



Full wwPDB EM Validation Report ⓘ

Nov 1, 2022 – 08:22 PM EDT

PDB ID : 5KCS
EMDB ID : EMD-8238
Title : Cryo-EM structure of the Escherichia coli 70S ribosome in complex with antibiotic Evernimycin, mRNA, TetM and P-site tRNA at 3.9Å resolution
Authors : Arenz, S.; Juette, M.F.; Graf, M.; Nguyen, F.; Huter, P.; Polikanov, Y.S.; Blanchard, S.C.; Wilson, D.N.
Deposited on : 2016-06-06
Resolution : 3.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

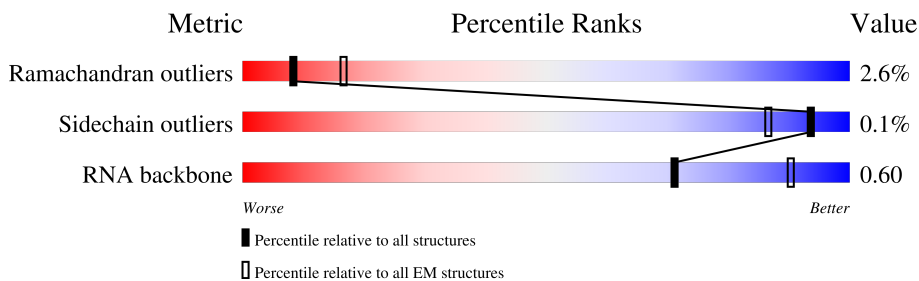
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1A	2904	9% (Upper red bar) 84% (Green) 15% (Yellow)
2	1B	120	8% (Upper red bar) 87% (Green) 13% (Yellow)
3	1D	273	15% (Upper red bar) 98% (Green) .. (Grey)
4	1E	209	25% (Upper red bar) 100% (Green)
5	1F	201	37% (Upper red bar) 99% (Green) . (Grey)
6	1G	179	61% (Upper red bar) 97% (Green) .. (Grey)
7	1H	177	46% (Upper red bar) 98% (Green) .. (Grey)
8	1L	121	56% (Upper red bar) 57% (Green) 43% (Grey)

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Mol	Chain	Length	Quality of chain
9	1I	149	92% 97%
10	1J	165	78% 76% 21%
11	1K	142	97% 94% 5%
12	1N	142	21% 99%
13	1O	123	27% 96%
14	1P	144	37% 96%
15	1Q	136	10% 96%
16	1R	127	17% 93% 6%
17	1S	117	52% 97%
18	1T	115	31% 99%
19	1U	118	15% 99%
20	1V	103	36% 96%
21	1W	110	21% 99%
22	1X	100	29% 91% 7%
23	1Y	104	47% 96%
24	1Z	94	38% 100%
25	10	85	18% 88% 12%
26	11	78	27% 99%
27	12	63	44% 100%
28	13	59	20% 98%
29	14	70	81% 93% 6%
30	15	57	23% 96%
31	16	55	91% 89% 9%
32	17	46	13% 100%
33	18	65	22% 97%

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Mol	Chain	Length	Quality of chain
34	19	38	13% 97%
35	1a	1539	15% 88% 12%
36	1b	241	78% 88% 10%
37	1c	233	46% 88% 12%
38	1d	206	73% 98%
39	1e	167	40% 89% 5% 6%
40	1f	135	31% 70% 26%
41	1g	179	54% 82% 16%
42	1h	130	31% 98%
43	1i	130	68% 93% 5%
44	1j	103	71% 89% 6% 5%
45	1k	129	49% 88% 10%
46	1l	124	64% 94% 6%
47	1m	118	49% 94%
48	1n	101	43% 92% 7%
49	1o	89	36% 94%
50	1p	82	50% 99%
51	1q	84	48% 92% 5%
52	1r	75	32% 83% 13%
53	1s	92	36% 85% 14%
54	1t	87	44% 98%
55	1u	71	86% 82% 8% 8%
56	1v	60	7% 13% 85%
57	1w	639	28% 95% 5%
58	1x	77	12% 82% 13% 5%

2 Entry composition i

There are 59 unique types of molecules in this entry. The entry contains 148945 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1A	2900	62276	27788	11459	20129	2900	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1A	1847	G	A	conflict	GB 802133627

- Molecule 2 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	1B	120	2570	1144	468	838	120	0	0

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1D	271	2082	1288	423	364	7	0	0

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1E	209	1565	979	288	294	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	1F	201	1552	974	283	290	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1G	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1H	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L7/L12.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	1L	69	Total	C	N	O	0	0
			276	138	69	69		

- Molecule 9 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 10 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 11 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1N	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 13 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1O	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 14 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1P	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 15 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1Q	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1R	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	1S	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1T	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	1U	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	1V	103	816	516	153	145	2	0	0

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	1W	110	857	532	166	156	3	0	0

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	1X	93	738	466	139	131	2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
23	1Y	102	779	492	146	141	0	0

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	1Z	94	753	479	137	134	3	0	0

- Molecule 25 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	10	75	575	356	116	102	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	11	77	625	388	129	106	2	0	0

- Molecule 27 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	12	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 28 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	13	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	14	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	15	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 31 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	16	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 32 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	17	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 33 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	18	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 34 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	19	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 35 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1a	1539	Total	C	N	O	P	0	0
			33029	14738	6052	10700	1539		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	1d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	1j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	1k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	1l	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	1m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1n	100	Total	C	N	O	S	0	0
			794	495	164	132	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	1o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	1p	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	1q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
52	1r	65	Total	C	N	O	0	0
			504	317	96	91		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1t	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 55 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	1u	65	Total	C	N	O	S	0	0
			495	307	100	87	1		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	1v	9	Total	C	N	O	P	0	0
			192	86	35	62	9		

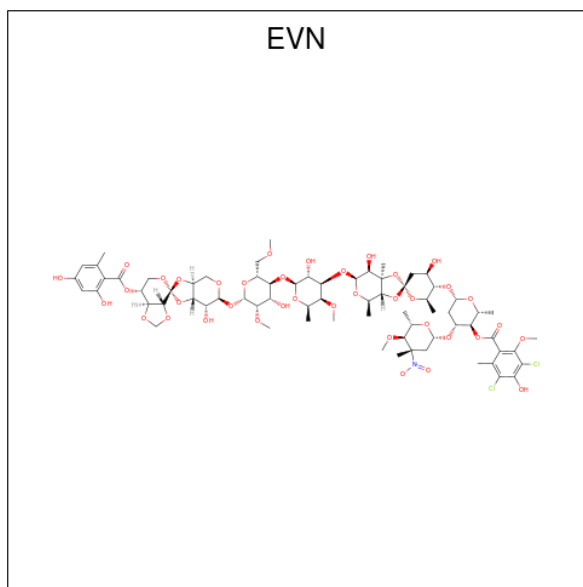
- Molecule 57 is a protein called Tetracycline resistance protein TetM from transposon Tn916.

Mol	Chain	Residues	Atoms				AltConf	Trace
57	1w	639	Total	C	N	O	0	0
			2590	1308	640	642		

- Molecule 58 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	1x	73	Total	C	N	O	P	0	0
			1567	699	285	510	73		

- Molecule 59 is (2R,3R,4R,6S)-6-{{(2R,3aR,4R,4'R,5'S,6S,6'R,7S,7aR)-6-{{(2S,3R,4R,5S,6R)-2-{{(2R,3S,4S,5S,6S)-6-{{(2R,3aS,3a'R,6S,7R,7'R,7aS,7a'S)-7'-[(2,4-dihydroxy-6-methylbenzoyl)oxy]-7-hydroxyoctahydro-4H-2,4'-spirobi[[1,3]dioxolo[4,5-c]pyran]-6-yl}oxy)-4-hydroxy-5-methoxy-2-(methoxymethyl)tetrahydro-2H-pyran-3-yl}oxy}-3-hydroxy-5-methoxy-6-methyltetrahydro-2H-pyran-4-yl}oxy}-4',7-dihydroxy-4,6',7a-trimethyloctahydro-4H-spiro[1,3-dioxolo[4,5-c]pyran-2,2'-pyran]-5'-yl}oxy}-4-{{(2R,4S,5R,6S)-5-methoxy-4,6-dimethyl-4-nitrotetrahydro-2H-pyran-2-yl}oxy}-2-methyltetrahydro-2H-pyran-3-yl 3,5-dichloro-4-hydroxy-2-methoxy-6-methylbenzoate (non-preferred name) (three-letter code: EVN) (formula: C₇₀H₉₇Cl₂NO₃₈).

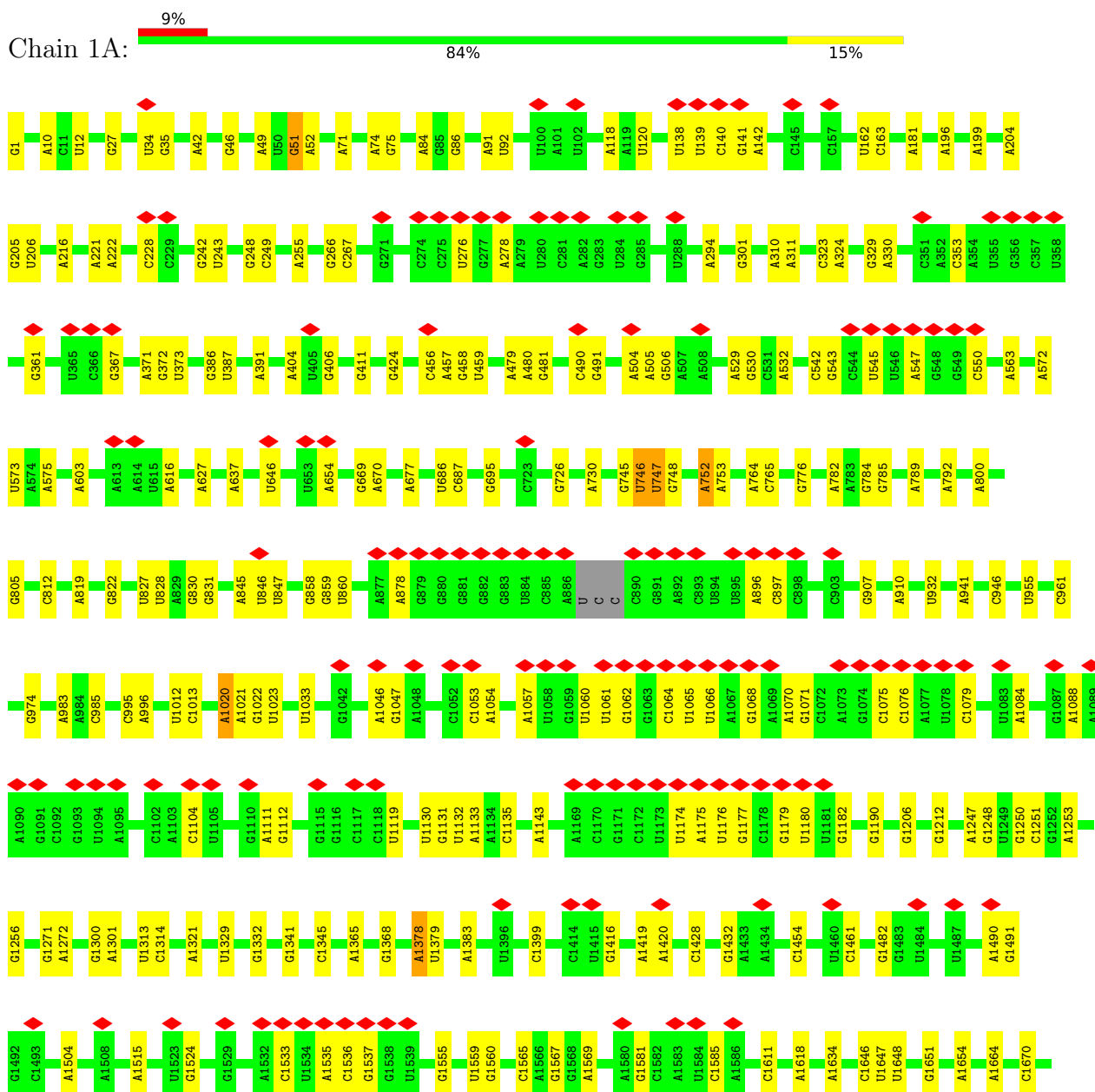


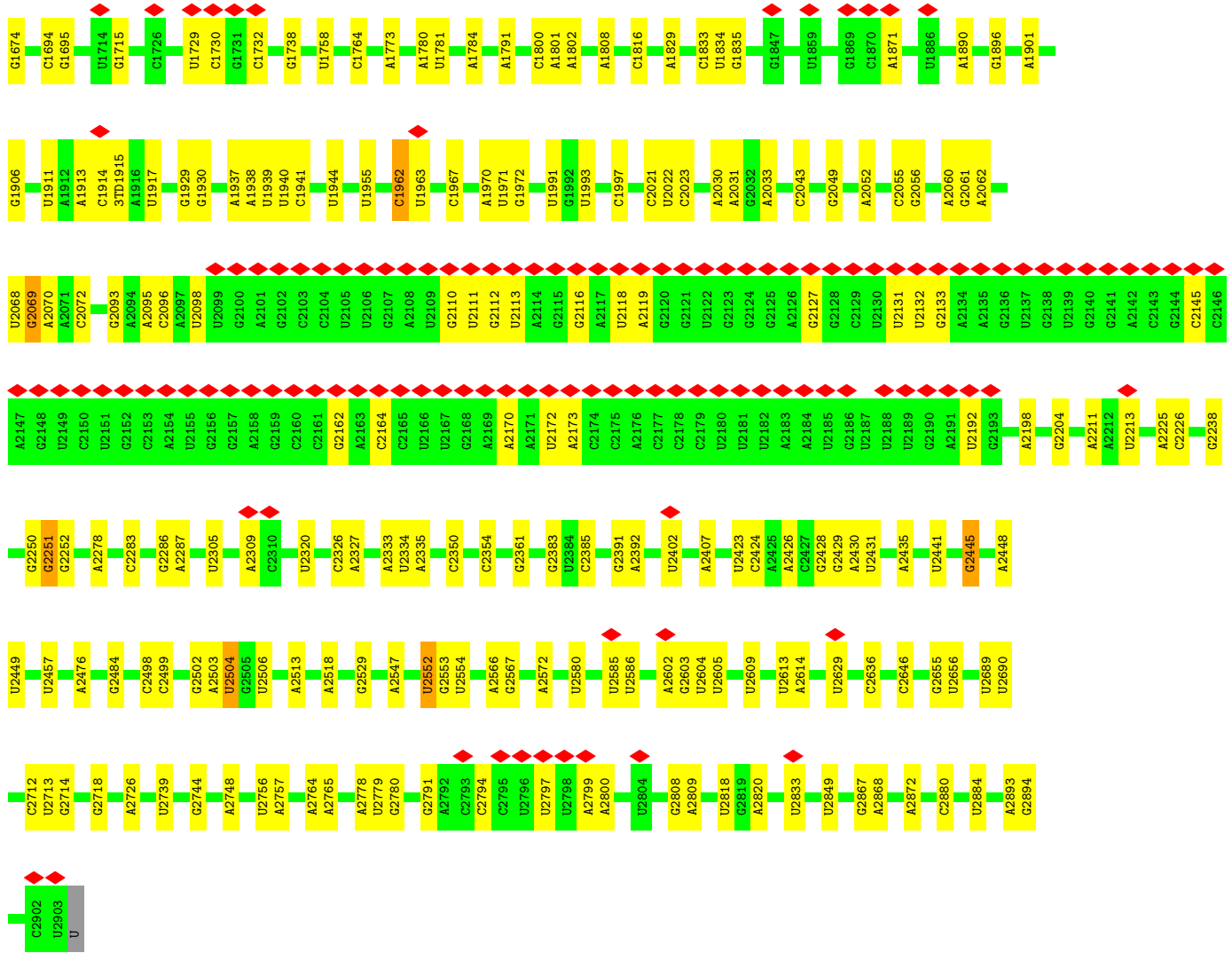
Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Cl	N		O
59	1A	1	111	70	2	1	38	0

3 Residue-property plots i

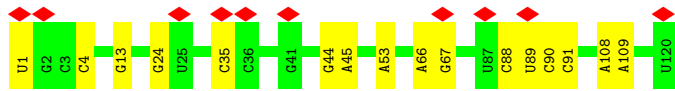
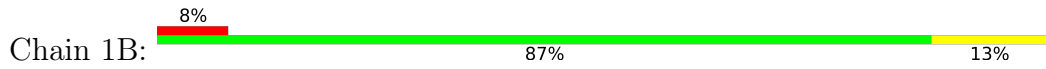
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 23S Ribosomal RNA

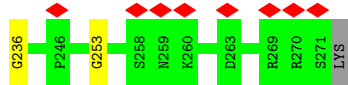
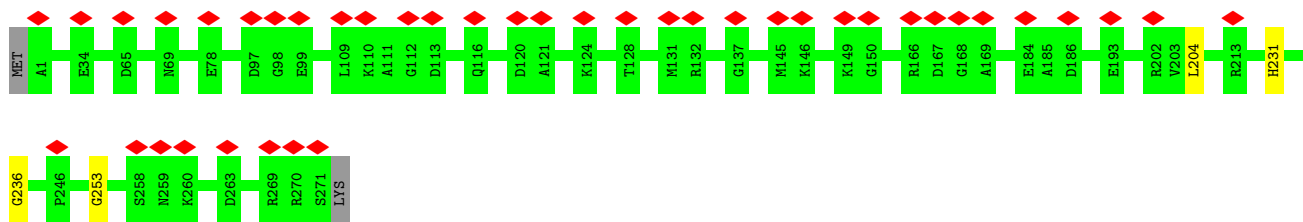




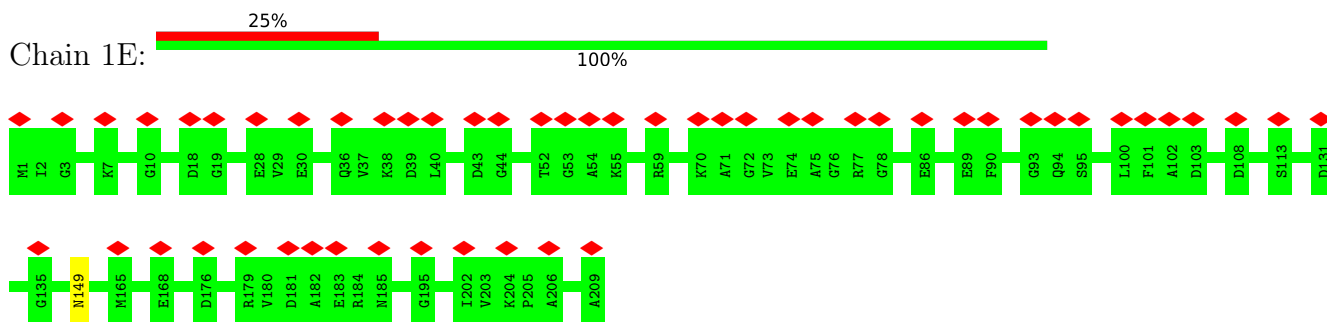
• Molecule 2: 5S Ribosomal RNA



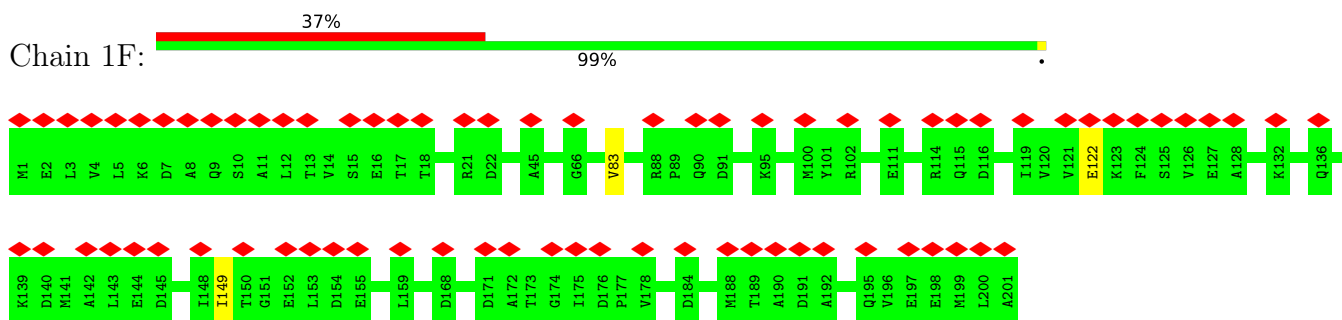
• Molecule 3: 50S ribosomal protein L2



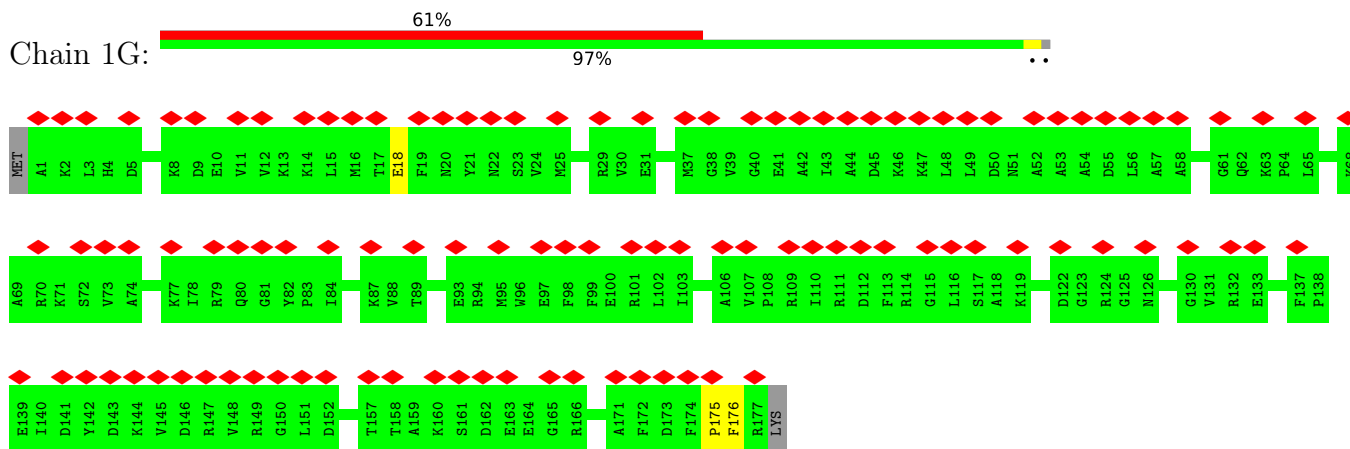
- Molecule 4: 50S ribosomal protein L3



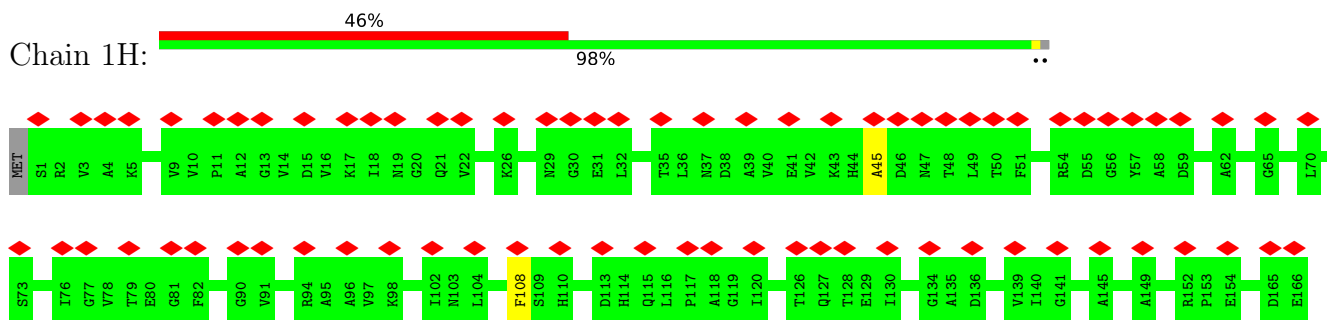
- Molecule 5: 50S ribosomal protein L4

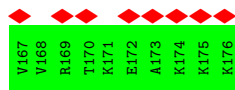


- Molecule 6: 50S ribosomal protein L5

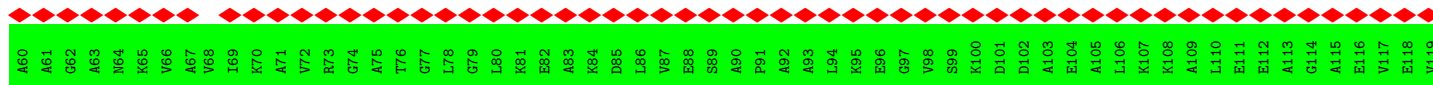
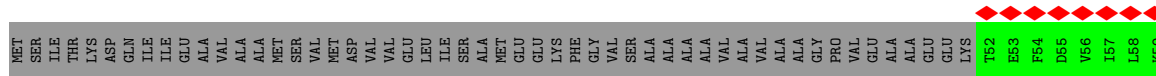


