Full wwPDB EM Validation Report (i)

May 26, 2024 – 03:42 AM EDT

PDB ID	:	7RYG
EMDB ID	:	EMD-24739
Title	:	A. baumannii Ribosome-TP-6076 complex: E-site tRNA 70S
Authors	:	Morgan, C.E.; Yu, E.W.
Deposited on	:	2021-08-25
Resolution	:	2.38 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:

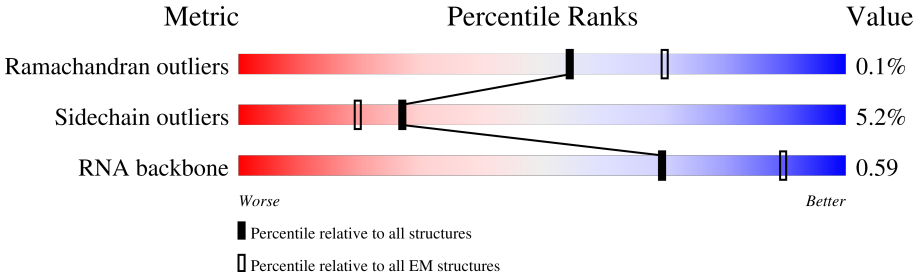
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.38 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	92% 8%
2	1	44	100%
3	2	64	94% 5%
4	3	38	95% 5%
5	A	2918	6% 78% 14% 8%
6	B	115	9% 85% 15%
7	C	274	98%
8	D	212	98%

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Mol	Chain	Length	Quality of chain
9	E	200	96%
10	F	178	76%, 85%, 13%
11	G	177	21%, 94%, 5%
12	H	148	13%, 37%, 59%
13	I	142	98%
14	J	122	96%
15	K	146	95%
16	L	137	96%
17	M	125	94%, 5%
18	N	116	5%, 95%
19	O	122	93%, 5%
20	P	119	98%
21	Q	103	96%
22	R	109	98%
23	S	106	5%, 84%, 14%
24	T	105	10%, 95%
25	U	98	93%, 6%
26	V	85	87%, 9%
27	W	78	96%
28	X	65	11%, 91%, 8%
29	Y	58	98%
30	Z	61	84%, 5%, 11%
31	a	1544	7%, 82%, 17%
32	b	250	56%, 83%, 7%, 10%
33	c	250	82%, 14%

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Mol	Chain	Length	Quality of chain
34	d	208	15% 96%
35	e	165	91% 6%
36	f	127	14% 74% 7% 18%
37	g	156	6% 79% 8% 13%
38	h	131	96%
39	i	128	96%
40	j	103	92% 5%
41	k	128	22% 86% 5% 9%
42	l	124	10% 94%
43	m	118	91% 7%
44	n	101	96%
45	o	89	98%
46	p	101	76% 5% 19%
47	q	85	87% 6% 7%
48	r	75	65% 31%
49	s	91	85% 5% 10%
50	t	88	95%
51	u	71	63% 76% 20%
52	v	77	57% 68% 27% 5%
53	w	3	67% 33%

2 Entry composition (i)

There are 56 unique types of molecules in this entry. The entry contains 137579 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	51	427	274	77	73	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	272	2111	1302	436	365	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	211	1572	972	297	300	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	142	1125	718	200	203	4	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	S		
23	S	91	710	452	128	129	1	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	79	621	390	116	114	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

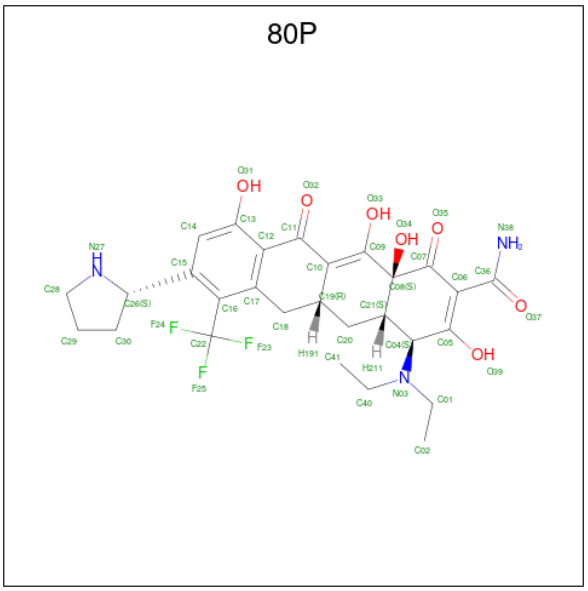
- Molecule 53 is a RNA chain called mRNA.

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).

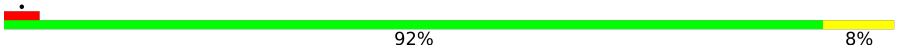
Mol	Chain	Residues	Atoms		AltConf
56	a	4	Total	Mg	0
			4	4	

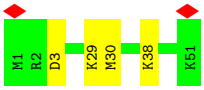
3 Residue-property plots (i)

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

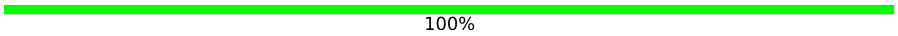
Chain 0:





• Molecule 2: 50S ribosomal protein L34

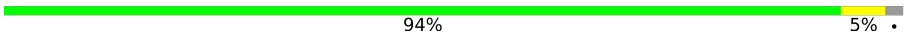
Chain 1:

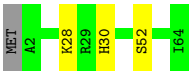


There are no outlier residues recorded for this chain.

• Molecule 3: 50S ribosomal protein L35

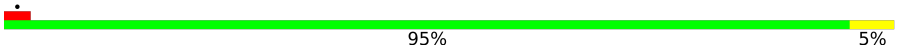
Chain 2:

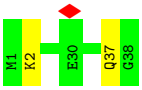




• Molecule 4: 50S ribosomal protein L36

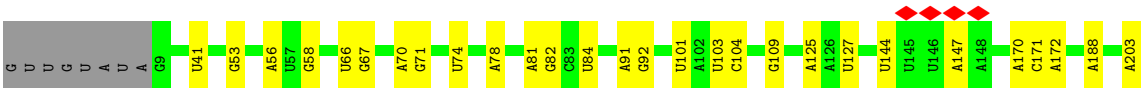
Chain 3:

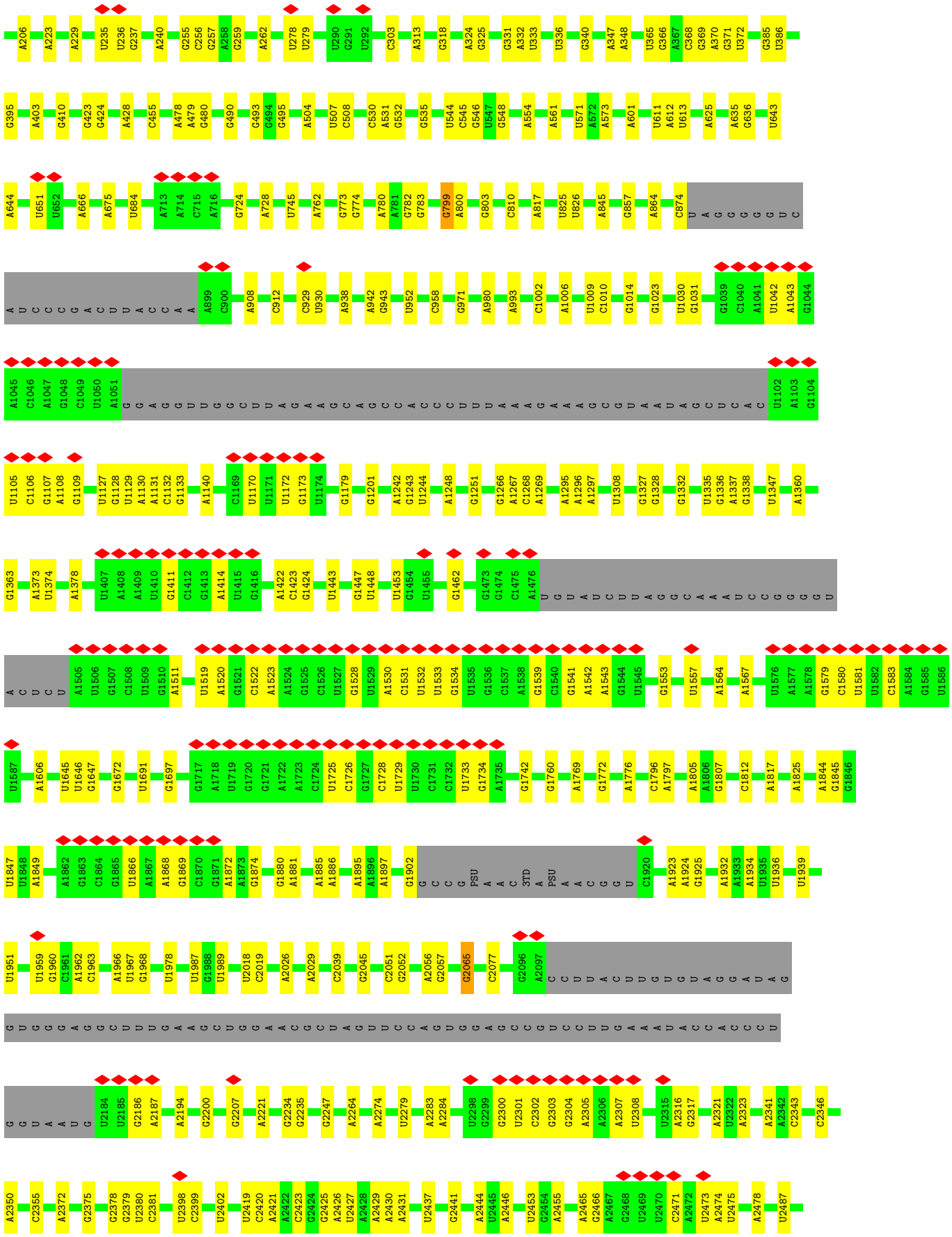




• Molecule 5: 23S ribosomal RNA

Chain A:

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G395 A403 G410 G423 G424 A428 C455 A478 A479 G480 G490 G493 G494 G495 A504 U507 C508 C530 A531 G532 G535 U544 C545 G546 U547 G548 A554 A561 U571 A572 A573 A601 U611 A612 U613 A625 A635 G636 U643
A644 U651 U652 A666 A675 U684 A713 A714 C715 A716 G724 A728 U745 A762 G773 G774 A780 A781 G782 G783 G799 A800 G803 C810 A817 U825 U826 A845 G857 A864 C874 U A G G G G U C
A U C C C G A C U U A C C A A899 C900 A908 C912 C929 U930 A938 A942 G943 U952 C958 G971 A980 A993 C1002 A1006 U1009 C1010 G1014 G1023 U1030 G1031 G1039 C1040 A1041 U1042 A1043 G1044
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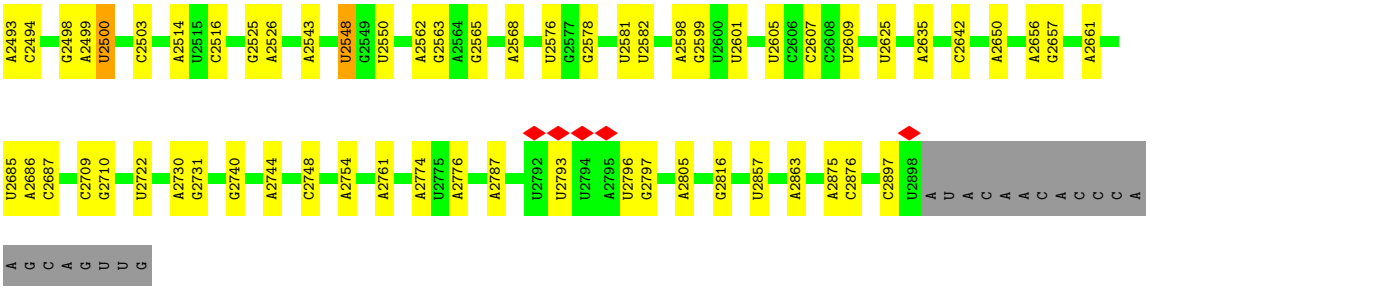
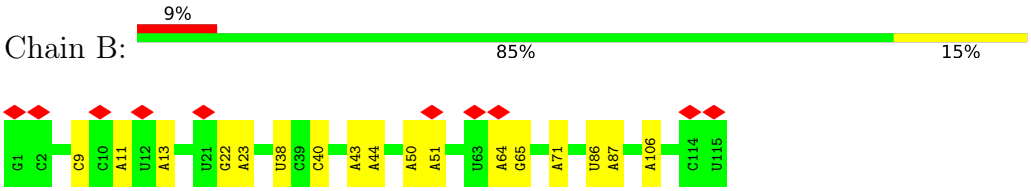


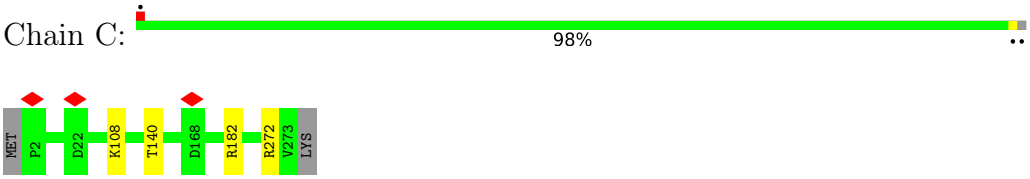
• Molecule 6: 5S ribosomal RNA

Chain B:



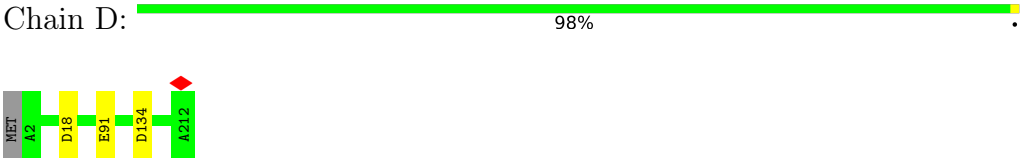
• Molecule 7: 50S ribosomal protein L2

Chain C:



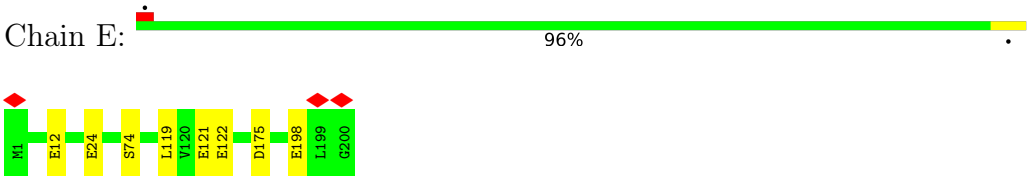
• Molecule 8: 50S ribosomal protein L3

Chain D:



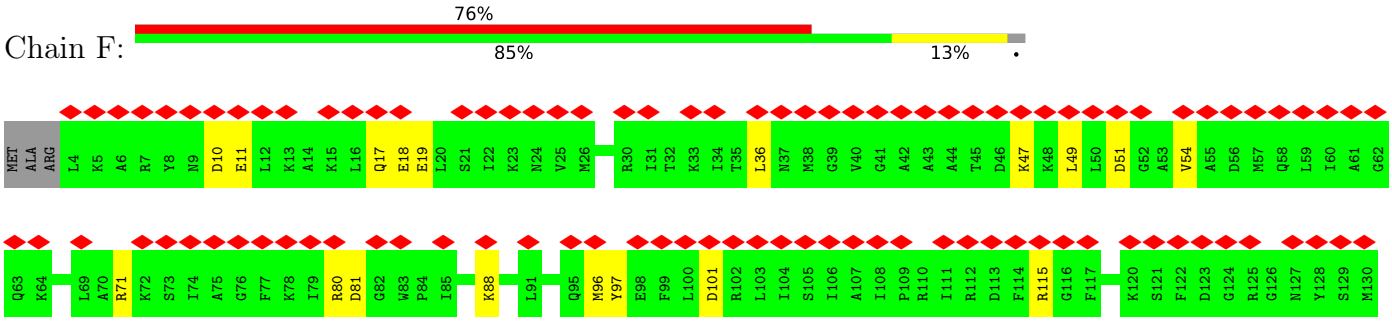
• Molecule 9: 50S ribosomal protein L4

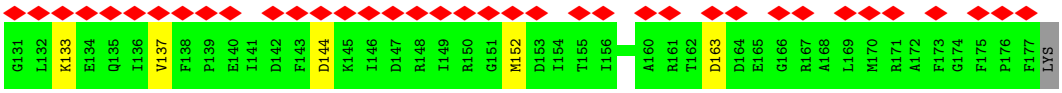
Chain E:



