Full wwPDB EM Validation Report ⓘ

Apr 30, 2024 – 03:18 PM EDT

PDB ID	:	8UU9
EMDB ID	:	EMD-42576
Title	:	Cryo-EM structure of the ratcheted Listeria innocua 70S ribosome (head-swiveled) in complex with HflXr and pe/E-tRNA (structure II-D)
Authors	:	Seely, S.M.; Basu, R.S.; Gagnon, M.G.
Deposited on	:	2023-10-31
Resolution	:	3.10 Å(reported)
Based on initial model	:	7NHN

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

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

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

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

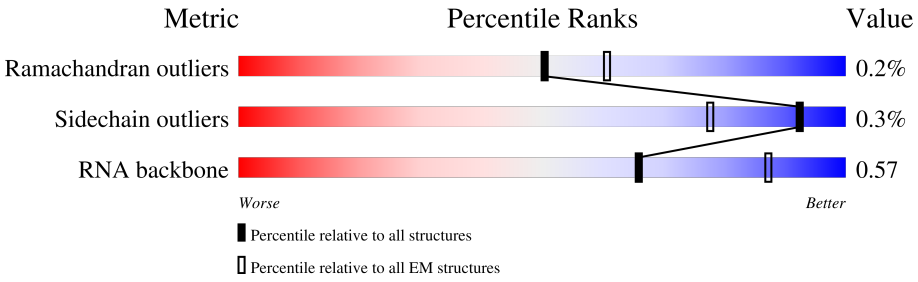
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	1550	79% 18%
2	b	249	17% 90% 10%
3	c	218	6% 93% 6%
4	d	200	100%
5	e	167	93% 7%
6	f	97	13% 96%
7	g	156	50% 94% 6%
8	h	132	99%

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Mol	Chain	Length	Quality of chain
9	i	130	17% 94% 5%
10	j	102	10% 93% 6%
11	k	129	12% 88% 12%
12	l	137	99%
13	m	121	54% 94% 6%
14	n	61	98%
15	o	89	98%
16	p	90	98%
17	q	87	93% 7%
18	r	79	81% 18%
19	s	92	55% 76% 20%
20	t	84	13% 95% 5%
21	x	76	63% 68% 26%
22	w	21	24% 14% 24% 62%
23	v	418	5% 99%
24	A	2932	6% 82% 17%
25	B	116	89% 9%
26	C	277	99%
27	D	209	99%
28	E	207	99%
29	F	179	22% 97%
30	G	178	99%
31	L	145	97%
32	M	122	100%
33	N	146	100%

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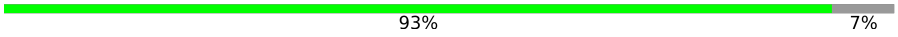
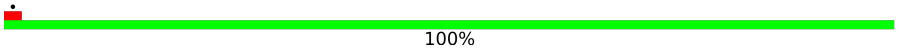
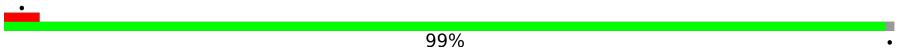
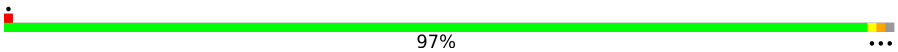
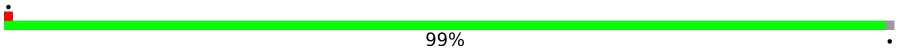
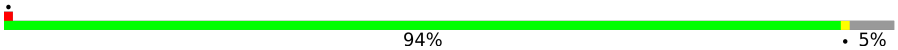
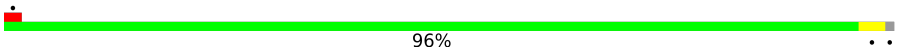
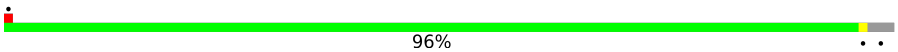
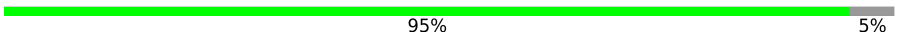
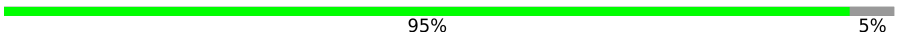
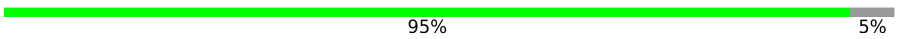
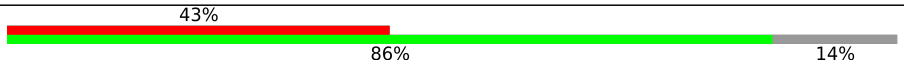
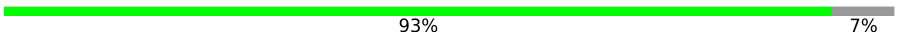
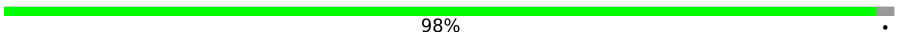
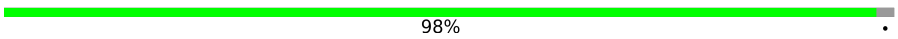
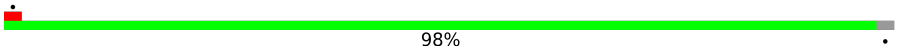
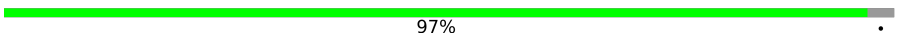
Mol	Chain	Length	Quality of chain
34	O	144	
35	P	135	
36	Q	119	
37	R	114	
38	S	119	
39	T	102	
40	U	118	
41	V	94	
42	W	103	
43	Y	96	
44	Z	62	
45	1	63	
46	2	59	
47	3	81	
48	4	57	
49	5	49	
50	6	44	
51	7	66	
52	8	37	

2 Entry composition

There are 56 unique types of molecules in this entry. The entry contains 142177 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1515	32493	14494	5955	10529	1515	0	0

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	224	1588	1011	279	292	6	0	0

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	204	1150	705	223	221	1	0	0

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	199	1537	961	286	288	2	0	0

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	155	1116	701	203	210	2	0	0

- Molecule 6 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	93	655	423	119	111	2	0	0

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	147	Total	C	N	O	S	0	0
			866	533	173	158	2		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	131	Total	C	N	O	S	0	0
			1022	651	180	189	2		

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	123	Total	C	N	O	S	0	0
			833	520	163	149	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	96	Total	C	N	O	S	0	0
			608	376	116	115	1		

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	114	Total	C	N	O	S	0	0
			824	508	158	155	3		

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	135	Total	C	N	O	S	0	0
			1002	621	198	181	2		

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	114	Total	C	N	O	S	0	0
			616	367	134	114	1		

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	60	Total	C	N	O	S	0	0
			445	283	84	73	5		

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	87	Total	C	N	O	S	0	0
			696	433	136	125	2		

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	88	Total	C	N	O	S	0	0
			711	450	132	126	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	81	Total	C	N	O	S	0	0
			629	396	120	112	1		

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	r	65	Total	C	N	O	S	0	0
			527	339	96	90	2		

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	s	74	Total	C	N	O	0	0
			459	279	96	84		

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	80	Total	C	N	O	S	0	0
			607	366	124	116	1		

- Molecule 21 is a RNA chain called pe/E Hybrid State Phenylalanine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	x	74	Total	C	N	O	P	S	0	0
			1591	713	285	517	74	2		

- Molecule 22 is a RNA chain called F-Stop mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	w	8	Total	C	N	O	P	0	0
			168	76	29	55	8		

- Molecule 23 is a protein called GTPase HflX.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	416	Total	C	N	O	S	0	0
			3200	2015	558	619	8		

- Molecule 24 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	A	2899	Total	C	N	O	P	0	0
			62278	27794	11524	20061	2899		

- Molecule 25 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	B	114	Total	C	N	O	P	0	0
			2428	1082	428	804	114		

- Molecule 26 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	C	273	Total	C	N	O	S	0	0
			2108	1307	415	379	7		

- Molecule 27 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	D	206	Total	C	N	O	S	0	0
			1545	974	287	280	4		

- Molecule 28 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	E	204	Total	C	N	O	0	0
			1564	989	288	287		

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	F	175	Total	C	N	O	S	0	0
			1232	785	211	231	5		

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	G	176	Total	C	N	O	S	0	0
			1318	830	244	243	1		

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	143	Total	C	N	O	S	0	0
			1128	715	205	205	3		

- Molecule 32 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	122	Total	C	N	O	S	0	0
			925	573	175	172	5		

- Molecule 33 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	N	146	Total	C	N	O	S	0	0
			1112	687	216	208	1		

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	O	134	Total	C	N	O	S	0	0
			1057	677	203	171	6		

- Molecule 35 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	P	123	Total	C	N	O	S	0	0
			986	618	194	173	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Q	119	Total	C	N	O	S	0	0
			867	530	172	164	1		

- Molecule 37 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	R	113	Total	C	N	O	S	0	0
			879	557	168	153	1		

- Molecule 38 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	S	118	Total	C	N	O	S	0	0
			953	605	188	156	4		

- Molecule 39 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	T	101	Total	C	N	O	S	0	0
			785	506	134	144	1		

- Molecule 40 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	U	112	Total	C	N	O	0	0
			864	544	162	158		

- Molecule 41 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	V	93	Total	C	N	O	S	0	0
			760	482	132	143	3		

- Molecule 42 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	W	100	Total	C	N	O	S	0	0
			734	465	137	129	3		

- Molecule 43 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Y	76	Total	C	N	O	S	0	0
			585	357	114	113	1		

- Molecule 44 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Z	59	Total	C	N	O	S	0	0
			462	286	97	77	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1	60	Total	C	N	O	S	0	0
			495	304	95	95	1		

- Molecule 46 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	2	56	Total	C	N	O	S	0	0
			433	272	82	78	1		

- Molecule 47 is a protein called Large ribosomal subunit protein bL31B.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	3	70	Total	C	N	O	0	0
			424	263	78	83		

- Molecule 48 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	4	53	Total	C	N	O	S	0	0
			425	259	87	74	5		

- Molecule 49 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	5	48	Total 394	C 241	N 79	O 70	S 4	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	6	43	Total 365	C 222	N 88	O 53	S 2	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	7	65	Total 529	C 328	N 116	O 80	S 5	0	0

- Molecule 52 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	8	36	Total 292	C 183	N 59	O 44	S 6	0	0

- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	a	202	Total 202	Mg 202	0
53	c	1	Total 1	Mg 1	0
53	e	1	Total 1	Mg 1	0
53	i	1	Total 1	Mg 1	0
53	l	1	Total 1	Mg 1	0
53	m	1	Total 1	Mg 1	0
53	q	1	Total 1	Mg 1	0
53	v	3	Total 3	Mg 3	0
53	A	256	Total 256	Mg 256	0

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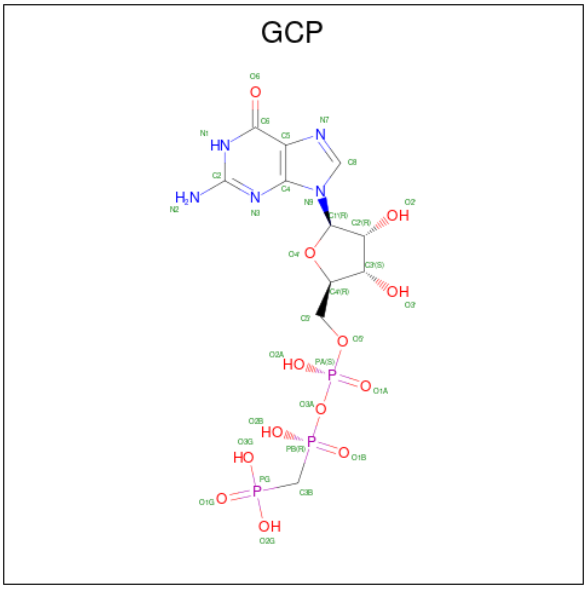
Mol	Chain	Residues	Atoms	AltConf
53	B	4	Total Mg 4 4	0
53	C	2	Total Mg 2 2	0
53	V	1	Total Mg 1 1	0
53	Y	1	Total Mg 1 1	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
54	n	1	Total Zn 1 1	0
54	4	1	Total Zn 1 1	0
54	5	1	Total Zn 1 1	0
54	8	1	Total Zn 1 1	0

- Molecule 55 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
55	v	1	Total C N O P 32 11 5 13 3	0

- Molecule 56 is water.

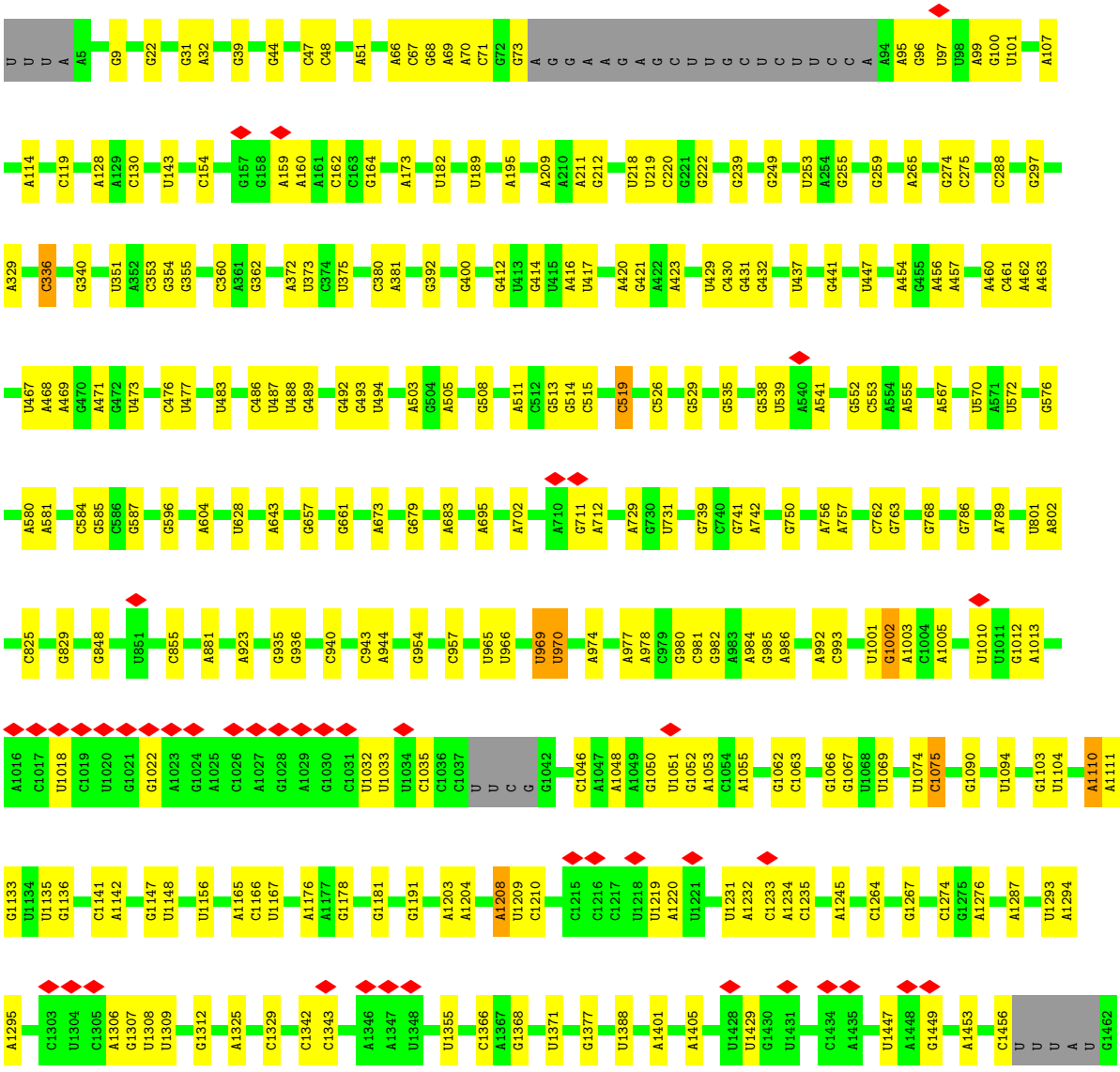
Mol	Chain	Residues	Atoms	AltConf
56	a	105	Total O 105 105	0
56	c	1	Total O 1 1	0
56	d	2	Total O 2 2	0
56	e	1	Total O 1 1	0
56	m	2	Total O 2 2	0
56	n	2	Total O 2 2	0
56	p	1	Total O 1 1	0
56	v	2	Total O 2 2	0
56	A	255	Total O 255 255	0
56	B	5	Total O 5 5	0
56	C	1	Total O 1 1	0
56	N	4	Total O 4 4	0
56	O	2	Total O 2 2	0
56	P	1	Total O 1 1	0
56	S	3	Total O 3 3	0
56	T	1	Total O 1 1	0
56	U	1	Total O 1 1	0
56	V	3	Total O 3 3	0
56	Y	1	Total O 1 1	0
56	Z	2	Total O 2 2	0
56	2	1	Total O 1 1	0

