Full wwPDB EM Validation Report (i)

May 26, 2024 – 03:02 AM EDT

PDB ID	:	7RYF
EMDB ID	:	EMD-24738
Title	:	A. baumannii Ribosome-TP-6076 complex: P-site tRNA 70S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-08-25
Resolution	:	2.65 Å(reported)

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

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

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

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

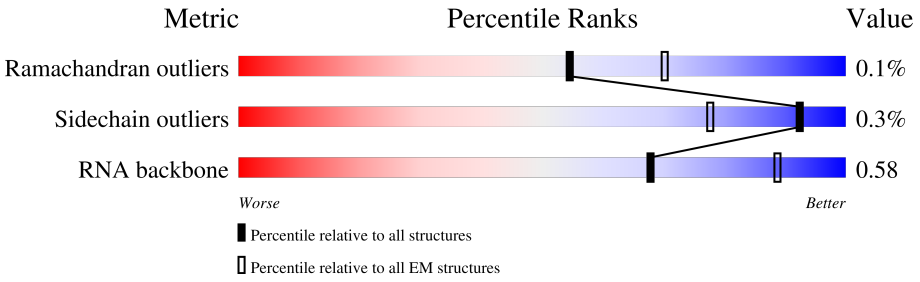
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.65 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	0	51	6%, 94%, 6%
2	1	44	100%
3	2	64	., 98%, .
4	3	38	24%, 100%
5	A	2918	9%, 77%, 15%, 8%
6	B	115	32%, 86%, 14%
7	C	274	., 99%, .
8	D	212	., 99%, .

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Mol	Chain	Length	Quality of chain
9	E	200	6% 100%
10	F	178	95% 97%
11	G	177	72% 97%
12	H	148	26% 41% 59%
13	I	142	99%
14	J	122	100%
15	K	146	99%
16	L	137	99%
17	M	125	95% 5%
18	N	116	23% 98%
19	O	122	7% 95% 5%
20	P	119	98%
21	Q	103	100%
22	R	109	100%
23	S	106	9% 85% 15%
24	T	105	14% 98%
25	U	98	7% 99%
26	V	85	91% 9%
27	W	78	99%
28	X	65	22% 92% 8%
29	Y	58	100%
30	Z	61	89% 11%
31	a	1544	11% 81% 17%
32	b	250	68% 89% 10%
33	c	250	84% 14%

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Mol	Chain	Length	Quality of chain
34	d	208	29% 99%
35	e	165	94% 6%
36	f	127	23% 81% 18%
37	g	156	14% 87% 13%
38	h	131	99%
39	i	128	98%
40	j	103	97%
41	k	128	34% 91% 9%
42	l	124	21% 98%
43	m	118	97%
44	n	101	99%
45	o	89	99%
46	p	101	81% 19%
47	q	85	92% 8%
48	r	75	5% 69% 31%
49	s	91	90% 10%
50	t	88	98%
51	u	71	63% 79% 20%
52	v	77	69% 61% 35%
53	w	3	100%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 137516 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	48	400	256	72	69	3	0	0

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	44	363	222	85	54	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	63	509	319	110	76	4	0	0

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	295	179	64	48	4	0	0

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	2685	57610	25715	10555	18655	2685	0	0

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	115	2450	1095	440	800	115	0	0

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	271	2104	1297	435	364	8	0	0

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	210	1566	969	296	298	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	200	1516	952	281	278	5	0	0

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	174	1370	871	243	248	8	0	0

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	174	1318	832	236	249	1	0	0

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	60	458	287	84	86	1	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	141	1117	713	199	202	3	0	0

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	122	946	592	180	169	5	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
15	K	144	1071	663	213	195	0	0

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	137	1087	687	210	185	5	0	0

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	119	942	590	186	163	3	0	0

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	114	857	528	173	155	1	0	0

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
19	O	116	913	575	176	162	0	0

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	117	934	589	197	146	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	103	807	506	155	143	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	109	826	514	158	150	4	0	0

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	S	90	702	447	127	128	0	0

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
24	T	103	766	476	142	148	0	0

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	U	97	760	477	143	139	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	V	77	581	360	112	107	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	W	77	632	395	130	105	2	0	0

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	X	60	486	302	93	90	1	0	0

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	Y	58	463	286	88	85	4	0	0

- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Z	54	447	265	100	81	1	0	0

- Molecule 31 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	a	1528	32782	14631	5994	10630	1527	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	1007	U	C	conflict	GB 1211343212
a	1034	C	U	conflict	GB 1211343212

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	b	225	1769	1110	328	325	6	0	0

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	c	215	1690	1065	318	299	8	0	0

- Molecule 34 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	d	207	1631	1017	313	299	2	0	0

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	e	155	1129	700	217	207	5	0	0

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	f	104	867	546	158	159	4	0	0

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	g	136	1073	671	201	194	7	0	0

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	h	130	985	615	177	187	6	0	0

- Molecule 39 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	i	126	991	618	197	175	1	0	0

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	j	100	801	500	150	148	3	0	0

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	k	117	862	535	167	159	1	0	0

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	l	122	945	580	193	167	5	0	0

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	m	115	903	558	184	158	3	0	0

- Molecule 44 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	n	100	792	493	158	137	4	0	0

- Molecule 45 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	o	88	705	434	144	126	1	0	0

- Molecule 46 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	p	82	644	403	128	112	1	0	0

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	q	78	614	386	115	112	1	0	0

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	r	52	426	273	74	79	0	0

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	s	82	646	412	125	107	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	t	86	663	409	139	113	2	0	0

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	u	57	473	294	96	82	1	0	0

- Molecule 52 is a RNA chain called tRNA-met.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
52	v	77	1636	733	291	535	76	1	0	0

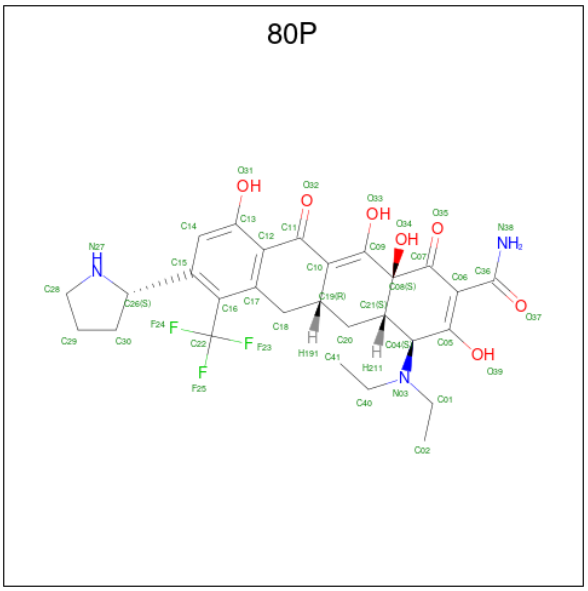
- Molecule 53 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
53	w	3	65	29	12	21	3	0	0

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

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
54	3	1	1	1	0

- Molecule 55 is (4S,4aS,5aR,12aS)-4-(diethylamino)-3,10,12,12a-tetrahydroxy-1,11-dioxo-8-[(2S)-pyrrolidin-2-yl]-7-(trifluoromethyl)-1,4,4a,5,5a,6,11,12a-octahydrotetracene-2-carboxamide (three-letter code: 80P) (formula: $C_{28}H_{32}F_3N_3O_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
55	a	1	Total	C	F	N	O	0
			41	28	3	3	7	
55	a	1	Total	C	F	N	O	0
			41	28	3	3	7	
55	a	1	Total	C	F	N	O	0
			41	28	3	3	7	

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

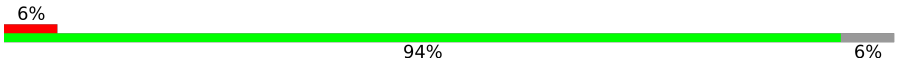
Mol	Chain	Residues	Atoms		AltConf
56	a	4	Total	Mg	0
			4	4	

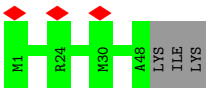
3 Residue-property plots (i)

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

- Molecule 1: 50S ribosomal protein L33

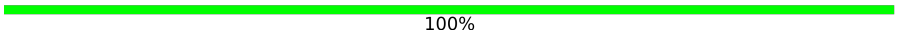
Chain 0:





- Molecule 2: 50S ribosomal protein L34

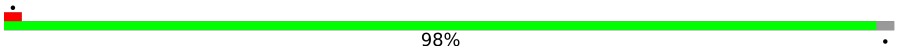
Chain 1:

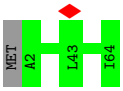


There are no outlier residues recorded for this chain.

- Molecule 3: 50S ribosomal protein L35

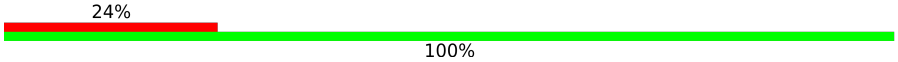
Chain 2:

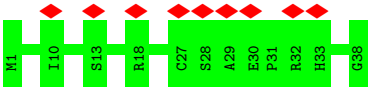




- Molecule 4: 50S ribosomal protein L36

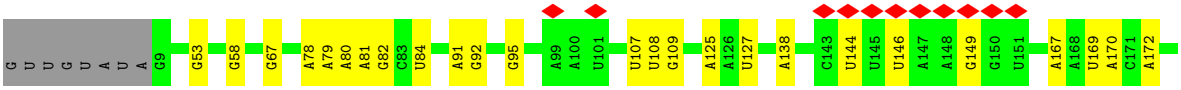
Chain 3:

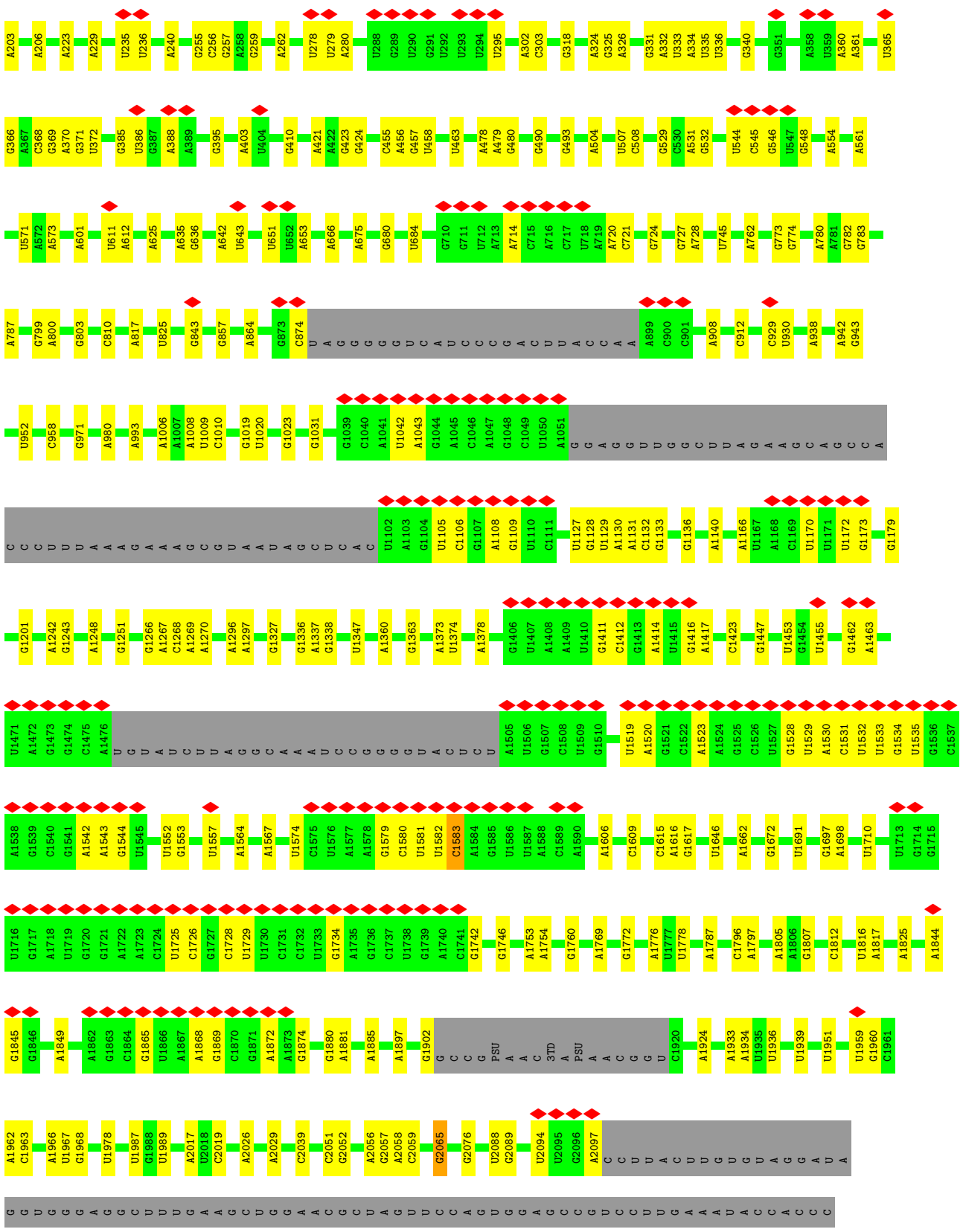




- Molecule 5: 23S ribosomal RNA

Chain A:




A203 A206 A223 A229 U235 U236 A240 G255 C256 G257 A258 C259 A262 U278 U279 A280 U288 G289 U290 G291 U292 U293 U294 U295 A302 C303 G318 A324 G325 A326 G331 A332 U333 A334 U335 U336 G340 G351 A358 U359 A360 A361 U365
G366 A367 C368 G369 A370 G371 U372 G385 U386 G387 A388 A389 G395 A403 U404 G410 A421 A422 G423 G424 C455 A456 G457 U458 U463 A478 A479 G480 G490 G493 A504 U507 C508 G529 C530 A531 G532 U544 C545 G546 U547 G548 A554 A561
U571 A572 A573 A601 U611 A612 A625 A635 G636 A642 U643 U651 U652 A653 A666 A675 G680 U684 G710 G711 U712 A713 A714 C715 A716 C717 U718 A719 A720 C721 G724 G727 A728 U745 A762 G773 G774 A780 A781 G782 G783
A787 G799 A800 G803 C810 A817 U825 G843 G857 A864 G873 C874 U A G G G G U C A U C C C G A C U U A C C A A A899 C900 C901 A908 C912 C929 U930 A938 A942 G943
U952 C958 G971 A980 A993 A1006 A1007 A1008 U1009 C1010 G1019 U1020 G1023 G1031 G1039 C1040 A1041 U1042 A1043 G1044 A1045 C1046 A1047 G1048 C1049 U1050 A1051 G G A G G U U G G C U U A G A A G C A G C C A
C C C U U U A A A G A A A A G C G U A A U A G C U C U C A U1102 A1103 G1104 U1105 C1106 G1107 A1108 G1109 U1110 C1111 U1127 G1128 U1129 A1130 A1131 C1132 G1133 G1136 A1140 A1166 U1167 A1168 C1169 U1170 U1171 U1172 G1173 G1179
G1201 A1242 G1243 A1248 G1251 G1266 A1267 C1268 A1269 A1270 A1296 A1297 G1327 G1336 A1337 G1338 U1347 A1360 G1363 A1373 U1374 A1378 G1406 U1407 A1408 A1409 U1410 G1411 C1412 G1413 A1414 U1415 G1416 A1417 C1423 G1447 U1453 G1454 U1455 G1462 A1463
U1471 A1472 G1473 G1474 C1475 A1476 U G U A U C U U A G G C A A A U C C G G G G U A C U U C U A1505 U1506 G1507 C1508 U1509 G1510 U1519 A1520 G1521 C1522 A1523 A1524 G1525 C1526 U1527 G1528 U1529 A1530 C1531 U1532 U1533 G1534 U1535 G1536 C1537
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G1845 G1846 A1849 A1862 G1863 C1864 G1865 U1866 A1867 A1868 G1869 C1870 G1871 A1872 A1873 G1874 G1880 A1881 A1885 A1897 G1902 G C C G PSU A A C 3TD A PSU A A C G G U C1920 A1924 A1933 A1934 U1935 U1936 U1939 U1951 U1959 G1960 C1961
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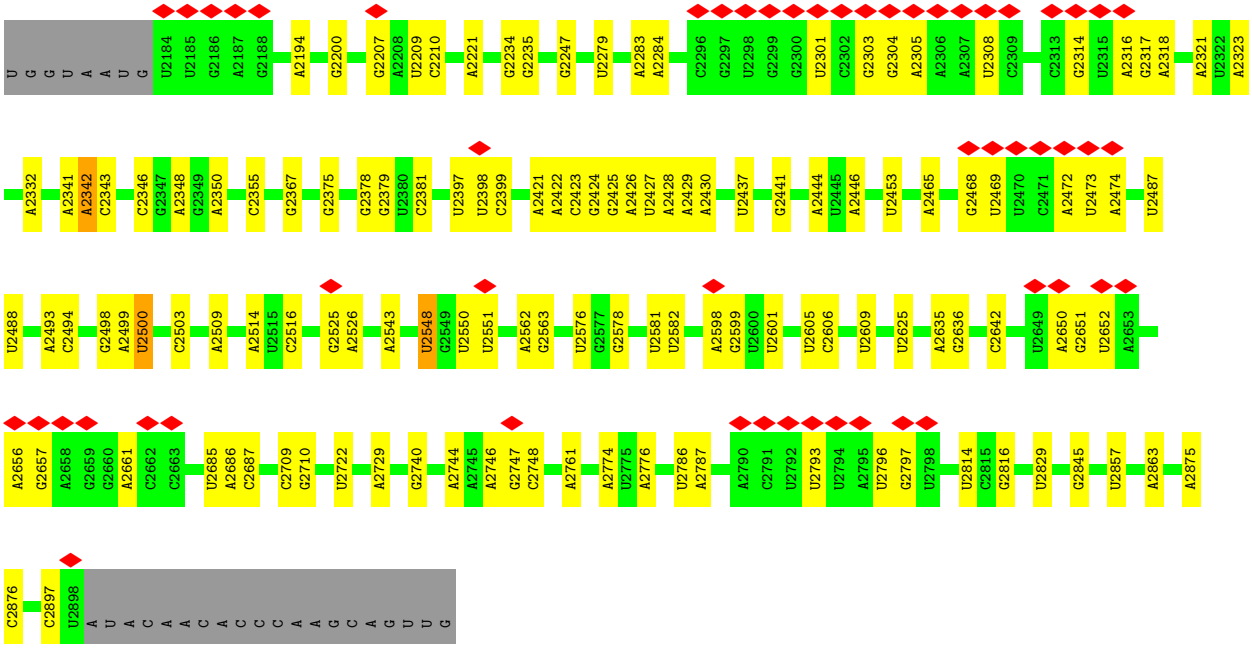
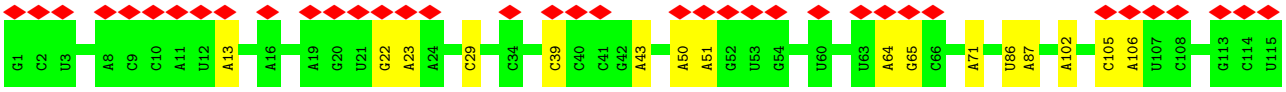