• Molecule 10: 50S ribosomal protein L5

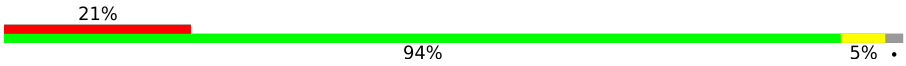
Chain F:

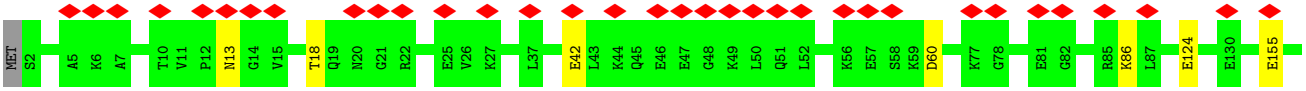


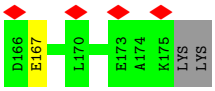


- Molecule 11: 50S ribosomal protein L6

Chain G:

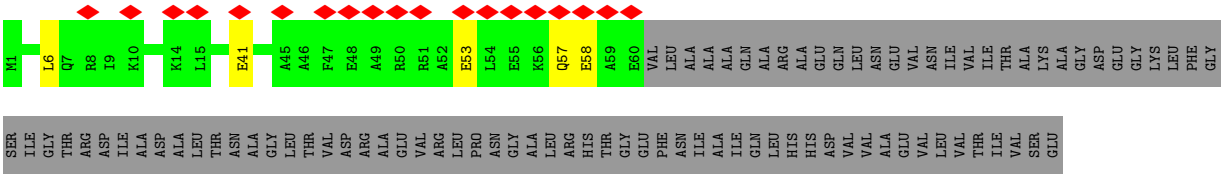






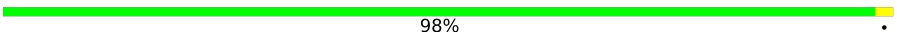
- Molecule 12: 50S ribosomal protein L9

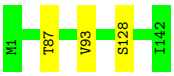
Chain H:



- Molecule 13: 50S ribosomal protein L13

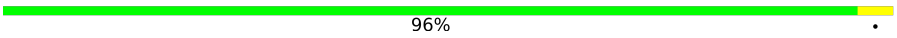
Chain I:





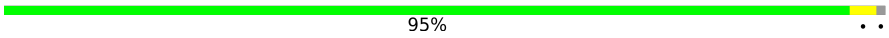
- Molecule 14: 50S ribosomal protein L14

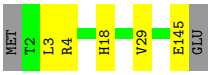
Chain J:



- Molecule 15: 50S ribosomal protein L15

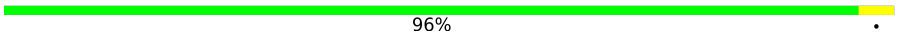
Chain K:



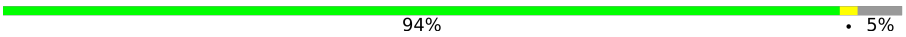


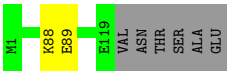
- Molecule 16: 50S ribosomal protein L16

Chain L:

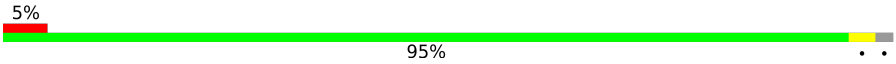


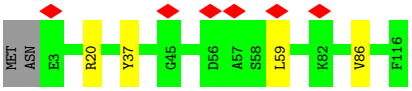
• Molecule 17: 50S ribosomal protein L17

Chain M: 

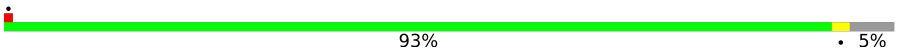


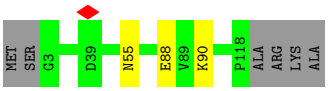
• Molecule 18: 50S ribosomal protein L18

Chain N: 

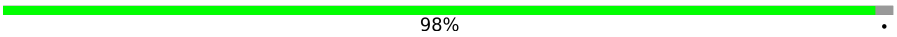


• Molecule 19: 50S ribosomal protein L19

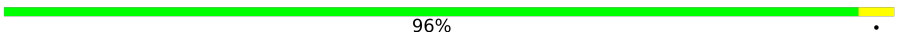
Chain O: 



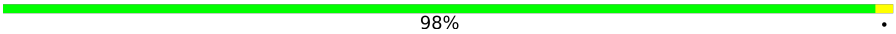
• Molecule 20: 50S ribosomal protein L20

Chain P: 

• Molecule 21: 50S ribosomal protein L21

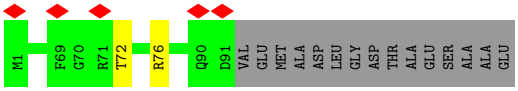
Chain Q: 

• Molecule 22: 50S ribosomal protein L22

Chain R: 

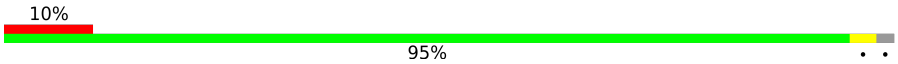
• Molecule 23: 50S ribosomal protein L23

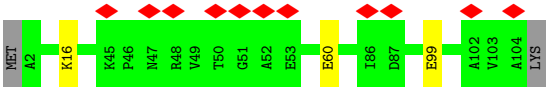
Chain S:



• Molecule 24: 50S ribosomal protein L24

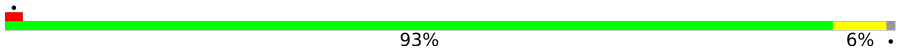
Chain T:





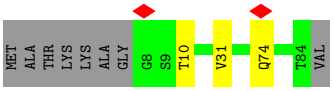
• Molecule 25: 50S ribosomal protein L25

Chain U:



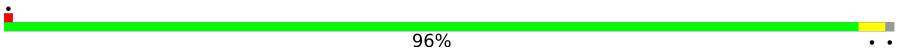
• Molecule 26: 50S ribosomal protein L27

Chain V:



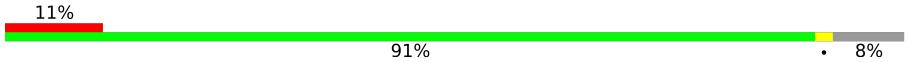
• Molecule 27: 50S ribosomal protein L28

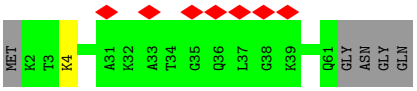
Chain W:



• Molecule 28: 50S ribosomal protein L29

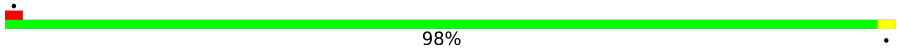
Chain X:

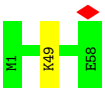




• Molecule 29: 50S ribosomal protein L30

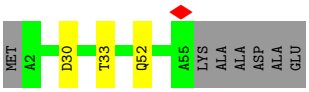
Chain Y:





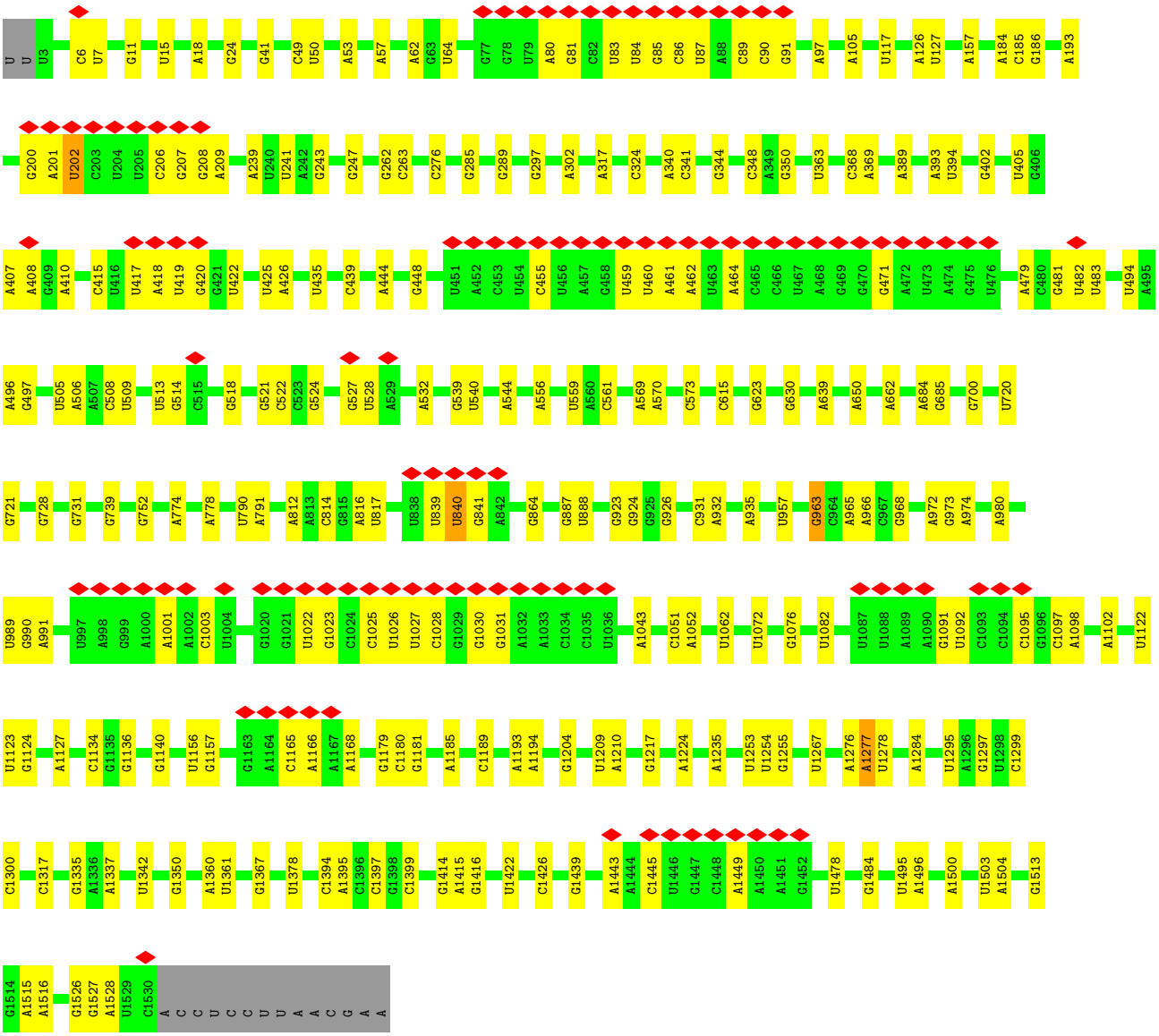
• Molecule 30: 50S ribosomal protein L32

Chain Z:



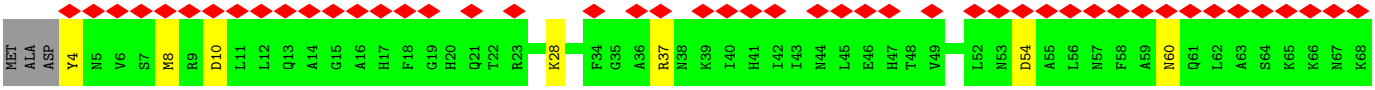
• Molecule 31: 16S Ribosomal RNA

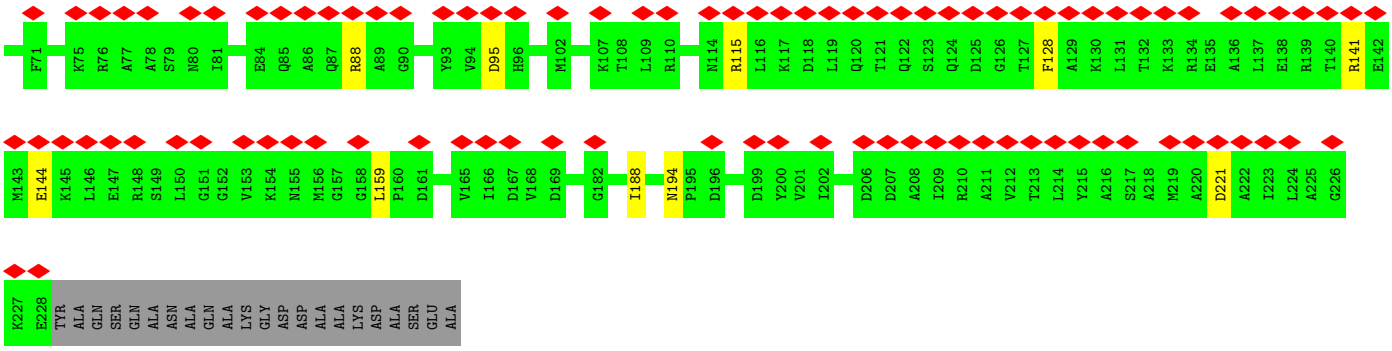
Chain a:



• Molecule 32: 30S ribosomal protein S2

Chain b:



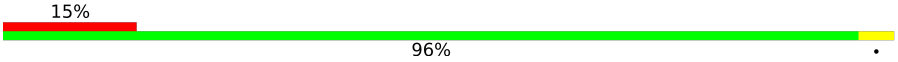


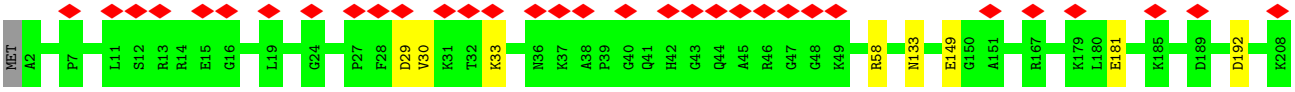
- Molecule 33: 30S ribosomal protein S3

Chain c:

- Molecule 34: 30S ribosomal protein S4

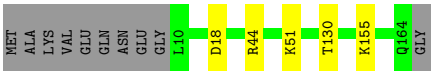
Chain d:





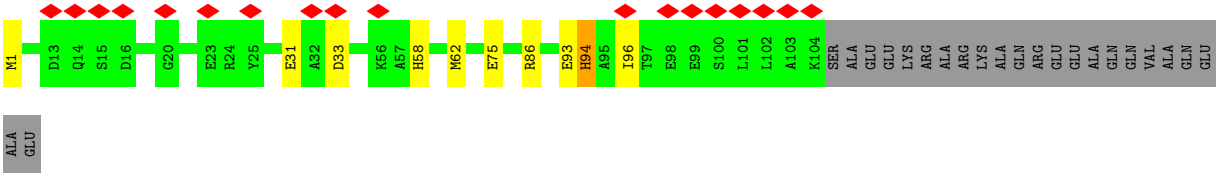
- Molecule 35: 30S ribosomal protein S5

Chain e:



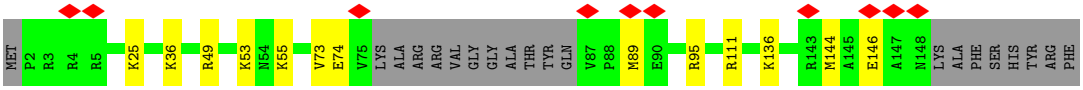
- Molecule 36: 30S ribosomal protein S6

Chain f:



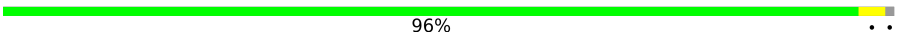
- Molecule 37: 30S ribosomal protein S7

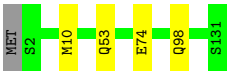
Chain g:



• Molecule 38: 30S ribosomal protein S8

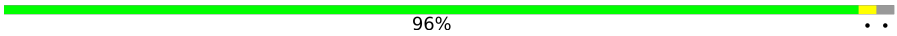
Chain h:

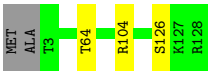




• Molecule 39: 30S ribosomal protein S9

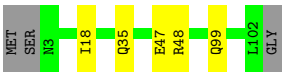
Chain i:





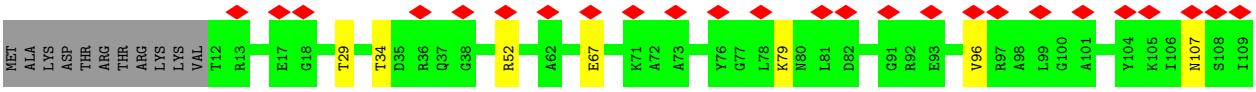
• Molecule 40: 30S ribosomal protein S10

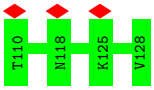
Chain j:



• Molecule 41: 30S ribosomal protein S11

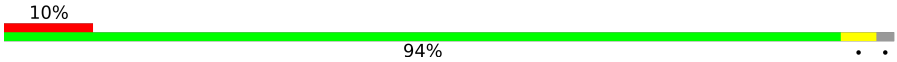
Chain k:

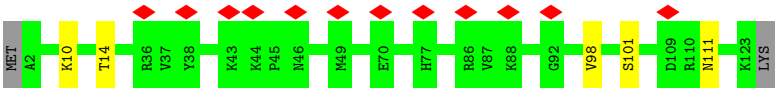




• Molecule 42: 30S ribosomal protein S12

Chain l:



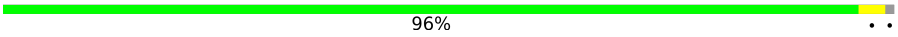


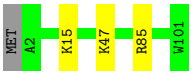
• Molecule 43: 30S ribosomal protein S13

Chain m:

• Molecule 44: 30S ribosomal protein S14

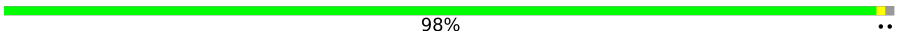
Chain n:





• Molecule 45: 30S ribosomal protein S15

Chain o:



• Molecule 46: 30S ribosomal protein S16

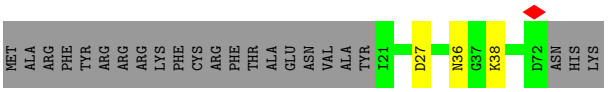
Chain p:

• Molecule 47: 30S ribosomal protein S17

Chain q:

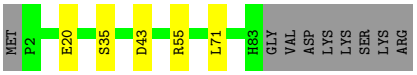
• Molecule 48: 30S ribosomal protein S18

Chain r:



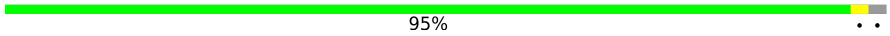
• Molecule 49: 30S ribosomal protein S19

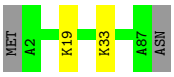
Chain s:



• Molecule 50: 30S ribosomal protein S20

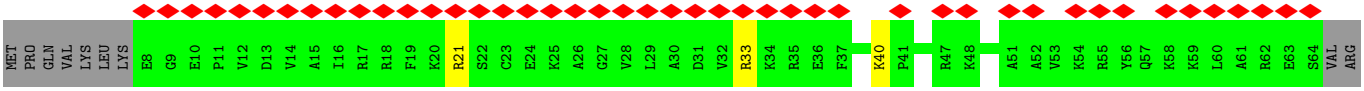
Chain t:





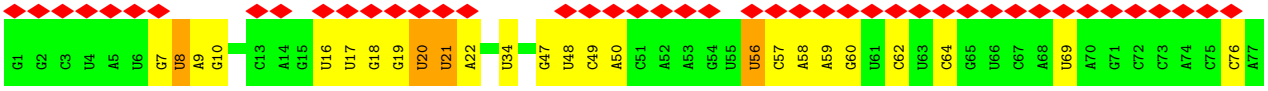
• Molecule 51: 30S ribosomal protein S21

Chain u:



- Molecule 52: tRNA-met

Chain v:



- Molecule 53: mRNA

Chain w:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	155853	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	6.067	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.046	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: 2MA, 7MG, 5MC, UR3, 80P, OMU, ZN, H2U, OMG, 5MU, PSU, 4OC, MA6, 4SU, 6MZ, 2MG, MG

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	0.29	0/434	0.58	0/573
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	0.61	0/389
5	A	0.20	0/64227	0.76	5/100172 (0.0%)
6	B	0.18	0/2739	0.75	0/4266
7	C	0.24	0/2152	0.58	0/2891
8	D	0.24	0/1590	0.54	0/2142
9	E	0.25	0/1537	0.51	0/2073
10	F	0.28	0/1390	0.64	0/1863
11	G	0.26	0/1337	0.51	0/1807
12	H	0.28	0/461	0.54	0/616
13	I	0.25	0/1151	0.47	0/1551
14	J	0.25	0/956	0.62	0/1286
15	K	0.25	0/1079	0.59	0/1439
16	L	0.26	0/1104	0.60	0/1475
17	M	0.25	0/956	0.57	0/1282
18	N	0.25	0/865	0.59	0/1156
19	O	0.24	0/925	0.55	0/1241
20	P	0.26	0/947	0.58	0/1262
21	Q	0.24	0/818	0.55	0/1094
22	R	0.24	0/831	0.52	0/1113
23	S	0.26	0/716	0.52	0/957
24	T	0.24	0/770	0.52	0/1034
25	U	0.24	0/770	0.54	0/1036
26	V	0.25	0/589	0.54	0/788
27	W	0.23	0/642	0.55	0/856
28	X	0.24	0/487	0.48	0/646
29	Y	0.25	0/468	0.51	0/624
30	Z	0.23	0/453	0.63	0/604
31	a	0.28	0/36476	0.77	5/56895 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	b	0.26	0/1799	0.55	0/2429
33	c	0.28	0/1714	0.59	0/2304
34	d	0.26	0/1653	0.56	0/2213
35	e	0.25	0/1141	0.55	0/1537
36	f	0.25	0/882	0.54	0/1189
37	g	0.25	0/1087	0.55	0/1456
38	h	0.26	0/993	0.53	0/1331
39	i	0.26	0/1002	0.60	0/1339
40	j	0.25	0/811	0.57	0/1096
41	k	0.25	0/878	0.53	0/1189
42	l	0.24	0/958	0.58	0/1284
43	m	0.25	0/913	0.62	0/1226
44	n	0.27	0/803	0.57	0/1071
45	o	0.26	0/715	0.56	0/958
46	p	0.25	0/655	0.57	0/879
47	q	0.24	0/628	0.57	0/847
48	r	0.25	0/432	0.54	0/583
49	s	0.26	0/664	0.53	0/897
50	t	0.28	0/669	0.55	0/892
51	u	0.25	0/478	0.53	0/631
52	v	0.20	0/1739	0.77	1/2709 (0.0%)
53	w	0.16	0/72	0.80	0/110
All	All	0.24	0/148734	0.72	11/222460 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1308	U	C2-N1-C1'	5.70	124.53	117.70
5	A	2300	G	N1-C6-O6	-5.63	116.52	119.90
31	a	202	U	C2-N1-C1'	5.61	124.43	117.70
31	a	482	U	C2-N1-C1'	5.35	124.12	117.70
31	a	439	C	C2-N1-C1'	5.25	124.57	118.80
31	a	840	U	C2-N1-C1'	5.20	123.94	117.70
5	A	2300	G	C5-C6-O6	5.16	131.70	128.60
31	a	1277	A	P-O3'-C3'	5.11	125.83	119.70
5	A	2307	A	C8-N9-C4	-5.08	103.77	105.80
52	v	21	U	C2-N1-C1'	5.06	123.77	117.70
5	A	799	G	P-O3'-C3'	5.05	125.77	119.70

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	49/51 (96%)	48 (98%)	1 (2%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	C	270/274 (98%)	260 (96%)	10 (4%)	0	100	100
8	D	209/212 (99%)	200 (96%)	9 (4%)	0	100	100
9	E	198/200 (99%)	198 (100%)	0	0	100	100
10	F	172/178 (97%)	157 (91%)	14 (8%)	1 (1%)	25	34
11	G	172/177 (97%)	166 (96%)	5 (3%)	1 (1%)	25	34
12	H	58/148 (39%)	56 (97%)	2 (3%)	0	100	100
13	I	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
14	J	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
15	K	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
16	L	135/137 (98%)	132 (98%)	2 (2%)	1 (1%)	22	30
17	M	117/125 (94%)	115 (98%)	2 (2%)	0	100	100
18	N	112/116 (97%)	109 (97%)	3 (3%)	0	100	100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	115/119 (97%)	114 (99%)	1 (1%)	0	100	100
21	Q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
23	S	89/106 (84%)	87 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	T	101/105 (96%)	99 (98%)	2 (2%)	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%)	56 (100%)	0	0	100	100
30	Z	52/61 (85%)	51 (98%)	1 (2%)	0	100	100
32	b	223/250 (89%)	216 (97%)	6 (3%)	1 (0%)	34	46
33	c	213/250 (85%)	203 (95%)	10 (5%)	0	100	100
34	d	205/208 (99%)	199 (97%)	6 (3%)	0	100	100
35	e	153/165 (93%)	151 (99%)	2 (1%)	0	100	100
36	f	102/127 (80%)	95 (93%)	5 (5%)	2 (2%)	7	8
37	g	132/156 (85%)	130 (98%)	2 (2%)	0	100	100
38	h	128/131 (98%)	123 (96%)	5 (4%)	0	100	100
39	i	124/128 (97%)	118 (95%)	6 (5%)	0	100	100
40	j	98/103 (95%)	94 (96%)	4 (4%)	0	100	100
41	k	115/128 (90%)	111 (96%)	4 (4%)	0	100	100
42	l	120/124 (97%)	113 (94%)	7 (6%)	0	100	100
43	m	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
44	n	98/101 (97%)	96 (98%)	2 (2%)	0	100	100
45	o	86/89 (97%)	86 (100%)	0	0	100	100
46	p	80/101 (79%)	79 (99%)	1 (1%)	0	100	100
47	q	77/85 (91%)	77 (100%)	0	0	100	100
48	r	50/75 (67%)	49 (98%)	1 (2%)	0	100	100
49	s	80/91 (88%)	79 (99%)	1 (1%)	0	100	100
50	t	84/88 (96%)	84 (100%)	0	0	100	100
51	u	55/71 (78%)	55 (100%)	0	0	100	100
All	All	5407/5872 (92%)	5258 (97%)	143 (3%)	6 (0%)	54	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	b	8	MET

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Mol	Chain	Res	Type
10	F	137	VAL
11	G	13	ASN
36	f	86	ARG
36	f	94	HIS
16	L	78	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/47 (100%)	43 (92%)	4 (8%)	10	14
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	49 (94%)	3 (6%)	20	30
4	3	33/33 (100%)	31 (94%)	2 (6%)	18	27
7	C	218/220 (99%)	214 (98%)	4 (2%)	59	75
8	D	166/167 (99%)	163 (98%)	3 (2%)	59	75
9	E	155/155 (100%)	147 (95%)	8 (5%)	23	35
10	F	144/147 (98%)	122 (85%)	22 (15%)	2	3
11	G	139/142 (98%)	132 (95%)	7 (5%)	24	37
12	H	45/112 (40%)	40 (89%)	5 (11%)	6	7
13	I	118/118 (100%)	115 (98%)	3 (2%)	47	65
14	J	103/103 (100%)	98 (95%)	5 (5%)	25	38
15	K	106/108 (98%)	101 (95%)	5 (5%)	26	39
16	L	113/113 (100%)	108 (96%)	5 (4%)	28	42
17	M	96/101 (95%)	94 (98%)	2 (2%)	53	70
18	N	83/85 (98%)	79 (95%)	4 (5%)	25	39
19	O	98/102 (96%)	95 (97%)	3 (3%)	40	57
20	P	85/86 (99%)	85 (100%)	0	100	100
21	Q	84/84 (100%)	80 (95%)	4 (5%)	25	39
22	R	88/88 (100%)	86 (98%)	2 (2%)	50	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	S	77/87 (88%)	75 (97%)	2 (3%)	46	64
24	T	83/85 (98%)	80 (96%)	3 (4%)	35	51
25	U	79/80 (99%)	73 (92%)	6 (8%)	13	18
26	V	59/64 (92%)	56 (95%)	3 (5%)	24	36
27	W	69/70 (99%)	67 (97%)	2 (3%)	42	60
28	X	53/56 (95%)	52 (98%)	1 (2%)	57	73
29	Y	54/54 (100%)	53 (98%)	1 (2%)	57	73
30	Z	46/50 (92%)	43 (94%)	3 (6%)	17	24
32	b	185/200 (92%)	169 (91%)	16 (9%)	10	14
33	c	175/198 (88%)	166 (95%)	9 (5%)	24	36
34	d	170/171 (99%)	162 (95%)	8 (5%)	26	39
35	e	113/120 (94%)	108 (96%)	5 (4%)	28	42
36	f	94/111 (85%)	85 (90%)	9 (10%)	8	11
37	g	113/128 (88%)	100 (88%)	13 (12%)	5	6
38	h	108/109 (99%)	104 (96%)	4 (4%)	34	50
39	i	99/100 (99%)	96 (97%)	3 (3%)	41	59
40	j	89/91 (98%)	84 (94%)	5 (6%)	21	31
41	k	88/98 (90%)	81 (92%)	7 (8%)	12	17
42	l	104/106 (98%)	99 (95%)	5 (5%)	25	39
43	m	95/98 (97%)	87 (92%)	8 (8%)	11	15
44	n	81/82 (99%)	78 (96%)	3 (4%)	34	50
45	o	71/72 (99%)	70 (99%)	1 (1%)	67	81
46	p	63/77 (82%)	58 (92%)	5 (8%)	12	17
47	q	71/76 (93%)	66 (93%)	5 (7%)	15	21
48	r	46/66 (70%)	43 (94%)	3 (6%)	17	24
49	s	70/78 (90%)	65 (93%)	5 (7%)	14	21
50	t	65/67 (97%)	63 (97%)	2 (3%)	40	57
51	u	48/62 (77%)	45 (94%)	3 (6%)	18	26
All	All	4477/4756 (94%)	4246 (95%)	231 (5%)	27	35

All (231) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	3	ASP
1	0	29	LYS
1	0	30	MET
1	0	38	LYS
3	2	28	LYS
3	2	30	HIS
3	2	52	SER
4	3	2	LYS
4	3	37	GLN
7	C	108	LYS
7	C	140	THR
7	C	182	ARG
7	C	272	ARG
8	D	18	ASP
8	D	91	GLU
8	D	134	ASP
9	E	12	GLU
9	E	24	GLU
9	E	74	SER
9	E	119	LEU
9	E	121	GLU
9	E	122	GLU
9	E	175	ASP
9	E	198	GLU
10	F	10	ASP
10	F	11	GLU
10	F	17	GLN
10	F	18	GLU
10	F	19	GLU
10	F	36	LEU
10	F	47	LYS
10	F	49	LEU
10	F	51	ASP
10	F	54	VAL
10	F	71	ARG
10	F	80	ARG
10	F	81	ASP
10	F	88	LYS
10	F	96	MET
10	F	97	TYR
10	F	101	ASP
10	F	115	ARG
10	F	133	LYS

