
7	A	413	A
7	A	414	G
7	A	428	A
7	A	429	A
7	A	446	A
7	A	447	G
7	A	454	U
7	A	472	C
7	A	473	C
7	A	475	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	478	G
7	A	480	A
7	A	495	G
7	A	500	G
7	A	544	U
7	A	545	U
7	A	570	G
7	A	592	G
7	A	593	A
7	A	595	U
7	A	596	A
7	A	597	C
7	A	616	A
7	A	618	U
7	A	619	C
7	A	620	C
7	A	621	G
7	A	665	G
7	A	674	A
7	A	675	G
7	A	676	A
7	A	677	A
7	A	689	G
7	A	693	G
7	A	694	G
7	A	706	A
7	A	718	G
7	A	719	U
7	A	738	G
7	A	741	A
7	A	749	U
7	A	757	C
7	A	758	C
7	A	759	C
7	A	760	A
7	A	764	G
7	A	765	C
7	A	766	G
7	A	769	U
7	A	770	A
7	A	771	C
7	A	772	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	773	C
7	A	777	U
7	A	778	G
7	A	779	U
7	A	780	G
7	A	781	A
7	A	782	A
7	A	783	U
7	A	815	U
7	A	843	U
7	A	846	G
7	A	852	G
7	A	855	G
7	A	859	C
7	A	876	U
7	A	886	G
7	A	893	A
7	A	904	G
7	A	905	G
7	A	911	A
7	A	913	G
7	A	914	G
7	A	934	G
7	A	941	C
7	A	956	U
7	A	988	G
7	A	1025	A
7	A	1026	C
7	A	1028	G
7	A	1036	C
7	A	1039	A
7	A	1043	C
7	A	1044	C
7	A	1059	A
7	A	1061	A
7	A	1074	G
7	A	1087	A
7	A	1089	G
7	A	1096	A
7	A	1103	A
7	A	1112	A
7	A	1118	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	1125	G
7	A	1142	G
7	A	1155	G
7	A	1162	U
7	A	1167	A
7	A	1187	G
7	A	1189	U
7	A	1195	U
7	A	1199	A
7	A	1200	G
7	A	1202	A
7	A	1205	C
7	A	1206	A
7	A	1207	C
7	A	1211	U
7	A	1212	G
7	A	1216	G
7	A	1217	A
7	A	1218	G
7	A	1227	A
7	A	1233	C
7	A	1240	A
7	A	1241	G
7	A	1243	G
7	A	1244	A
7	A	1249	G
7	A	1257	A
7	A	1258	A
7	A	1261	U
7	A	1262	A
7	A	1264	C
7	A	1271	C
7	A	1273	A
7	A	1301	A
7	A	1302	C
7	A	1304	U
7	A	1306	G
7	A	1307	U
7	A	1308	G
7	A	1309	G
7	A	1313	G
7	A	1342	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	1384	A
7	A	1386	U
7	A	1387	G
7	A	1402	G
7	A	1403	A
7	A	1406	A
7	A	1425	C
7	A	1431	A
7	A	1432	A
7	A	1452	C
7	A	1456	C
7	A	1483	U
7	A	1491	G
7	A	1496	A
7	A	1509	A
7	A	1510	U
7	A	1515	A
7	A	1534	A
7	A	1656	G
7	A	1657	A
7	A	1665	A
7	A	1666	C
7	A	1675	G
7	A	1689	C
7	A	1690	A
7	A	1692	U
7	A	1693	G
7	A	1697	A
7	A	1698	C
7	A	1699	A
7	A	1714	U
7	A	1720	G
7	A	1722	G
7	A	1727	A
7	A	1730	C
7	A	1734	U
7	A	1746	U
7	A	1747	A
7	A	1754	A
7	A	1755	G
7	A	1770	C
7	A	1773	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	1774	U
7	A	1775	G
7	A	1777	G
7	A	1802	C
7	A	1803	A
7	A	1806	A
7	A	1821	G
7	A	1830	C
7	A	1832	G
7	A	1833	C
7	A	1842	C
7	A	1843	A
7	A	1845	A
7	A	1869	C
7	A	1881	U
7	A	1883	C
7	A	1888	U
7	A	1889	A
7	A	1909	G
7	A	1910	C
7	A	1949	U
7	A	1950	A
7	A	1962	C
7	A	1964	U
7	A	1992	A
7	A	1998	U
7	A	2007	A
7	A	2010	G
7	A	2015	C
7	A	2020	A
7	A	2034	C
7	A	2035	G
7	A	2041	G
7	A	2043	A
7	A	2050	U
7	A	2063	A
7	A	2092	G
7	A	2105	G
7	A	2107	A
7	A	2108	A
7	A	2109	G
7	A	2114	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	2144	G
7	A	2150	A
7	A	2152	C
7	A	2167	G
7	A	2168	G
7	A	2175	A
7	A	2176	A
7	A	2193	U
7	A	2205	C
7	A	2208	A
7	A	2209	U
7	A	2210	G
7	A	2229	U
7	A	2230	G
7	A	2231	U
7	A	2261	A
7	A	2269	A
7	A	2270	G
7	A	2281	C
7	A	2293	C
7	A	2294	G
7	A	2296	A
7	A	2297	A
7	A	2298	A
7	A	2299	G
7	A	2330	G
7	A	2333	G
7	A	2435	A
7	A	2449	A
7	A	2463	A
7	A	2476	G
7	A	2477	G
7	A	2489	OMG
7	A	2517	G
7	A	2521	C
7	A	2525	A
7	A	2543	A
7	A	2546	G
7	A	2547	C
7	A	2558	C
7	A	2563	G
7	A	2573	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	2585	C
7	A	2588	C
7	A	2615	A
7	A	2621	G
7	A	2623	A
7	A	2641	C
7	A	2644	A
7	A	2661	U
7	A	2663	A
7	A	2667	G
7	A	2668	A
7	A	2674	G
7	A	2679	C
7	A	2686	A
7	A	2714	A
7	A	2716	A
7	A	2736	C
7	A	2740	G
7	A	2743	G
7	A	2751	G
7	A	2756	A
7	A	2767	G
7	A	2773	G
7	A	2804	A
7	A	2805	G
7	A	2811	C
7	A	2840	A
7	A	2851	U
7	A	2868	A
7	A	2884	C
7	A	2901	G
7	A	2911	G
7	A	2952	G
7	A	2962	C
7	A	2964	C
7	A	2971	U
7	A	2982	G
7	A	2986	A
7	A	2995	A
7	A	2996	A
7	A	3003	A
7	A	3016	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	A	3018	C
7	A	3037	G
7	A	3038	U
7	A	3040	G
7	A	3041	G
7	A	3043	U
7	A	3053	C
7	A	3056	A
7	A	3058	A
7	A	3070	A
7	A	3071	U
7	A	3107	A
7	A	3114	G
7	A	3118	A
7	A	3119	C
7	A	3120	C
7	A	3128	A
7	A	3129	A
8	B	2	U
8	B	3	A
8	B	4	C
8	B	6	G
8	B	7	C
8	B	33	G
8	B	36	C
8	B	41	C
8	B	55	U
8	B	56	A
8	B	65	A
8	B	68	G
8	B	88	G
8	B	101	G
8	B	105	A
8	B	109	C
8	B	110	C
8	B	113	A
8	B	115	A
32	a	10	G
32	a	12	G
32	a	21	C
32	a	25	G
32	a	35	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	42	G
32	a	51	U
32	a	54	A
32	a	74	A
32	a	80	U
32	a	86	G
32	a	89	A
32	a	90	U
32	a	91	A
32	a	93	U
32	a	99	G
32	a	111	A
32	a	115	A
32	a	116	C
32	a	125	G
32	a	127	U
32	a	137	A
32	a	140	U
32	a	142	G
32	a	144	G
32	a	146	U
32	a	164	U
32	a	169	U
32	a	174	G
32	a	178	G
32	a	179	G
32	a	185	G
32	a	187	G
32	a	189	U
32	a	191	C
32	a	192	A
32	a	194	G
32	a	198	U
32	a	204	G
32	a	206	A
32	a	213	U
32	a	214	U
32	a	215	U
32	a	216	A
32	a	217	G
32	a	219	G
32	a	224	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	244	C
32	a	246	G
32	a	247	C
32	a	250	G
32	a	255	U
32	a	265	G
32	a	266	C
32	a	279	C
32	a	288	G
32	a	308	G
32	a	320	A
32	a	326	A
32	a	328	A
32	a	329	C
32	a	339	U
32	a	343	A
32	a	346	G
32	a	350	G
32	a	351	C
32	a	355	A
32	a	362	A
32	a	366	U
32	a	371	C
32	a	391	C
32	a	396	A
32	a	397	C
32	a	405	G
32	a	411	U
32	a	412	G
32	a	420	U
32	a	421	C
32	a	422	G
32	a	427	G
32	a	428	U
32	a	449	G
32	a	451	A
32	a	452	G
32	a	453	G
32	a	456	C
32	a	459	G
32	a	460	U
32	a	462	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	465	U
32	a	467	G
32	a	473	A
32	a	476	G
32	a	485	G
32	a	487	A
32	a	488	G
32	a	493	A
32	a	497	G
32	a	500	A
32	a	502	C
32	a	509	C
32	a	512	G
32	a	516	C
32	a	517	C
32	a	518	G7M
32	a	523	A
32	a	524	A
32	a	536	C
32	a	538	A
32	a	550	A
32	a	553	U
32	a	558	G
32	a	563	A
32	a	564	A
32	a	567	A
32	a	568	G
32	a	587	C
32	a	598	A
32	a	606	C
32	a	610	U
32	a	616	G
32	a	623	U
32	a	624	G
32	a	630	G
32	a	640	G
32	a	644	A
32	a	656	G
32	a	676	G
32	a	678	A
32	a	682	G
32	a	686	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	694	G
32	a	709	A
32	a	712	G
32	a	714	U
32	a	740	A
32	a	746	G
32	a	768	A
32	a	784	U
32	a	785	A
32	a	790	G
32	a	803	G
32	a	806	A
32	a	808	C
32	a	812	G
32	a	820	G
32	a	830	U
32	a	833	U
32	a	834	U
32	a	835	C
32	a	836	C
32	a	837	U
32	a	838	U
32	a	839	G
32	a	848	G
32	a	883	G
32	a	895	G
32	a	900	A
32	a	907	A
32	a	910	G
32	a	911	A
32	a	915	G
32	a	919	G
32	a	927	C
32	a	928	A
32	a	951	A
32	a	953	U
32	a	959	2MG
32	a	962	A
32	a	964	G
32	a	968	A
32	a	969	G
32	a	970	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	971	A
32	a	985	U
32	a	986	G
32	a	987	A
32	a	994	C
32	a	997	G
32	a	1016	G
32	a	1019	C
32	a	1021	C
32	a	1022	U
32	a	1023	U
32	a	1036	C
32	a	1044	G
32	a	1047	U
32	a	1056	U
32	a	1061	U
32	a	1085	G
32	a	1086	U
32	a	1090	G
32	a	1092	A
32	a	1099	G
32	a	1115	G
32	a	1128	A
32	a	1129	A
32	a	1131	G
32	a	1132	G
32	a	1138	A
32	a	1141	C
32	a	1143	U
32	a	1146	G
32	a	1149	A
32	a	1151	U
32	a	1160	C
32	a	1163	C
32	a	1174	G
32	a	1176	G
32	a	1188	A
32	a	1189	A
32	a	1192	C
32	a	1205	A
32	a	1206	U
32	a	1228	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	a	1230	A
32	a	1249	U
32	a	1250	G
32	a	1252	G
32	a	1270	G
32	a	1272	A
32	a	1278	A
32	a	1279	A
32	a	1282	G
32	a	1292	G
32	a	1297	G
32	a	1304	G
32	a	1315	G
32	a	1329	G
32	a	1338	A
32	a	1345	G
32	a	1355	A
32	a	1356	A
32	a	1357	C
32	a	1363	G
32	a	1368	A
32	a	1369	U
32	a	1370	A
32	a	1387	A
32	a	1390	C
32	a	1391	A
32	a	1399	U
32	a	1427	A
32	a	1435	G
32	a	1439	A
32	a	1480	G
32	a	1485	A
32	a	1486	A
32	a	1490	G
32	a	1492	A
32	a	1496	A
32	a	1510	G
32	a	1522	G
32	a	1523	G
52	u	77	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	759	C
7	A	763	C
7	A	913	G
7	A	2994	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
32	G7M	a	518	32	20,26,27	2.80	8 (40%)	17,39,42	1.06	1 (5%)
7	5MU	A	2177	7	19,22,23	7.21	8 (42%)	28,32,35	3.60	10 (35%)
32	4OC	a	1395	32	20,23,24	3.09	8 (40%)	26,32,35	0.97	1 (3%)
7	OMG	A	2489	52,7	18,26,27	2.49	8 (44%)	19,38,41	1.45	4 (21%)
32	MA6	a	1511	32	18,26,27	1.10	2 (11%)	19,38,41	4.86	3 (15%)
32	5MC	a	960	32	18,22,23	3.71	8 (44%)	26,32,35	1.04	2 (7%)
7	OMG	A	2791	7	18,26,27	2.48	8 (44%)	19,38,41	1.45	4 (21%)
32	MA6	a	1512	32	18,26,27	1.04	2 (11%)	19,38,41	4.92	3 (15%)
32	2MG	a	959	32	18,26,27	2.47	7 (38%)	16,38,41	1.41	3 (18%)
32	UR3	a	1491	32	19,22,23	2.73	7 (36%)	26,32,35	1.29	1 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	G7M	a	518	32	-	0/3/25/26	0/3/3/3
7	5MU	A	2177	7	-	0/7/25/26	0/2/2/2
32	4OC	a	1395	32	-	0/9/29/30	0/2/2/2
7	OMG	A	2489	52,7	-	3/5/27/28	0/3/3/3
32	MA6	a	1511	32	-	2/7/29/30	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	5MC	a	960	32	-	0/7/25/26	0/2/2/2
7	OMG	A	2791	7	-	1/5/27/28	0/3/3/3
32	MA6	a	1512	32	-	2/7/29/30	0/3/3/3
32	2MG	a	959	32	-	2/5/27/28	0/3/3/3
32	UR3	a	1491	32	-	0/7/25/26	0/2/2/2