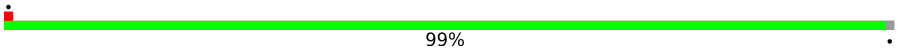
- Molecule 6: 5S ribosomal RNA

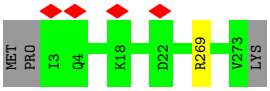
Chain B:



- Molecule 7: 50S ribosomal protein L2

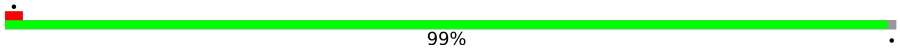
Chain C:

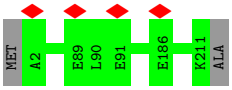




- Molecule 8: 50S ribosomal protein L3

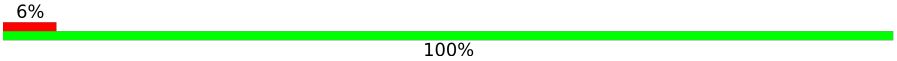
Chain D:

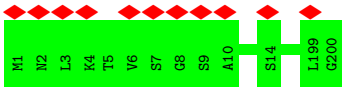




- Molecule 9: 50S ribosomal protein L4

Chain E:





- Molecule 10: 50S ribosomal protein L5

Chain F: 95% 97%

MET ALA ARG L4 K5 A6 R7 Y8 N9 D10 E11 L12 K13 A14 K15 L16 Q17 E18 E19 L20 S21 I22 K23 N24 V25 M26 E27 I28 P29 R30 I31 T32 K33 I34 T35 L36 N37 M38 G39 V40 G41 A42 A43 A44 T45 D46 K47 K48 L49 L50 D51 G52 A53 V54 A55 D56 M57 Q58 L59 I60

A61 G62 Q63 K64 P65 V66 V67 T68 L69 A70 R71 K72 S73 A74 A75 G76 F77 K78 I79 R80 D81 G82 W83 P84 I85 G86 C87 K88 V89 T90 L91 R92 G93 D94 Q95 M96 Y97 E98 F99 L100 D101 R102 L103 I104 S105 I106 A107 I108 P109 R110 I111 R112 D113 F114 R115 G116 F117 S118 A119 K120

S121 F122 D123 G124 R125 G126 N127 Y128 S129 M130 G131 L132 K133 E134 Q135 I136 V137 F138 P139 E140 I141 D142 F143 D144 K145 I146 D147 R148 I149 R150 G151 M152 D153 I154 T155 I156 T157 T158 T159 A160 R161 T162 D163 D164 E165 G166 R167 A168 L169 M170 R171 A172 F173 G174 F175 P176 F177 LYS

- Molecule 11: 50S ribosomal protein L6

Chain G: 72% 97%

MET S2 R3 V4 A5 K6 A7 P8 V9 T10 V11 P12 N13 G14 V15 T16 V17 T18 Q19 N20 G21 R22 Q23 V24 E25 V26 K27 G28 S29 K30 G31 T32 L33 S34 F35 N36 L37 H38 A39 L40 V41 E42 L43 K44 Q45 E46 E47 G48 K49 L50 Q51 L52 A53 P54 A55 K56 E57 S58 K59 D60

A61 W62 M63 G66 T67 A68 R69 L72 N73 N74 L75 V76 K77 G78 V79 S80 E81 G82 F83 E84 R85 K86 L87 Q88 L89 V90 G91 V92 G93 Y94 K95 A96 A97 V98 K99 G100 T101 N104 L105 N106 L107 G108 Y109 S110 H111 P112 I113 D114 Y115 A123 E124 T127 A128 T129 E130

I131 I132 L133 K134 S135 A136 N137 K138 L141 A150 Y151 R152 E155 P156 Y157 K158 R163 Y164 S165 D166 E167 V168 I169 L170 R171 K172 E173 A174 K175 LYS LYS

- Molecule 12: 50S ribosomal protein L9

Chain H: 26% 41% 59%

M1 D2 V3 I4 L5 L6 Q7 R8 I9 K10 N11 L12 G13 K14 L15 G16 D17 K18 Q33 A38 A39 T40 E41 A42 N43 T44 A45 A46 F47 E48 A49 R50 R51 A52 E53 L54 E55 K56 Q57 E58 A59 E60 VAL LEU ALA ALA ALA GLN ALA ARG ALA GLU GLN LEU ASN GLU VAL ASN

ILE VAL ILE THR ALA LYS ALA GLY ASP GLU GLY LYS LEU PHE GLY SER ILE GLY THR ARG ASP ILE ALA ASP ALA LEU THR ASN ALA GLY LEU THR VAL ASP ARG ALA GLU VAL ARG LEU PRO ASN GLY ALA LEU ARG HIS THR GLY GLU PHE ASN ILE ALA ILE GLN LEU HIS HIS ASP

VAL VAL ALA GLU VAL LEU VAL THR ILE VAL SER GLU

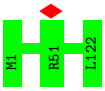
- Molecule 13: 50S ribosomal protein L13

Chain I: 99%

MET K2 H95 I142

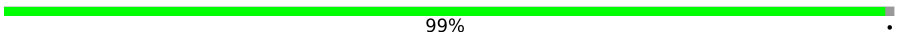
- Molecule 14: 50S ribosomal protein L14

Chain J: 100%



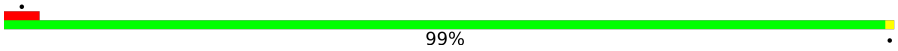
• Molecule 15: 50S ribosomal protein L15

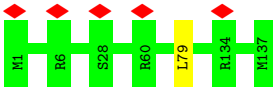
Chain K:



• Molecule 16: 50S ribosomal protein L16

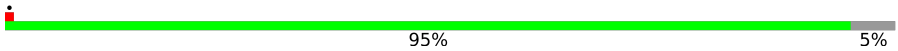
Chain L:

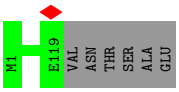




• Molecule 17: 50S ribosomal protein L17

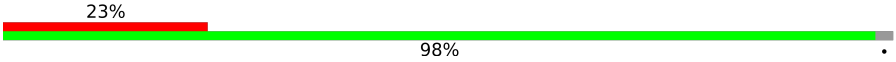
Chain M:

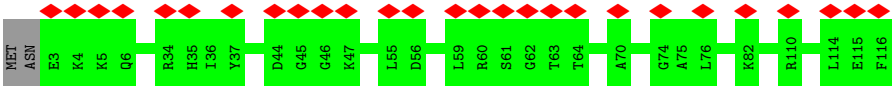




• Molecule 18: 50S ribosomal protein L18

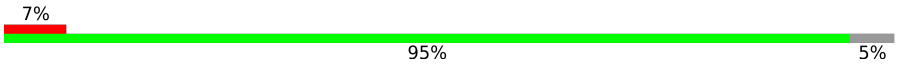
Chain N:

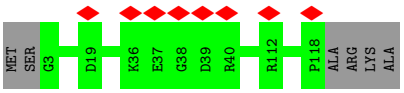




• Molecule 19: 50S ribosomal protein L19

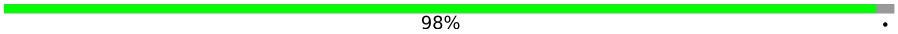
Chain O:



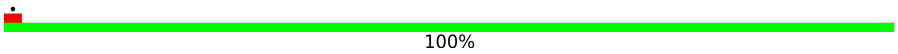


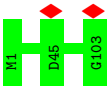
• Molecule 20: 50S ribosomal protein L20

Chain P:

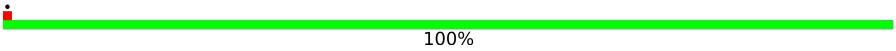


• Molecule 21: 50S ribosomal protein L21

Chain Q: 

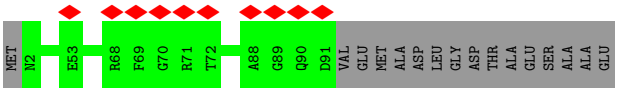


• Molecule 22: 50S ribosomal protein L22

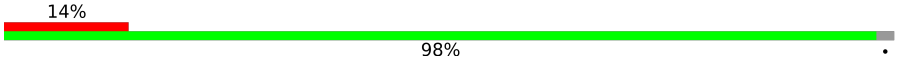
Chain R: 

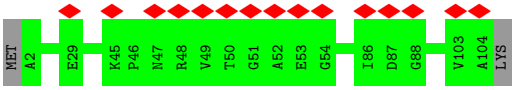
• Molecule 23: 50S ribosomal protein L23

Chain S:

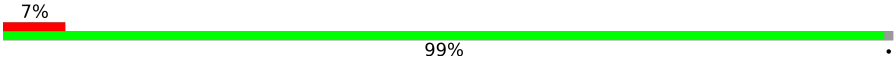


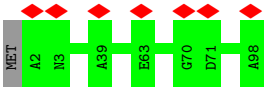
• Molecule 24: 50S ribosomal protein L24

Chain T: 



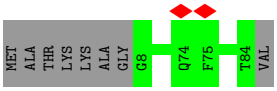
• Molecule 25: 50S ribosomal protein L25

Chain U: 

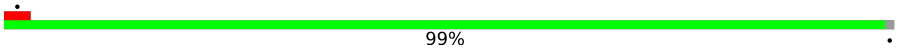


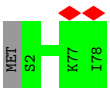
• Molecule 26: 50S ribosomal protein L27

Chain V:



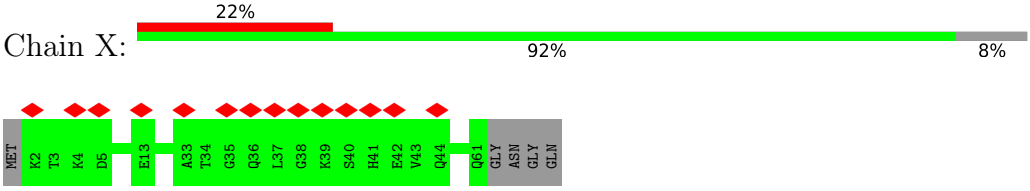
• Molecule 27: 50S ribosomal protein L28

Chain W: 



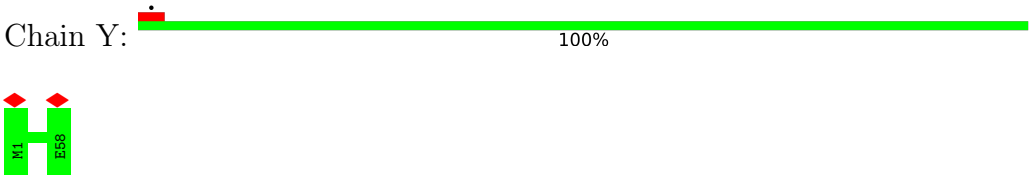
- Molecule 28: 50S ribosomal protein L29

Chain X:



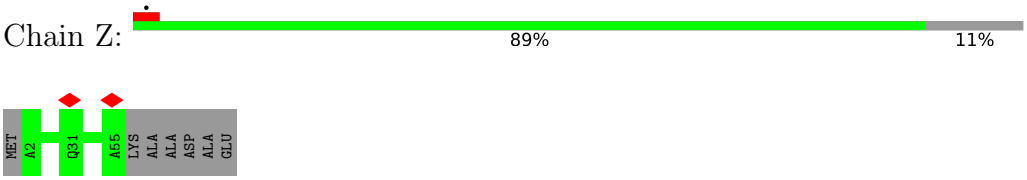
- Molecule 29: 50S ribosomal protein L30

Chain Y:



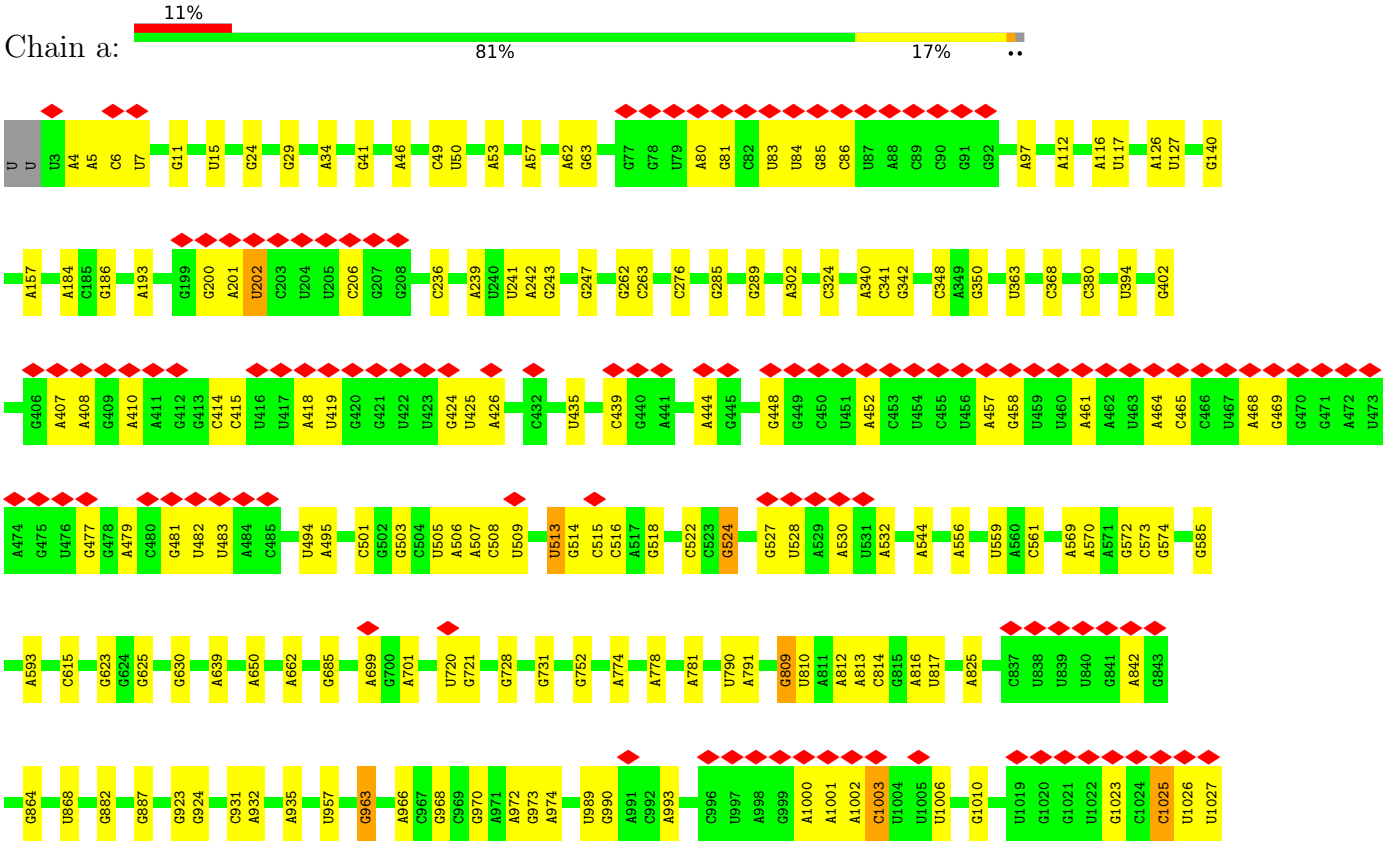
- Molecule 30: 50S ribosomal protein L32