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Mol	Chain	Res	Type
10	F	144	ASP
10	F	152	MET
10	F	163	ASP
11	G	18	THR
11	G	42	GLU
11	G	60	ASP
11	G	86	LYS
11	G	124	GLU
11	G	155	GLU
11	G	167	GLU
12	H	6	LEU
12	H	41	GLU
12	H	53	GLU
12	H	57	GLN
12	H	58	GLU
13	I	87	THR
13	I	93	VAL
13	I	128	SER
14	J	1	MET
14	J	53	LYS
14	J	54	LYS
14	J	89	ASN
14	J	112	MET
15	K	3	LEU
15	K	4	ARG
15	K	18	HIS
15	K	29	VAL
15	K	145	GLU
16	L	5	LYS
16	L	14	LYS
16	L	28	SER
16	L	56	ARG
16	L	134	ARG
17	M	88	LYS
17	M	89	GLU
18	N	20	ARG
18	N	37	TYR
18	N	59	LEU
18	N	86	VAL
19	O	55	ASN
19	O	88	GLU
19	O	90	LYS

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Mol	Chain	Res	Type
21	Q	29	SER
21	Q	36	ASP
21	Q	43	ASN
21	Q	97	LYS
22	R	13	SER
22	R	105	VAL
23	S	72	THR
23	S	76	ARG
24	T	16	LYS
24	T	60	GLU
24	T	99	GLU
25	U	15	LYS
25	U	53	LYS
25	U	57	SER
25	U	69	VAL
25	U	71	ASP
25	U	75	ASN
26	V	10	THR
26	V	31	VAL
26	V	74	GLN
27	W	48	ARG
27	W	51	LEU
28	X	4	LYS
29	Y	49	LYS
30	Z	30	ASP
30	Z	33	THR
30	Z	52	GLN
32	b	4	TYR
32	b	10	ASP
32	b	28	LYS
32	b	37	ARG
32	b	54	ASP
32	b	60	ASN
32	b	88	ARG
32	b	95	ASP
32	b	115	ARG
32	b	128	PHE
32	b	141	ARG
32	b	144	GLU
32	b	159	LEU
32	b	188	ILE
32	b	194	ASN

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Mol	Chain	Res	Type
32	b	221	ASP
33	c	45	LYS
33	c	49	ASN
33	c	108	ARG
33	c	114	ARG
33	c	118	GLU
33	c	122	SER
33	c	142	MET
33	c	154	SER
33	c	172	ARG
34	d	29	ASP
34	d	30	VAL
34	d	33	LYS
34	d	58	ARG
34	d	133	ASN
34	d	149	GLU
34	d	181	GLU
34	d	192	ASP
35	e	18	ASP
35	e	44	ARG
35	e	51	LYS
35	e	130	THR
35	e	155	LYS
36	f	1	MET
36	f	31	GLU
36	f	33	ASP
36	f	58	HIS
36	f	62	MET
36	f	75	GLU
36	f	93	GLU
36	f	94	HIS
36	f	96	ILE
37	g	25	LYS
37	g	36	LYS
37	g	49	ARG
37	g	53	LYS
37	g	55	LYS
37	g	73	VAL
37	g	74	GLU
37	g	89	MET
37	g	95	ARG
37	g	111	ARG

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Mol	Chain	Res	Type
37	g	136	LYS
37	g	144	MET
37	g	146	GLU
38	h	10	MET
38	h	53	GLN
38	h	74	GLU
38	h	98	GLN
39	i	64	THR
39	i	104	ARG
39	i	126	SER
40	j	18	ILE
40	j	35	GLN
40	j	47	GLU
40	j	48	ARG
40	j	99	GLN
41	k	29	THR
41	k	34	THR
41	k	52	ARG
41	k	67	GLU
41	k	79	LYS
41	k	96	VAL
41	k	107	ASN
42	l	10	LYS
42	l	14	THR
42	l	98	VAL
42	l	101	SER
42	l	111	ASN
43	m	11	ASP
43	m	27	ARG
43	m	29	THR
43	m	75	MET
43	m	78	LYS
43	m	89	LEU
43	m	107	ARG
43	m	114	LYS
44	n	15	LYS
44	n	47	LYS
44	n	85	ARG
45	o	75	HIS
46	p	19	MET
46	p	47	ASP
46	p	53	ARG

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Mol	Chain	Res	Type
46	p	73	ASP
46	p	91	SER
47	q	24	VAL
47	q	28	ARG
47	q	69	SER
47	q	75	THR
47	q	81	GLU
48	r	27	ASP
48	r	36	ASN
48	r	38	LYS
49	s	20	GLU
49	s	35	SER
49	s	43	ASP
49	s	55	ARG
49	s	71	LEU
50	t	19	LYS
50	t	33	LYS
51	u	21	ARG
51	u	33	ARG
51	u	40	LYS

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

Mol	Chain	Res	Type
27	W	36	HIS
29	Y	14	HIS
33	c	28	GLN
36	f	94	HIS
37	g	29	HIS
40	j	58	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
31	a	1524/1544 (98%)	250 (16%)	0
5	A	2677/2918 (91%)	390 (14%)	30 (1%)
52	v	76/77 (98%)	25 (32%)	0
53	w	2/3 (66%)	1 (50%)	0
6	B	114/115 (99%)	16 (14%)	2 (1%)
All	All	4393/4657 (94%)	682 (15%)	32 (0%)

All (682) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	41	U
5	A	53	G
5	A	56	A
5	A	58	G
5	A	66	U
5	A	67	G
5	A	70	A
5	A	71	G
5	A	74	U
5	A	78	A
5	A	81	A
5	A	82	G
5	A	92	G
5	A	101	U
5	A	103	U
5	A	104	C
5	A	109	G
5	A	125	A
5	A	127	U
5	A	144	U
5	A	147	A
5	A	170	A
5	A	171	C
5	A	172	A
5	A	188	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	237	G
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	303	C
5	A	313	A
5	A	318	G

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Mol	Chain	Res	Type
5	A	325	G
5	A	331	G
5	A	332	A
5	A	333	U
5	A	336	U
5	A	340	G
5	A	347	A
5	A	348	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	395	G
5	A	403	A
5	A	410	G
5	A	423	G
5	A	428	A
5	A	455	C
5	A	479	A
5	A	480	G
5	A	490	G
5	A	493	G
5	A	495	G
5	A	504	A
5	A	507	U
5	A	508	C
5	A	530	C
5	A	531	A
5	A	532	G
5	A	535	G
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

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Mol	Chain	Res	Type
5	A	601	A
5	A	611	U
5	A	612	A
5	A	613	U
5	A	625	A
5	A	635	A
5	A	636	G
5	A	643	U
5	A	644	A
5	A	651	U
5	A	666	A
5	A	675	A
5	A	684	U
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	800	A
5	A	803	G
5	A	810	C
5	A	817	A
5	A	825	U
5	A	826	U
5	A	845	A
5	A	857	G
5	A	864	A
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

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Mol	Chain	Res	Type
5	A	993	A
5	A	1002	C
5	A	1006	A
5	A	1009	U
5	A	1010	C
5	A	1014	G
5	A	1023	G
5	A	1030	U
5	A	1031	G
5	A	1042	U
5	A	1043	A
5	A	1105	U
5	A	1106	C
5	A	1107	G
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	1140	A
5	A	1170	U
5	A	1173	G
5	A	1201	G
5	A	1242	A
5	A	1243	G
5	A	1244	U
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	1295	A
5	A	1296	A
5	A	1297	A
5	A	1327	G
5	A	1328	G
5	A	1332	G
5	A	1336	G

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Mol	Chain	Res	Type
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	1414	A
5	A	1422	A
5	A	1423	C
5	A	1424	G
5	A	1443	U
5	A	1447	G
5	A	1448	U
5	A	1453	U
5	A	1462	G
5	A	1511	A
5	A	1519	U
5	A	1520	A
5	A	1522	C
5	A	1523	A
5	A	1528	G
5	A	1530	A
5	A	1531	C
5	A	1532	U
5	A	1533	U
5	A	1534	G
5	A	1539	G
5	A	1541	G
5	A	1542	A
5	A	1543	A
5	A	1553	G
5	A	1557	U
5	A	1564	A
5	A	1567	A
5	A	1579	G
5	A	1580	C
5	A	1581	U
5	A	1583	C
5	A	1606	A
5	A	1645	U

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Mol	Chain	Res	Type
5	A	1646	U
5	A	1647	G
5	A	1672	G
5	A	1691	U
5	A	1697	G
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	1760	G
5	A	1769	A
5	A	1772	G
5	A	1776	A
5	A	1796	C
5	A	1797	A
5	A	1805	A
5	A	1807	G
5	A	1812	C
5	A	1817	A
5	A	1825	A
5	A	1845	G
5	A	1847	U
5	A	1849	A
5	A	1866	U
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	1886	A
5	A	1895	A
5	A	1897	A
5	A	1902	G
5	A	1923	A
5	A	1924	A
5	A	1925	G
5	A	1932	A
5	A	1934	A
5	A	1936	U

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Mol	Chain	Res	Type
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	2018	U
5	A	2019	C
5	A	2029	A
5	A	2039	C
5	A	2045	G
5	A	2051	C
5	A	2052	G
5	A	2056	A
5	A	2057	G
5	A	2065	7MG
5	A	2077	C
5	A	2186	G
5	A	2187	A
5	A	2194	A
5	A	2200	G
5	A	2207	G
5	A	2221	A
5	A	2234	G
5	A	2235	G
5	A	2264	A
5	A	2274	A
5	A	2279	U
5	A	2283	A
5	A	2284	A
5	A	2301	U
5	A	2302	C
5	A	2303	G
5	A	2304	G
5	A	2305	A
5	A	2308	U

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Mol	Chain	Res	Type
5	A	2316	A
5	A	2317	G
5	A	2321	A
5	A	2323	A
5	A	2341	A
5	A	2343	C
5	A	2346	C
5	A	2350	A
5	A	2355	C
5	A	2372	A
5	A	2375	G
5	A	2378	G
5	A	2379	G
5	A	2380	U
5	A	2381	C
5	A	2398	U
5	A	2399	C
5	A	2402	U
5	A	2420	C
5	A	2421	A
5	A	2423	C
5	A	2425	G
5	A	2426	A
5	A	2427	U
5	A	2429	A
5	A	2430	A
5	A	2431	A
5	A	2437	U
5	A	2444	A
5	A	2446	A
5	A	2455	A
5	A	2465	A
5	A	2466	G
5	A	2471	C
5	A	2473	U
5	A	2474	A
5	A	2475	U
5	A	2478	A
5	A	2487	U
5	A	2493	A
5	A	2494	C
5	A	2498	G

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Mol	Chain	Res	Type
5	A	2500	PSU
5	A	2503	C
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	2562	A
5	A	2563	G
5	A	2565	G
5	A	2568	A
5	A	2578	G
5	A	2581	U
5	A	2582	U
5	A	2598	A
5	A	2599	G
5	A	2605	U
5	A	2607	C
5	A	2609	U
5	A	2625	U
5	A	2635	A
5	A	2642	C
5	A	2650	A
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	2730	A
5	A	2731	G
5	A	2740	G
5	A	2744	A
5	A	2748	C
5	A	2754	A
5	A	2761	A
5	A	2774	A

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Mol	Chain	Res	Type
5	A	2776	A
5	A	2787	A
5	A	2793	U
5	A	2796	U
5	A	2797	G
5	A	2805	A
5	A	2816	G
5	A	2857	U
5	A	2863	A
5	A	2875	A
5	A	2876	C
5	A	2897	C
6	B	9	C
6	B	11	A
6	B	13	A
6	B	22	G
6	B	23	A
6	B	38	U
6	B	40	C
6	B	43	A
6	B	44	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	106	A
31	a	6	C
31	a	7	U
31	a	11	G
31	a	15	U
31	a	18	A
31	a	24	G
31	a	41	G
31	a	49	C
31	a	50	U
31	a	53	A
31	a	57	A
31	a	62	A
31	a	64	U
31	a	80	A

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Mol	Chain	Res	Type
31	a	81	G
31	a	83	U
31	a	84	U
31	a	85	G
31	a	86	C
31	a	87	U
31	a	89	C
31	a	90	C
31	a	91	G
31	a	97	A
31	a	105	A
31	a	117	U
31	a	126	A
31	a	127	U
31	a	157	A
31	a	184	A
31	a	185	C
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	207	G
31	a	208	G
31	a	209	A
31	a	239	A
31	a	241	U
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	297	G
31	a	302	A
31	a	317	A
31	a	324	C
31	a	340	A
31	a	341	C
31	a	344	G

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Mol	Chain	Res	Type
31	a	348	C
31	a	350	G
31	a	363	U
31	a	368	C
31	a	369	A
31	a	389	A
31	a	393	A
31	a	394	U
31	a	402	G
31	a	405	U
31	a	407	A
31	a	408	A
31	a	410	A
31	a	415	C
31	a	417	U
31	a	418	A
31	a	419	U
31	a	420	G
31	a	422	U
31	a	425	U
31	a	426	A
31	a	435	U
31	a	444	A
31	a	448	G
31	a	455	C
31	a	459	U
31	a	460	U
31	a	461	A
31	a	462	A
31	a	464	A
31	a	471	G
31	a	479	A
31	a	481	G
31	a	483	U
31	a	494	U
31	a	496	A
31	a	497	G
31	a	505	U
31	a	506	A
31	a	508	C
31	a	509	U
31	a	514	G

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Mol	Chain	Res	Type
31	a	518	G
31	a	521	G
31	a	522	C
31	a	527	G
31	a	528	U
31	a	532	A
31	a	539	G
31	a	540	U
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	573	C
31	a	615	C
31	a	623	G
31	a	630	G
31	a	639	A
31	a	650	A
31	a	662	A
31	a	684	A
31	a	685	G
31	a	700	G
31	a	720	U
31	a	721	G
31	a	728	G
31	a	731	G
31	a	739	G
31	a	752	G
31	a	774	A
31	a	778	A
31	a	790	U
31	a	791	A
31	a	812	A
31	a	814	C
31	a	816	A
31	a	817	U
31	a	839	U
31	a	840	U
31	a	841	G
31	a	864	G

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Mol	Chain	Res	Type
31	a	887	G
31	a	888	U
31	a	923	G
31	a	924	G
31	a	926	G
31	a	931	C
31	a	932	A
31	a	935	A
31	a	957	U
31	a	963	2MG
31	a	965	A
31	a	966	A
31	a	968	G
31	a	972	A
31	a	973	G
31	a	974	A
31	a	980	A
31	a	989	U
31	a	990	G
31	a	991	A
31	a	1001	A
31	a	1003	C
31	a	1022	U
31	a	1023	G
31	a	1025	C
31	a	1026	U
31	a	1027	U
31	a	1028	C
31	a	1030	G
31	a	1031	G
31	a	1043	A
31	a	1051	C
31	a	1052	A
31	a	1062	U
31	a	1072	U
31	a	1076	G
31	a	1082	U
31	a	1091	G
31	a	1092	U
31	a	1095	C
31	a	1097	C
31	a	1098	A

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Mol	Chain	Res	Type
31	a	1102	A
31	a	1122	U
31	a	1123	U
31	a	1124	G
31	a	1127	A
31	a	1134	C
31	a	1136	G
31	a	1140	G
31	a	1156	U
31	a	1157	G
31	a	1165	C
31	a	1166	A
31	a	1168	A
31	a	1179	G
31	a	1180	C
31	a	1181	G
31	a	1185	A
31	a	1189	C
31	a	1193	A
31	a	1194	A
31	a	1209	U
31	a	1210	A
31	a	1217	G
31	a	1224	A
31	a	1235	A
31	a	1253	U
31	a	1254	U
31	a	1255	G
31	a	1267	U
31	a	1276	A
31	a	1277	A
31	a	1278	U
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	1337	A
31	a	1342	U
31	a	1350	G

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Mol	Chain	Res	Type
31	a	1360	A
31	a	1361	U
31	a	1367	G
31	a	1378	U
31	a	1394	C
31	a	1395	A
31	a	1397	C
31	a	1414	G
31	a	1415	A
31	a	1416	G
31	a	1422	U
31	a	1426	C
31	a	1439	G
31	a	1443	A
31	a	1445	C
31	a	1449	A
31	a	1478	U
31	a	1484	G
31	a	1496	A
31	a	1500	A
31	a	1503	U
31	a	1504	A
31	a	1513	G
31	a	1526	G
31	a	1527	G
31	a	1528	A
52	v	7	G
52	v	8	4SU
52	v	9	A
52	v	10	G
52	v	16	U
52	v	17	U
52	v	18	G
52	v	19	G
52	v	20	H2U
52	v	21	U
52	v	22	A
52	v	34	U
52	v	47	G
52	v	48	U
52	v	49	C
52	v	50	A