- Molecule 7: 50S ribosomal protein L6

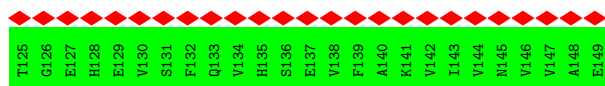
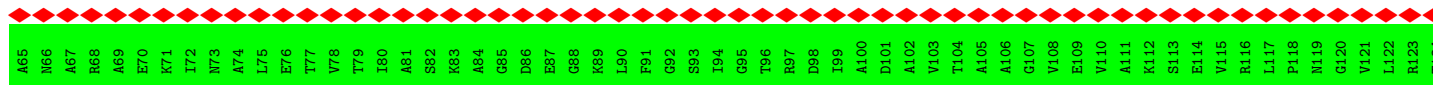
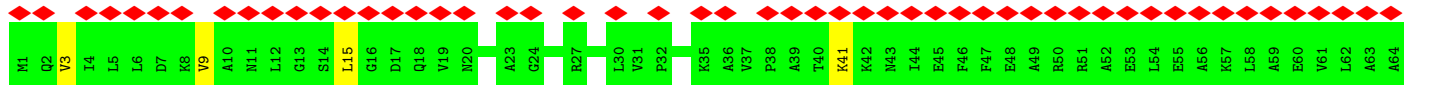
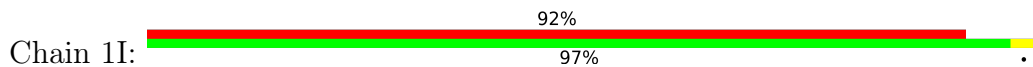




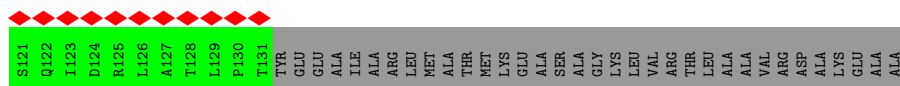
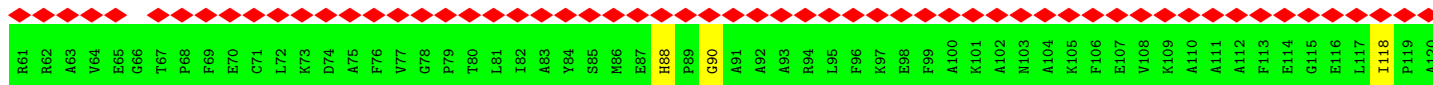
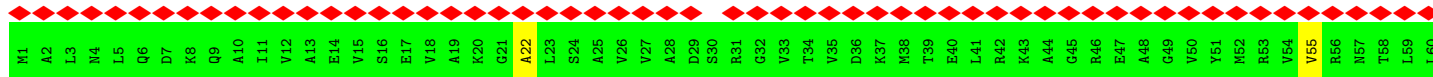
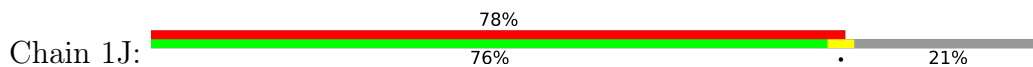
• Molecule 8: 50S ribosomal protein L7/L12



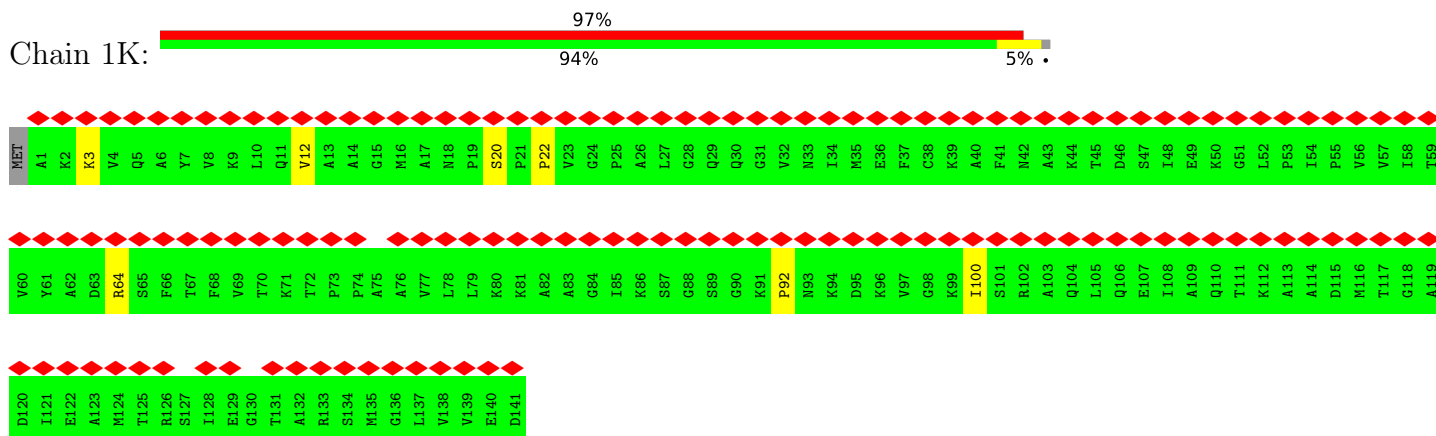
• Molecule 9: 50S ribosomal protein L9



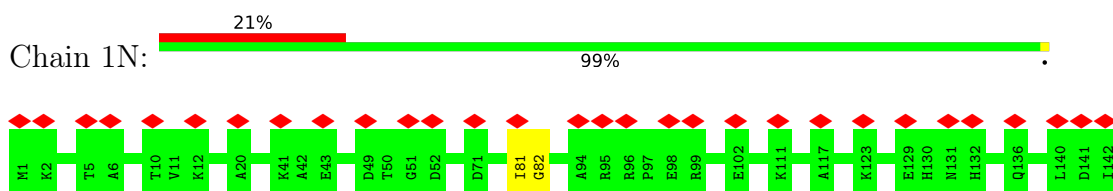
• Molecule 10: 50S ribosomal protein L10



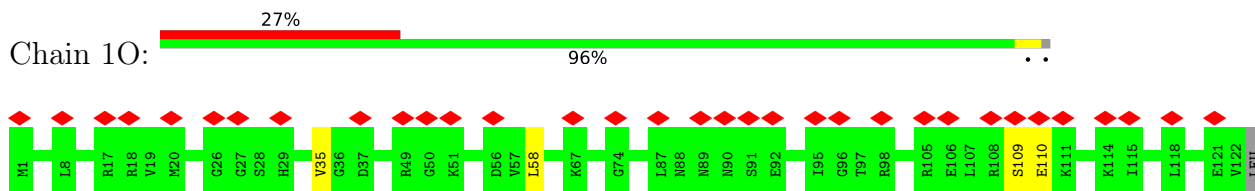
• Molecule 11: 50S ribosomal protein L11



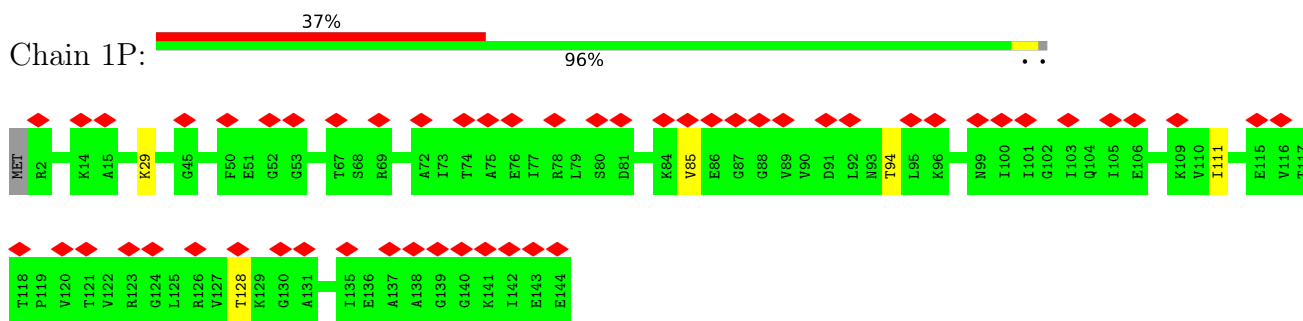
- Molecule 12: 50S ribosomal protein L13



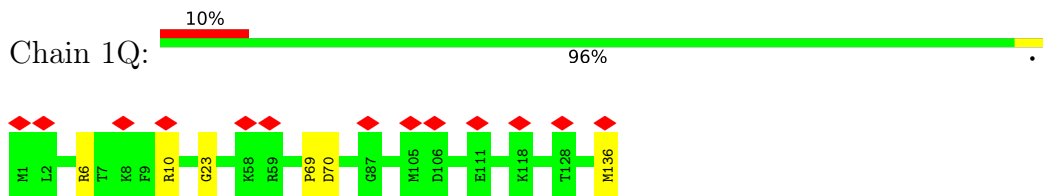
- Molecule 13: 50S ribosomal protein L14



- Molecule 14: 50S ribosomal protein L15

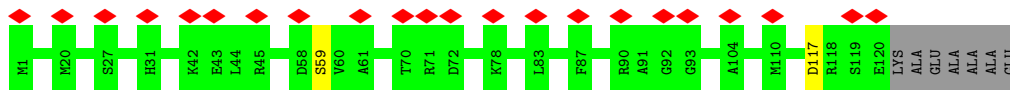


- Molecule 15: 50S ribosomal protein L16



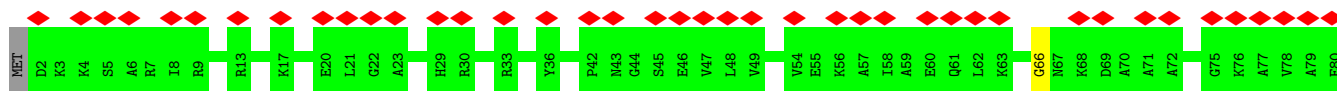
- Molecule 16: 50S ribosomal protein L17





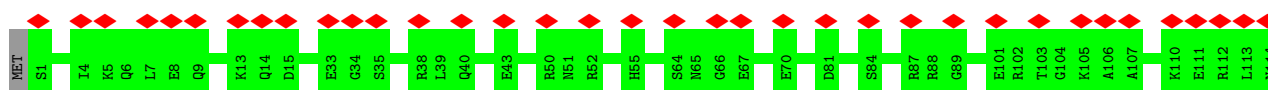
- Molecule 17: 50S ribosomal protein L18

Chain 1S: 52%
 97%



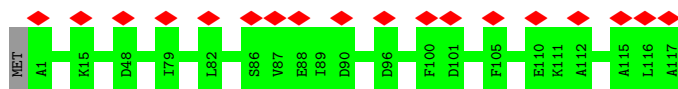
- Molecule 18: 50S ribosomal protein L19

Chain 1T: 31%
 99%



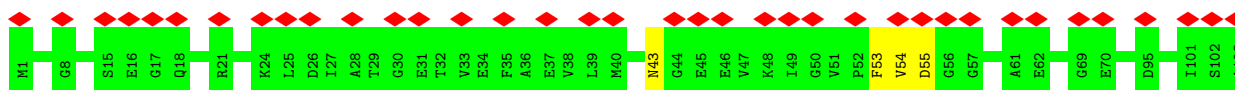
- Molecule 19: 50S ribosomal protein L20

Chain 1U: 15%
 99%



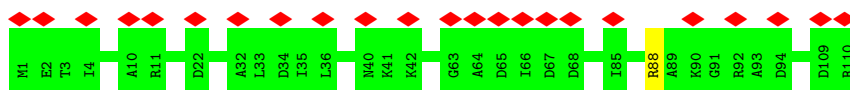
- Molecule 20: 50S ribosomal protein L21

Chain 1V: 36%
 96%



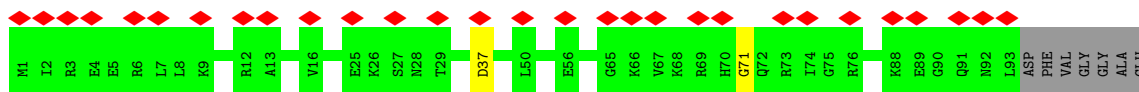
- Molecule 21: 50S ribosomal protein L22

Chain 1W: 21%
 99%

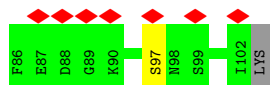
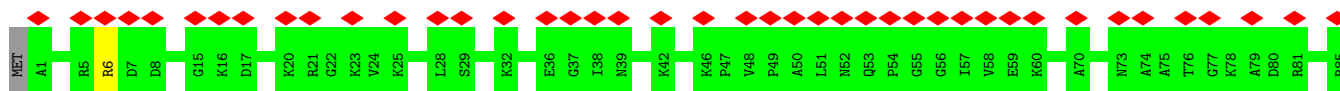


- Molecule 22: 50S ribosomal protein L23

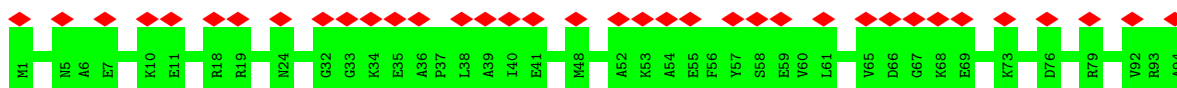
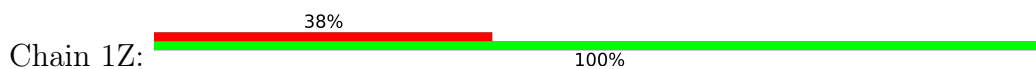
Chain 1X: 29%
 91% 7%



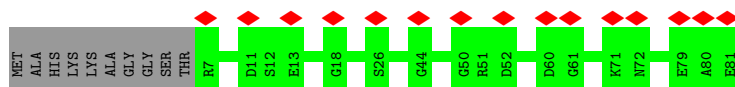
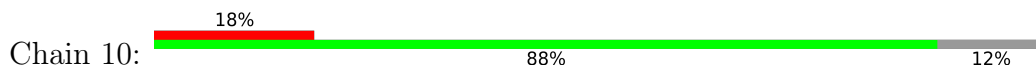
- Molecule 23: 50S ribosomal protein L24



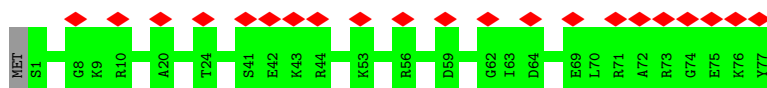
- Molecule 24: 50S ribosomal protein L25



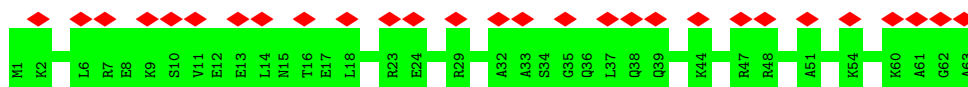
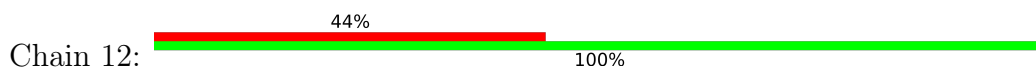
- Molecule 25: 50S ribosomal protein L27



- Molecule 26: 50S ribosomal protein L28

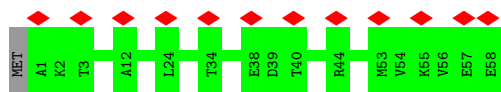


- Molecule 27: 50S ribosomal protein L29

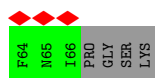
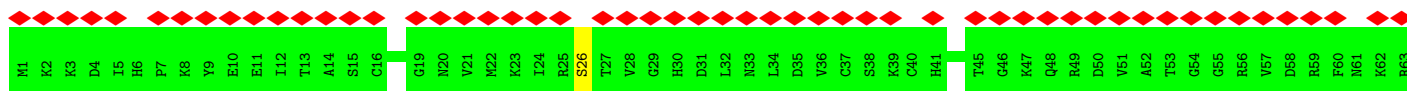
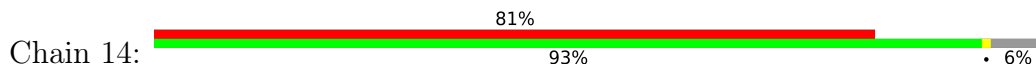


- Molecule 28: 50S ribosomal protein L30

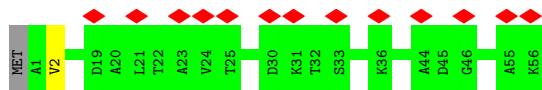




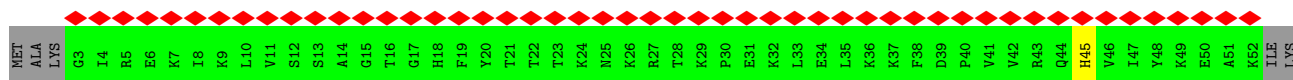
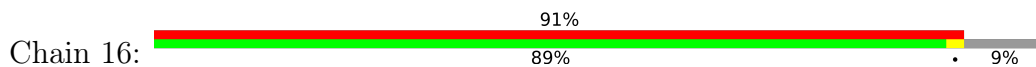
- Molecule 29: 50S ribosomal protein L31



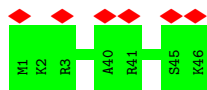
- Molecule 30: 50S ribosomal protein L32