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	2177	5MU	C4-C5	20.94	1.79	1.44
7	A	2177	5MU	C6-N1	16.24	1.65	1.38
7	A	2177	5MU	C4-N3	-11.07	1.18	1.38
7	A	2177	5MU	C6-C5	-10.62	1.17	1.34
32	a	960	5MC	C6-C5	9.35	1.50	1.34
32	a	1491	UR3	C2-N1	6.95	1.48	1.38
32	a	1395	4OC	C4-N3	6.79	1.44	1.32
32	a	960	5MC	C2-N3	6.59	1.49	1.36
32	a	518	G7M	C2-N2	6.55	1.49	1.34
32	a	960	5MC	C4-N3	6.26	1.44	1.34
32	a	1395	4OC	C6-C5	6.23	1.49	1.35
32	a	1491	UR3	C6-C5	6.19	1.49	1.35
32	a	1395	4OC	C2-N3	5.85	1.48	1.36
32	a	518	G7M	C2-N3	5.82	1.47	1.33
32	a	959	2MG	C2-N2	5.62	1.45	1.33
7	A	2489	OMG	C2-N3	5.32	1.46	1.33
7	A	2791	OMG	C2-N3	5.25	1.46	1.33
32	a	518	G7M	C4-N3	5.21	1.50	1.37
32	a	960	5MC	C2-N1	5.16	1.51	1.40
32	a	1491	UR3	C2-N3	4.97	1.48	1.39
7	A	2177	5MU	C2-N3	4.87	1.46	1.38
7	A	2489	OMG	C4-N3	4.79	1.49	1.37
7	A	2791	OMG	C4-N3	4.64	1.48	1.37
7	A	2791	OMG	C2-N2	4.63	1.45	1.34
32	a	960	5MC	C6-N1	4.62	1.45	1.38
32	a	959	2MG	C2-N1	4.59	1.44	1.36
7	A	2489	OMG	C2-N2	4.54	1.45	1.34
32	a	959	2MG	C4-N3	4.52	1.48	1.37
32	a	1395	4OC	C4-N4	4.50	1.45	1.35
32	a	518	G7M	C6-N1	4.45	1.44	1.37
32	a	960	5MC	C4-N4	4.40	1.45	1.34
32	a	1395	4OC	C5-C4	3.97	1.49	1.40
32	a	1395	4OC	C2-N1	3.90	1.48	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	959	2MG	C6-N1	3.53	1.43	1.37
32	a	518	G7M	C5-C6	3.47	1.54	1.45
7	A	2791	OMG	C6-N1	3.34	1.42	1.37
7	A	2489	OMG	C6-N1	3.22	1.42	1.37
32	a	1395	4OC	O2-C2	-3.12	1.17	1.23
32	a	1395	4OC	C6-N1	3.09	1.45	1.38
32	a	518	G7M	C2-N1	3.05	1.45	1.37
32	a	1491	UR3	C6-N1	2.98	1.45	1.38
7	A	2177	5MU	O2-C2	-2.92	1.17	1.23
32	a	1511	MA6	C5-C4	-2.84	1.33	1.40
7	A	2177	5MU	C2-N1	2.78	1.42	1.38
7	A	2791	OMG	C5-C6	2.78	1.53	1.47
7	A	2489	OMG	C5-C6	2.78	1.53	1.47
32	a	1512	MA6	C5-C4	-2.77	1.33	1.40
7	A	2177	5MU	O4-C4	-2.75	1.18	1.23
7	A	2791	OMG	C5-C4	-2.71	1.36	1.43
7	A	2489	OMG	C5-C4	-2.68	1.36	1.43
32	a	959	2MG	O6-C6	-2.65	1.17	1.23
7	A	2791	OMG	C2-N1	2.52	1.43	1.37
7	A	2489	OMG	C2-N1	2.52	1.43	1.37
32	a	959	2MG	C5-C6	2.43	1.52	1.47
7	A	2489	OMG	O6-C6	-2.40	1.18	1.23
7	A	2791	OMG	O6-C6	-2.38	1.18	1.23
32	a	1511	MA6	C2-N3	2.30	1.35	1.32
32	a	1491	UR3	O4-C4	-2.29	1.18	1.23
32	a	960	5MC	CM5-C5	2.25	1.56	1.50
32	a	1491	UR3	C5-C4	2.25	1.49	1.43
32	a	959	2MG	C5-C4	-2.23	1.37	1.43
32	a	1512	MA6	C2-N3	2.22	1.35	1.32
32	a	1491	UR3	O2-C2	-2.21	1.18	1.22
32	a	518	G7M	O6-C6	-2.09	1.19	1.23
32	a	518	G7M	C8-N7	2.06	1.36	1.33
32	a	960	5MC	O2-C2	-2.02	1.20	1.23