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Mol	Chain	Res	Type
52	v	56	PSU
52	v	57	C
52	v	58	A
52	v	59	A
52	v	60	G
52	v	62	C
52	v	64	C
52	v	69	U
52	v	76	C
53	w	2	U

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	84	U
5	A	91	A
5	A	256	C
5	A	324	A
5	A	365	U
5	A	368	C
5	A	371	G
5	A	424	G
5	A	478	A
5	A	507	U
5	A	782	G
5	A	799	G
5	A	1106	C
5	A	1127	U
5	A	1172	U
5	A	1179	G
5	A	1267	A
5	A	1268	C
5	A	1296	A
5	A	1335	U
5	A	1337	A
5	A	1519	U
5	A	1733	U
5	A	1844	A
5	A	1880	G
5	A	1923	A
5	A	1924	A
5	A	2379	G

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Mol	Chain	Res	Type
5	A	2419	U
5	A	2525	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	$\#\|Z\| > 2$
31	UR3	a	1495	31	19,22,23	2.91	6 (31%)	26,32,35	1.30	2 (7%)
31	4OC	a	1399	31	20,23,24	3.18	8 (40%)	26,32,35	0.90	1 (3%)
5	PSU	A	2453	5	18,21,22	1.07	1 (5%)	22,30,33	1.82	6 (27%)
52	5MU	v	55	52	19,22,23	0.42	0	28,32,35	0.45	0
5	PSU	A	2576	5	18,21,22	1.10	1 (5%)	22,30,33	1.79	5 (22%)
5	2MG	A	2441	5	18,26,27	1.13	2 (11%)	16,38,41	0.84	1 (6%)
31	2MG	a	1204	31	18,26,27	1.16	2 (11%)	16,38,41	0.92	1 (6%)
52	H2U	v	20	52	18,21,22	0.57	0	21,30,33	1.30	3 (14%)
31	7MG	a	524	31	22,26,27	1.20	1 (4%)	29,39,42	0.81	1 (3%)
5	7MG	A	2065	5	22,26,27	1.18	1 (4%)	29,39,42	0.80	1 (3%)
5	PSU	A	2601	5	18,21,22	1.09	1 (5%)	22,30,33	1.79	5 (22%)
31	PSU	a	513	31	18,21,22	1.08	1 (5%)	22,30,33	1.78	4 (18%)
5	OMG	A	2247	5	18,26,27	1.10	2 (11%)	19,38,41	0.91	1 (5%)
5	OMU	A	2548	5	19,22,23	3.08	8 (42%)	26,31,34	1.70	5 (19%)
31	2MG	a	963	31	18,26,27	1.17	2 (11%)	16,38,41	0.96	1 (6%)
5	PSU	A	952	5	18,21,22	1.07	1 (5%)	22,30,33	1.77	4 (18%)
52	4SU	v	8	52	18,21,22	4.31	8 (44%)	26,30,33	2.21	5 (19%)
31	MA6	a	1516	31	18,26,27	1.03	2 (11%)	19,38,41	3.50	2 (10%)
5	5MU	A	1935	5	19,22,23	0.41	0	28,32,35	0.54	0
31	MA6	a	1515	31	18,26,27	1.01	2 (11%)	19,38,41	3.36	2 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
52	PSU	v	56	52	18,21,22	1.09	1 (5%)	22,30,33	1.78	5 (22%)
5	2MA	A	2499	5	17,25,26	2.53	5 (29%)	17,37,40	1.36	2 (11%)
5	PSU	A	2500	5	18,21,22	1.09	1 (5%)	22,30,33	1.78	5 (22%)
5	6MZ	A	2026	5	18,25,26	1.86	3 (16%)	16,36,39	3.40	4 (25%)
31	5MC	a	964	31	18,22,23	0.57	0	26,32,35	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	UR3	a	1495	31	-	0/7/25/26	0/2/2/2
31	4OC	a	1399	31	-	2/9/29/30	0/2/2/2
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
52	5MU	v	55	52	-	4/7/25/26	0/2/2/2
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	0/5/27/28	0/3/3/3
31	2MG	a	1204	31	-	0/5/27/28	0/3/3/3
52	H2U	v	20	52	-	5/7/38/39	0/2/2/2
31	7MG	a	524	31	-	1/7/37/38	0/3/3/3
5	7MG	A	2065	5	-	3/7/37/38	0/3/3/3
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
31	PSU	a	513	31	-	0/7/25/26	0/2/2/2
5	OMG	A	2247	5	-	1/5/27/28	0/3/3/3
5	OMU	A	2548	5	-	3/9/27/28	0/2/2/2
31	2MG	a	963	31	-	1/5/27/28	0/3/3/3
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
52	4SU	v	8	52	-	4/7/25/26	0/2/2/2
31	MA6	a	1516	31	-	1/7/29/30	0/3/3/3
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
31	MA6	a	1515	31	-	0/7/29/30	0/3/3/3
52	PSU	v	56	52	-	3/7/25/26	0/2/2/2
5	2MA	A	2499	5	-	3/3/25/26	0/3/3/3
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	1/5/27/28	0/3/3/3
31	5MC	a	964	31	-	0/7/25/26	0/2/2/2

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	8	4SU	C2-N1	9.33	1.53	1.38
52	v	8	4SU	C4-N3	8.63	1.46	1.37
5	A	2499	2MA	C2-N3	7.38	1.46	1.31
5	A	2548	OMU	C2-N1	7.27	1.50	1.38
31	a	1495	UR3	C2-N1	7.04	1.48	1.38
52	v	8	4SU	C2-N3	7.02	1.50	1.38
31	a	1399	4OC	C4-N3	6.89	1.44	1.32
52	v	8	4SU	C5-C4	6.83	1.51	1.42
31	a	1495	UR3	C6-C5	6.80	1.50	1.35
5	A	2548	OMU	C2-N3	6.71	1.49	1.38
5	A	2026	6MZ	C6-N6	6.57	1.45	1.35
52	v	8	4SU	C6-C5	6.49	1.50	1.35
31	a	1399	4OC	C6-C5	6.27	1.49	1.35
31	a	1399	4OC	C2-N3	6.12	1.48	1.36
5	A	2548	OMU	C6-C5	5.81	1.48	1.35
31	a	1495	UR3	C2-N3	5.79	1.50	1.39
5	A	2499	2MA	C4-N3	5.21	1.50	1.37
31	a	1399	4OC	C4-N4	4.96	1.46	1.35
5	A	2065	7MG	C5-N7	4.96	1.41	1.35
31	a	524	7MG	C5-N7	4.95	1.41	1.35
52	v	8	4SU	C4-S4	-4.39	1.60	1.68
31	a	1399	4OC	C2-N1	4.24	1.49	1.40
5	A	2548	OMU	C4-N3	4.23	1.46	1.38
31	a	1399	4OC	C5-C4	3.89	1.49	1.40
5	A	2500	PSU	C6-C5	3.58	1.39	1.35
52	v	56	PSU	C6-C5	3.58	1.39	1.35
5	A	2601	PSU	C6-C5	3.57	1.39	1.35
5	A	2576	PSU	C6-C5	3.56	1.39	1.35
31	a	513	PSU	C6-C5	3.53	1.39	1.35
5	A	952	PSU	C6-C5	3.51	1.39	1.35
5	A	2453	PSU	C6-C5	3.45	1.39	1.35
31	a	1495	UR3	C6-N1	3.40	1.46	1.38
31	a	1399	4OC	C6-N1	3.35	1.46	1.38
31	a	963	2MG	C8-N7	-3.11	1.29	1.35
5	A	2441	2MG	C8-N7	-3.00	1.29	1.35
5	A	2548	OMU	C6-N1	2.97	1.45	1.38
31	a	1204	2MG	C8-N7	-2.96	1.30	1.35
5	A	2499	2MA	C6-N1	2.89	1.44	1.38
5	A	2548	OMU	O4-C4	-2.86	1.18	1.24
52	v	8	4SU	C6-N1	2.71	1.44	1.38
5	A	2247	OMG	C8-N7	-2.71	1.30	1.35
31	a	1399	4OC	O2-C2	-2.64	1.18	1.23
31	a	1516	MA6	C5-C4	-2.61	1.34	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2499	2MA	C5-C4	-2.60	1.36	1.43
31	a	1516	MA6	C2-N3	2.59	1.36	1.32
31	a	1515	MA6	C5-C4	-2.56	1.34	1.40
52	v	8	4SU	O2-C2	-2.55	1.18	1.23
5	A	2548	OMU	C5-C4	2.55	1.49	1.43
31	a	1515	MA6	C2-N3	2.53	1.36	1.32
5	A	2499	2MA	C2-N1	2.49	1.44	1.36
5	A	2026	6MZ	C5-C4	-2.40	1.34	1.40
31	a	963	2MG	C5-C6	-2.36	1.42	1.47
31	a	1495	UR3	C4-N3	2.35	1.46	1.40
31	a	1204	2MG	C5-C6	-2.33	1.42	1.47
5	A	2548	OMU	O2-C2	-2.32	1.18	1.23
31	a	1495	UR3	C5-C4	2.28	1.49	1.43
5	A	2026	6MZ	C2-N3	2.25	1.35	1.32
5	A	2441	2MG	C5-C6	-2.24	1.42	1.47
5	A	2247	OMG	C5-C6	-2.21	1.42	1.47

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	1516	MA6	N1-C6-N6	-13.97	102.35	117.06
31	a	1515	MA6	N1-C6-N6	-13.38	102.98	117.06
5	A	2026	6MZ	C1'-N9-C4	-11.41	106.59	126.64
52	v	8	4SU	C4-N3-C2	-7.68	119.88	127.34
5	A	2026	6MZ	N3-C2-N1	-5.64	119.87	128.68
31	a	1516	MA6	N3-C2-N1	-5.53	120.03	128.68
31	a	1515	MA6	N3-C2-N1	-5.45	120.16	128.68
52	v	8	4SU	C5-C4-N3	5.34	119.64	114.69
5	A	2548	OMU	C4-N3-C2	-5.19	119.73	126.58
31	a	1495	UR3	C4-N3-C2	-4.74	120.10	124.56
31	a	513	PSU	C4-N3-C2	-4.71	119.56	126.34
5	A	952	PSU	C4-N3-C2	-4.66	119.62	126.34
5	A	2601	PSU	C4-N3-C2	-4.65	119.63	126.34
5	A	2453	PSU	C4-N3-C2	-4.62	119.69	126.34
5	A	2453	PSU	N1-C2-N3	4.60	120.34	115.13
5	A	2500	PSU	C4-N3-C2	-4.58	119.73	126.34
52	v	56	PSU	C4-N3-C2	-4.55	119.78	126.34
5	A	2601	PSU	N1-C2-N3	4.53	120.26	115.13
5	A	952	PSU	N1-C2-N3	4.50	120.23	115.13
52	v	56	PSU	N1-C2-N3	4.49	120.22	115.13
31	a	513	PSU	N1-C2-N3	4.48	120.21	115.13
5	A	2500	PSU	N1-C2-N3	4.47	120.20	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	2576	PSU	C4-N3-C2	-4.39	120.01	126.34
5	A	2576	PSU	N1-C2-N3	4.38	120.10	115.13
5	A	2548	OMU	N3-C2-N1	3.85	120.00	114.89
52	v	8	4SU	N3-C2-N1	3.80	119.94	114.89
52	v	20	H2U	C5-C4-N3	-3.68	112.51	116.65
5	A	2499	2MA	C5-C6-N1	3.64	120.29	114.02
5	A	2026	6MZ	C2-N1-C6	3.38	119.49	116.59
52	v	8	4SU	C5-C4-S4	-3.33	120.17	124.47
5	A	2548	OMU	C5-C4-N3	3.31	119.78	114.84
5	A	2499	2MA	C8-N7-C5	2.93	108.57	102.99
5	A	2500	PSU	O2-C2-N1	-2.84	119.67	122.79
52	v	20	H2U	O2-C2-N1	2.81	126.63	123.11
5	A	2548	OMU	O4-C4-C5	-2.76	120.31	125.16
5	A	2576	PSU	O2-C2-N1	-2.75	119.77	122.79
5	A	2247	OMG	O6-C6-C5	2.60	129.46	124.37
31	a	513	PSU	O2-C2-N1	-2.59	119.94	122.79
5	A	952	PSU	O2-C2-N1	-2.59	119.94	122.79
52	v	56	PSU	O2-C2-N1	-2.56	119.97	122.79
5	A	2453	PSU	O2-C2-N1	-2.53	120.01	122.79
5	A	2576	PSU	O4'-C1'-C2'	2.45	108.60	105.14
31	a	1399	4OC	C6-C5-C4	2.44	119.94	116.96
5	A	2601	PSU	O2-C2-N1	-2.38	120.17	122.79
31	a	1204	2MG	O6-C6-C5	2.37	129.00	124.37
5	A	2453	PSU	C6-C5-C4	2.28	119.79	118.20
52	v	56	PSU	C6-N1-C2	-2.22	120.41	122.68
5	A	2441	2MG	O6-C6-C5	2.22	128.71	124.37
5	A	2576	PSU	C6-N1-C2	-2.21	120.42	122.68
52	v	56	PSU	O4'-C1'-C2'	2.21	108.26	105.14
31	a	524	7MG	C5-C4-N9	2.21	109.21	106.35
52	v	20	H2U	O2-C2-N3	-2.18	117.44	121.50
5	A	2548	OMU	O2-C2-N1	-2.17	119.90	122.79
5	A	2453	PSU	C6-N1-C2	-2.16	120.47	122.68
31	a	963	2MG	O6-C6-C5	2.16	128.59	124.37
5	A	2065	7MG	C4-C5-N7	2.13	108.49	105.53
5	A	2601	PSU	C6-C5-C4	2.10	119.66	118.20
5	A	2453	PSU	O4'-C1'-C2'	2.09	108.09	105.14
5	A	2601	PSU	C6-N1-C2	-2.07	120.56	122.68
5	A	2500	PSU	C6-C5-C4	2.07	119.65	118.20
31	a	1495	UR3	C6-N1-C2	-2.06	119.94	121.79
5	A	2026	6MZ	C9-N6-C6	-2.05	121.11	122.87
5	A	952	PSU	C6-N1-C2	-2.03	120.60	122.68
5	A	2500	PSU	C6-N1-C2	-2.03	120.61	122.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a	513	PSU	C6-C5-C4	2.02	119.61	118.20
52	v	8	4SU	O2-C2-N1	-2.01	120.11	122.79

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
52	v	20	H2U	C3'-C4'-C5'-O5'
52	v	55	5MU	C2'-C1'-N1-C2
52	v	55	5MU	C2'-C1'-N1-C6
52	v	56	PSU	C2'-C1'-C5-C4
5	A	2247	OMG	C1'-C2'-O2'-CM2
5	A	2499	2MA	O4'-C4'-C5'-O5'
5	A	2548	OMU	C3'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C2
31	a	1399	4OC	O4'-C4'-C5'-O5'
5	A	2548	OMU	O4'-C4'-C5'-O5'
52	v	20	H2U	O4'-C4'-C5'-O5'
52	v	56	PSU	C3'-C4'-C5'-O5'
5	A	2499	2MA	C3'-C4'-C5'-O5'
52	v	20	H2U	C2'-C1'-N1-C6
31	a	1399	4OC	C3'-C4'-C5'-O5'
52	v	56	PSU	O4'-C4'-C5'-O5'
52	v	8	4SU	O4'-C1'-N1-C6
52	v	8	4SU	C4'-C5'-O5'-P
5	A	2499	2MA	C4'-C5'-O5'-P
5	A	2065	7MG	O4'-C4'-C5'-O5'
31	a	963	2MG	C4'-C5'-O5'-P
52	v	20	H2U	C4'-C5'-O5'-P
52	v	55	5MU	O4'-C1'-N1-C6
31	a	524	7MG	C3'-C4'-C5'-O5'
52	v	55	5MU	O4'-C1'-N1-C2
52	v	8	4SU	O4'-C1'-N1-C2
31	a	1516	MA6	C5-C6-N6-C9
5	A	2065	7MG	C4'-C5'-O5'-P
52	v	8	4SU	C2'-C1'-N1-C2
5	A	2026	6MZ	O4'-C4'-C5'-O5'
5	A	2065	7MG	C3'-C4'-C5'-O5'
5	A	2548	OMU	C3'-C2'-O2'-CM2