- Molecule 31: 50S ribosomal protein L33



- Molecule 32: 50S ribosomal protein L34

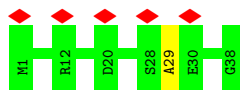


- Molecule 33: 50S ribosomal protein L35

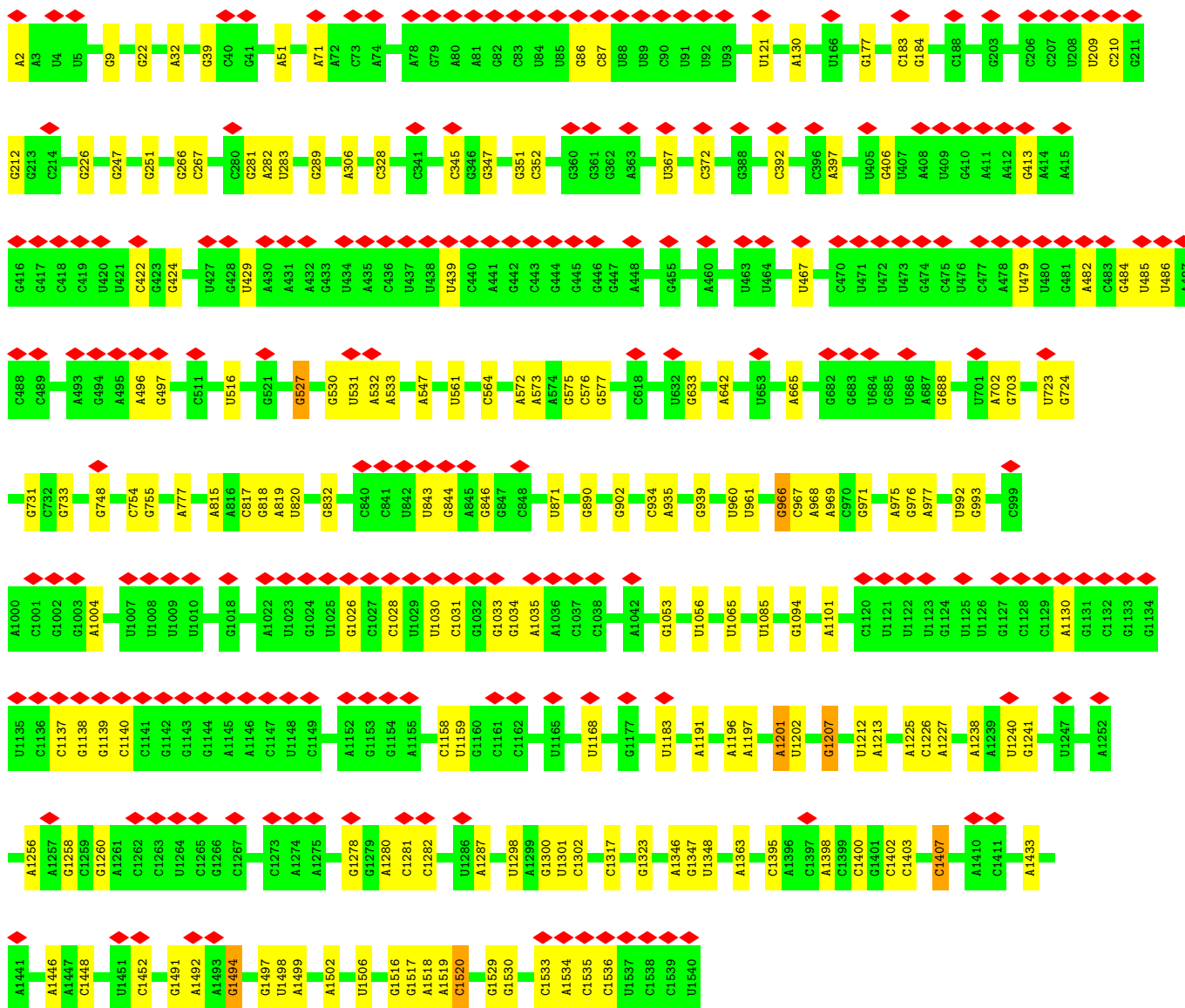
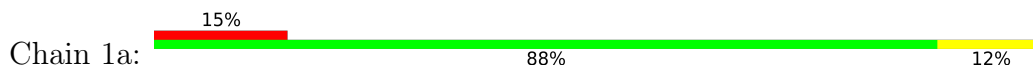


- Molecule 34: 50S ribosomal protein L36

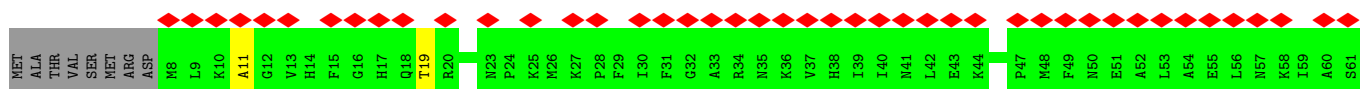
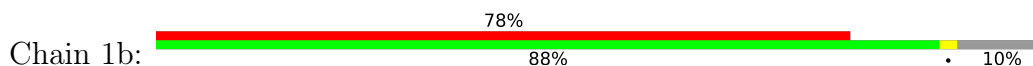


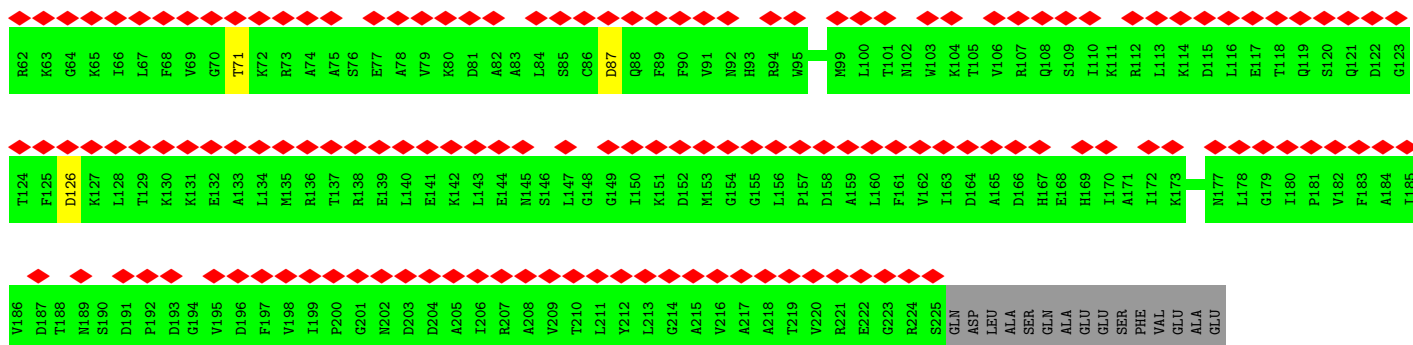


• Molecule 35: 16S Ribosomal RNA

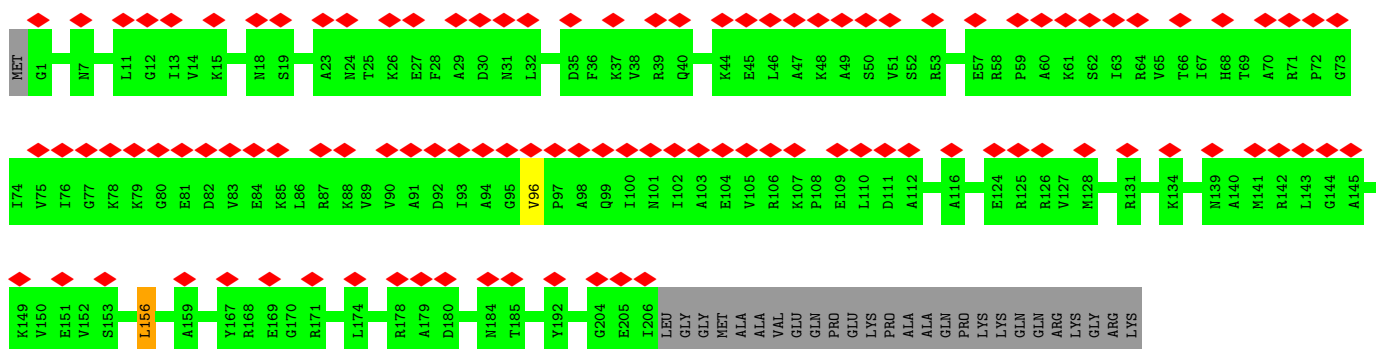
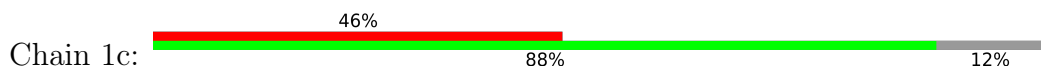


• Molecule 36: 30S ribosomal protein S2

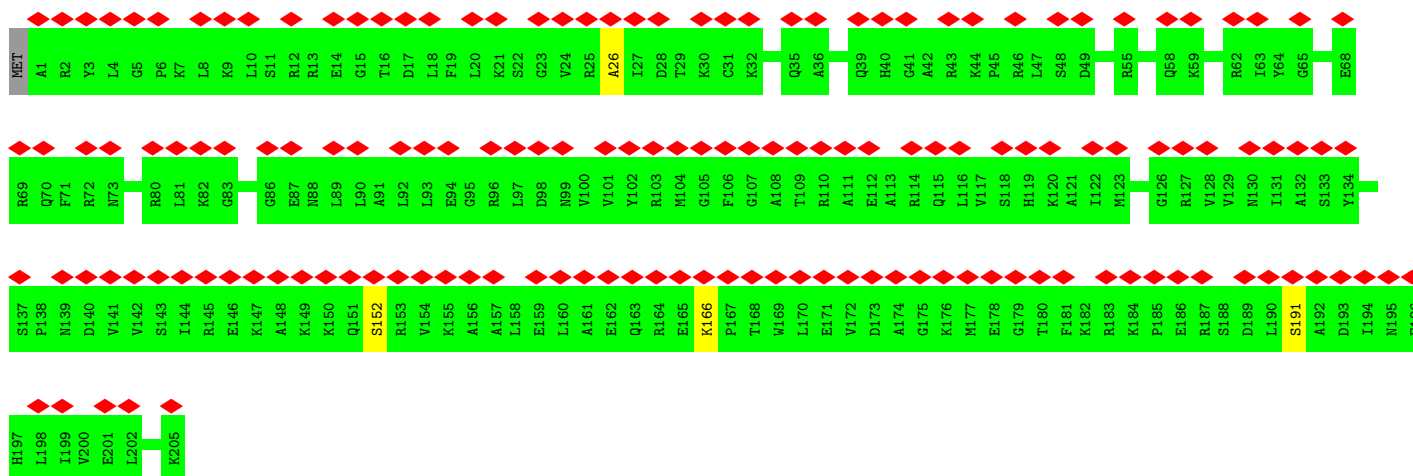
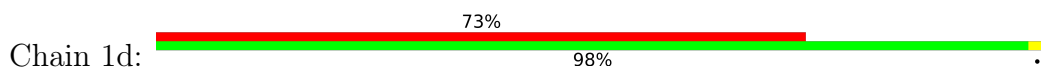




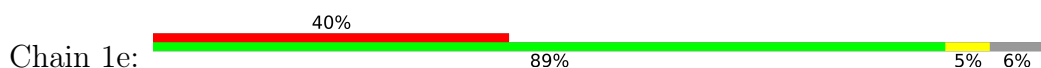
• Molecule 37: 30S ribosomal protein S3

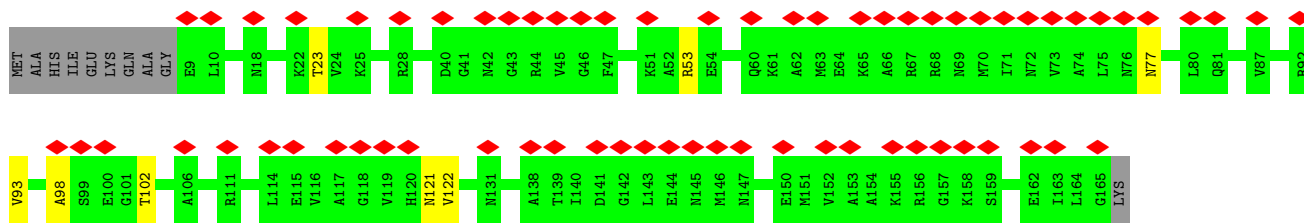


• Molecule 38: 30S ribosomal protein S4

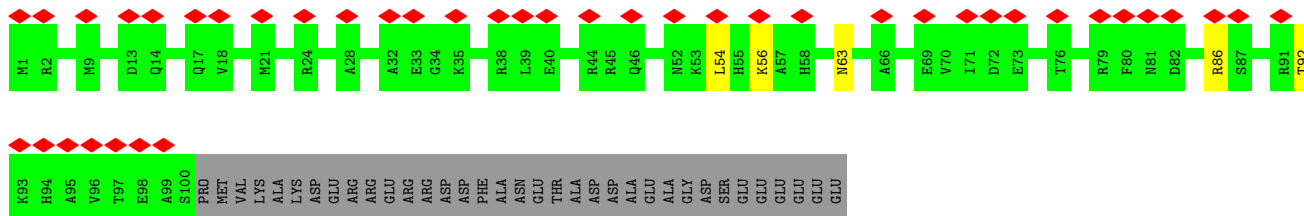


• Molecule 39: 30S ribosomal protein S5

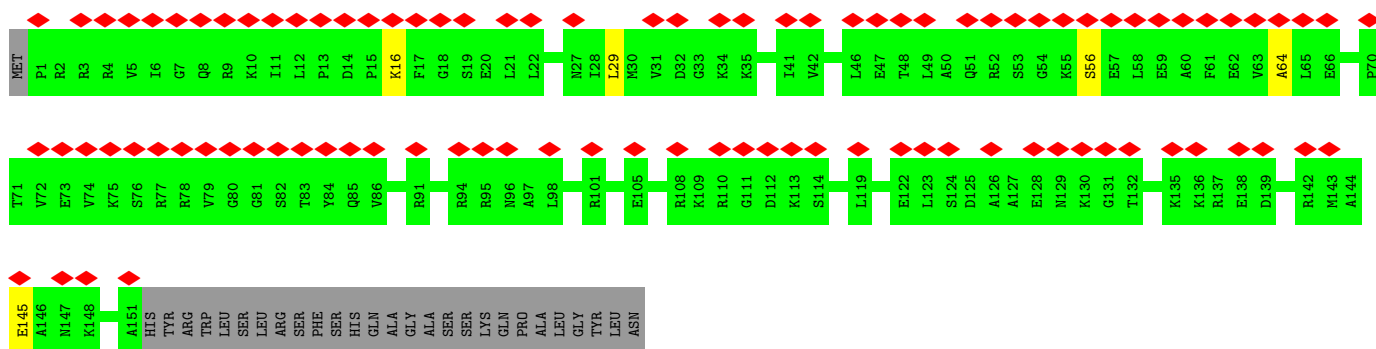
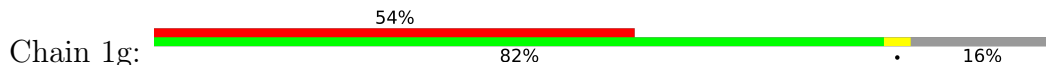




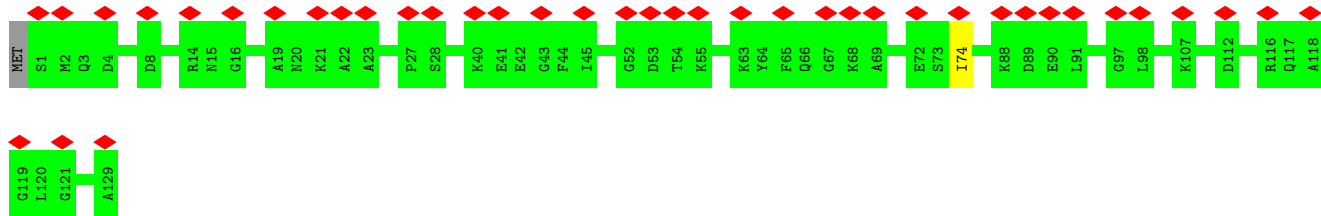
• Molecule 40: 30S ribosomal protein S6



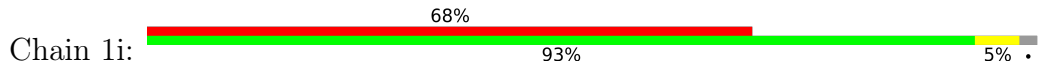
• Molecule 41: 30S ribosomal protein S7

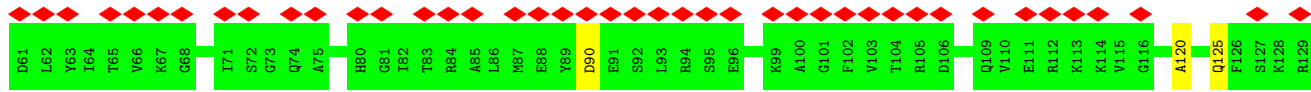
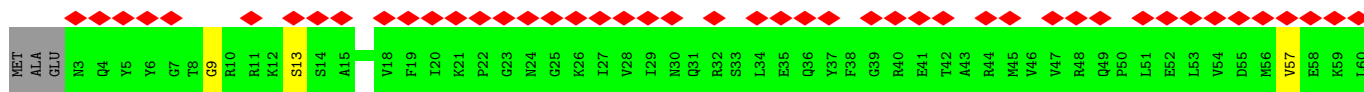


• Molecule 42: 30S ribosomal protein S8

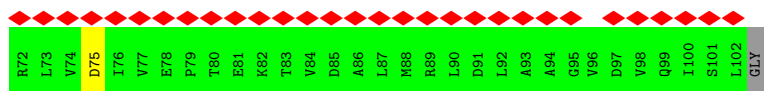
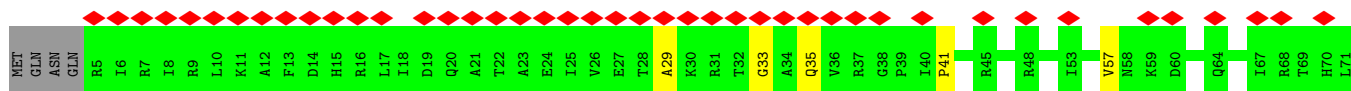
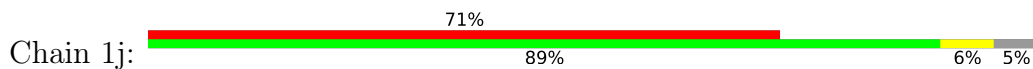


• Molecule 43: 30S ribosomal protein S9

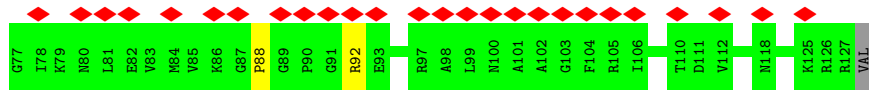
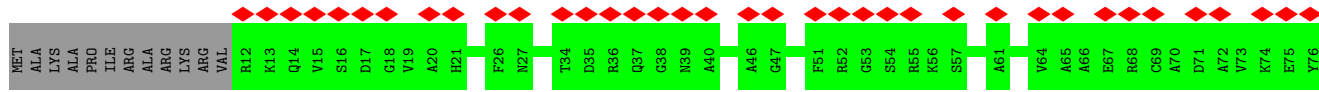
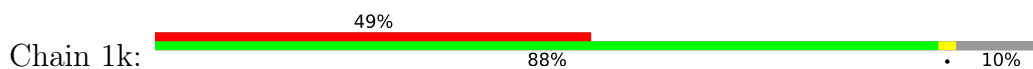




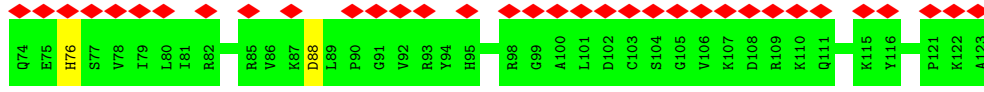
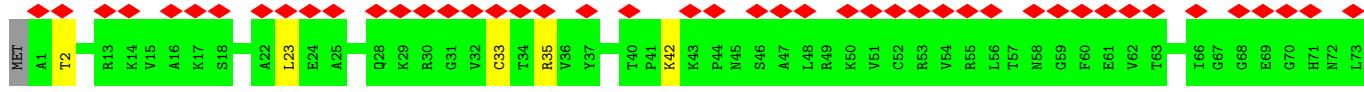
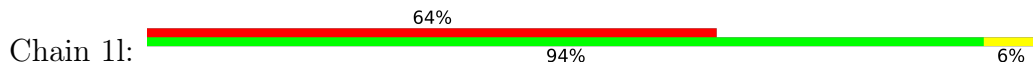
• Molecule 44: 30S ribosomal protein S10



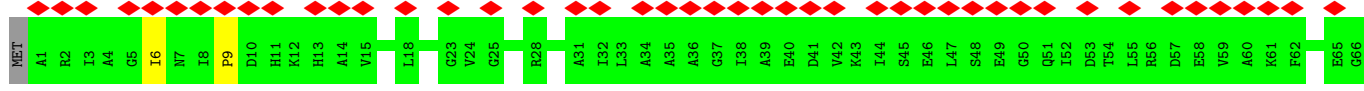
• Molecule 45: 30S ribosomal protein S11

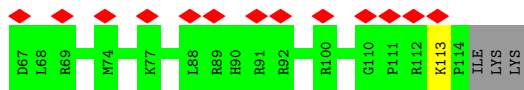


• Molecule 46: 30S ribosomal protein S12

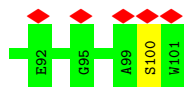
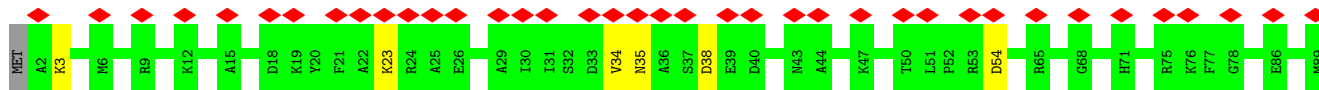
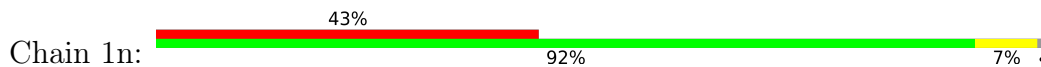


• Molecule 47: 30S ribosomal protein S13

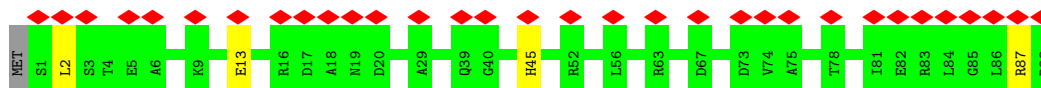




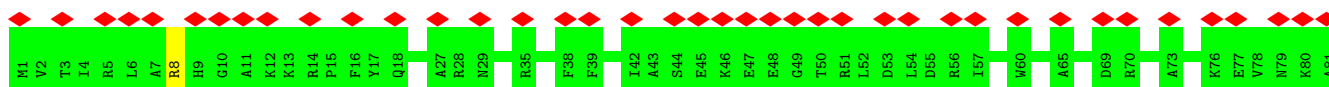
- Molecule 48: 30S ribosomal protein S14



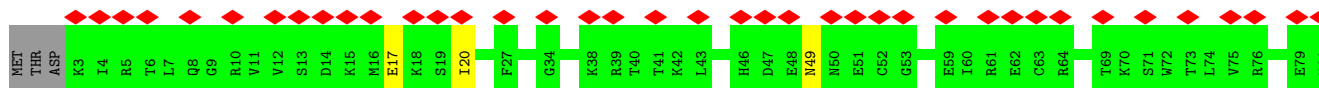
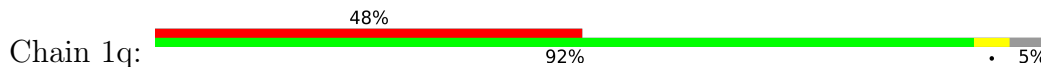
- Molecule 49: 30S ribosomal protein S15