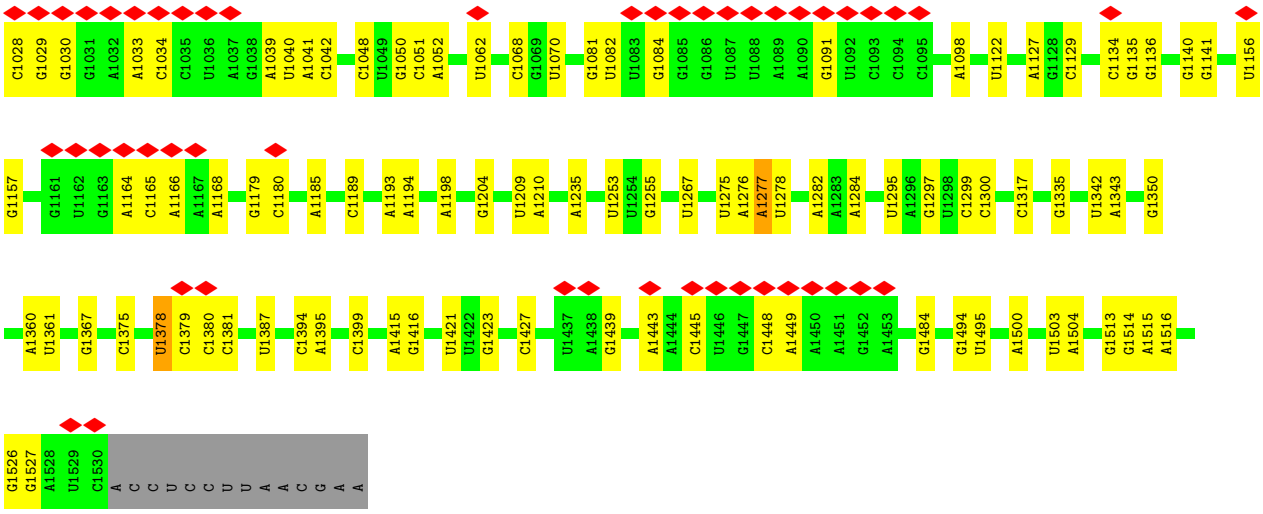
Chain Z:



- Molecule 31: 16S Ribosomal RNA

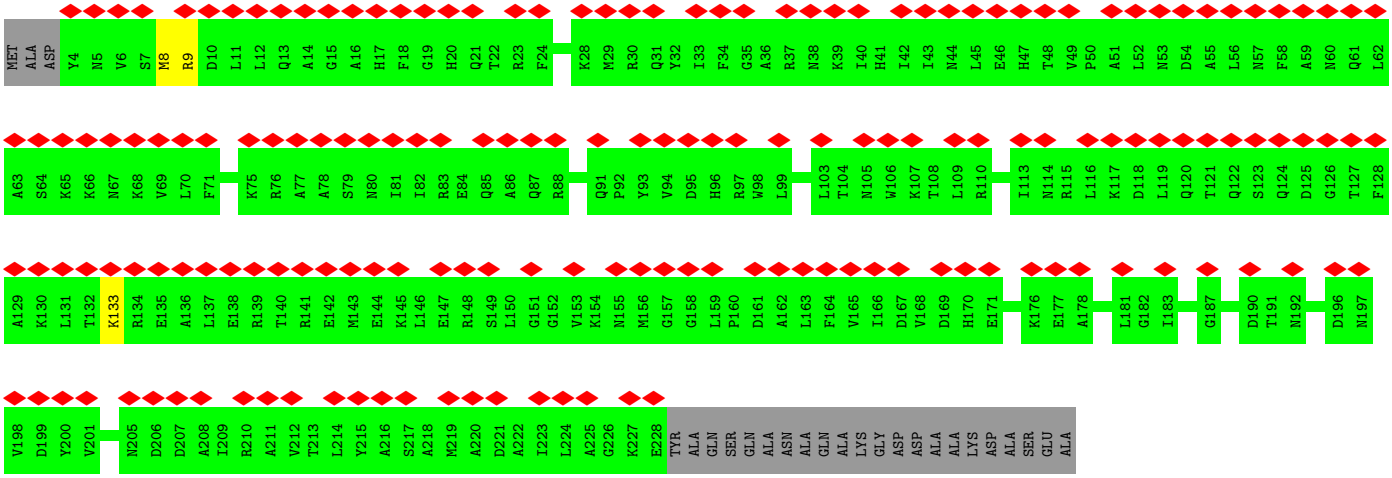
Chain a:





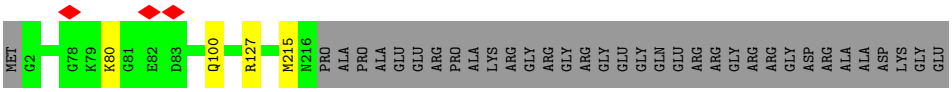
- Molecule 32: 30S ribosomal protein S2

Chain b:



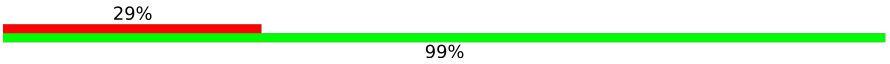
- Molecule 33: 30S ribosomal protein S3

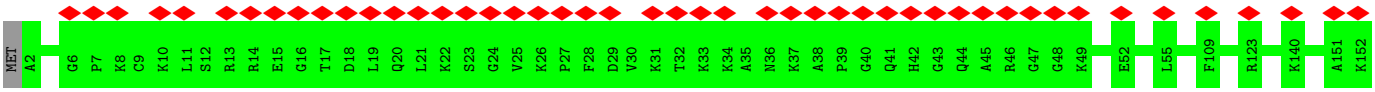
Chain c:

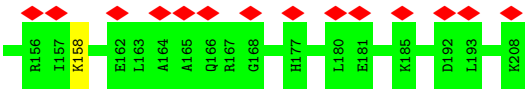


- Molecule 34: 30S ribosomal protein S4

Chain d:

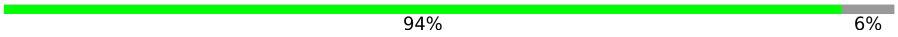


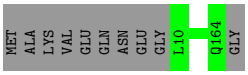




• Molecule 35: 30S ribosomal protein S5

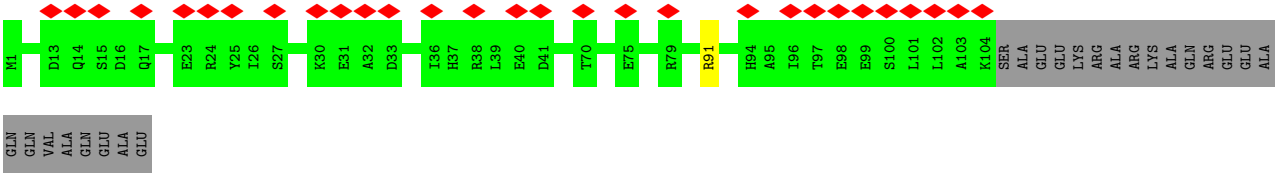
Chain e:





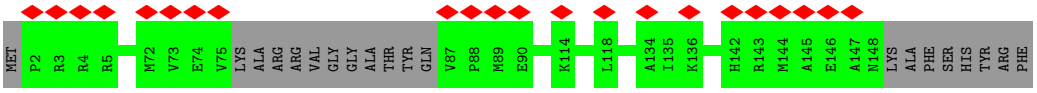
• Molecule 36: 30S ribosomal protein S6

Chain f:



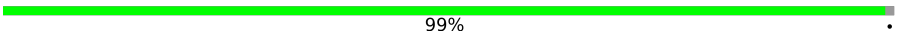
• Molecule 37: 30S ribosomal protein S7

Chain g:



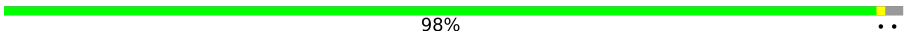
• Molecule 38: 30S ribosomal protein S8

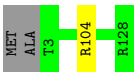
Chain h:



• Molecule 39: 30S ribosomal protein S9

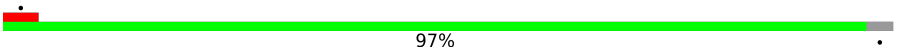
Chain i:

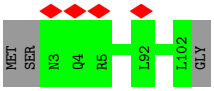




• Molecule 40: 30S ribosomal protein S10

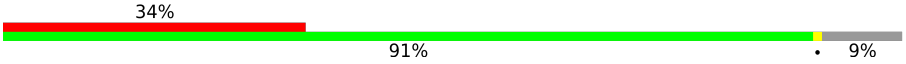
Chain j:

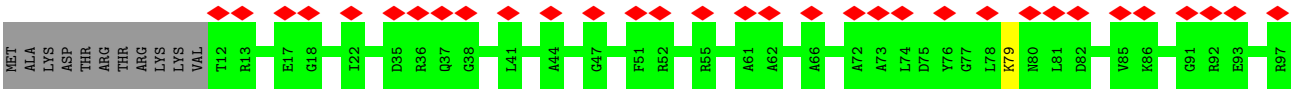


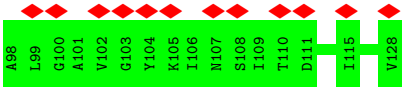


• Molecule 41: 30S ribosomal protein S11

Chain k:

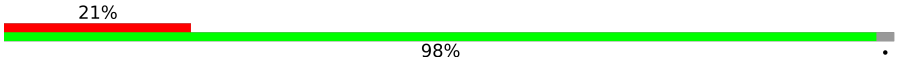


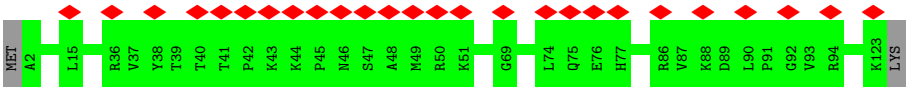




• Molecule 42: 30S ribosomal protein S12

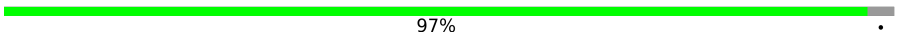
Chain l:

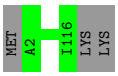




• Molecule 43: 30S ribosomal protein S13

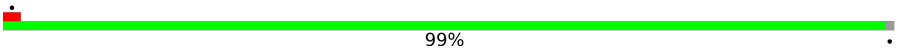
Chain m:

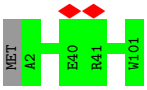




• Molecule 44: 30S ribosomal protein S14

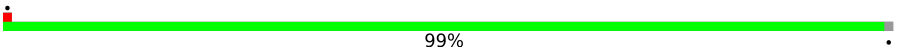
Chain n:

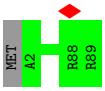




• Molecule 45: 30S ribosomal protein S15

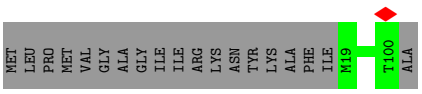
Chain o:





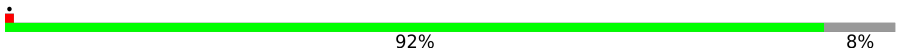
• Molecule 46: 30S ribosomal protein S16

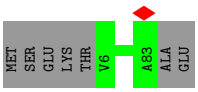
Chain p:



• Molecule 47: 30S ribosomal protein S17

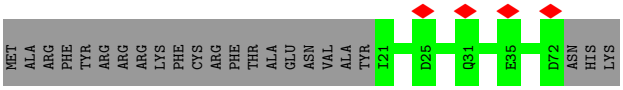
Chain q:





• Molecule 48: 30S ribosomal protein S18

Chain r:

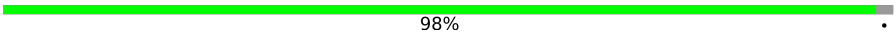


• Molecule 49: 30S ribosomal protein S19

Chain s:

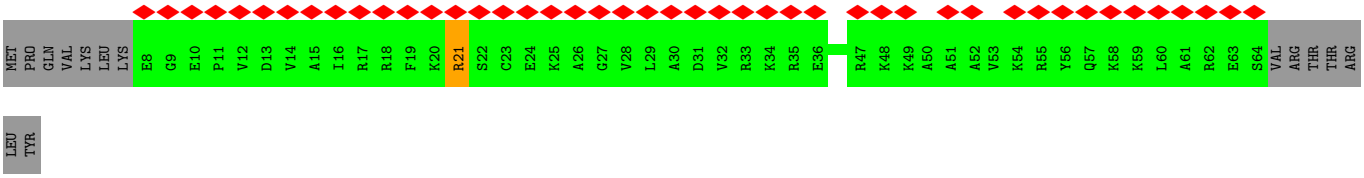
• Molecule 50: 30S ribosomal protein S20

Chain t:



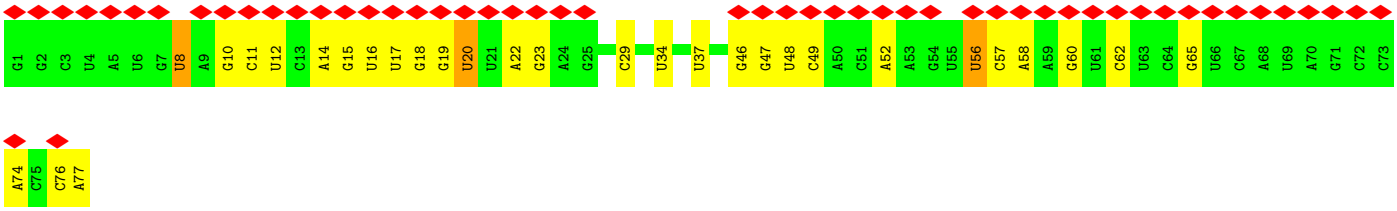
• Molecule 51: 30S ribosomal protein S21

Chain u:



• Molecule 52: tRNA-met

Chain v:



• Molecule 53: mRNA

Chain w: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47011	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	4.322	Depositor
Minimum map value	-0.094	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.1	Depositor
Map size (Å)	557.568, 557.568, 557.568	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.089, 1.089, 1.089	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: ZN, UR3, MA6, 6MZ, 80P, OMG, PSU, OMU, H2U, 5MU, MG, 7MG, 4OC, 2MA, 4SU, 5MC, 2MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	0	0.27	0/407	0.51	0/540
2	1	0.24	0/367	0.66	0/481
3	2	0.24	0/515	0.61	0/678
4	3	0.25	0/296	0.59	0/389
5	A	0.21	0/64227	0.76	3/100172 (0.0%)
6	B	0.18	0/2739	0.74	0/4266
7	C	0.24	0/2144	0.58	0/2880
8	D	0.24	0/1584	0.56	0/2135
9	E	0.25	0/1537	0.51	0/2073
10	F	0.26	0/1390	0.59	0/1863
11	G	0.27	0/1337	0.53	0/1807
12	H	0.27	0/461	0.53	0/616
13	I	0.25	0/1143	0.49	0/1541
14	J	0.25	0/956	0.59	0/1286
15	K	0.24	0/1079	0.58	0/1439
16	L	0.25	0/1104	0.58	0/1475
17	M	0.24	0/956	0.57	0/1282
18	N	0.26	0/865	0.58	0/1156
19	O	0.25	0/925	0.57	0/1241
20	P	0.26	0/947	0.59	0/1262
21	Q	0.24	0/818	0.55	0/1094
22	R	0.24	0/831	0.51	0/1113
23	S	0.25	0/708	0.54	0/947
24	T	0.24	0/770	0.51	0/1034
25	U	0.25	0/770	0.55	0/1036
26	V	0.25	0/589	0.53	0/788
27	W	0.24	0/642	0.56	0/856
28	X	0.24	0/487	0.47	0/646
29	Y	0.26	0/468	0.53	0/624
30	Z	0.24	0/453	0.63	0/604
31	a	0.29	0/36476	0.77	10/56895 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.25	0/1799	0.52	0/2429
33	c	0.28	0/1714	0.59	1/2304 (0.0%)
34	d	0.27	0/1653	0.56	0/2213
35	e	0.26	0/1141	0.58	0/1537
36	f	0.25	0/882	0.53	0/1189
37	g	0.26	0/1087	0.56	0/1456
38	h	0.25	0/993	0.52	0/1331
39	i	0.27	0/1002	0.59	0/1339
40	j	0.26	0/811	0.54	0/1096
41	k	0.24	0/878	0.52	0/1189
42	l	0.24	0/958	0.58	0/1284
43	m	0.25	0/913	0.59	0/1226
44	n	0.29	0/803	0.61	0/1071
45	o	0.25	0/715	0.52	0/958
46	p	0.25	0/655	0.56	0/879
47	q	0.24	0/621	0.53	0/837
48	r	0.25	0/432	0.51	0/583
49	s	0.27	0/664	0.52	0/897
50	t	0.26	0/669	0.52	0/892
51	u	0.30	0/478	0.63	1/631 (0.2%)
52	v	0.19	0/1739	0.76	0/2709
53	w	0.15	0/72	0.72	0/110
All	All	0.25	0/148670	0.71	15/222379 (0.0%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	415	C	N3-C2-O2	-7.00	117.00	121.90
31	a	1379	C	C2-N1-C1'	6.81	126.29	118.80
31	a	202	U	C2-N1-C1'	6.47	125.47	117.70
31	a	1378	U	C2-N1-C1'	6.18	125.12	117.70
5	A	1583	C	C2-N1-C1'	5.80	125.18	118.80
31	a	1025	C	N3-C2-O2	-5.57	118.00	121.90
31	a	809	G	P-O3'-C3'	5.45	126.25	119.70
5	A	727	G	O4'-C1'-N9	5.44	112.55	108.20
33	c	215	MET	CA-CB-CG	5.44	122.55	113.30
5	A	2342	A	P-O3'-C3'	5.40	126.18	119.70
31	a	1277	A	P-O3'-C3'	5.35	126.12	119.70
51	u	21	ARG	CB-CG-CD	5.32	125.44	111.60
31	a	439	C	C2-N1-C1'	5.21	124.53	118.80
31	a	414	C	N1-C2-O2	5.20	122.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1003	C	N3-C2-O2	-5.00	118.40	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	46/51 (90%)	45 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
3	2	61/64 (95%)	59 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
7	C	269/274 (98%)	261 (97%)	8 (3%)	0	100	100
8	D	208/212 (98%)	200 (96%)	8 (4%)	0	100	100
9	E	198/200 (99%)	197 (100%)	1 (0%)	0	100	100
10	F	172/178 (97%)	163 (95%)	8 (5%)	1 (1%)	25	37
11	G	172/177 (97%)	170 (99%)	1 (1%)	1 (1%)	25	37
12	H	58/148 (39%)	56 (97%)	2 (3%)	0	100	100
13	I	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
14	J	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
15	K	142/146 (97%)	137 (96%)	5 (4%)	0	100	100
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	22	33
17	M	117/125 (94%)	115 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	N	112/116 (97%)	112 (100%)	0	0	100	100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	115 (100%)	0	0	100	100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	R	107/109 (98%)	103 (96%)	4 (4%)	0	100	100
23	S	88/106 (83%)	88 (100%)	0	0	100	100
24	T	101/105 (96%)	96 (95%)	5 (5%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	75 (100%)	0	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	211 (95%)	11 (5%)	1 (0%)	34	48
33	c	213/250 (85%)	202 (95%)	11 (5%)	0	100	100
34	d	205/208 (99%)	198 (97%)	7 (3%)	0	100	100
35	e	153/165 (93%)	151 (99%)	2 (1%)	0	100	100
36	f	102/127 (80%)	96 (94%)	6 (6%)	0	100	100
37	g	132/156 (85%)	130 (98%)	2 (2%)	0	100	100
38	h	128/131 (98%)	124 (97%)	4 (3%)	0	100	100
39	i	124/128 (97%)	121 (98%)	3 (2%)	0	100	100
40	j	98/103 (95%)	94 (96%)	4 (4%)	0	100	100
41	k	115/128 (90%)	112 (97%)	3 (3%)	0	100	100
42	l	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	94 (96%)	4 (4%)	0	100	100
45	o	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
46	p	80/101 (79%)	80 (100%)	0	0	100	100
47	q	76/85 (89%)	76 (100%)	0	0	100	100
48	r	50/75 (67%)	50 (100%)	0	0	100	100
49	s	80/91 (88%)	80 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	55/71 (78%)	52 (94%)	3 (6%)	0	100	100
All	All	5399/5872 (92%)	5260 (97%)	135 (2%)	4 (0%)	54	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	F	137	VAL
11	G	13	ASN
16	L	79	LEU
32	b	8	MET