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	3.16	18 (40%)	52,72,72	2.46	18 (34%)
55	80P	a	1602	56	44,45,45	3.65	20 (45%)	52,72,72	2.53	17 (32%)
55	80P	a	1603	56	44,45,45	3.65	22 (50%)	52,72,72	2.45	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	-	15/22/87/87	0/5/5/5
55	80P	a	1602	56	-	6/22/87/87	0/5/5/5
55	80P	a	1603	56	-	11/22/87/87	0/5/5/5

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1602	80P	C08-C09	13.05	1.63	1.52
55	a	1603	80P	C08-C09	12.24	1.62	1.52
55	a	1601	80P	C08-C09	10.38	1.61	1.52
55	a	1602	80P	C08-C21	9.28	1.61	1.53
55	a	1603	80P	C08-C21	8.91	1.61	1.53
55	a	1603	80P	C04-N03	7.72	1.55	1.47
55	a	1602	80P	C04-N03	7.07	1.54	1.47
55	a	1601	80P	C08-C21	7.05	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1603	80P	C06-C07	6.74	1.63	1.45
55	a	1602	80P	C06-C07	6.61	1.62	1.45
55	a	1603	80P	C06-C36	6.45	1.60	1.47
55	a	1602	80P	C06-C36	6.39	1.60	1.47
55	a	1601	80P	C04-N03	6.34	1.53	1.47
55	a	1601	80P	C04-C05	5.92	1.63	1.51
55	a	1601	80P	C06-C07	5.64	1.60	1.45
55	a	1601	80P	C06-C36	5.42	1.58	1.47
55	a	1603	80P	C04-C05	5.24	1.62	1.51
55	a	1602	80P	C08-C07	5.12	1.61	1.55
55	a	1602	80P	C04-C05	5.06	1.62	1.51
55	a	1603	80P	C08-C07	4.63	1.61	1.55
55	a	1601	80P	C18-C19	4.15	1.63	1.52
55	a	1602	80P	C18-C19	4.10	1.63	1.52
55	a	1603	80P	C18-C19	4.01	1.63	1.52
55	a	1603	80P	C18-C17	3.87	1.57	1.51
55	a	1603	80P	C15-C26	3.78	1.57	1.52
55	a	1602	80P	C12-C11	3.68	1.55	1.46
55	a	1601	80P	C18-C17	3.65	1.57	1.51
55	a	1602	80P	C10-C11	3.62	1.55	1.47
55	a	1602	80P	C22-C16	3.47	1.59	1.51
55	a	1602	80P	C18-C17	3.40	1.56	1.51
55	a	1603	80P	C22-C16	3.38	1.59	1.51
55	a	1603	80P	C12-C11	3.35	1.55	1.46
55	a	1601	80P	C16-C17	3.33	1.46	1.40
55	a	1603	80P	C10-C11	3.31	1.54	1.47
55	a	1601	80P	C08-C07	3.31	1.59	1.55
55	a	1601	80P	C22-C16	3.29	1.58	1.51
55	a	1602	80P	C16-C17	3.26	1.45	1.40
55	a	1603	80P	C16-C17	3.10	1.45	1.40
55	a	1602	80P	C12-C13	3.04	1.46	1.41
55	a	1601	80P	C12-C11	3.01	1.54	1.46
55	a	1603	80P	C19-C10	2.96	1.54	1.51
55	a	1602	80P	C15-C26	2.79	1.56	1.52
55	a	1603	80P	C30-C26	2.76	1.57	1.54
55	a	1601	80P	C19-C10	2.72	1.54	1.51
55	a	1602	80P	C36-N38	2.71	1.40	1.33
55	a	1601	80P	C36-N38	2.71	1.40	1.33
55	a	1603	80P	C12-C13	2.70	1.45	1.41
55	a	1601	80P	C12-C13	2.68	1.45	1.41
55	a	1603	80P	C36-N38	2.65	1.40	1.33
55	a	1603	80P	C16-C15	2.62	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	a	1601	80P	C15-C26	2.57	1.55	1.52
55	a	1601	80P	C10-C11	2.49	1.52	1.47
55	a	1603	80P	C40-N03	2.38	1.54	1.47
55	a	1603	80P	C14-C15	2.32	1.43	1.39
55	a	1602	80P	C19-C10	2.30	1.54	1.51
55	a	1602	80P	C14-C15	2.12	1.43	1.39
55	a	1603	80P	C20-C19	2.10	1.58	1.53
55	a	1601	80P	C40-N03	2.09	1.53	1.47
55	a	1602	80P	C16-C15	2.05	1.43	1.40
55	a	1602	80P	O39-C05	2.04	1.39	1.33

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	a	1602	80P	C11-C10-C09	9.40	126.24	118.80
55	a	1603	80P	C11-C10-C09	8.53	125.55	118.80
55	a	1601	80P	C11-C10-C09	8.02	125.14	118.80
55	a	1602	80P	C08-C21-C04	5.71	119.44	111.64
55	a	1603	80P	C36-C06-C07	-5.48	114.49	120.97
55	a	1603	80P	C12-C11-C10	5.06	127.14	118.53
55	a	1602	80P	C12-C11-C10	4.93	126.92	118.53
55	a	1601	80P	C12-C11-C10	4.88	126.85	118.53
55	a	1603	80P	C08-C21-C04	4.87	118.30	111.64
55	a	1601	80P	C36-C06-C07	-4.78	115.31	120.97
55	a	1602	80P	O33-C09-C10	4.76	130.41	123.90
55	a	1603	80P	O33-C09-C10	4.60	130.20	123.90
55	a	1601	80P	O33-C09-C10	4.58	130.17	123.90
55	a	1602	80P	O33-C09-C08	-4.54	106.80	113.37
55	a	1601	80P	C08-C21-C04	4.52	117.82	111.64
55	a	1602	80P	C36-C06-C07	-4.44	115.71	120.97
55	a	1603	80P	O33-C09-C08	-4.39	107.02	113.37
55	a	1601	80P	O33-C09-C08	-4.14	107.37	113.37
55	a	1601	80P	C12-C17-C16	-4.09	117.13	120.75
55	a	1601	80P	C13-C12-C17	4.07	123.63	119.05
55	a	1603	80P	C13-C12-C17	3.67	123.19	119.05
55	a	1602	80P	C13-C12-C17	3.62	123.13	119.05
55	a	1602	80P	C12-C17-C16	-3.52	117.63	120.75
55	a	1601	80P	C18-C17-C16	3.43	126.92	120.94
55	a	1601	80P	C13-C12-C11	-3.26	116.69	121.47
55	a	1601	80P	O32-C11-C10	-3.22	115.84	120.78
55	a	1603	80P	C12-C17-C16	-3.20	117.91	120.75
55	a	1603	80P	O32-C11-C10	-3.20	115.87	120.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	a	1602	80P	O32-C11-C10	-3.11	116.01	120.78
55	a	1603	80P	C13-C12-C11	-3.07	116.97	121.47
55	a	1602	80P	F25-C22-C16	3.04	119.54	112.34
55	a	1601	80P	F23-C22-C16	2.97	119.38	112.34
55	a	1602	80P	C13-C12-C11	-2.89	117.24	121.47
55	a	1601	80P	C21-C04-N03	-2.86	104.45	111.30
55	a	1602	80P	C18-C17-C16	2.82	125.85	120.94
55	a	1601	80P	C14-C13-C12	-2.78	117.71	120.93
55	a	1603	80P	F25-C22-C16	2.76	118.89	112.34
55	a	1603	80P	C14-C13-C12	-2.69	117.81	120.93
55	a	1603	80P	O32-C11-C12	-2.65	116.98	121.99
55	a	1602	80P	O37-C36-N38	-2.61	116.78	122.88
55	a	1602	80P	O32-C11-C12	-2.60	117.07	121.99
55	a	1602	80P	C14-C13-C12	-2.59	117.92	120.93
55	a	1603	80P	O37-C36-N38	-2.57	116.88	122.88
55	a	1601	80P	O37-C36-N38	-2.53	116.95	122.88
55	a	1601	80P	O32-C11-C12	-2.47	117.31	121.99
55	a	1603	80P	C15-C26-N27	2.42	116.16	112.06
55	a	1601	80P	C21-C08-C07	-2.42	108.27	111.05
55	a	1603	80P	C18-C17-C16	2.37	125.07	120.94
55	a	1603	80P	C08-C07-C06	2.32	119.44	115.75
55	a	1602	80P	C08-C07-C06	2.17	119.21	115.75
55	a	1601	80P	F25-C22-C16	2.17	117.48	112.34
55	a	1603	80P	F23-C22-C16	2.15	117.44	112.34
55	a	1602	80P	F23-C22-C16	2.11	117.34	112.34

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	a	1601	80P	C05-C04-N03-C01
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	1601	80P	C41-C40-N03-C04
55	a	1603	80P	C05-C04-N03-C01
55	a	1603	80P	C05-C04-N03-C40
55	a	1603	80P	C16-C15-C26-C30
55	a	1603	80P	C41-C40-N03-C01
55	a	1603	80P	C41-C40-N03-C04
55	a	1602	80P	C41-C40-N03-C01
55	a	1601	80P	C21-C04-N03-C40

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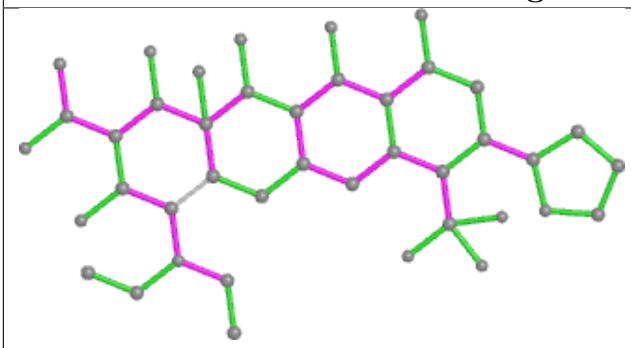
Mol	Chain	Res	Type	Atoms
55	a	1603	80P	C21-C04-N03-C01
55	a	1603	80P	C21-C04-N03-C40
55	a	1602	80P	C41-C40-N03-C04
55	a	1603	80P	C02-C01-N03-C04
55	a	1603	80P	C07-C06-C36-O37
55	a	1601	80P	C07-C06-C36-N38
55	a	1603	80P	C16-C15-C26-N27
55	a	1601	80P	C21-C04-N03-C01
55	a	1601	80P	C15-C16-C22-F23
55	a	1602	80P	C15-C16-C22-F25
55	a	1601	80P	C14-C15-C26-C30
55	a	1601	80P	C41-C40-N03-C01
55	a	1601	80P	C15-C16-C22-F24
55	a	1601	80P	C17-C16-C22-F23
55	a	1602	80P	C15-C16-C22-F24
55	a	1602	80P	C15-C16-C22-F23
55	a	1601	80P	C15-C16-C22-F25
55	a	1601	80P	C17-C16-C22-F25
55	a	1602	80P	C17-C16-C22-F23
55	a	1603	80P	C14-C15-C26-N27

There are no ring outliers.

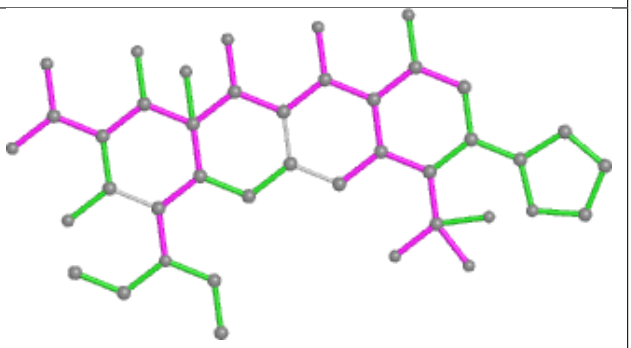
No monomer is involved in short contacts.

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.