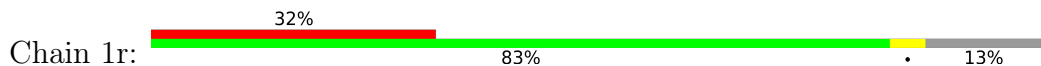
- Molecule 50: 30S ribosomal protein S16

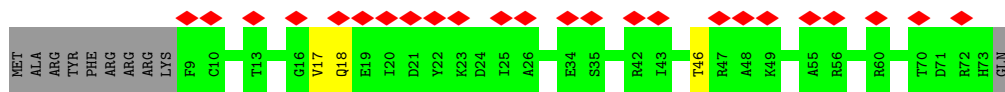


- Molecule 51: 30S ribosomal protein S17

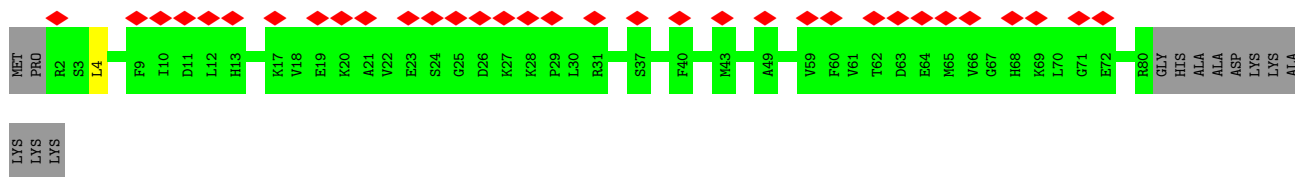
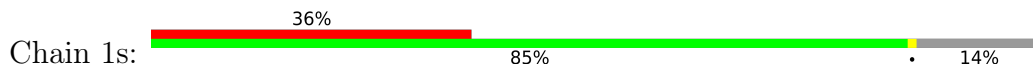


- Molecule 52: 30S ribosomal protein S18

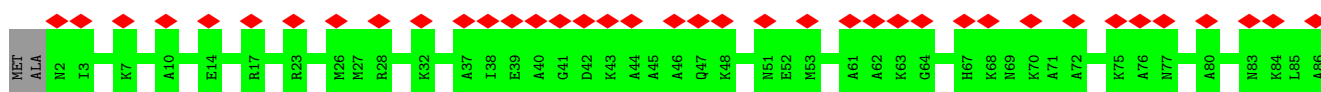




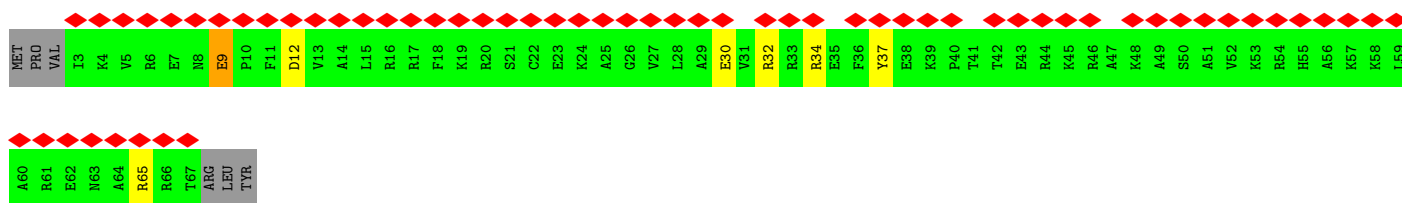
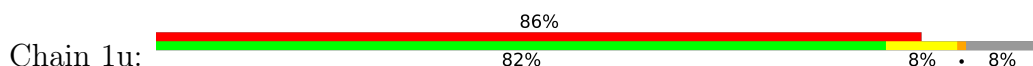
• Molecule 53: 30S ribosomal protein S19



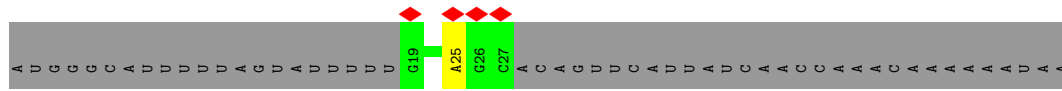
• Molecule 54: 30S ribosomal protein S20



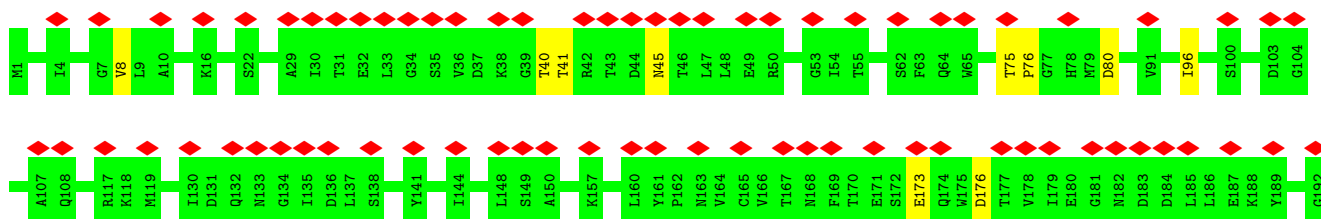
• Molecule 55: 30S ribosomal protein S21

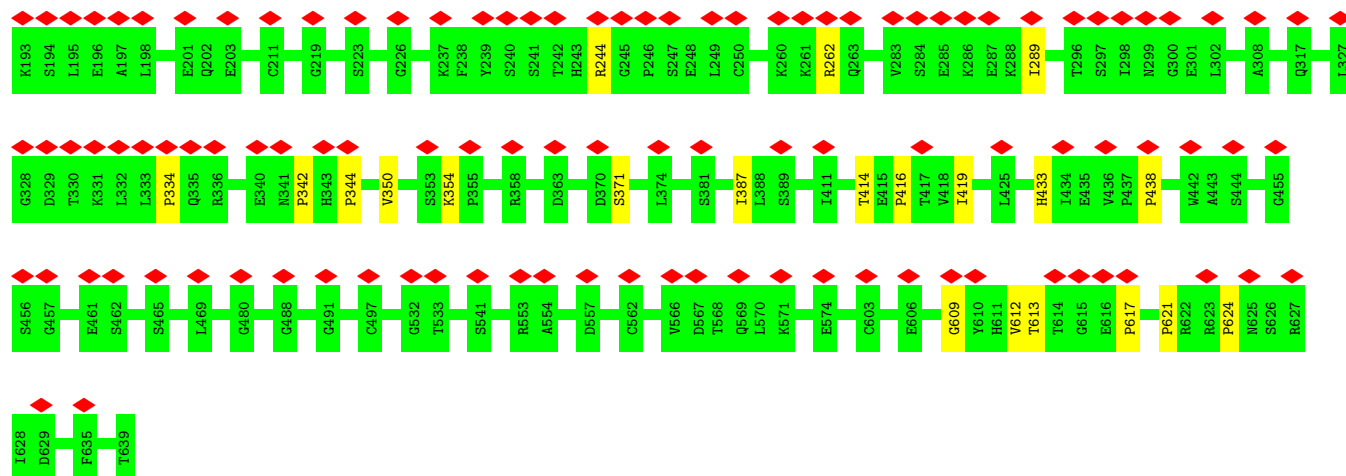


• Molecule 56: mRNA

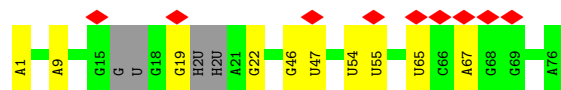
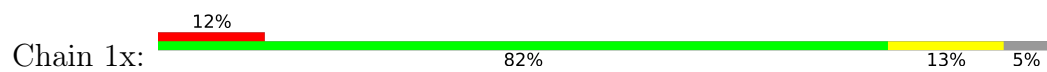


• Molecule 57: Tetracycline resistance protein TetM from transposon Tn916





- Molecule 58: P-site tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	78186	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 ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.018	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00307	Depositor
Map size (\AA)	407.74402, 407.74402, 407.74402	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.108, 1.108, 1.108	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, OMG, G7M, H2U, 3TD, 6MZ, UR3, 7MG, 1MG, 2MA, EVN, 5MU, 4OC, 5MC, MA6, OMC, PSU, OMU

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	1A	0.19	1/69174 (0.0%)	0.69	11/107910 (0.0%)
2	1B	0.26	1/2873 (0.0%)	0.68	0/4478
3	1D	0.28	0/2121	0.47	0/2852
4	1E	0.27	0/1586	0.46	0/2134
5	1F	0.25	0/1571	0.41	0/2113
6	1G	0.27	0/1434	0.42	0/1926
7	1H	0.26	0/1343	0.44	0/1816
8	1L	0.25	0/275	0.43	0/342
9	1I	0.27	0/1122	0.43	0/1515
10	1J	0.29	0/1001	0.47	0/1350
11	1K	0.27	0/1046	0.44	0/1410
12	1N	0.25	0/1152	0.42	0/1551
13	1O	0.26	0/947	0.45	0/1268
14	1P	0.27	0/1054	0.45	0/1403
15	1Q	0.30	0/1093	0.49	0/1460
16	1R	0.25	0/973	0.41	0/1301
17	1S	0.26	0/902	0.39	0/1209
18	1T	0.26	0/929	0.46	0/1242
19	1U	0.25	0/960	0.35	0/1278
20	1V	0.27	0/829	0.45	0/1107
21	1W	0.26	0/864	0.44	0/1156
22	1X	0.26	0/744	0.42	0/994
23	1Y	0.27	0/787	0.45	0/1051
24	1Z	0.28	0/766	0.42	0/1025
25	10	0.27	0/582	0.42	0/769
26	11	0.25	0/635	0.41	0/848
27	12	0.24	0/510	0.40	0/677
28	13	0.24	0/453	0.45	0/605
29	14	0.28	0/531	0.43	0/709
30	15	0.24	0/450	0.43	0/599
31	16	0.26	0/416	0.43	0/554

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	17	0.25	0/380	0.43	0/498
33	18	0.26	0/513	0.44	0/676
34	19	0.25	0/303	0.40	0/397
35	1a	0.19	1/36701 (0.0%)	0.70	13/57246 (0.0%)
36	1b	0.26	0/1735	0.41	0/2338
37	1c	0.26	0/1651	0.44	0/2225
38	1d	0.26	0/1665	0.42	0/2227
39	1e	0.26	0/1154	0.44	0/1554
40	1f	0.25	0/835	0.43	0/1128
41	1g	0.26	0/1195	0.42	0/1602
42	1h	0.26	0/989	0.46	0/1326
43	1i	0.26	0/1034	0.45	0/1375
44	1j	0.25	0/796	0.47	0/1077
45	1k	0.26	0/885	0.43	0/1195
46	1l	0.26	0/969	0.46	0/1300
47	1m	0.25	0/892	0.43	0/1193
48	1n	0.26	0/806	0.43	0/1074
49	1o	0.24	0/722	0.38	0/964
50	1p	0.26	0/659	0.42	0/884
51	1q	0.28	0/657	0.46	0/881
52	1r	0.26	0/511	0.42	0/689
53	1s	0.25	0/652	0.40	0/877
54	1t	0.26	0/671	0.37	0/888
55	1u	0.38	1/500 (0.2%)	0.40	0/668
56	1v	0.53	0/214	1.10	3/331 (0.9%)
57	1w	0.26	0/2594	0.47	0/3251
58	1x	0.36	1/1656 (0.1%)	0.72	0/2575
All	All	0.22	5/160462 (0.0%)	0.63	27/239091 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	1x	1	A	OP3-P	-10.60	1.48	1.61
35	1a	2	A	OP3-P	-10.55	1.48	1.61
2	1B	1	U	OP3-P	-10.46	1.48	1.61
1	1A	1	G	OP3-P	-10.44	1.48	1.61
55	1u	9	GLU	C-N	5.99	1.45	1.34

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1a	754	C	C2-N1-C1'	8.93	128.63	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1a	754	C	N1-C2-O2	8.83	124.20	118.90
35	1a	1158	C	C2-N1-C1'	8.63	128.30	118.80
35	1a	1158	C	N1-C2-O2	8.58	124.05	118.90
1	1A	2884	U	C2-N1-C1'	7.77	127.02	117.70
1	1A	1313	U	C2-N1-C1'	7.42	126.60	117.70
1	1A	1313	U	N1-C2-O2	7.38	127.97	122.80
35	1a	1158	C	N3-C2-O2	-7.25	116.83	121.90
1	1A	2884	U	N1-C2-O2	7.06	127.74	122.80
1	1A	1313	U	N3-C2-O2	-6.98	117.32	122.20
56	1v	25	A	C2-N3-C4	-6.92	107.14	110.60
35	1a	754	C	N3-C2-O2	-6.85	117.10	121.90
1	1A	2884	U	N3-C2-O2	-6.54	117.62	122.20
35	1a	754	C	C6-N1-C1'	-6.44	113.07	120.80
35	1a	1158	C	C6-N1-C2	-6.35	117.76	120.30
1	1A	1378	A	OP1-P-O3'	5.98	118.36	105.20
1	1A	51	G	OP2-P-O3'	5.87	118.12	105.20
35	1a	1158	C	C6-N1-C1'	-5.77	113.87	120.80
1	1A	752	A	OP2-P-O3'	5.55	117.42	105.20
56	1v	25	A	C5-N7-C8	-5.37	101.22	103.90
35	1a	1494	G	N3-C4-C5	5.29	131.24	128.60
35	1a	1520	C	C2-N3-C4	5.20	122.50	119.90
1	1A	752	A	P-O3'-C3'	5.15	125.89	119.70
35	1a	754	C	C6-N1-C2	-5.14	118.24	120.30
56	1v	25	A	N3-C4-C5	5.08	130.36	126.80
35	1a	1201	A	P-O3'-C3'	5.04	125.74	119.70
1	1A	1020	A	P-O3'-C3'	5.01	125.72	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	
3	1D	269/273 (98%)	242 (90%)	23 (9%)	4 (2%)	10	45
4	1E	207/209 (99%)	187 (90%)	19 (9%)	1 (0%)	29	67
5	1F	199/201 (99%)	185 (93%)	11 (6%)	3 (2%)	10	45
6	1G	175/179 (98%)	153 (87%)	19 (11%)	3 (2%)	9	43
7	1H	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	14	51
8	1L	67/121 (55%)	64 (96%)	3 (4%)	0	100	100
9	1I	147/149 (99%)	130 (88%)	13 (9%)	4 (3%)	5	35
10	1J	129/165 (78%)	101 (78%)	23 (18%)	5 (4%)	3	28
11	1K	139/142 (98%)	118 (85%)	14 (10%)	7 (5%)	2	23
12	1N	140/142 (99%)	132 (94%)	6 (4%)	2 (1%)	11	46
13	1O	120/123 (98%)	106 (88%)	11 (9%)	3 (2%)	5	36
14	1P	141/144 (98%)	120 (85%)	16 (11%)	5 (4%)	3	30
15	1Q	134/136 (98%)	120 (90%)	9 (7%)	5 (4%)	3	29
16	1R	118/127 (93%)	103 (87%)	13 (11%)	2 (2%)	9	43
17	1S	114/117 (97%)	103 (90%)	9 (8%)	2 (2%)	8	42
18	1T	112/115 (97%)	105 (94%)	7 (6%)	0	100	100
19	1U	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
20	1V	101/103 (98%)	89 (88%)	8 (8%)	4 (4%)	3	27
21	1W	108/110 (98%)	96 (89%)	12 (11%)	0	100	100
22	1X	91/100 (91%)	80 (88%)	9 (10%)	2 (2%)	6	38
23	1Y	100/104 (96%)	86 (86%)	12 (12%)	2 (2%)	7	40
24	1Z	92/94 (98%)	87 (95%)	5 (5%)	0	100	100
25	10	73/85 (86%)	68 (93%)	5 (7%)	0	100	100
26	11	75/78 (96%)	71 (95%)	4 (5%)	0	100	100
27	12	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
28	13	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
29	14	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	9	44
30	15	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	8	41
31	16	48/55 (87%)	42 (88%)	5 (10%)	1 (2%)	7	39
32	17	44/46 (96%)	42 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	18	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
34	19	36/38 (95%)	30 (83%)	5 (14%)	1 (3%)	5	34
36	1b	216/241 (90%)	187 (87%)	24 (11%)	5 (2%)	6	38
37	1c	204/233 (88%)	190 (93%)	12 (6%)	2 (1%)	15	52
38	1d	203/206 (98%)	179 (88%)	20 (10%)	4 (2%)	7	40
39	1e	155/167 (93%)	136 (88%)	11 (7%)	8 (5%)	2	23
40	1f	98/135 (73%)	87 (89%)	6 (6%)	5 (5%)	2	23
41	1g	149/179 (83%)	129 (87%)	15 (10%)	5 (3%)	3	31
42	1h	127/130 (98%)	115 (91%)	11 (9%)	1 (1%)	19	57
43	1i	125/130 (96%)	107 (86%)	12 (10%)	6 (5%)	2	24
44	1j	96/103 (93%)	80 (83%)	10 (10%)	6 (6%)	1	19
45	1k	114/129 (88%)	98 (86%)	14 (12%)	2 (2%)	8	42
46	1l	121/124 (98%)	100 (83%)	14 (12%)	7 (6%)	1	21
47	1m	112/118 (95%)	102 (91%)	7 (6%)	3 (3%)	5	35
48	1n	98/101 (97%)	83 (85%)	9 (9%)	6 (6%)	1	20
49	1o	86/89 (97%)	76 (88%)	6 (7%)	4 (5%)	2	24
50	1p	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	12	48
51	1q	78/84 (93%)	65 (83%)	10 (13%)	3 (4%)	3	28
52	1r	63/75 (84%)	57 (90%)	3 (5%)	3 (5%)	2	24
53	1s	77/92 (84%)	70 (91%)	6 (8%)	1 (1%)	12	48
54	1t	83/87 (95%)	78 (94%)	5 (6%)	0	100	100
55	1u	63/71 (89%)	45 (71%)	11 (18%)	7 (11%)	0	8
57	1w	637/639 (100%)	548 (86%)	58 (9%)	31 (5%)	2	24
All	All	6550/6980 (94%)	5803 (89%)	577 (9%)	170 (3%)	8	35

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1G	18	GLU
7	1H	108	PHE
11	1K	22	PRO
11	1K	92	PRO
12	1N	81	ILE
14	1P	85	VAL

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Mol	Chain	Res	Type
15	1Q	6	ARG
20	1V	55	ASP
37	1c	96	VAL
37	1c	156	LEU
39	1e	122	VAL
40	1f	92	THR
41	1g	16	LYS
43	1i	90	ASP
52	1r	17	VAL
57	1w	8	VAL
57	1w	76	PRO
57	1w	96	ILE
57	1w	176	ASP
57	1w	334	PRO
57	1w	342	PRO
57	1w	344	PRO
57	1w	416	PRO
57	1w	433	HIS
57	1w	438	PRO
57	1w	612	VAL
57	1w	617	PRO
57	1w	624	PRO
9	1I	9	VAL
10	1J	55	VAL
10	1J	90	GLY
11	1K	12	VAL
11	1K	64	ARG
12	1N	82	GLY
14	1P	111	ILE
14	1P	128	THR
15	1Q	10	ARG
15	1Q	23	GLY
20	1V	43	ASN
22	1X	71	GLY
23	1Y	6	ARG
38	1d	26	ALA
38	1d	152	SER
41	1g	29	LEU
41	1g	145	GLU
42	1h	74	ILE
43	1i	57	VAL
43	1i	120	ALA

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Mol	Chain	Res	Type
44	1j	57	VAL
45	1k	88	PRO
46	1l	33	CYS
47	1m	6	ILE
48	1n	35	ASN
48	1n	54	ASP
55	1u	12	ASP
55	1u	32	ARG
57	1w	80	ASP
3	1D	204	LEU
11	1K	20	SER
14	1P	94	THR
16	1R	59	SER
16	1R	117	ASP
17	1S	66	GLY
23	1Y	97	SER
36	1b	71	THR
41	1g	56	SER
41	1g	64	ALA
43	1i	13	SER
43	1i	125	GLN
44	1j	35	GLN
44	1j	75	ASP
45	1k	92	ARG
46	1l	23	LEU
46	1l	76	HIS
47	1m	113	LYS
48	1n	3	LYS
48	1n	38	ASP
49	1o	2	LEU
49	1o	45	HIS
51	1q	49	ASN
52	1r	18	GLN
55	1u	30	GLU
55	1u	37	TYR
57	1w	40	THR
57	1w	262	ARG
3	1D	231	HIS
5	1F	83	VAL
5	1F	122	GLU
6	1G	176	PHE
9	1I	41	LYS

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Mol	Chain	Res	Type
10	1J	22	ALA
10	1J	88	HIS
11	1K	100	ILE
13	1O	109	SER
13	1O	110	GLU
14	1P	29	LYS
17	1S	100	HIS
22	1X	37	ASP
29	14	26	SER
31	16	45	HIS
34	19	29	ALA
36	1b	11	ALA
36	1b	126	ASP
38	1d	166	LYS
38	1d	191	SER
39	1e	53	ARG
39	1e	98	ALA
40	1f	54	LEU
40	1f	56	LYS
40	1f	63	ASN
40	1f	86	ARG
44	1j	29	ALA
46	1l	2	THR
46	1l	35	ARG
49	1o	13	GLU
50	1p	8	ARG
53	1s	4	LEU
55	1u	34	ARG
55	1u	65	ARG
57	1w	45	ASN
57	1w	173	GLU
57	1w	244	ARG
57	1w	289	ILE
57	1w	354	LYS
57	1w	414	THR
57	1w	609	GLY
4	1E	149	ASN
5	1F	149	ILE
7	1H	45	ALA
9	1I	3	VAL
9	1I	15	LEU
10	1J	118	ILE

