Full wwPDB EM Validation Report ⓘ

Apr 14, 2022 – 04:46 am BST

PDB ID	:	7P7T
EMDB ID	:	EMD-13244
Title	:	PoxtA-EQ2 antibiotic resistance ABCF bound to E. faecalis 70S ribosome, state III
Authors	:	Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on	:	2021-07-20
Resolution	:	2.90 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 ⓘ symbol.

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

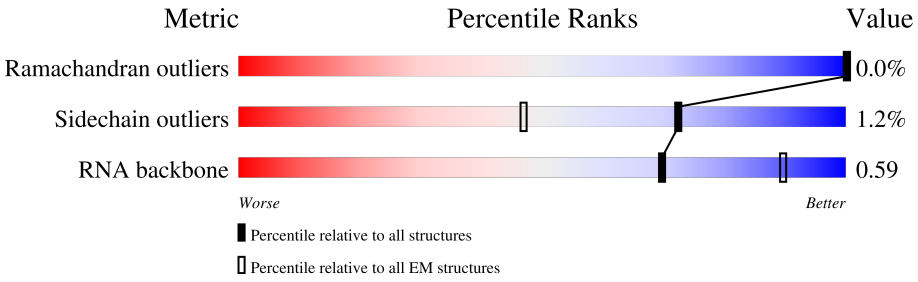
EMDB validation analysis	:	0.0.0.dev97
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.27

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 2.90 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.



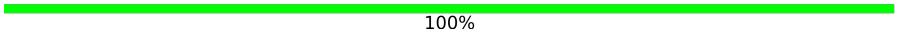
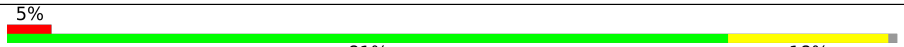
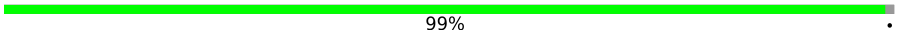
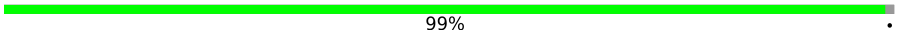
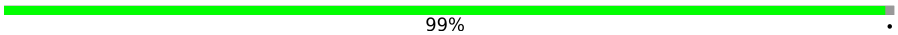
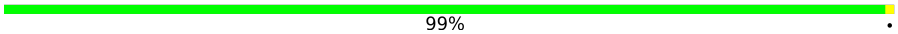
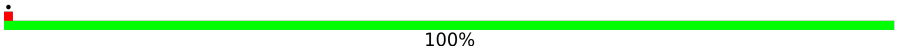
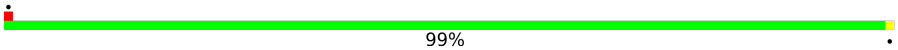
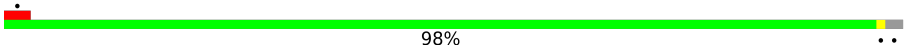
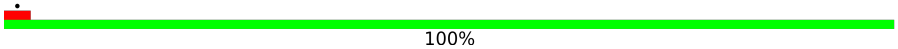
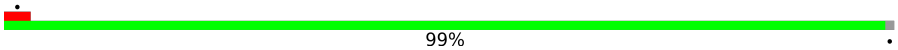
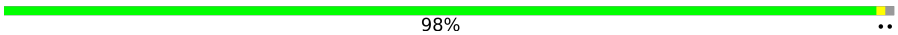
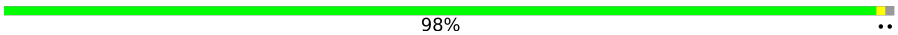
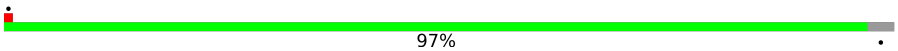
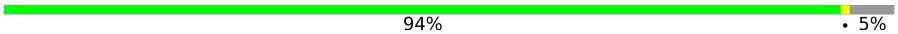
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	586	16% 90% · 9%
2	1	62	92% · 5%
3	2	59	· 97% ·
4	3	89	51% 89% · 10%
5	4	59	88% · 10%
6	5	49	96% · ·
7	6	44	· 100%
8	7	66	95% · ·

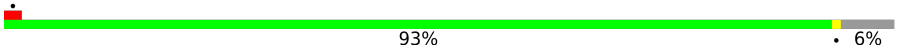
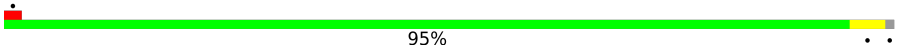
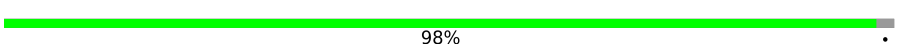
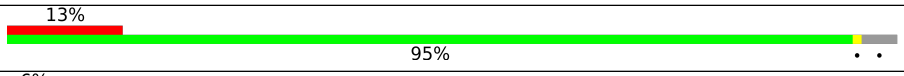
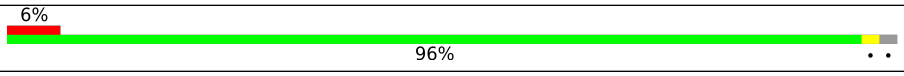
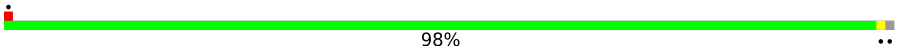
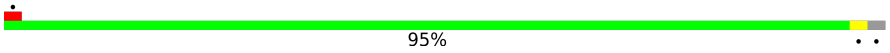
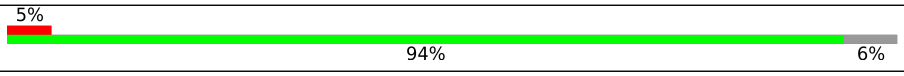
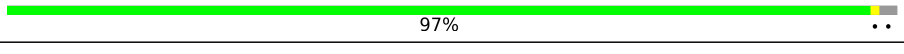
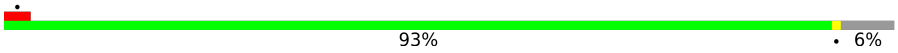
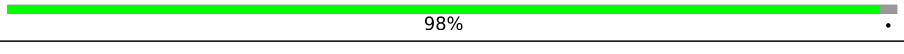
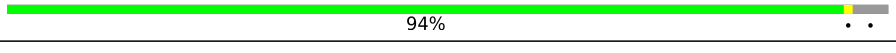
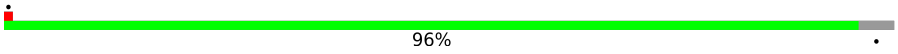
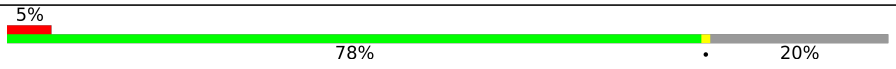
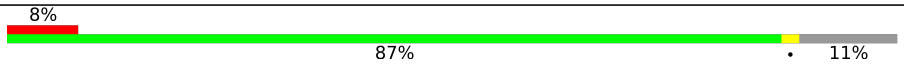
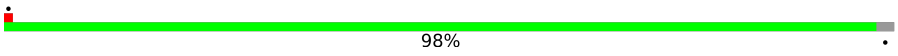
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	8	38	
10	A	2912	
11	B	116	
12	C	76	
13	D	77	
14	F	229	
15	G	276	
16	H	209	
17	I	207	
18	J	179	
19	K	178	
20	M	147	
21	N	122	
22	O	146	
23	P	144	
24	Q	127	
25	R	118	
26	S	115	
27	T	119	
28	U	102	
29	V	115	
30	W	96	
31	X	103	
32	Y	95	
33	Z	62	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	a	1558	
35	b	19	
36	c	261	
37	d	218	
38	e	203	
39	f	166	
40	g	100	
41	h	156	
42	i	132	
43	j	130	
44	k	102	
45	l	129	
46	m	137	
47	n	121	
48	o	61	
49	p	89	
50	q	91	
51	r	88	
52	s	79	
53	t	92	
54	u	83	

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 149080 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 ARE-ABC-F family resistance factor PoxtA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	534	Total	C	N	O	S	0	0
			4347	2789	720	823	15		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			491	307	91	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			428	266	80	81	1		

- Molecule 4 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	80	Total	C	N	O	S	0	0
			647	409	110	126	2		

- Molecule 5 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	53	Total	C	N	O	S	0	0
			406	248	84	69	5		

- Molecule 6 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	48	Total	C	N	O	S	0	0
			410	247	84	75	4		

- Molecule 7 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	44	Total	C	N	O	S	0	0
			374	227	91	54	2		

- Molecule 8 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	64	Total	C	N	O	S	0	0
			522	320	122	78	2		

- Molecule 9 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	38	Total	C	N	O	S	0	0
			305	188	66	45	6		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	A	2901	Total	C	N	O	P	0	0
			62268	27794	11451	20122	2901		

- Molecule 11 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	B	114	Total	C	N	O	P	0	0
			2439	1088	439	798	114		

- Molecule 12 is a RNA chain called A-site tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	C	72	Total	C	N	O	P	S	0	0
			1546	692	273	508	72	1		

- Molecule 13 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	D	76	Total	C	N	O	P	0	0
			1624	724	295	529	76		

- Molecule 14 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	226	Total	C	N	O	S	0	0
			1693	1073	287	327	6		

- Molecule 15 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	274	Total	C	N	O	S	0	0
			2106	1305	414	380	7		

- Molecule 16 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	206	Total	C	N	O	S	0	0
			1572	990	291	287	4		

- Molecule 17 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	205	Total	C	N	O	S	0	0
			1572	984	289	297	2		

- Molecule 18 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	177	Total	C	N	O	S	0	0
			1392	887	239	260	6		

- Molecule 19 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	174	Total	C	N	O	S	0	0
			1335	838	242	251	4		

- Molecule 20 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	147	Total	C	N	O	S	0	0
			1146	726	207	209	4		

- Molecule 21 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	122	Total	C	N	O	S	0	0
			923	574	176	171	2		

- Molecule 22 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	146	Total	C	N	O	S	0	0
			1096	677	212	206	1		

- Molecule 23 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	134	Total	C	N	O	S	0	0
			1070	683	209	173	5		

- Molecule 24 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	125	Total	C	N	O	S	0	0
			997	615	192	187	3		

- Molecule 25 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	118	Total	C	N	O	S	0	0
			908	561	176	169	2		

- Molecule 26 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	S	114	Total	C	N	O	0	0
			925	582	185	158		

- Molecule 27 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	118	Total	C	N	O	S	0	0
			950	602	184	160	4		

- Molecule 28 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	101	Total	C	N	O	S	0	0
			779	497	138	142	2		

- Molecule 29 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	V	111	Total	C	N	O	S	0	0
			841	527	154	158	2		

- Molecule 30 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	W	91	Total	C	N	O	S	0	0
			736	469	129	134	4		

- Molecule 31 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	X	101	Total	C	N	O	S	0	0
			763	486	135	140	2		

- Molecule 32 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Y	74	Total	C	N	O	0	0
			559	344	107	108		

- Molecule 33 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	61	Total	C	N	O	S	0	0
			480	299	97	82	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1521	Total	C	N	O	P	0	0
			32595	14542	5954	10578	1521		

- Molecule 35 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	13	Total	C	N	O	P	0	0
			287	128	59	87	13		

- Molecule 36 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	c	222	Total	C	N	O	S	0	0
			1773	1126	312	326	9		

- Molecule 37 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	d	205	Total	C	N	O	S	0	0
			1618	1018	304	293	3		

- Molecule 38 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	200	Total	C	N	O	S	0	0
			1611	1010	301	296	4		

- Molecule 39 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	163	Total	C	N	O	S	0	0
			1204	759	222	221	2		

- Molecule 40 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	96	Total	C	N	O	S	0	0
			786	496	135	152	3		

- Molecule 41 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	h	153	Total	C	N	O	S	0	0
			1218	759	232	221	6		

- Molecule 42 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	i	131	Total	C	N	O	S	0	0
			1041	662	184	193	2		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	127	Total	C	N	O	S	0	0
			980	610	195	174	1		

- Molecule 44 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	96	Total	C	N	O	S	0	0
			773	487	142	142	2		

- Molecule 45 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	116	Total	C	N	O	S	0	0
			854	527	163	160	4		

- Molecule 46 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	134	Total	C	N	O	S	0	0
			1051	652	211	186	2		

- Molecule 47 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	114	Total	C	N	O	S	0	0
			902	552	183	166	1		

- Molecule 48 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	o	60	Total	C	N	O	S	0	0
			492	310	100	77	5		

- Molecule 49 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	p	85	Total	C	N	O	S	0	0
			716	440	146	129	1		

- Molecule 50 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	87	Total	C	N	O	S	0	0
			692	437	128	125	2		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	80	Total	C	N	O	S	0	0
			660	414	124	119	3		

- Molecule 52 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	63	Total	C	N	O	S	0	0
			511	328	95	87	1		

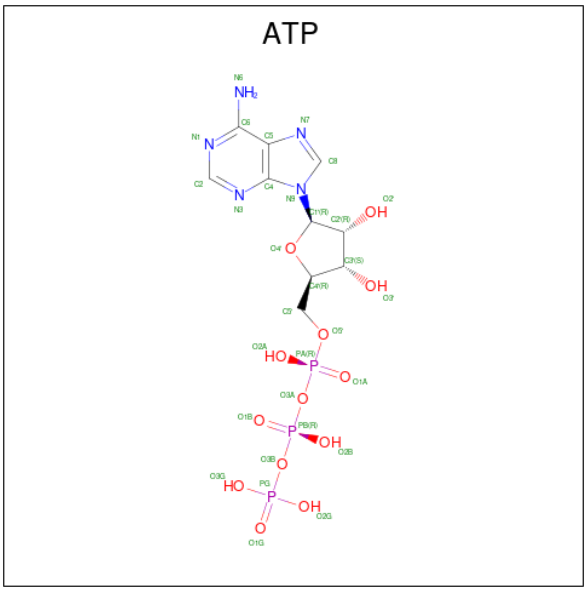
- Molecule 53 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	82	Total	C	N	O	S	0	0
			663	426	122	113	2		

- Molecule 54 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	81	Total	C	N	O	S	0	0
			608	371	118	117	2		

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
55	0	1	Total	C	N	O	P	0
			62	20	10	26	6	
55	0	1	Total	C	N	O	P	0
			62	20	10	26	6	

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

Mol	Chain	Residues	Atoms		AltConf
56	0	2	Total	Mg	0
			2	2	
56	A	117	Total	Mg	0
			117	117	
56	B	1	Total	Mg	0
			1	1	
56	G	1	Total	Mg	0
			1	1	
56	a	39	Total	Mg	0
			39	39	
56	n	1	Total	Mg	0
			1	1	

- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	4	1	Total	Zn	0
			1	1	

Continued on next page...

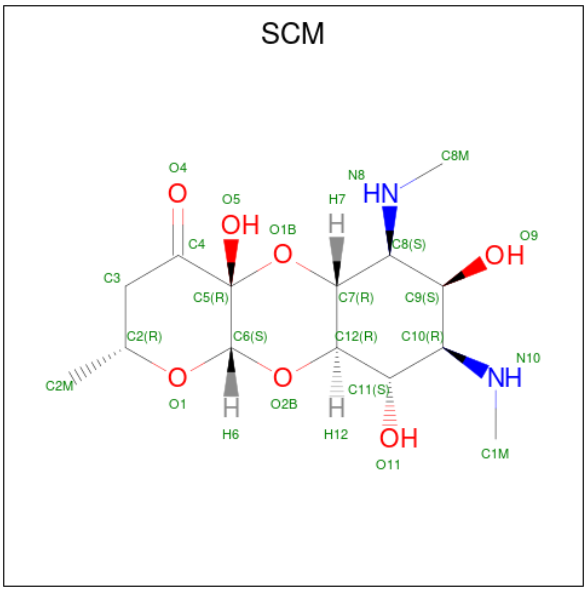
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
57	5	1	Total Zn 1 1	0
57	8	1	Total Zn 1 1	0
57	o	1	Total Zn 1 1	0

- Molecule 58 is POTASSIUM ION (three-letter code: K) (formula: K).