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	44/47 (94%)	44 (100%)	0	100	100
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	217/220 (99%)	216 (100%)	1 (0%)	88	94
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	155/155 (100%)	155 (100%)	0	100	100
10	F	144/147 (98%)	144 (100%)	0	100	100
11	G	139/142 (98%)	138 (99%)	1 (1%)	84	91
12	H	45/112 (40%)	45 (100%)	0	100	100
13	I	117/118 (99%)	116 (99%)	1 (1%)	78	87
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	106 (100%)	0	100	100
16	L	113/113 (100%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	98/102 (96%)	98 (100%)	0	100	100
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	76/87 (87%)	76 (100%)	0	100	100
24	T	83/85 (98%)	83 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	59/64 (92%)	59 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	53 (100%)	0	100	100
29	Y	54/54 (100%)	54 (100%)	0	100	100
30	Z	46/50 (92%)	46 (100%)	0	100	100
32	b	185/200 (92%)	183 (99%)	2 (1%)	73	85
33	c	175/198 (88%)	172 (98%)	3 (2%)	60	77
34	d	170/171 (99%)	169 (99%)	1 (1%)	86	92
35	e	113/120 (94%)	113 (100%)	0	100	100
36	f	94/111 (85%)	93 (99%)	1 (1%)	73	85
37	g	113/128 (88%)	113 (100%)	0	100	100
38	h	108/109 (99%)	108 (100%)	0	100	100
39	i	99/100 (99%)	98 (99%)	1 (1%)	76	86
40	j	89/91 (98%)	89 (100%)	0	100	100
41	k	88/98 (90%)	87 (99%)	1 (1%)	73	85
42	l	104/106 (98%)	104 (100%)	0	100	100
43	m	95/98 (97%)	95 (100%)	0	100	100
44	n	81/82 (99%)	81 (100%)	0	100	100
45	o	71/72 (99%)	71 (100%)	0	100	100
46	p	63/77 (82%)	63 (100%)	0	100	100
47	q	70/76 (92%)	70 (100%)	0	100	100
48	r	46/66 (70%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	s	70/78 (90%)	70 (100%)	0	100	100
50	t	65/67 (97%)	65 (100%)	0	100	100
51	u	48/62 (77%)	47 (98%)	1 (2%)	53	72
All	All	4470/4756 (94%)	4457 (100%)	13 (0%)	92	96

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	C	269	ARG
11	G	86	LYS
13	I	95	HIS
32	b	9	ARG
32	b	133	LYS
33	c	80	LYS
33	c	100	GLN
33	c	127	ARG
34	d	158	LYS
36	f	91	ARG
39	i	104	ARG
41	k	79	LYS
51	u	21	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
9	E	162	ASN
16	L	46	GLN
20	P	101	HIS
32	b	61	GLN
37	g	29	HIS
40	j	56	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1524/1544 (98%)	267 (17%)	0
5	A	2677/2918 (91%)	412 (15%)	37 (1%)
52	v	76/77 (98%)	30 (39%)	0
53	w	2/3 (66%)	0	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	B	114/115 (99%)	15 (13%)	2 (1%)
All	All	4393/4657 (94%)	724 (16%)	39 (0%)

All (724) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	53	G
5	A	58	G
5	A	67	G
5	A	78	A
5	A	80	A
5	A	81	A
5	A	82	G
5	A	92	G
5	A	95	G
5	A	107	U
5	A	108	U
5	A	109	G
5	A	125	A
5	A	127	U
5	A	138	A
5	A	144	U
5	A	146	U
5	A	149	G
5	A	167	A
5	A	169	U
5	A	170	A
5	A	172	A
5	A	203	A
5	A	206	A
5	A	223	A
5	A	229	A
5	A	235	U
5	A	236	U
5	A	240	A
5	A	255	G
5	A	257	G
5	A	259	G
5	A	262	A
5	A	278	U
5	A	279	U
5	A	280	A

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Mol	Chain	Res	Type
5	A	295	U
5	A	302	A
5	A	303	C
5	A	318	G
5	A	325	G
5	A	326	A
5	A	331	G
5	A	332	A
5	A	333	U
5	A	335	U
5	A	336	U
5	A	340	G
5	A	360	A
5	A	361	A
5	A	365	U
5	A	366	G
5	A	369	G
5	A	370	A
5	A	371	G
5	A	372	U
5	A	385	G
5	A	386	U
5	A	388	A
5	A	395	G
5	A	403	A
5	A	410	G
5	A	421	A
5	A	423	G
5	A	455	C
5	A	456	A
5	A	457	G
5	A	458	U
5	A	479	A
5	A	480	G
5	A	490	G
5	A	493	G
5	A	504	A
5	A	507	U
5	A	508	C
5	A	529	G
5	A	531	A
5	A	532	G

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Mol	Chain	Res	Type
5	A	544	U
5	A	545	C
5	A	546	G
5	A	548	G
5	A	554	A
5	A	561	A
5	A	571	U
5	A	573	A
5	A	601	A
5	A	611	U
5	A	612	A
5	A	625	A
5	A	635	A
5	A	636	G
5	A	643	U
5	A	651	U
5	A	653	A
5	A	666	A
5	A	675	A
5	A	680	G
5	A	684	U
5	A	714	A
5	A	721	C
5	A	724	G
5	A	728	A
5	A	745	U
5	A	762	A
5	A	773	G
5	A	774	G
5	A	780	A
5	A	782	G
5	A	783	G
5	A	787	A
5	A	799	G
5	A	800	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	843	G
5	A	857	G
5	A	864	A

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Mol	Chain	Res	Type
5	A	874	C
5	A	908	A
5	A	912	C
5	A	929	C
5	A	930	U
5	A	938	A
5	A	942	A
5	A	943	G
5	A	958	C
5	A	971	G
5	A	980	A
5	A	993	A
5	A	1006	A
5	A	1008	A
5	A	1009	U
5	A	1010	C
5	A	1019	G
5	A	1020	U
5	A	1023	G
5	A	1031	G
5	A	1042	U
5	A	1043	A
5	A	1105	U
5	A	1106	C
5	A	1108	A
5	A	1109	G
5	A	1128	G
5	A	1129	U
5	A	1130	A
5	A	1131	A
5	A	1132	C
5	A	1133	G
5	A	1136	G
5	A	1140	A
5	A	1166	A
5	A	1170	U
5	A	1172	U
5	A	1173	G
5	A	1179	G
5	A	1201	G
5	A	1242	A
5	A	1243	G

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Mol	Chain	Res	Type
5	A	1248	A
5	A	1251	G
5	A	1266	G
5	A	1267	A
5	A	1268	C
5	A	1269	A
5	A	1270	A
5	A	1296	A
5	A	1297	A
5	A	1327	G
5	A	1336	G
5	A	1338	G
5	A	1347	U
5	A	1360	A
5	A	1363	G
5	A	1373	A
5	A	1374	U
5	A	1378	A
5	A	1411	G
5	A	1412	C
5	A	1414	A
5	A	1416	G
5	A	1417	A
5	A	1423	C
5	A	1447	G
5	A	1453	U
5	A	1455	U
5	A	1462	G
5	A	1463	A
5	A	1519	U
5	A	1520	A
5	A	1523	A
5	A	1528	G
5	A	1529	U
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1535	U
5	A	1542	A
5	A	1543	A

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Mol	Chain	Res	Type
5	A	1544	G
5	A	1552	U
5	A	1553	G
5	A	1557	U
5	A	1564	A
5	A	1567	A
5	A	1574	U
5	A	1579	G
5	A	1580	C
5	A	1581	U
5	A	1582	U
5	A	1583	C
5	A	1606	A
5	A	1609	C
5	A	1615	C
5	A	1616	A
5	A	1617	G
5	A	1646	U
5	A	1662	A
5	A	1672	G
5	A	1691	U
5	A	1697	G
5	A	1698	A
5	A	1710	U
5	A	1725	U
5	A	1726	C
5	A	1728	C
5	A	1729	U
5	A	1734	G
5	A	1742	G
5	A	1746	G
5	A	1753	A
5	A	1754	A
5	A	1760	G
5	A	1769	A
5	A	1772	G
5	A	1776	A
5	A	1778	U
5	A	1787	A
5	A	1796	C
5	A	1797	A
5	A	1805	A

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Mol	Chain	Res	Type
5	A	1807	G
5	A	1812	C
5	A	1817	A
5	A	1825	A
5	A	1844	A
5	A	1845	G
5	A	1849	A
5	A	1865	G
5	A	1868	A
5	A	1869	G
5	A	1872	A
5	A	1874	G
5	A	1881	A
5	A	1885	A
5	A	1897	A
5	A	1902	G
5	A	1924	A
5	A	1933	A
5	A	1934	A
5	A	1936	U
5	A	1939	U
5	A	1951	U
5	A	1959	U
5	A	1960	G
5	A	1962	A
5	A	1963	C
5	A	1966	A
5	A	1967	U
5	A	1968	G
5	A	1978	U
5	A	1987	U
5	A	1989	U
5	A	2017	A
5	A	2019	C
5	A	2029	A
5	A	2039	C
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2058	A
5	A	2059	C

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Mol	Chain	Res	Type
5	A	2065	7MG
5	A	2076	G
5	A	2089	G
5	A	2094	U
5	A	2097	A
5	A	2194	A
5	A	2200	G
5	A	2207	G
5	A	2210	C
5	A	2221	A
5	A	2234	G
5	A	2235	G
5	A	2279	U
5	A	2283	A
5	A	2284	A
5	A	2301	U
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2308	U
5	A	2314	G
5	A	2316	A
5	A	2317	G
5	A	2318	A
5	A	2321	A
5	A	2323	A
5	A	2332	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2348	A
5	A	2350	A
5	A	2355	C
5	A	2367	G
5	A	2375	G
5	A	2378	G
5	A	2379	G
5	A	2381	C
5	A	2397	U
5	A	2398	U
5	A	2399	C
5	A	2421	A

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Mol	Chain	Res	Type
5	A	2422	A
5	A	2423	C
5	A	2424	G
5	A	2425	G
5	A	2426	A
5	A	2427	U
5	A	2428	A
5	A	2429	A
5	A	2430	A
5	A	2437	U
5	A	2444	A
5	A	2446	A
5	A	2465	A
5	A	2468	G
5	A	2469	U
5	A	2472	A
5	A	2473	U
5	A	2474	A
5	A	2487	U
5	A	2488	U
5	A	2493	A
5	A	2494	C
5	A	2498	G
5	A	2500	PSU
5	A	2503	C
5	A	2509	A
5	A	2514	A
5	A	2516	C
5	A	2525	G
5	A	2526	A
5	A	2543	A
5	A	2548	OMU
5	A	2550	U
5	A	2551	U
5	A	2562	A
5	A	2563	G
5	A	2578	G
5	A	2581	U
5	A	2582	U
5	A	2598	A
5	A	2599	G
5	A	2605	U

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Mol	Chain	Res	Type
5	A	2606	C
5	A	2609	U
5	A	2625	U
5	A	2635	A
5	A	2636	G
5	A	2642	C
5	A	2650	A
5	A	2651	G
5	A	2652	U
5	A	2656	A
5	A	2657	G
5	A	2661	A
5	A	2685	U
5	A	2686	A
5	A	2687	C
5	A	2709	C
5	A	2710	G
5	A	2722	U
5	A	2729	A
5	A	2740	G
5	A	2744	A
5	A	2746	A
5	A	2748	C
5	A	2761	A
5	A	2774	A
5	A	2776	A
5	A	2786	U
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2814	U
5	A	2816	G
5	A	2829	U
5	A	2845	G
5	A	2857	U
5	A	2863	A
5	A	2875	A
5	A	2876	C
5	A	2897	C
6	B	13	A
6	B	22	G

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Mol	Chain	Res	Type
6	B	23	A
6	B	29	C
6	B	39	C
6	B	43	A
6	B	51	A
6	B	64	A
6	B	65	G
6	B	71	A
6	B	86	U
6	B	87	A
6	B	102	A
6	B	105	C
6	B	106	A
31	a	4	A
31	a	5	A
31	a	6	C
31	a	7	U
31	a	11	G
31	a	15	U
31	a	24	G
31	a	29	G
31	a	34	A
31	a	41	G
31	a	46	A
31	a	49	C
31	a	50	U
31	a	53	A
31	a	57	A
31	a	62	A
31	a	63	G
31	a	80	A
31	a	81	G
31	a	83	U
31	a	84	U
31	a	85	G
31	a	86	C
31	a	97	A
31	a	112	A
31	a	116	A
31	a	117	U
31	a	126	A
31	a	127	U

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Mol	Chain	Res	Type
31	a	140	G
31	a	157	A
31	a	184	A
31	a	186	G
31	a	193	A
31	a	200	G
31	a	201	A
31	a	202	U
31	a	206	C
31	a	236	C
31	a	239	A
31	a	241	U
31	a	242	A
31	a	243	G
31	a	247	G
31	a	262	G
31	a	263	C
31	a	276	C
31	a	285	G
31	a	289	G
31	a	302	A
31	a	324	C
31	a	340	A
31	a	341	C
31	a	342	G
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	380	C
31	a	394	U
31	a	402	G
31	a	407	A
31	a	408	A
31	a	410	A
31	a	418	A
31	a	419	U
31	a	424	G
31	a	425	U
31	a	426	A
31	a	435	U
31	a	444	A

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Mol	Chain	Res	Type
31	a	448	G
31	a	452	A
31	a	457	A
31	a	458	G
31	a	461	A
31	a	464	A
31	a	465	C
31	a	468	A
31	a	469	G
31	a	477	G
31	a	479	A
31	a	481	G
31	a	482	U
31	a	483	U
31	a	494	U
31	a	495	A
31	a	501	C
31	a	503	G
31	a	505	U
31	a	506	A
31	a	507	A
31	a	508	C
31	a	509	U
31	a	513	PSU
31	a	514	G
31	a	515	C
31	a	516	C
31	a	518	G
31	a	522	C
31	a	524	7MG
31	a	527	G
31	a	528	U
31	a	530	A
31	a	532	A
31	a	544	A
31	a	556	A
31	a	559	U
31	a	561	C
31	a	569	A
31	a	570	A
31	a	572	G
31	a	573	C

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Mol	Chain	Res	Type
31	a	574	G
31	a	585	G
31	a	593	A
31	a	615	C
31	a	623	G
31	a	625	G
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	685	G
31	a	699	A
31	a	701	A
31	a	720	U
31	a	721	G
31	a	728	G
31	a	731	G
31	a	752	G
31	a	774	A
31	a	778	A
31	a	781	A
31	a	790	U
31	a	791	A
31	a	809	G
31	a	810	U
31	a	812	A
31	a	813	A
31	a	814	C
31	a	816	A
31	a	817	U
31	a	825	A
31	a	842	A
31	a	864	G
31	a	868	U
31	a	882	G
31	a	887	G
31	a	923	G
31	a	924	G
31	a	931	C
31	a	932	A
31	a	935	A
31	a	957	U