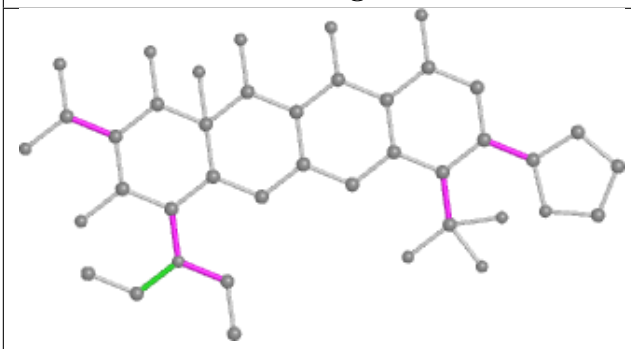
Ligand 80P a 1601



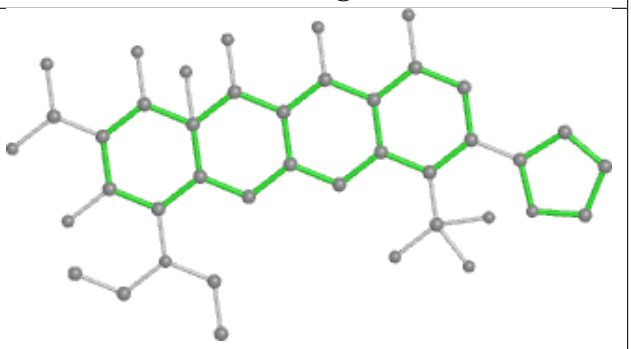
Bond lengths



Bond angles

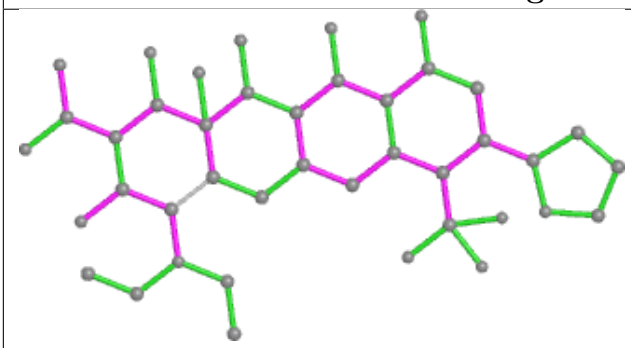


Torsions

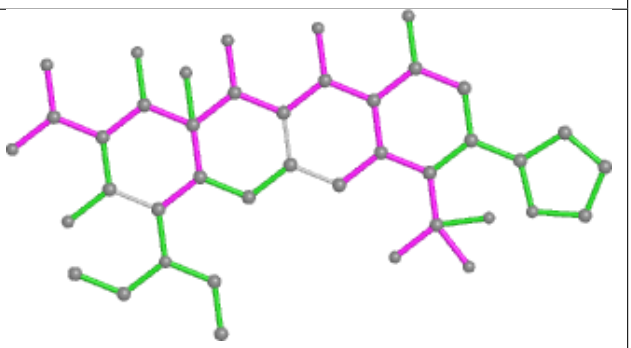


Rings

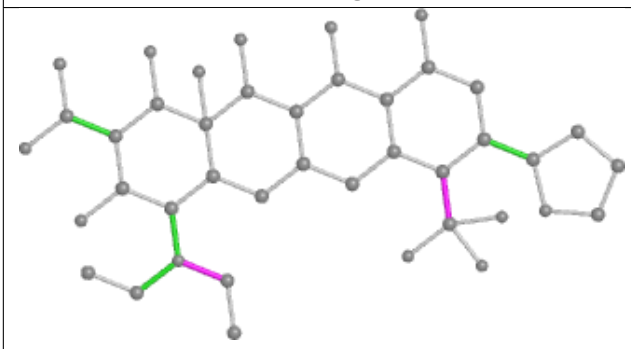
Ligand 80P a 1602



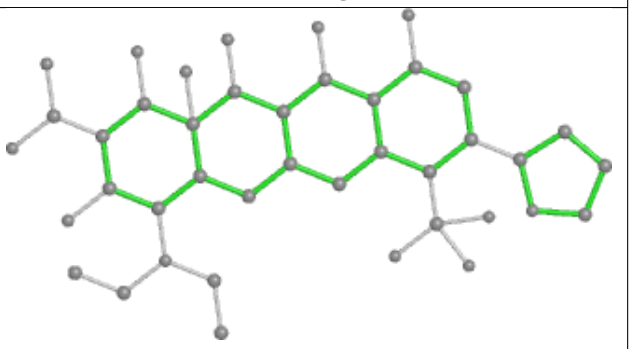
Bond lengths



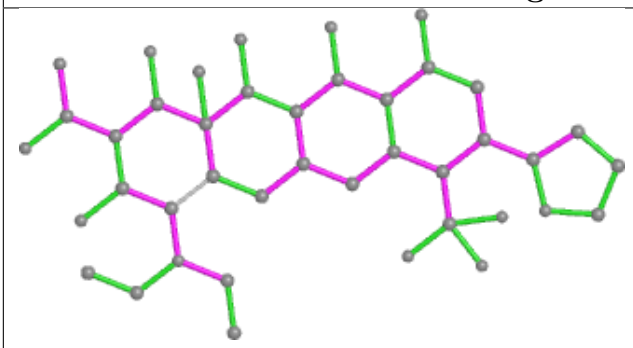
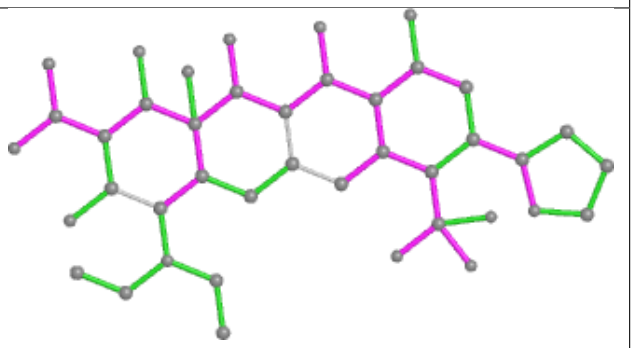
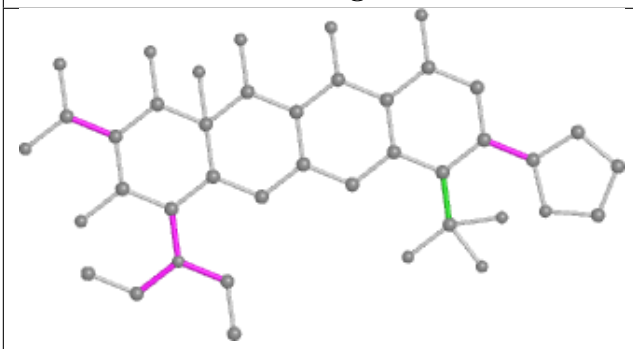
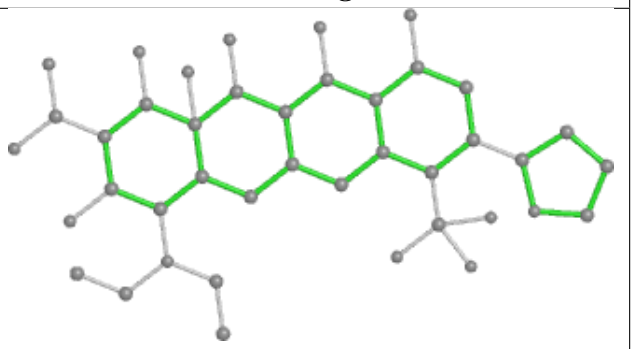
Bond angles



Torsions



Rings

Ligand 80P a 1603	
 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.

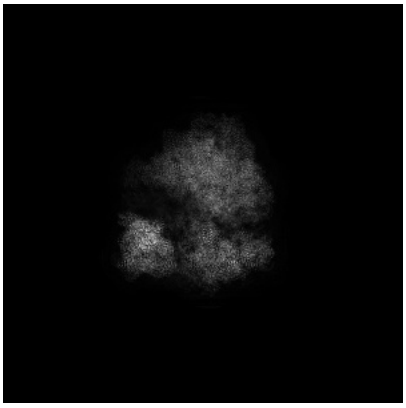
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-24739. These allow visual inspection of the internal detail of the map and identification of artifacts.

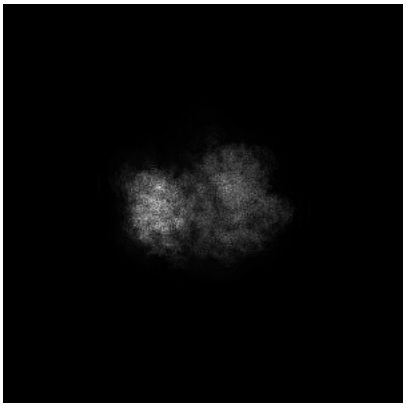
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

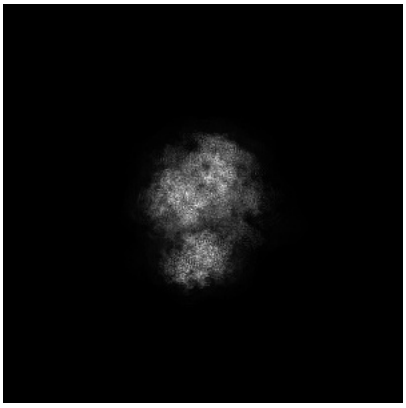
6.1.1 Primary map



X



Y

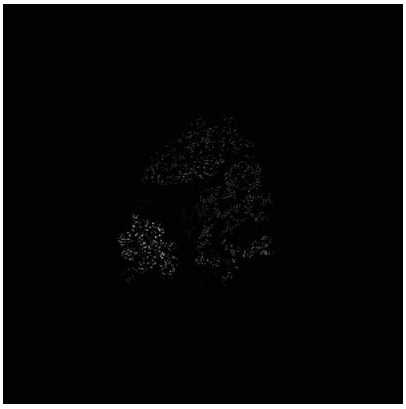


Z

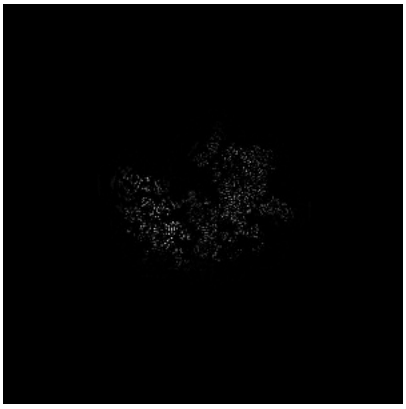
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

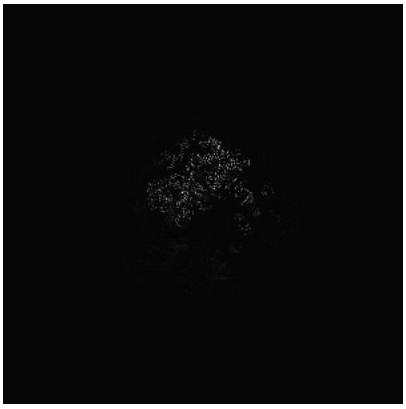
6.2.1 Primary map



X Index: 256



Y Index: 256



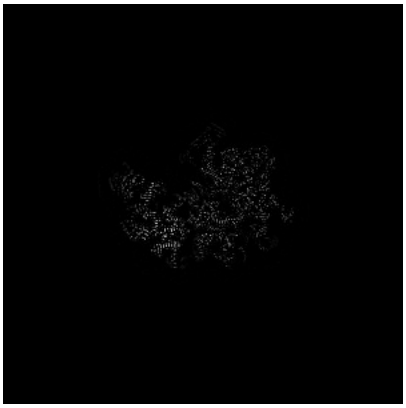
Z Index: 256

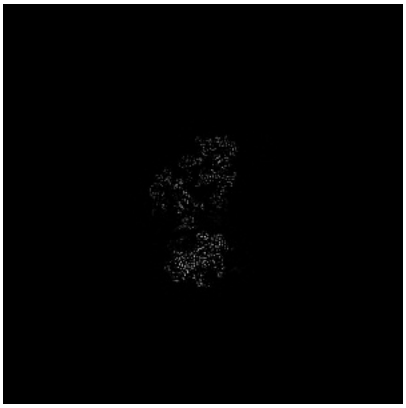
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 248

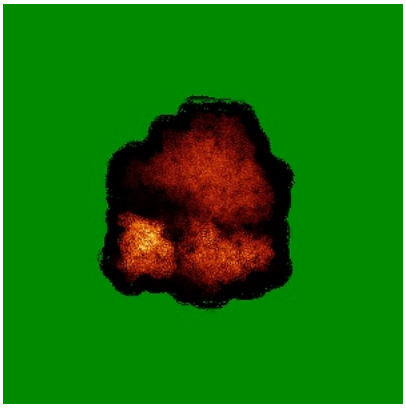

Y Index: 267

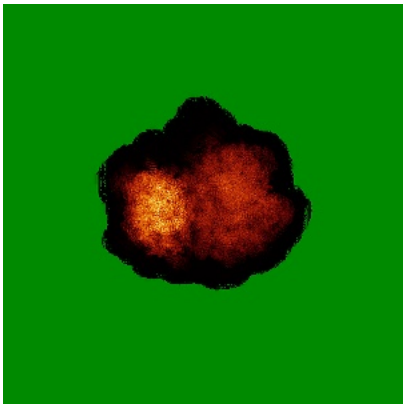

Z Index: 200

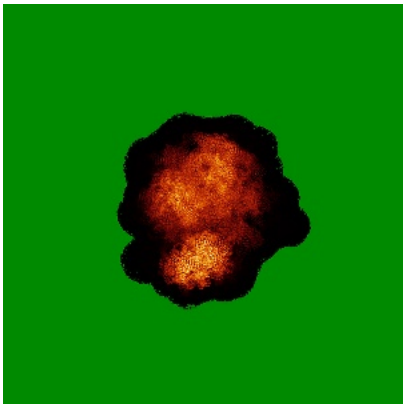
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X


Y


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

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

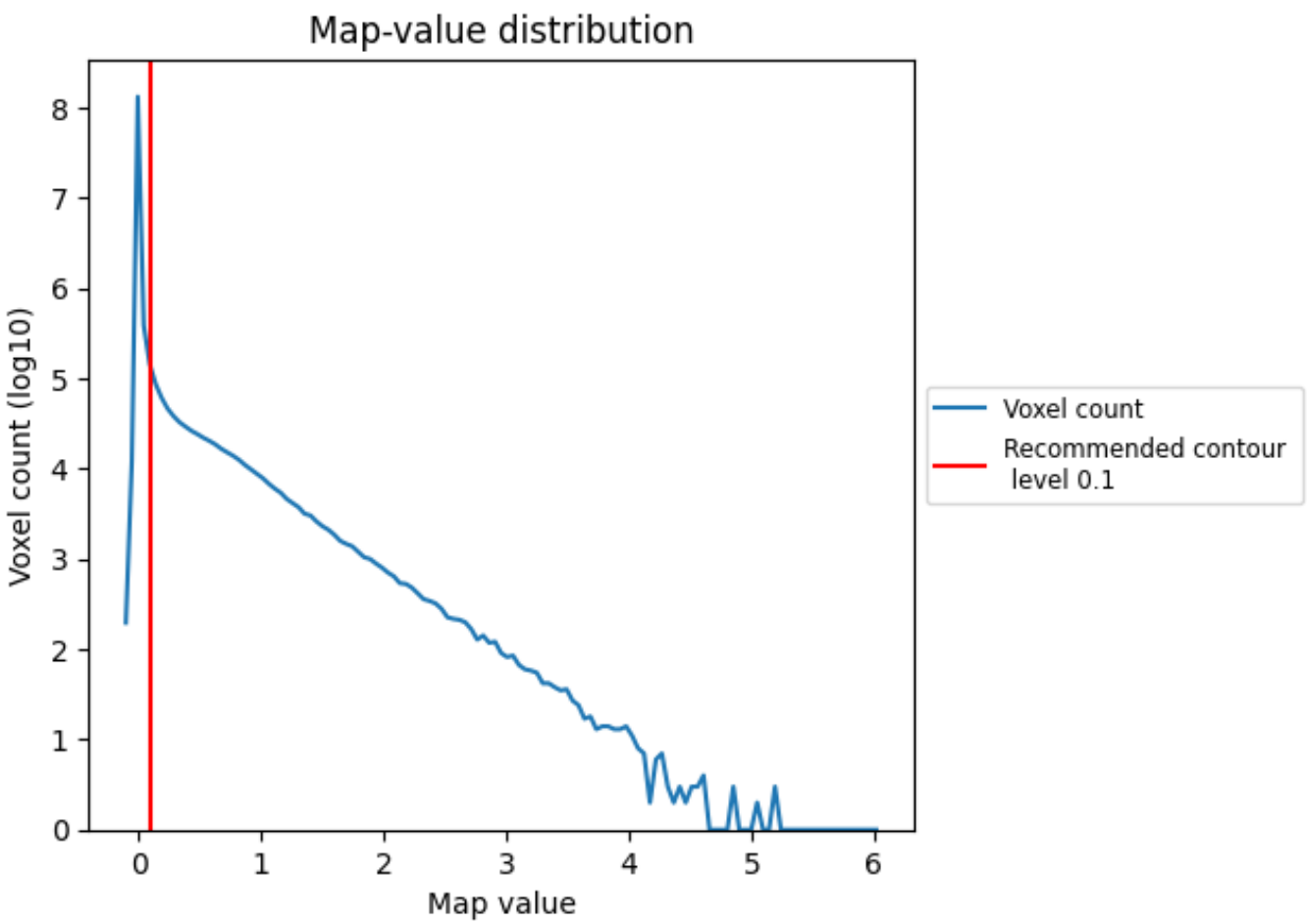
6.6 Mask visualisation (i)

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

7 Map analysis (i)

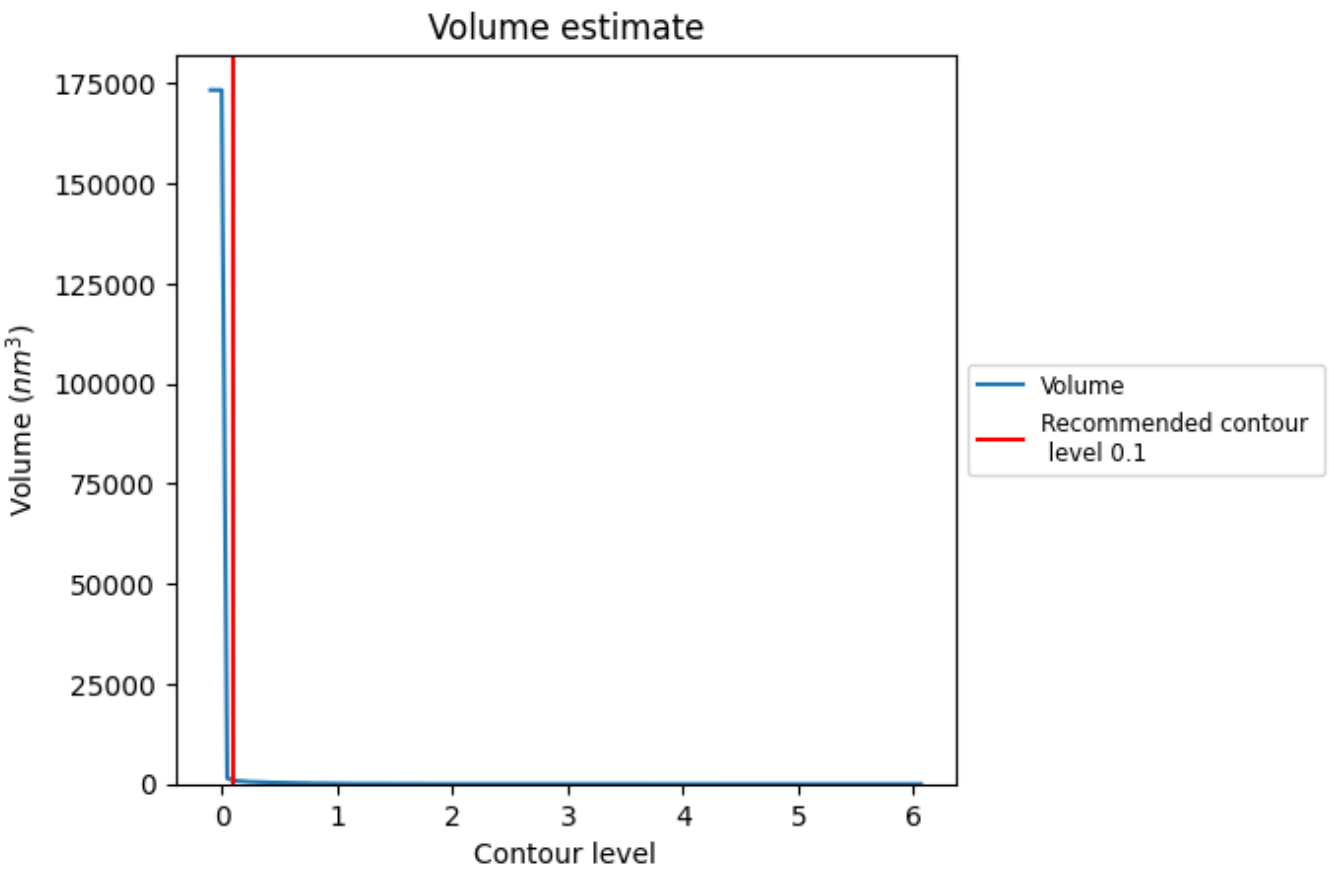
This section contains the results of statistical analysis of the map.