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Mol	Chain	Res	Type
15	1Q	70	ASP
20	1V	53	PHE
30	15	2	VAL
36	1b	19	THR
39	1e	23	THR
39	1e	77	ASN
39	1e	121	ASN
44	1j	33	GLY
46	1l	42	LYS
46	1l	88	ASP
48	1n	23	LYS
48	1n	100	SER
49	1o	87	ARG
51	1q	17	GLU
52	1r	46	THR
57	1w	350	VAL
57	1w	371	SER
57	1w	419	ILE
57	1w	613	THR
11	1K	3	LYS
20	1V	54	VAL
36	1b	87	ASP
39	1e	102	THR
43	1i	9	GLY
57	1w	41	THR
15	1Q	69	PRO
51	1q	20	ILE
57	1w	75	THR
3	1D	236	GLY
3	1D	253	GLY
39	1e	93	VAL
44	1j	41	PRO
57	1w	621	PRO
13	1O	35	VAL
47	1m	9	PRO
6	1G	175	PRO
55	1u	9	GLU
57	1w	387	ILE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	1D	216/218 (99%)	216 (100%)	0	100	100
4	1E	164/164 (100%)	164 (100%)	0	100	100
5	1F	165/165 (100%)	165 (100%)	0	100	100
6	1G	148/150 (99%)	148 (100%)	0	100	100
7	1H	137/138 (99%)	137 (100%)	0	100	100
9	1I	114/114 (100%)	114 (100%)	0	100	100
10	1J	100/123 (81%)	100 (100%)	0	100	100
11	1K	109/110 (99%)	109 (100%)	0	100	100
12	1N	116/116 (100%)	116 (100%)	0	100	100
13	1O	103/104 (99%)	102 (99%)	1 (1%)	76	86
14	1P	102/103 (99%)	102 (100%)	0	100	100
15	1Q	109/109 (100%)	108 (99%)	1 (1%)	78	87
16	1R	100/103 (97%)	100 (100%)	0	100	100
17	1S	86/87 (99%)	86 (100%)	0	100	100
18	1T	99/100 (99%)	99 (100%)	0	100	100
19	1U	89/90 (99%)	89 (100%)	0	100	100
20	1V	84/84 (100%)	84 (100%)	0	100	100
21	1W	93/93 (100%)	92 (99%)	1 (1%)	73	84
22	1X	80/84 (95%)	80 (100%)	0	100	100
23	1Y	83/85 (98%)	83 (100%)	0	100	100
24	1Z	78/78 (100%)	78 (100%)	0	100	100
25	10	57/63 (90%)	57 (100%)	0	100	100
26	11	67/68 (98%)	67 (100%)	0	100	100
27	12	55/55 (100%)	55 (100%)	0	100	100
28	13	48/49 (98%)	48 (100%)	0	100	100
29	14	59/62 (95%)	59 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	15	47/48 (98%)	47 (100%)	0	100	100
31	16	45/49 (92%)	45 (100%)	0	100	100
32	17	38/38 (100%)	38 (100%)	0	100	100
33	18	51/52 (98%)	50 (98%)	1 (2%)	55	74
34	19	34/34 (100%)	34 (100%)	0	100	100
36	1b	180/199 (90%)	180 (100%)	0	100	100
37	1c	170/190 (90%)	169 (99%)	1 (1%)	86	91
38	1d	172/173 (99%)	172 (100%)	0	100	100
39	1e	114/126 (90%)	114 (100%)	0	100	100
40	1f	87/116 (75%)	87 (100%)	0	100	100
41	1g	124/147 (84%)	124 (100%)	0	100	100
42	1h	104/105 (99%)	104 (100%)	0	100	100
43	1i	105/107 (98%)	105 (100%)	0	100	100
44	1j	86/90 (96%)	86 (100%)	0	100	100
45	1k	89/99 (90%)	89 (100%)	0	100	100
46	1l	103/104 (99%)	103 (100%)	0	100	100
47	1m	92/96 (96%)	92 (100%)	0	100	100
48	1n	79/84 (94%)	78 (99%)	1 (1%)	69	82
49	1o	76/77 (99%)	76 (100%)	0	100	100
50	1p	65/65 (100%)	65 (100%)	0	100	100
51	1q	74/78 (95%)	74 (100%)	0	100	100
52	1r	48/65 (74%)	48 (100%)	0	100	100
53	1s	70/79 (89%)	70 (100%)	0	100	100
54	1t	65/66 (98%)	65 (100%)	0	100	100
55	1u	44/61 (72%)	44 (100%)	0	100	100
57	1w	6/576 (1%)	6 (100%)	0	100	100
All	All	4829/5639 (86%)	4823 (100%)	6 (0%)	93	97

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	1O	58	LEU
15	1Q	136	MET

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Mol	Chain	Res	Type
21	1W	88	ARG
33	18	61	LEU
37	1c	156	LEU
48	1n	34	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
3	1D	36	ASN
3	1D	45	ASN
3	1D	85	ASN
3	1D	225	ASN
4	1E	32	ASN
4	1E	49	GLN
4	1E	150	GLN
4	1E	173	GLN
5	1F	41	GLN
6	1G	4	HIS
7	1H	44	HIS
7	1H	72	ASN
7	1H	103	ASN
7	1H	138	GLN
10	1J	4	ASN
10	1J	88	HIS
12	1N	40	HIS
13	1O	3	GLN
15	1Q	13	HIS
16	1R	9	GLN
18	1T	2	ASN
18	1T	11	GLN
21	1W	7	HIS
21	1W	40	ASN
21	1W	61	ASN
22	1X	15	HIS
24	1Z	87	GLN
25	10	42	HIS
26	11	16	ASN
27	12	25	GLN
27	12	27	ASN
31	16	18	HIS
36	1b	18	GLN
36	1b	41	ASN

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Mol	Chain	Res	Type
38	1d	125	ASN
38	1d	197	HIS
39	1e	145	ASN
40	1f	11	HIS
40	1f	58	HIS
41	1g	141	HIS
42	1h	3	GLN
42	1h	20	ASN
44	1j	70	HIS
49	1o	39	GLN
50	1p	79	ASN
51	1q	30	HIS
53	1s	51	HIS
53	1s	55	GLN
53	1s	68	HIS
54	1t	2	ASN
54	1t	60	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1A	2894/2904 (99%)	424 (14%)	33 (1%)
2	1B	119/120 (99%)	14 (11%)	2 (1%)
35	1a	1535/1539 (99%)	179 (11%)	0
56	1v	8/60 (13%)	0	0
58	1x	70/77 (90%)	5 (7%)	0
All	All	4626/4700 (98%)	622 (13%)	35 (0%)

All (622) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1A	10	A
1	1A	12	U
1	1A	27	G
1	1A	34	U
1	1A	35	G
1	1A	42	A
1	1A	46	G
1	1A	49	A
1	1A	51	G
1	1A	52	A

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Mol	Chain	Res	Type
1	1A	71	A
1	1A	74	A
1	1A	75	G
1	1A	84	A
1	1A	91	A
1	1A	92	U
1	1A	118	A
1	1A	120	U
1	1A	138	U
1	1A	139	U
1	1A	140	C
1	1A	141	G
1	1A	142	A
1	1A	162	U
1	1A	163	C
1	1A	181	A
1	1A	196	A
1	1A	199	A
1	1A	205	G
1	1A	206	U
1	1A	216	A
1	1A	221	A
1	1A	222	A
1	1A	228	C
1	1A	242	G
1	1A	243	U
1	1A	248	G
1	1A	249	C
1	1A	255	A
1	1A	266	G
1	1A	267	C
1	1A	276	U
1	1A	278	A
1	1A	294	A
1	1A	301	G
1	1A	310	A
1	1A	311	A
1	1A	323	C
1	1A	324	A
1	1A	329	G
1	1A	330	A
1	1A	353	C

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Mol	Chain	Res	Type
1	1A	361	G
1	1A	367	G
1	1A	371	A
1	1A	372	G
1	1A	373	U
1	1A	386	G
1	1A	387	U
1	1A	391	A
1	1A	404	A
1	1A	406	G
1	1A	411	G
1	1A	424	G
1	1A	456	C
1	1A	457	A
1	1A	458	G
1	1A	459	U
1	1A	480	A
1	1A	481	G
1	1A	491	G
1	1A	504	A
1	1A	505	A
1	1A	506	G
1	1A	529	A
1	1A	530	G
1	1A	532	A
1	1A	542	C
1	1A	543	G
1	1A	545	U
1	1A	547	A
1	1A	550	C
1	1A	563	A
1	1A	572	A
1	1A	573	U
1	1A	575	A
1	1A	603	A
1	1A	616	A
1	1A	627	A
1	1A	637	A
1	1A	646	U
1	1A	654	A
1	1A	669	G
1	1A	670	A

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Mol	Chain	Res	Type
1	1A	677	A
1	1A	686	U
1	1A	687	C
1	1A	695	G
1	1A	726	G
1	1A	730	A
1	1A	746	PSU
1	1A	747	5MU
1	1A	748	G
1	1A	752	A
1	1A	753	A
1	1A	764	A
1	1A	765	C
1	1A	776	G
1	1A	782	A
1	1A	784	G
1	1A	785	G
1	1A	789	A
1	1A	792	A
1	1A	800	A
1	1A	805	G
1	1A	812	C
1	1A	819	A
1	1A	822	G
1	1A	827	U
1	1A	828	U
1	1A	830	G
1	1A	831	G
1	1A	845	A
1	1A	846	U
1	1A	847	U
1	1A	858	G
1	1A	859	G
1	1A	860	U
1	1A	878	A
1	1A	896	A
1	1A	897	C
1	1A	907	G
1	1A	910	A
1	1A	932	U
1	1A	941	A
1	1A	946	C

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Mol	Chain	Res	Type
1	1A	961	C
1	1A	974	G
1	1A	983	A
1	1A	985	C
1	1A	995	C
1	1A	996	A
1	1A	1012	U
1	1A	1013	C
1	1A	1021	A
1	1A	1022	G
1	1A	1023	U
1	1A	1033	U
1	1A	1046	A
1	1A	1047	G
1	1A	1053	C
1	1A	1054	A
1	1A	1057	A
1	1A	1060	U
1	1A	1061	U
1	1A	1062	G
1	1A	1064	C
1	1A	1065	U
1	1A	1066	U
1	1A	1068	G
1	1A	1070	A
1	1A	1071	G
1	1A	1075	C
1	1A	1076	C
1	1A	1079	C
1	1A	1084	A
1	1A	1088	A
1	1A	1104	C
1	1A	1111	A
1	1A	1112	G
1	1A	1119	U
1	1A	1130	U
1	1A	1131	G
1	1A	1132	U
1	1A	1133	A
1	1A	1135	C
1	1A	1143	A
1	1A	1174	U

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Mol	Chain	Res	Type
1	1A	1175	A
1	1A	1176	U
1	1A	1177	G
1	1A	1179	G
1	1A	1180	U
1	1A	1206	G
1	1A	1212	G
1	1A	1247	A
1	1A	1248	G
1	1A	1250	G
1	1A	1251	C
1	1A	1253	A
1	1A	1256	G
1	1A	1271	G
1	1A	1272	A
1	1A	1300	G
1	1A	1301	A
1	1A	1314	C
1	1A	1321	A
1	1A	1329	U
1	1A	1332	G
1	1A	1341	G
1	1A	1345	C
1	1A	1365	A
1	1A	1368	G
1	1A	1378	A
1	1A	1379	U
1	1A	1383	A
1	1A	1416	G
1	1A	1419	A
1	1A	1420	A
1	1A	1428	C
1	1A	1454	C
1	1A	1461	C
1	1A	1482	G
1	1A	1490	A
1	1A	1491	G
1	1A	1504	A
1	1A	1515	A
1	1A	1524	G
1	1A	1533	C
1	1A	1535	A

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Mol	Chain	Res	Type
1	1A	1536	C
1	1A	1537	G
1	1A	1555	G
1	1A	1559	U
1	1A	1560	G
1	1A	1565	C
1	1A	1567	G
1	1A	1569	A
1	1A	1581	G
1	1A	1585	C
1	1A	1611	C
1	1A	1634	A
1	1A	1646	C
1	1A	1647	U
1	1A	1648	U
1	1A	1651	G
1	1A	1654	A
1	1A	1664	A
1	1A	1670	C
1	1A	1674	G
1	1A	1694	C
1	1A	1695	G
1	1A	1715	G
1	1A	1729	U
1	1A	1730	C
1	1A	1732	C
1	1A	1738	G
1	1A	1758	U
1	1A	1764	C
1	1A	1773	A
1	1A	1780	A
1	1A	1781	U
1	1A	1784	A
1	1A	1791	A
1	1A	1800	C
1	1A	1801	A
1	1A	1802	A
1	1A	1808	A
1	1A	1816	C
1	1A	1829	A
1	1A	1833	C
1	1A	1834	U

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Mol	Chain	Res	Type
1	1A	1871	A
1	1A	1890	A
1	1A	1896	G
1	1A	1901	A
1	1A	1906	G
1	1A	1913	A
1	1A	1914	C
1	1A	1929	G
1	1A	1930	G
1	1A	1937	A
1	1A	1938	A
1	1A	1940	U
1	1A	1941	C
1	1A	1944	U
1	1A	1955	U
1	1A	1962	5MC
1	1A	1963	U
1	1A	1967	C
1	1A	1970	A
1	1A	1971	U
1	1A	1972	G
1	1A	1991	U
1	1A	1993	U
1	1A	1997	C
1	1A	2021	C
1	1A	2022	U
1	1A	2023	C
1	1A	2031	A
1	1A	2033	A
1	1A	2043	C
1	1A	2049	G
1	1A	2052	A
1	1A	2055	C
1	1A	2056	G
1	1A	2060	A
1	1A	2061	G
1	1A	2062	A
1	1A	2068	U
1	1A	2069	G7M
1	1A	2070	A
1	1A	2072	C
1	1A	2093	G

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Mol	Chain	Res	Type
1	1A	2095	A
1	1A	2096	C
1	1A	2098	U
1	1A	2110	G
1	1A	2111	U
1	1A	2112	G
1	1A	2113	U
1	1A	2116	G
1	1A	2118	U
1	1A	2119	A
1	1A	2127	G
1	1A	2131	U
1	1A	2132	U
1	1A	2133	G
1	1A	2145	C
1	1A	2162	G
1	1A	2164	C
1	1A	2170	A
1	1A	2172	U
1	1A	2173	A
1	1A	2192	U
1	1A	2198	A
1	1A	2204	G
1	1A	2211	A
1	1A	2213	U
1	1A	2225	A
1	1A	2226	C
1	1A	2238	G
1	1A	2250	G
1	1A	2251	OMG
1	1A	2252	G
1	1A	2278	A
1	1A	2283	C
1	1A	2287	A
1	1A	2305	U
1	1A	2309	A
1	1A	2320	U
1	1A	2327	A
1	1A	2334	U
1	1A	2335	A
1	1A	2350	C
1	1A	2354	C

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Mol	Chain	Res	Type
1	1A	2361	G
1	1A	2383	G
1	1A	2385	C
1	1A	2391	G
1	1A	2392	A
1	1A	2402	U
1	1A	2407	A
1	1A	2423	U
1	1A	2424	C
1	1A	2426	A
1	1A	2428	G
1	1A	2429	G
1	1A	2430	A
1	1A	2431	U
1	1A	2435	A
1	1A	2441	U
1	1A	2445	2MG
1	1A	2448	A
1	1A	2476	A
1	1A	2484	G
1	1A	2499	C
1	1A	2502	G
1	1A	2504	PSU
1	1A	2506	U
1	1A	2513	A
1	1A	2518	A
1	1A	2529	G
1	1A	2547	A
1	1A	2552	OMU
1	1A	2553	G
1	1A	2554	U
1	1A	2567	G
1	1A	2572	A
1	1A	2585	U
1	1A	2586	U
1	1A	2602	A
1	1A	2603	G
1	1A	2609	U
1	1A	2613	U
1	1A	2614	A
1	1A	2629	U
1	1A	2636	C

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Mol	Chain	Res	Type
1	1A	2646	C
1	1A	2655	G
1	1A	2656	U
1	1A	2689	U
1	1A	2690	U
1	1A	2712	C
1	1A	2713	U
1	1A	2714	G
1	1A	2718	G
1	1A	2726	A
1	1A	2739	U
1	1A	2744	G
1	1A	2748	A
1	1A	2757	A
1	1A	2764	A
1	1A	2765	A
1	1A	2778	A
1	1A	2779	U
1	1A	2780	G
1	1A	2791	G
1	1A	2794	C
1	1A	2797	U
1	1A	2799	A
1	1A	2800	A
1	1A	2808	G
1	1A	2809	A
1	1A	2818	U
1	1A	2820	A
1	1A	2833	U
1	1A	2849	U
1	1A	2867	G
1	1A	2868	A
1	1A	2872	A
1	1A	2880	C
1	1A	2893	A
1	1A	2894	G
2	1B	4	C
2	1B	13	G
2	1B	24	G
2	1B	35	C
2	1B	44	G
2	1B	45	A

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Mol	Chain	Res	Type
2	1B	53	A
2	1B	67	G
2	1B	88	C
2	1B	89	U
2	1B	90	C
2	1B	91	C
2	1B	108	A
2	1B	109	A
35	1a	9	G
35	1a	22	G
35	1a	32	A
35	1a	39	G
35	1a	51	A
35	1a	71	A
35	1a	86	G
35	1a	87	C
35	1a	121	U
35	1a	130	A
35	1a	177	G
35	1a	183	C
35	1a	184	G
35	1a	209	U
35	1a	210	C
35	1a	212	G
35	1a	226	G
35	1a	247	G
35	1a	251	G
35	1a	266	G
35	1a	267	C
35	1a	281	G
35	1a	282	A
35	1a	283	U
35	1a	289	G
35	1a	306	A
35	1a	328	C
35	1a	345	C
35	1a	347	G
35	1a	351	G
35	1a	352	C
35	1a	367	U
35	1a	372	C
35	1a	392	C

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Mol	Chain	Res	Type
35	1a	397	A
35	1a	406	G
35	1a	413	G
35	1a	422	C
35	1a	424	G
35	1a	429	U
35	1a	439	U
35	1a	467	U
35	1a	479	U
35	1a	482	A
35	1a	484	G
35	1a	485	U
35	1a	486	U
35	1a	496	A
35	1a	497	G
35	1a	527	7MG
35	1a	530	G
35	1a	531	U
35	1a	532	A
35	1a	533	A
35	1a	547	A
35	1a	561	U
35	1a	564	C
35	1a	572	A
35	1a	573	A
35	1a	575	G
35	1a	576	C
35	1a	577	G
35	1a	633	G
35	1a	642	A
35	1a	665	A
35	1a	688	G
35	1a	702	A
35	1a	703	G
35	1a	723	U
35	1a	724	G
35	1a	731	G
35	1a	733	G
35	1a	748	G
35	1a	755	G
35	1a	777	A
35	1a	815	A

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Mol	Chain	Res	Type
35	1a	817	C
35	1a	818	G
35	1a	819	A
35	1a	820	U
35	1a	832	G
35	1a	843	U
35	1a	844	G
35	1a	846	G
35	1a	871	U
35	1a	890	G
35	1a	902	G
35	1a	934	C
35	1a	935	A
35	1a	939	G
35	1a	960	U
35	1a	961	U
35	1a	966	2MG
35	1a	968	A
35	1a	969	A
35	1a	971	G
35	1a	975	A
35	1a	976	G
35	1a	977	A
35	1a	992	U
35	1a	993	G
35	1a	1004	A
35	1a	1026	G
35	1a	1028	C
35	1a	1030	U
35	1a	1031	C
35	1a	1033	G
35	1a	1034	G
35	1a	1035	A
35	1a	1053	G
35	1a	1056	U
35	1a	1065	U
35	1a	1085	U
35	1a	1094	G
35	1a	1101	A
35	1a	1130	A
35	1a	1137	C
35	1a	1138	G

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Mol	Chain	Res	Type
35	1a	1139	G
35	1a	1140	C
35	1a	1159	U
35	1a	1168	U
35	1a	1183	U
35	1a	1191	A
35	1a	1196	A
35	1a	1197	A
35	1a	1201	A
35	1a	1202	U
35	1a	1207	2MG
35	1a	1212	U
35	1a	1213	A
35	1a	1225	A
35	1a	1226	C
35	1a	1227	A
35	1a	1238	A
35	1a	1240	U
35	1a	1241	G
35	1a	1256	A
35	1a	1258	G
35	1a	1260	G
35	1a	1278	G
35	1a	1280	A
35	1a	1281	C
35	1a	1282	C
35	1a	1287	A
35	1a	1298	U
35	1a	1300	G
35	1a	1301	U
35	1a	1302	C
35	1a	1317	C
35	1a	1323	G
35	1a	1346	A
35	1a	1347	G
35	1a	1348	U
35	1a	1363	A
35	1a	1395	C
35	1a	1398	A
35	1a	1400	C
35	1a	1403	C
35	1a	1407	5MC

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Mol	Chain	Res	Type
35	1a	1433	A
35	1a	1446	A
35	1a	1448	C
35	1a	1452	C
35	1a	1491	G
35	1a	1492	A
35	1a	1494	G
35	1a	1497	G
35	1a	1499	A
35	1a	1502	A
35	1a	1506	U
35	1a	1517	G
35	1a	1520	C
35	1a	1529	G
35	1a	1530	G
35	1a	1533	C
35	1a	1534	A
35	1a	1535	C
35	1a	1536	C
58	1x	9	A
58	1x	19	G
58	1x	22	G
58	1x	47	U
58	1x	67	A

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1A	51	G
1	1A	86	G
1	1A	204	A
1	1A	242	G
1	1A	372	G
1	1A	458	G
1	1A	479	A
1	1A	490	C
1	1A	747	5MU
1	1A	752	A
1	1A	858	G
1	1A	859	G
1	1A	1020	A
1	1A	1022	G

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Mol	Chain	Res	Type
1	1A	1070	A
1	1A	1111	A
1	1A	1130	U
1	1A	1182	G
1	1A	1190	G
1	1A	1300	G
1	1A	1378	A
1	1A	1399	C
1	1A	1432	G
1	1A	1940	U
1	1A	2251	OMG
1	1A	2286	G
1	1A	2326	C
1	1A	2333	A
1	1A	2391	G
1	1A	2566	A
1	1A	2655	G
1	1A	2756	U
1	1A	2808	G
2	1B	66	A
2	1B	88	C