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	1512	MA6	N1-C6-N6	-18.40	97.69	117.06
32	a	1511	MA6	N1-C6-N6	-17.63	98.51	117.06
7	A	2177	5MU	C5-C4-N3	10.78	124.52	115.31
32	a	1511	MA6	C1'-N9-C4	-10.21	108.71	126.64
7	A	2177	5MU	C5-C6-N1	-9.33	113.74	123.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	a	1512	MA6	C1'-N9-C4	-9.27	110.36	126.64
7	A	2177	5MU	C4-N3-C2	-7.57	117.55	127.35
32	a	1512	MA6	N3-C2-N1	-5.44	120.17	128.68
32	a	1511	MA6	N3-C2-N1	-5.33	120.35	128.68
7	A	2177	5MU	N3-C2-N1	4.96	121.47	114.89
32	a	1491	UR3	C4-N3-C2	-4.88	119.97	124.56
7	A	2177	5MU	C5M-C5-C6	-4.34	117.05	122.85
7	A	2177	5MU	O4-C4-C5	-3.82	120.47	124.90
32	a	960	5MC	C5-C6-N1	-3.75	119.48	123.34
7	A	2177	5MU	C6-C5-C4	3.60	121.04	118.03
7	A	2489	OMG	C5-C6-N1	3.43	120.00	113.95
32	a	959	2MG	C5-C6-N1	3.40	119.96	113.95
7	A	2791	OMG	C5-C6-N1	3.37	119.90	113.95
7	A	2489	OMG	C2-N1-C6	-3.17	119.26	125.10
7	A	2791	OMG	C2-N1-C6	-3.00	119.58	125.10
7	A	2177	5MU	O2-C2-N1	-3.00	118.80	122.79
32	a	518	G7M	C2-N1-C6	-2.87	119.81	125.10
7	A	2177	5MU	C5M-C5-C4	2.85	121.91	118.77
32	a	959	2MG	C8-N7-C5	2.78	108.28	102.99
7	A	2177	5MU	O4-C4-N3	-2.66	115.01	120.12
32	a	1395	4OC	C6-C5-C4	2.56	120.10	116.96
7	A	2489	OMG	C8-N7-C5	2.53	107.81	102.99
7	A	2791	OMG	C8-N7-C5	2.51	107.78	102.99
7	A	2489	OMG	O6-C6-C5	-2.29	119.90	124.37
7	A	2791	OMG	O6-C6-C5	-2.19	120.10	124.37
32	a	959	2MG	O6-C6-C5	-2.17	120.14	124.37
32	a	960	5MC	CM5-C5-C6	-2.12	120.01	122.85

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	2489	OMG	O4'-C4'-C5'-O5'
7	A	2489	OMG	C1'-C2'-O2'-CM2
32	a	959	2MG	O4'-C4'-C5'-O5'
32	a	959	2MG	C3'-C4'-C5'-O5'
7	A	2489	OMG	C3'-C4'-C5'-O5'
32	a	1512	MA6	O4'-C4'-C5'-O5'
32	a	1511	MA6	O4'-C4'-C5'-O5'
32	a	1511	MA6	C3'-C4'-C5'-O5'
7	A	2791	OMG	C3'-C2'-O2'-CM2
32	a	1512	MA6	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 447 ligands modelled in this entry, 446 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
55	A1L32	A	3501	-	85,87,87	2.28	15 (17%)	122,130,130	1.53	22 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	A1L32	A	3501	-	-	23/91/146/146	0/7/7/7

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3501	A1L32	C45-C44	9.20	1.55	1.38
55	A	3501	A1L32	C54-C46	7.58	1.53	1.38
55	A	3501	A1L32	C55-C43	7.23	1.54	1.38
55	A	3501	A1L32	O2-C13	6.11	1.48	1.34
55	A	3501	A1L32	N6-N3	-5.69	1.28	1.37
55	A	3501	A1L32	C48-N5	5.23	1.48	1.36
55	A	3501	A1L32	O1-C1	-4.38	1.36	1.44
55	A	3501	A1L32	C6-C7	4.17	1.61	1.54
55	A	3501	A1L32	C42-C43	3.56	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	A	3501	A1L32	N5-N6	3.43	1.40	1.34
55	A	3501	A1L32	C49-C48	3.02	1.53	1.48
55	A	3501	A1L32	C44-C43	-2.96	1.32	1.38
55	A	3501	A1L32	C45-C46	-2.79	1.32	1.38
55	A	3501	A1L32	C55-C54	-2.41	1.34	1.38
55	A	3501	A1L32	O11-C7	-2.22	1.40	1.44

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	A	3501	A1L32	C49-C48-N5	4.18	127.64	120.96
55	A	3501	A1L32	O2-C13-C12	3.87	120.06	111.56
55	A	3501	A1L32	C1-C2-C3	-3.84	107.01	115.80
55	A	3501	A1L32	O12-C2-C1	3.72	110.98	106.39
55	A	3501	A1L32	C7-C9-C10	-3.64	108.89	114.05
55	A	3501	A1L32	C15-C14-C1	-3.56	108.46	115.20
55	A	3501	A1L32	C38-O14-C56	3.10	119.78	113.69
55	A	3501	A1L32	O6-C21-C20	3.02	108.29	103.81
55	A	3501	A1L32	C6-C5-C4	-3.02	107.76	112.06
55	A	3501	A1L32	C21-C20-C19	-2.72	106.96	111.14
55	A	3501	A1L32	C42-O13-C41	2.62	119.01	114.22
55	A	3501	A1L32	C46-N3-N6	2.61	122.48	117.19
55	A	3501	A1L32	C37-C3-C2	-2.49	110.60	113.68
55	A	3501	A1L32	O5-C19-C25	2.37	111.82	106.70
55	A	3501	A1L32	C4-N1-C3	-2.33	108.09	112.05
55	A	3501	A1L32	O16-C40-C39	-2.31	105.00	110.35
55	A	3501	A1L32	C5-C4-N1	-2.29	109.27	113.95
55	A	3501	A1L32	O13-C41-C40	2.27	114.57	109.83
55	A	3501	A1L32	O8-C9-C10	-2.16	108.31	111.54
55	A	3501	A1L32	C7-C6-C5	-2.11	111.21	117.06
55	A	3501	A1L32	C58-C1-C14	-2.08	108.38	111.31
55	A	3501	A1L32	C36-N1-C3	-2.02	109.91	113.59

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	A	3501	A1L32	C2-C3-N1-C4
55	A	3501	A1L32	C37-C3-N1-C4
55	A	3501	A1L32	C2-C3-N1-C36
55	A	3501	A1L32	C37-C3-N1-C36
55	A	3501	A1L32	C54-C46-N3-C47

Continued on next page...