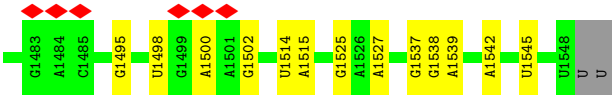
3 Residue-property plots (i)

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: 16S Ribosomal RNA

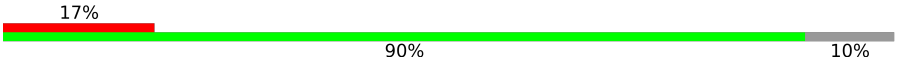
Chain a:

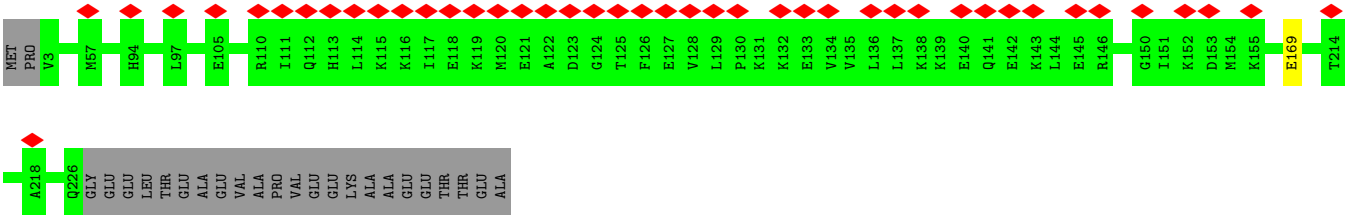




• Molecule 2: Small ribosomal subunit protein uS2

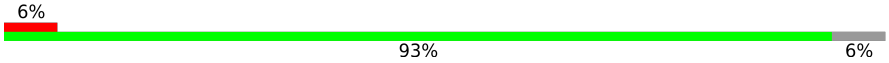
Chain b:

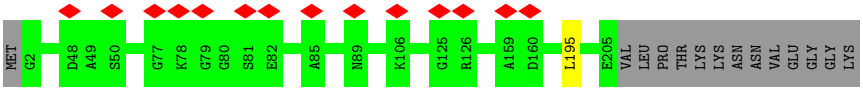




• Molecule 3: Small ribosomal subunit protein uS3

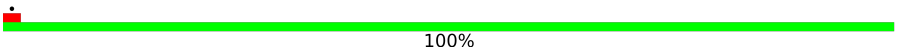
Chain c:

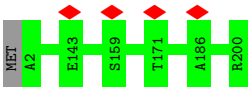




• Molecule 4: Small ribosomal subunit protein uS4

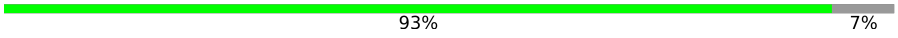
Chain d:

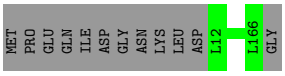




• Molecule 5: Small ribosomal subunit protein uS5

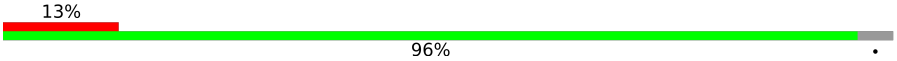
Chain e:

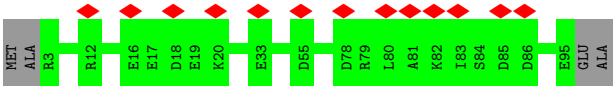




• Molecule 6: Small ribosomal subunit protein bS6

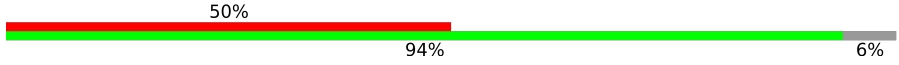
Chain f:

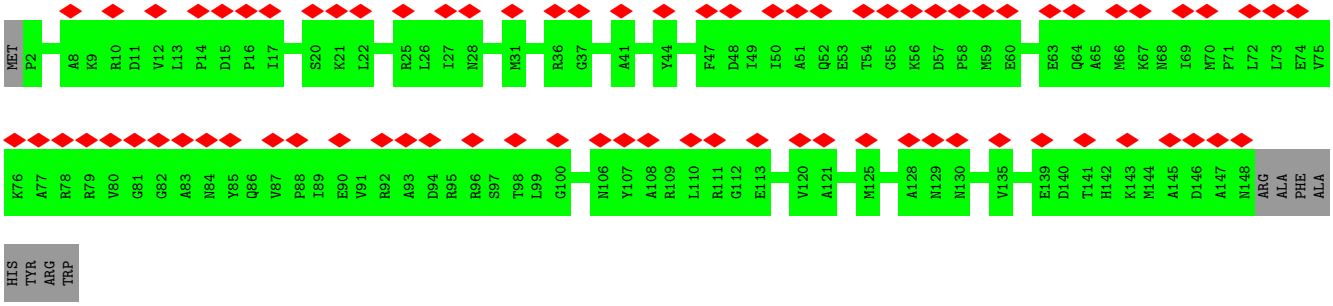




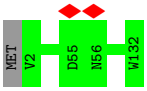
• Molecule 7: Small ribosomal subunit protein uS7

Chain g:

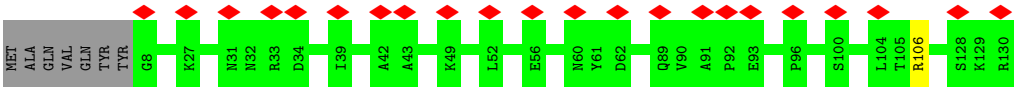




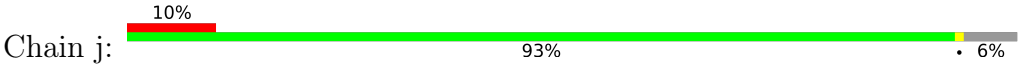
• Molecule 8: Small ribosomal subunit protein uS8

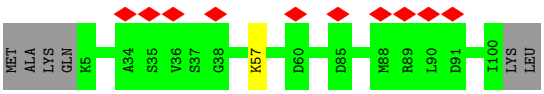


• Molecule 9: Small ribosomal subunit protein uS9

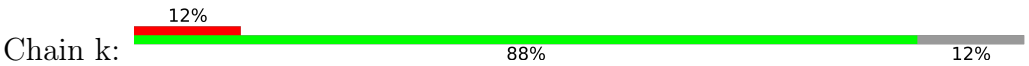


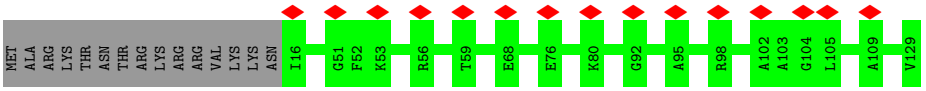
• Molecule 10: Small ribosomal subunit protein uS10



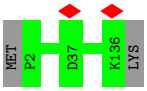


• Molecule 11: Small ribosomal subunit protein uS11



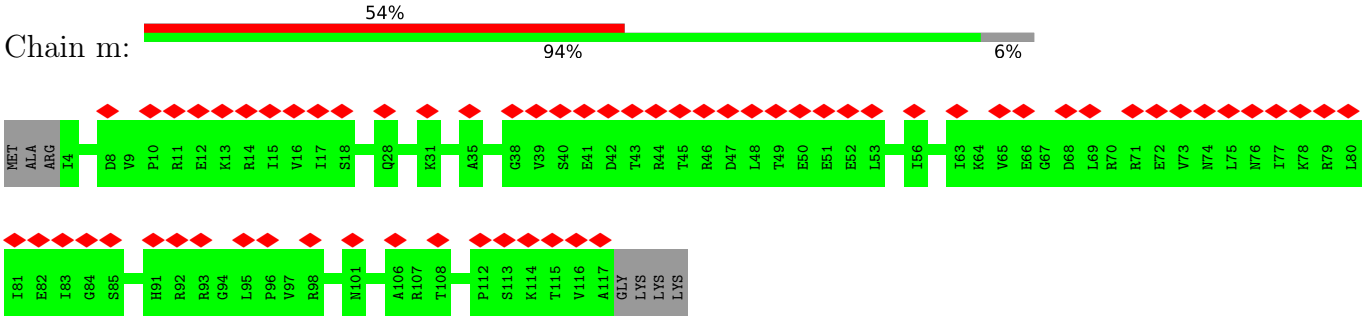


• Molecule 12: Small ribosomal subunit protein uS12



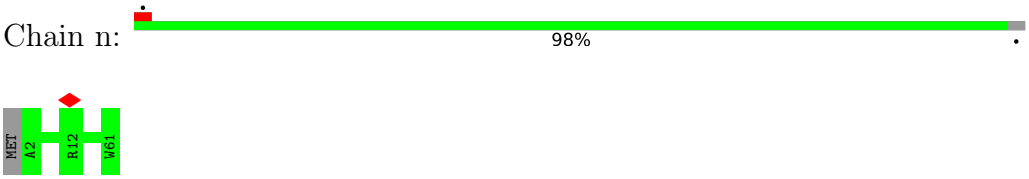
• Molecule 13: Small ribosomal subunit protein uS13

Chain m:



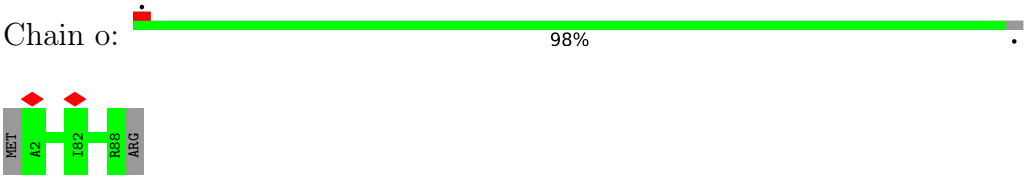
• Molecule 14: Small ribosomal subunit protein uS14

Chain n:



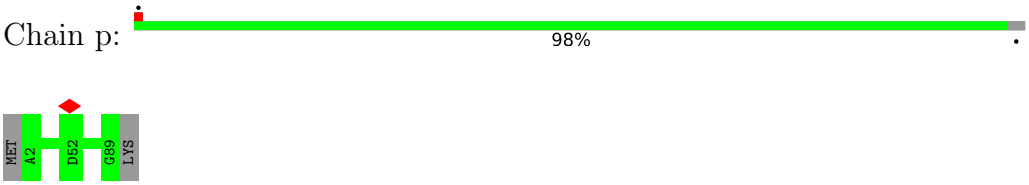
• Molecule 15: Small ribosomal subunit protein uS15

Chain o:



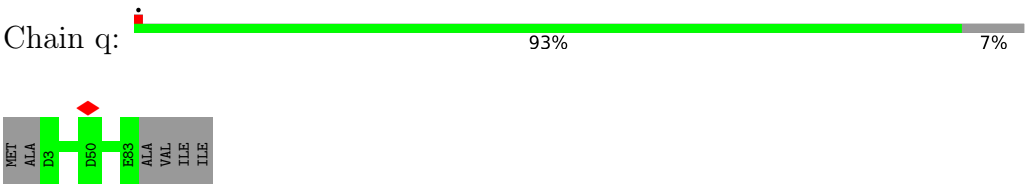
• Molecule 16: Small ribosomal subunit protein bS16

Chain p:



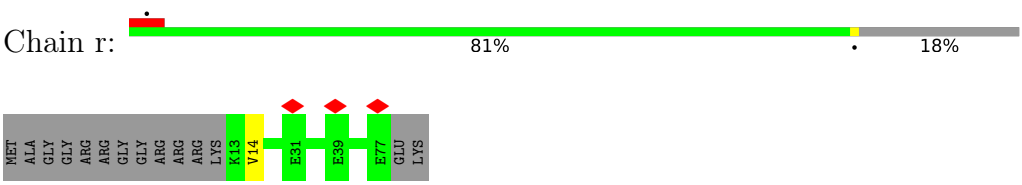
• Molecule 17: Small ribosomal subunit protein uS17

Chain q:



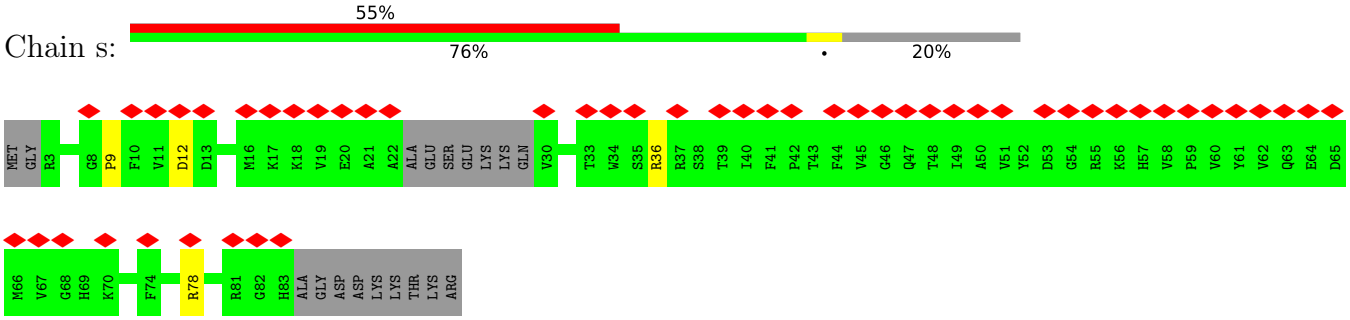
• Molecule 18: Small ribosomal subunit protein bS18

Chain r:



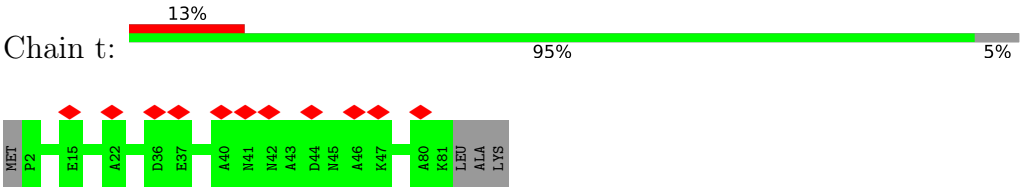
• Molecule 19: Small ribosomal subunit protein uS19

Chain s:



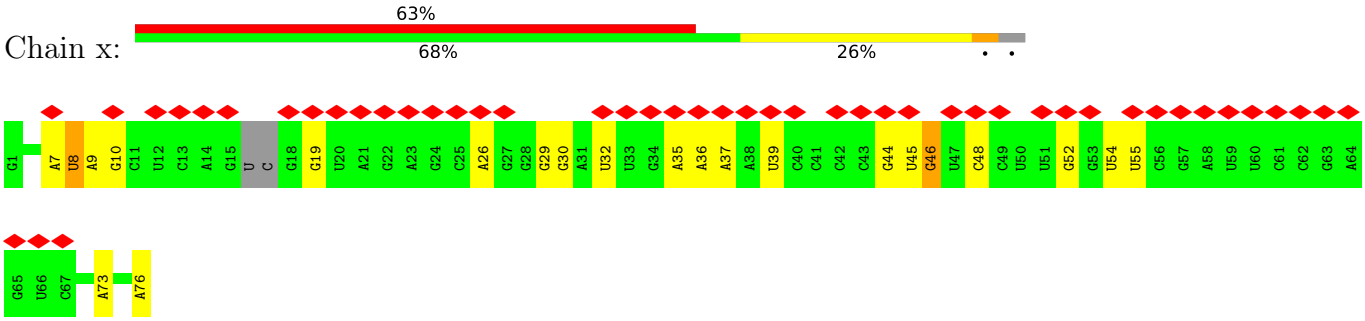
• Molecule 20: Small ribosomal subunit protein bS20

Chain t:



• Molecule 21: pe/E Hybrid State Phenylalanine tRNA

Chain x:

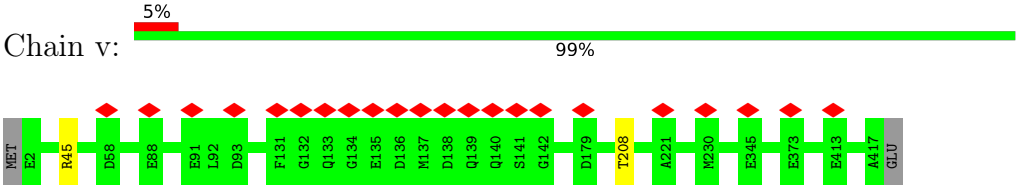


• Molecule 22: F-Stop mRNA

Chain w:

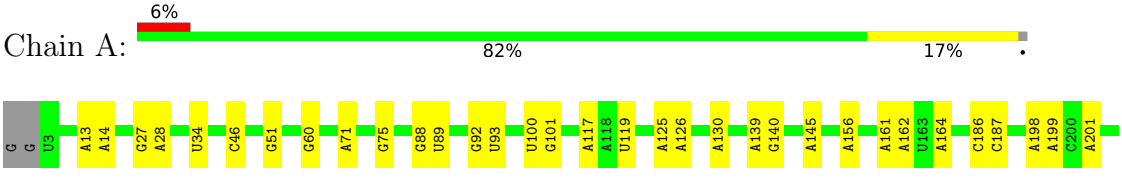
• Molecule 23: GTPase HflX

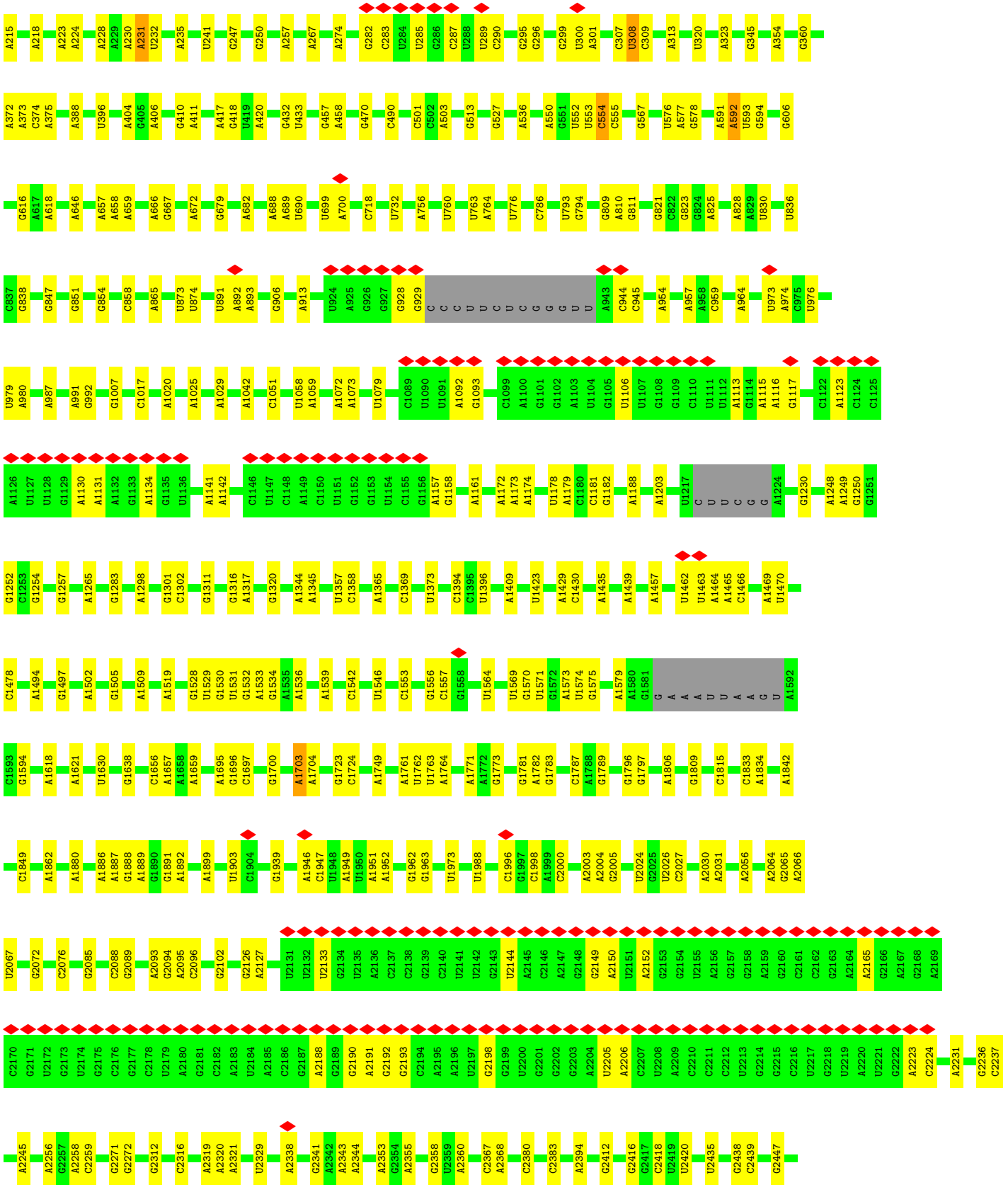
Chain v:

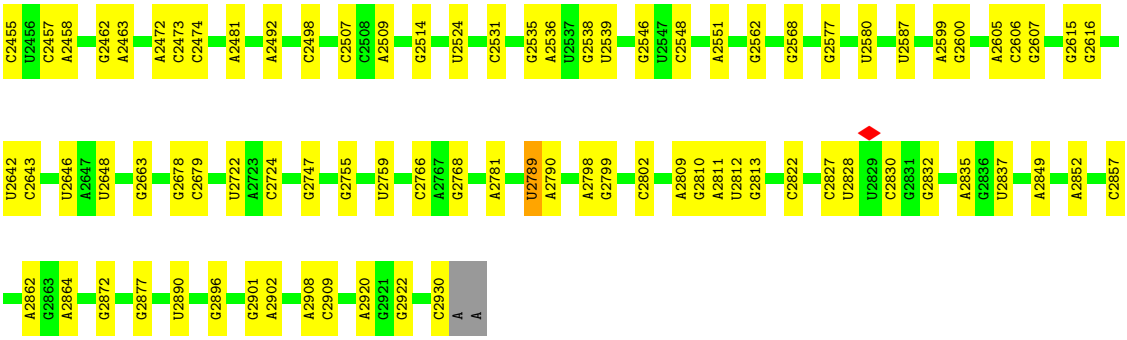


• Molecule 24: 23S Ribosomal RNA

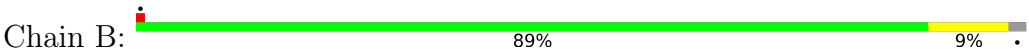
Chain A:



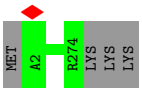

A215 A218 A223 A224 A228 A229 A230 A231 U232 A235 U241 G247 G250 A257 A267 A274 G282 C283 U284 U285 G286 C287 U288 U289 C290 G295 G296 G299 U300 A301 C307 U308 C309 A313 U320 A323 G345 A354 G360
A372 A373 C374 A375 A388 U396 A404 G405 A406 G410 A411 A417 G418 U419 A420 G432 U433 G457 A458 G470 C490 C501 C502 A503 G513 G527 A536 A550 G551 U552 U553 C554 C555 G567 U576 A577 G578 A591 A592 U593 G594 G606
G616 A617 A618 A646 A657 A658 A659 A666 G667 A672 G679 A682 A688 A689 U690 U699 A700 C718 U732 A756 U760 U763 A764 U776 C786 U793 G794 G809 A810 G811 G821 C822 G823 G824 A825 A828 A829 U830 U836
C837 G838 G847 G851 G854 C858 A865 U873 U874 U891 A892 A893 G906 A913 U924 A925 G926 G927 G928 G929 C C C U U C U C G G G U U A943 C944 C945 A954 A957 A958 C959 A964 U973 A974 G975 U976
U979 A980 A987 A991 G992 C1007 C1017 A1020 A1025 A1029 A1042 C1051 U1058 A1059 A1072 A1073 U1079 C1089 U1090 U1091 A1092 G1093 C1099 A1100 C1101 G1102 A1103 U1104 G1105 U1106 U1107 C1108 G1109 C1110 U1111 U1112 A1113 G1114 A1115 A1116 G1117 C1122 A1123 C1124 C1125
A1126 U1127 U1128 G1129 A1130 A1131 A1132 G1133 A1134 G1135 U1136 A1141 A1142 C1146 U1147 C1148 A1149 C1150 U1151 G1152 G1153 U1164 C1155 G1156 A1157 G1158 A1161 A1172 A1173 A1174 U1178 A1179 C1180 C1181 G1182 A1188 A1203 U1217 C U U C G G A1224 G1230 A1248 A1249 G1250 G1251
G1252 C1253 G1254 G1257 A1265 G1283 A1298 G1301 C1302 G1311 G1316 A1317 G1320 A1344 A1345 U1357 C1358 A1365 C1369 U1373 C1394 C1395 U1396 A1409 U1423 A1429 C1430 A1435 A1439 A1457 U1462 U1463 A1464 A1465 C1466 A1469 U1470
C1478 A1494 G1497 A1502 G1505 A1509 A1519 G1528 U1529 G1530 U1531 G1532 A1533 G1534 A1535 A1536 A1539 C1542 U1546 C1553 G1556 C1557 G1558 U1564 U1569 G1570 U1571 G1572 A1573 U1574 G1575 A1579 A1580 G1581 G A A A U U A A G U A1592
C1593 G1594 A1618 A1621 U1630 G1638 C1656 A1657 A1658 A1659 A1695 G1696 C1697 G1700 A1703 A1704 G1723 C1724 A1749 A1761 U1762 U1763 A1764 A1771 A1772 G1773 G1781 A1782 G1783 C1787 A1788 G1789 G1796 G1797 A1806 G1809 C1815 C1833 A1834 A1842
C1849 A1862 A1880 A1886 A1887 G1888 A1889 G1890 G1891 A1892 A1899 U1903 C1904 G1939 A1946 C1947 U1948 A1949 U1950 A1951 A1952 G1962 G1963 U1973 U1988 C1996 G1997 C1998 A1999 C2000 A2003 A2004 G2005 U2024 G2025 U2026 C2027 A2030 A2031 A2056 A2064 G2065 A2066
U2067 G2072 C2076 G2085 C2088 G2089 A2093 G2094 A2095 C2096 G2102 G2126 A2127 U2131 U2132 U2133 G2134 U2135 A2136 C2137 C2138 G2139 C2140 U2141 U2142 G2143 U2144 A2145 C2146 A2147 G2148 G2149 A2150 U2151 A2152 G2153 G2154 U2155 A2156 G2157 G2158 A2159 G2160 C2161 C2162 G2163 A2164 A2165 G2166 A2167 G2168 A2169
C2170 G2171 U2172 G2173 U2174 G2175 C2176 G2177 C2178 U2179 A2180 G2181 C2182 A2183 U2184 A2185 C2186 G2187 A2188 G2189 G2190 A2191 G2192 G2193 C2194 A2195 A2196 U2197 G2198 G2199 U2200 G2201 G2202 G2203 A2204 U2205 A2206 C2207 U2208 A2209 C2210 C2211 C2212 U2213 G2214 G2215 C2216 U2217 G2218 U2219 A2220 U2221 G2222 A2223 C2224 A2231 G2236 C2237
A2245 A2256 G2257 A2258 C2259 G2271 G2272 G2312 C2316 A2319 A2320 A2321 U2329 A2338 G2341 A2342 A2343 A2344 A2353 G2354 A2355 G2358 U2359 A2360 C2367 A2368 C2380 C2383 A2394 G2412 G2416 G2417 C2418 U2419 U2420 U2435 G2438 C2439 G2447



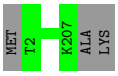
• Molecule 25: 5S Ribosomal RNA



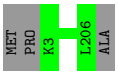
• Molecule 26: Large ribosomal subunit protein uL2



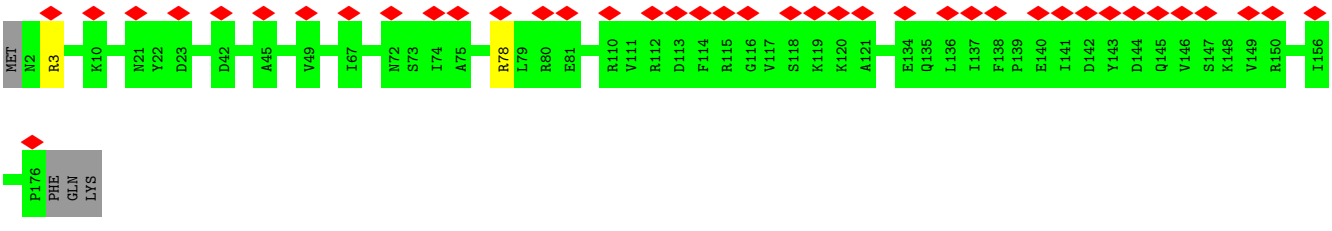
• Molecule 27: Large ribosomal subunit protein uL3



• Molecule 28: Large ribosomal subunit protein uL4

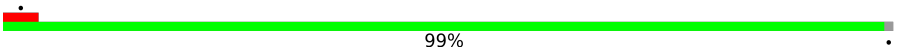


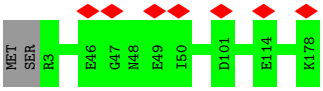
• Molecule 29: Large ribosomal subunit protein uL5



• Molecule 30: Large ribosomal subunit protein uL6

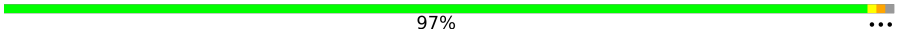
Chain G:

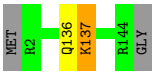




• Molecule 31: Large ribosomal subunit protein uL13

Chain L:





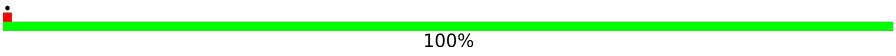
• Molecule 32: Large ribosomal subunit protein uL14

Chain M:

There are no outlier residues recorded for this chain.

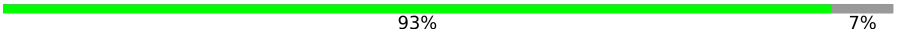
• Molecule 33: Large ribosomal subunit protein uL15

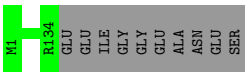
Chain N:



• Molecule 34: Large ribosomal subunit protein uL16

Chain O:



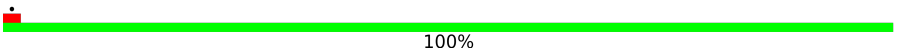


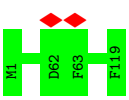
• Molecule 35: Large ribosomal subunit protein bL17

Chain P:

• Molecule 36: Large ribosomal subunit protein uL18

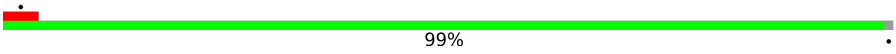
Chain Q:

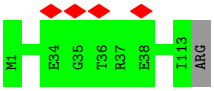




• Molecule 37: Large ribosomal subunit protein bL19

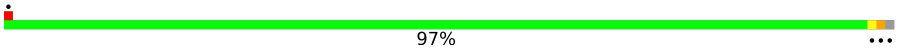
Chain R:

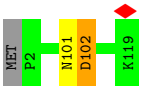




• Molecule 38: Large ribosomal subunit protein bL20

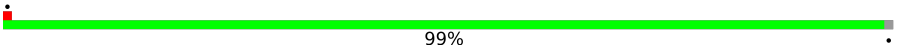
Chain S:

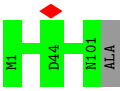




• Molecule 39: Large ribosomal subunit protein bL21

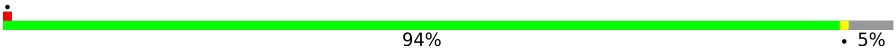
Chain T:

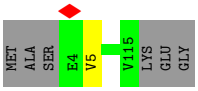




• Molecule 40: Large ribosomal subunit protein uL22

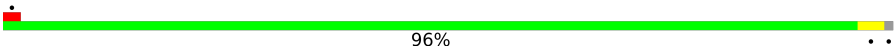
Chain U:

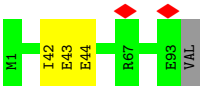




• Molecule 41: Large ribosomal subunit protein uL23

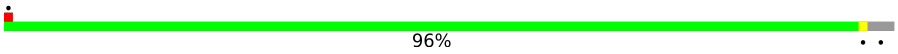
Chain V:

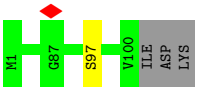




• Molecule 42: Large ribosomal subunit protein uL24

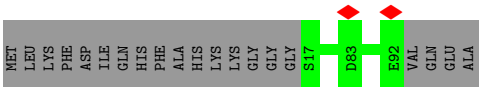
Chain W:





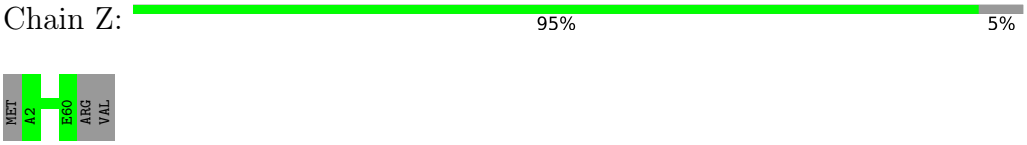
• Molecule 43: Large ribosomal subunit protein bL27

Chain Y:



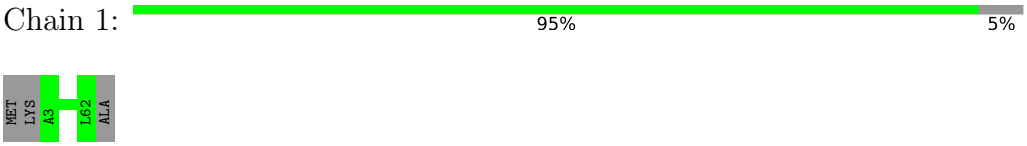
• Molecule 44: Large ribosomal subunit protein bL28

Chain Z:



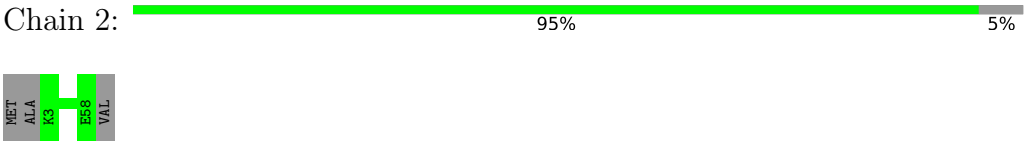
• Molecule 45: Large ribosomal subunit protein uL29