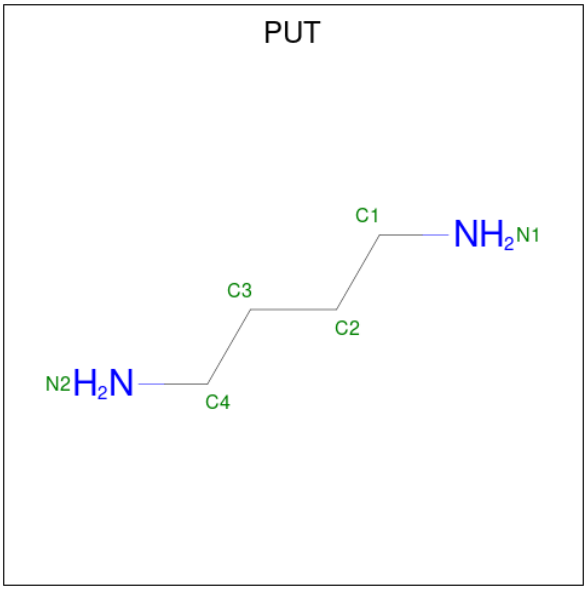
Mol	Chain	Residues	Atoms	AltConf
58	7	2	Total K 2 2	0
58	A	92	Total K 92 92	0
58	B	3	Total K 3 3	0
58	G	3	Total K 3 3	0
58	P	1	Total K 1 1	0
58	a	35	Total K 35 35	0
58	g	1	Total K 1 1	0
58	o	1	Total K 1 1	0

- Molecule 59 is SPECTINOMYCIN (three-letter code: SCM) (formula: $C_{14}H_{24}N_2O_7$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
59	a	1	23	14	2	7	0

- Molecule 60 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
60	a	1	6	4	2	0

- Molecule 61 is water.

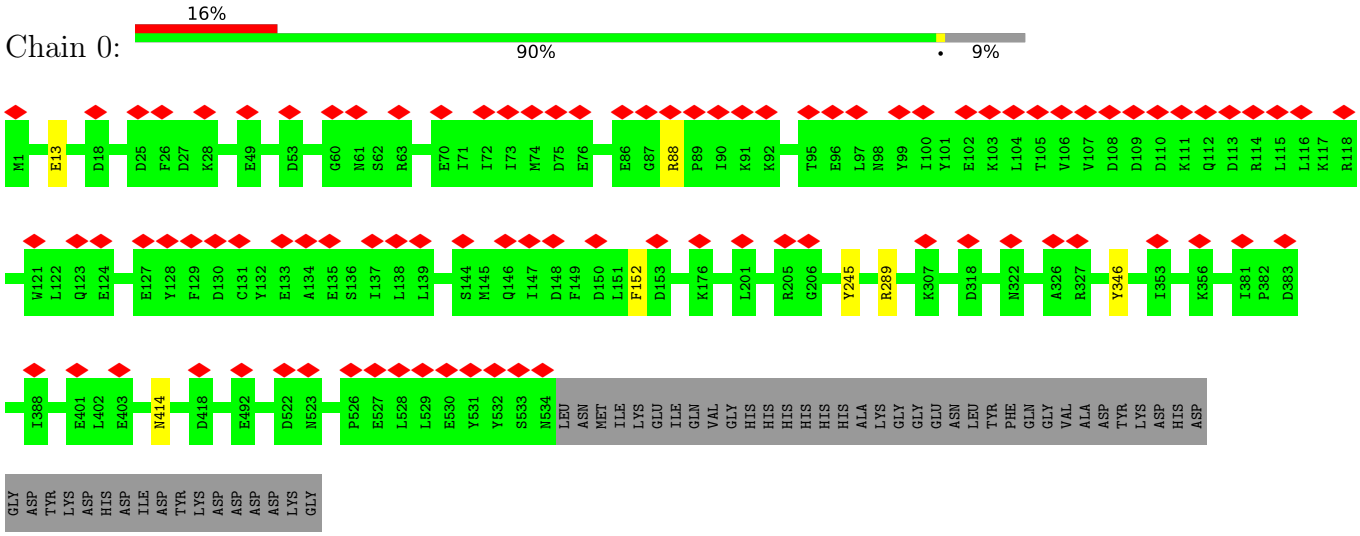
Mol	Chain	Residues	Atoms	AltConf
61	D	1	Total O 1 1	0

3 Residue-property plots (i)

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

• Molecule 1: ARE-ABC-F family resistance factor PoxtA

Chain 0:



• Molecule 2: 50S ribosomal protein L29

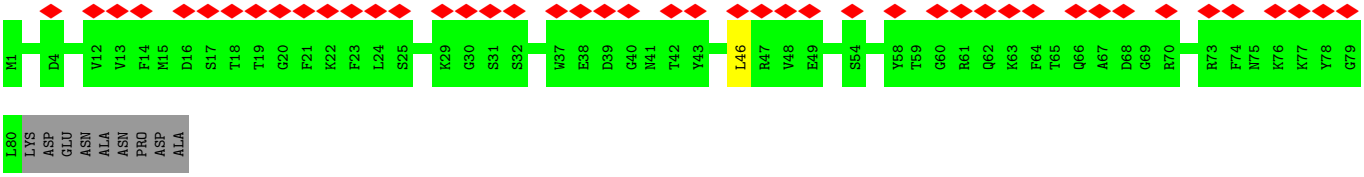
Chain 1:

• Molecule 3: 50S ribosomal protein L30

Chain 2:

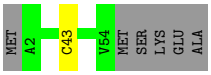
• Molecule 4: 50S ribosomal protein L31 type B

Chain 3:



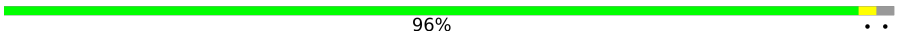
• Molecule 5: 50S ribosomal protein L32

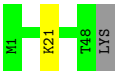
Chain 4:



• Molecule 6: 50S ribosomal protein L33

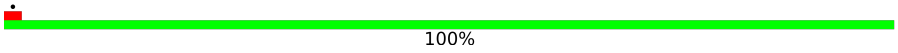
Chain 5:





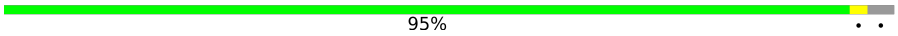
• Molecule 7: 50S ribosomal protein L34

Chain 6:



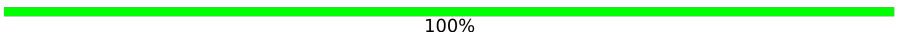
• Molecule 8: 50S ribosomal protein L35

Chain 7:



• Molecule 9: 50S ribosomal protein L36

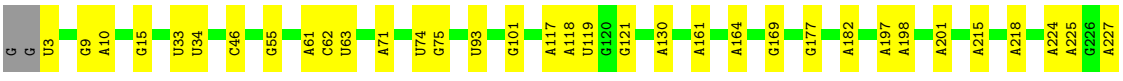
Chain 8:

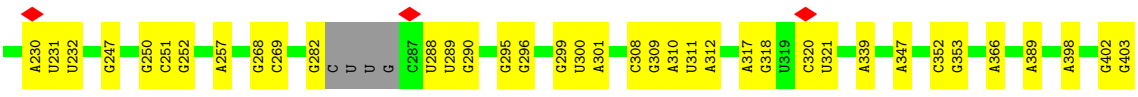


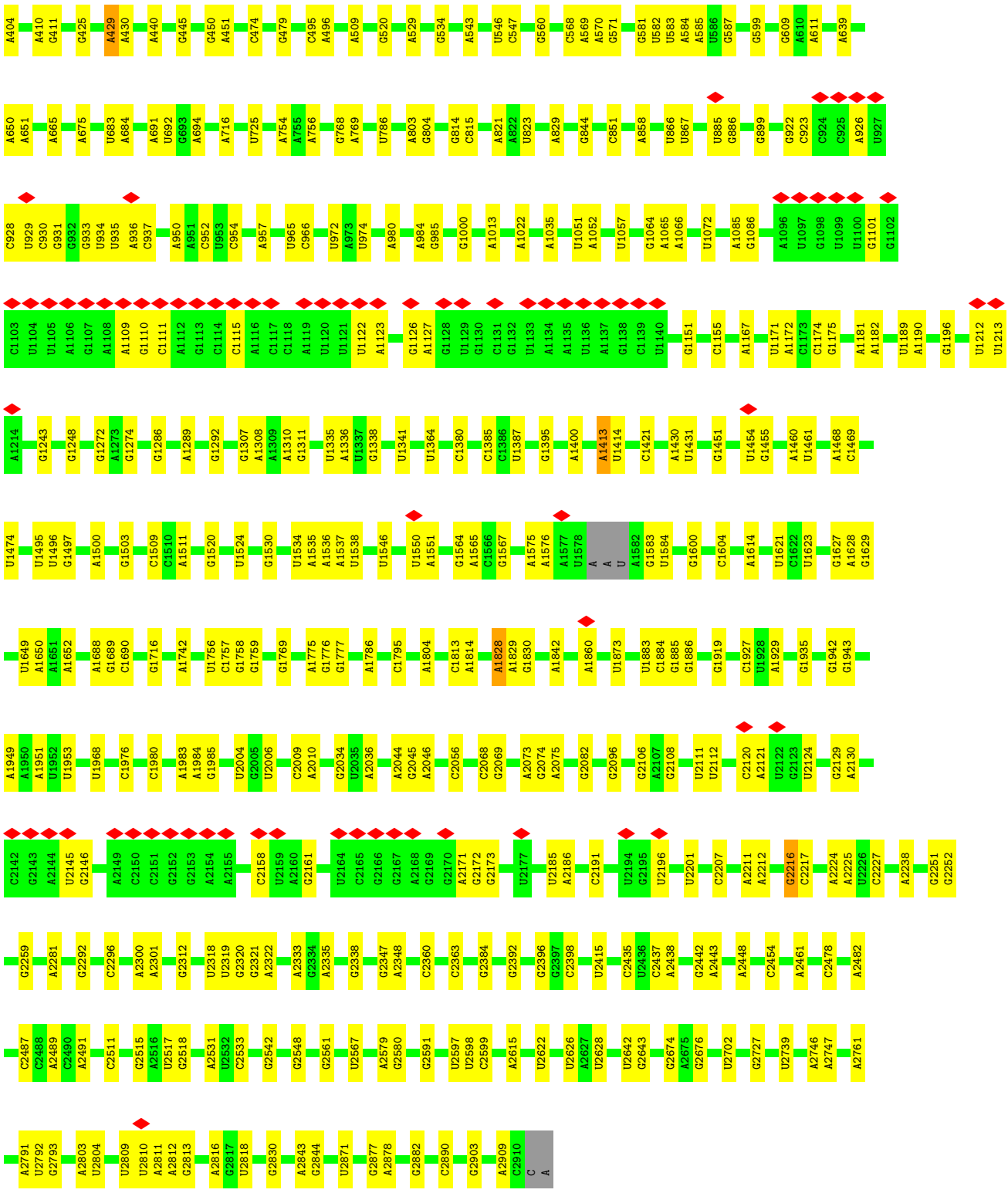
There are no outlier residues recorded for this chain.

• Molecule 10: 23S rRNA

Chain A:

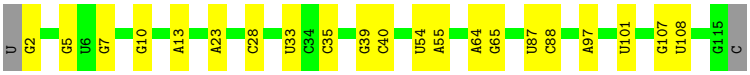






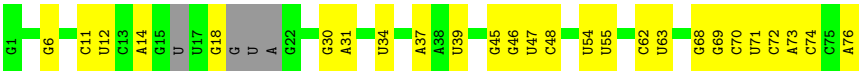
• Molecule 11: 5S rRNA

Chain B:



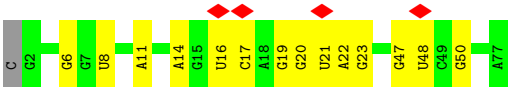
• Molecule 12: A-site tRNA

Chain C:



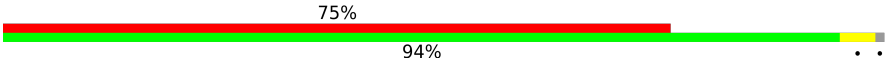
• Molecule 13: tRNA-fMet

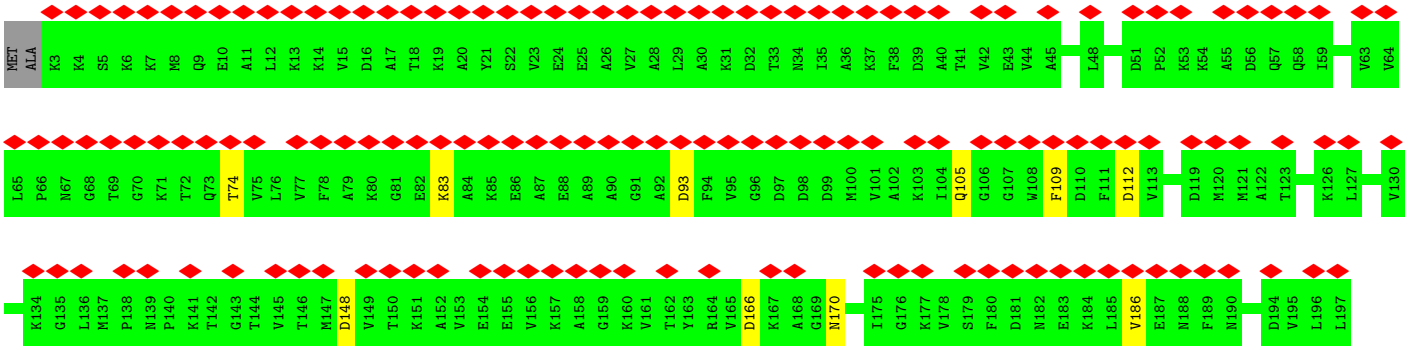
Chain D:



• Molecule 14: 50S ribosomal protein L1

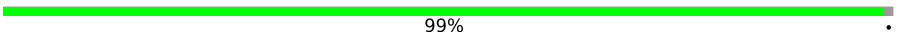
Chain F:





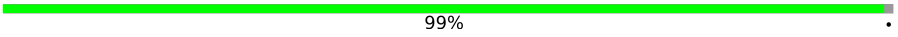
• Molecule 15: 50S ribosomal protein L2

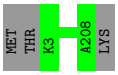
Chain G:



• Molecule 16: 50S ribosomal protein L3

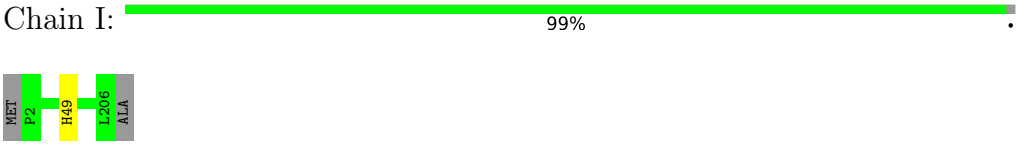
Chain H:





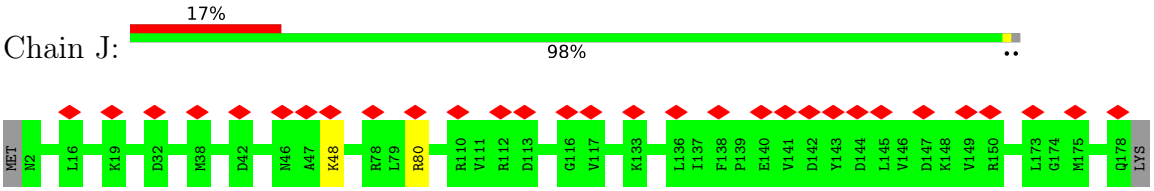
• Molecule 17: 50S ribosomal protein L4

Chain I:



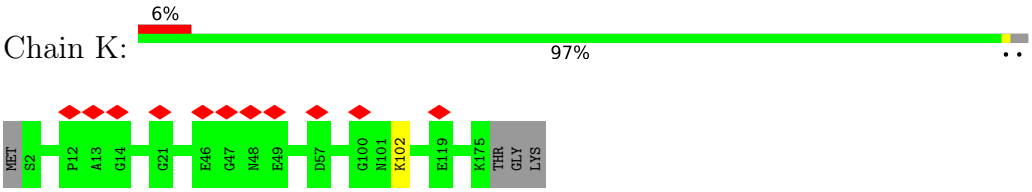
• Molecule 18: 50S ribosomal protein L5

Chain J:



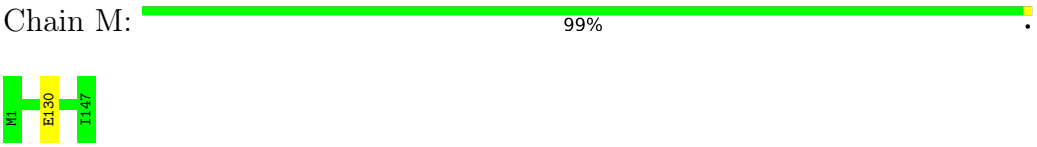
• Molecule 19: 50S ribosomal protein L6

Chain K:



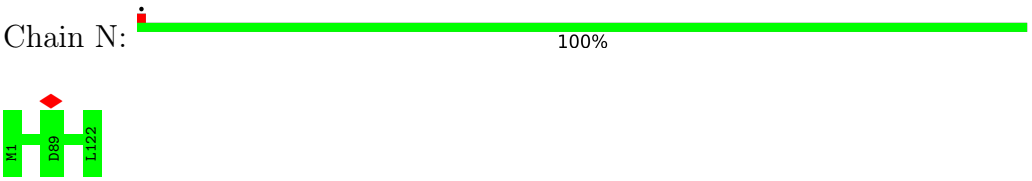
• Molecule 20: 50S ribosomal protein L13

Chain M:



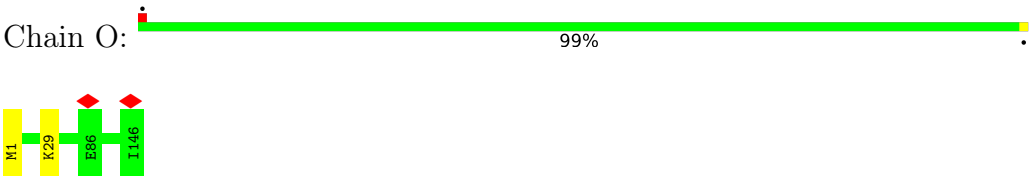
• Molecule 21: 50S ribosomal protein L14

Chain N:



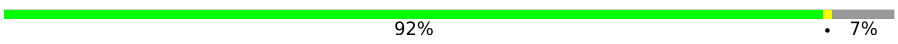
• Molecule 22: 50S ribosomal protein L15

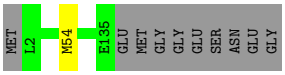
Chain O:



• Molecule 23: 50S ribosomal protein L16

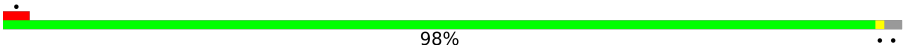
Chain P:

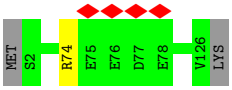




• Molecule 24: 50S ribosomal protein L17

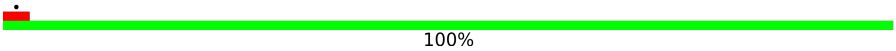
Chain Q:

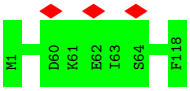




• Molecule 25: 50S ribosomal protein L18

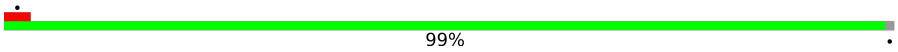
Chain R:

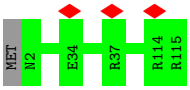




• Molecule 26: 50S ribosomal protein L19

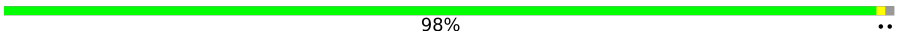
Chain S:





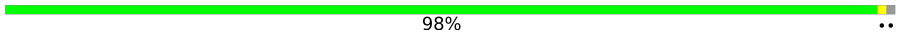
• Molecule 27: 50S ribosomal protein L20

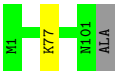
Chain T:



• Molecule 28: 50S ribosomal protein L21

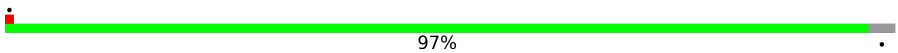
Chain U:

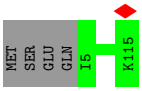




• Molecule 29: 50S ribosomal protein L22

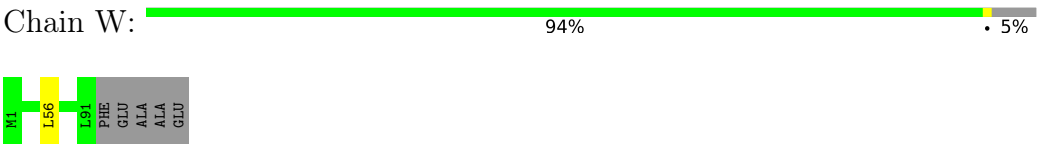
Chain V:





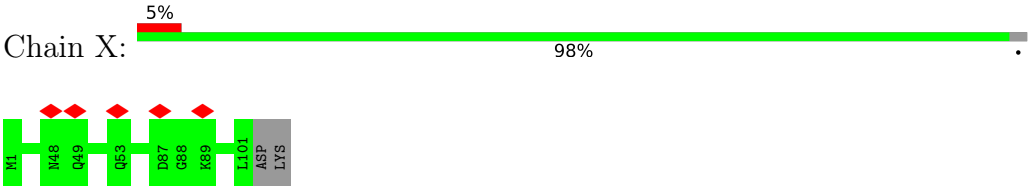
• Molecule 30: 50S ribosomal protein L23

Chain W:



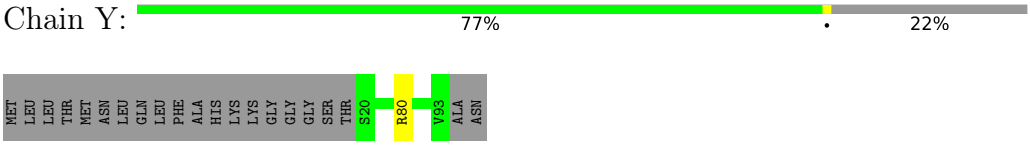
• Molecule 31: 50S ribosomal protein L24

Chain X:



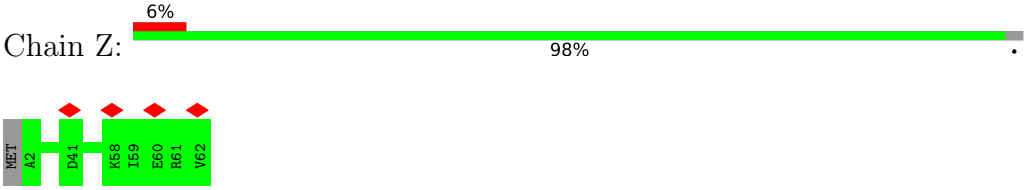
• Molecule 32: 50S ribosomal protein L27

Chain Y:



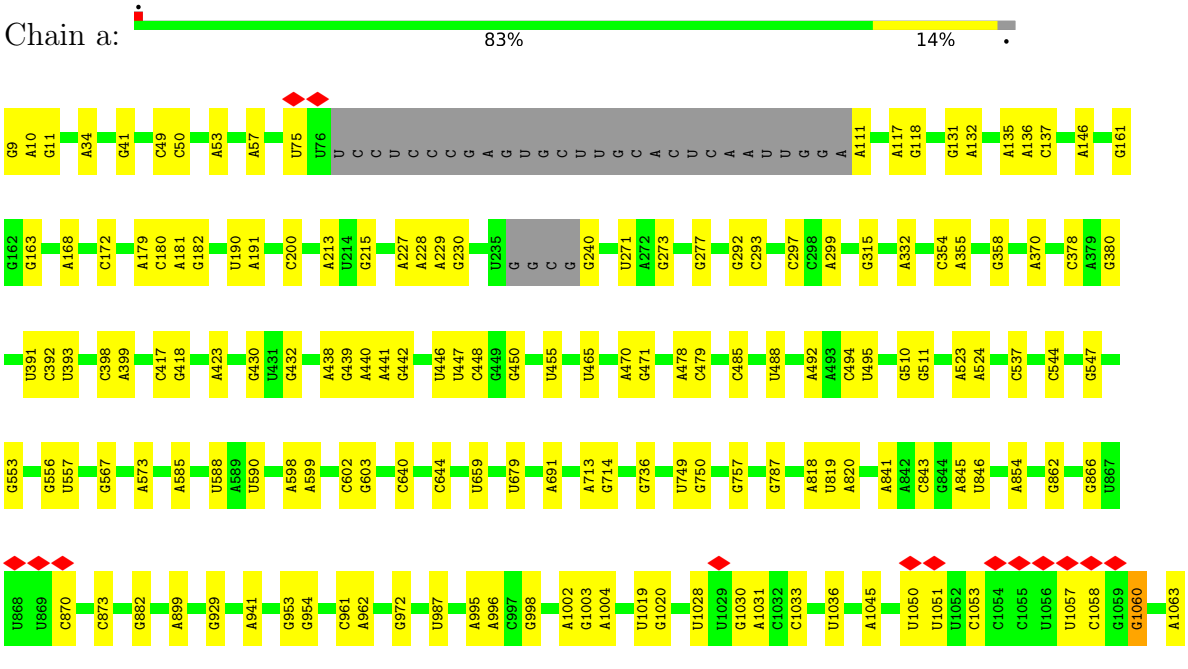
• Molecule 33: 50S ribosomal protein L28

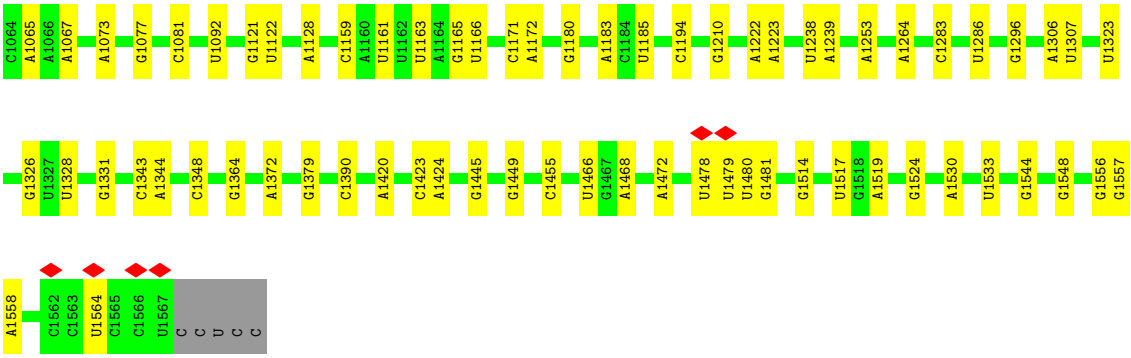
Chain Z:



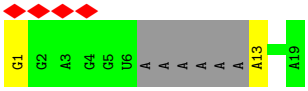
• Molecule 34: 16S rRNA

Chain a:

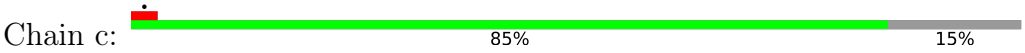


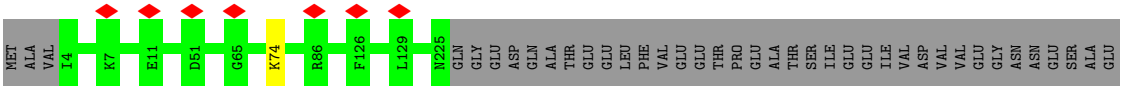


• Molecule 35: mRNA

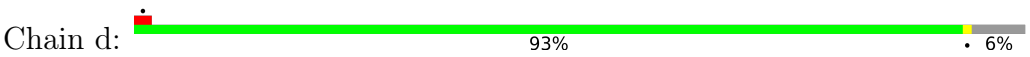


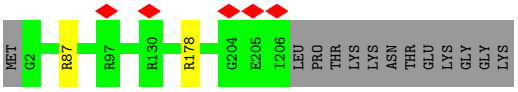
• Molecule 36: 30S ribosomal protein S2



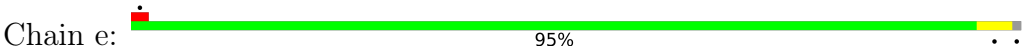


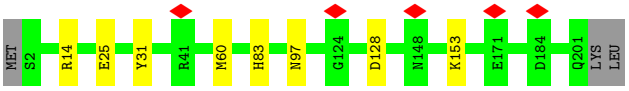
• Molecule 37: 30S ribosomal protein S3



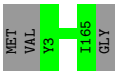


• Molecule 38: 30S ribosomal protein S4



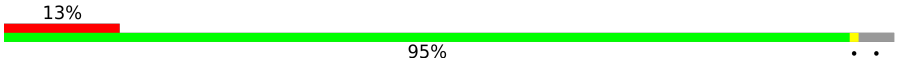


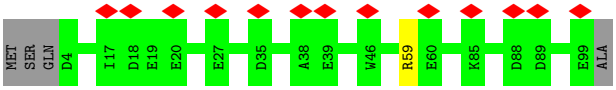
• Molecule 39: 30S ribosomal protein S5



• Molecule 40: 30S ribosomal protein S6

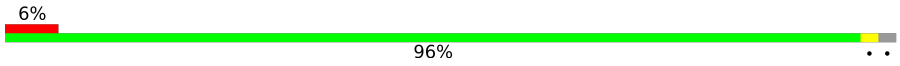
Chain g:

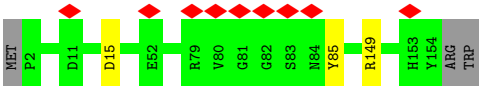




• Molecule 41: 30S ribosomal protein S7

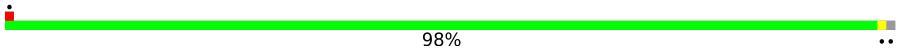
Chain h:

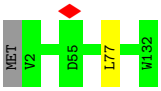




• Molecule 42: 30S ribosomal protein S8

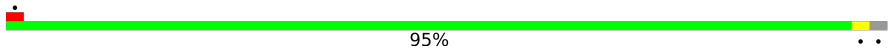
Chain i:

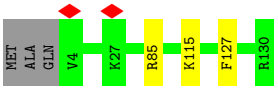




• Molecule 43: 30S ribosomal protein S9

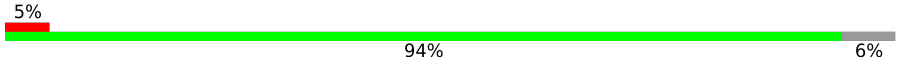
Chain j:

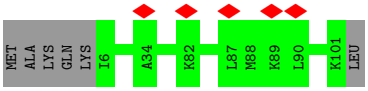




• Molecule 44: 30S ribosomal protein S10

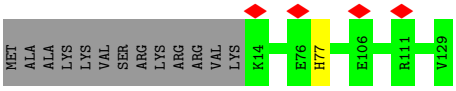
Chain k:





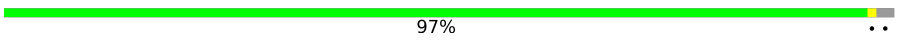
• Molecule 45: 30S ribosomal protein S11

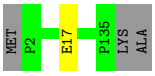
Chain l:



• Molecule 46: 30S ribosomal protein S12

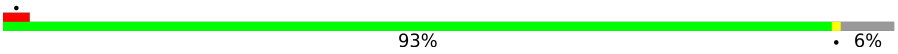
Chain m:

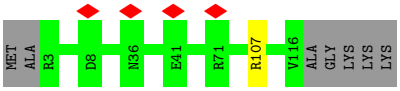




• Molecule 47: 30S ribosomal protein S13

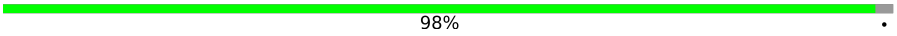
Chain n:





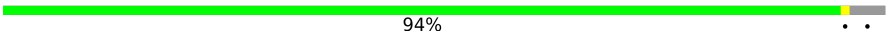
• Molecule 48: 30S ribosomal protein S14 type Z

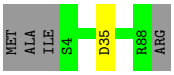
Chain o:



• Molecule 49: 30S ribosomal protein S15

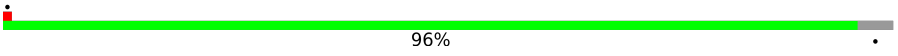
Chain p:

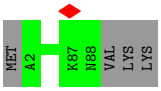




• Molecule 50: 30S ribosomal protein S16

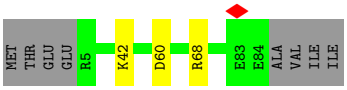
Chain q:





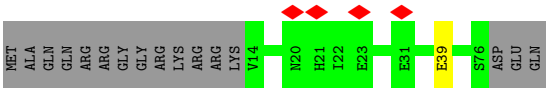
• Molecule 51: 30S ribosomal protein S17

Chain r:



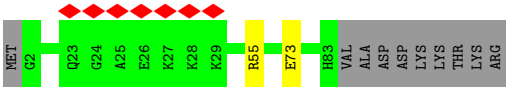
• Molecule 52: 30S ribosomal protein S18

Chain s:



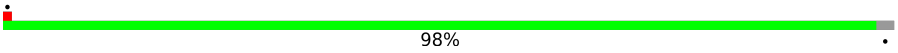
• Molecule 53: 30S ribosomal protein S19

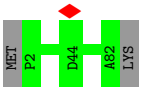
Chain t:



• Molecule 54: 30S ribosomal protein S20

Chain u:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23806	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 ($e^-/Å^2$)	30.255	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.010	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	344.4, 344.4, 344.4	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, PSU, MG, PUT, U8U, ATP, ZN, T6A, K, SCM