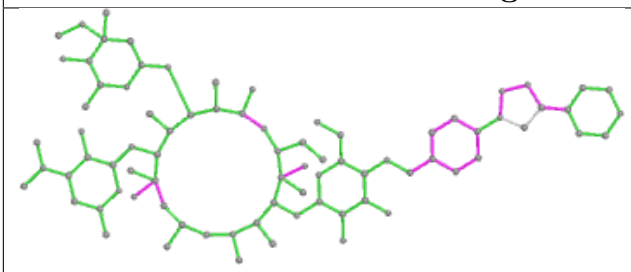
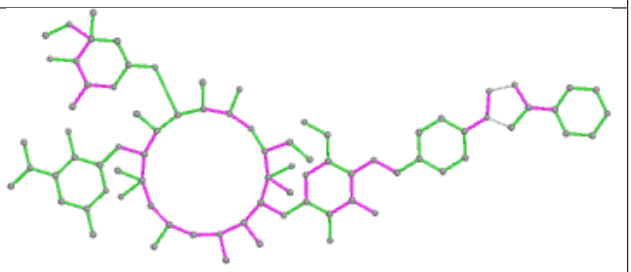
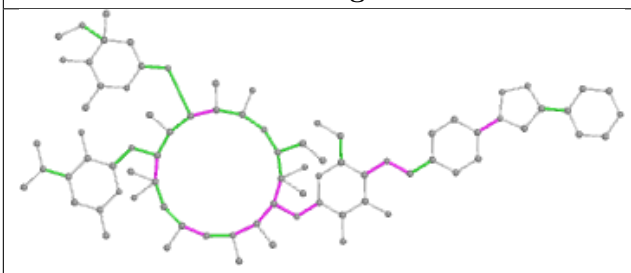
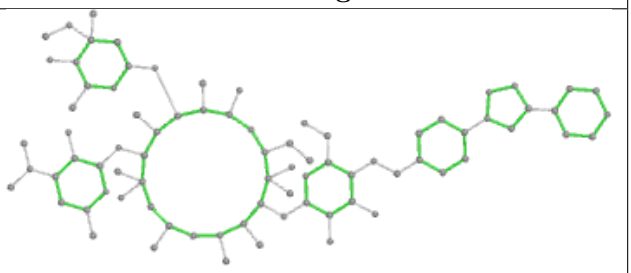
Continued from previous page...

Mol	Chain	Res	Type	Atoms
55	A	3501	A1L32	N1-C4-C5-C6
55	A	3501	A1L32	N1-C4-C5-C35
55	A	3501	A1L32	C58-C1-C2-O12
55	A	3501	A1L32	O1-C1-C2-O12
55	A	3501	A1L32	C40-C41-O13-C42
55	A	3501	A1L32	O14-C38-O12-C2
55	A	3501	A1L32	C39-C38-O12-C2
55	A	3501	A1L32	C14-C1-C2-O12
55	A	3501	A1L32	C58-C1-C2-C3
55	A	3501	A1L32	C3-C2-O12-C38
55	A	3501	A1L32	C1-C2-C3-N1
55	A	3501	A1L32	O12-C2-C3-N1
55	A	3501	A1L32	C1-C2-O12-C38
55	A	3501	A1L32	C45-C46-N3-C47
55	A	3501	A1L32	C8-C7-C9-C10
55	A	3501	A1L32	C1-C2-C3-C37
55	A	3501	A1L32	C10-C11-C12-C17
55	A	3501	A1L32	C43-C42-O13-C41

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 A1L32 A 3501	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

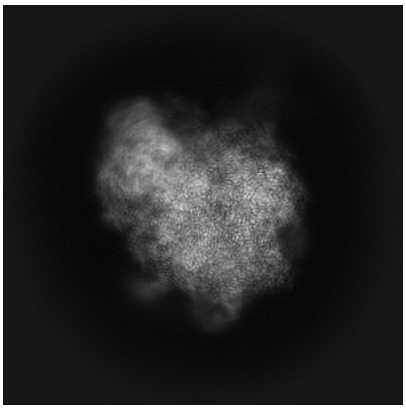
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-61076. These allow visual inspection of the internal detail of the map and identification of artifacts.

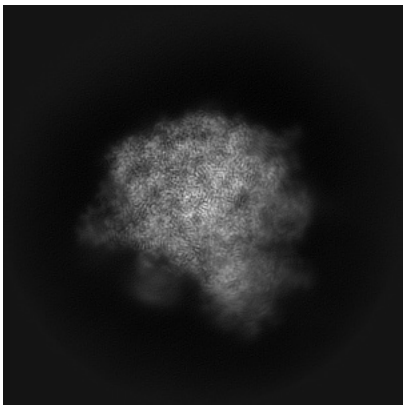
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

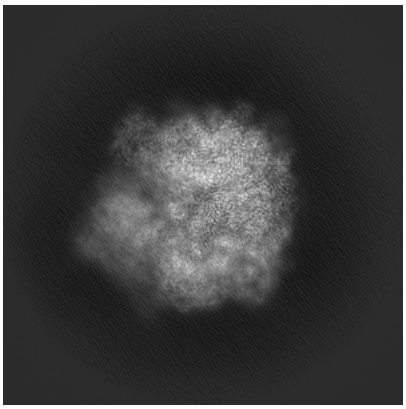
6.1.1 Primary map



X

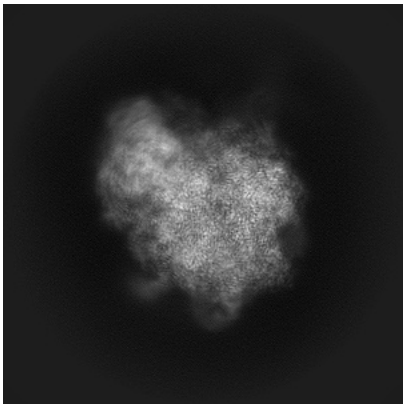


Y

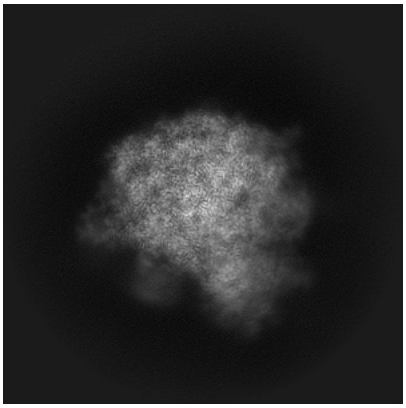


Z

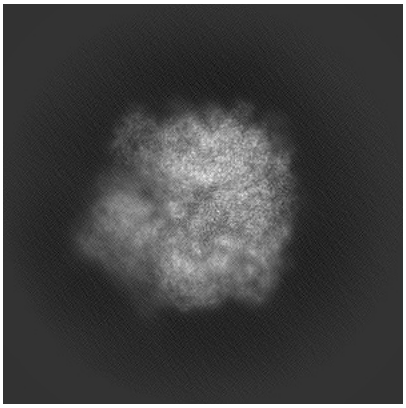
6.1.2 Raw map



X



Y

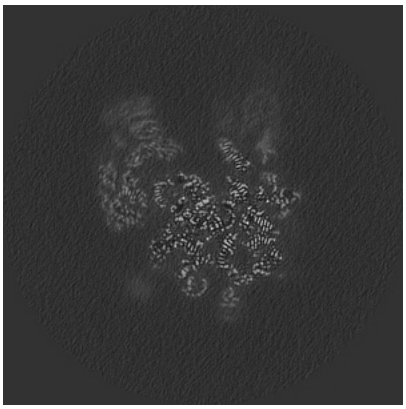


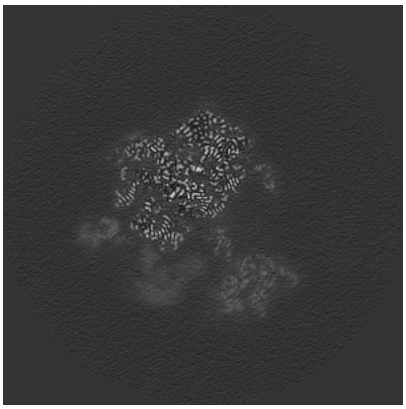
Z

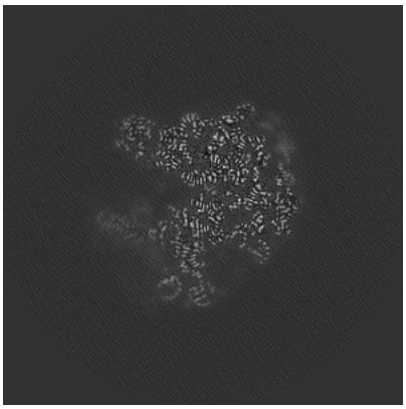
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