Chain 1:



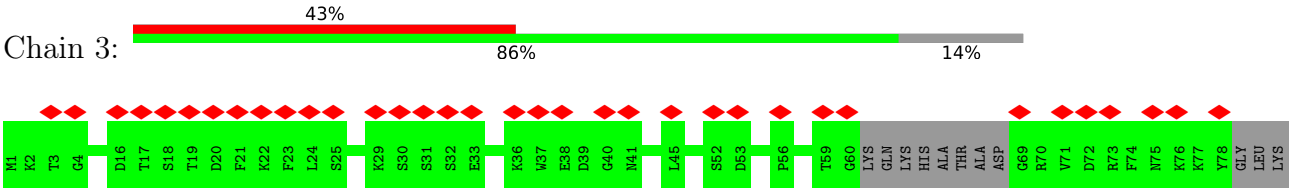
• Molecule 46: Large ribosomal subunit protein uL30

Chain 2:



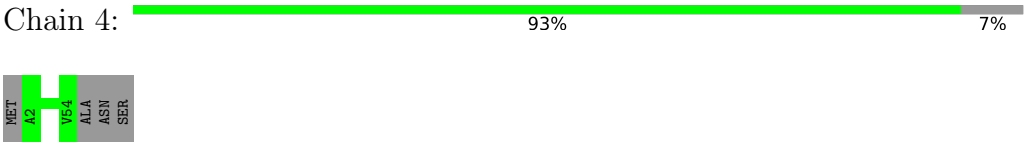
• Molecule 47: Large ribosomal subunit protein bL31B

Chain 3:



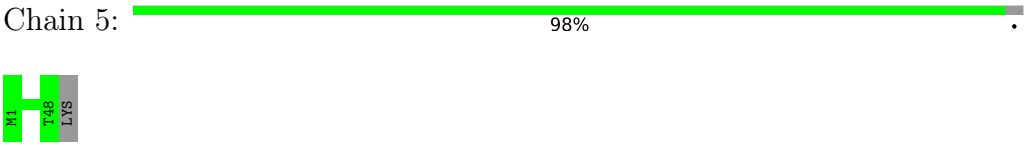
• Molecule 48: Large ribosomal subunit protein bL32

Chain 4:



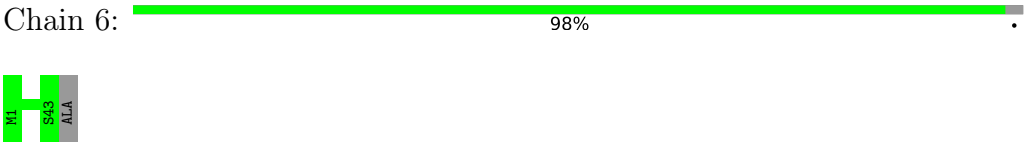
• Molecule 49: Large ribosomal subunit protein bL33

Chain 5:



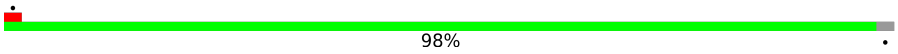
• Molecule 50: Large ribosomal subunit protein bL34

Chain 6:



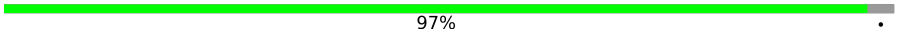
• Molecule 51: Large ribosomal subunit protein bL35

Chain 7:



• Molecule 52: Large ribosomal subunit protein bL36

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	80381	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40.0	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	31.784	Depositor
Minimum map value	-18.322	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	1.115	Depositor
Recommended contour level	3.4	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	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: PSU, 4SU, MG, MIA, GCP, ZN, 5MU, 7MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	a	0.58	0/36378	0.87	25/56739 (0.0%)
2	b	0.28	0/1612	0.46	0/2195
3	c	0.31	0/1160	0.55	1/1601 (0.1%)
4	d	0.33	0/1564	0.53	0/2109
5	e	0.33	0/1129	0.57	0/1530
6	f	0.29	0/666	0.52	0/909
7	g	0.28	0/871	0.55	0/1190
8	h	0.38	0/1035	0.56	0/1392
9	i	0.35	0/845	0.58	0/1146
10	j	0.37	0/617	0.55	0/845
11	k	0.28	0/838	0.53	0/1132
12	l	0.37	0/1017	0.61	0/1375
13	m	0.25	0/617	0.49	0/843
14	n	0.40	0/453	0.56	0/608
15	o	0.29	0/706	0.59	0/952
16	p	0.37	0/724	0.56	0/970
17	q	0.31	0/638	0.53	0/860
18	r	0.31	0/535	0.55	0/716
19	s	0.31	0/466	0.62	0/636
20	t	0.28	0/610	0.52	0/813
21	x	0.28	0/1605	0.82	0/2497
22	w	0.38	0/187	1.10	0/288
23	v	0.31	0/3240	0.52	0/4380
24	A	0.51	0/69775	0.80	10/108849 (0.0%)
25	B	0.31	0/2711	0.76	0/4224
26	C	0.32	0/2144	0.56	0/2875
27	D	0.34	0/1567	0.55	0/2111
28	E	0.31	0/1584	0.53	0/2134
29	F	0.28	0/1249	0.55	0/1704
30	G	0.28	0/1339	0.51	0/1811
31	L	0.33	0/1151	0.54	1/1546 (0.1%)
32	M	0.32	0/932	0.56	0/1248

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	N	0.30	0/1123	0.55	0/1492
34	O	0.32	0/1079	0.54	0/1442
35	P	0.32	0/997	0.60	1/1333 (0.1%)
36	Q	0.27	0/874	0.55	0/1175
37	R	0.31	0/891	0.55	0/1199
38	S	0.36	0/966	0.53	0/1284
39	T	0.35	0/798	0.49	0/1071
40	U	0.32	0/874	0.55	0/1182
41	V	0.35	0/769	0.56	0/1029
42	W	0.30	0/744	0.49	0/998
43	Y	0.35	0/592	0.60	0/788
44	Z	0.29	0/467	0.58	0/619
45	1	0.27	0/496	0.55	0/662
46	2	0.28	0/436	0.56	0/585
47	3	0.24	0/431	0.48	0/591
48	4	0.34	0/433	0.59	0/577
49	5	0.30	0/398	0.58	0/534
50	6	0.32	0/368	0.64	0/479
51	7	0.31	0/536	0.64	0/696
52	8	0.32	0/295	0.56	0/387
All	All	0.48	0/153532	0.76	38/230351 (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
19	s	0	1
31	L	0	1
All	All	0	2

There are no bond length outliers.

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	A	308	U	C2-N1-C1'	6.86	125.93	117.70
1	a	970	U	C2-N3-C4	-6.73	122.96	127.00
24	A	1357	U	C2-N1-C1'	6.68	125.72	117.70
1	a	519	C	C2-N1-C1'	-6.61	111.53	118.80
1	a	1075	C	C2-N1-C1'	6.52	125.98	118.80
1	a	762	C	C2-N1-C1'	6.38	125.82	118.80

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	969	U	C2-N1-C1'	6.32	125.28	117.70
24	A	1703	A	O4'-C1'-N9	6.25	113.20	108.20
3	c	195	LEU	CA-CB-CG	6.08	129.27	115.30
1	a	1166	C	C2-N1-C1'	6.02	125.42	118.80
1	a	1366	C	C5-C6-N1	6.01	124.01	121.00
1	a	1366	C	C6-N1-C2	-5.98	117.91	120.30
1	a	970	U	N1-C2-N3	5.86	118.42	114.90
1	a	969	U	N1-C2-O2	5.73	126.81	122.80
24	A	554	C	C2-N1-C1'	5.65	125.01	118.80
24	A	231	A	O4'-C1'-N9	5.61	112.69	108.20
1	a	336	C	N1-C2-O2	5.52	122.21	118.90
1	a	993	C	C6-N1-C2	-5.50	118.10	120.30
1	a	67	C	C6-N1-C2	-5.46	118.12	120.30
1	a	1136	G	C4-N9-C1'	5.45	133.58	126.50
1	a	1208	A	P-O3'-C3'	5.44	126.23	119.70
24	A	2539	U	C2-N1-C1'	5.42	124.20	117.70
24	A	1358	C	C2-N1-C1'	5.39	124.73	118.80
1	a	336	C	C2-N1-C1'	5.33	124.67	118.80
1	a	1002	G	N3-C4-N9	5.28	129.17	126.00
24	A	2789	U	P-O3'-C3'	5.26	126.01	119.70
1	a	1136	G	C8-N9-C1'	-5.25	120.17	127.00
1	a	477	U	N3-C2-O2	-5.20	118.56	122.20
31	L	136	GLN	C-N-CA	5.19	134.67	121.70
35	P	134	LEU	CA-CB-CG	5.17	127.19	115.30
1	a	756	A	P-O3'-C3'	5.15	125.88	119.70
1	a	519	C	C6-N1-C1'	5.13	126.96	120.80
1	a	476	C	C2-N1-C1'	5.13	124.44	118.80
24	A	592	A	N1-C6-N6	-5.10	115.54	118.60
1	a	1110	A	P-O3'-C3'	5.07	125.78	119.70
1	a	1166	C	N1-C2-O2	5.07	121.94	118.90
1	a	1210	C	C5-C6-N1	5.07	123.53	121.00
24	A	308	U	C6-N1-C1'	-5.02	114.17	121.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	L	137	LYS	Peptide
19	s	36	ARG	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/249 (89%)	207 (93%)	15 (7%)	0	100	100
3	c	202/218 (93%)	171 (85%)	31 (15%)	0	100	100
4	d	197/200 (98%)	180 (91%)	17 (9%)	0	100	100
5	e	153/167 (92%)	142 (93%)	11 (7%)	0	100	100
6	f	91/97 (94%)	84 (92%)	7 (8%)	0	100	100
7	g	145/156 (93%)	122 (84%)	23 (16%)	0	100	100
8	h	129/132 (98%)	124 (96%)	5 (4%)	0	100	100
9	i	121/130 (93%)	111 (92%)	10 (8%)	0	100	100
10	j	94/102 (92%)	83 (88%)	10 (11%)	1 (1%)	14	46
11	k	112/129 (87%)	102 (91%)	10 (9%)	0	100	100
12	l	133/137 (97%)	126 (95%)	7 (5%)	0	100	100
13	m	112/121 (93%)	100 (89%)	12 (11%)	0	100	100
14	n	58/61 (95%)	52 (90%)	6 (10%)	0	100	100
15	o	85/89 (96%)	83 (98%)	2 (2%)	0	100	100
16	p	86/90 (96%)	82 (95%)	4 (5%)	0	100	100
17	q	79/87 (91%)	74 (94%)	5 (6%)	0	100	100
18	r	63/79 (80%)	59 (94%)	3 (5%)	1 (2%)	9	37
19	s	70/92 (76%)	54 (77%)	14 (20%)	2 (3%)	4	24
20	t	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
23	v	414/418 (99%)	384 (93%)	30 (7%)	0	100	100
26	C	271/277 (98%)	258 (95%)	13 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	D	204/209 (98%)	193 (95%)	11 (5%)	0	100	100
28	E	202/207 (98%)	189 (94%)	13 (6%)	0	100	100
29	F	173/179 (97%)	161 (93%)	12 (7%)	0	100	100
30	G	174/178 (98%)	163 (94%)	11 (6%)	0	100	100
31	L	141/145 (97%)	137 (97%)	3 (2%)	1 (1%)	22	57
32	M	120/122 (98%)	114 (95%)	6 (5%)	0	100	100
33	N	144/146 (99%)	137 (95%)	7 (5%)	0	100	100
34	O	132/144 (92%)	128 (97%)	4 (3%)	0	100	100
35	P	119/135 (88%)	113 (95%)	5 (4%)	1 (1%)	19	54
36	Q	117/119 (98%)	111 (95%)	6 (5%)	0	100	100
37	R	111/114 (97%)	106 (96%)	5 (4%)	0	100	100
38	S	116/119 (98%)	111 (96%)	4 (3%)	1 (1%)	17	52
39	T	99/102 (97%)	92 (93%)	7 (7%)	0	100	100
40	U	110/118 (93%)	105 (96%)	4 (4%)	1 (1%)	17	52
41	V	91/94 (97%)	84 (92%)	7 (8%)	0	100	100
42	W	98/103 (95%)	95 (97%)	2 (2%)	1 (1%)	15	49
43	Y	74/96 (77%)	67 (90%)	7 (10%)	0	100	100
44	Z	57/62 (92%)	52 (91%)	5 (9%)	0	100	100
45	1	58/63 (92%)	55 (95%)	3 (5%)	0	100	100
46	2	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
47	3	66/81 (82%)	53 (80%)	13 (20%)	0	100	100
48	4	51/57 (90%)	48 (94%)	3 (6%)	0	100	100
49	5	46/49 (94%)	46 (100%)	0	0	100	100
50	6	41/44 (93%)	41 (100%)	0	0	100	100
51	7	63/66 (96%)	58 (92%)	5 (8%)	0	100	100
52	8	34/37 (92%)	33 (97%)	1 (3%)	0	100	100
All	All	5610/5963 (94%)	5217 (93%)	384 (7%)	9 (0%)	50	79

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	s	9	PRO
31	L	137	LYS

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Mol	Chain	Res	Type
10	j	57	LYS
18	r	14	VAL
38	S	102	ASP
35	P	3	TYR
42	W	97	SER
19	s	12	ASP
40	U	5	VAL

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
2	b	138/214 (64%)	137 (99%)	1 (1%)	84 93
3	c	41/177 (23%)	41 (100%)	0	100 100
4	d	154/170 (91%)	154 (100%)	0	100 100
5	e	116/131 (88%)	116 (100%)	0	100 100
6	f	50/85 (59%)	50 (100%)	0	100 100
7	g	38/130 (29%)	38 (100%)	0	100 100
8	h	109/110 (99%)	109 (100%)	0	100 100
9	i	63/102 (62%)	62 (98%)	1 (2%)	62 84
10	j	35/93 (38%)	35 (100%)	0	100 100
11	k	83/100 (83%)	83 (100%)	0	100 100
12	l	105/118 (89%)	105 (100%)	0	100 100
13	m	13/102 (13%)	13 (100%)	0	100 100
14	n	41/52 (79%)	41 (100%)	0	100 100
15	o	72/81 (89%)	72 (100%)	0	100 100
16	p	78/80 (98%)	78 (100%)	0	100 100
17	q	65/78 (83%)	65 (100%)	0	100 100
18	r	58/67 (87%)	58 (100%)	0	100 100
19	s	21/78 (27%)	20 (95%)	1 (5%)	25 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
20	t	62/66 (94%)	62 (100%)	0	100 100
23	v	329/365 (90%)	327 (99%)	2 (1%)	86 94
26	C	221/225 (98%)	221 (100%)	0	100 100
27	D	159/171 (93%)	159 (100%)	0	100 100
28	E	170/174 (98%)	170 (100%)	0	100 100
29	F	114/155 (74%)	112 (98%)	2 (2%)	59 82
30	G	136/147 (92%)	136 (100%)	0	100 100
31	L	120/121 (99%)	120 (100%)	0	100 100
32	M	101/101 (100%)	101 (100%)	0	100 100
33	N	115/115 (100%)	115 (100%)	0	100 100
34	O	105/113 (93%)	105 (100%)	0	100 100
35	P	102/111 (92%)	102 (100%)	0	100 100
36	Q	83/97 (86%)	83 (100%)	0	100 100
37	R	92/99 (93%)	92 (100%)	0	100 100
38	S	96/97 (99%)	94 (98%)	2 (2%)	53 79
39	T	82/82 (100%)	82 (100%)	0	100 100
40	U	93/97 (96%)	93 (100%)	0	100 100
41	V	83/84 (99%)	80 (96%)	3 (4%)	35 67
42	W	78/88 (89%)	78 (100%)	0	100 100
43	Y	61/76 (80%)	61 (100%)	0	100 100
44	Z	50/53 (94%)	50 (100%)	0	100 100
45	1	53/55 (96%)	53 (100%)	0	100 100
46	2	50/52 (96%)	50 (100%)	0	100 100
47	3	27/73 (37%)	27 (100%)	0	100 100
48	4	47/50 (94%)	47 (100%)	0	100 100
49	5	44/48 (92%)	44 (100%)	0	100 100
50	6	39/39 (100%)	39 (100%)	0	100 100
51	7	55/56 (98%)	55 (100%)	0	100 100
52	8	35/35 (100%)	35 (100%)	0	100 100
All	All	4082/5013 (81%)	4070 (100%)	12 (0%)	92 96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	169	GLU
9	i	106	ARG
19	s	78	ARG
23	v	45	ARG
23	v	208	THR
29	F	3	ARG
29	F	78	ARG
38	S	101	ASN
38	S	102	ASP
41	V	42	ILE
41	V	43	GLU
41	V	44	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	15	HIS
4	d	59	HIS
4	d	73	ASN
4	d	85	ASN
4	d	96	ASN
4	d	112	GLN
4	d	116	HIS
5	e	71	ASN
8	h	22	HIS
9	i	81	HIS
12	l	86	ASN
15	o	18	HIS
16	p	85	ASN
17	q	5	ASN
17	q	49	HIS
18	r	56	GLN
19	s	69	HIS
20	t	21	ASN
20	t	24	GLN
23	v	67	GLN
23	v	117	GLN
23	v	119	GLN
23	v	148	ASN
23	v	203	ASN
23	v	264	HIS
26	C	53	HIS
26	C	194	GLN