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	0.24	0/4421	0.44	0/5951
2	1	0.23	0/492	0.49	0/654
3	2	0.23	0/430	0.48	0/579
4	3	0.26	0/664	0.48	0/896
5	4	0.26	0/413	0.53	0/549
6	5	0.25	0/414	0.57	0/552
7	6	0.24	0/377	0.65	0/491
8	7	0.25	0/528	0.62	0/689
9	8	0.29	0/310	0.55	0/409
10	A	0.26	0/69752	0.69	9/108803 (0.0%)
11	B	0.20	0/2728	0.67	1/4252 (0.0%)
12	C	0.20	0/1595	0.69	0/2477
13	D	0.21	0/1815	0.67	0/2828
14	F	0.25	0/1717	0.43	0/2318
15	G	0.25	0/2141	0.53	0/2881
16	H	0.26	0/1594	0.51	0/2140
17	I	0.25	0/1595	0.49	0/2157
18	J	0.25	0/1411	0.48	0/1897
19	K	0.25	0/1355	0.51	0/1825
20	M	0.25	0/1167	0.49	0/1576
21	N	0.26	0/930	0.57	0/1247
22	O	0.26	0/1106	0.53	0/1474
23	P	0.25	0/1093	0.53	0/1457
24	Q	0.24	0/1006	0.55	0/1349
25	R	0.25	0/917	0.53	0/1226
26	S	0.25	0/939	0.58	0/1262
27	T	0.25	0/963	0.48	0/1280
28	U	0.27	0/791	0.47	0/1061
29	V	0.25	0/850	0.51	0/1145
30	W	0.26	0/743	0.49	0/993
31	X	0.26	0/772	0.46	0/1035
32	Y	0.26	0/565	0.54	0/755

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	Z	0.23	0/486	0.53	0/648
34	a	0.23	0/36487	0.68	7/56905 (0.0%)
35	b	0.22	0/322	0.76	2/499 (0.4%)
36	c	0.24	0/1803	0.46	0/2430
37	d	0.25	0/1643	0.52	0/2208
38	e	0.25	0/1641	0.50	0/2206
39	f	0.25	0/1217	0.52	0/1641
40	g	0.24	0/798	0.49	0/1075
41	h	0.24	0/1238	0.50	0/1668
42	i	0.24	0/1054	0.51	0/1417
43	j	0.24	0/993	0.54	0/1331
44	k	0.24	0/785	0.51	0/1059
45	l	0.24	0/869	0.51	0/1174
46	m	0.25	0/1068	0.57	0/1435
47	n	0.24	0/908	0.57	0/1219
48	o	0.25	0/504	0.51	0/669
49	p	0.23	0/726	0.51	0/969
50	q	0.24	0/704	0.51	0/945
51	r	0.24	0/668	0.53	0/891
52	s	0.24	0/518	0.51	0/694
53	t	0.25	0/680	0.50	0/911
54	u	0.23	0/611	0.46	0/818
All	All	0.25	0/161317	0.64	19/241020 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	1	G	OP1-P-OP2	-6.83	109.36	119.60
10	A	3	U	OP1-P-OP2	-6.81	109.38	119.60
11	B	2	G	OP1-P-OP2	-6.80	109.40	119.60
34	a	1060	G	OP1-P-OP2	-6.79	109.41	119.60
35	b	13	A	OP1-P-OP2	-6.75	109.47	119.60
34	a	111	A	OP1-P-OP2	-6.74	109.48	119.60
10	A	429	A	OP1-P-OP2	-6.73	109.50	119.60
34	a	240	G	OP1-P-OP2	-6.72	109.52	119.60
10	A	980	A	OP1-P-OP2	-6.71	109.54	119.60
34	a	131	G	OP1-P-OP2	-6.71	109.54	119.60
10	A	121	G	OP1-P-OP2	-6.70	109.55	119.60
10	A	2216	G	OP1-P-OP2	-6.68	109.58	119.60
10	A	1413	A	OP1-P-OP2	-6.67	109.60	119.60
34	a	9	G	OP1-P-OP2	-6.67	109.60	119.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	845	A	OP1-P-OP2	-6.59	109.72	119.60
10	A	2384	G	OP1-P-OP2	-6.58	109.72	119.60
34	a	1548	G	OP1-P-OP2	-6.52	109.82	119.60
10	A	1828	A	OP1-P-OP2	-6.51	109.84	119.60
10	A	197	A	OP1-P-OP2	-6.39	110.02	119.60

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	532/586 (91%)	521 (98%)	11 (2%)	0	100	100
2	1	57/62 (92%)	57 (100%)	0	0	100	100
3	2	55/59 (93%)	53 (96%)	2 (4%)	0	100	100
4	3	78/89 (88%)	77 (99%)	1 (1%)	0	100	100
5	4	51/59 (86%)	49 (96%)	2 (4%)	0	100	100
6	5	46/49 (94%)	43 (94%)	3 (6%)	0	100	100
7	6	42/44 (96%)	42 (100%)	0	0	100	100
8	7	62/66 (94%)	62 (100%)	0	0	100	100
9	8	36/38 (95%)	36 (100%)	0	0	100	100
14	F	224/229 (98%)	216 (96%)	8 (4%)	0	100	100
15	G	272/276 (99%)	265 (97%)	6 (2%)	1 (0%)	34	66
16	H	204/209 (98%)	194 (95%)	10 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	I	203/207 (98%)	200 (98%)	3 (2%)	0	100	100
18	J	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
19	K	172/178 (97%)	165 (96%)	7 (4%)	0	100	100
20	M	145/147 (99%)	144 (99%)	1 (1%)	0	100	100
21	N	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
22	O	144/146 (99%)	138 (96%)	5 (4%)	1 (1%)	22	54
23	P	132/144 (92%)	132 (100%)	0	0	100	100
24	Q	123/127 (97%)	120 (98%)	3 (2%)	0	100	100
25	R	116/118 (98%)	113 (97%)	3 (3%)	0	100	100
26	S	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
27	T	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
28	U	99/102 (97%)	96 (97%)	3 (3%)	0	100	100
29	V	109/115 (95%)	108 (99%)	1 (1%)	0	100	100
30	W	89/96 (93%)	88 (99%)	1 (1%)	0	100	100
31	X	99/103 (96%)	94 (95%)	5 (5%)	0	100	100
32	Y	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
33	Z	59/62 (95%)	57 (97%)	2 (3%)	0	100	100
36	c	220/261 (84%)	214 (97%)	6 (3%)	0	100	100
37	d	203/218 (93%)	200 (98%)	3 (2%)	0	100	100
38	e	198/203 (98%)	195 (98%)	3 (2%)	0	100	100
39	f	161/166 (97%)	158 (98%)	3 (2%)	0	100	100
40	g	94/100 (94%)	92 (98%)	2 (2%)	0	100	100
41	h	151/156 (97%)	149 (99%)	2 (1%)	0	100	100
42	i	129/132 (98%)	125 (97%)	4 (3%)	0	100	100
43	j	125/130 (96%)	120 (96%)	5 (4%)	0	100	100
44	k	94/102 (92%)	92 (98%)	2 (2%)	0	100	100
45	l	114/129 (88%)	111 (97%)	3 (3%)	0	100	100
46	m	132/137 (96%)	126 (96%)	6 (4%)	0	100	100
47	n	112/121 (93%)	108 (96%)	4 (4%)	0	100	100
48	o	58/61 (95%)	55 (95%)	3 (5%)	0	100	100
49	p	83/89 (93%)	82 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	q	85/91 (93%)	81 (95%)	4 (5%)	0	100	100
51	r	78/88 (89%)	75 (96%)	3 (4%)	0	100	100
52	s	61/79 (77%)	59 (97%)	2 (3%)	0	100	100
53	t	80/92 (87%)	78 (98%)	2 (2%)	0	100	100
54	u	79/83 (95%)	78 (99%)	1 (1%)	0	100	100
All	All	6001/6379 (94%)	5845 (97%)	154 (3%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
22	O	29	LYS
15	G	155	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	489/533 (92%)	482 (99%)	7 (1%)	67	89
2	1	54/56 (96%)	52 (96%)	2 (4%)	34	68
3	2	48/50 (96%)	48 (100%)	0	100	100
4	3	72/79 (91%)	71 (99%)	1 (1%)	67	89
5	4	43/48 (90%)	42 (98%)	1 (2%)	50	80
6	5	48/49 (98%)	47 (98%)	1 (2%)	53	81
7	6	39/39 (100%)	39 (100%)	0	100	100
8	7	51/53 (96%)	50 (98%)	1 (2%)	55	82
9	8	35/35 (100%)	35 (100%)	0	100	100
14	F	181/183 (99%)	171 (94%)	10 (6%)	21	53
15	G	224/226 (99%)	224 (100%)	0	100	100
16	H	169/172 (98%)	169 (100%)	0	100	100
17	I	172/173 (99%)	171 (99%)	1 (1%)	86	96

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	J	154/156 (99%)	152 (99%)	2 (1%)	69	90
19	K	145/148 (98%)	144 (99%)	1 (1%)	84	95
20	M	124/124 (100%)	123 (99%)	1 (1%)	81	94
21	N	98/98 (100%)	98 (100%)	0	100	100
22	O	112/112 (100%)	111 (99%)	1 (1%)	78	93
23	P	107/114 (94%)	106 (99%)	1 (1%)	78	93
24	Q	107/109 (98%)	106 (99%)	1 (1%)	78	93
25	R	92/92 (100%)	92 (100%)	0	100	100
26	S	97/98 (99%)	97 (100%)	0	100	100
27	T	94/95 (99%)	93 (99%)	1 (1%)	73	92
28	U	83/83 (100%)	82 (99%)	1 (1%)	71	91
29	V	94/98 (96%)	94 (100%)	0	100	100
30	W	82/85 (96%)	81 (99%)	1 (1%)	71	91
31	X	85/87 (98%)	85 (100%)	0	100	100
32	Y	59/75 (79%)	58 (98%)	1 (2%)	60	86
33	Z	54/55 (98%)	54 (100%)	0	100	100
36	c	187/220 (85%)	186 (100%)	1 (0%)	88	96
37	d	163/174 (94%)	161 (99%)	2 (1%)	71	91
38	e	174/177 (98%)	166 (95%)	8 (5%)	27	60
39	f	126/128 (98%)	126 (100%)	0	100	100
40	g	85/88 (97%)	84 (99%)	1 (1%)	71	91
41	h	130/133 (98%)	127 (98%)	3 (2%)	50	80
42	i	112/113 (99%)	111 (99%)	1 (1%)	78	93
43	j	100/102 (98%)	97 (97%)	3 (3%)	41	75
44	k	87/92 (95%)	87 (100%)	0	100	100
45	l	90/101 (89%)	89 (99%)	1 (1%)	73	92
46	m	117/119 (98%)	116 (99%)	1 (1%)	78	93
47	n	98/102 (96%)	97 (99%)	1 (1%)	76	92
48	o	51/52 (98%)	51 (100%)	0	100	100
49	p	76/79 (96%)	75 (99%)	1 (1%)	69	90
50	q	77/81 (95%)	77 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
51	r	74/81 (91%)	71 (96%)	3 (4%)	30 64
52	s	54/67 (81%)	53 (98%)	1 (2%)	57 84
53	t	70/79 (89%)	68 (97%)	2 (3%)	42 76
54	u	62/64 (97%)	62 (100%)	0	100 100
All	All	5145/5377 (96%)	5081 (99%)	64 (1%)	72 91

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	13	GLU
1	0	88	ARG
1	0	152	PHE
1	0	245	TYR
1	0	289	ARG
1	0	346	TYR
1	0	414	ASN
2	1	19	LYS
2	1	58	ARG
4	3	46	LEU
5	4	43	CYS
6	5	21	LYS
8	7	31	HIS
14	F	74	THR
14	F	83	LYS
14	F	93	ASP
14	F	105	GLN
14	F	109	PHE
14	F	112	ASP
14	F	148	ASP
14	F	166	ASP
14	F	170	ASN
14	F	186	VAL
17	I	49	HIS
18	J	48	LYS
18	J	80	ARG
19	K	102	LYS
20	M	130	GLU
22	O	1	MET
23	P	54	MET
24	Q	74	ARG
27	T	51	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	U	77	LYS
30	W	56	LEU
32	Y	80	ARG
36	c	74	LYS
37	d	87	ARG
37	d	178	ARG
38	e	14	ARG
38	e	25	GLU
38	e	31	TYR
38	e	60	MET
38	e	83	HIS
38	e	97	ASN
38	e	128	ASP
38	e	153	LYS
40	g	59	ARG
41	h	15	ASP
41	h	85	TYR
41	h	149	ARG
42	i	77	LEU
43	j	85	ARG
43	j	115	LYS
43	j	127	PHE
45	l	77	HIS
46	m	17	GLU
47	n	107	ARG
49	p	35	ASP
51	r	42	LYS
51	r	60	ASP
51	r	68	ARG
52	s	39	GLU
53	t	55	ARG
53	t	73	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	475	HIS
45	l	64	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	2898/2912 (99%)	433 (14%)	21 (0%)
11	B	113/116 (97%)	20 (17%)	0
12	C	68/76 (89%)	20 (29%)	1 (1%)
13	D	75/77 (97%)	13 (17%)	1 (1%)
34	a	1518/1558 (97%)	218 (14%)	0
35	b	11/19 (57%)	0	0
All	All	4683/4758 (98%)	704 (15%)	23 (0%)