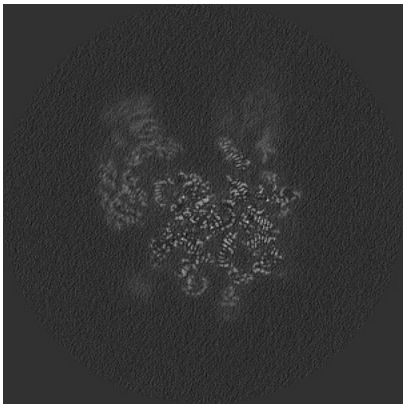
6.2.1 Primary map

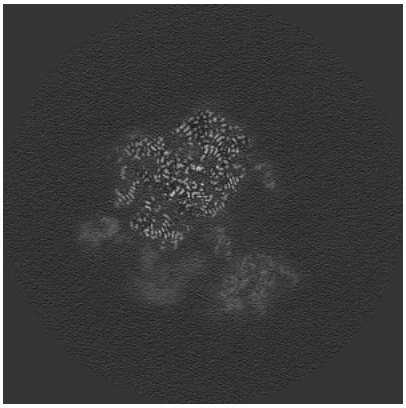

X Index: 256

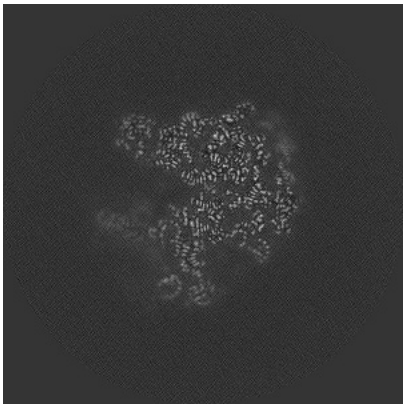

Y Index: 256


Z Index: 256

6.2.2 Raw map


X Index: 256

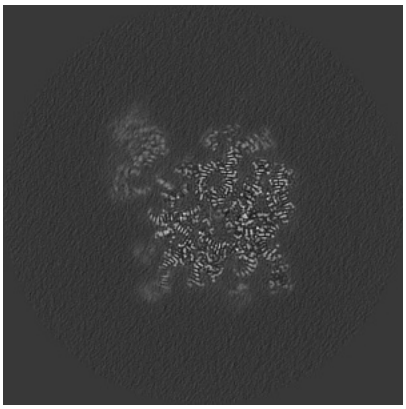

Y Index: 256

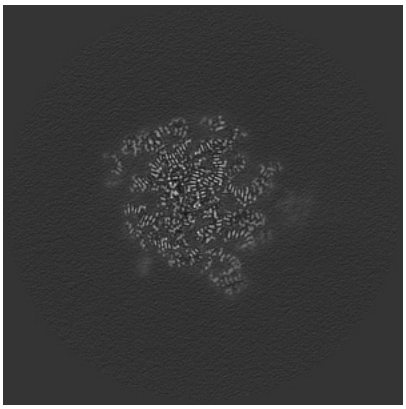

Z Index: 256

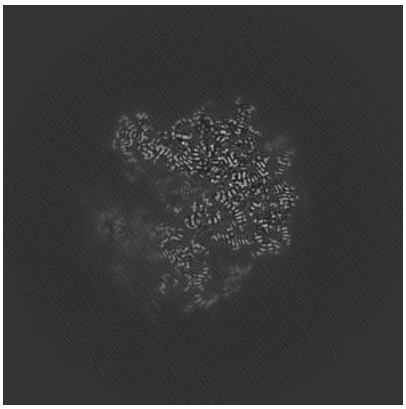
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

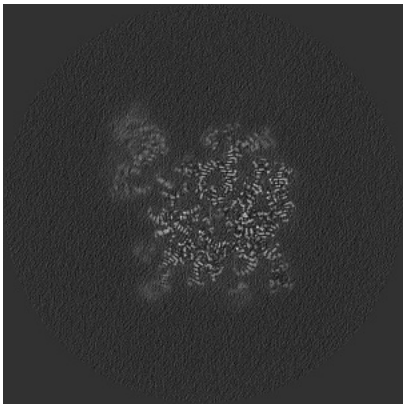
6.3.1 Primary map

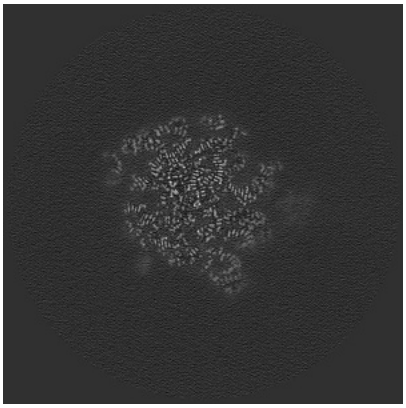

X Index: 288

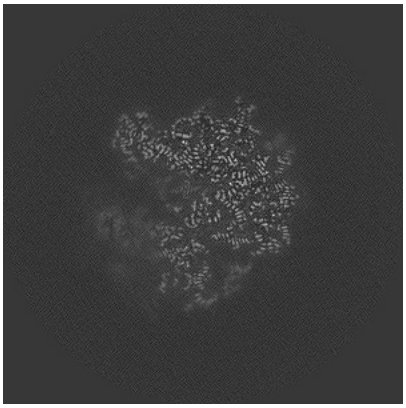

Y Index: 314


Z Index: 266

6.3.2 Raw map


X Index: 288

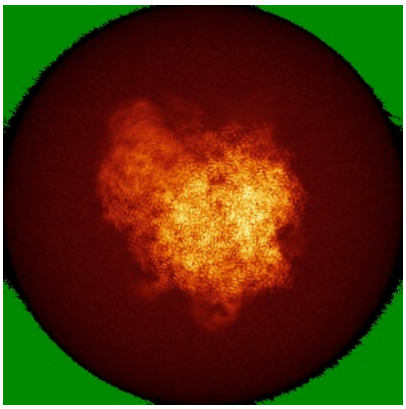

Y Index: 314

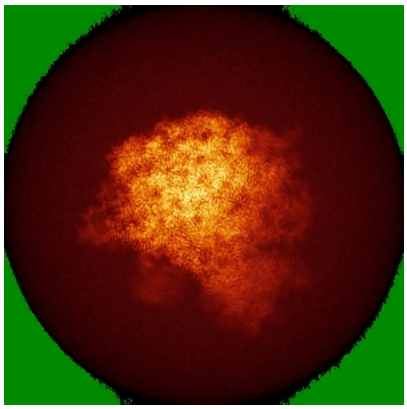

Z Index: 266

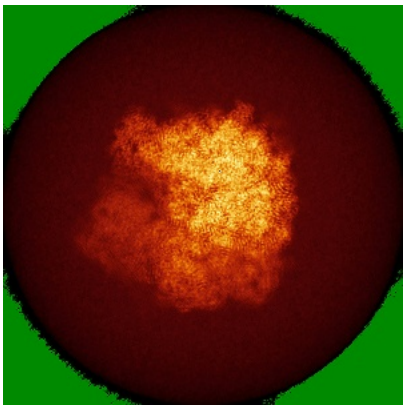
The images above show the largest variance slices of the map in three orthogonal directions.

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

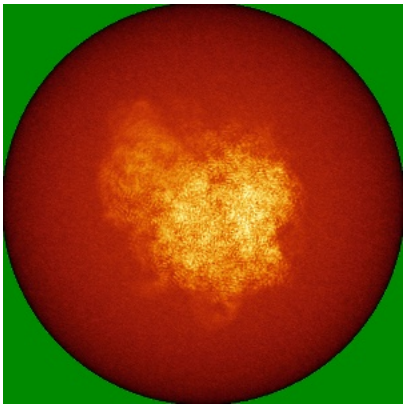
6.4.1 Primary map

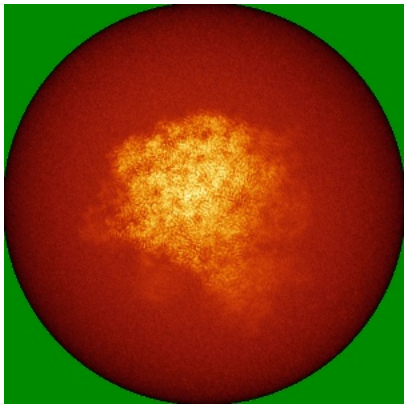

X

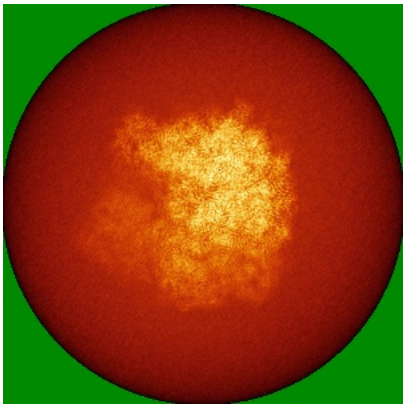

Y


Z

6.4.2 Raw map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0085. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