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Mol	Chain	Res	Type
27	D	50	GLN
27	D	68	HIS
27	D	152	ASN
28	E	119	ASN
30	G	20	ASN
30	G	51	ASN
30	G	97	GLN
31	L	97	ASN
31	L	136	GLN
32	M	4	GLN
33	N	27	ASN
39	T	90	GLN
40	U	107	HIS
41	V	73	ASN
42	W	67	ASN
43	Y	20	ASN
44	Z	16	ASN
44	Z	34	GLN
47	3	55	HIS
49	5	16	ASN
49	5	26	ASN
51	7	35	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1511/1550 (97%)	281 (18%)	0
21	x	71/76 (93%)	17 (23%)	0
22	w	7/21 (33%)	5 (71%)	0
24	A	2895/2932 (98%)	473 (16%)	28 (0%)
25	B	113/116 (97%)	11 (9%)	0
All	All	4597/4695 (97%)	787 (17%)	28 (0%)

All (787) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	22	G
1	a	31	G
1	a	32	A
1	a	39	G

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Mol	Chain	Res	Type
1	a	44	G
1	a	47	C
1	a	48	C
1	a	51	A
1	a	66	A
1	a	68	G
1	a	69	A
1	a	70	A
1	a	71	C
1	a	73	G
1	a	95	A
1	a	96	G
1	a	97	U
1	a	99	A
1	a	100	G
1	a	101	U
1	a	107	A
1	a	114	A
1	a	119	C
1	a	128	A
1	a	130	C
1	a	143	U
1	a	154	C
1	a	159	A
1	a	160	A
1	a	162	C
1	a	164	G
1	a	173	A
1	a	182	U
1	a	189	U
1	a	195	A
1	a	209	A
1	a	211	A
1	a	212	G
1	a	218	U
1	a	219	U
1	a	220	C
1	a	222	G
1	a	239	G
1	a	249	G
1	a	253	U
1	a	255	G

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Mol	Chain	Res	Type
1	a	259	G
1	a	265	A
1	a	274	G
1	a	275	C
1	a	288	C
1	a	297	G
1	a	329	A
1	a	336	C
1	a	340	G
1	a	351	U
1	a	353	C
1	a	354	G
1	a	355	G
1	a	360	C
1	a	362	G
1	a	372	A
1	a	373	U
1	a	375	U
1	a	380	C
1	a	381	A
1	a	392	G
1	a	400	G
1	a	412	G
1	a	414	G
1	a	416	A
1	a	417	U
1	a	420	A
1	a	421	G
1	a	423	A
1	a	429	U
1	a	430	C
1	a	431	G
1	a	432	G
1	a	437	U
1	a	441	G
1	a	447	U
1	a	454	A
1	a	456	A
1	a	457	A
1	a	460	A
1	a	461	C
1	a	462	A

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Mol	Chain	Res	Type
1	a	463	A
1	a	467	U
1	a	468	A
1	a	469	A
1	a	471	A
1	a	473	U
1	a	483	U
1	a	486	C
1	a	487	U
1	a	488	U
1	a	489	G
1	a	492	G
1	a	493	G
1	a	494	U
1	a	503	A
1	a	505	A
1	a	508	G
1	a	511	A
1	a	513	G
1	a	514	G
1	a	515	C
1	a	519	C
1	a	526	C
1	a	529	G
1	a	535	G
1	a	538	G
1	a	539	U
1	a	541	A
1	a	552	G
1	a	553	C
1	a	555	A
1	a	567	A
1	a	570	U
1	a	572	U
1	a	576	G
1	a	580	A
1	a	581	A
1	a	584	C
1	a	585	G
1	a	587	G
1	a	596	G
1	a	604	A

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Mol	Chain	Res	Type
1	a	628	U
1	a	643	A
1	a	657	G
1	a	661	G
1	a	673	A
1	a	679	G
1	a	683	A
1	a	695	A
1	a	702	A
1	a	711	G
1	a	712	A
1	a	729	A
1	a	731	U
1	a	739	G
1	a	741	G
1	a	742	A
1	a	750	G
1	a	757	A
1	a	763	G
1	a	768	G
1	a	786	G
1	a	789	A
1	a	801	U
1	a	802	A
1	a	825	C
1	a	829	G
1	a	848	G
1	a	855	C
1	a	881	A
1	a	923	A
1	a	935	G
1	a	936	G
1	a	940	C
1	a	943	C
1	a	944	A
1	a	954	G
1	a	957	C
1	a	965	U
1	a	966	U
1	a	969	U
1	a	970	U
1	a	974	A

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Mol	Chain	Res	Type
1	a	977	A
1	a	978	A
1	a	980	G
1	a	981	C
1	a	982	G
1	a	984	A
1	a	985	G
1	a	986	A
1	a	992	A
1	a	1001	U
1	a	1002	G
1	a	1003	A
1	a	1005	A
1	a	1010	U
1	a	1012	G
1	a	1013	A
1	a	1018	U
1	a	1022	G
1	a	1032	U
1	a	1033	U
1	a	1035	C
1	a	1046	C
1	a	1048	A
1	a	1050	G
1	a	1051	U
1	a	1052	G
1	a	1053	A
1	a	1055	A
1	a	1062	G
1	a	1063	C
1	a	1066	G
1	a	1067	G
1	a	1069	U
1	a	1074	U
1	a	1075	C
1	a	1090	G
1	a	1094	U
1	a	1103	G
1	a	1104	U
1	a	1110	A
1	a	1111	A
1	a	1133	G

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Mol	Chain	Res	Type
1	a	1135	U
1	a	1141	C
1	a	1142	A
1	a	1147	G
1	a	1148	U
1	a	1156	U
1	a	1165	A
1	a	1167	U
1	a	1176	A
1	a	1178	G
1	a	1181	G
1	a	1191	G
1	a	1203	A
1	a	1204	A
1	a	1208	A
1	a	1209	U
1	a	1219	U
1	a	1220	A
1	a	1231	U
1	a	1232	A
1	a	1233	C
1	a	1234	A
1	a	1235	C
1	a	1245	A
1	a	1264	C
1	a	1267	G
1	a	1274	C
1	a	1276	A
1	a	1287	A
1	a	1293	U
1	a	1294	A
1	a	1295	A
1	a	1306	A
1	a	1307	G
1	a	1308	U
1	a	1309	U
1	a	1312	G
1	a	1325	A
1	a	1329	C
1	a	1342	C
1	a	1343	C
1	a	1355	U

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Mol	Chain	Res	Type
1	a	1368	G
1	a	1371	U
1	a	1377	G
1	a	1388	U
1	a	1401	A
1	a	1405	A
1	a	1429	U
1	a	1447	U
1	a	1449	G
1	a	1453	A
1	a	1456	C
1	a	1495	G
1	a	1498	U
1	a	1500	A
1	a	1502	G
1	a	1514	U
1	a	1515	A
1	a	1525	G
1	a	1527	A
1	a	1537	G
1	a	1538	G
1	a	1539	A
1	a	1542	A
1	a	1545	U
21	x	7	A
21	x	8	4SU
21	x	9	A
21	x	10	G
21	x	19	G
21	x	26	A
21	x	29	G
21	x	30	G
21	x	35	A
21	x	36	A
21	x	44	G
21	x	45	U
21	x	46	7MG
21	x	48	C
21	x	52	G
21	x	73	A
21	x	76	A
22	w	12	A

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Mol	Chain	Res	Type
22	w	14	U
22	w	16	C
22	w	17	U
22	w	18	A
24	A	13	A
24	A	14	A
24	A	28	A
24	A	34	U
24	A	46	C
24	A	51	G
24	A	60	G
24	A	71	A
24	A	75	G
24	A	89	U
24	A	93	U
24	A	100	U
24	A	101	G
24	A	117	A
24	A	119	U
24	A	125	A
24	A	126	A
24	A	130	A
24	A	139	A
24	A	140	G
24	A	145	A
24	A	156	A
24	A	161	A
24	A	162	A
24	A	164	A
24	A	186	C
24	A	187	C
24	A	198	A
24	A	199	A
24	A	201	A
24	A	215	A
24	A	218	A
24	A	223	A
24	A	224	A
24	A	228	A
24	A	230	A
24	A	231	A
24	A	232	U

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Mol	Chain	Res	Type
24	A	235	A
24	A	241	U
24	A	247	G
24	A	250	G
24	A	257	A
24	A	267	A
24	A	274	A
24	A	282	G
24	A	283	C
24	A	285	U
24	A	287	C
24	A	289	U
24	A	290	C
24	A	295	G
24	A	296	G
24	A	299	G
24	A	300	U
24	A	301	A
24	A	307	C
24	A	308	U
24	A	309	C
24	A	313	A
24	A	320	U
24	A	323	A
24	A	345	G
24	A	354	A
24	A	360	G
24	A	372	A
24	A	373	A
24	A	374	C
24	A	375	A
24	A	388	A
24	A	396	U
24	A	404	A
24	A	406	A
24	A	410	G
24	A	411	A
24	A	417	A
24	A	418	G
24	A	420	A
24	A	432	G
24	A	433	U

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Mol	Chain	Res	Type
24	A	457	G
24	A	458	A
24	A	470	G
24	A	490	C
24	A	501	C
24	A	503	A
24	A	513	G
24	A	527	G
24	A	536	A
24	A	550	A
24	A	552	U
24	A	553	U
24	A	554	C
24	A	555	C
24	A	567	G
24	A	576	U
24	A	577	A
24	A	578	G
24	A	591	A
24	A	592	A
24	A	593	U
24	A	594	G
24	A	606	G
24	A	616	G
24	A	618	A
24	A	646	A
24	A	657	A
24	A	658	A
24	A	659	A
24	A	666	A
24	A	667	G
24	A	672	A
24	A	679	G
24	A	682	A
24	A	689	A
24	A	690	U
24	A	699	U
24	A	700	A
24	A	718	C
24	A	732	U
24	A	760	U
24	A	763	U

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Mol	Chain	Res	Type
24	A	764	A
24	A	776	U
24	A	786	C
24	A	793	U
24	A	794	G
24	A	810	A
24	A	811	G
24	A	821	G
24	A	823	G
24	A	825	A
24	A	828	A
24	A	830	U
24	A	836	U
24	A	838	G
24	A	851	G
24	A	858	C
24	A	865	A
24	A	873	U
24	A	874	U
24	A	891	U
24	A	892	A
24	A	893	A
24	A	906	G
24	A	913	A
24	A	928	G
24	A	929	G
24	A	944	C
24	A	945	C
24	A	954	A
24	A	957	A
24	A	959	C
24	A	964	A
24	A	973	U
24	A	974	A
24	A	976	U
24	A	979	U
24	A	980	A
24	A	987	A
24	A	991	A
24	A	992	G
24	A	1007	G
24	A	1020	A

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Mol	Chain	Res	Type
24	A	1025	A
24	A	1029	A
24	A	1042	A
24	A	1051	C
24	A	1058	U
24	A	1059	A
24	A	1072	A
24	A	1073	A
24	A	1079	U
24	A	1092	A
24	A	1093	G
24	A	1106	U
24	A	1113	A
24	A	1115	A
24	A	1116	A
24	A	1117	G
24	A	1123	A
24	A	1130	A
24	A	1131	A
24	A	1134	A
24	A	1141	A
24	A	1142	A
24	A	1157	A
24	A	1158	G
24	A	1161	A
24	A	1173	A
24	A	1174	A
24	A	1178	U
24	A	1179	A
24	A	1181	C
24	A	1182	G
24	A	1188	A
24	A	1203	A
24	A	1230	G
24	A	1249	A
24	A	1250	G
24	A	1252	G
24	A	1254	G
24	A	1257	G
24	A	1265	A
24	A	1283	G
24	A	1298	A

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Mol	Chain	Res	Type
24	A	1301	G
24	A	1302	C
24	A	1311	G
24	A	1316	G
24	A	1317	A
24	A	1320	G
24	A	1344	A
24	A	1345	A
24	A	1365	A
24	A	1369	C
24	A	1373	U
24	A	1394	C
24	A	1396	U
24	A	1409	A
24	A	1423	U
24	A	1429	A
24	A	1430	C
24	A	1435	A
24	A	1439	A
24	A	1457	A
24	A	1462	U
24	A	1463	U
24	A	1464	A
24	A	1465	A
24	A	1466	C
24	A	1469	A
24	A	1470	U
24	A	1478	C
24	A	1494	A
24	A	1502	A
24	A	1505	G
24	A	1509	A
24	A	1519	A
24	A	1528	G
24	A	1529	U
24	A	1530	G
24	A	1531	U
24	A	1532	G
24	A	1533	A
24	A	1534	G
24	A	1536	A
24	A	1539	A

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Mol	Chain	Res	Type
24	A	1542	C
24	A	1546	U
24	A	1553	C
24	A	1556	G
24	A	1557	C
24	A	1564	U
24	A	1570	G
24	A	1571	U
24	A	1573	A
24	A	1574	U
24	A	1575	G
24	A	1579	A
24	A	1594	G
24	A	1618	A
24	A	1621	A
24	A	1630	U
24	A	1638	G
24	A	1656	C
24	A	1657	A
24	A	1659	A
24	A	1695	A
24	A	1696	G
24	A	1697	C
24	A	1700	G
24	A	1703	A
24	A	1704	A
24	A	1723	G
24	A	1724	C
24	A	1749	A
24	A	1761	A
24	A	1762	U
24	A	1763	U
24	A	1764	A
24	A	1771	A
24	A	1773	G
24	A	1781	G
24	A	1782	A
24	A	1783	G
24	A	1787	C
24	A	1789	G
24	A	1796	G
24	A	1797	G

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Mol	Chain	Res	Type
24	A	1806	A
24	A	1809	G
24	A	1815	C
24	A	1833	C
24	A	1834	A
24	A	1842	A
24	A	1849	C
24	A	1862	A
24	A	1880	A
24	A	1886	A
24	A	1887	A
24	A	1889	A
24	A	1891	G
24	A	1892	A
24	A	1899	A
24	A	1903	U
24	A	1939	G
24	A	1946	A
24	A	1947	C
24	A	1949	A
24	A	1951	A
24	A	1952	A
24	A	1962	G
24	A	1963	G
24	A	1973	U
24	A	1988	U
24	A	1996	C
24	A	1998	C
24	A	2000	C
24	A	2003	A
24	A	2004	A
24	A	2005	G
24	A	2024	U
24	A	2026	U
24	A	2027	C
24	A	2030	A
24	A	2031	A
24	A	2056	A
24	A	2064	A
24	A	2065	G
24	A	2066	A
24	A	2067	U

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Mol	Chain	Res	Type
24	A	2072	G
24	A	2076	C
24	A	2085	G
24	A	2088	C
24	A	2089	G
24	A	2093	A
24	A	2094	G
24	A	2095	A
24	A	2096	C
24	A	2102	G
24	A	2126	G
24	A	2127	A
24	A	2133	U
24	A	2144	U
24	A	2149	G
24	A	2150	A
24	A	2152	A
24	A	2165	A
24	A	2188	A
24	A	2190	G
24	A	2191	A
24	A	2192	G
24	A	2193	G
24	A	2198	G
24	A	2205	U
24	A	2206	A
24	A	2223	A
24	A	2224	C
24	A	2231	A
24	A	2236	G
24	A	2237	C
24	A	2245	A
24	A	2256	A
24	A	2258	A
24	A	2259	C
24	A	2271	G
24	A	2272	G
24	A	2312	G
24	A	2316	C
24	A	2319	A
24	A	2320	A
24	A	2321	A

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Mol	Chain	Res	Type
24	A	2329	U
24	A	2338	A
24	A	2341	G
24	A	2343	A
24	A	2344	A
24	A	2353	A
24	A	2355	A
24	A	2358	G
24	A	2360	A
24	A	2367	C
24	A	2368	A
24	A	2380	C
24	A	2383	C
24	A	2394	A
24	A	2412	G
24	A	2416	G
24	A	2418	C
24	A	2420	U
24	A	2435	U
24	A	2439	C
24	A	2447	G
24	A	2455	C
24	A	2457	C
24	A	2458	A
24	A	2462	G
24	A	2463	A
24	A	2473	C
24	A	2474	C
24	A	2481	A
24	A	2492	A
24	A	2498	C
24	A	2507	C
24	A	2509	A
24	A	2514	G
24	A	2524	U
24	A	2531	C
24	A	2535	G
24	A	2536	A
24	A	2538	G
24	A	2546	G
24	A	2548	C
24	A	2551	A