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

39 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
1	PSU	1A	2605	1	18,21,22	1.38	2 (11%)	22,30,33	1.97	3 (13%)
35	UR3	1a	1498	35	19,22,23	1.06	2 (10%)	26,32,35	1.57	4 (15%)
35	5MC	1a	1407	35	18,22,23	0.89	2 (11%)	26,32,35	1.12	2 (7%)
58	7MG	1x	46	58	22,26,27	1.29	2 (9%)	29,39,42	2.65	7 (24%)
1	PSU	1A	955	1	18,21,22	1.40	2 (11%)	22,30,33	2.05	3 (13%)
58	PSU	1x	65	58	18,21,22	1.37	3 (16%)	22,30,33	1.98	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
35	2MG	1a	966	35	18,26,27	0.96	1 (5%)	16,38,41	1.24	2 (12%)
58	5MU	1x	54	58	19,22,23	1.41	5 (26%)	28,32,35	2.13	8 (28%)
35	MA6	1a	1518	35	19,26,27	1.01	1 (5%)	18,38,41	1.90	6 (33%)
1	PSU	1A	1911	1	18,21,22	1.38	2 (11%)	22,30,33	2.04	3 (13%)
35	4OC	1a	1402	35	20,23,24	0.88	0	26,32,35	1.43	4 (15%)
35	PSU	1a	516	35	18,21,22	1.38	2 (11%)	22,30,33	2.04	3 (13%)
1	6MZ	1A	1618	1	18,25,26	0.86	1 (5%)	16,36,39	2.06	4 (25%)
1	5MU	1A	1939	1	19,22,23	1.46	6 (31%)	28,32,35	2.20	6 (21%)
1	PSU	1A	2580	1	18,21,22	1.36	2 (11%)	22,30,33	2.06	3 (13%)
1	6MZ	1A	2030	1	18,25,26	0.89	1 (5%)	16,36,39	2.34	4 (25%)
1	PSU	1A	2457	1	18,21,22	1.35	2 (11%)	22,30,33	2.12	3 (13%)
1	5MC	1A	1962	1	18,22,23	0.94	2 (11%)	26,32,35	1.33	4 (15%)
1	2MG	1A	1835	1	18,26,27	0.97	1 (5%)	16,38,41	1.29	2 (12%)
1	3TD	1A	1915	1	18,22,23	1.50	3 (16%)	22,32,35	2.18	5 (22%)
1	G7M	1A	2069	1	20,26,27	1.30	2 (10%)	17,39,42	0.80	1 (5%)
1	H2U	1A	2449	1	18,21,22	1.11	2 (11%)	21,30,33	1.63	3 (14%)
35	2MG	1a	1516	35	18,26,27	0.96	1 (5%)	16,38,41	1.19	1 (6%)
1	5MU	1A	747	1	19,22,23	1.50	5 (26%)	28,32,35	2.48	8 (28%)
1	1MG	1A	745	1	18,26,27	0.82	0	19,39,42	1.19	2 (10%)
1	PSU	1A	2604	1	18,21,22	1.38	2 (11%)	22,30,33	2.03	3 (13%)
35	5MC	1a	967	35	18,22,23	1.00	2 (11%)	26,32,35	1.40	5 (19%)
1	PSU	1A	1917	1	18,21,22	1.37	2 (11%)	22,30,33	1.98	3 (13%)
58	PSU	1x	55	58	18,21,22	1.37	2 (11%)	22,30,33	1.95	4 (18%)
1	PSU	1A	746	1	18,21,22	1.46	3 (16%)	22,30,33	1.96	4 (18%)
1	OMC	1A	2498	1	19,22,23	0.83	0	26,31,34	0.91	1 (3%)
1	2MG	1A	2445	1	18,26,27	0.89	1 (5%)	16,38,41	1.31	2 (12%)
35	7MG	1a	527	35	22,26,27	1.59	3 (13%)	29,39,42	2.52	8 (27%)
35	2MG	1a	1207	35	18,26,27	0.89	1 (5%)	16,38,41	1.40	3 (18%)
1	PSU	1A	2504	1	18,21,22	1.39	2 (11%)	22,30,33	2.02	3 (13%)
1	OMG	1A	2251	58,1	18,26,27	0.88	1 (5%)	19,38,41	1.23	2 (10%)
1	OMU	1A	2552	1	19,22,23	1.26	3 (15%)	26,31,34	1.82	6 (23%)
1	2MA	1A	2503	1	17,25,26	1.00	1 (5%)	17,37,40	1.13	2 (11%)
35	MA6	1a	1519	35	19,26,27	0.96	1 (5%)	18,38,41	1.81	6 (33%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	1A	2605	1	-	0/7/25/26	0/2/2/2
35	UR3	1a	1498	35	-	2/7/25/26	0/2/2/2
35	5MC	1a	1407	35	-	2/7/25/26	0/2/2/2
58	7MG	1x	46	58	-	2/7/37/38	0/3/3/3
1	PSU	1A	955	1	-	0/7/25/26	0/2/2/2
58	PSU	1x	65	58	-	0/7/25/26	0/2/2/2
35	2MG	1a	966	35	-	3/5/27/28	0/3/3/3
58	5MU	1x	54	58	-	0/7/25/26	0/2/2/2
35	MA6	1a	1518	35	-	2/7/29/30	0/3/3/3
1	PSU	1A	1911	1	-	0/7/25/26	0/2/2/2
35	4OC	1a	1402	35	-	3/9/29/30	0/2/2/2
35	PSU	1a	516	35	-	0/7/25/26	0/2/2/2
1	6MZ	1A	1618	1	-	1/5/27/28	0/3/3/3
1	5MU	1A	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	1A	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	1A	2030	1	-	2/5/27/28	0/3/3/3
1	PSU	1A	2457	1	-	2/7/25/26	0/2/2/2
1	5MC	1A	1962	1	-	4/7/25/26	0/2/2/2
1	2MG	1A	1835	1	-	0/5/27/28	0/3/3/3
1	3TD	1A	1915	1	-	4/7/25/26	0/2/2/2
1	G7M	1A	2069	1	-	2/3/25/26	0/3/3/3
1	H2U	1A	2449	1	-	0/7/38/39	0/2/2/2
35	2MG	1a	1516	35	-	0/5/27/28	0/3/3/3
1	5MU	1A	747	1	-	4/7/25/26	0/2/2/2
1	1MG	1A	745	1	-	0/3/25/26	0/3/3/3
1	PSU	1A	2604	1	-	0/7/25/26	0/2/2/2
35	5MC	1a	967	35	-	0/7/25/26	0/2/2/2
1	PSU	1A	1917	1	-	0/7/25/26	0/2/2/2
58	PSU	1x	55	58	-	2/7/25/26	0/2/2/2
1	PSU	1A	746	1	-	2/7/25/26	0/2/2/2
1	OMC	1A	2498	1	-	0/9/27/28	0/2/2/2
1	2MG	1A	2445	1	-	1/5/27/28	0/3/3/3
35	7MG	1a	527	35	-	3/7/37/38	0/3/3/3
35	2MG	1a	1207	35	-	2/5/27/28	0/3/3/3
1	PSU	1A	2504	1	-	2/7/25/26	0/2/2/2
1	OMG	1A	2251	58,1	-	4/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMU	1A	2552	1	-	3/9/27/28	0/2/2/2
1	2MA	1A	2503	1	-	2/3/25/26	0/3/3/3
35	MA6	1a	1519	35	-	1/7/29/30	0/3/3/3

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	1a	527	7MG	C4-N9	-4.77	1.32	1.37
1	1A	2605	PSU	C6-C5	3.71	1.39	1.35
58	1x	55	PSU	C6-C5	3.70	1.39	1.35
1	1A	955	PSU	C6-C5	3.60	1.39	1.35
1	1A	2504	PSU	C6-C5	3.57	1.39	1.35
1	1A	2069	G7M	C5-C4	3.56	1.46	1.39
1	1A	2604	PSU	C6-C5	3.53	1.39	1.35
35	1a	516	PSU	C6-C5	3.49	1.39	1.35
1	1A	2580	PSU	C6-C5	3.47	1.39	1.35
1	1A	1917	PSU	C6-C5	3.44	1.39	1.35
1	1A	747	5MU	C6-C5	3.43	1.40	1.34
1	1A	1911	PSU	C6-C5	3.42	1.39	1.35
1	1A	2457	PSU	C6-C5	3.35	1.39	1.35
1	1A	746	PSU	O4'-C1'	-3.18	1.39	1.43
1	1A	746	PSU	C6-C5	3.18	1.39	1.35
58	1x	46	7MG	C5-C4	3.13	1.48	1.38
1	1A	1915	3TD	C6-C5	3.11	1.38	1.35
1	1A	1915	3TD	C4-N3	-3.05	1.33	1.40
35	1a	527	7MG	C5-C4	2.98	1.47	1.38
1	1A	1835	2MG	C6-N1	-2.96	1.33	1.37
1	1A	1917	PSU	C4-N3	-2.94	1.33	1.38
1	1A	955	PSU	C4-N3	-2.94	1.33	1.38
1	1A	2504	PSU	C4-N3	-2.92	1.33	1.38
1	1A	1911	PSU	C4-N3	-2.89	1.33	1.38
1	1A	747	5MU	C4-N3	-2.89	1.33	1.38
1	1A	2457	PSU	C4-N3	-2.88	1.33	1.38
1	1A	2605	PSU	C4-N3	-2.88	1.33	1.38
1	1A	2449	H2U	C2-N3	-2.87	1.32	1.38
35	1a	516	PSU	C4-N3	-2.87	1.33	1.38
1	1A	2604	PSU	C4-N3	-2.87	1.33	1.38
35	1a	966	2MG	C6-N1	-2.86	1.33	1.37
1	1A	1939	5MU	C4-N3	-2.85	1.33	1.38
1	1A	2580	PSU	C4-N3	-2.85	1.33	1.38
1	1A	2552	OMU	C4-N3	-2.85	1.33	1.38
58	1x	55	PSU	C4-N3	-2.81	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1A	1939	5MU	C6-C5	2.80	1.39	1.34
58	1x	65	PSU	C6-C5	2.78	1.38	1.35
58	1x	54	5MU	C4-N3	-2.76	1.33	1.38
1	1A	2030	6MZ	C5-C4	2.67	1.48	1.40
58	1x	65	PSU	C4-N3	-2.64	1.33	1.38
35	1a	1498	UR3	C2-N1	2.62	1.42	1.38
1	1A	1915	3TD	O4'-C1'	-2.60	1.40	1.43
35	1a	967	5MC	C6-C5	2.59	1.38	1.34
1	1A	2449	H2U	C4-N3	-2.58	1.33	1.37
35	1a	1518	MA6	C5-C4	2.54	1.47	1.40
35	1a	1519	MA6	C5-C4	2.53	1.47	1.40
1	1A	746	PSU	C4-N3	-2.51	1.34	1.38
35	1a	1207	2MG	C6-N1	-2.49	1.34	1.37
1	1A	1618	6MZ	C5-C4	2.47	1.47	1.40
1	1A	2445	2MG	C6-N1	-2.47	1.34	1.37
1	1A	2069	G7M	C6-N1	-2.44	1.34	1.37
58	1x	54	5MU	C6-N1	-2.43	1.33	1.38
58	1x	54	5MU	C6-C5	2.43	1.38	1.34
1	1A	1939	5MU	C4-C5	2.43	1.48	1.44
58	1x	46	7MG	C6-N1	-2.42	1.34	1.38
58	1x	54	5MU	C2-N1	2.40	1.42	1.38
35	1a	967	5MC	C6-N1	-2.40	1.34	1.38
58	1x	65	PSU	O4'-C1'	-2.39	1.40	1.43
1	1A	1962	5MC	C6-N1	-2.39	1.34	1.38
35	1a	1407	5MC	C6-N1	-2.33	1.34	1.38
1	1A	1939	5MU	C6-N1	-2.32	1.34	1.38
1	1A	1962	5MC	C6-C5	2.32	1.38	1.34
35	1a	527	7MG	C6-N1	-2.31	1.34	1.38
35	1a	1407	5MC	C6-C5	2.28	1.38	1.34
1	1A	1939	5MU	C2-N1	2.24	1.42	1.38
1	1A	747	5MU	C4-C5	2.23	1.48	1.44
35	1a	1516	2MG	C6-N1	-2.22	1.34	1.37
1	1A	1939	5MU	C2-N3	-2.22	1.34	1.38
1	1A	2251	OMG	C6-N1	-2.22	1.34	1.37
1	1A	747	5MU	C2-N1	2.16	1.41	1.38
58	1x	54	5MU	C4-C5	2.13	1.48	1.44
1	1A	747	5MU	C2-N3	-2.10	1.34	1.38
1	1A	2503	2MA	C2-N3	2.08	1.35	1.31
35	1a	1498	UR3	C6-C5	2.06	1.39	1.35
1	1A	2552	OMU	C5-C4	-2.02	1.39	1.43
1	1A	2552	OMU	C2-N3	-2.02	1.34	1.38

All (147) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1x	46	7MG	N9-C4-N3	9.54	139.74	125.47
35	1a	527	7MG	N9-C4-N3	8.22	137.76	125.47
1	1A	1915	3TD	N1-C2-N3	7.44	122.01	116.14
1	1A	2457	PSU	N1-C2-N3	6.51	122.51	115.13
1	1A	2580	PSU	N1-C2-N3	6.45	122.43	115.13
35	1a	516	PSU	N1-C2-N3	6.33	122.30	115.13
1	1A	1911	PSU	N1-C2-N3	6.32	122.29	115.13
1	1A	955	PSU	N1-C2-N3	6.32	122.29	115.13
1	1A	2504	PSU	N1-C2-N3	6.30	122.27	115.13
1	1A	2604	PSU	N1-C2-N3	6.29	122.26	115.13
35	1a	527	7MG	N9-C8-N7	-6.18	94.54	103.38
1	1A	1917	PSU	N1-C2-N3	6.14	122.09	115.13
1	1A	2605	PSU	N1-C2-N3	6.10	122.04	115.13
58	1x	55	PSU	N1-C2-N3	6.02	121.95	115.13
58	1x	65	PSU	N1-C2-N3	6.00	121.93	115.13
1	1A	747	5MU	N3-C2-N1	5.92	122.75	114.89
1	1A	747	5MU	C4-N3-C2	-5.89	119.72	127.35
1	1A	746	PSU	N1-C2-N3	5.76	121.65	115.13
1	1A	1618	6MZ	C2-N1-C6	5.76	121.53	116.59
58	1x	46	7MG	C5-C4-N3	-5.73	117.21	128.13
1	1A	2030	6MZ	C9-N6-C6	-5.72	117.94	122.87
1	1A	2030	6MZ	C2-N1-C6	5.69	121.47	116.59
35	1a	1498	UR3	C4-N3-C2	-5.51	119.38	124.56
1	1A	1939	5MU	C4-N3-C2	-5.47	120.27	127.35
1	1A	747	5MU	C5-C6-N1	-5.22	117.97	123.34
1	1A	1939	5MU	N3-C2-N1	5.18	121.76	114.89
58	1x	54	5MU	C4-N3-C2	-5.15	120.68	127.35
35	1a	527	7MG	C5-C4-N3	-5.04	118.52	128.13
58	1x	46	7MG	N9-C8-N7	-4.83	96.48	103.38
1	1A	2552	OMU	C4-N3-C2	-4.81	120.24	126.58
1	1A	1939	5MU	C5-C4-N3	4.73	119.35	115.31
1	1A	2449	H2U	C4-N3-C2	-4.71	121.89	125.79
58	1x	54	5MU	C5-C4-N3	4.69	119.32	115.31
1	1A	2457	PSU	C4-N3-C2	-4.69	119.59	126.34
58	1x	54	5MU	N3-C2-N1	4.66	121.08	114.89
1	1A	747	5MU	C5-C4-N3	4.66	119.29	115.31
1	1A	2504	PSU	C4-N3-C2	-4.54	119.80	126.34
1	1A	2580	PSU	C4-N3-C2	-4.54	119.80	126.34
35	1a	516	PSU	C4-N3-C2	-4.50	119.86	126.34
1	1A	1911	PSU	C4-N3-C2	-4.47	119.90	126.34
1	1A	1917	PSU	C4-N3-C2	-4.41	119.99	126.34
1	1A	955	PSU	C4-N3-C2	-4.39	120.01	126.34
1	1A	2604	PSU	C4-N3-C2	-4.38	120.03	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	2605	PSU	C4-N3-C2	-4.35	120.06	126.34
1	1A	1939	5MU	C5-C6-N1	-4.26	118.96	123.34
58	1x	54	5MU	O4-C4-C5	-4.24	119.99	124.90
58	1x	46	7MG	C2-N3-C4	4.18	119.75	112.30
1	1A	2552	OMU	N3-C2-N1	4.18	120.44	114.89
1	1A	747	5MU	O4-C4-C5	-4.09	120.17	124.90
58	1x	55	PSU	C4-N3-C2	-4.07	120.47	126.34
35	1a	527	7MG	C2-N3-C4	4.06	119.53	112.30
58	1x	65	PSU	O2-C2-N1	-4.02	118.37	122.79
1	1A	2457	PSU	O2-C2-N1	-3.99	118.40	122.79
1	1A	1618	6MZ	C9-N6-C6	-3.96	119.46	122.87
58	1x	65	PSU	C4-N3-C2	-3.94	120.66	126.34
1	1A	1939	5MU	O4-C4-C5	-3.91	120.36	124.90
35	1a	1519	MA6	C10-N6-C6	-3.86	107.83	119.51
1	1A	2604	PSU	O2-C2-N1	-3.83	118.58	122.79
1	1A	1911	PSU	O2-C2-N1	-3.71	118.71	122.79
35	1a	1402	4OC	C1'-N1-C2	3.69	126.66	118.42
1	1A	955	PSU	O2-C2-N1	-3.68	118.74	122.79
1	1A	746	PSU	C4-N3-C2	-3.67	121.05	126.34
35	1a	1407	5MC	C5-C6-N1	-3.67	119.56	123.34
1	1A	1915	3TD	C4-N3-C2	-3.65	120.64	124.61
1	1A	2449	H2U	N3-C2-N1	3.64	120.50	116.65
1	1A	2580	PSU	O2-C2-N1	-3.63	118.79	122.79
35	1a	967	5MC	C5-C6-N1	-3.60	119.64	123.34
35	1a	1518	MA6	C4-C5-N7	-3.56	105.69	109.40
1	1A	2552	OMU	C5-C4-N3	3.55	120.16	114.84
35	1a	516	PSU	O2-C2-N1	-3.48	118.96	122.79
58	1x	54	5MU	C5-C6-N1	-3.47	119.77	123.34
1	1A	746	PSU	O2-C2-N1	-3.43	119.01	122.79
1	1A	2504	PSU	O2-C2-N1	-3.38	119.07	122.79
35	1a	1519	MA6	N3-C2-N1	-3.37	123.41	128.68
1	1A	1915	3TD	O4'-C1'-C2'	3.37	109.90	105.14
35	1a	1518	MA6	C10-N6-C6	-3.37	109.32	119.51
35	1a	1518	MA6	N3-C2-N1	-3.30	123.53	128.68
1	1A	2030	6MZ	C4-C5-N7	-3.29	105.97	109.40
58	1x	55	PSU	O2-C2-N1	-3.29	119.17	122.79
1	1A	1917	PSU	O2-C2-N1	-3.28	119.18	122.79
35	1a	1519	MA6	C4-C5-N7	-3.18	106.09	109.40
1	1A	747	5MU	O2-C2-N1	-3.17	118.57	122.79
1	1A	2605	PSU	O2-C2-N1	-3.14	119.33	122.79
35	1a	527	7MG	C5-C6-N1	3.10	116.45	110.99
1	1A	1962	5MC	C5-C6-N1	-3.08	120.17	123.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1A	1939	5MU	O2-C2-N1	-2.97	118.84	122.79
35	1a	967	5MC	C1'-N1-C6	-2.96	116.19	121.12
35	1a	1402	4OC	C1'-N1-C6	-2.96	114.40	120.84
35	1a	1518	MA6	C10-N6-C9	-2.95	106.61	116.12
1	1A	2552	OMU	O2-C2-N1	-2.94	118.87	122.79
1	1A	2030	6MZ	N3-C2-N1	-2.87	124.19	128.68
1	1A	2449	H2U	O2-C2-N1	-2.83	119.55	123.11
1	1A	746	PSU	O4'-C1'-C2'	2.81	109.10	105.14
1	1A	1962	5MC	C5-C4-N3	-2.78	118.67	121.67
1	1A	1962	5MC	C1'-N1-C6	-2.74	116.56	121.12
1	1A	2503	2MA	C8-N7-C5	2.73	108.19	102.99
58	1x	46	7MG	C5-C6-N1	2.70	115.74	110.99
1	1A	745	1MG	C5-C6-N1	2.69	117.94	113.90
58	1x	65	PSU	O4'-C1'-C2'	2.67	108.90	105.14
1	1A	1618	6MZ	C4-C5-N7	-2.65	106.64	109.40
1	1A	2503	2MA	C5-C6-N1	2.64	118.58	114.02
1	1A	1618	6MZ	N3-C2-N1	-2.63	124.57	128.68
1	1A	1962	5MC	CM5-C5-C6	-2.60	119.37	122.85
35	1a	1498	UR3	C6-N1-C2	-2.55	119.51	121.79
58	1x	46	7MG	C5-C4-N9	-2.54	103.05	106.35
1	1A	2498	OMC	CM2-O2'-C2'	-2.54	107.85	114.52
35	1a	1402	4OC	O2-C2-N3	-2.53	118.22	122.33
1	1A	2552	OMU	O4-C4-C5	-2.47	120.81	125.16
35	1a	1519	MA6	C10-N6-C9	-2.47	108.18	116.12
1	1A	1835	2MG	C5-C6-N1	2.45	118.28	113.95
35	1a	1519	MA6	C9-N6-C6	-2.44	112.13	119.51
35	1a	1498	UR3	C1'-N1-C2	2.39	121.02	116.99
35	1a	1207	2MG	O6-C6-C5	-2.36	119.75	124.37
1	1A	2251	OMG	C8-N7-C5	2.36	107.50	102.99
1	1A	1835	2MG	C8-N7-C5	2.36	107.49	102.99
58	1x	54	5MU	O2-C2-N1	-2.34	119.68	122.79
35	1a	967	5MC	C5-C4-N3	-2.34	119.15	121.67
35	1a	1498	UR3	O2-C2-N3	-2.34	118.05	121.34
1	1A	745	1MG	C8-N7-C5	2.33	107.43	102.99
35	1a	1207	2MG	C5-C6-N1	2.32	118.04	113.95
58	1x	46	7MG	O6-C6-C5	-2.30	121.89	127.54
1	1A	1915	3TD	C5-C6-N1	-2.30	118.66	122.11
1	1A	1915	3TD	C3'-C2'-C1'	2.27	104.28	101.64
58	1x	54	5MU	C5M-C5-C4	2.24	121.23	118.77
1	1A	2445	2MG	C8-N7-C5	2.23	107.24	102.99
35	1a	966	2MG	C8-N7-C5	2.22	107.22	102.99
1	1A	2251	OMG	C5-C6-N1	2.22	117.86	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	1a	1402	4OC	C6-C5-C4	2.19	119.64	116.96
35	1a	527	7MG	O6-C6-C5	-2.18	122.20	127.54
1	1A	2445	2MG	C5-C6-N1	2.18	117.80	113.95
35	1a	1518	MA6	N1-C6-N6	2.15	119.32	117.06
35	1a	967	5MC	O2-C2-N3	-2.14	118.85	122.33
35	1a	1407	5MC	C5-C4-N3	-2.13	119.38	121.67
58	1x	54	5MU	C1'-N1-C2	2.13	121.43	117.57
35	1a	966	2MG	C5-C6-N1	2.10	117.67	113.95
35	1a	1519	MA6	N1-C6-N6	2.09	119.26	117.06
35	1a	1518	MA6	C9-N6-C6	-2.09	113.20	119.51
1	1A	747	5MU	C1'-N1-C6	2.08	124.60	121.12
1	1A	2069	G7M	C3'-C2'-C1'	2.06	104.08	100.98
1	1A	2552	OMU	C5-C6-N1	-2.06	118.36	121.81
35	1a	1207	2MG	C8-N7-C5	2.04	106.87	102.99
35	1a	527	7MG	C5-C4-N9	-2.03	103.71	106.35
35	1a	1516	2MG	CM2-N2-C2	-2.03	119.39	123.86
58	1x	55	PSU	C6-C5-C4	-2.02	116.78	118.20
35	1a	527	7MG	C6-C5-N7	2.02	135.09	131.91
1	1A	747	5MU	C2'-C3'-C4'	2.01	106.55	102.64
35	1a	967	5MC	CM5-C5-C6	-2.00	120.17	122.85