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.

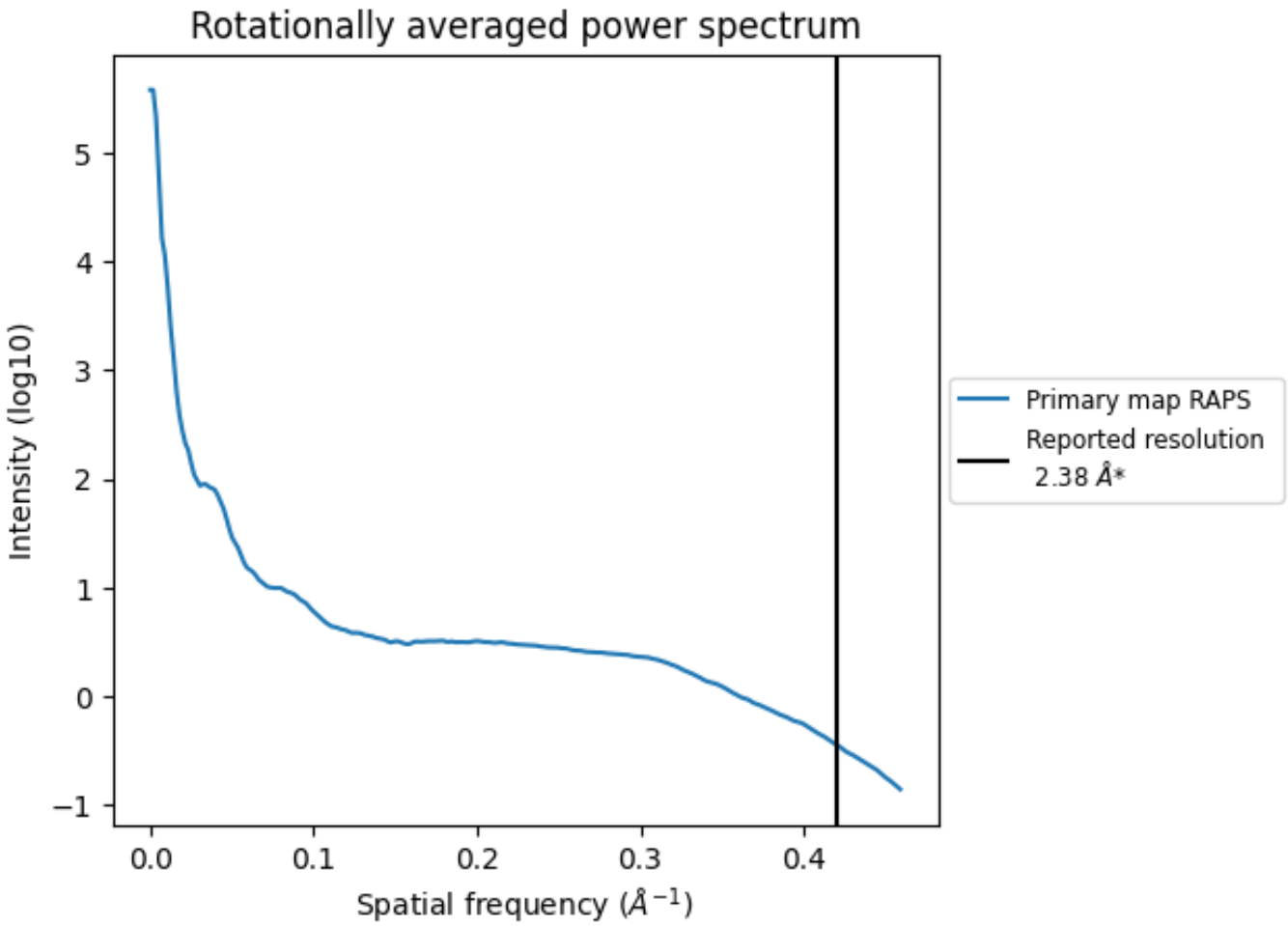
7.2 Volume estimate (i)



The volume at the recommended contour level is 894 nm^3; this corresponds to an approximate mass of 807 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 0.420 Å^{-1}

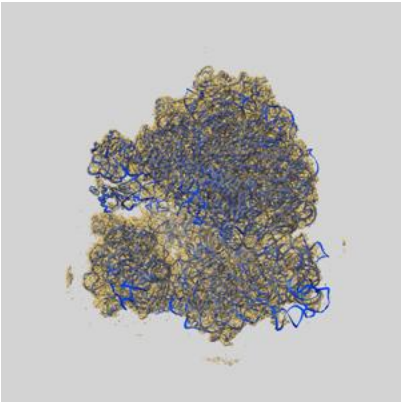
8 Fourier-Shell correlation (i)

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

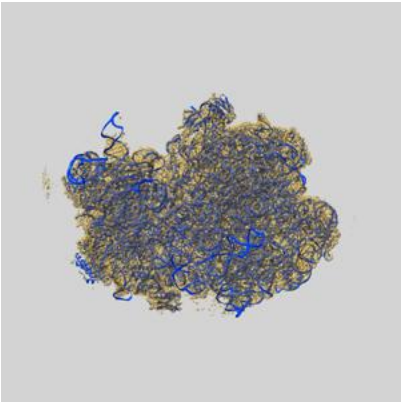
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24739 and PDB model 7RYG. Per-residue inclusion information can be found in section 3 on page 14.

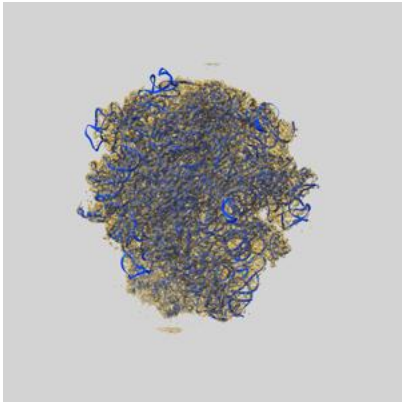
9.1 Map-model overlay (i)



X



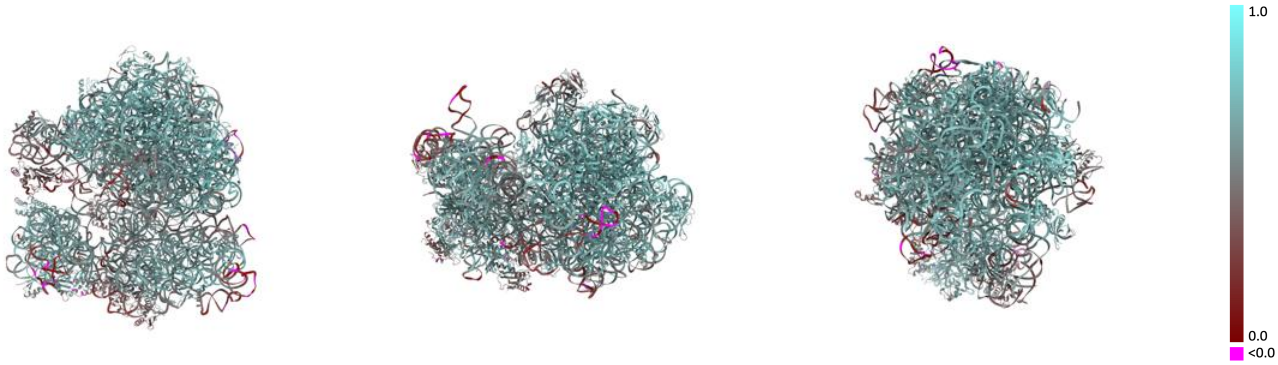
Y



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.

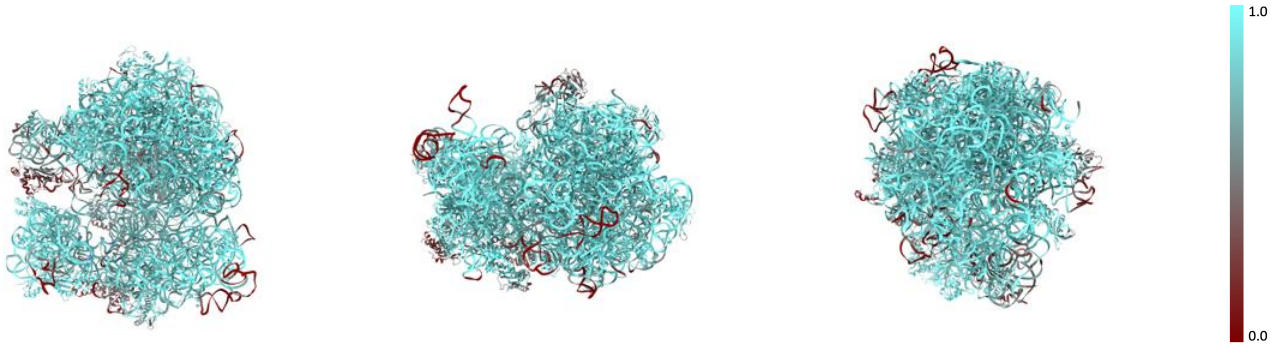
9.2 Q-score mapped to coordinate model (i)



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.

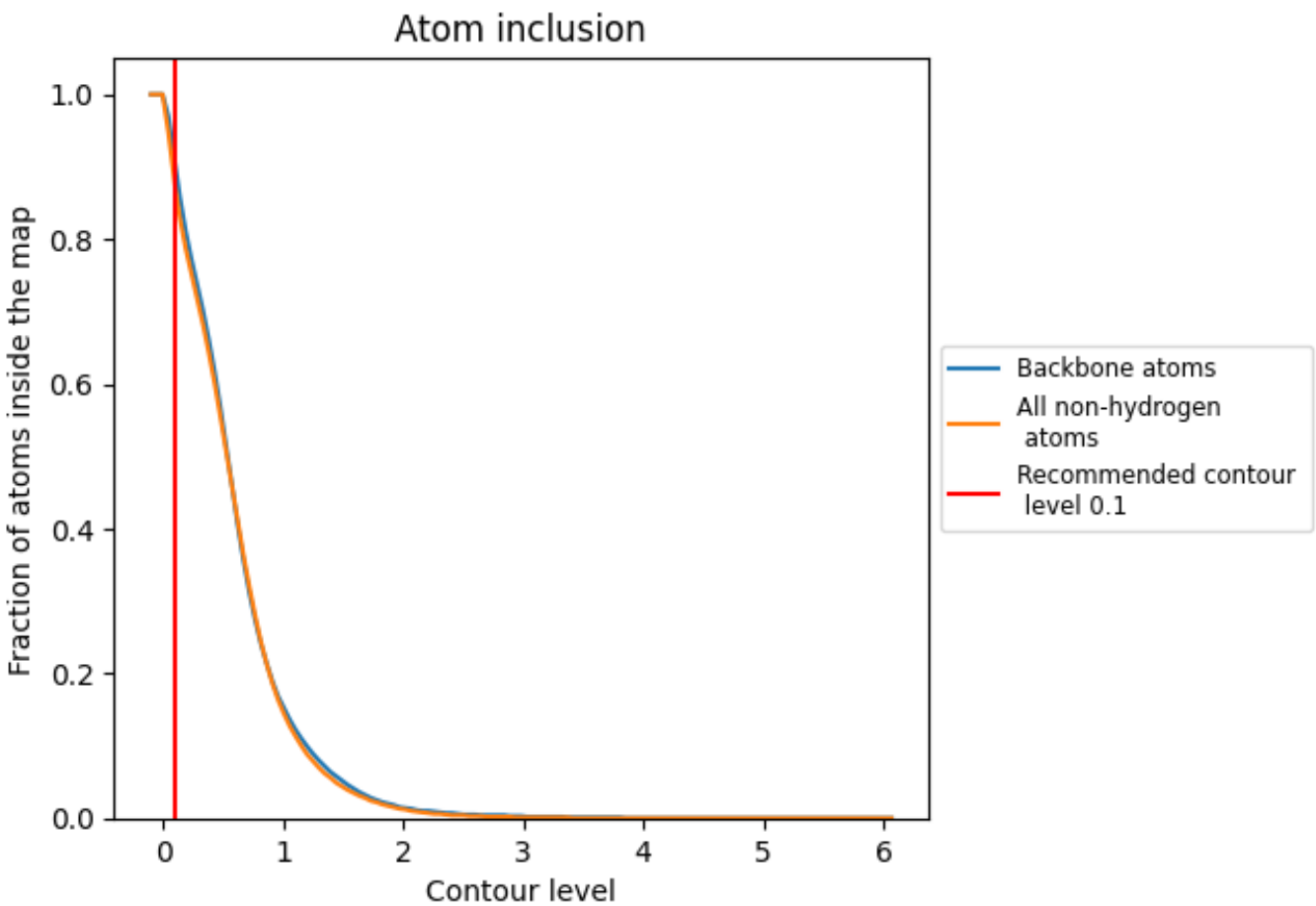
9.3 Atom inclusion mapped to coordinate model (i)



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, 90% of all backbone atoms, 87% 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	0.8730	0.5960
0	0.8750	0.6340
1	0.9800	0.7360
2	0.9840	0.7180
3	0.8250	0.5900
A	0.9090	0.6260
B	0.7270	0.4930
C	0.9620	0.6900
D	0.9660	0.7220
E	0.9270	0.6880
F	0.2510	0.3340
G	0.5580	0.4820
H	0.5590	0.4720
I	0.9720	0.7180
J	0.9620	0.6810
K	0.9620	0.7100
L	0.9290	0.6660
M	0.9900	0.7330
N	0.7760	0.5340
O	0.9320	0.6700
P	0.9930	0.7300
Q	0.9540	0.7020
R	0.9630	0.7150
S	0.8810	0.6560
T	0.8310	0.6180
U	0.8690	0.6280
V	0.9420	0.7080
W	0.9310	0.6860
X	0.7540	0.5610
Y	0.9400	0.6990
Z	0.9300	0.6850
a	0.8850	0.5580
b	0.3370	0.3450
c	0.9650	0.6220
d	0.6890	0.4320

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Chain	Atom inclusion	Q-score
e	0.9530	0.6220
f	0.6590	0.4130
g	0.8270	0.4880
h	0.9660	0.6680
i	0.9860	0.6630
j	0.9510	0.6200
k	0.5700	0.3900
l	0.7560	0.5290
m	0.9860	0.6370
n	0.9690	0.6610
o	0.9680	0.6290
p	0.9580	0.6670
q	0.9310	0.6120
r	0.8350	0.5090
s	0.9860	0.6560
t	0.9640	0.6410
u	0.2100	0.3140
v	0.4330	0.2890
w	0.8310	0.3420