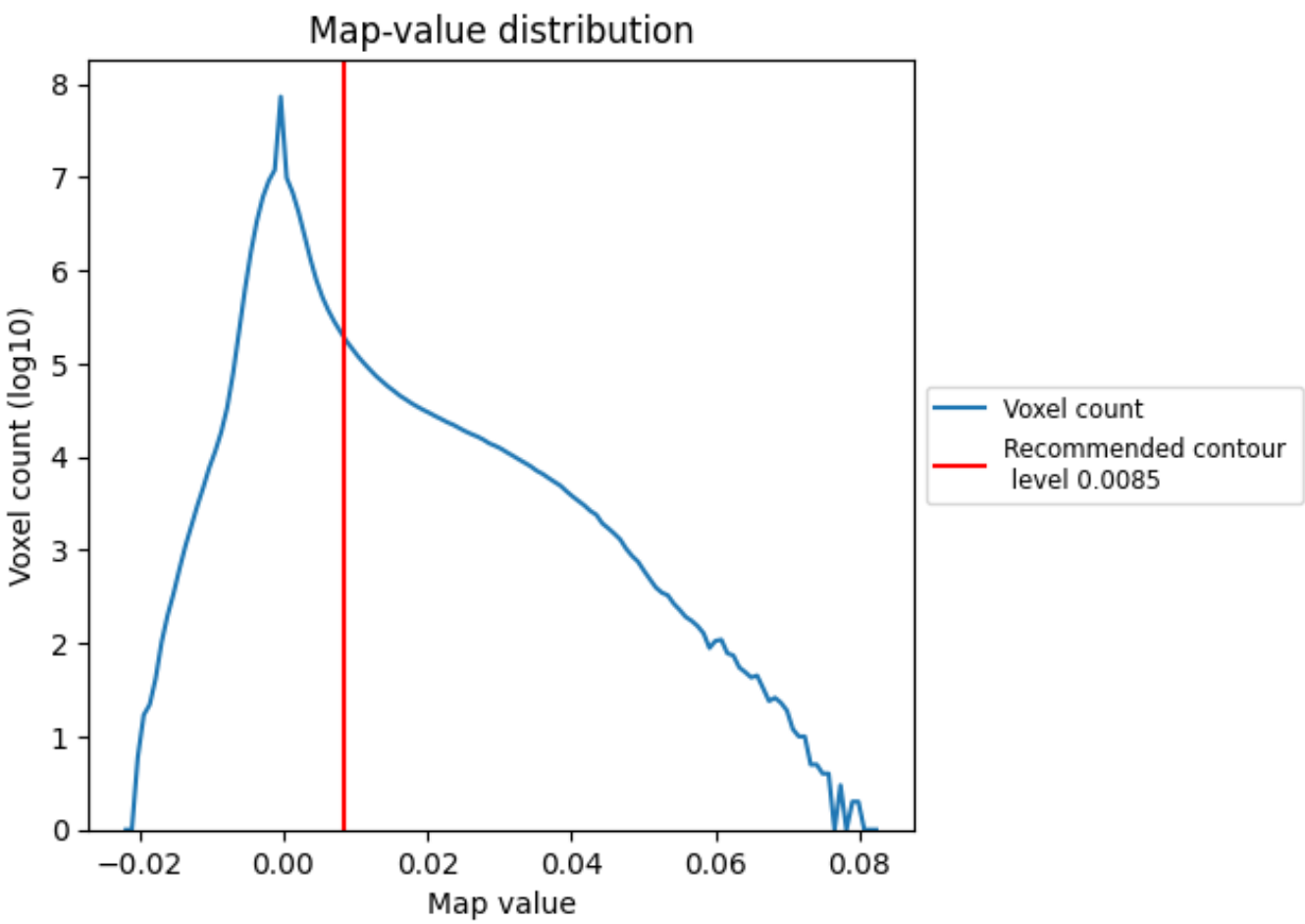
6.6 Mask visualisation (i)

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

7 Map analysis (i)

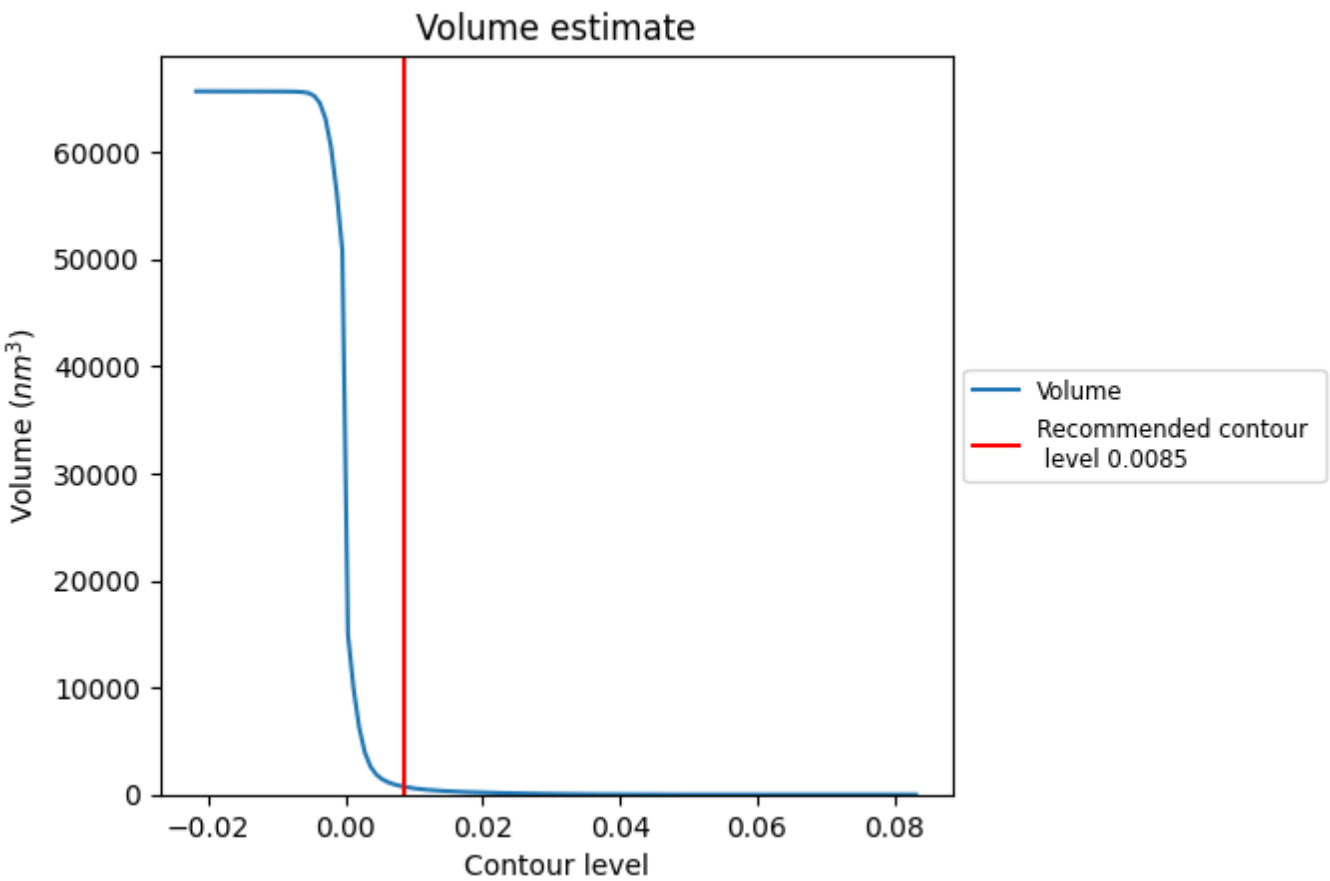
This section contains the results of statistical analysis of the map.

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.