All (704) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
10	A	10	A
10	A	15	G
10	A	34	U
10	A	46	C
10	A	55	G
10	A	61	A
10	A	62	C
10	A	63	U
10	A	71	A
10	A	74	U
10	A	75	G
10	A	93	U
10	A	101	G
10	A	117	A
10	A	118	A
10	A	119	U
10	A	130	A
10	A	161	A
10	A	164	A
10	A	169	G
10	A	177	G
10	A	182	A
10	A	198	A
10	A	201	A
10	A	215	A
10	A	218	A
10	A	224	A
10	A	225	A
10	A	230	A
10	A	231	U
10	A	232	U
10	A	247	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	250	G
10	A	251	C
10	A	252	G
10	A	257	A
10	A	268	G
10	A	269	C
10	A	282	G
10	A	289	U
10	A	290	G
10	A	295	G
10	A	296	G
10	A	299	G
10	A	300	U
10	A	301	A
10	A	308	C
10	A	309	G
10	A	310	A
10	A	311	U
10	A	312	A
10	A	317	A
10	A	318	G
10	A	320	C
10	A	321	U
10	A	339	A
10	A	347	A
10	A	352	C
10	A	353	G
10	A	366	A
10	A	389	A
10	A	398	A
10	A	402	G
10	A	403	G
10	A	404	A
10	A	410	A
10	A	411	G
10	A	425	G
10	A	430	A
10	A	440	A
10	A	445	G
10	A	450	G
10	A	451	A
10	A	474	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	479	G
10	A	495	C
10	A	496	A
10	A	509	A
10	A	520	G
10	A	529	A
10	A	534	G
10	A	543	A
10	A	546	U
10	A	547	C
10	A	560	G
10	A	568	C
10	A	569	A
10	A	570	A
10	A	571	G
10	A	581	G
10	A	582	U
10	A	583	U
10	A	584	A
10	A	585	A
10	A	587	G
10	A	599	G
10	A	609	G
10	A	611	A
10	A	639	A
10	A	650	A
10	A	651	A
10	A	665	A
10	A	675	A
10	A	683	U
10	A	684	A
10	A	691	A
10	A	692	U
10	A	694	A
10	A	716	A
10	A	725	U
10	A	754	A
10	A	756	A
10	A	768	G
10	A	769	A
10	A	786	U
10	A	803	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	804	G
10	A	814	G
10	A	815	C
10	A	821	A
10	A	823	U
10	A	829	A
10	A	844	G
10	A	851	C
10	A	858	A
10	A	866	U
10	A	867	U
10	A	885	U
10	A	886	G
10	A	899	G
10	A	922	G
10	A	923	C
10	A	926	A
10	A	928	C
10	A	929	U
10	A	930	C
10	A	931	G
10	A	933	G
10	A	934	U
10	A	935	U
10	A	936	A
10	A	937	C
10	A	950	A
10	A	952	C
10	A	954	C
10	A	957	A
10	A	965	U
10	A	966	C
10	A	972	U
10	A	974	U
10	A	984	A
10	A	985	G
10	A	1000	G
10	A	1013	A
10	A	1022	A
10	A	1035	A
10	A	1051	U
10	A	1052	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1064	G
10	A	1065	A
10	A	1066	A
10	A	1072	U
10	A	1085	A
10	A	1086	G
10	A	1101	G
10	A	1109	A
10	A	1110	G
10	A	1111	C
10	A	1115	C
10	A	1122	U
10	A	1123	A
10	A	1126	G
10	A	1127	A
10	A	1151	G
10	A	1155	C
10	A	1167	A
10	A	1171	U
10	A	1172	A
10	A	1174	C
10	A	1175	G
10	A	1181	A
10	A	1182	A
10	A	1190	A
10	A	1196	G
10	A	1212	U
10	A	1213	U
10	A	1243	G
10	A	1248	G
10	A	1272	G
10	A	1274	G
10	A	1286	G
10	A	1289	A
10	A	1292	G
10	A	1307	G
10	A	1308	A
10	A	1310	A
10	A	1311	G
10	A	1335	U
10	A	1336	A
10	A	1338	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1341	U
10	A	1364	U
10	A	1380	C
10	A	1385	C
10	A	1387	U
10	A	1395	G
10	A	1400	A
10	A	1413	A
10	A	1414	U
10	A	1421	C
10	A	1430	A
10	A	1431	U
10	A	1451	G
10	A	1454	U
10	A	1455	G
10	A	1460	A
10	A	1461	U
10	A	1468	A
10	A	1469	C
10	A	1474	U
10	A	1495	U
10	A	1496	U
10	A	1497	G
10	A	1500	A
10	A	1503	G
10	A	1509	C
10	A	1511	A
10	A	1520	G
10	A	1524	U
10	A	1530	G
10	A	1534	U
10	A	1535	A
10	A	1536	A
10	A	1537	A
10	A	1538	U
10	A	1546	U
10	A	1550	U
10	A	1551	A
10	A	1564	G
10	A	1565	A
10	A	1567	G
10	A	1575	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1576	A
10	A	1583	G
10	A	1584	U
10	A	1600	G
10	A	1604	C
10	A	1614	A
10	A	1621	U
10	A	1623	U
10	A	1627	G
10	A	1628	A
10	A	1629	G
10	A	1649	U
10	A	1650	A
10	A	1652	A
10	A	1688	A
10	A	1689	G
10	A	1690	C
10	A	1716	G
10	A	1742	A
10	A	1756	U
10	A	1757	C
10	A	1758	G
10	A	1759	G
10	A	1769	G
10	A	1775	A
10	A	1776	G
10	A	1777	G
10	A	1786	A
10	A	1795	C
10	A	1804	A
10	A	1813	C
10	A	1814	A
10	A	1828	A
10	A	1829	A
10	A	1830	G
10	A	1842	A
10	A	1860	A
10	A	1873	U
10	A	1883	U
10	A	1884	C
10	A	1885	G
10	A	1886	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	1919	G
10	A	1929	A
10	A	1935	G
10	A	1942	G
10	A	1943	G
10	A	1949	A
10	A	1951	A
10	A	1953	U
10	A	1968	U
10	A	1976	C
10	A	1980	C
10	A	1983	A
10	A	1984	A
10	A	1985	G
10	A	2004	U
10	A	2006	U
10	A	2009	C
10	A	2010	A
10	A	2034	G
10	A	2036	A
10	A	2044	A
10	A	2045	G
10	A	2046	A
10	A	2056	C
10	A	2068	C
10	A	2069	G
10	A	2073	A
10	A	2074	G
10	A	2075	A
10	A	2082	G
10	A	2096	G
10	A	2106	G
10	A	2108	G
10	A	2112	U
10	A	2120	C
10	A	2121	A
10	A	2124	U
10	A	2129	G
10	A	2130	A
10	A	2145	U
10	A	2146	G
10	A	2158	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	2161	G
10	A	2171	A
10	A	2172	G
10	A	2173	G
10	A	2185	U
10	A	2186	A
10	A	2191	C
10	A	2196	U
10	A	2201	U
10	A	2207	C
10	A	2211	A
10	A	2212	A
10	A	2216	G
10	A	2217	C
10	A	2224	A
10	A	2225	A
10	A	2227	C
10	A	2238	A
10	A	2251	G
10	A	2252	G
10	A	2259	G
10	A	2281	A
10	A	2292	G
10	A	2296	C
10	A	2300	A
10	A	2301	A
10	A	2312	G
10	A	2318	U
10	A	2319	U
10	A	2320	G
10	A	2321	G
10	A	2322	A
10	A	2333	A
10	A	2335	A
10	A	2338	G
10	A	2347	G
10	A	2348	A
10	A	2360	C
10	A	2363	C
10	A	2392	G
10	A	2396	G
10	A	2398	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	2415	U
10	A	2435	C
10	A	2437	C
10	A	2438	A
10	A	2442	G
10	A	2443	A
10	A	2448	A
10	A	2454	C
10	A	2461	A
10	A	2478	C
10	A	2482	A
10	A	2487	C
10	A	2489	A
10	A	2491	A
10	A	2511	C
10	A	2515	G
10	A	2517	U
10	A	2518	G
10	A	2531	A
10	A	2533	C
10	A	2542	G
10	A	2548	G
10	A	2561	G
10	A	2567	U
10	A	2579	A
10	A	2580	G
10	A	2591	G
10	A	2597	U
10	A	2599	C
10	A	2615	A
10	A	2622	U
10	A	2626	U
10	A	2628	U
10	A	2642	U
10	A	2643	G
10	A	2674	G
10	A	2676	G
10	A	2702	U
10	A	2727	G
10	A	2739	U
10	A	2746	A
10	A	2747	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	A	2761	A
10	A	2791	A
10	A	2792	U
10	A	2793	G
10	A	2803	A
10	A	2804	U
10	A	2809	U
10	A	2810	U
10	A	2811	A
10	A	2812	A
10	A	2813	G
10	A	2816	A
10	A	2818	U
10	A	2830	G
10	A	2843	A
10	A	2844	G
10	A	2871	U
10	A	2877	G
10	A	2878	A
10	A	2882	G
10	A	2890	C
10	A	2903	G
10	A	2909	A
11	B	5	G
11	B	7	G
11	B	10	G
11	B	13	A
11	B	23	A
11	B	28	C
11	B	33	U
11	B	35	C
11	B	39	G
11	B	40	C
11	B	54	U
11	B	55	A
11	B	64	A
11	B	65	G
11	B	87	U
11	B	88	C
11	B	97	A
11	B	101	U
11	B	107	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	B	108	U
12	C	6	G
12	C	11	C
12	C	12	U
12	C	14	A
12	C	18	G
12	C	30	G
12	C	31	A
12	C	45	G
12	C	46	G
12	C	47	U
12	C	48	C
12	C	62	C
12	C	63	U
12	C	68	G
12	C	70	C
12	C	71	U
12	C	72	C
12	C	73	A
12	C	74	C
12	C	76	A
13	D	6	G
13	D	8	U
13	D	11	A
13	D	14	A
13	D	16	U
13	D	17	C
13	D	19	G
13	D	21	U
13	D	22	A
13	D	23	G
13	D	47	G
13	D	48	U
13	D	50	G
34	a	10	A
34	a	11	G
34	a	34	A
34	a	41	G
34	a	49	C
34	a	50	C
34	a	53	A
34	a	57	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	75	U
34	a	117	A
34	a	118	G
34	a	132	A
34	a	135	A
34	a	136	A
34	a	137	C
34	a	146	A
34	a	161	G
34	a	163	G
34	a	168	A
34	a	172	C
34	a	179	A
34	a	180	C
34	a	181	A
34	a	182	G
34	a	190	U
34	a	191	A
34	a	200	C
34	a	213	A
34	a	215	G
34	a	227	A
34	a	228	A
34	a	229	A
34	a	230	G
34	a	271	U
34	a	273	G
34	a	277	G
34	a	292	G
34	a	293	C
34	a	297	C
34	a	299	A
34	a	315	G
34	a	332	A
34	a	354	C
34	a	355	A
34	a	358	G
34	a	370	A
34	a	378	C
34	a	380	G
34	a	391	U
34	a	392	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	393	U
34	a	398	C
34	a	399	A
34	a	417	C
34	a	418	G
34	a	423	A
34	a	430	G
34	a	432	G
34	a	438	A
34	a	439	G
34	a	440	A
34	a	441	A
34	a	442	G
34	a	446	U
34	a	447	U
34	a	448	C
34	a	450	G
34	a	455	U
34	a	465	U
34	a	470	A
34	a	471	G
34	a	478	A
34	a	479	C
34	a	485	C
34	a	488	U
34	a	492	A
34	a	494	C
34	a	495	U
34	a	510	G
34	a	511	G
34	a	523	A
34	a	524	A
34	a	537	C
34	a	544	C
34	a	547	G
34	a	553	G
34	a	556	G
34	a	557	U
34	a	567	G
34	a	573	A
34	a	585	A
34	a	588	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	590	U
34	a	598	A
34	a	599	A
34	a	602	C
34	a	603	G
34	a	640	C
34	a	644	C
34	a	659	U
34	a	679	U
34	a	691	A
34	a	713	A
34	a	714	G
34	a	736	G
34	a	749	U
34	a	750	G
34	a	757	G
34	a	787	G
34	a	818	A
34	a	819	U
34	a	820	A
34	a	841	A
34	a	843	C
34	a	846	U
34	a	854	A
34	a	862	G
34	a	866	G
34	a	870	C
34	a	873	C
34	a	882	G
34	a	899	A
34	a	929	G
34	a	941	A
34	a	953	G
34	a	954	G
34	a	961	C
34	a	962	A
34	a	972	G
34	a	987	U
34	a	995	A
34	a	996	A
34	a	998	G
34	a	1002	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	1003	G
34	a	1004	A
34	a	1019	U
34	a	1020	G
34	a	1028	U
34	a	1030	G
34	a	1031	A
34	a	1033	C
34	a	1036	U
34	a	1045	A
34	a	1050	U
34	a	1051	U
34	a	1053	C
34	a	1057	U
34	a	1058	C
34	a	1060	G
34	a	1063	A
34	a	1065	A
34	a	1067	A
34	a	1073	A
34	a	1077	G
34	a	1081	C
34	a	1092	U
34	a	1121	G
34	a	1122	U
34	a	1128	A
34	a	1159	C
34	a	1161	U
34	a	1163	U
34	a	1165	G
34	a	1166	U
34	a	1171	C
34	a	1172	A
34	a	1180	G
34	a	1183	A
34	a	1185	U
34	a	1194	C
34	a	1210	G
34	a	1222	A
34	a	1223	A
34	a	1238	U
34	a	1239	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	a	1253	A
34	a	1264	A
34	a	1283	C
34	a	1286	U
34	a	1296	G
34	a	1306	A
34	a	1307	U
34	a	1323	U
34	a	1326	G
34	a	1328	U
34	a	1331	G
34	a	1343	C
34	a	1344	A
34	a	1348	C
34	a	1364	G
34	a	1372	A
34	a	1379	G
34	a	1390	C
34	a	1420	A
34	a	1423	C
34	a	1424	A
34	a	1445	G
34	a	1449	G
34	a	1455	C
34	a	1466	U
34	a	1468	A
34	a	1472	A
34	a	1478	U
34	a	1479	U
34	a	1480	U
34	a	1481	G
34	a	1514	G
34	a	1517	U
34	a	1519	A
34	a	1524	G
34	a	1530	A
34	a	1533	U
34	a	1544	G
34	a	1556	G
34	a	1557	G
34	a	1558	A
34	a	1564	U

All (23) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	9	G
10	A	33	U
10	A	227	A
10	A	251	C
10	A	288	U
10	A	295	G
10	A	429	A
10	A	683	U
10	A	1057	U
10	A	1189	U
10	A	1413	A
10	A	1536	A
10	A	1583	G
10	A	1828	A
10	A	1927	C
10	A	2111	U
10	A	2216	G
10	A	2318	U
10	A	2598	U
10	A	2810	U
10	A	2877	G
12	C	69	G
13	D	20	G

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

5 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	$\#\|Z\| > 2$
12	T6A	C	37	12	24,34,35	2.34	5 (20%)	24,49,52	6.34	8 (33%)
12	PSU	C	39	12	17,21,22	3.81	8 (47%)	20,30,33	3.09	5 (25%)
12	PSU	C	55	12	17,21,22	3.77	9 (52%)	20,30,33	3.17	6 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	5MU	C	54	12	15,22,23	5.89	5 (33%)	16,32,35	2.02	2 (12%)
12	U8U	C	34	12,35	17,24,25	2.57	4 (23%)	19,34,37	1.52	3 (15%)

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
12	T6A	C	37	12	-	1/15/41/42	0/3/3/3
12	PSU	C	39	12	-	2/7/25/26	0/2/2/2
12	PSU	C	55	12	-	0/7/25/26	0/2/2/2
12	5MU	C	54	12	-	0/5/25/26	0/2/2/2
12	U8U	C	34	12,35	-	0/7/28/29	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	54	5MU	C5-C4	18.18	1.80	1.41
12	C	54	5MU	C6-C5	-9.13	1.14	1.40
12	C	54	5MU	C4-N3	-8.45	1.18	1.33
12	C	34	U8U	C4-N3	7.72	1.46	1.33
12	C	55	PSU	C4-N3	7.26	1.45	1.33
12	C	39	PSU	C4-N3	7.21	1.45	1.33
12	C	39	PSU	C6-C5	7.02	1.49	1.38
12	C	55	PSU	C6-C5	6.98	1.49	1.38
12	C	37	T6A	C6-N6	6.96	1.48	1.36
12	C	39	PSU	C2-N3	6.90	1.51	1.38
12	C	55	PSU	C2-N3	6.84	1.51	1.38
12	C	39	PSU	C2-N1	5.66	1.49	1.38
12	C	55	PSU	C2-N1	5.62	1.49	1.38
12	C	37	T6A	C10-N11	5.44	1.47	1.35
12	C	55	PSU	C6-N1	5.16	1.45	1.34
12	C	39	PSU	C6-N1	5.13	1.45	1.34
12	C	37	T6A	C10-N6	5.00	1.47	1.37
12	C	34	U8U	C2-S2	-4.66	1.56	1.66
12	C	34	U8U	C6-C5	4.38	1.47	1.37
12	C	54	5MU	C2-N3	4.16	1.46	1.38
12	C	39	PSU	C5-C1'	3.73	1.55	1.52
12	C	54	5MU	C5M-C5	3.71	1.58	1.51
12	C	39	PSU	C5-C4	3.63	1.49	1.41
12	C	55	PSU	C5-C1'	3.60	1.55	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	C	55	PSU	C5-C4	3.54	1.49	1.41
12	C	37	T6A	C2-N3	2.75	1.36	1.32
12	C	34	U8U	C5-C4	2.64	1.47	1.41
12	C	37	T6A	C5-C4	-2.42	1.34	1.40
12	C	39	PSU	O4'-C1'	-2.39	1.41	1.44
12	C	55	PSU	O4'-C1'	-2.06	1.41	1.44
12	C	55	PSU	O4-C4	-2.02	1.19	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	C	37	T6A	N6-C6-N1	-27.17	82.33	118.72
12	C	55	PSU	N3-C2-N1	-10.79	119.85	128.43
12	C	39	PSU	N3-C2-N1	-10.66	119.96	128.43
12	C	37	T6A	N6-C10-N11	10.33	128.18	113.76
12	C	54	5MU	C5-C6-N1	-6.02	115.71	122.19
12	C	55	PSU	C2-N3-C4	5.47	119.76	115.14
12	C	37	T6A	C12-N11-C10	-5.39	116.99	122.75
12	C	39	PSU	C2-N3-C4	5.37	119.68	115.14
12	C	54	5MU	C2-N3-C4	5.06	119.42	115.14
12	C	37	T6A	N3-C2-N1	-4.88	121.05	128.68
12	C	37	T6A	O10-C10-N6	-4.72	115.64	123.62
12	C	55	PSU	C5-C4-N3	-4.42	119.66	125.36
12	C	39	PSU	C5-C4-N3	-4.40	119.69	125.36
12	C	34	U8U	C4-N3-C2	4.22	120.25	115.93
12	C	37	T6A	C1'-N9-C4	-4.03	119.56	126.64
12	C	34	U8U	C5-C4-N3	-3.86	119.59	125.25
12	C	37	T6A	O10-C10-N11	-3.54	116.18	122.62
12	C	37	T6A	C2-N1-C6	3.30	119.42	116.59
12	C	55	PSU	C5-C6-N1	-3.29	120.40	124.44
12	C	39	PSU	C5-C6-N1	-3.22	120.47	124.44
12	C	55	PSU	C5-C1'-C2'	-2.89	110.16	115.32
12	C	34	U8U	C6-C5-C4	2.77	120.01	115.73
12	C	55	PSU	C6-N1-C2	2.65	119.74	115.36
12	C	39	PSU	C6-N1-C2	2.60	119.65	115.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	C	37	T6A	C5-C6-N6-C10
12	C	39	PSU	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
12	C	39	PSU	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 307 ligands modelled in this entry, 303 are monoatomic - leaving 4 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	ATP	0	602	56	26,33,33	3.43	10 (38%)	31,52,52	2.41	9 (29%)
59	SCM	a	1615	-	23,25,25	7.02	12 (52%)	26,39,39	1.25	3 (11%)
60	PUT	a	1627	-	5,5,5	0.26	0	4,4,4	0.45	0
55	ATP	0	601	56	26,33,33	3.44	10 (38%)	31,52,52	2.38	9 (29%)