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Mol	Chain	Res	Type
24	A	2562	G
24	A	2568	G
24	A	2577	G
24	A	2580	U
24	A	2587	U
24	A	2599	A
24	A	2600	G
24	A	2605	A
24	A	2606	C
24	A	2607	G
24	A	2615	G
24	A	2616	G
24	A	2642	U
24	A	2643	C
24	A	2646	U
24	A	2648	U
24	A	2663	G
24	A	2678	G
24	A	2679	C
24	A	2722	U
24	A	2724	C
24	A	2747	G
24	A	2755	G
24	A	2759	U
24	A	2766	C
24	A	2768	G
24	A	2781	A
24	A	2790	A
24	A	2798	A
24	A	2799	G
24	A	2802	C
24	A	2810	G
24	A	2811	A
24	A	2812	U
24	A	2813	G
24	A	2822	C
24	A	2827	C
24	A	2828	U
24	A	2830	C
24	A	2832	G
24	A	2835	A
24	A	2837	U

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Mol	Chain	Res	Type
24	A	2849	A
24	A	2852	A
24	A	2857	C
24	A	2862	A
24	A	2864	A
24	A	2872	G
24	A	2877	G
24	A	2890	U
24	A	2896	G
24	A	2901	G
24	A	2902	A
24	A	2909	C
24	A	2920	A
24	A	2922	G
24	A	2930	C
25	B	10	U
25	B	23	U
25	B	24	C
25	B	33	U
25	B	40	C
25	B	54	U
25	B	55	A
25	B	84	G
25	B	87	U
25	B	88	C
25	B	107	G

All (28) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	A	27	G
24	A	88	G
24	A	92	G
24	A	139	A
24	A	553	U
24	A	688	A
24	A	756	A
24	A	809	G
24	A	847	G
24	A	854	G
24	A	1017	C
24	A	1172	A

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Mol	Chain	Res	Type
24	A	1248	A
24	A	1249	A
24	A	1497	G
24	A	1528	G
24	A	1532	G
24	A	1533	A
24	A	1569	U
24	A	1886	A
24	A	1888	G
24	A	2320	A
24	A	2438	G
24	A	2472	A
24	A	2615	G
24	A	2789	U
24	A	2809	A
24	A	2908	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
21	5MU	x	54	21	19,22,23	1.39	5 (26%)	28,32,35	2.02	6 (21%)
21	PSU	x	39	21	18,21,22	1.27	2 (11%)	22,30,33	2.08	4 (18%)
21	PSU	x	55	21	18,21,22	1.33	2 (11%)	22,30,33	1.90	3 (13%)
21	MIA	x	37	21	24,31,32	2.22	3 (12%)	26,44,47	2.52	9 (34%)
21	7MG	x	46	21	22,26,27	1.31	3 (13%)	29,39,42	2.58	7 (24%)
21	PSU	x	32	21	18,21,22	1.34	2 (11%)	22,30,33	1.89	3 (13%)
21	4SU	x	8	21	18,21,22	1.77	5 (27%)	26,30,33	2.34	5 (19%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	5MU	x	54	21	-	0/7/25/26	0/2/2/2
21	PSU	x	39	21	-	0/7/25/26	0/2/2/2
21	PSU	x	55	21	-	0/7/25/26	0/2/2/2
21	MIA	x	37	21	-	2/11/33/34	0/3/3/3
21	7MG	x	46	21	-	5/7/37/38	0/3/3/3
21	PSU	x	32	21	-	0/7/25/26	0/2/2/2
21	4SU	x	8	21	-	0/7/25/26	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	x	37	MIA	C13-C14	7.11	1.52	1.32
21	x	37	MIA	C2-S10	-6.84	1.69	1.75
21	x	8	4SU	C4-S4	-4.56	1.59	1.68
21	x	8	4SU	C4-N3	-3.30	1.34	1.37
21	x	55	PSU	C6-C5	3.12	1.39	1.35
21	x	46	7MG	C5-C4	2.99	1.47	1.38
21	x	39	PSU	C6-C5	2.89	1.38	1.35
21	x	32	PSU	C6-C5	2.76	1.38	1.35
21	x	46	7MG	C4-N9	-2.76	1.34	1.37
21	x	54	5MU	C6-C5	2.69	1.39	1.34
21	x	32	PSU	C4-N3	-2.64	1.33	1.38
21	x	55	PSU	C4-N3	-2.61	1.34	1.38
21	x	54	5MU	C4-N3	-2.57	1.34	1.38
21	x	8	4SU	C5-C4	-2.51	1.39	1.42
21	x	37	MIA	C5-C4	2.50	1.47	1.40
21	x	46	7MG	C6-N1	-2.39	1.34	1.38
21	x	54	5MU	C2-N1	2.32	1.42	1.38
21	x	39	PSU	C4-N3	-2.31	1.34	1.38
21	x	54	5MU	C4-C5	2.24	1.48	1.44
21	x	54	5MU	C6-N1	-2.17	1.34	1.38
21	x	8	4SU	C2-N1	2.11	1.41	1.38
21	x	8	4SU	C2-N3	-2.08	1.34	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	x	46	7MG	N9-C4-N3	9.14	139.14	125.47
21	x	37	MIA	C12-C13-C14	-8.03	111.52	127.14
21	x	8	4SU	C4-N3-C2	-7.13	120.41	127.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	x	39	PSU	N1-C2-N3	6.32	122.29	115.13
21	x	8	4SU	C5-C4-N3	6.02	120.27	114.69
21	x	55	PSU	N1-C2-N3	5.94	121.86	115.13
21	x	32	PSU	N1-C2-N3	5.88	121.79	115.13
21	x	46	7MG	C5-C4-N3	-5.60	117.45	128.13
21	x	46	7MG	N9-C8-N7	-5.08	96.12	103.38
21	x	54	5MU	C4-N3-C2	-4.94	120.95	127.35
21	x	54	5MU	N3-C2-N1	4.83	121.31	114.89
21	x	39	PSU	C4-N3-C2	-4.59	119.72	126.34
21	x	46	7MG	C2-N3-C4	4.37	120.09	112.30
21	x	37	MIA	C2-N3-C4	4.29	121.24	115.32
21	x	39	PSU	O2-C2-N1	-4.23	118.13	122.79
21	x	54	5MU	C5-C4-N3	4.23	118.92	115.31
21	x	8	4SU	N3-C2-N1	4.19	120.45	114.89
21	x	37	MIA	C16-C14-C13	-4.08	110.86	122.65
21	x	54	5MU	O4-C4-C5	-4.06	120.20	124.90
21	x	55	PSU	C4-N3-C2	-4.04	120.51	126.34
21	x	8	4SU	C5-C4-S4	-4.01	119.31	124.47
21	x	37	MIA	C15-C14-C13	-3.96	111.21	122.65
21	x	32	PSU	O2-C2-N1	-3.87	118.53	122.79
21	x	32	PSU	C4-N3-C2	-3.82	120.84	126.34
21	x	37	MIA	C5-C6-N1	-3.63	117.79	120.81
21	x	55	PSU	O2-C2-N1	-3.46	118.98	122.79
21	x	54	5MU	C5-C6-N1	-3.38	119.86	123.34
21	x	37	MIA	C4-C5-N7	-2.76	106.52	109.40
21	x	46	7MG	C5-C6-N1	2.76	115.86	110.99
21	x	37	MIA	C11-S10-C2	-2.73	100.23	102.27
21	x	37	MIA	C2-N1-C6	2.65	121.93	117.19
21	x	46	7MG	C5-C4-N9	-2.27	103.40	106.35
21	x	37	MIA	N3-C2-N1	-2.23	122.88	126.98
21	x	46	7MG	O6-C6-C5	-2.19	122.18	127.54
21	x	39	PSU	C5-C6-N1	-2.03	119.07	122.11
21	x	8	4SU	C3'-C2'-C1'	2.02	105.27	101.43
21	x	54	5MU	O2-C2-N1	-2.00	120.12	122.79

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	x	37	MIA	C12-C13-C14-C16
21	x	46	7MG	O4'-C4'-C5'-O5'
21	x	46	7MG	O4'-C1'-N9-C4

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Mol	Chain	Res	Type	Atoms
21	x	46	7MG	C3'-C4'-C5'-O5'
21	x	46	7MG	O4'-C1'-N9-C8
21	x	37	MIA	N6-C12-C13-C14
21	x	46	7MG	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 480 ligands modelled in this entry, 479 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	GCP	v	502	53	27,34,34	1.42	5 (18%)	34,54,54	1.87	7 (20%)

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	GCP	v	502	53	-	5/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	502	GCP	C5-C6	3.77	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	502	GCP	PG-O3G	2.87	1.61	1.54
55	v	502	GCP	PG-O2G	2.67	1.61	1.54
55	v	502	GCP	PB-O3A	2.34	1.61	1.58
55	v	502	GCP	C5-C4	2.16	1.46	1.40

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	v	502	GCP	C2-N3-C4	4.39	120.37	115.36
55	v	502	GCP	C4-C5-C6	-4.30	116.69	120.80
55	v	502	GCP	C2-N1-C6	4.06	122.39	115.93
55	v	502	GCP	C5-C6-N1	-3.98	117.99	123.43
55	v	502	GCP	PB-O3A-PA	-3.43	121.69	132.56
55	v	502	GCP	N3-C2-N1	-3.20	122.96	127.22
55	v	502	GCP	C4-C5-N7	-2.58	106.71	109.40

There are no chirality outliers.

All (5) torsion outliers are listed below:

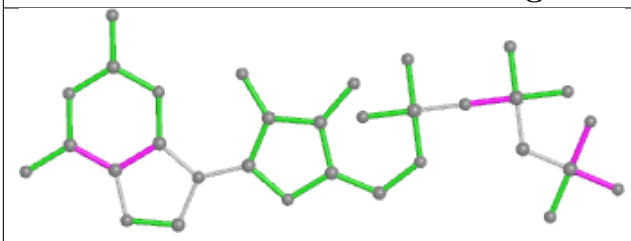
Mol	Chain	Res	Type	Atoms
55	v	502	GCP	C5'-O5'-PA-O1A
55	v	502	GCP	C3'-C4'-C5'-O5'
55	v	502	GCP	O4'-C4'-C5'-O5'
55	v	502	GCP	C5'-O5'-PA-O3A
55	v	502	GCP	C5'-O5'-PA-O2A

There are no ring outliers.

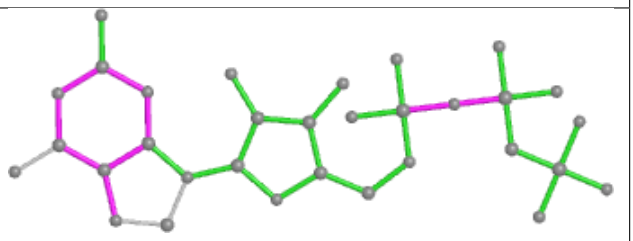
No monomer is involved in short contacts.

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.

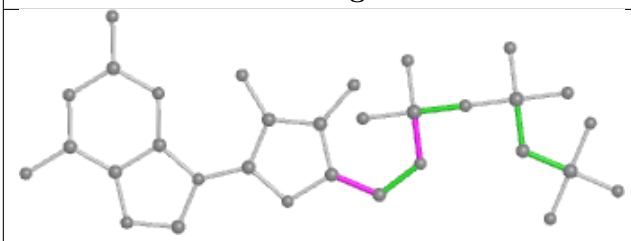
Ligand GCP v 502



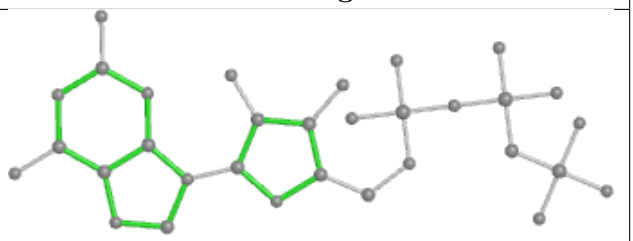
Bond lengths



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.

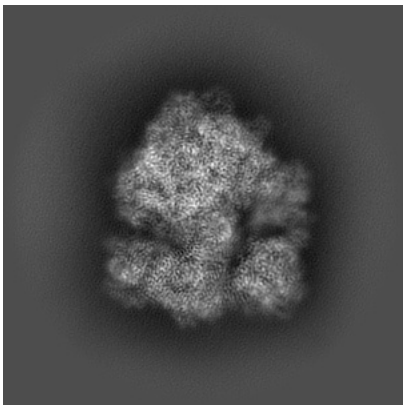
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42576. These allow visual inspection of the internal detail of the map and identification of artifacts.

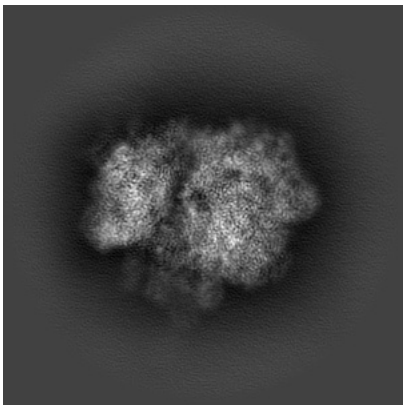
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

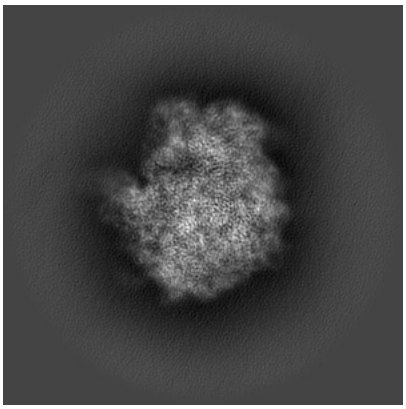
6.1.1 Primary map



X

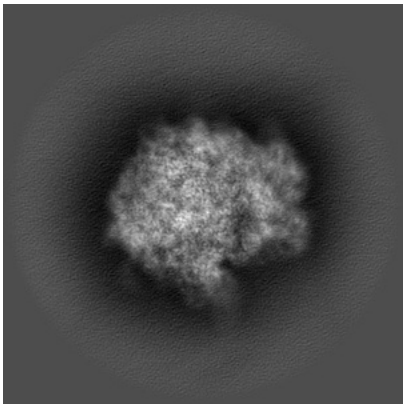


Y

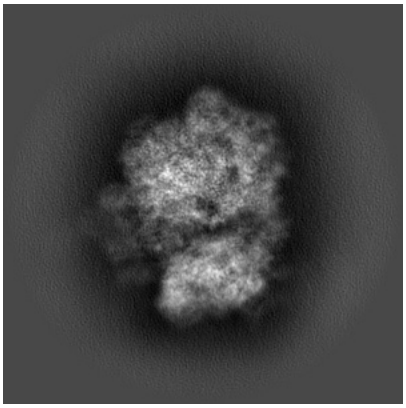


Z

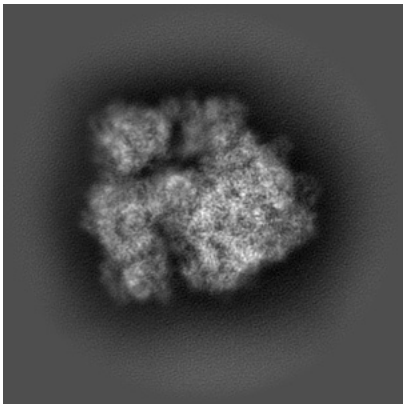
6.1.2 Raw map



X



Y

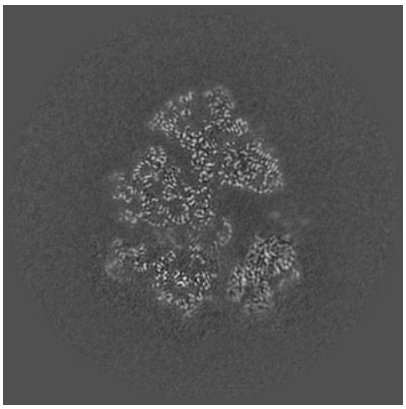


Z

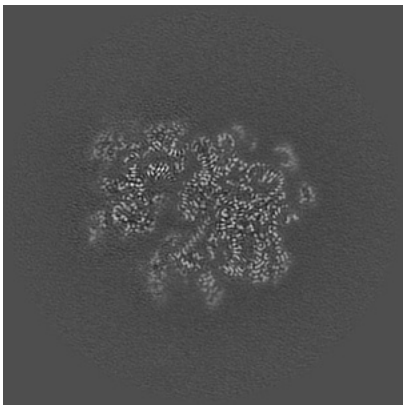
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