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	746	PSU	O4'-C4'-C5'-O5'
1	1A	747	5MU	C2'-C1'-N1-C2
1	1A	747	5MU	C2'-C1'-N1-C6
1	1A	1618	6MZ	N1-C6-N6-C9
1	1A	1915	3TD	C2'-C1'-C5-C6
1	1A	1915	3TD	O4'-C1'-C5-C6
1	1A	1915	3TD	C3'-C4'-C5'-O5'
1	1A	1962	5MC	O4'-C4'-C5'-O5'
1	1A	1962	5MC	C3'-C4'-C5'-O5'
1	1A	2251	OMG	O4'-C4'-C5'-O5'
1	1A	2251	OMG	C3'-C4'-C5'-O5'
1	1A	2251	OMG	C1'-C2'-O2'-CM2
1	1A	2504	PSU	C3'-C4'-C5'-O5'
1	1A	2504	PSU	O4'-C4'-C5'-O5'
35	1a	527	7MG	C3'-C4'-C5'-O5'
35	1a	1207	2MG	C3'-C4'-C5'-O5'
35	1a	1402	4OC	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
35	1a	1407	5MC	O4'-C4'-C5'-O5'
35	1a	1407	5MC	C3'-C4'-C5'-O5'
35	1a	1498	UR3	O4'-C1'-N1-C6
35	1a	1498	UR3	O4'-C1'-N1-C2
35	1a	1518	MA6	C5-C6-N6-C9
58	1x	55	PSU	O4'-C1'-C5-C4
58	1x	55	PSU	O4'-C1'-C5-C6
1	1A	746	PSU	C3'-C4'-C5'-O5'
1	1A	2030	6MZ	O4'-C4'-C5'-O5'
1	1A	2030	6MZ	C3'-C4'-C5'-O5'
58	1x	46	7MG	O4'-C4'-C5'-O5'
1	1A	1915	3TD	O4'-C4'-C5'-O5'
1	1A	2552	OMU	C4'-C5'-O5'-P
35	1a	527	7MG	O4'-C4'-C5'-O5'
35	1a	527	7MG	C4'-C5'-O5'-P
35	1a	1207	2MG	O4'-C4'-C5'-O5'
58	1x	46	7MG	C3'-C4'-C5'-O5'
35	1a	1518	MA6	N1-C6-N6-C9
1	1A	2251	OMG	C4'-C5'-O5'-P
1	1A	2445	2MG	C4'-C5'-O5'-P
1	1A	2552	OMU	O4'-C4'-C5'-O5'
1	1A	2552	OMU	C3'-C4'-C5'-O5'
35	1a	1519	MA6	C5-C6-N6-C9
1	1A	747	5MU	O4'-C1'-N1-C6
1	1A	1962	5MC	C2'-C1'-N1-C6
1	1A	2503	2MA	C4'-C5'-O5'-P
35	1a	966	2MG	C4'-C5'-O5'-P
35	1a	966	2MG	C3'-C4'-C5'-O5'
1	1A	2069	G7M	O4'-C4'-C5'-O5'
1	1A	2457	PSU	O4'-C1'-C5-C4
1	1A	1962	5MC	O4'-C1'-N1-C6
35	1a	1402	4OC	C2'-C1'-N1-C6
1	1A	2069	G7M	C4'-C5'-O5'-P
35	1a	966	2MG	O4'-C4'-C5'-O5'
35	1a	1402	4OC	C2'-C1'-N1-C2
1	1A	747	5MU	O4'-C1'-N1-C2
1	1A	2457	PSU	O4'-C1'-C5-C6
1	1A	2503	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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$
59	EVN	1A	3001	1	117,123,123	1.94	19 (16%)	155,191,191	1.91	34 (21%)

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
59	EVN	1A	3001	1	-	23/50/234/234	1/13/13/13

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	3001	EVN	ODS-NDQ	10.70	1.45	1.22
59	1A	3001	EVN	CDN-CAC	-6.50	1.38	1.51
59	1A	3001	EVN	OCW-CCQ	5.84	1.45	1.40
59	1A	3001	EVN	CEG-CDI	-5.70	1.39	1.51
59	1A	3001	EVN	CDD-CDB	-4.50	1.39	1.50
59	1A	3001	EVN	CAD-CAJ	-4.27	1.40	1.50
59	1A	3001	EVN	ODT-CAX	3.87	1.49	1.42
59	1A	3001	EVN	OCZ-CCY	3.53	1.47	1.41
59	1A	3001	EVN	OCX-CCY	3.49	1.47	1.41
59	1A	3001	EVN	CCT-CCS	-2.86	1.48	1.53
59	1A	3001	EVN	OCN-CCM	2.76	1.48	1.43
59	1A	3001	EVN	OBX-CBW	2.39	1.48	1.43
59	1A	3001	EVN	CAY-NDQ	-2.22	1.48	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	1A	3001	EVN	OBE-CBD	2.17	1.43	1.41
59	1A	3001	EVN	OCN-CCI	2.12	1.46	1.41
59	1A	3001	EVN	OBQ-CBM	2.09	1.47	1.41
59	1A	3001	EVN	OAL-CAJ	2.08	1.38	1.34
59	1A	3001	EVN	OBK-CBD	2.02	1.45	1.41
59	1A	3001	EVN	CBI-CBJ	-2.01	1.48	1.54

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	3001	EVN	OCX-CCS-CCT	-9.11	99.01	106.63
59	1A	3001	EVN	OCZ-CCT-CCS	-6.12	98.47	106.41
59	1A	3001	EVN	CAE-CAF-CLAG	5.67	128.17	118.90
59	1A	3001	EVN	CAF-CAA-CAB	5.39	123.19	117.81
59	1A	3001	EVN	OCR-CCL-CCK	-5.30	94.64	103.49
59	1A	3001	EVN	CAA-CAB-CAC	-4.25	120.09	122.79
59	1A	3001	EVN	O1-CCI-OCN	3.93	117.83	109.08
59	1A	3001	EVN	OBK-CBJ-CBI	-3.92	96.90	104.14
59	1A	3001	EVN	CAP-OAQ-CAR	-3.55	104.28	113.84
59	1A	3001	EVN	CDM-ODL-CAE	3.42	124.15	114.78
59	1A	3001	EVN	CAA-CAF-CAE	-3.40	115.65	120.63
59	1A	3001	EVN	CBD-OBE-CBF	-3.38	109.09	112.16
59	1A	3001	EVN	CCY-OCZ-CCT	-3.31	101.27	106.31
59	1A	3001	EVN	OBE-CBF-CDW	3.27	109.92	105.85
59	1A	3001	EVN	OCP-CCK-CCL	-3.24	98.90	103.47
59	1A	3001	EVN	CDW-CBF-CBA	-2.92	108.95	113.41
59	1A	3001	EVN	ODL-CAE-CAD	-2.64	113.95	120.18
59	1A	3001	EVN	CEF-O2-C2	-2.61	107.68	114.52
59	1A	3001	EVN	ODJ-CDE-CDD	-2.50	116.47	121.14
59	1A	3001	EVN	CCM-CCL-CCK	-2.48	107.47	112.49
59	1A	3001	EVN	CBV-O4-C4	-2.47	111.85	117.96
59	1A	3001	EVN	CAP-OAS-CBA	-2.40	109.80	114.66
59	1A	3001	EVN	OCW-CCQ-OCR	2.36	114.32	109.91
59	1A	3001	EVN	OAL-CAM-CAR	2.36	112.53	107.83
59	1A	3001	EVN	ODL-CAE-CAF	2.21	123.33	120.05
59	1A	3001	EVN	O1-C1-C2	2.17	113.50	109.10
59	1A	3001	EVN	OBQ-CBR-CBW	2.15	113.01	107.28
59	1A	3001	EVN	CDX-CBO-CBJ	-2.15	109.23	113.52
59	1A	3001	EVN	CDY-CBI-CBJ	-2.15	108.55	114.85
59	1A	3001	EVN	OAV-CAW-CDP	2.09	111.21	106.70
59	1A	3001	EVN	O2-C2-C3	-2.08	105.31	110.29
59	1A	3001	EVN	O4-C4-C3	2.04	112.71	107.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	1A	3001	EVN	CDP-CAW-CAX	-2.03	109.47	113.52
59	1A	3001	EVN	OAL-CAM-CAN	2.02	112.27	108.22

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	3001	EVN	C2-C1-O1-CCI
59	1A	3001	EVN	CAO-CAP-OAS-CBA
59	1A	3001	EVN	OAQ-CAP-OAS-CBA
59	1A	3001	EVN	CAW-CAX-ODT-CDU
59	1A	3001	EVN	OAK-CAJ-OAL-CAM
59	1A	3001	EVN	CAD-CAJ-OAL-CAM
59	1A	3001	EVN	CAF-CAE-ODL-CDM
59	1A	3001	EVN	C3-C4-O4-CBV
59	1A	3001	EVN	OAV-CAU-OAT-CAN
59	1A	3001	EVN	CAZ-CAU-OAT-CAN
59	1A	3001	EVN	CBF-CBA-OAS-CAP
59	1A	3001	EVN	O5-C5-C6-O6
59	1A	3001	EVN	CAD-CAE-ODL-CDM
59	1A	3001	EVN	CBW-CBR-OBQ-CBM
59	1A	3001	EVN	CBB-CBA-OAS-CAP
59	1A	3001	EVN	CBS-CBR-OBQ-CBM
59	1A	3001	EVN	C5-C6-O6-CED
59	1A	3001	EVN	CAR-CAM-OAL-CAJ
59	1A	3001	EVN	OCN-CCI-O1-C1
59	1A	3001	EVN	C5-C4-O4-CBV
59	1A	3001	EVN	OBN-CBM-OBQ-CBR
59	1A	3001	EVN	CBL-CBM-OBQ-CBR
59	1A	3001	EVN	CAZ-CAY-NDQ-ODS

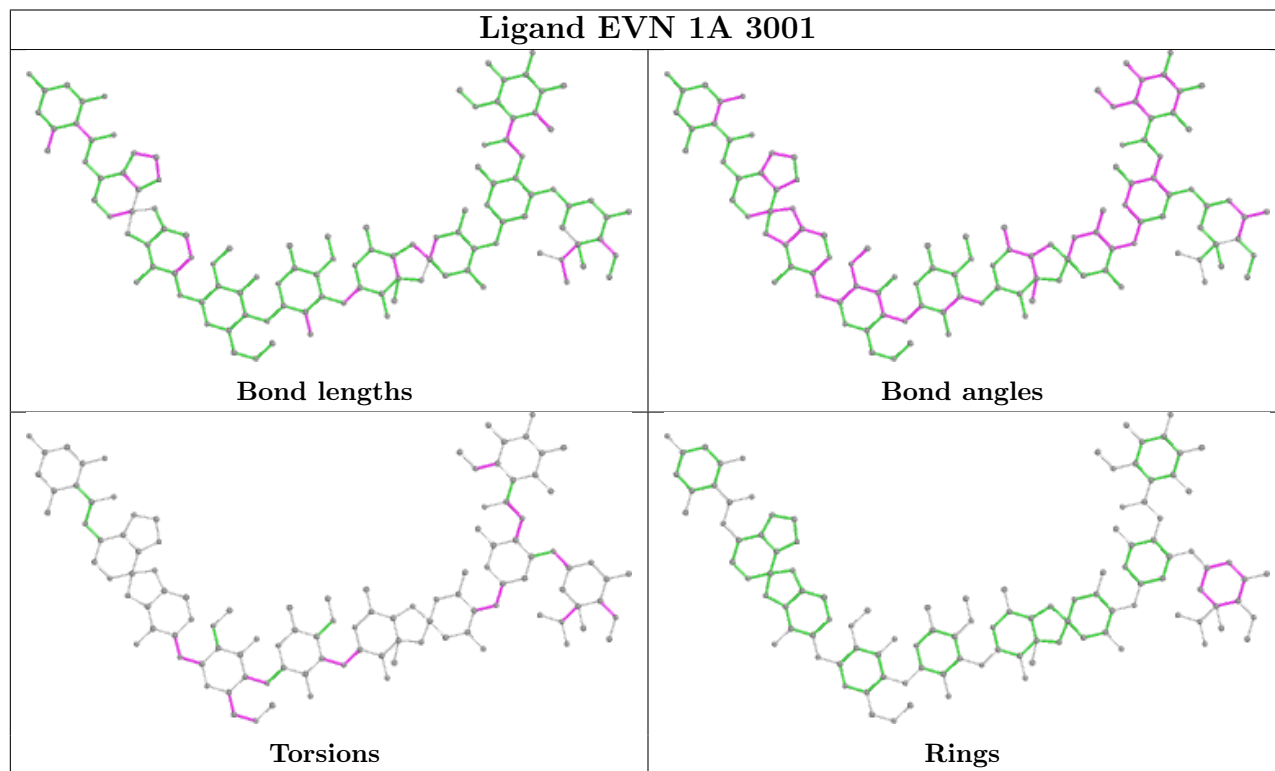
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1A	3001	EVN	CAU-CAW-CAX-CAY-CAZ-OAV

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 than 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.



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.

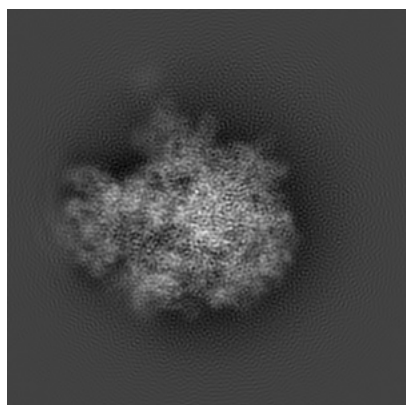
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8238. These allow visual inspection of the internal detail of the map and identification of artifacts.

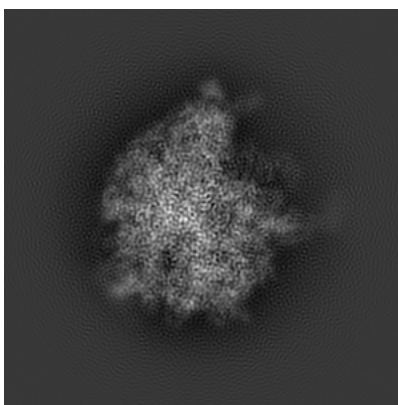
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

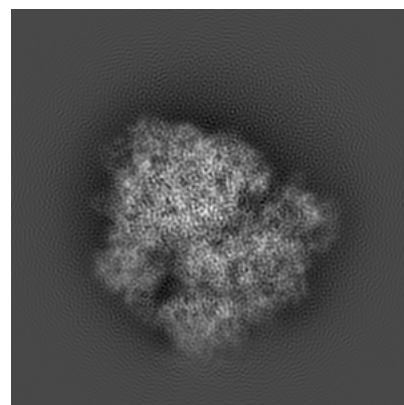
6.1.1 Primary map



X



Y

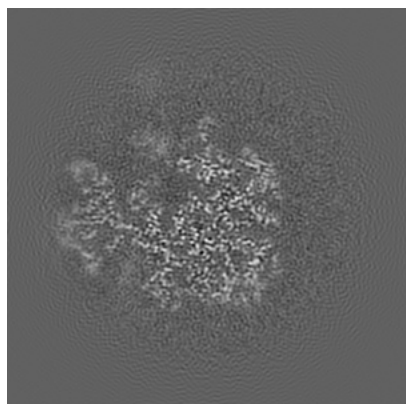


Z

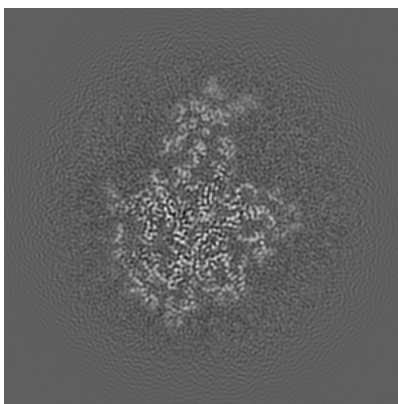
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

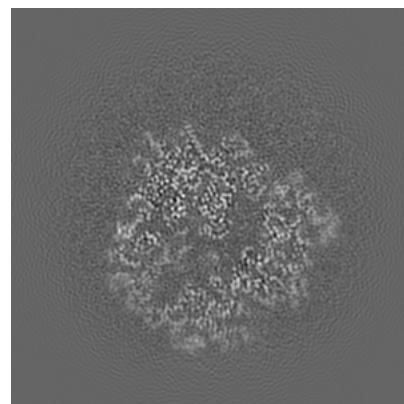
6.2.1 Primary map



X Index: 184



Y Index: 184

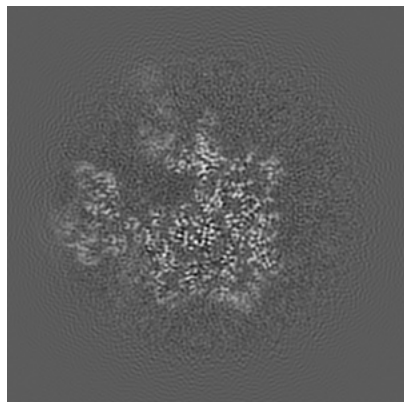


Z Index: 184

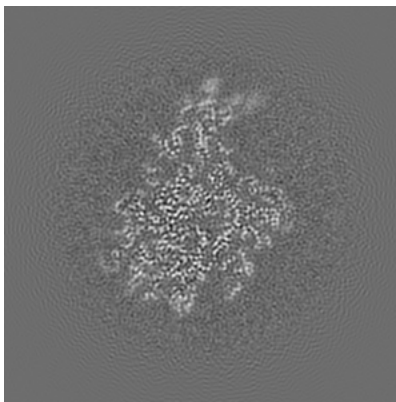
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

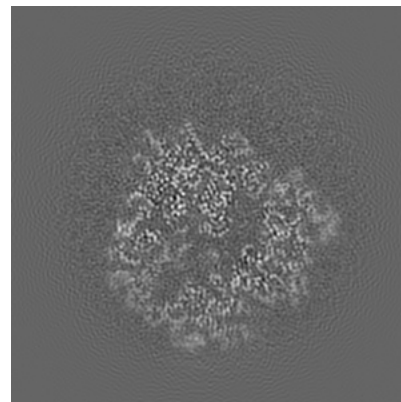
6.3.1 Primary map



X Index: 179



Y Index: 177



Z Index: 184

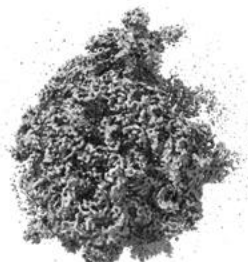
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00307. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