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	ATP	0	602	56	-	5/18/38/38	0/3/3/3
59	SCM	a	1615	-	-	0/4/57/57	0/3/3/3
60	PUT	a	1627	-	-	0/3/3/3	-
55	ATP	0	601	56	-	9/18/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	a	1615	SCM	O2B-C12	-27.35	1.01	1.44
59	a	1615	SCM	O1-C2	-15.20	1.15	1.44
55	0	601	ATP	C2'-C3'	-10.52	1.24	1.53
55	0	602	ATP	C2'-C3'	-10.45	1.24	1.53
55	0	602	ATP	O4'-C1'	6.99	1.50	1.41
55	0	601	ATP	O4'-C1'	6.98	1.50	1.41
55	0	602	ATP	O4'-C4'	-6.62	1.30	1.45
55	0	601	ATP	O4'-C4'	-6.49	1.30	1.45
55	0	601	ATP	C3'-C4'	5.67	1.67	1.53
55	0	602	ATP	C3'-C4'	5.50	1.67	1.53
59	a	1615	SCM	C2M-C2	5.46	1.72	1.51
59	a	1615	SCM	C9-C8	4.58	1.61	1.53
55	0	602	ATP	C2'-C1'	4.57	1.60	1.53
55	0	601	ATP	C2'-C1'	4.53	1.60	1.53
59	a	1615	SCM	C8-N8	-4.19	1.40	1.47
59	a	1615	SCM	C11-C12	4.15	1.63	1.52
59	a	1615	SCM	O1B-C7	3.86	1.50	1.44
59	a	1615	SCM	C12-C7	-3.50	1.45	1.52
59	a	1615	SCM	O11-C11	-3.49	1.34	1.43
55	0	602	ATP	O2'-C2'	3.33	1.50	1.43
55	0	601	ATP	O2'-C2'	3.26	1.50	1.43
55	0	601	ATP	C6-N6	3.25	1.45	1.34
55	0	602	ATP	C6-N6	3.24	1.45	1.34
59	a	1615	SCM	C3-C2	-3.14	1.44	1.51
55	0	601	ATP	C5-C4	-2.79	1.33	1.40
55	0	602	ATP	C5-C4	-2.72	1.33	1.40
55	0	602	ATP	C2-N3	2.25	1.35	1.32
55	0	601	ATP	C2-N3	2.20	1.35	1.32
55	0	601	ATP	O3'-C3'	2.15	1.48	1.43
55	0	602	ATP	O3'-C3'	2.11	1.47	1.43
59	a	1615	SCM	C9-C10	-2.07	1.49	1.53
59	a	1615	SCM	C3-C4	2.05	1.54	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	0	602	ATP	C5-C6-N6	6.56	130.32	120.35
55	0	601	ATP	C5-C6-N6	6.48	130.20	120.35
55	0	601	ATP	C1'-N9-C4	6.18	137.51	126.64
55	0	602	ATP	C1'-N9-C4	6.17	137.49	126.64
55	0	602	ATP	N3-C2-N1	-5.52	120.06	128.68
55	0	601	ATP	N3-C2-N1	-5.51	120.07	128.68
55	0	602	ATP	N6-C6-N1	-4.51	109.21	118.57

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	0	601	ATP	N6-C6-N1	-4.41	109.43	118.57
59	a	1615	SCM	C1M-N10-C10	-3.42	109.40	114.38
55	0	602	ATP	C3'-C2'-C1'	3.37	106.05	100.98
55	0	601	ATP	C3'-C2'-C1'	2.89	105.33	100.98
55	0	601	ATP	C2'-C3'-C4'	2.78	108.04	102.64
55	0	601	ATP	PA-O3A-PB	-2.76	123.35	132.83
55	0	602	ATP	PB-O3B-PG	-2.70	123.55	132.83
55	0	602	ATP	PA-O3A-PB	-2.60	123.91	132.83
55	0	601	ATP	PB-O3B-PG	-2.58	123.97	132.83
55	0	602	ATP	C2'-C3'-C4'	2.56	107.61	102.64
59	a	1615	SCM	C2M-C2-C3	-2.29	108.76	113.22
55	0	602	ATP	O4'-C1'-C2'	-2.20	103.72	106.93
59	a	1615	SCM	C8M-N8-C8	-2.19	111.20	114.38
55	0	601	ATP	O4'-C1'-C2'	-2.00	104.00	106.93

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	0	601	ATP	PB-O3B-PG-O2G
55	0	601	ATP	C5'-O5'-PA-O1A
55	0	601	ATP	C5'-O5'-PA-O2A
55	0	601	ATP	C5'-O5'-PA-O3A
55	0	601	ATP	O4'-C4'-C5'-O5'
55	0	602	ATP	C5'-O5'-PA-O3A
55	0	601	ATP	C3'-C4'-C5'-O5'
55	0	602	ATP	C5'-O5'-PA-O1A
55	0	602	ATP	C5'-O5'-PA-O2A
55	0	601	ATP	PG-O3B-PB-O2B
55	0	602	ATP	PA-O3A-PB-O2B
55	0	601	ATP	PB-O3B-PG-O1G
55	0	601	ATP	PG-O3B-PB-O1B
55	0	602	ATP	O4'-C4'-C5'-O5'

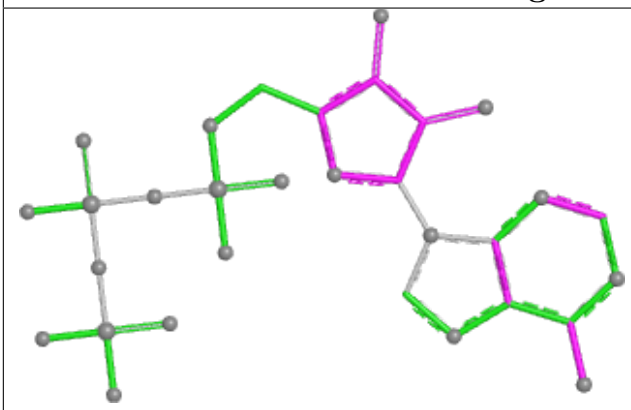
There are no ring outliers.

No monomer is involved in short contacts.

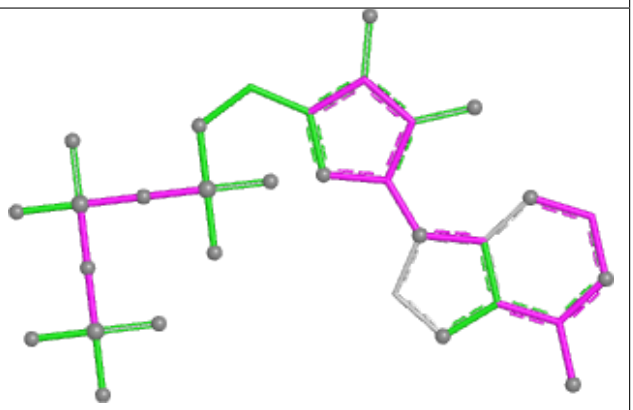
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

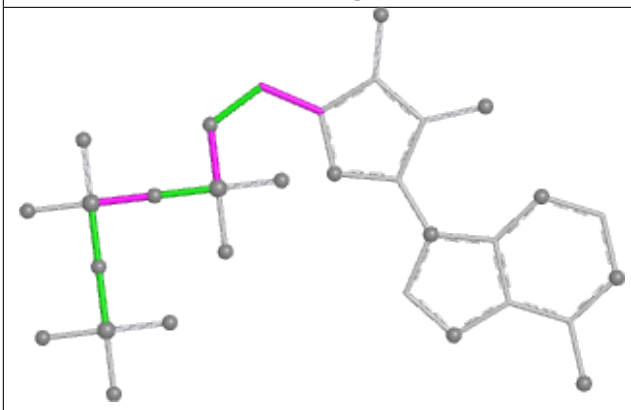
Ligand ATP 0 602



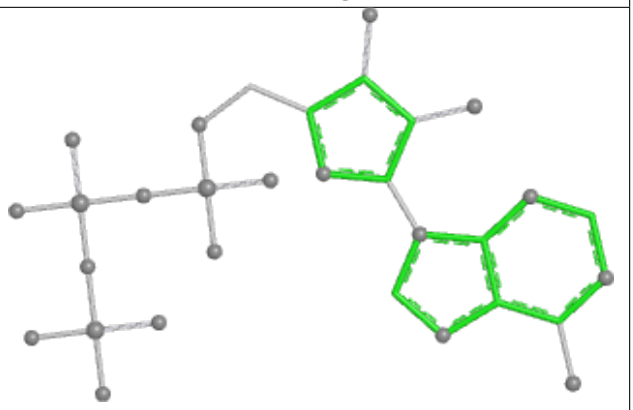
Bond lengths



Bond angles

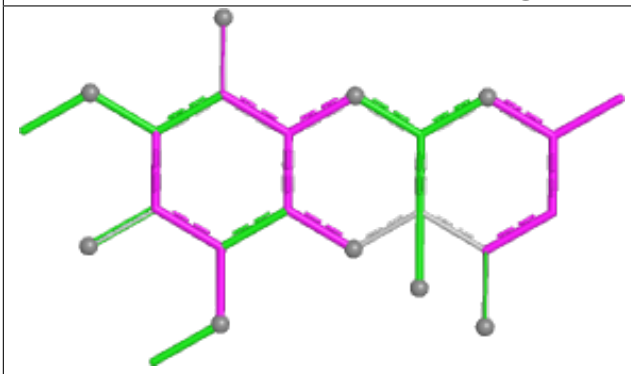


Torsions

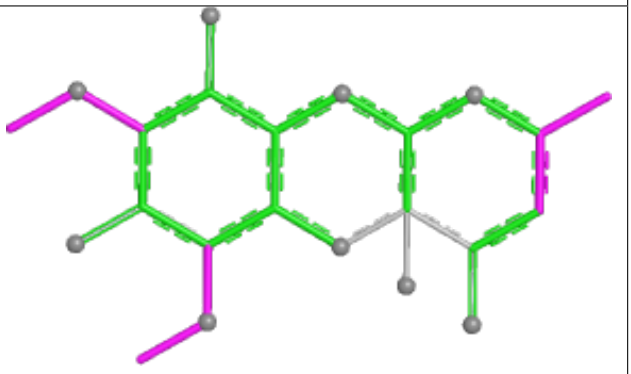


Rings

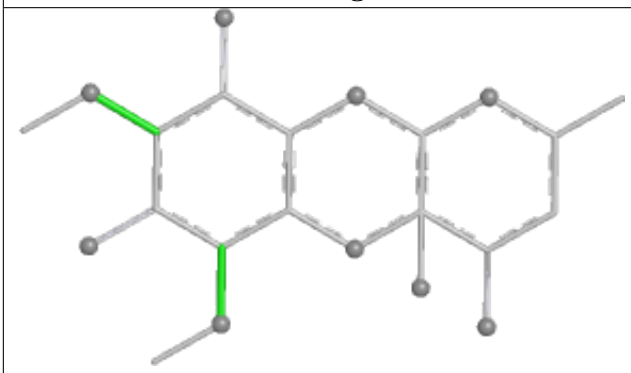
Ligand SCM a 1615



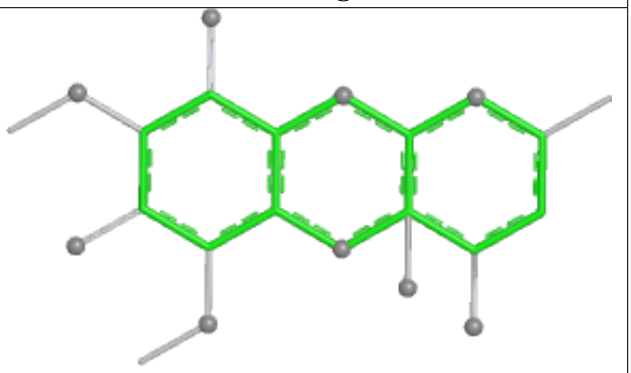
Bond lengths



Bond angles

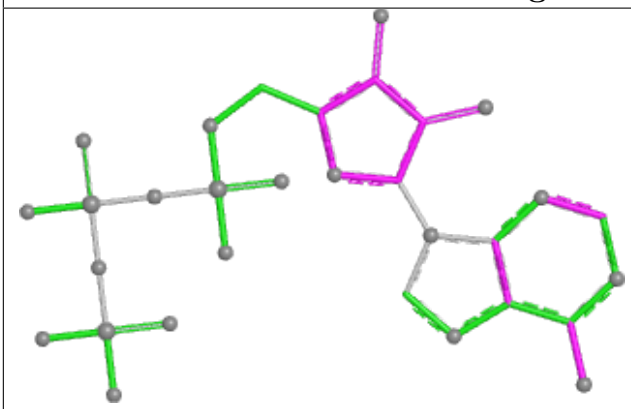


Torsions

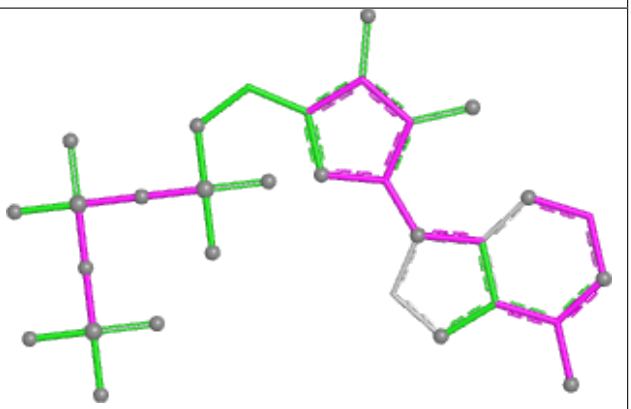


Rings

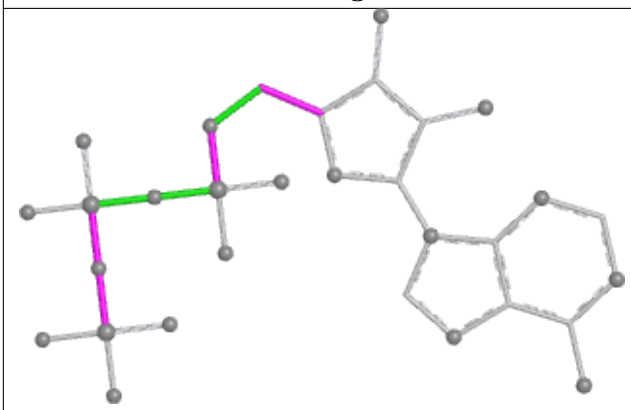
Ligand ATP 0 601



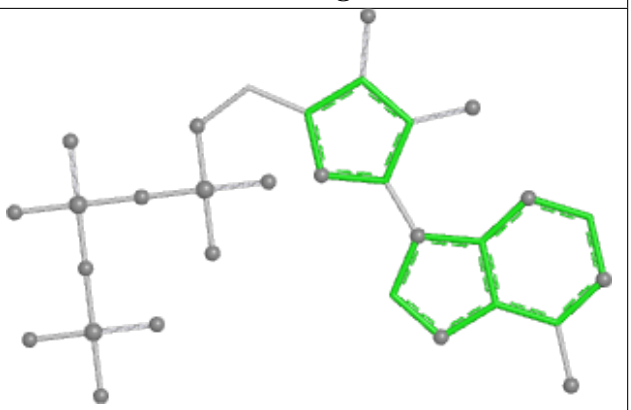
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

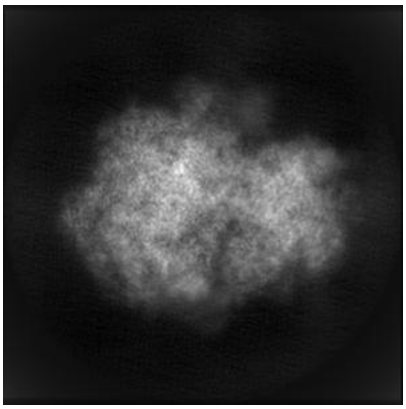
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13244. These allow visual inspection of the internal detail of the map and identification of artifacts.