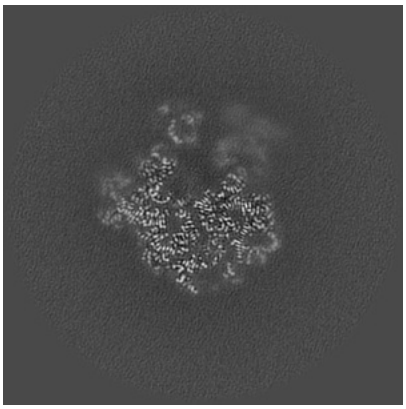
6.2.1 Primary map



X Index: 256

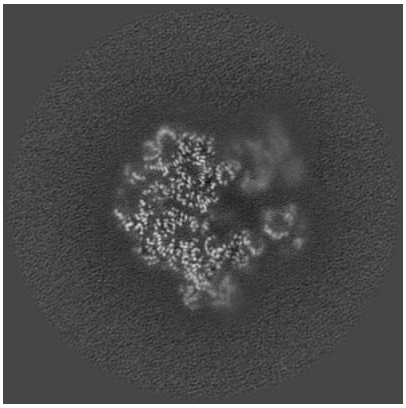


Y Index: 256

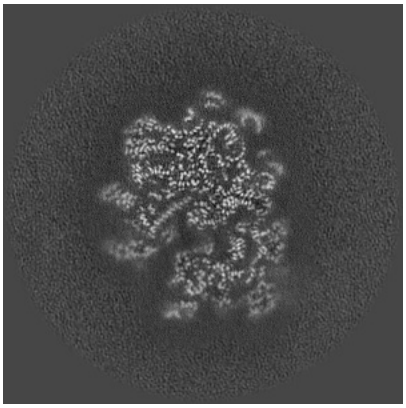


Z Index: 256

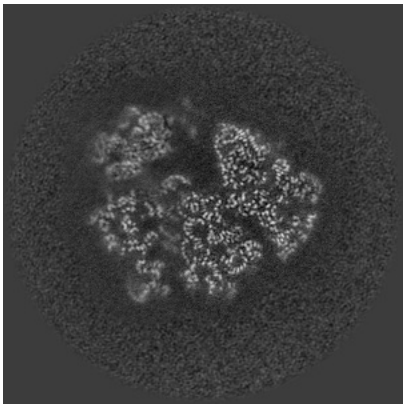
6.2.2 Raw map



X Index: 256



Y Index: 256

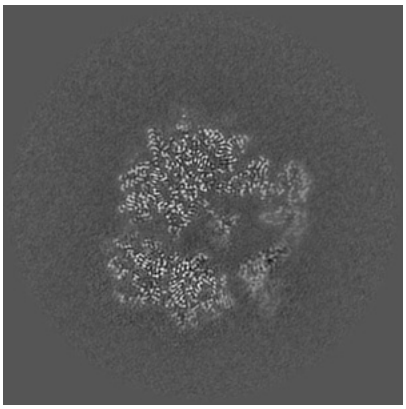


Z Index: 256

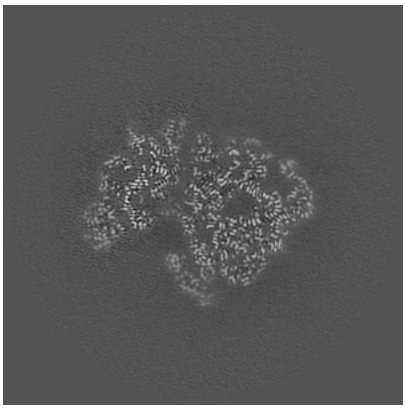
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

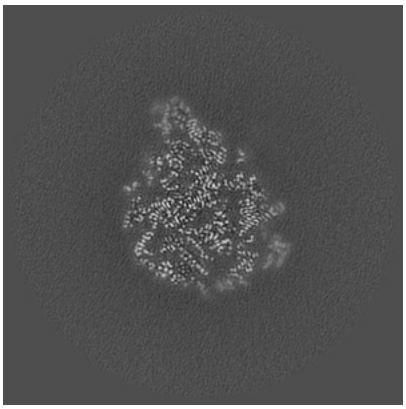
6.3.1 Primary map



X Index: 230

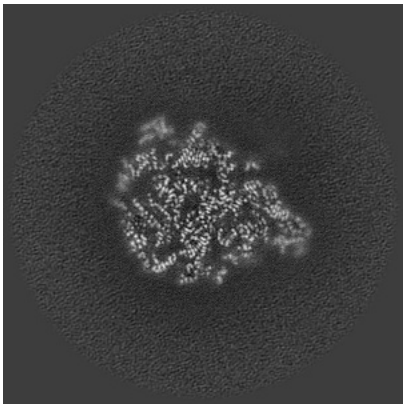


Y Index: 235

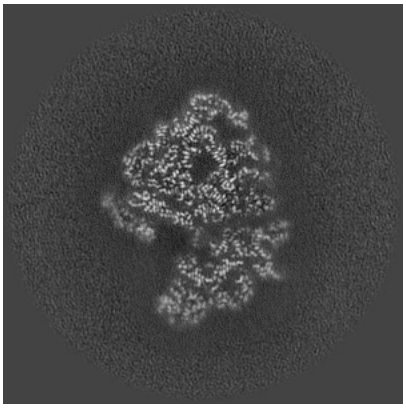


Z Index: 296

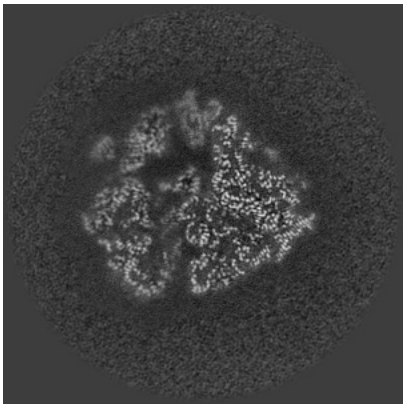
6.3.2 Raw map



X Index: 296



Y Index: 234

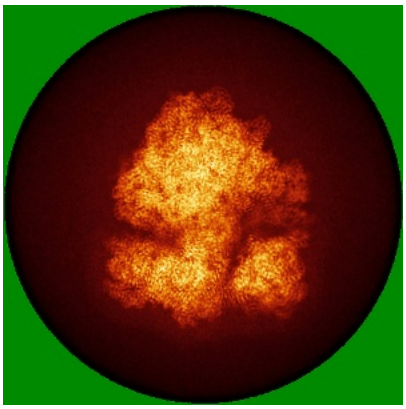


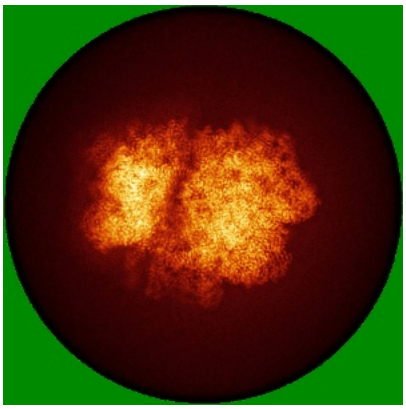
Z Index: 244

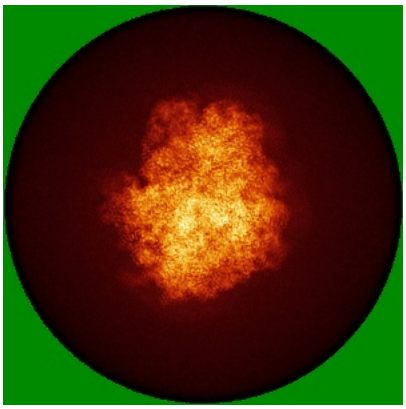
The images above show the largest variance slices of the map in three orthogonal directions.

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

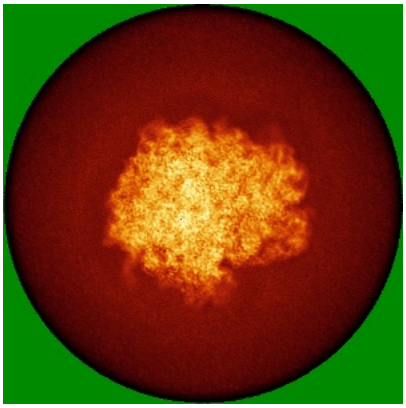
6.4.1 Primary map

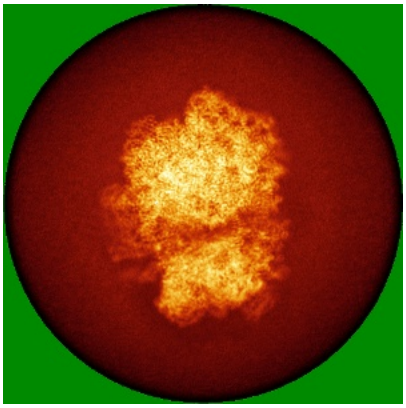

X

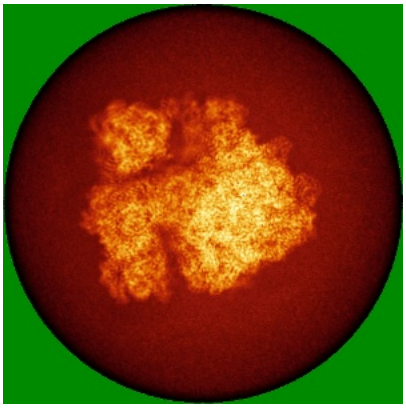

Y


Z

6.4.2 Raw map


X

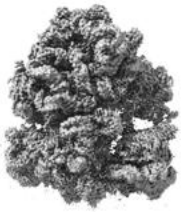

Y


Z

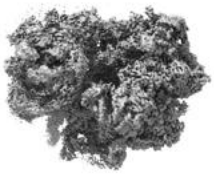
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

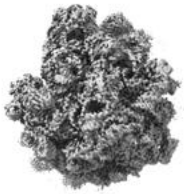
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.4. 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.

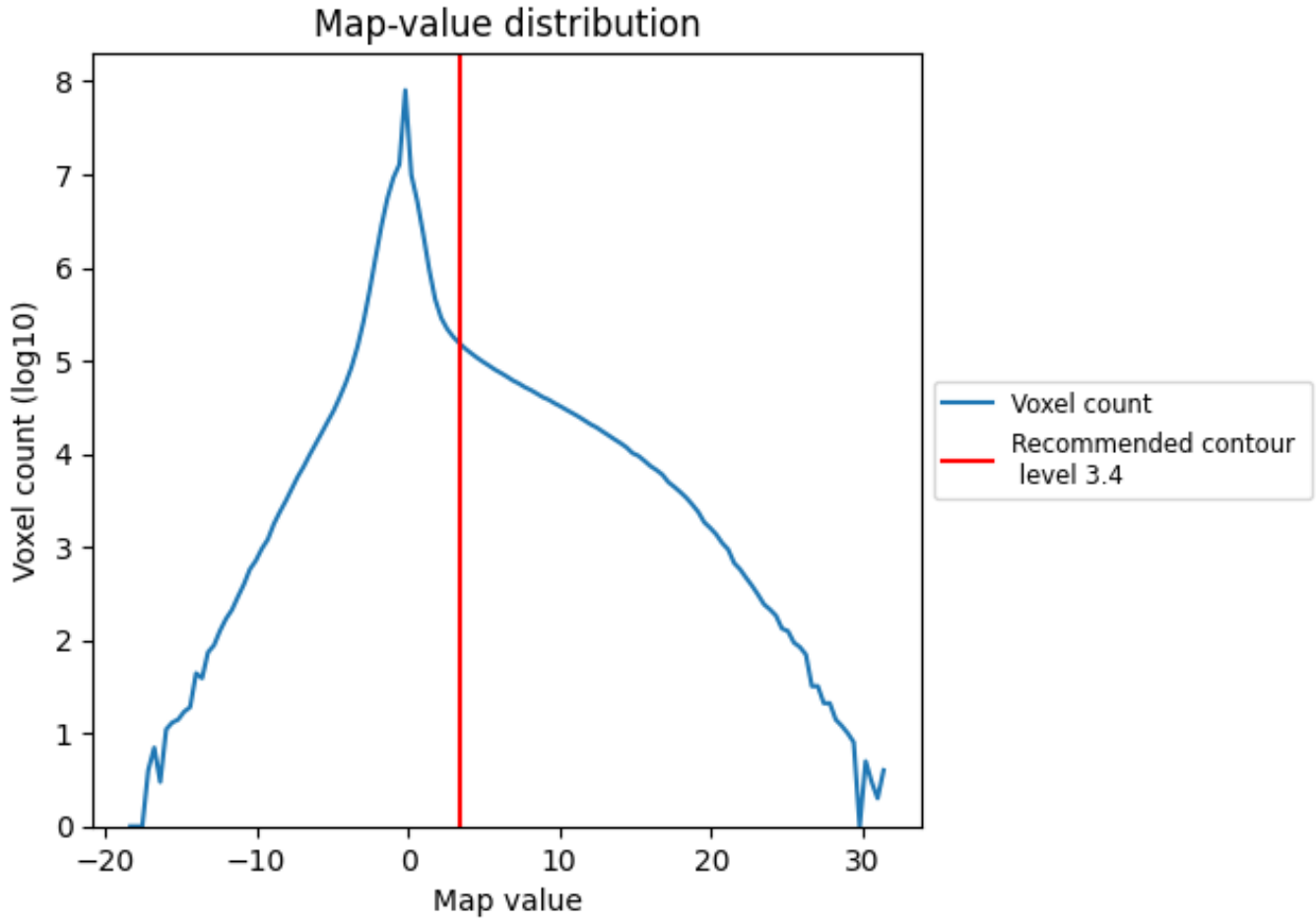
6.6 Mask visualisation (i)

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

7 Map analysis

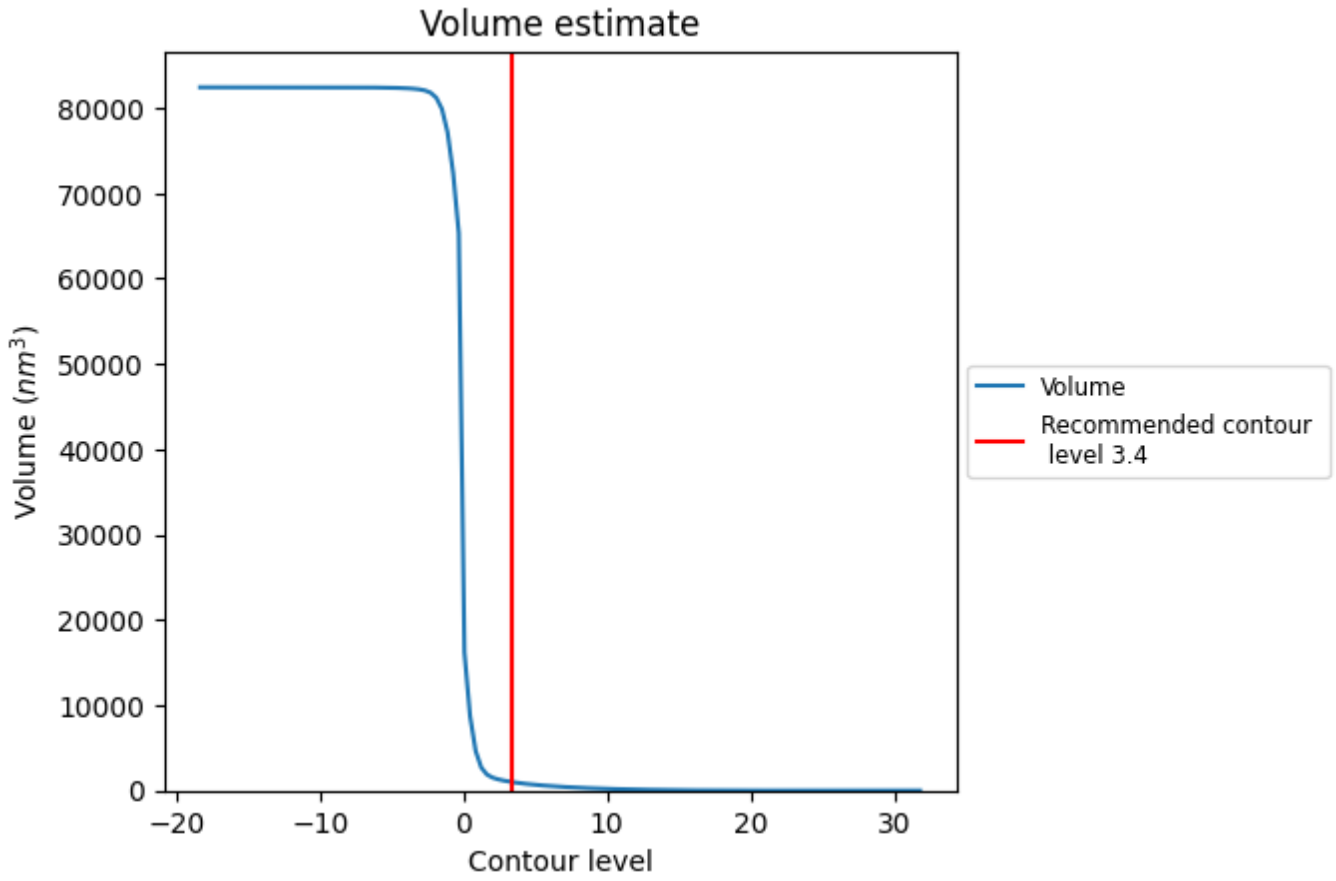
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