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Mol	Chain	Res	Type
31	a	963	2MG
31	a	966	A
31	a	968	G
31	a	970	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	989	U
31	a	990	G
31	a	993	A
31	a	1000	A
31	a	1001	A
31	a	1002	A
31	a	1003	C
31	a	1006	U
31	a	1010	G
31	a	1023	G
31	a	1025	C
31	a	1026	U
31	a	1027	U
31	a	1028	C
31	a	1029	G
31	a	1030	G
31	a	1033	A
31	a	1034	C
31	a	1039	A
31	a	1040	U
31	a	1041	A
31	a	1042	C
31	a	1048	C
31	a	1050	G
31	a	1051	C
31	a	1052	A
31	a	1062	U
31	a	1068	C
31	a	1070	U
31	a	1081	G
31	a	1082	U
31	a	1084	G
31	a	1091	G
31	a	1098	A
31	a	1122	U

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Mol	Chain	Res	Type
31	a	1127	A
31	a	1129	C
31	a	1134	C
31	a	1135	G
31	a	1136	G
31	a	1140	G
31	a	1141	G
31	a	1156	U
31	a	1157	G
31	a	1164	A
31	a	1165	C
31	a	1166	A
31	a	1168	A
31	a	1179	G
31	a	1180	C
31	a	1185	A
31	a	1189	C
31	a	1193	A
31	a	1194	A
31	a	1198	A
31	a	1209	U
31	a	1210	A
31	a	1235	A
31	a	1253	U
31	a	1255	G
31	a	1267	U
31	a	1275	U
31	a	1276	A
31	a	1277	A
31	a	1278	U
31	a	1282	A
31	a	1284	A
31	a	1295	U
31	a	1297	G
31	a	1299	C
31	a	1300	C
31	a	1317	C
31	a	1335	G
31	a	1342	U
31	a	1343	A
31	a	1350	G
31	a	1360	A

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Mol	Chain	Res	Type
31	a	1361	U
31	a	1367	G
31	a	1375	C
31	a	1378	U
31	a	1380	C
31	a	1381	C
31	a	1387	U
31	a	1394	C
31	a	1395	A
31	a	1415	A
31	a	1416	G
31	a	1421	U
31	a	1423	G
31	a	1427	C
31	a	1439	G
31	a	1443	A
31	a	1445	C
31	a	1448	C
31	a	1449	A
31	a	1484	G
31	a	1494	G
31	a	1500	A
31	a	1503	U
31	a	1504	A
31	a	1513	G
31	a	1514	G
31	a	1526	G
31	a	1527	G
52	v	8	4SU
52	v	10	G
52	v	11	C
52	v	12	U
52	v	14	A
52	v	15	G
52	v	16	U
52	v	17	U
52	v	18	G
52	v	19	G
52	v	20	H2U
52	v	22	A
52	v	23	G
52	v	29	C

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Mol	Chain	Res	Type
52	v	34	U
52	v	37	U
52	v	46	G
52	v	47	G
52	v	48	U
52	v	49	C
52	v	52	A
52	v	56	PSU
52	v	57	C
52	v	58	A
52	v	60	G
52	v	62	C
52	v	65	G
52	v	74	A
52	v	76	C
52	v	77	A

All (39) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	79	A
5	A	84	U
5	A	91	A
5	A	256	C
5	A	324	A
5	A	332	A
5	A	334	A
5	A	365	U
5	A	368	C
5	A	371	G
5	A	424	G
5	A	457	G
5	A	463	U
5	A	478	A
5	A	507	U
5	A	642	A
5	A	720	A
5	A	782	G
5	A	799	G
5	A	929	C
5	A	1127	U
5	A	1179	G

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Mol	Chain	Res	Type
5	A	1267	A
5	A	1268	C
5	A	1296	A
5	A	1337	A
5	A	1519	U
5	A	1697	G
5	A	1816	U
5	A	1880	G
5	A	2088	U
5	A	2209	U
5	A	2342	A
5	A	2422	A
5	A	2525	G
5	A	2651	G
5	A	2747	G
6	B	50	A
6	B	86	U

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

25 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	$\#\|Z\| > 2$
52	5MU	v	55	52	19,22,23	0.40	0	28,32,35	0.57	0
31	5MC	a	964	31	18,22,23	0.57	0	26,32,35	0.59	0
52	PSU	v	56	52	18,21,22	1.09	1 (5%)	22,30,33	1.79	5 (22%)
5	PSU	A	2500	5	18,21,22	1.11	1 (5%)	22,30,33	1.81	5 (22%)
5	PSU	A	2576	5	18,21,22	1.12	1 (5%)	22,30,33	1.77	5 (22%)
31	4OC	a	1399	31	20,23,24	3.16	8 (40%)	26,32,35	0.88	1 (3%)
5	6MZ	A	2026	5	18,25,26	1.84	3 (16%)	16,36,39	3.39	5 (31%)
5	OMG	A	2247	52,5	18,26,27	1.11	2 (11%)	19,38,41	0.86	1 (5%)
31	2MG	a	1204	31	18,26,27	1.14	2 (11%)	16,38,41	0.94	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
52	H2U	v	20	52	18,21,22	0.56	0	21,30,33	1.12	1 (4%)
31	2MG	a	963	31	18,26,27	1.14	2 (11%)	16,38,41	1.00	1 (6%)
52	4SU	v	8	52	18,21,22	4.36	8 (44%)	26,30,33	2.32	8 (30%)
5	PSU	A	952	5	18,21,22	1.08	1 (5%)	22,30,33	1.78	5 (22%)
31	PSU	a	513	31	18,21,22	1.05	1 (5%)	22,30,33	1.72	3 (13%)
5	PSU	A	2601	5	18,21,22	1.06	1 (5%)	22,30,33	1.78	4 (18%)
5	5MU	A	1935	5	19,22,23	0.43	0	28,32,35	0.53	0
5	2MG	A	2441	5	18,26,27	1.14	2 (11%)	16,38,41	0.90	1 (6%)
5	7MG	A	2065	5	22,26,27	1.19	1 (4%)	29,39,42	0.83	2 (6%)
31	UR3	a	1495	31	19,22,23	2.89	6 (31%)	26,32,35	1.31	2 (7%)
5	OMU	A	2548	5	19,22,23	3.06	8 (42%)	26,31,34	1.68	5 (19%)
31	MA6	a	1516	31	18,26,27	1.05	2 (11%)	19,38,41	3.59	2 (10%)
31	7MG	a	524	31	22,26,27	1.22	1 (4%)	29,39,42	0.81	2 (6%)
5	2MA	A	2499	5	17,25,26	2.54	5 (29%)	17,37,40	1.35	2 (11%)
5	PSU	A	2453	5	18,21,22	1.09	1 (5%)	22,30,33	1.82	6 (27%)
31	MA6	a	1515	31	18,26,27	1.01	2 (11%)	19,38,41	3.61	2 (10%)

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
52	5MU	v	55	52	-	3/7/25/26	0/2/2/2
31	5MC	a	964	31	-	2/7/25/26	0/2/2/2
52	PSU	v	56	52	-	2/7/25/26	0/2/2/2
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
5	6MZ	A	2026	5	-	1/5/27/28	0/3/3/3
5	OMG	A	2247	52,5	-	1/5/27/28	0/3/3/3
31	2MG	a	1204	31	-	2/5/27/28	0/3/3/3
52	H2U	v	20	52	-	4/7/38/39	0/2/2/2
31	2MG	a	963	31	-	2/5/27/28	0/3/3/3
52	4SU	v	8	52	-	5/7/25/26	0/2/2/2
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	0/5/27/28	0/3/3/3
5	7MG	A	2065	5	-	1/7/37/38	0/3/3/3
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	2/9/27/28	0/2/2/2
31	MA6	a	1516	31	-	5/7/29/30	0/3/3/3
31	7MG	a	524	31	-	2/7/37/38	0/3/3/3
5	2MA	A	2499	5	-	3/3/25/26	0/3/3/3
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
31	MA6	a	1515	31	-	3/7/29/30	0/3/3/3

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	8	4SU	C2-N1	10.04	1.54	1.38
52	v	8	4SU	C4-N3	8.38	1.46	1.37
5	A	2499	2MA	C2-N3	7.39	1.46	1.31
5	A	2548	OMU	C2-N1	7.19	1.50	1.38
31	a	1495	UR3	C2-N1	7.04	1.48	1.38
52	v	8	4SU	C2-N3	6.99	1.50	1.38
31	a	1399	4OC	C4-N3	6.89	1.44	1.32
5	A	2548	OMU	C2-N3	6.77	1.50	1.38
31	a	1495	UR3	C6-C5	6.71	1.50	1.35
52	v	8	4SU	C5-C4	6.67	1.51	1.42
52	v	8	4SU	C6-C5	6.48	1.50	1.35
5	A	2026	6MZ	C6-N6	6.44	1.45	1.35
31	a	1399	4OC	C6-C5	6.29	1.49	1.35
31	a	1399	4OC	C2-N3	6.13	1.48	1.36
5	A	2548	OMU	C6-C5	5.77	1.48	1.35
31	a	1495	UR3	C2-N3	5.75	1.50	1.39
5	A	2499	2MA	C4-N3	5.23	1.50	1.37
31	a	524	7MG	C5-N7	4.99	1.41	1.35
5	A	2065	7MG	C5-N7	4.98	1.41	1.35
31	a	1399	4OC	C4-N4	4.92	1.46	1.35
52	v	8	4SU	C4-S4	-4.33	1.60	1.68
5	A	2548	OMU	C4-N3	4.16	1.46	1.38
31	a	1399	4OC	C2-N1	4.09	1.48	1.40
31	a	1399	4OC	C5-C4	3.80	1.48	1.40
5	A	2500	PSU	C6-C5	3.66	1.39	1.35
52	v	56	PSU	C6-C5	3.60	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2576	PSU	C6-C5	3.59	1.39	1.35
5	A	952	PSU	C6-C5	3.48	1.39	1.35
5	A	2453	PSU	C6-C5	3.47	1.39	1.35
31	a	513	PSU	C6-C5	3.45	1.39	1.35
5	A	2601	PSU	C6-C5	3.42	1.39	1.35
31	a	1495	UR3	C6-N1	3.40	1.46	1.38
31	a	1399	4OC	C6-N1	3.32	1.46	1.38
5	A	2441	2MG	C8-N7	-3.02	1.29	1.35
31	a	963	2MG	C8-N7	-2.98	1.29	1.35
31	a	1204	2MG	C8-N7	-2.93	1.30	1.35
5	A	2548	OMU	O4-C4	-2.90	1.18	1.24
5	A	2548	OMU	C6-N1	2.90	1.45	1.38
5	A	2499	2MA	C6-N1	2.89	1.44	1.38
5	A	2247	OMG	C8-N7	-2.83	1.30	1.35
52	v	8	4SU	C6-N1	2.72	1.44	1.38
31	a	1516	MA6	C5-C4	-2.69	1.33	1.40
31	a	1399	4OC	O2-C2	-2.66	1.18	1.23
52	v	8	4SU	O2-C2	-2.64	1.18	1.23
31	a	1515	MA6	C5-C4	-2.60	1.34	1.40
5	A	2499	2MA	C5-C4	-2.59	1.36	1.43
5	A	2026	6MZ	C5-C4	-2.55	1.34	1.40
31	a	1516	MA6	C2-N3	2.54	1.36	1.32
5	A	2499	2MA	C2-N1	2.53	1.44	1.36
5	A	2548	OMU	C5-C4	2.53	1.49	1.43
31	a	1515	MA6	C2-N3	2.48	1.36	1.32
31	a	1204	2MG	C5-C6	-2.35	1.42	1.47
31	a	1495	UR3	C4-N3	2.34	1.46	1.40
31	a	963	2MG	C5-C6	-2.33	1.42	1.47
5	A	2548	OMU	O2-C2	-2.31	1.18	1.23
5	A	2441	2MG	C5-C6	-2.30	1.42	1.47
5	A	2247	OMG	C5-C6	-2.20	1.42	1.47
31	a	1495	UR3	C5-C4	2.16	1.49	1.43
5	A	2026	6MZ	C2-N3	2.16	1.35	1.32

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1515	MA6	N1-C6-N6	-14.49	101.81	117.06
31	a	1516	MA6	N1-C6-N6	-14.41	101.89	117.06
5	A	2026	6MZ	C1'-N9-C4	-11.40	106.61	126.64
52	v	8	4SU	C4-N3-C2	-7.12	120.42	127.34
31	a	1515	MA6	N3-C2-N1	-5.54	120.02	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	N3-C2-N1	-5.52	120.05	128.68
5	A	2026	6MZ	N3-C2-N1	-5.50	120.08	128.68
5	A	2548	OMU	C4-N3-C2	-5.16	119.78	126.58
52	v	8	4SU	C5-C4-N3	5.04	119.36	114.69
31	a	1495	UR3	C4-N3-C2	-4.70	120.14	124.56
5	A	2453	PSU	C4-N3-C2	-4.70	119.57	126.34
52	v	8	4SU	C1'-N1-C2	4.64	125.97	117.57
31	a	513	PSU	C4-N3-C2	-4.63	119.66	126.34
5	A	2601	PSU	C4-N3-C2	-4.62	119.68	126.34
5	A	2500	PSU	N1-C2-N3	4.60	120.34	115.13
5	A	2453	PSU	N1-C2-N3	4.60	120.34	115.13
5	A	2500	PSU	C4-N3-C2	-4.58	119.74	126.34
5	A	952	PSU	C4-N3-C2	-4.57	119.75	126.34
52	v	56	PSU	N1-C2-N3	4.56	120.30	115.13
52	v	56	PSU	C4-N3-C2	-4.55	119.78	126.34
5	A	952	PSU	N1-C2-N3	4.50	120.23	115.13
5	A	2601	PSU	N1-C2-N3	4.46	120.19	115.13
5	A	2576	PSU	C4-N3-C2	-4.43	119.96	126.34
31	a	513	PSU	N1-C2-N3	4.38	120.09	115.13
5	A	2576	PSU	N1-C2-N3	4.35	120.06	115.13
52	v	8	4SU	N3-C2-N1	3.85	120.00	114.89
5	A	2548	OMU	N3-C2-N1	3.83	119.97	114.89
5	A	2499	2MA	C5-C6-N1	3.61	120.24	114.02
5	A	2548	OMU	C5-C4-N3	3.23	119.68	114.84
52	v	8	4SU	C5-C4-S4	-3.22	120.32	124.47
52	v	20	H2U	C5-C4-N3	-3.09	113.18	116.65
5	A	2026	6MZ	C2-N1-C6	3.00	119.16	116.59
5	A	2499	2MA	C8-N7-C5	2.96	108.62	102.99
52	v	56	PSU	O2-C2-N1	-2.81	119.69	122.79
5	A	2548	OMU	O4-C4-C5	-2.73	120.37	125.16
5	A	2500	PSU	O2-C2-N1	-2.72	119.80	122.79
5	A	2601	PSU	O2-C2-N1	-2.70	119.82	122.79
5	A	2453	PSU	O2-C2-N1	-2.63	119.90	122.79
31	a	513	PSU	O2-C2-N1	-2.58	119.95	122.79
5	A	2576	PSU	O2-C2-N1	-2.55	119.98	122.79
5	A	2026	6MZ	C9-N6-C6	-2.54	120.69	122.87
5	A	2500	PSU	C6-C5-C4	2.47	119.92	118.20
31	a	1204	2MG	O6-C6-C5	2.46	129.17	124.37
5	A	2247	OMG	O6-C6-C5	2.43	129.11	124.37
52	v	8	4SU	C1'-N1-C6	-2.39	115.62	120.84
5	A	2576	PSU	O4'-C1'-C2'	2.36	108.47	105.14
31	a	963	2MG	O6-C6-C5	2.34	128.94	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2441	2MG	O6-C6-C5	2.33	128.92	124.37
5	A	952	PSU	O2-C2-N1	-2.32	120.24	122.79
52	v	56	PSU	C6-N1-C2	-2.27	120.36	122.68
31	a	1399	4OC	C6-C5-C4	2.22	119.68	116.96
31	a	1495	UR3	C6-N1-C2	-2.22	119.80	121.79
5	A	952	PSU	C6-C5-C4	2.19	119.73	118.20
52	v	56	PSU	O4'-C1'-C2'	2.17	108.20	105.14
31	a	524	7MG	C5-C4-N9	2.16	109.15	106.35
5	A	2453	PSU	C6-N1-C2	-2.15	120.48	122.68
52	v	8	4SU	O2-C2-N3	-2.15	117.50	121.50
5	A	952	PSU	C6-N1-C2	-2.14	120.50	122.68
5	A	2453	PSU	C6-C5-C4	2.12	119.68	118.20
5	A	2576	PSU	C6-N1-C2	-2.10	120.53	122.68
5	A	2601	PSU	C6-N1-C2	-2.10	120.54	122.68
5	A	2548	OMU	O2-C2-N1	-2.08	120.02	122.79
5	A	2065	7MG	C5-C4-N9	2.07	109.04	106.35
5	A	2500	PSU	C6-N1-C2	-2.05	120.59	122.68
52	v	8	4SU	C6-N1-C2	-2.03	118.40	120.99
5	A	2065	7MG	C4-C5-N7	2.02	108.33	105.53
31	a	524	7MG	C4-C5-N7	2.01	108.33	105.53
5	A	2453	PSU	O4'-C1'-C2'	2.01	107.98	105.14
5	A	2026	6MZ	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	a	513	PSU	C3'-C4'-C5'-O5'
31	a	513	PSU	O4'-C4'-C5'-O5'
31	a	524	7MG	C3'-C4'-C5'-O5'
31	a	963	2MG	O4'-C4'-C5'-O5'
31	a	1399	4OC	O4'-C4'-C5'-O5'
31	a	1399	4OC	C3'-C4'-C5'-O5'
31	a	1515	MA6	C5-C6-N6-C9
31	a	1515	MA6	N1-C6-N6-C9
31	a	1516	MA6	C5-C6-N6-C9
31	a	1516	MA6	C5-C6-N6-C10
52	v	8	4SU	C3'-C4'-C5'-O5'
52	v	8	4SU	O4'-C4'-C5'-O5'
52	v	56	PSU	C2'-C1'-C5-C4
5	A	2247	OMG	C1'-C2'-O2'-CM2
5	A	2548	OMU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	A	2548	OMU	O4'-C4'-C5'-O5'
52	v	8	4SU	C2'-C1'-N1-C6
52	v	8	4SU	C2'-C1'-N1-C2
31	a	963	2MG	C3'-C4'-C5'-O5'
31	a	1204	2MG	O4'-C4'-C5'-O5'
5	A	2499	2MA	O4'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
31	a	1516	MA6	N1-C6-N6-C9
31	a	524	7MG	O4'-C4'-C5'-O5'
31	a	1204	2MG	C3'-C4'-C5'-O5'
31	a	1516	MA6	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
52	v	55	5MU	C3'-C4'-C5'-O5'
52	v	56	PSU	C4'-C5'-O5'-P
31	a	1515	MA6	C5-C6-N6-C10
31	a	964	5MC	C3'-C4'-C5'-O5'
52	v	55	5MU	O4'-C4'-C5'-O5'
31	a	964	5MC	O4'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C6
52	v	8	4SU	C4'-C5'-O5'-P
52	v	20	H2U	C3'-C4'-C5'-O5'
5	A	2065	7MG	O4'-C4'-C5'-O5'
5	A	2499	2MA	C4'-C5'-O5'-P
52	v	20	H2U	C2'-C1'-N1-C2
52	v	55	5MU	C2'-C1'-N1-C2
31	a	1516	MA6	C3'-C4'-C5'-O5'
5	A	2026	6MZ	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 5 are monoatomic - leaving 3 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	80P	a	1601	56	44,45,45	3.40	20 (45%)	52,72,72	2.45	15 (28%)
55	80P	a	1603	56	44,45,45	3.53	21 (47%)	52,72,72	2.46	17 (32%)
55	80P	a	1602	56	44,45,45	3.82	22 (50%)	52,72,72	2.47	18 (34%)