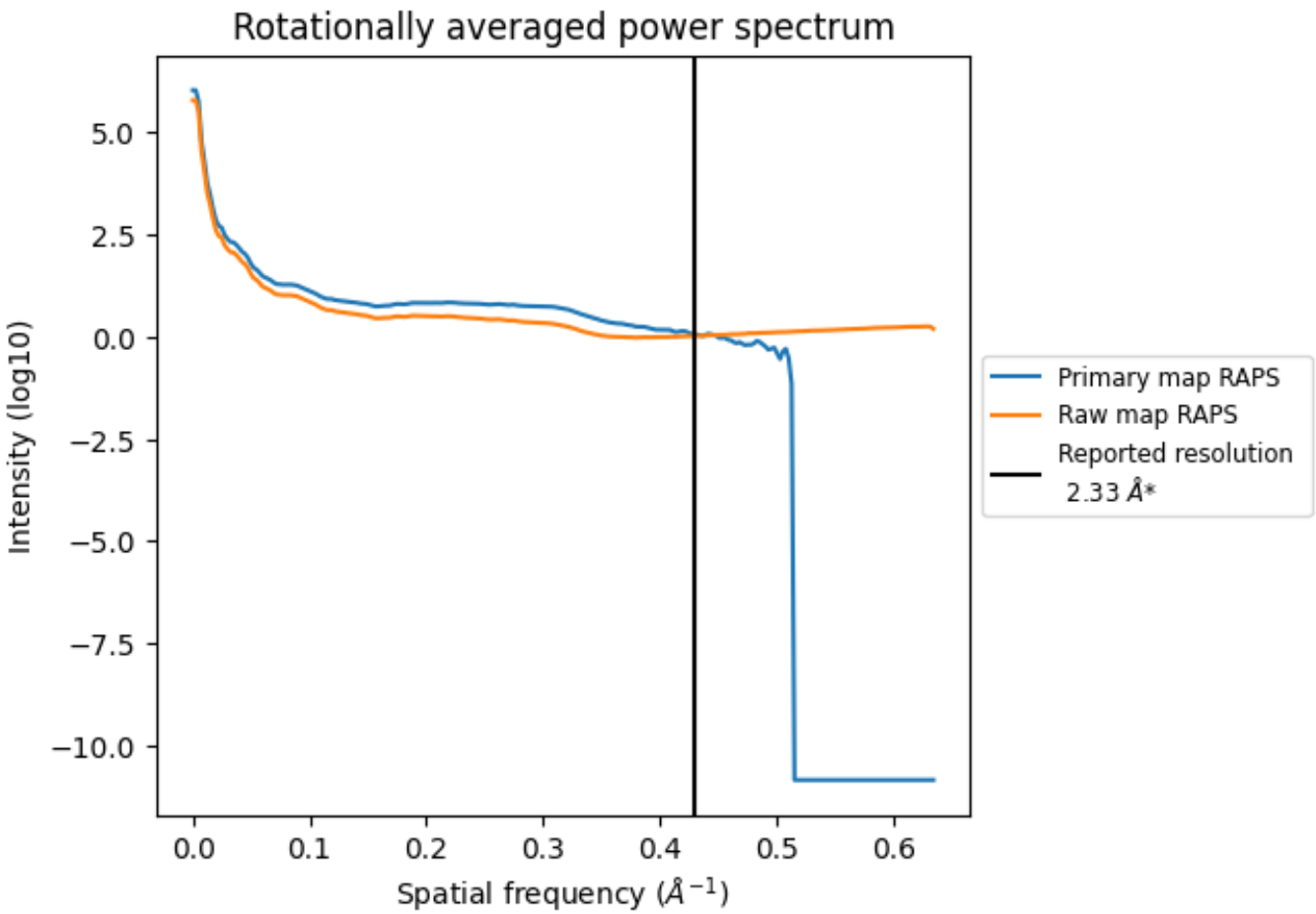
7.2 Volume estimate (i)



The volume at the recommended contour level is 731 nm^3; this corresponds to an approximate mass of 660 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)

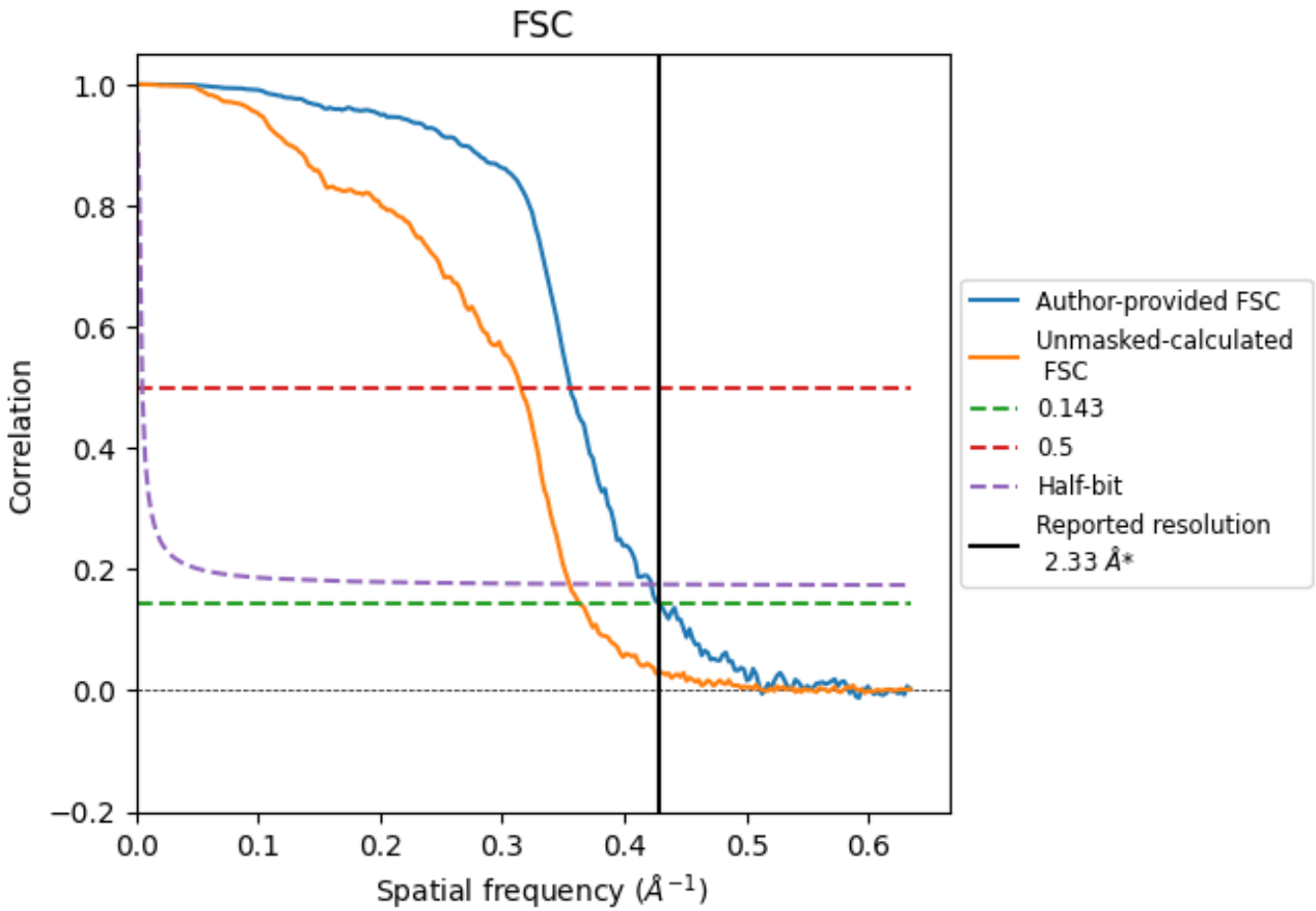


*Reported resolution corresponds to spatial frequency of 0.429 Å^{-1}

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 0.429 Å^{-1}

8.2 Resolution estimates (i)

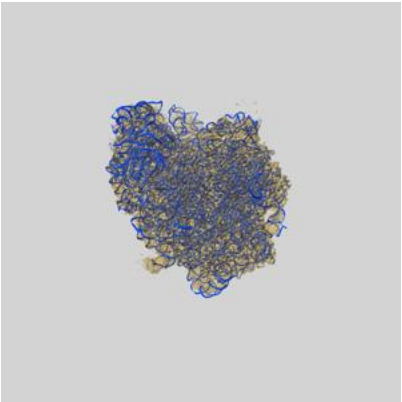
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.33	-	-
Author-provided FSC curve	2.33	2.81	2.37
Unmasked-calculated*	2.75	3.17	2.82

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.75 differs from the reported value 2.33 by more than 10 %

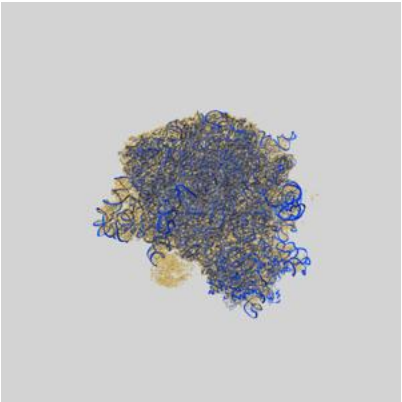
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-61076 and PDB model 9J1M. Per-residue inclusion information can be found in section 3 on page 14.