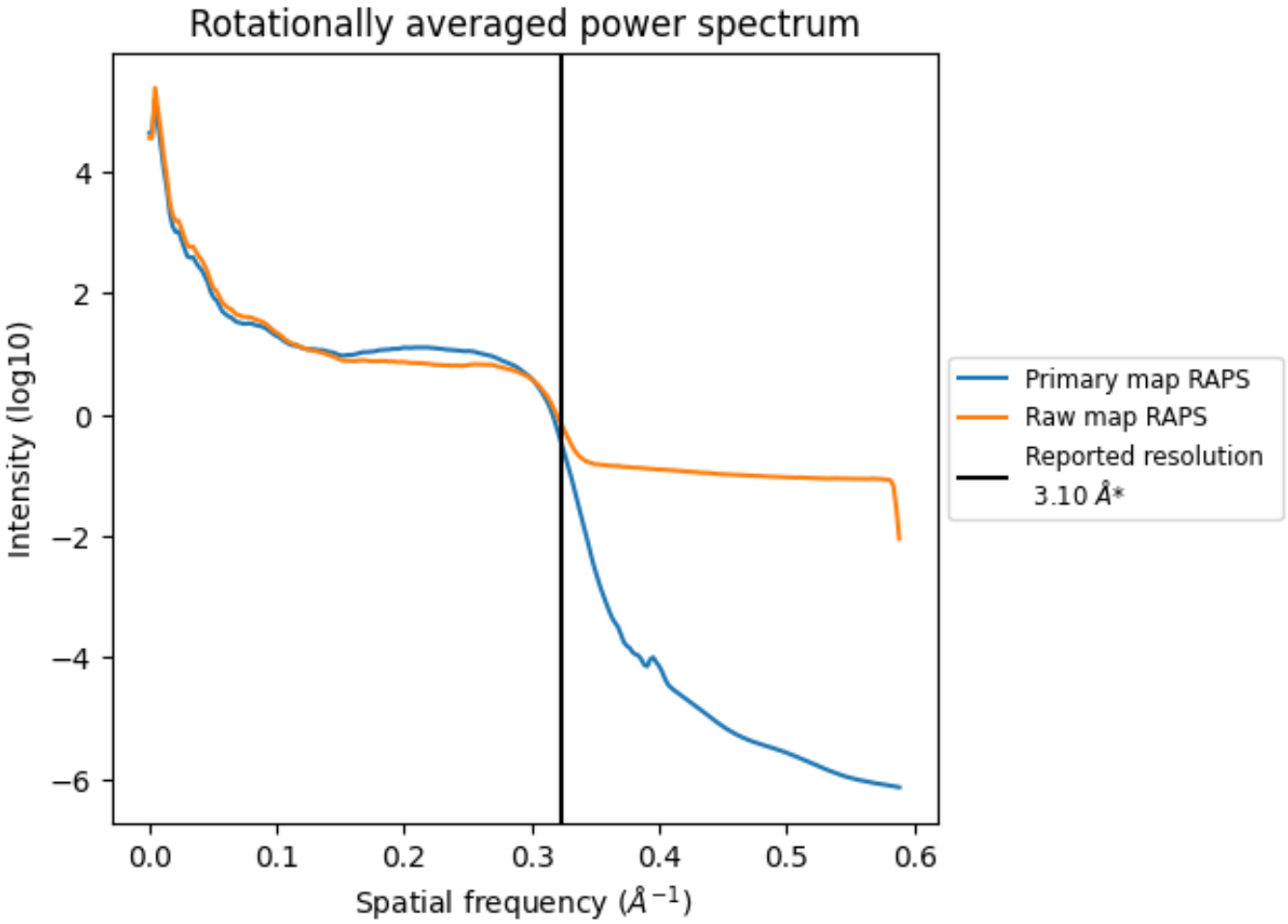
7.2 Volume estimate



The volume at the recommended contour level is 997 nm^3; this corresponds to an approximate mass of 901 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)

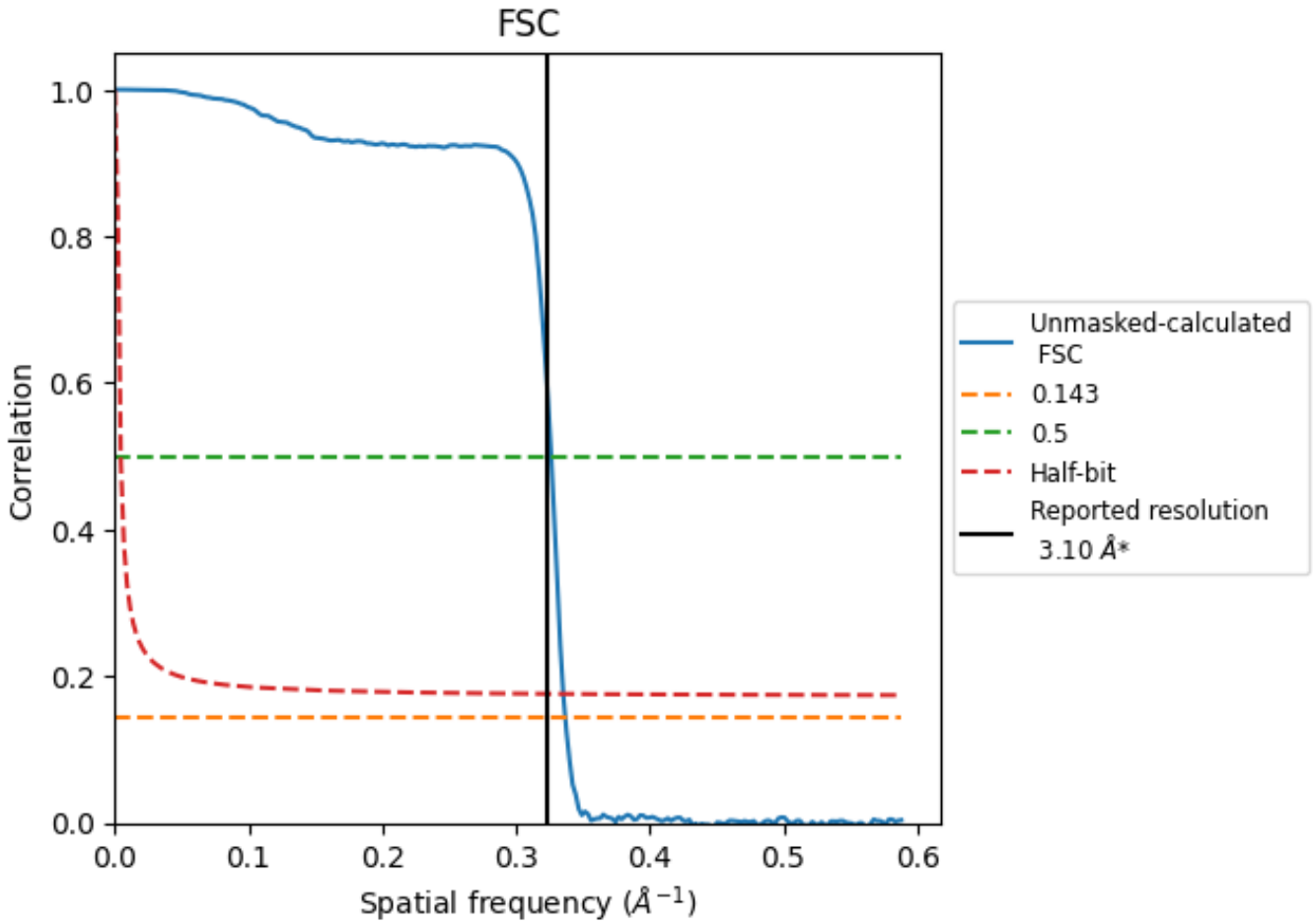


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

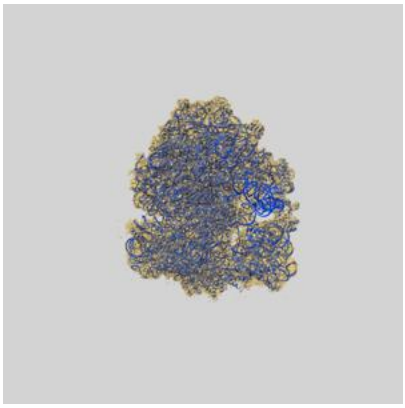
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	2.97	3.06	2.98

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

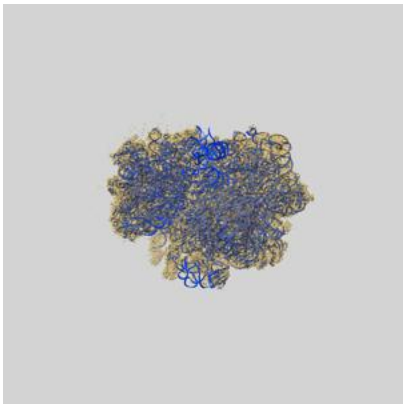
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42576 and PDB model 8UU9. Per-residue inclusion information can be found in section 3 on page 15.

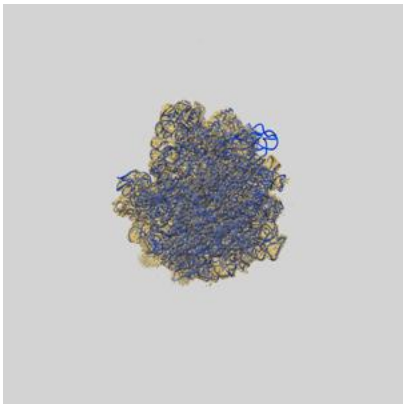
9.1 Map-model overlay



X



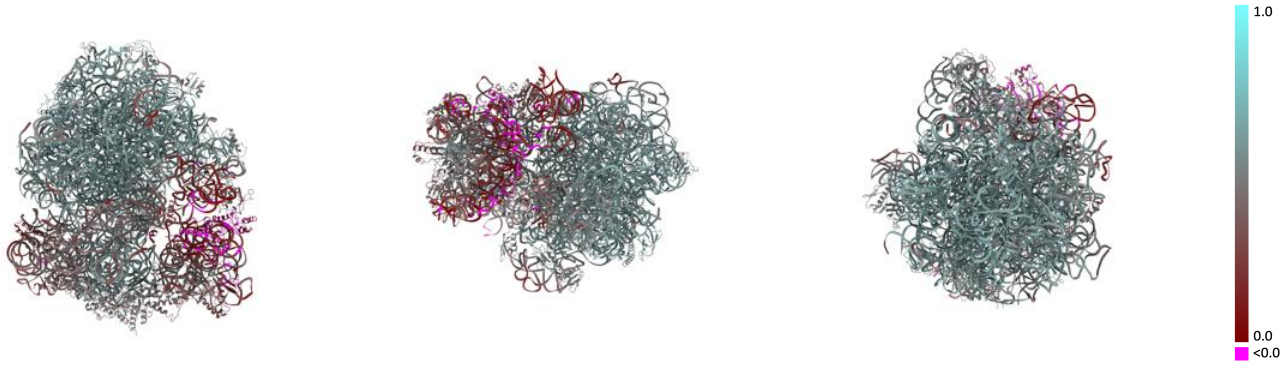
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.4 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.

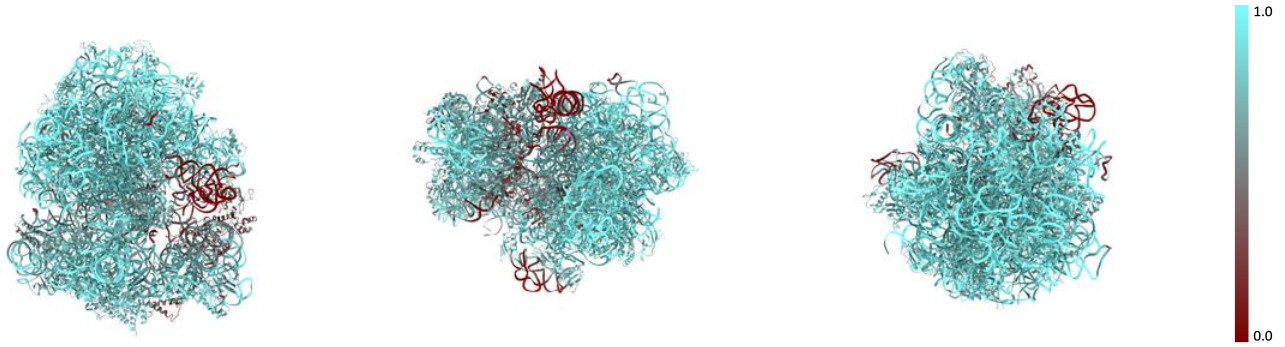
9.2 Q-score mapped to coordinate model



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.

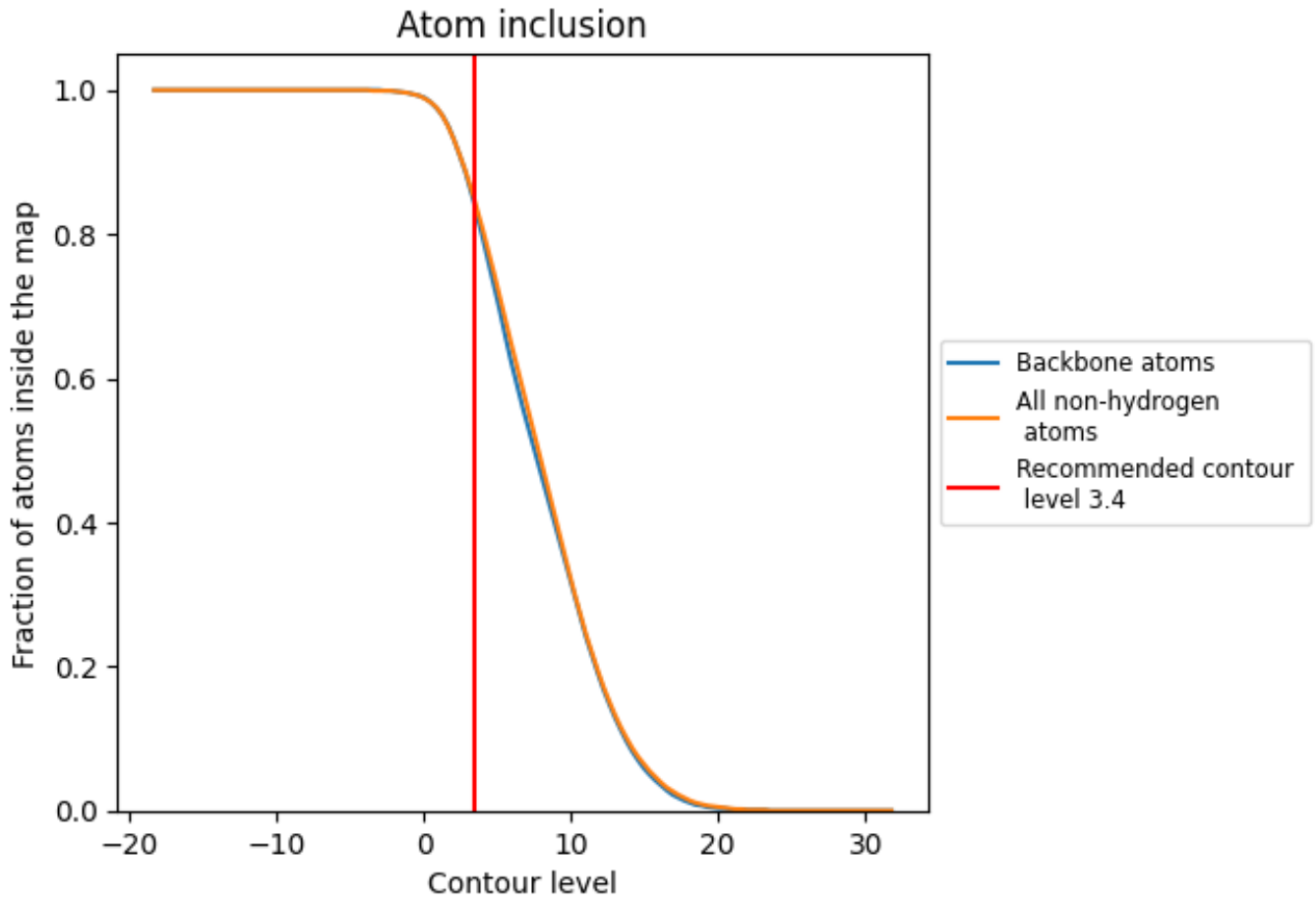
9.3 Atom inclusion mapped to coordinate model



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 (3.4).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 85% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.4950
1	0.8620	0.5420
2	0.8940	0.5740
3	0.4420	0.3260
4	0.8860	0.5630
5	0.8970	0.5780
6	0.9390	0.6050
7	0.9220	0.6050
8	0.8990	0.5820
A	0.9170	0.5600
B	0.9350	0.5130
C	0.8930	0.5940
D	0.9220	0.5880
E	0.8850	0.5720
F	0.5740	0.4020
G	0.7650	0.5040
L	0.9140	0.5930
M	0.8220	0.5750
N	0.8610	0.5650
O	0.8940	0.5850
P	0.8920	0.5810
Q	0.8180	0.5200
R	0.8480	0.5760
S	0.9230	0.5910
T	0.9110	0.5880
U	0.8910	0.5860
V	0.8520	0.5620
W	0.8420	0.5490
Y	0.9110	0.5750
Z	0.8640	0.5700
a	0.8150	0.3880
b	0.6720	0.4670
c	0.8160	0.4320
d	0.7840	0.4280
e	0.8550	0.5450

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.7170	0.3850
g	0.4440	0.1330
h	0.8600	0.5120
i	0.6920	0.2370
j	0.8110	0.4170
k	0.6440	0.3450
l	0.8610	0.5340
m	0.4220	0.0750
n	0.8370	0.4080
o	0.7150	0.4320
p	0.7400	0.3670
q	0.8090	0.4140
r	0.7680	0.4390
s	0.3210	0.0980
t	0.6540	0.2830
v	0.7920	0.5180
w	0.2740	0.1830
x	0.3410	0.2300