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	80P	a	1601	56	-	12/22/87/87	0/5/5/5
55	80P	a	1603	56	-	13/22/87/87	0/5/5/5
55	80P	a	1602	56	-	12/22/87/87	0/5/5/5

All (63) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1602	80P	C08-C09	13.07	1.63	1.52
55	a	1603	80P	C08-C09	11.93	1.62	1.52
55	a	1601	80P	C08-C09	11.75	1.62	1.52
55	a	1602	80P	C08-C21	9.94	1.62	1.53
55	a	1601	80P	C08-C21	8.34	1.60	1.53
55	a	1603	80P	C06-C07	7.30	1.64	1.45
55	a	1602	80P	C06-C07	7.21	1.64	1.45
55	a	1603	80P	C08-C21	7.12	1.59	1.53
55	a	1602	80P	C06-C36	6.88	1.61	1.47
55	a	1602	80P	C04-N03	6.85	1.54	1.47
55	a	1603	80P	C04-N03	6.80	1.54	1.47
55	a	1601	80P	C04-N03	6.73	1.54	1.47
55	a	1603	80P	C06-C36	6.67	1.61	1.47
55	a	1602	80P	C08-C07	6.49	1.63	1.55
55	a	1601	80P	C06-C07	5.79	1.60	1.45
55	a	1601	80P	C06-C36	5.72	1.59	1.47
55	a	1601	80P	C04-C05	5.60	1.63	1.51
55	a	1601	80P	C08-C07	5.36	1.62	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1603	80P	C08-C07	5.24	1.62	1.55
55	a	1603	80P	C04-C05	4.80	1.61	1.51
55	a	1602	80P	C18-C19	4.77	1.65	1.52
55	a	1602	80P	C04-C05	4.51	1.61	1.51
55	a	1603	80P	C18-C19	4.41	1.64	1.52
55	a	1603	80P	C18-C17	4.36	1.58	1.51
55	a	1602	80P	C18-C17	4.22	1.58	1.51
55	a	1601	80P	C18-C19	3.98	1.63	1.52
55	a	1601	80P	C18-C17	3.66	1.57	1.51
55	a	1603	80P	C12-C11	3.61	1.55	1.46
55	a	1602	80P	C16-C17	3.58	1.46	1.40
55	a	1603	80P	C16-C17	3.56	1.46	1.40
55	a	1602	80P	C12-C11	3.49	1.55	1.46
55	a	1602	80P	C10-C11	3.47	1.55	1.47
55	a	1602	80P	C22-C16	3.39	1.59	1.51
55	a	1603	80P	C22-C16	3.33	1.59	1.51
55	a	1601	80P	C12-C11	3.22	1.54	1.46
55	a	1603	80P	C10-C11	3.18	1.54	1.47
55	a	1601	80P	C16-C17	3.18	1.45	1.40
55	a	1603	80P	C19-C10	2.97	1.54	1.51
55	a	1602	80P	C15-C26	2.93	1.56	1.52
55	a	1602	80P	C12-C13	2.92	1.46	1.41
55	a	1603	80P	C15-C26	2.77	1.56	1.52
55	a	1601	80P	C22-C16	2.76	1.57	1.51
55	a	1602	80P	C36-N38	2.76	1.40	1.33
55	a	1603	80P	C36-N38	2.71	1.40	1.33
55	a	1603	80P	C12-C13	2.68	1.45	1.41
55	a	1601	80P	C15-C26	2.66	1.56	1.52
55	a	1601	80P	C10-C11	2.59	1.53	1.47
55	a	1602	80P	C19-C10	2.59	1.54	1.51
55	a	1601	80P	C36-N38	2.53	1.40	1.33
55	a	1603	80P	C20-C19	2.48	1.59	1.53
55	a	1601	80P	C12-C13	2.44	1.45	1.41
55	a	1602	80P	C20-C19	2.41	1.58	1.53
55	a	1603	80P	C40-N03	2.38	1.54	1.47
55	a	1601	80P	C19-C10	2.34	1.54	1.51
55	a	1602	80P	C40-N03	2.28	1.54	1.47
55	a	1603	80P	C16-C15	2.24	1.43	1.40
55	a	1602	80P	C16-C15	2.16	1.43	1.40
55	a	1601	80P	C14-C15	2.13	1.43	1.39
55	a	1601	80P	C20-C19	2.13	1.58	1.53
55	a	1602	80P	C14-C15	2.11	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1602	80P	O39-C05	2.07	1.39	1.33
55	a	1603	80P	O39-C05	2.07	1.39	1.33
55	a	1601	80P	C40-N03	2.04	1.53	1.47

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	a	1603	80P	C11-C10-C09	8.82	125.77	118.80
55	a	1601	80P	C11-C10-C09	8.68	125.66	118.80
55	a	1602	80P	C11-C10-C09	8.44	125.47	118.80
55	a	1601	80P	C08-C21-C04	5.17	118.71	111.64
55	a	1602	80P	C12-C11-C10	5.15	127.30	118.53
55	a	1603	80P	C36-C06-C07	-4.88	115.19	120.97
55	a	1603	80P	C12-C11-C10	4.82	126.75	118.53
55	a	1603	80P	O33-C09-C10	4.70	130.34	123.90
55	a	1602	80P	O33-C09-C08	-4.68	106.59	113.37
55	a	1601	80P	C12-C11-C10	4.60	126.36	118.53
55	a	1602	80P	O33-C09-C10	4.56	130.14	123.90
55	a	1602	80P	C36-C06-C07	-4.54	115.60	120.97
55	a	1601	80P	O33-C09-C10	4.37	129.88	123.90
55	a	1602	80P	C08-C21-C04	4.35	117.59	111.64
55	a	1603	80P	O33-C09-C08	-4.27	107.19	113.37
55	a	1601	80P	C36-C06-C07	-4.12	116.10	120.97
55	a	1601	80P	C13-C12-C17	4.07	123.63	119.05
55	a	1601	80P	O33-C09-C08	-4.02	107.55	113.37
55	a	1602	80P	C12-C17-C16	-3.97	117.23	120.75
55	a	1602	80P	C13-C12-C17	3.93	123.48	119.05
55	a	1601	80P	C12-C17-C16	-3.90	117.29	120.75
55	a	1603	80P	C12-C17-C16	-3.90	117.29	120.75
55	a	1603	80P	C13-C12-C17	3.90	123.44	119.05
55	a	1601	80P	C18-C17-C16	3.81	127.57	120.94
55	a	1603	80P	C08-C21-C04	3.73	116.74	111.64
55	a	1603	80P	C18-C17-C16	3.52	127.06	120.94
55	a	1602	80P	C18-C17-C16	3.27	126.64	120.94
55	a	1602	80P	O32-C11-C10	-3.23	115.82	120.78
55	a	1601	80P	O32-C11-C10	-3.19	115.88	120.78
55	a	1603	80P	O32-C11-C10	-3.19	115.89	120.78
55	a	1602	80P	C13-C12-C11	-3.13	116.89	121.47
55	a	1603	80P	C13-C12-C11	-3.08	116.95	121.47
55	a	1603	80P	F25-C22-C16	3.04	119.53	112.34
55	a	1602	80P	F25-C22-C16	3.02	119.50	112.34
55	a	1601	80P	F23-C22-C16	2.97	119.37	112.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	a	1602	80P	C08-C07-C06	2.90	120.36	115.75
55	a	1601	80P	C13-C12-C11	-2.86	117.28	121.47
55	a	1602	80P	O32-C11-C12	-2.71	116.88	121.99
55	a	1601	80P	C14-C13-C12	-2.70	117.79	120.93
55	a	1601	80P	O37-C36-N38	-2.67	116.64	122.88
55	a	1602	80P	O37-C36-N38	-2.56	116.90	122.88
55	a	1602	80P	C14-C13-C12	-2.55	117.97	120.93
55	a	1603	80P	C14-C13-C12	-2.54	117.98	120.93
55	a	1603	80P	O37-C36-N38	-2.53	116.95	122.88
55	a	1603	80P	O32-C11-C12	-2.45	117.36	121.99
55	a	1603	80P	C08-C07-C06	2.40	119.57	115.75
55	a	1601	80P	O32-C11-C12	-2.24	117.76	121.99
55	a	1603	80P	F23-C22-C16	2.13	117.39	112.34
55	a	1602	80P	F23-C22-C16	2.12	117.35	112.34
55	a	1602	80P	O35-C07-C08	-2.01	115.14	119.08

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	a	1601	80P	C05-C04-N03-C01
55	a	1601	80P	C21-C04-N03-C40
55	a	1601	80P	C14-C15-C26-N27
55	a	1601	80P	C16-C15-C26-C30
55	a	1601	80P	C16-C15-C26-N27
55	a	1602	80P	C05-C06-C36-N38
55	a	1602	80P	C05-C06-C36-O37
55	a	1602	80P	C07-C06-C36-N38
55	a	1602	80P	C07-C06-C36-O37
55	a	1602	80P	C41-C40-N03-C04
55	a	1603	80P	C05-C04-N03-C40
55	a	1603	80P	C05-C06-C36-N38
55	a	1603	80P	C05-C06-C36-O37
55	a	1603	80P	C16-C15-C26-C30
55	a	1601	80P	C21-C04-N03-C01
55	a	1601	80P	C41-C40-N03-C01
55	a	1602	80P	C41-C40-N03-C01
55	a	1601	80P	C05-C04-N03-C40
55	a	1602	80P	C05-C04-N03-C40
55	a	1603	80P	C21-C04-N03-C40
55	a	1603	80P	C15-C16-C22-F25
55	a	1601	80P	C41-C40-N03-C04

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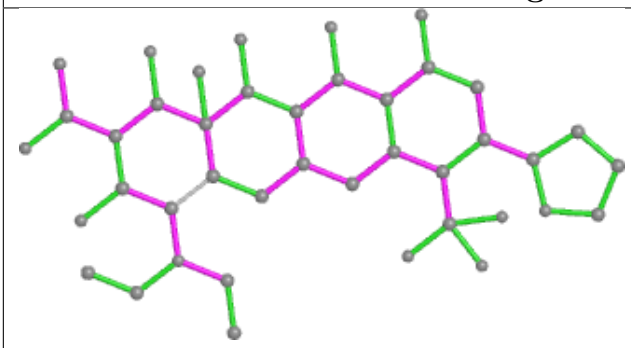
Mol	Chain	Res	Type	Atoms
55	a	1603	80P	C17-C16-C22-F25
55	a	1603	80P	C14-C15-C26-N27
55	a	1603	80P	C21-C04-N03-C01
55	a	1601	80P	C15-C16-C22-F23
55	a	1602	80P	C15-C16-C22-F25
55	a	1603	80P	C15-C16-C22-F24
55	a	1601	80P	C15-C16-C22-F24
55	a	1602	80P	C15-C16-C22-F24
55	a	1603	80P	C15-C16-C22-F23
55	a	1603	80P	C17-C16-C22-F23
55	a	1602	80P	C15-C16-C22-F23
55	a	1602	80P	C17-C16-C22-F23
55	a	1602	80P	C17-C16-C22-F25
55	a	1603	80P	C17-C16-C22-F24
55	a	1601	80P	C15-C16-C22-F25

There are no ring outliers.

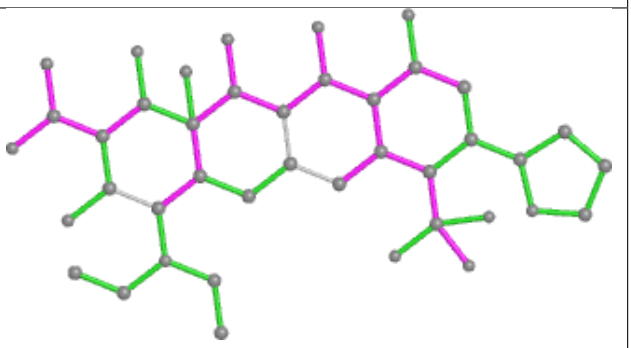
No monomer is involved in short contacts.

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.