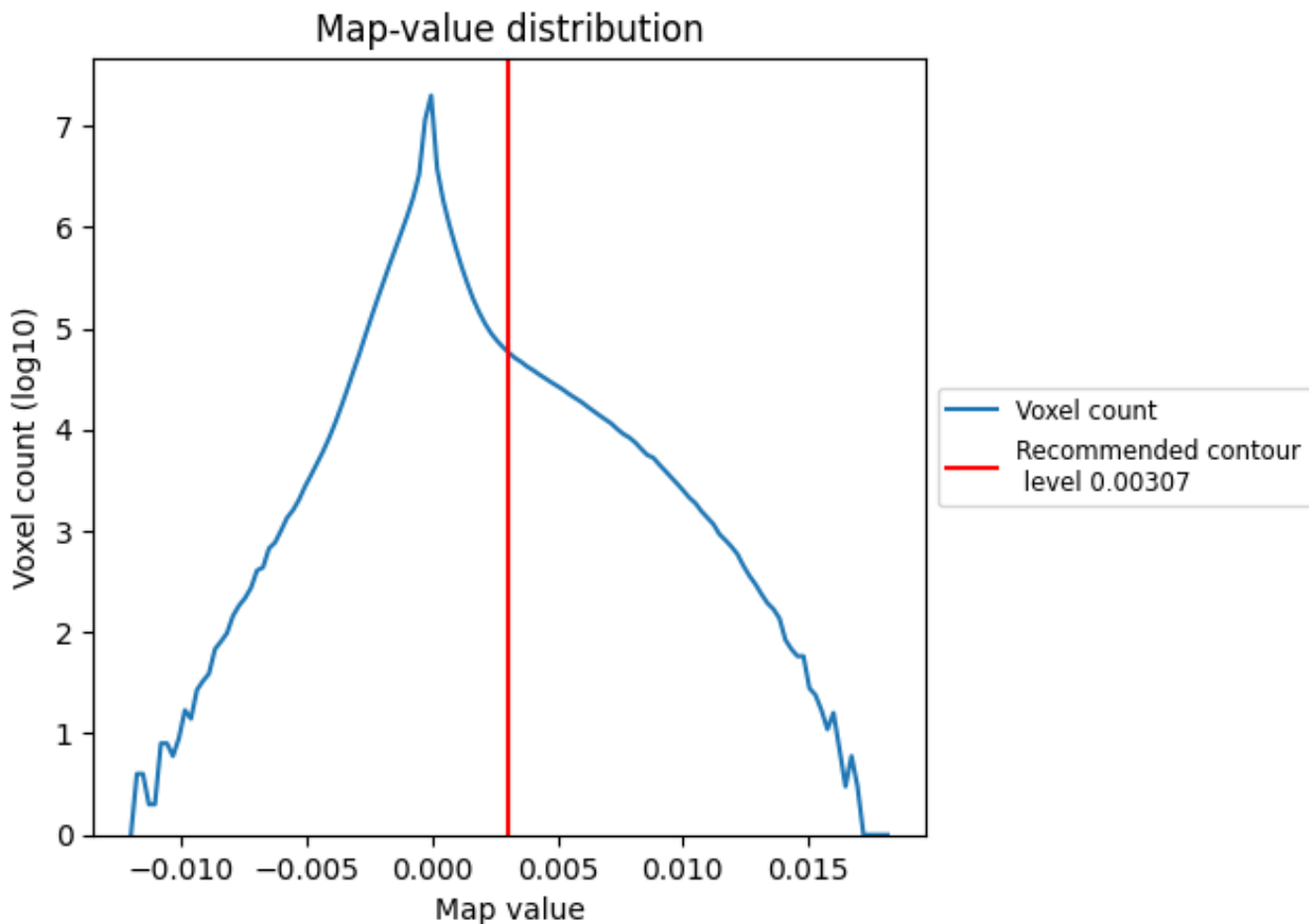
6.5 Mask visualisation

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

7 Map analysis [i](#)

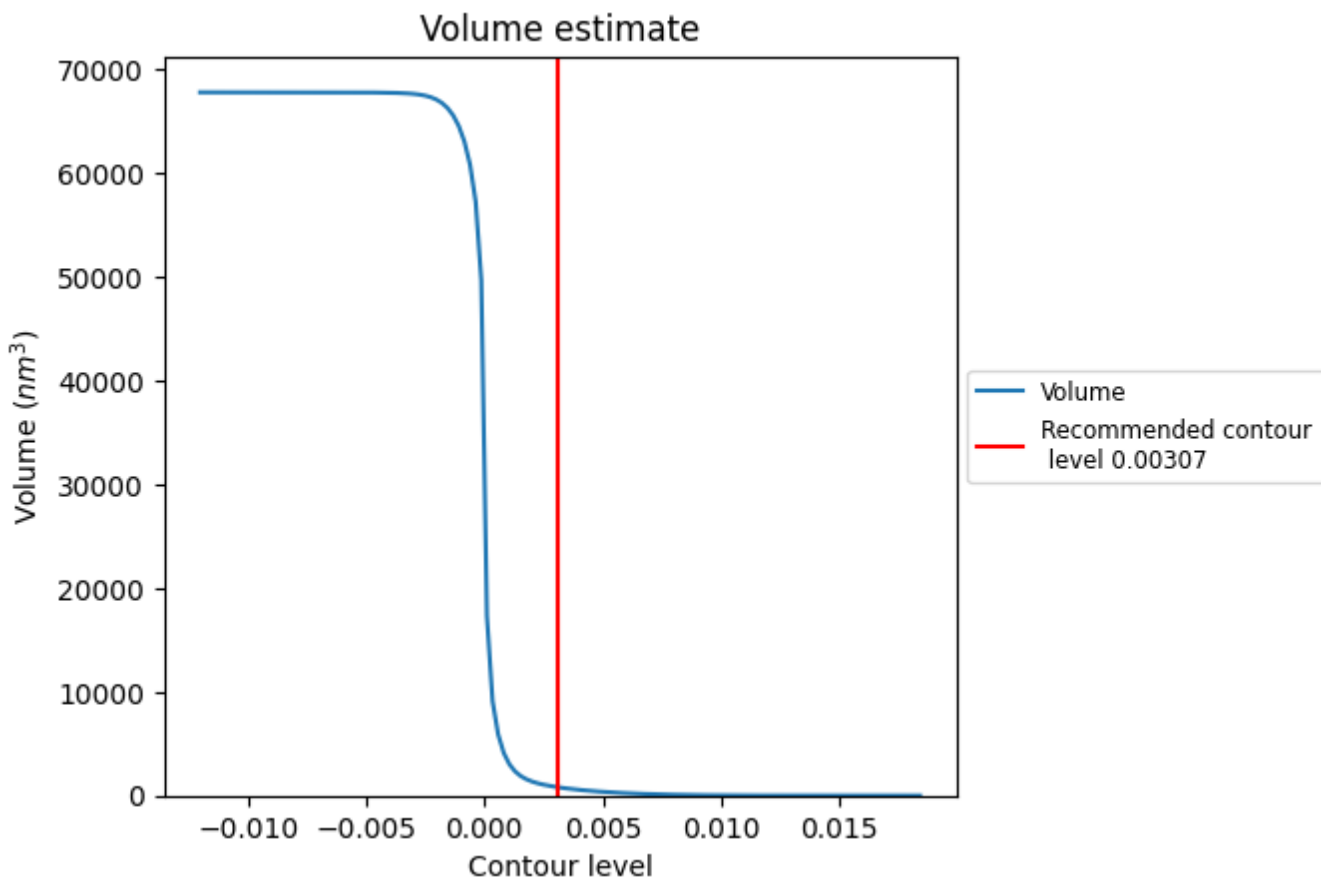
This section contains the results of statistical analysis of the map.

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.

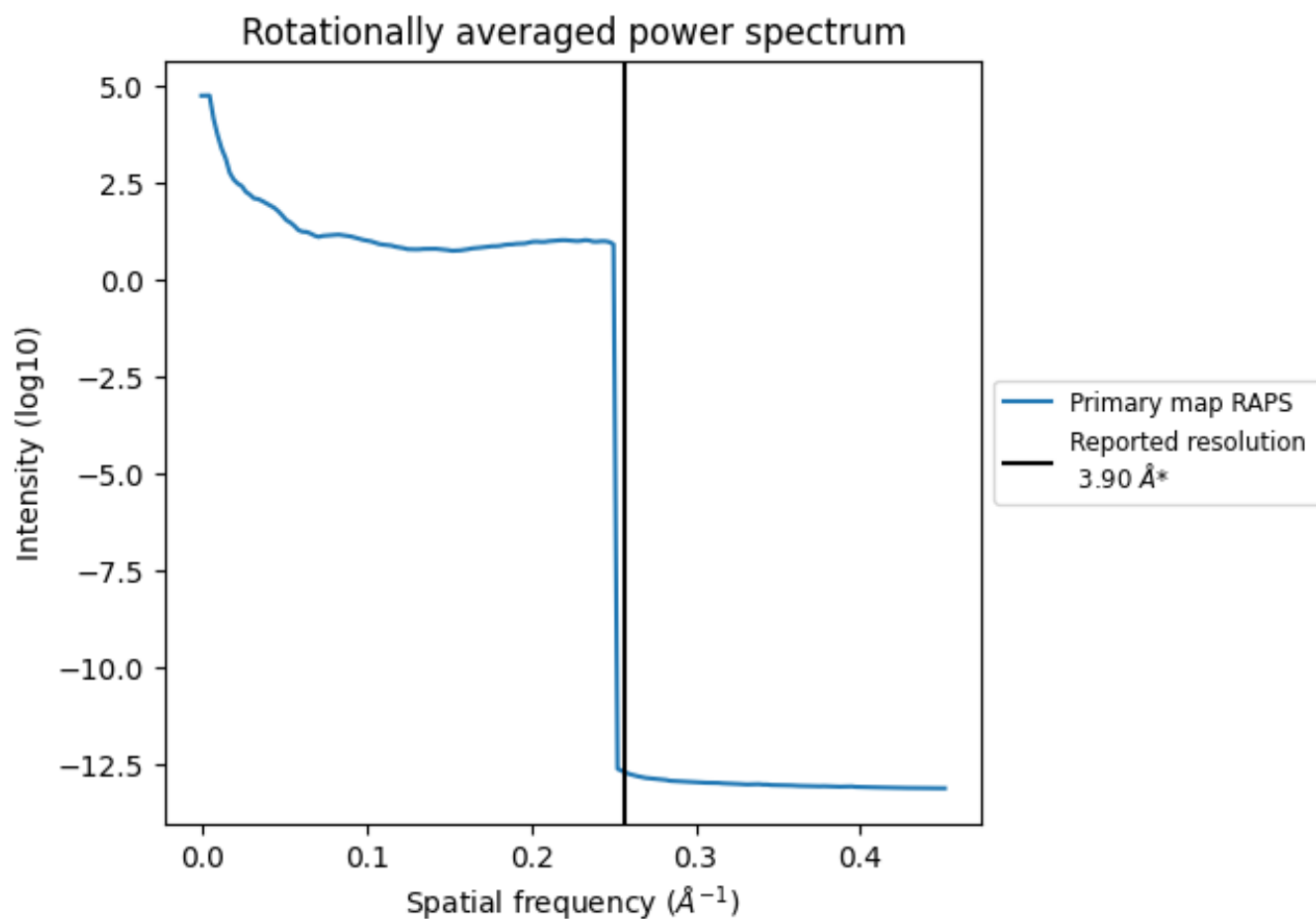
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 816 nm³; this corresponds to an approximate mass of 737 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 0.256 \AA^{-1}

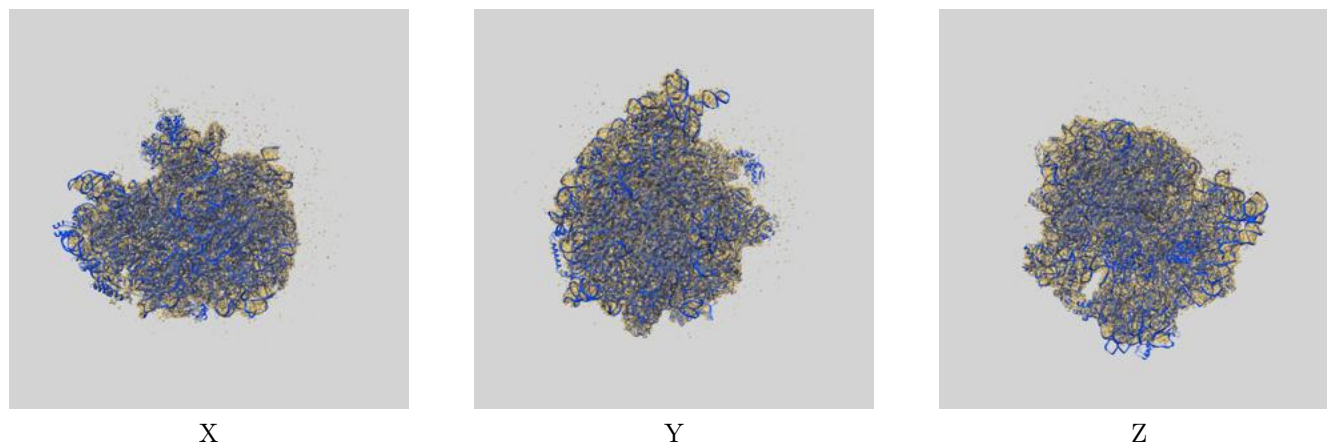
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

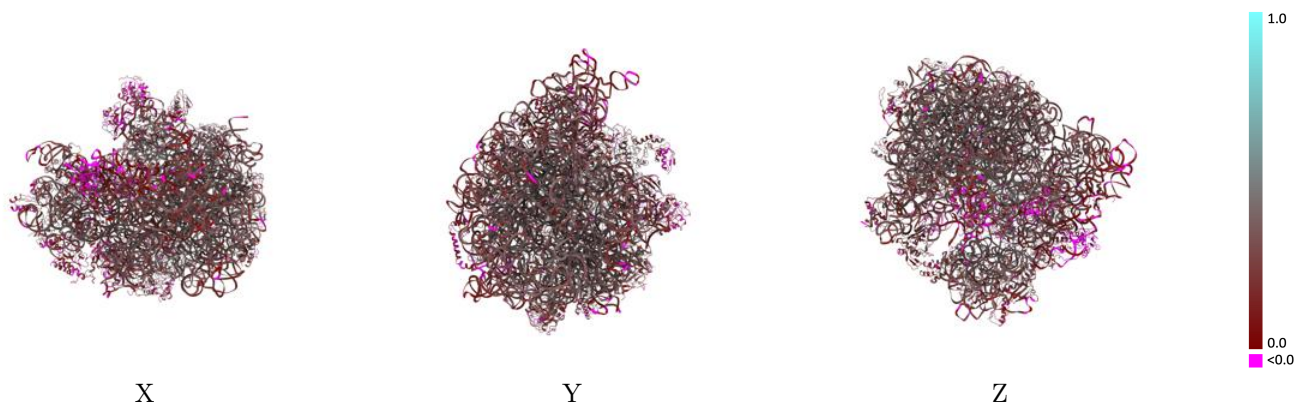
This section contains information regarding the fit between EMDB map EMD-8238 and PDB model 5KCS. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



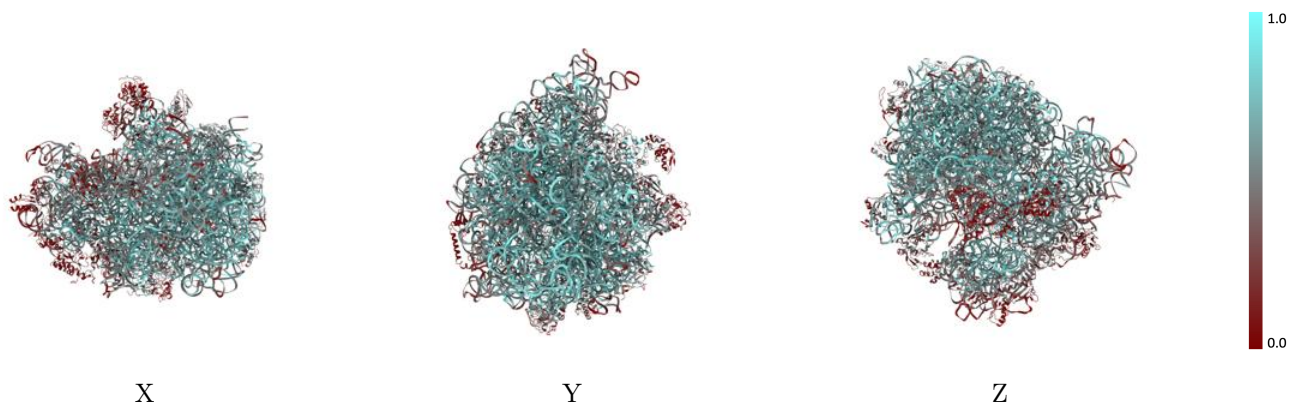
The images above show the 3D surface view of the map at the recommended contour level 0.00307 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



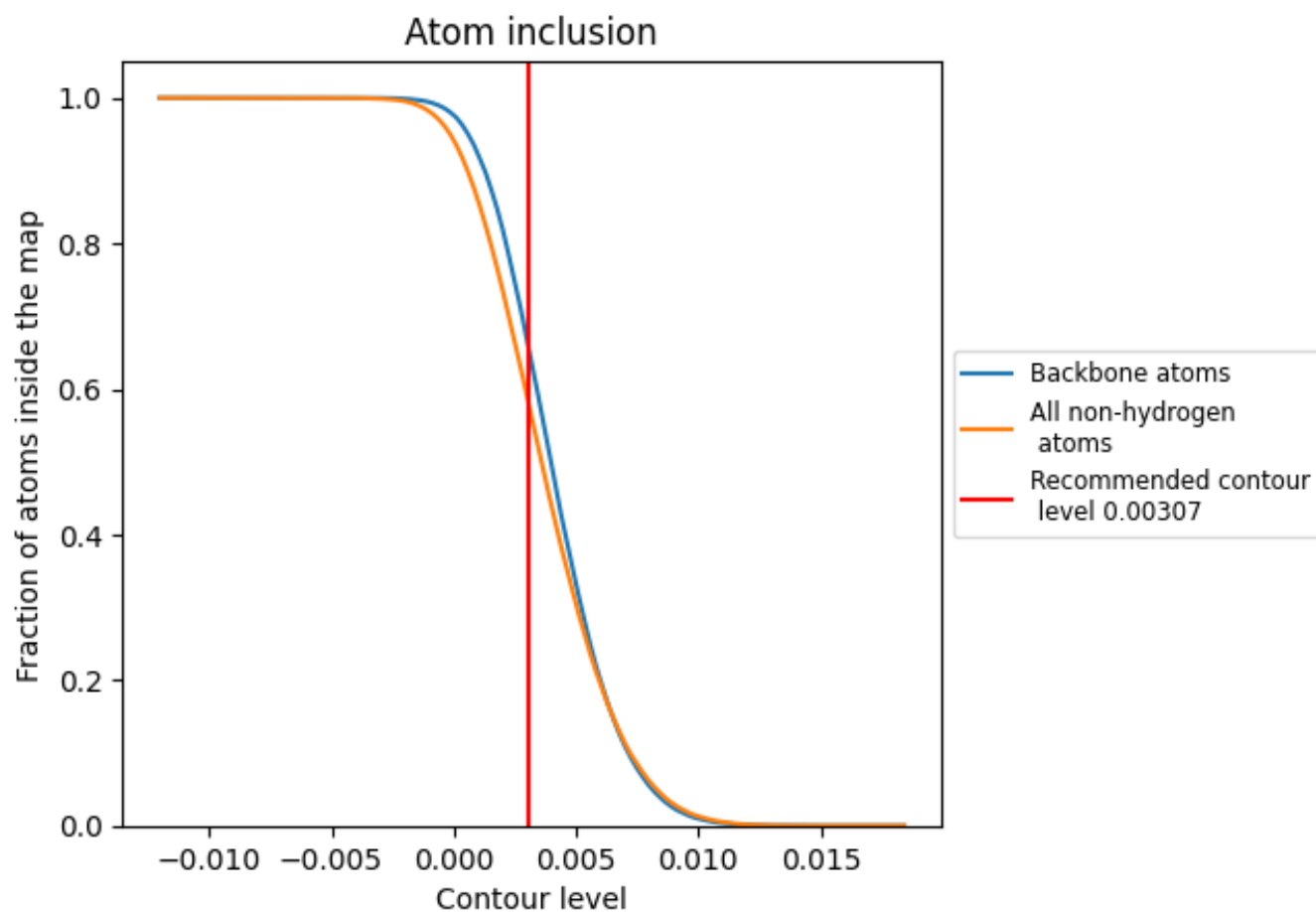
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.00307).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

















































The table lists the average atom inclusion at the recommended contour level (0.00307) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5784	 0.2930
10	 0.5778	 0.3400
11	 0.5291	 0.3340
12	 0.4326	 0.2550
13	 0.5263	 0.3310
14	 0.2114	 0.1720
15	 0.5421	 0.3270
16	 0.0923	 0.1900
17	 0.6254	 0.3430
18	 0.5804	 0.3540
19	 0.5890	 0.3360
1A	 0.6815	 0.3250
1B	 0.6482	 0.2900
1D	 0.5863	 0.3510
1E	 0.5364	 0.3240
1F	 0.4671	 0.2970
1G	 0.3678	 0.2320
1H	 0.4025	 0.2420
1I	 0.0967	 0.1240
1J	 0.0640	 0.0470
1K	 0.0763	 0.0790
1L	 0.0507	 0.0670
1N	 0.5645	 0.3080
1O	 0.5170	 0.3210
1P	 0.4833	 0.2900
1Q	 0.5864	 0.3890
1R	 0.5662	 0.3360
1S	 0.4009	 0.2380
1T	 0.5101	 0.2950
1U	 0.6189	 0.3520
1V	 0.4918	 0.2850
1W	 0.5478	 0.3350
1X	 0.4834	 0.2990
1Y	 0.4198	 0.2820
1Z	 0.4729	 0.2870



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Chain	Atom inclusion	Q-score
1a	 0.6148	 0.2830
1b	 0.1875	 0.1630
1c	 0.3859	 0.2920
1d	 0.2748	 0.0620
1e	 0.4272	 0.2330
1f	 0.4121	 0.2290
1g	 0.3208	 0.2650
1h	 0.4760	 0.2870
1i	 0.2625	 0.2500
1j	 0.2181	 0.2390
1k	 0.3799	 0.1990
1l	 0.3051	 0.0930
1m	 0.3772	 0.2740
1n	 0.4364	 0.3030
1o	 0.4942	 0.2860
1p	 0.4242	 0.1710
1q	 0.4209	 0.2330
1r	 0.4887	 0.3050
1s	 0.4412	 0.2780
1t	 0.4523	 0.2520
1u	 0.1513	 0.1390
1v	 0.4635	 0.2870
1w	 0.5508	 0.3290
1x	 0.5839	 0.3020