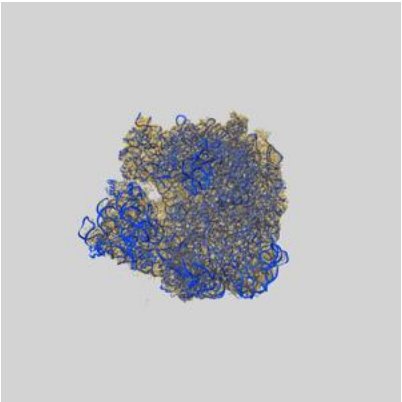
9.1 Map-model overlay (i)



X



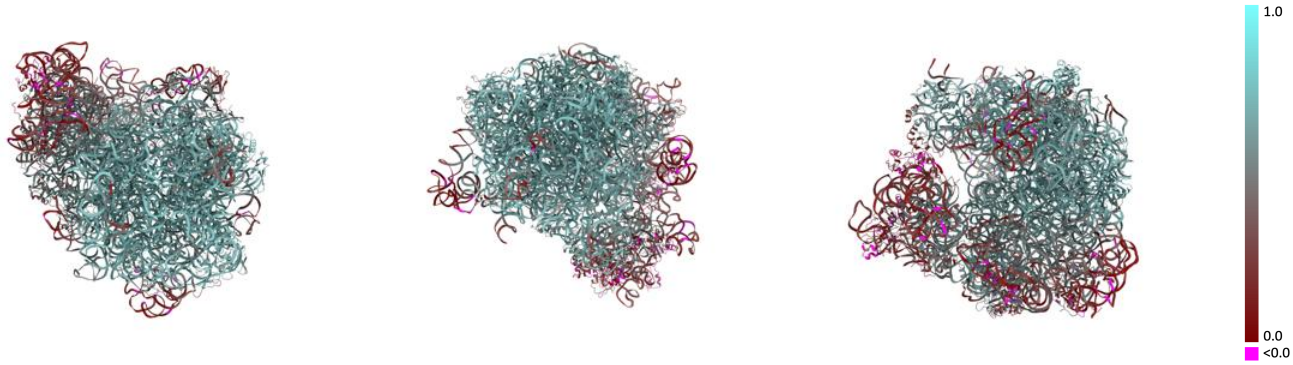
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0085 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.

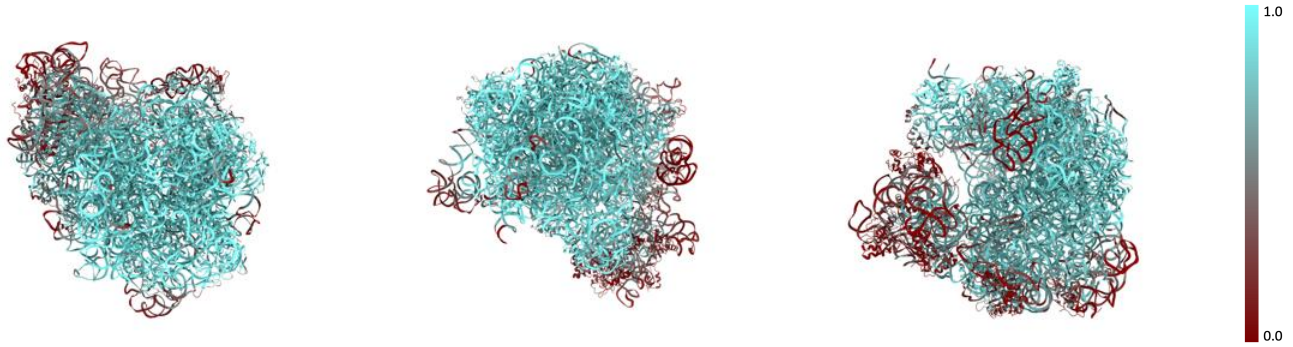
9.2 Q-score mapped to coordinate model (i)



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.

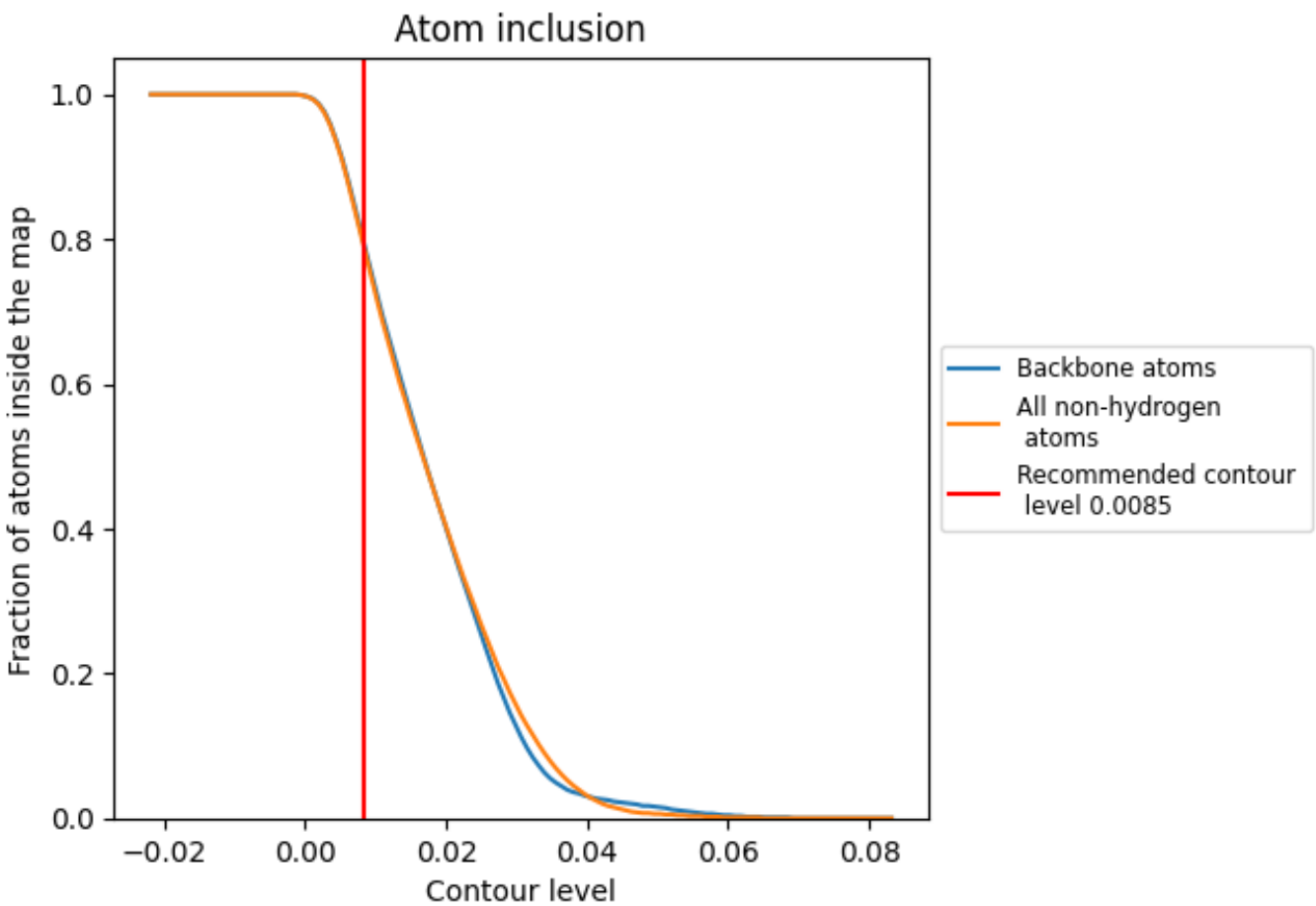
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0085).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 78% 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 (0.0085) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7840	0.5520
0	0.9000	0.6620
1	0.9020	0.6430
2	0.9880	0.7180
3	0.9830	0.7150
4	0.9170	0.6460
7	0.9890	0.6910
A	0.9060	0.6310
B	0.9000	0.5810
C	0.9580	0.6930
D	0.9170	0.6680
E	0.9150	0.6640
F	0.5710	0.4130
G	0.6230	0.4850
H	0.5160	0.4600
J	0.9490	0.6870
K	0.9380	0.6690
L	0.9160	0.6570
M	0.9350	0.6630
N	0.9640	0.6930
O	0.8950	0.6250
P	0.8570	0.6380
Q	0.9670	0.7070
R	0.8940	0.6590
S	0.9610	0.6920
T	0.8640	0.6340
U	0.7590	0.5550
V	0.5690	0.4570
W	0.9340	0.6660
X	0.9690	0.6960
Y	0.8290	0.5840
Z	0.9300	0.6750
a	0.6810	0.4430
c	0.2510	0.3750
d	0.0960	0.2050

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	0.6340	0.5290
f	0.5900	0.5080
g	0.2460	0.2600
h	0.6920	0.5290
i	0.2330	0.2400
j	0.1950	0.2430
k	0.6610	0.5090
l	0.4710	0.3970
m	0.1810	0.1740
n	0.4530	0.4590
o	0.7060	0.5290
p	0.3380	0.3070
q	0.4140	0.3120
r	0.6930	0.5320
s	0.1170	0.1640
t	0.3660	0.2070
u	0.9210	0.6560
x	0.6880	0.5640