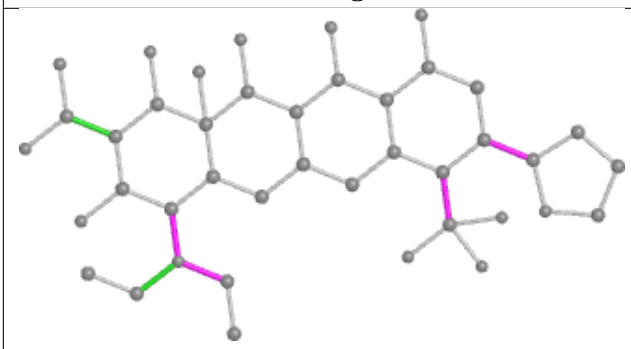
Ligand 80P a 1601



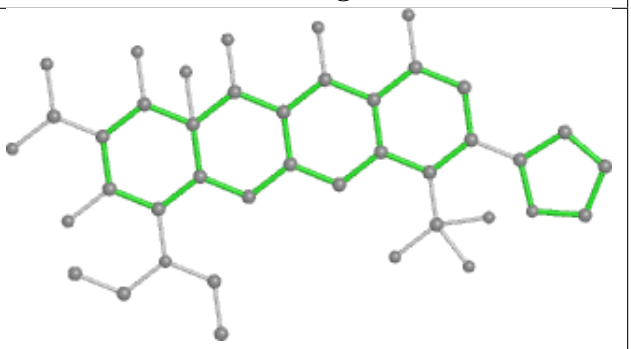
Bond lengths



Bond angles

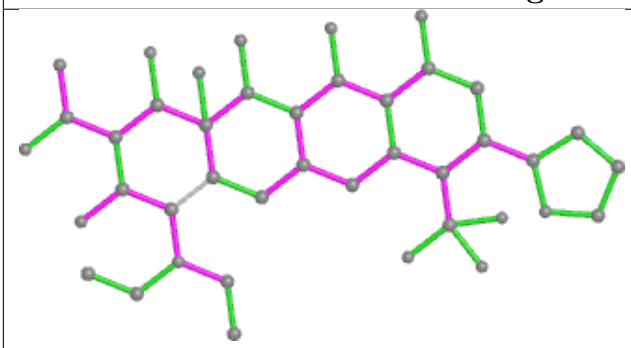


Torsions

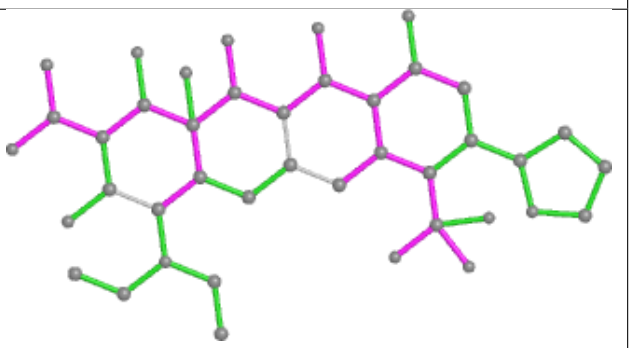


Rings

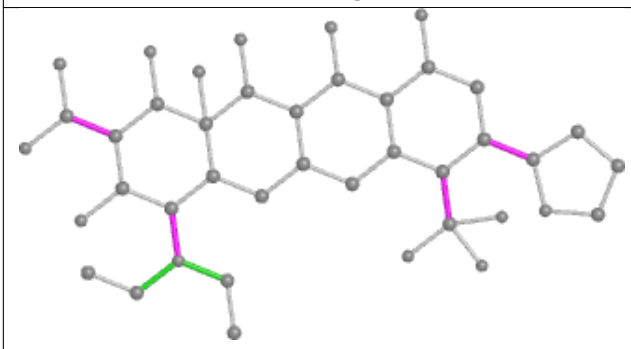
Ligand 80P a 1603



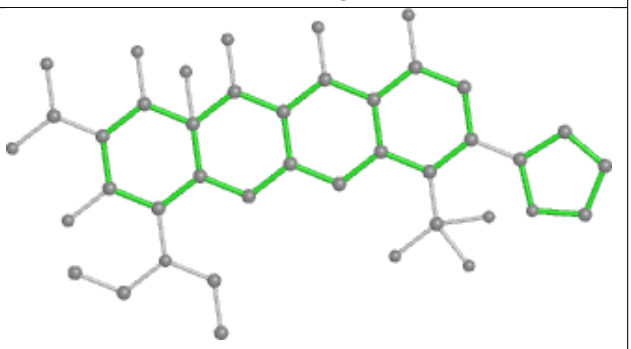
Bond lengths



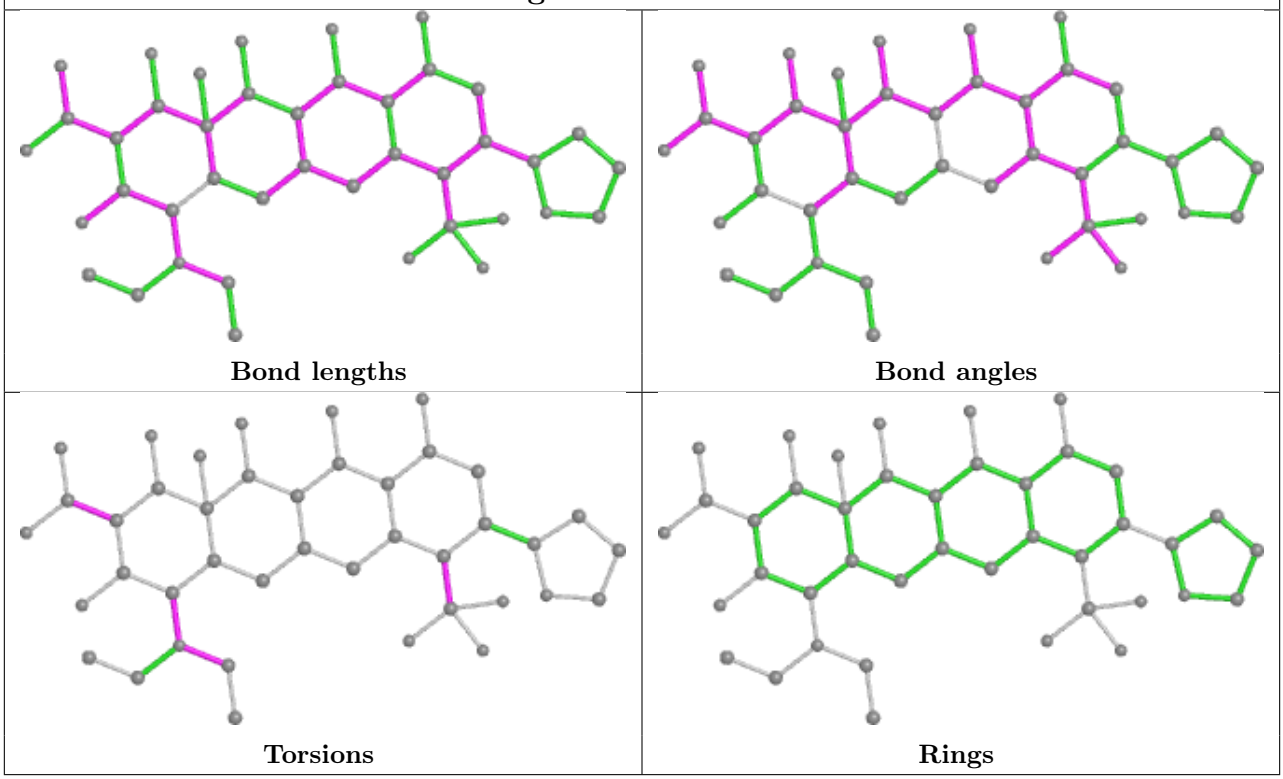
Bond angles



Torsions



Rings

Ligand 80P a 1602	
	
Bond lengths	Bond angles
Torsions	Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

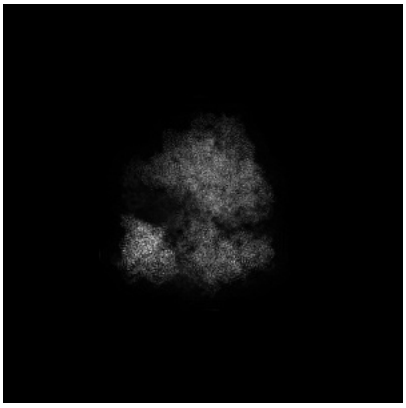
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24738. These allow visual inspection of the internal detail of the map and identification of artifacts.

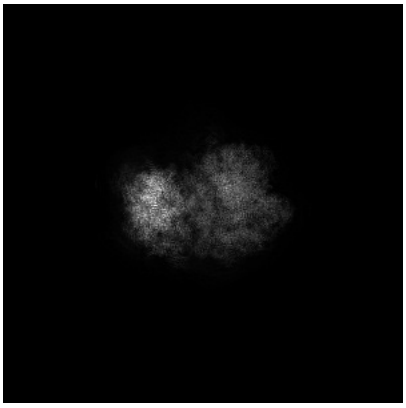
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

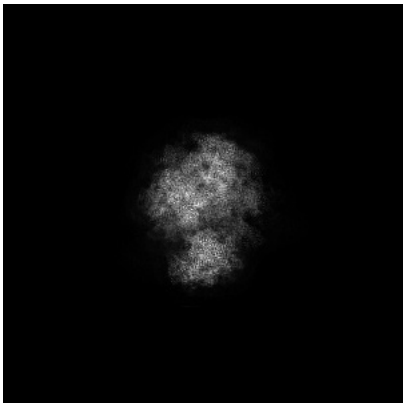
6.1.1 Primary map



X



Y

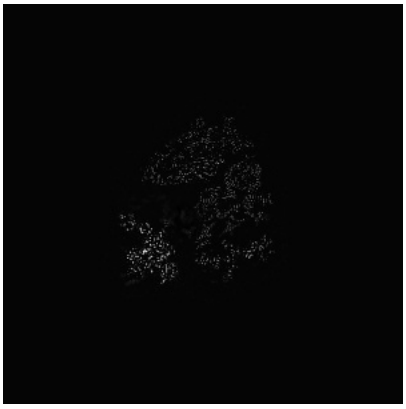


Z

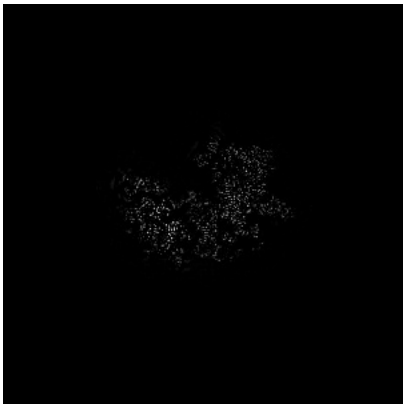
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

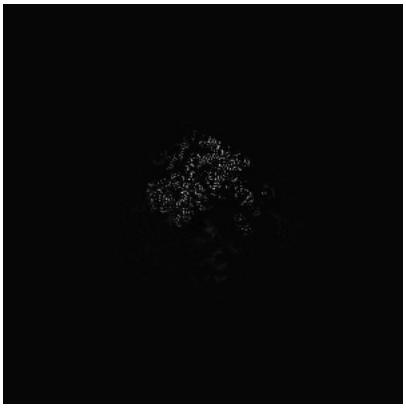
6.2.1 Primary map



X Index: 256



Y Index: 256



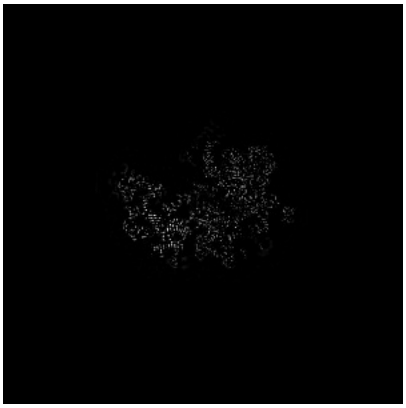
Z Index: 256

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

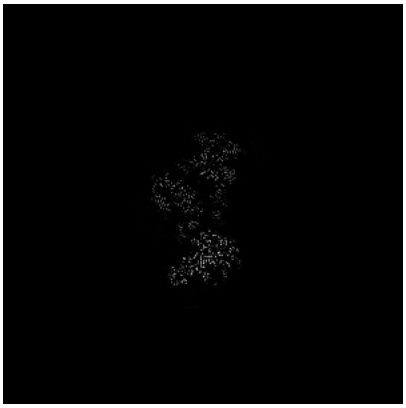
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 263



Y Index: 265

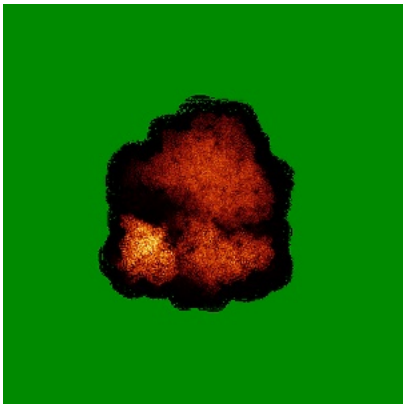


Z Index: 194

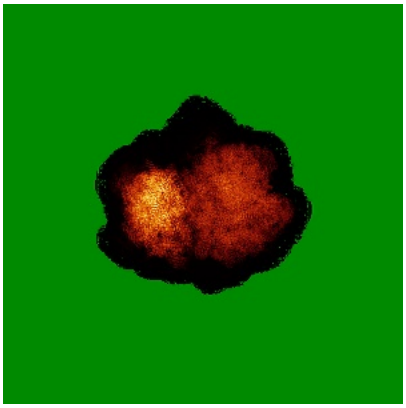
The images above show the largest variance slices of the map in three orthogonal directions.

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

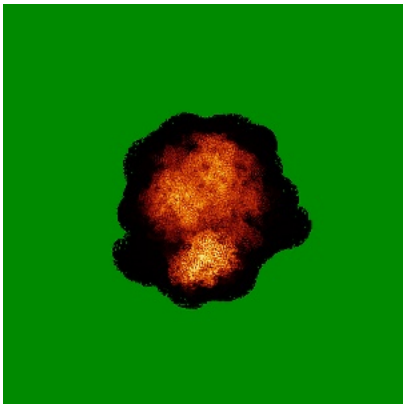
6.4.1 Primary map



X



Y

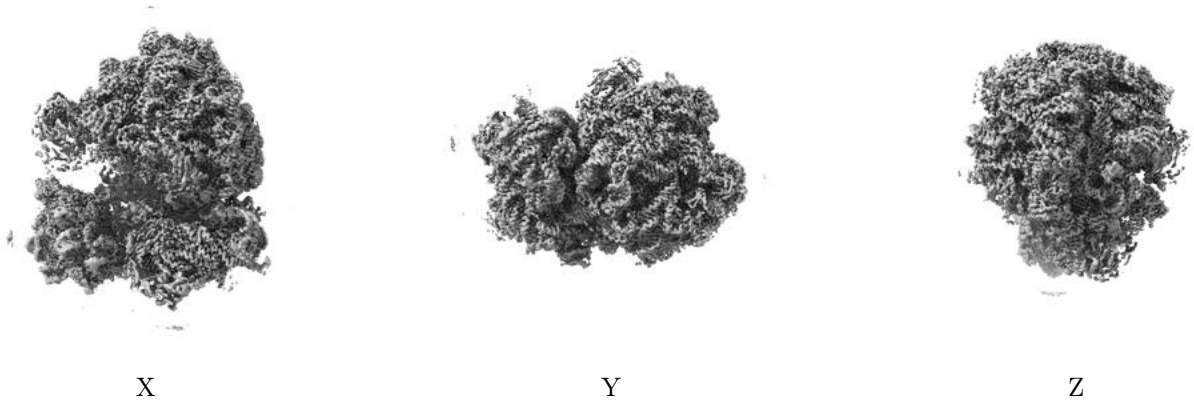


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

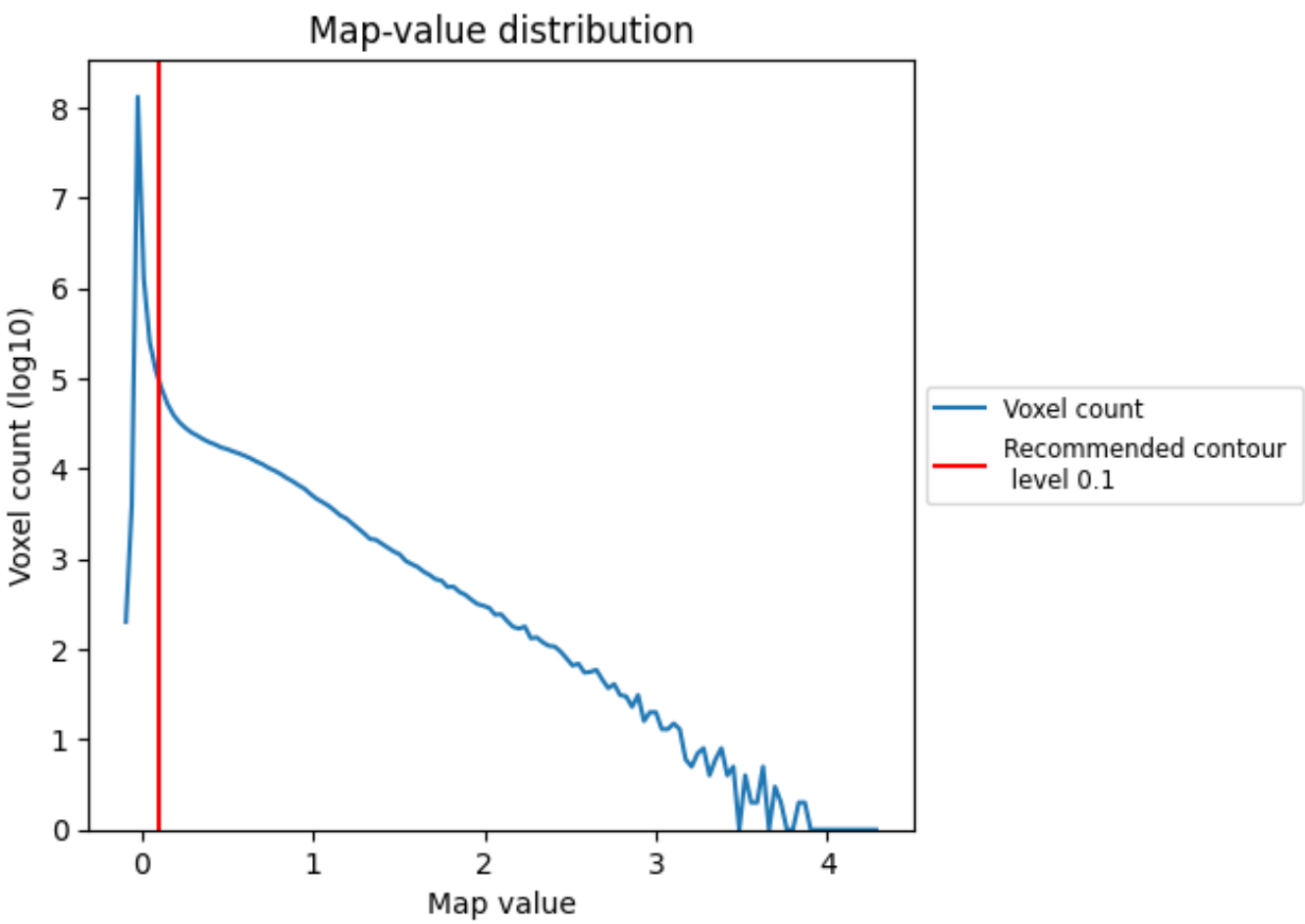
6.6 Mask visualisation (i)