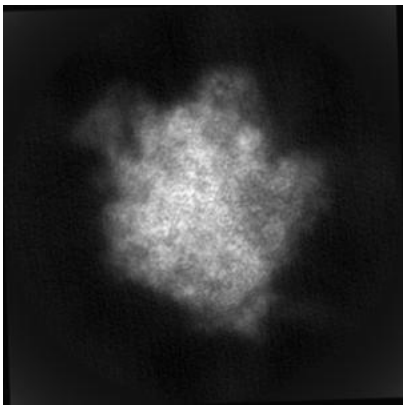
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

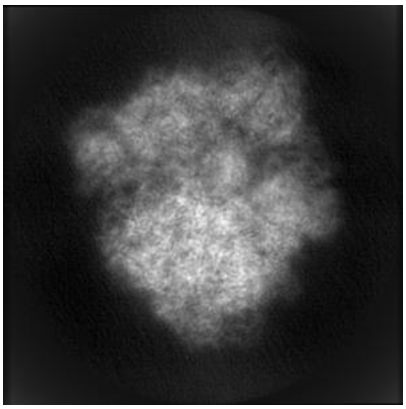
6.1.1 Primary map



X

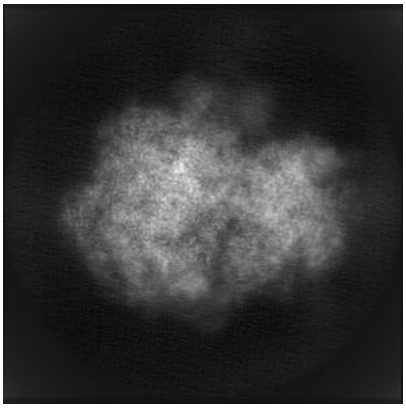


Y

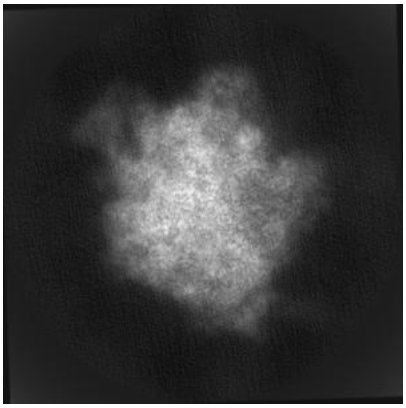


Z

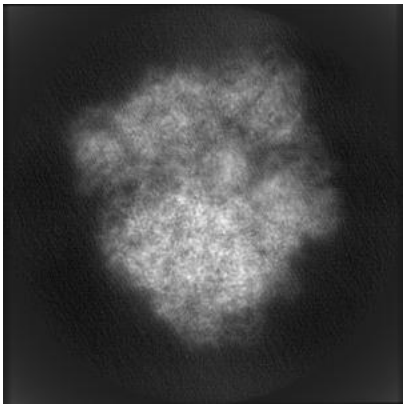
6.1.2 Raw map



X



Y

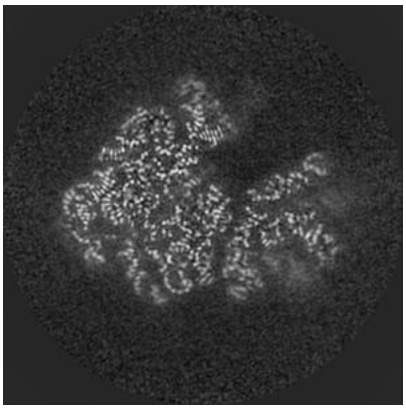


Z

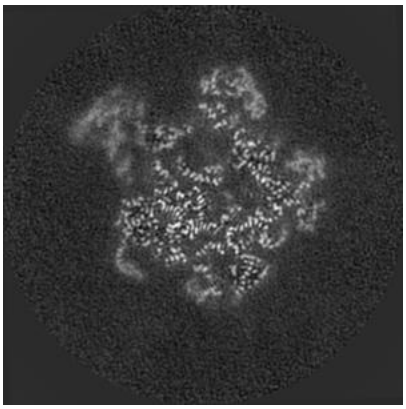
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

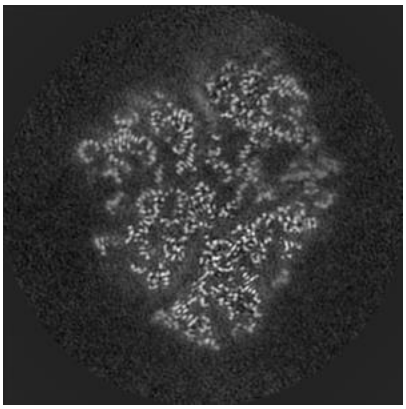
6.2.1 Primary map



X Index: 210

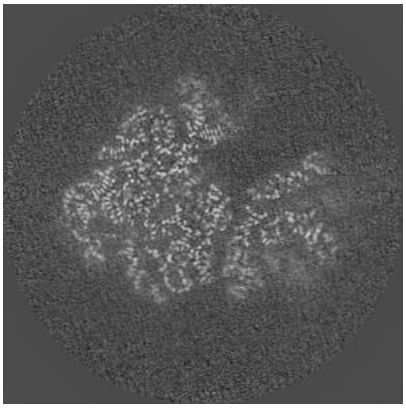


Y Index: 210

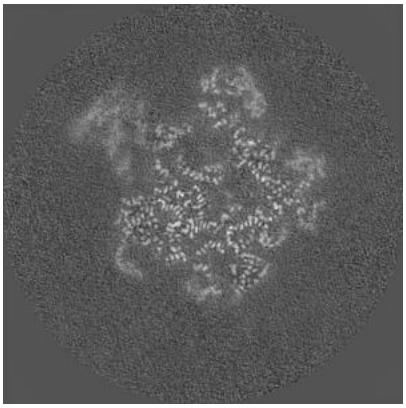


Z Index: 210

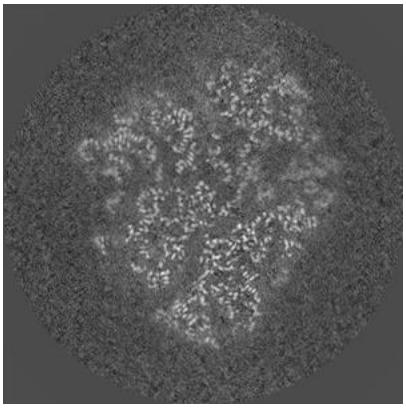
6.2.2 Raw map



X Index: 210



Y Index: 210

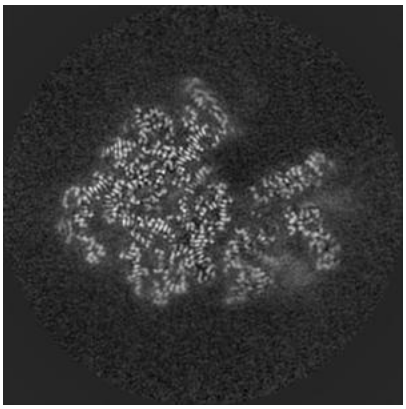


Z Index: 210

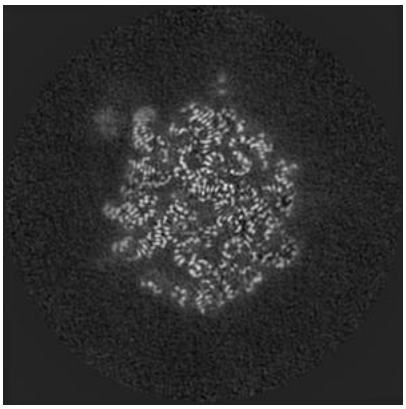
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

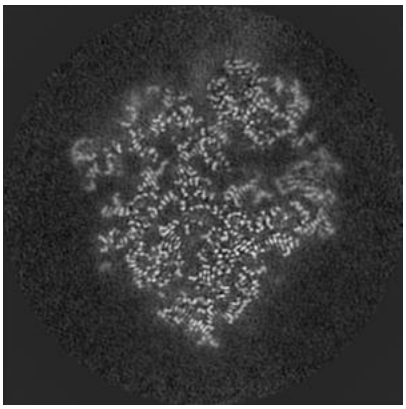
6.3.1 Primary map



X Index: 206

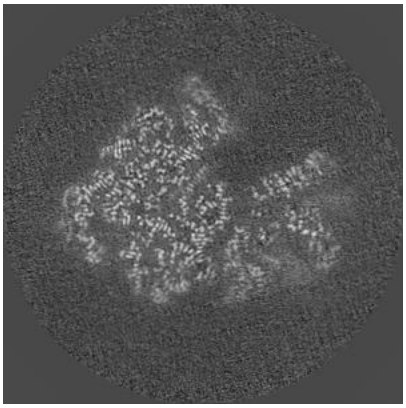


Y Index: 170

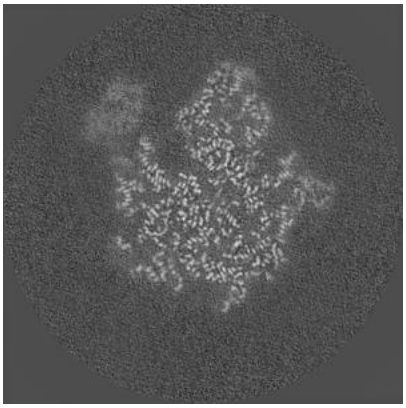


Z Index: 217

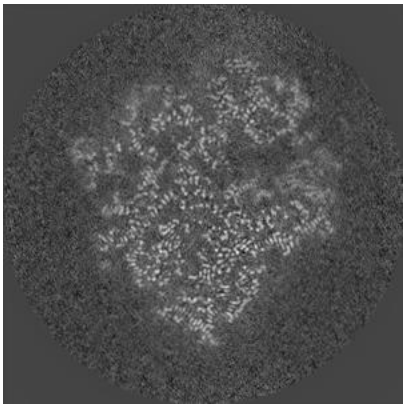
6.3.2 Raw map



X Index: 207



Y Index: 191

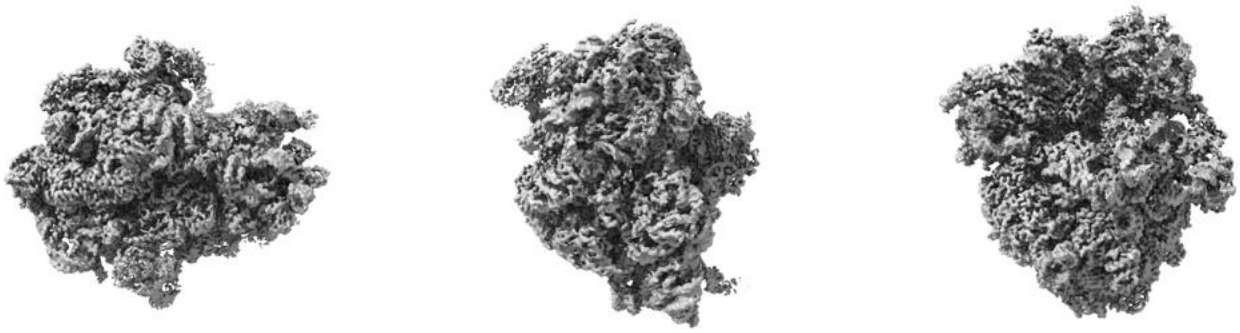


Z Index: 217

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.014. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

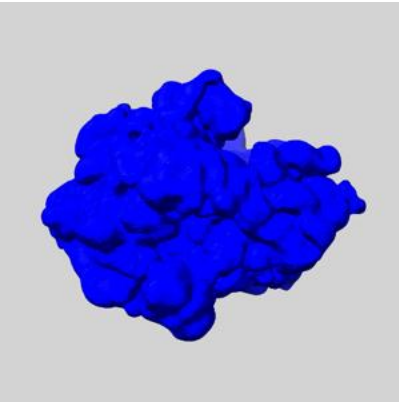
6.5 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

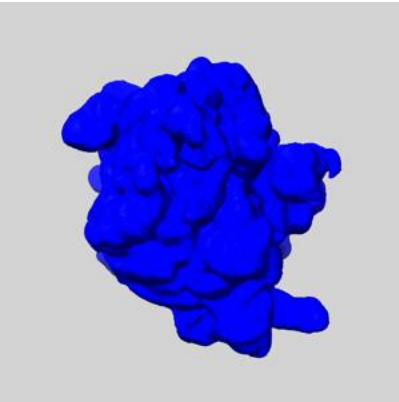
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

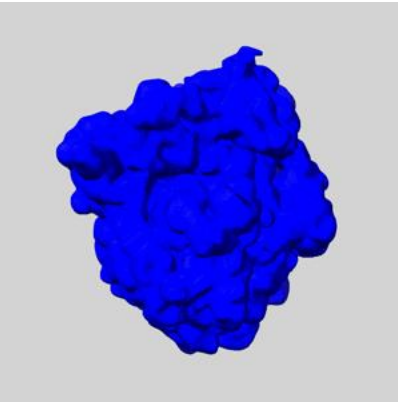
6.5.1 emd_13244_msk_1.map (i)