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

7 Map analysis (i)

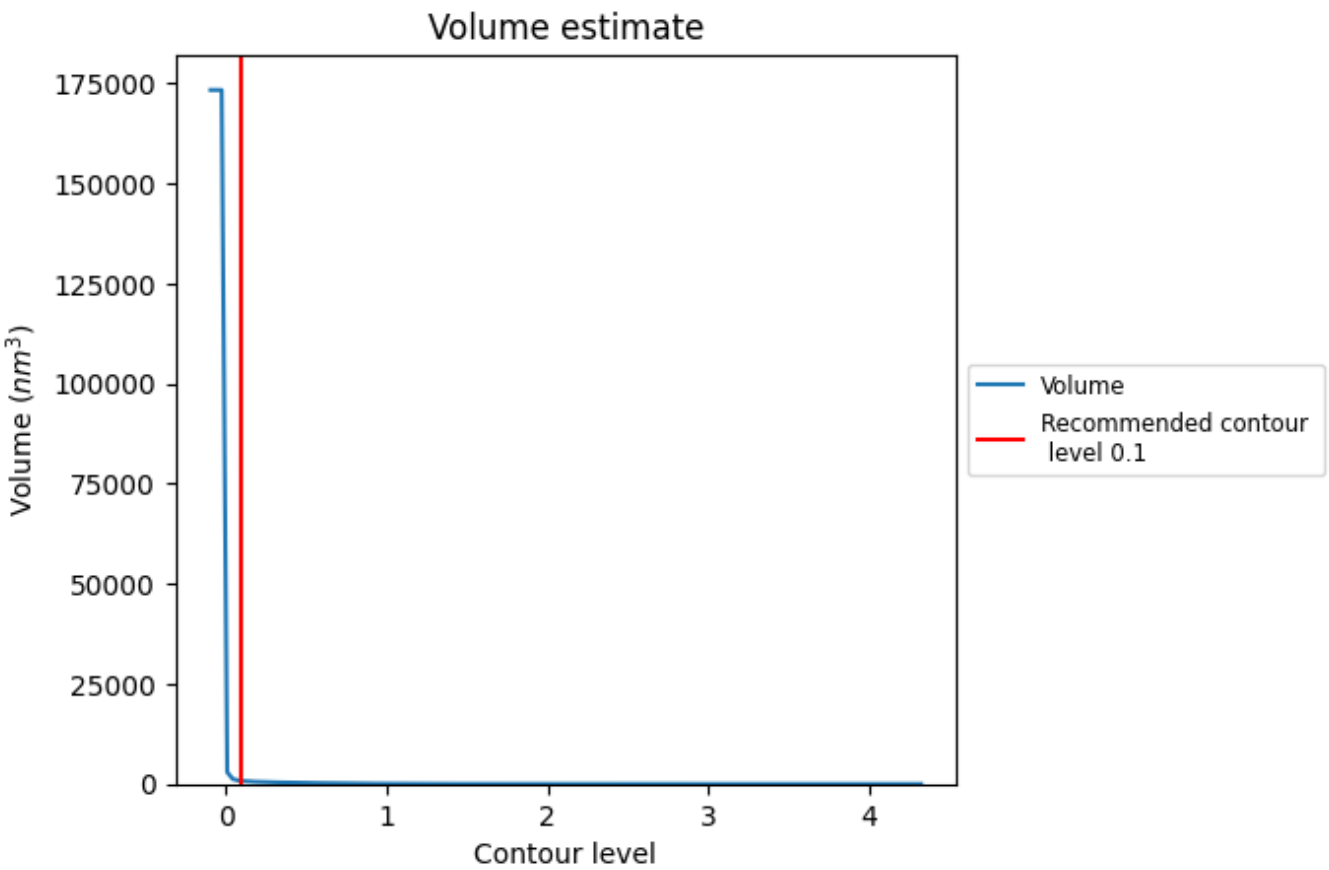
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

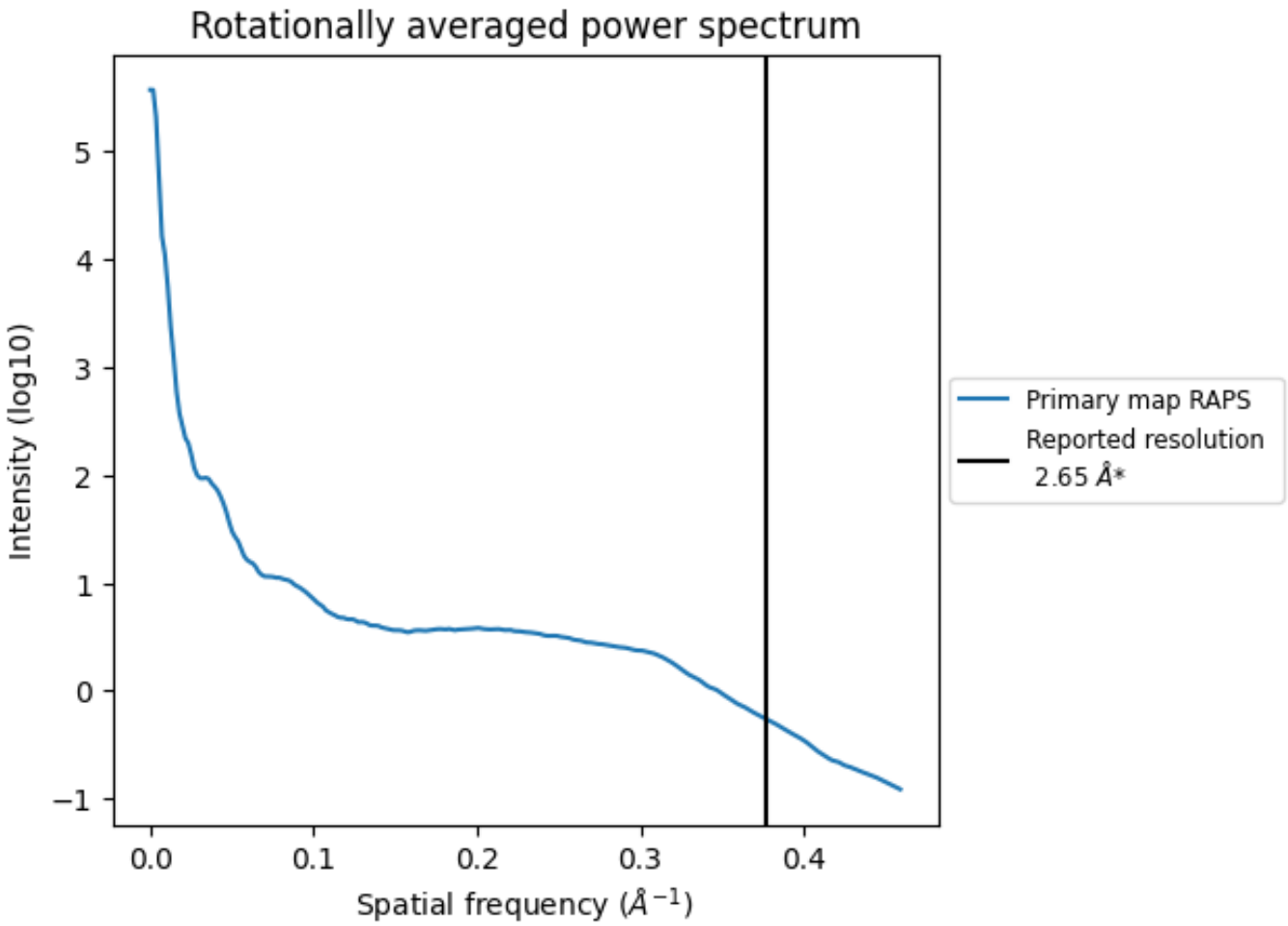
7.2 Volume estimate (i)



The volume at the recommended contour level is 789 nm^3; this corresponds to an approximate mass of 713 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 0.377 Å^{-1}

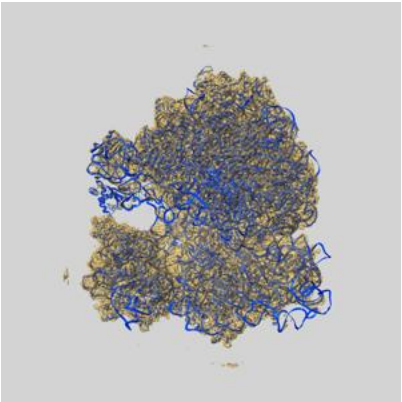
8 Fourier-Shell correlation (i)

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

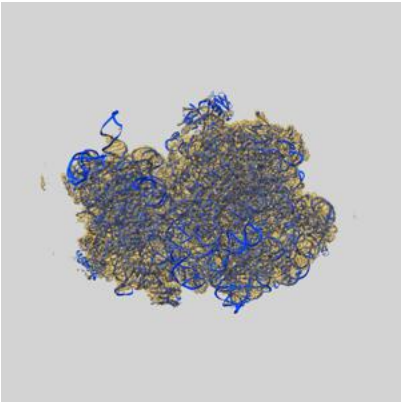
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24738 and PDB model 7RYF. Per-residue inclusion information can be found in section 3 on page 14.

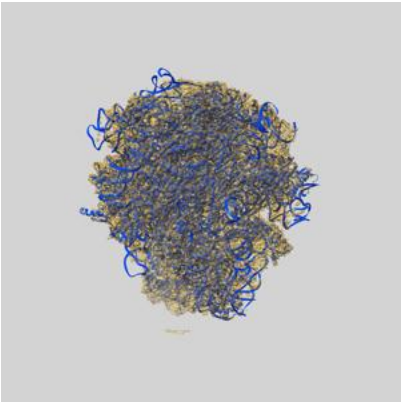
9.1 Map-model overlay (i)



X



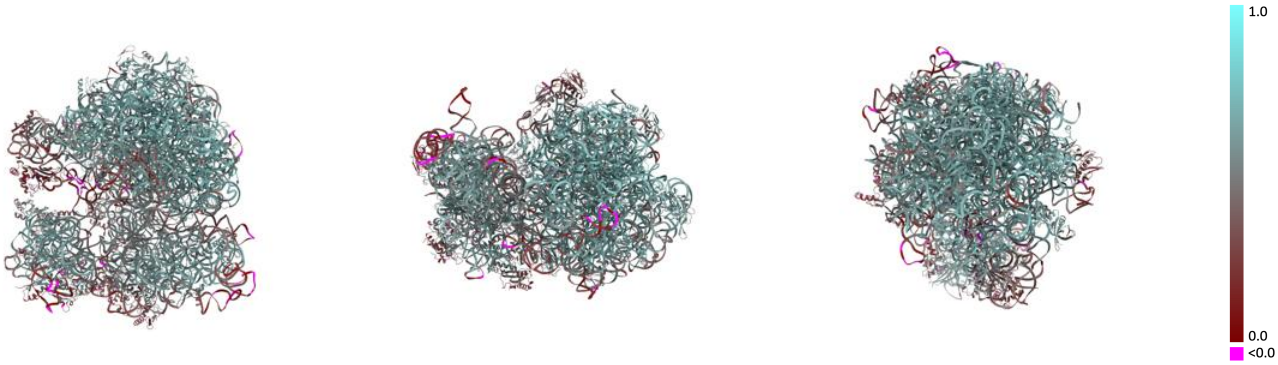
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

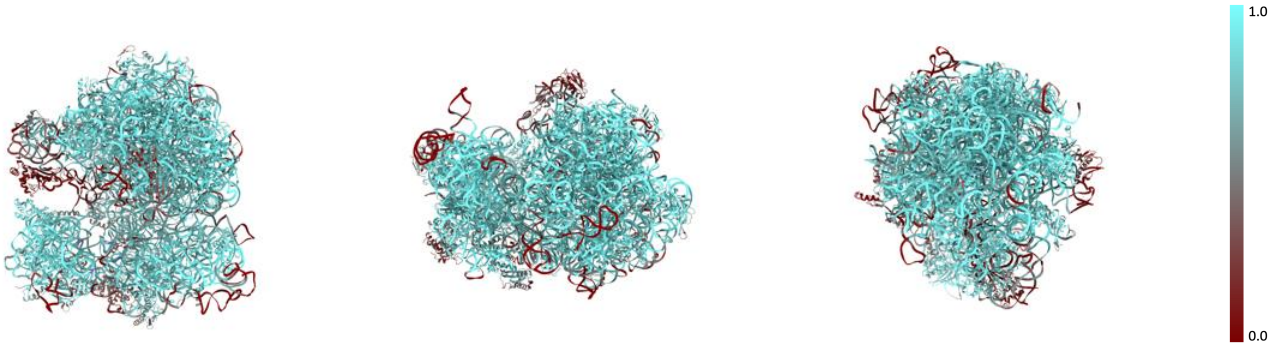
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

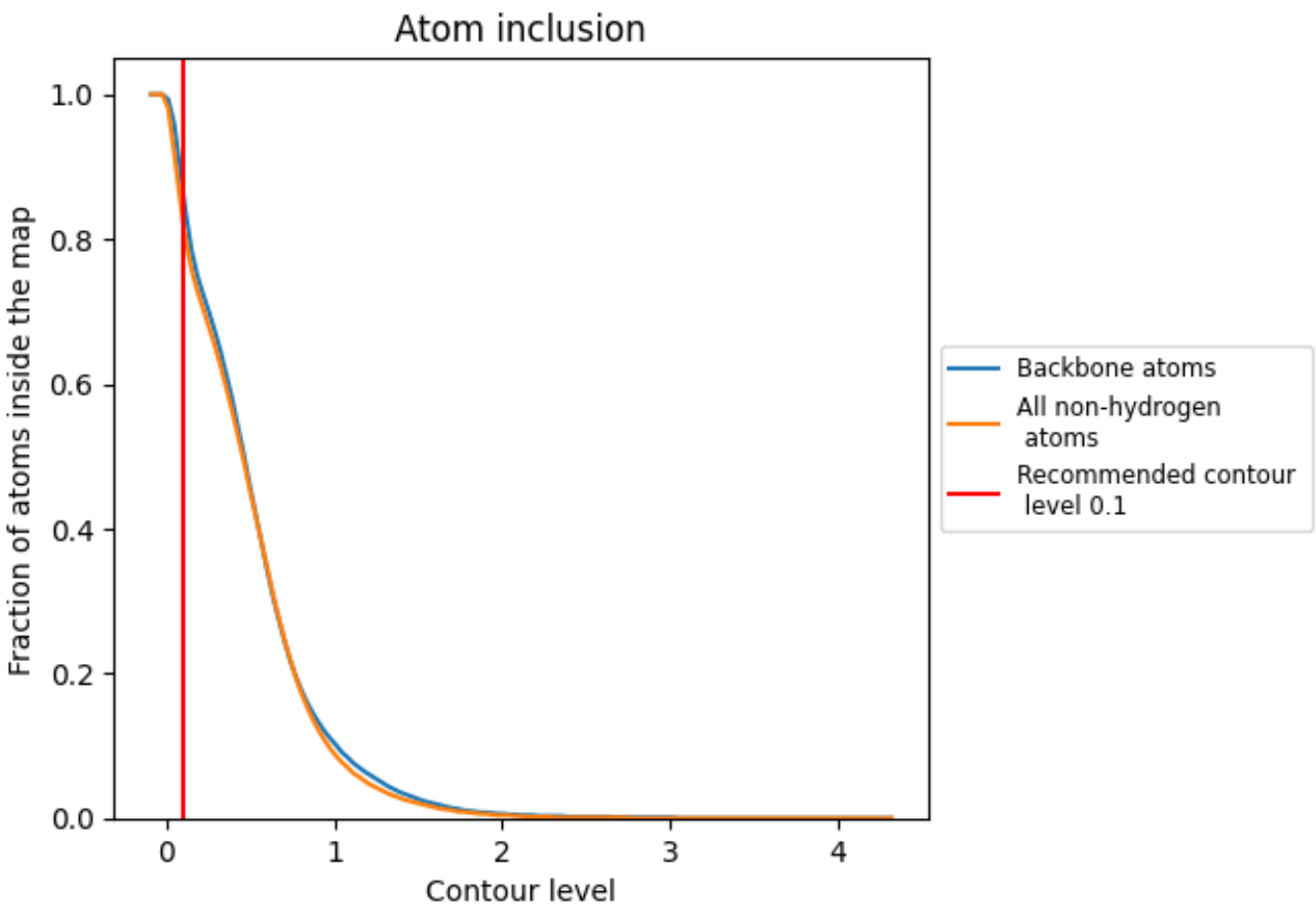
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.1).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8180	0.5410
0	0.7690	0.5310
1	0.9710	0.6830
2	0.8690	0.5990
3	0.6470	0.4940
A	0.8720	0.5910
B	0.5650	0.4400
C	0.9210	0.6280
D	0.9380	0.6570
E	0.8600	0.6160
F	0.0690	0.2250
G	0.2760	0.3480
H	0.3540	0.3450
I	0.9370	0.6580
J	0.9150	0.6250
K	0.9380	0.6450
L	0.8570	0.5830
M	0.9710	0.6830
N	0.5900	0.4030
O	0.8670	0.5880
P	0.9730	0.6920
Q	0.9050	0.6270
R	0.9260	0.6570
S	0.7700	0.5630
T	0.7100	0.5410
U	0.7990	0.5550
V	0.9140	0.6500
W	0.8860	0.6140
X	0.5900	0.4520
Y	0.8980	0.6240
Z	0.8760	0.6180
a	0.8400	0.5080
b	0.2730	0.2740
c	0.8860	0.5030
d	0.5550	0.3520

Continued on next page...

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Chain	Atom inclusion	Q-score
e	0.8980	0.5460
f	0.5620	0.3430
g	0.6950	0.3510
h	0.9440	0.5970
i	0.9520	0.5770
j	0.8730	0.5130
k	0.5110	0.3240
l	0.6490	0.4530
m	0.9170	0.5150
n	0.9290	0.5680
o	0.9060	0.5580
p	0.9080	0.5970
q	0.8430	0.5070
r	0.7870	0.4540
s	0.9560	0.5670
t	0.9170	0.5620
u	0.1720	0.2610
v	0.2930	0.1800
w	0.7690	0.3290