X



Y

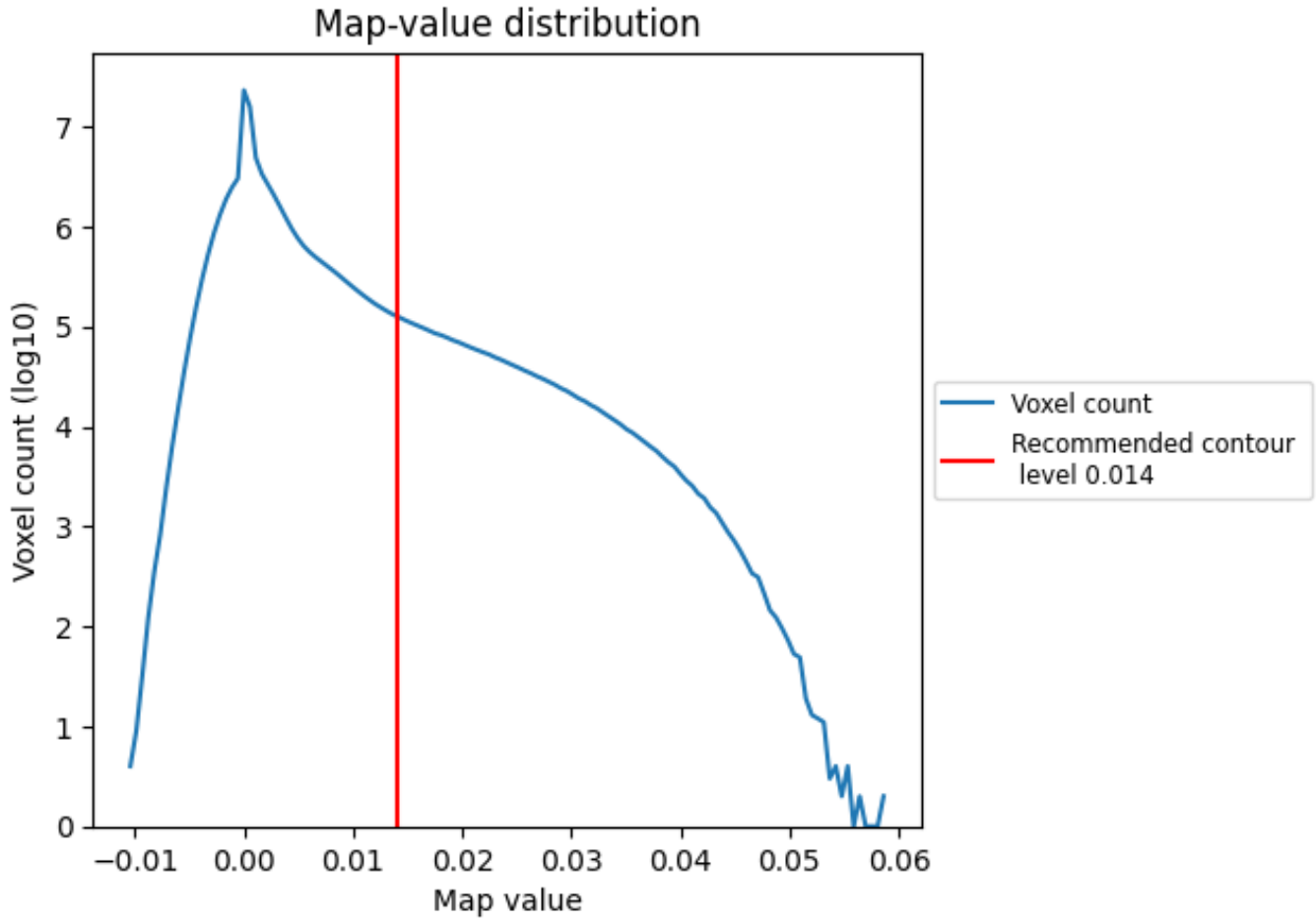


Z

7 Map analysis

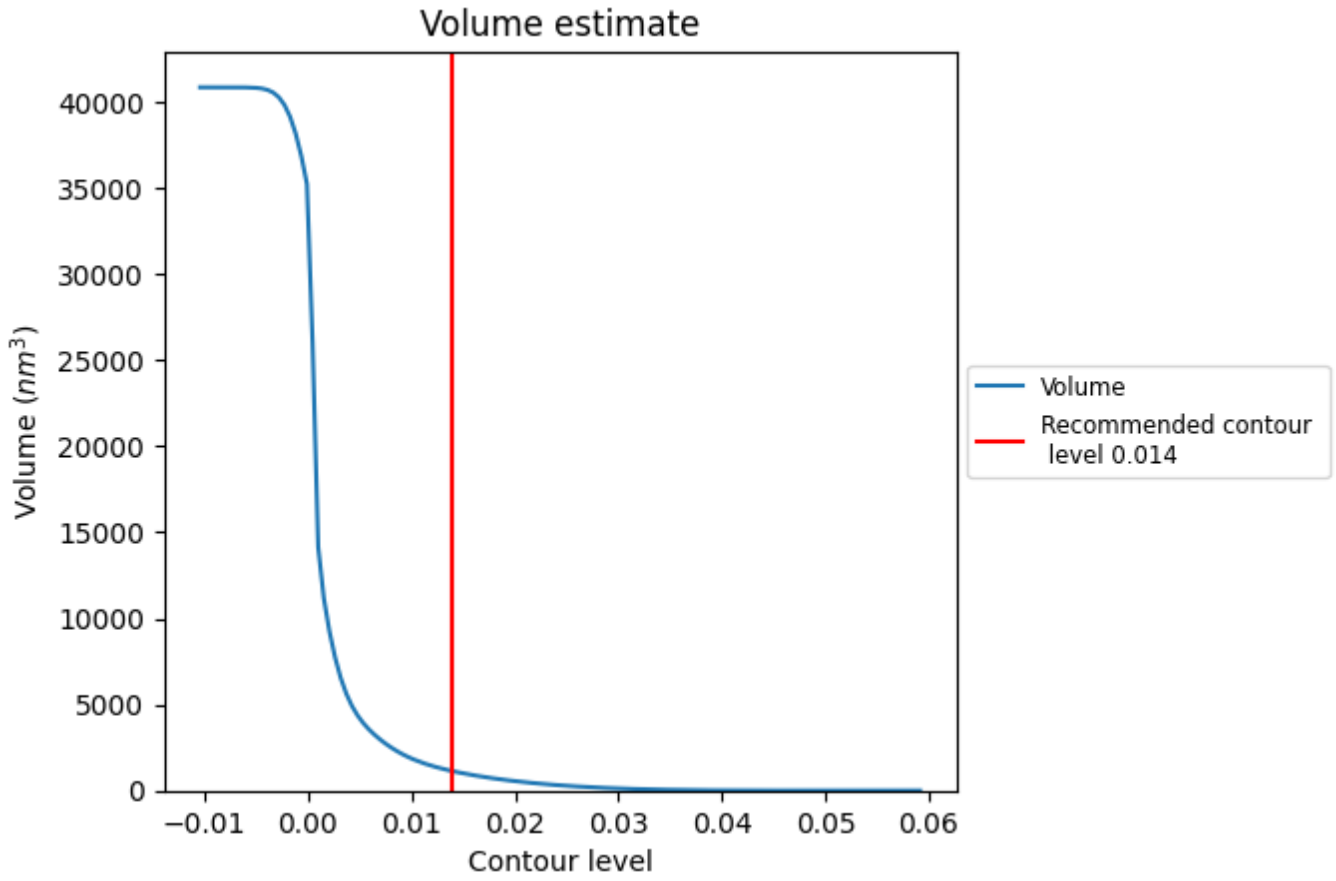
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

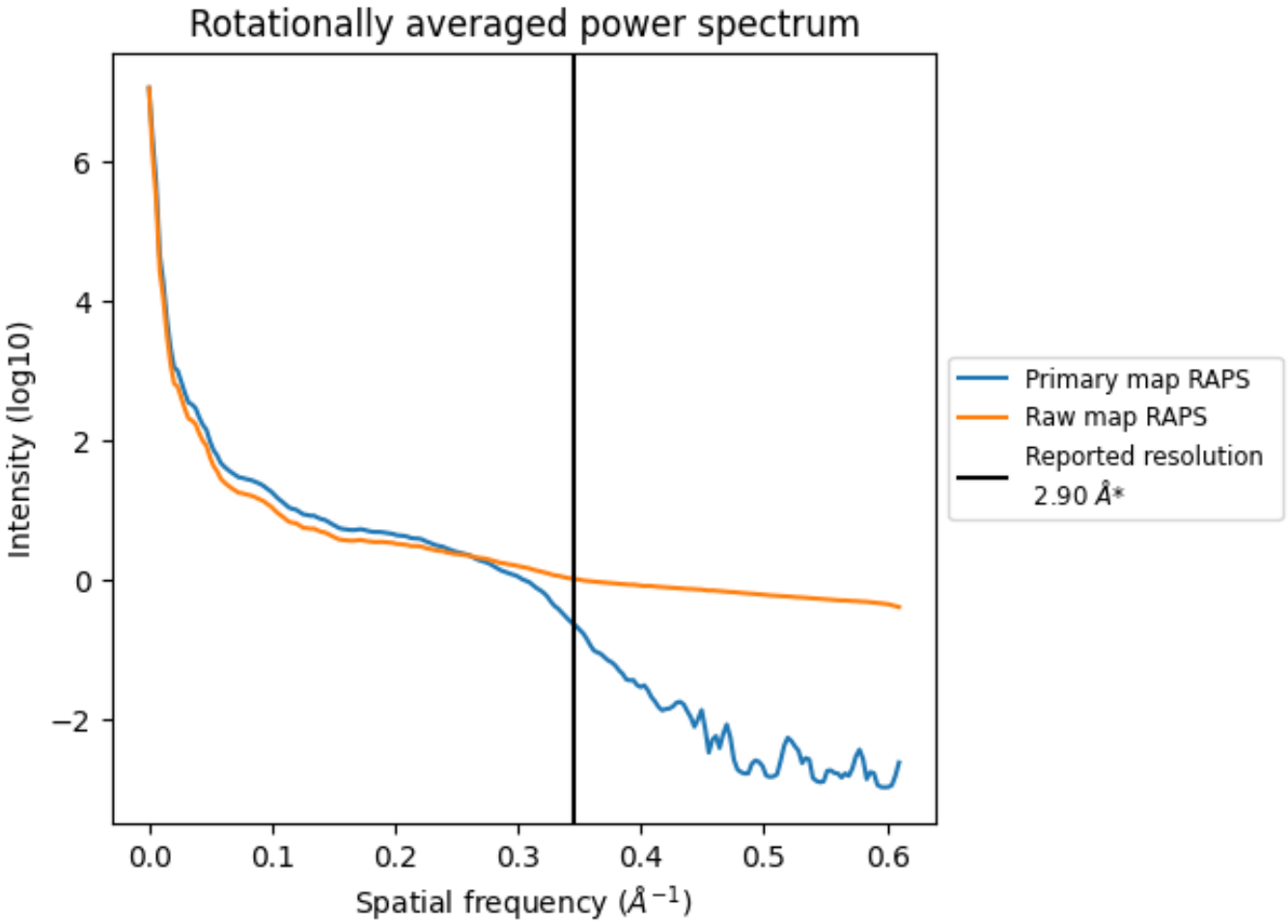
7.2 Volume estimate



The volume at the recommended contour level is 1125 nm^3; this corresponds to an approximate mass of 1016 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)

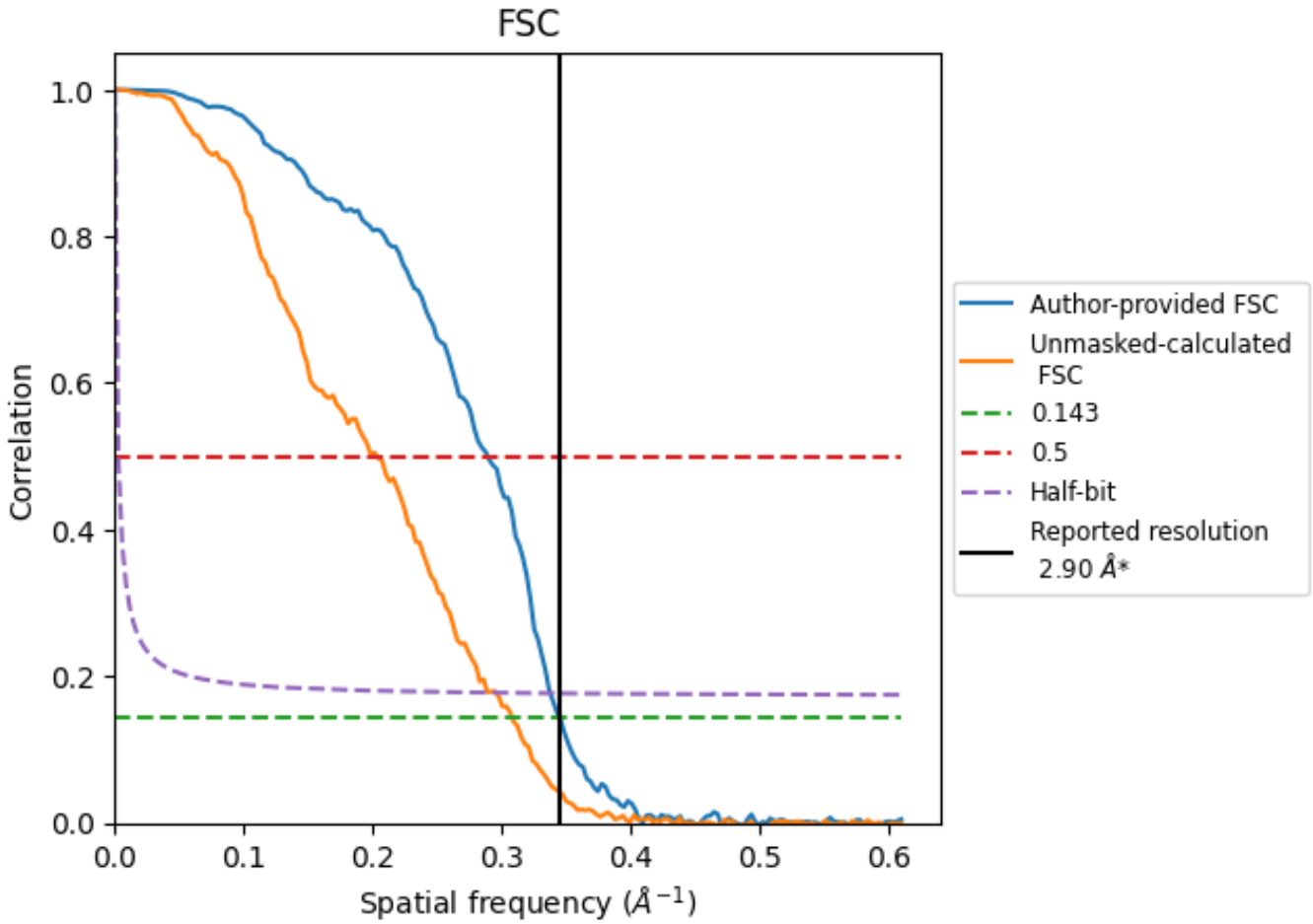


*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

8.2 Resolution estimates (i)

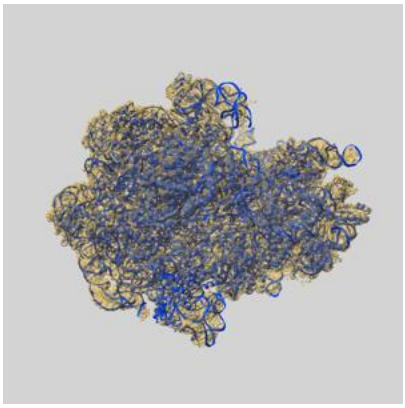
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.90	3.46	2.96
Unmasked-calculated*	3.25	4.92	3.38

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.25 differs from the reported value 2.9 by more than 10 %

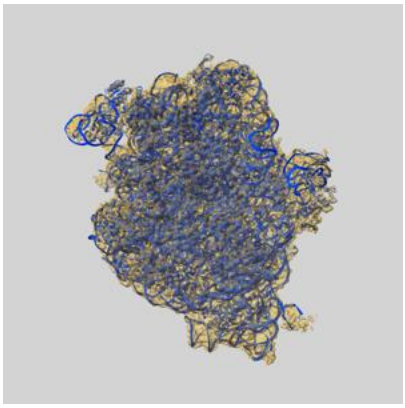
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13244 and PDB model 7P7T. Per-residue inclusion information can be found in section 3 on page 17.

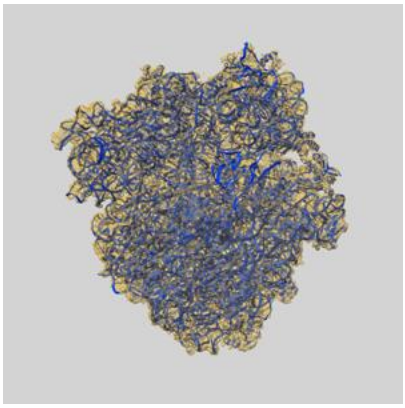
9.1 Map-model overlay



X



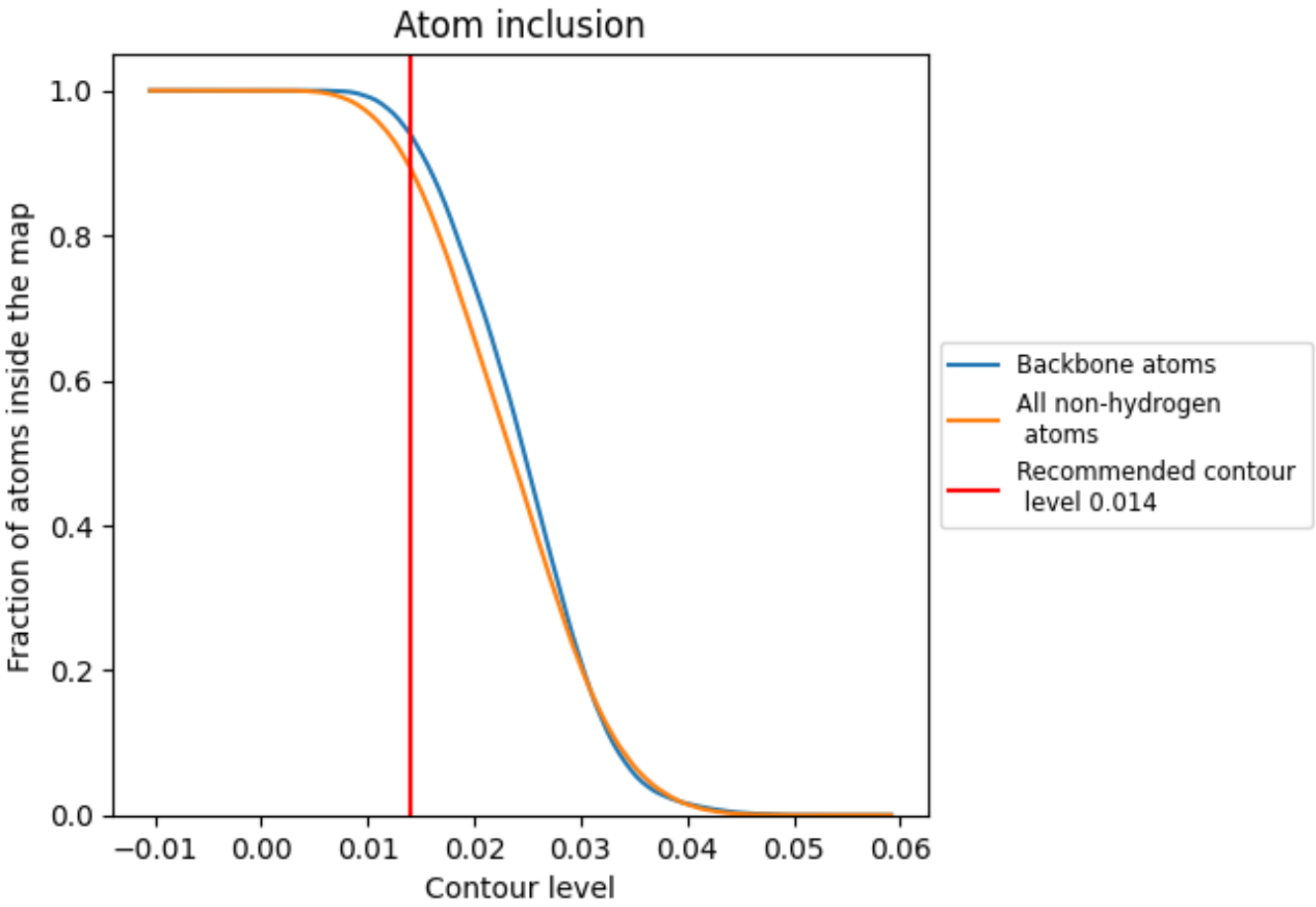
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.014 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 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 89% of all non-hydrogen atoms, are inside the map.