



Full wwPDB EM Validation Report ⓘ

Dec 11, 2022 – 11:39 am GMT

PDB ID : 5AFI
EMDB ID : EMD-2847
Title : 2.9Å Structure of E. coli ribosome-EF-TU complex by cs-corrected cryo-EM
Authors : Fischer, N.; Neumann, P.; Konevega, A.L.; Bock, L.V.; Ficner, R.; Rodnina, M.V.; Stark, H.
Deposited on : 2015-01-22
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

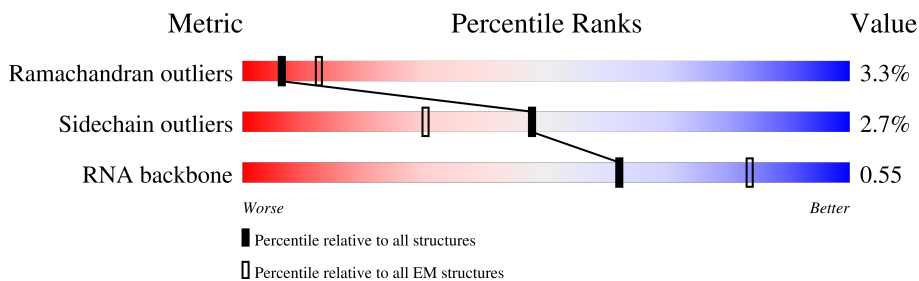
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	a	1539	
2	b	240	
3	c	233	
4	d	206	
5	e	167	
6	f	135	
7	g	179	
8	h	130	

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Mol	Chain	Length	Quality of chain
9	i	130	10% 88% 10%
10	j	103	22% 87% 8% 5%
11	k	129	5% 84% 6% 10%
12	l	124	9% 93% 6%
13	m	118	16% 91% 6%
14	n	102	11% 90% 9%
15	o	89	6% 91% 8%
16	p	82	11% 93% 7%
17	q	84	10% 86% 10% 5%
18	r	75	11% 79% 8% 13%
19	s	92	7% 85% 14%
20	t	87	5% 93% 5%
21	u	71	30% 82% 10% 8%
22	v	77	6% 74% 23%
22	w	77	47% 35% 49% 16%
23	x	11	9% 82% 18%
24	y	77	6% 68% 27% 5%
25	z	393	13% 91% 6%
26	A	2903	5% 79% 20%
27	B	120	. 84% 16%
28	C	273	. 95% 5%
29	D	209	5% 98% .
30	E	201	8% 94% 6%
31	F	179	16% 92% 7%
32	G	177	14% 97% ..

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Mol	Chain	Length	Quality of chain
33	H	149	80% 97%
34	I	142	85% 91% 8%
35	J	142	5% 97%
36	K	123	93% 7%
37	L	144	6% 90% 9%
38	M	136	97%
39	N	127	91% 6%
40	O	117	11% 97%
41	P	115	10% 96%
42	Q	118	97%
43	R	103	8% 97%
44	S	110	6% 93% 6%
45	T	100	9% 87% 5% 7%
46	U	104	17% 94%
47	V	94	11% 97%
48	W	85	5% 86% 12%
49	X	78	8% 97%
50	Y	63	16% 97%
51	Z	59	7% 98%
52	0	57	7% 93% 5%
53	1	55	15% 89% 9%
54	2	46	7% 100%
55	3	65	5% 95%
56	4	38	100%
57	5	165	73% 73% 6% 21%

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Mol	Chain	Length	Quality of chain
58	6	70	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '36%', a green segment in the middle labeled '91%', and a yellow/grey segment on the right labeled '6%'. The green segment is the largest, followed by the red segment, and the yellow/grey segment is the smallest.</p>

2 Entry composition [i](#)

There are 66 unique types of molecules in this entry. The entry contains 152717 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

- Molecule 2 is a protein called 30S ribosomal protein S2.

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

- Molecule 3 is a protein called 30S ribosomal protein S3.

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

- Molecule 4 is a protein called 30S ribosomal protein S4.

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

- Molecule 5 is a protein called 30S ribosomal protein S5.

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

- Molecule 6 is a protein called 30S ribosomal protein S6.

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

- Molecule 7 is a protein called 30S ribosomal protein S7.

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

- Molecule 8 is a protein called 30S ribosomal protein S8.

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

- Molecule 9 is a protein called 30S ribosomal protein S9.

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

- Molecule 10 is a protein called 30S ribosomal protein S10.

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

- Molecule 11 is a protein called 30S ribosomal protein S11.

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

- Molecule 12 is a protein called 30S ribosomal protein S12.

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

- Molecule 13 is a protein called 30S ribosomal protein S13.

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

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	101	799	498	165	133	3	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 15 is a protein called 30S ribosomal protein S15.

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

- Molecule 16 is a protein called 30S ribosomal protein S16.

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

- Molecule 17 is a protein called 30S ribosomal protein S17.

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

- Molecule 18 is a protein called 30S ribosomal protein S18.

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

- Molecule 19 is a protein called 30S ribosomal protein S19.

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

- Molecule 20 is a protein called 30S ribosomal protein S20.

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

- Molecule 21 is a protein called 30S ribosomal protein S21.

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

- Molecule 22 is a RNA chain called P-site fMet-tRNA^{fMet}.

Mol	Chain	Residues	Atoms					AltConf	Trace	
22	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		
22	w	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	x	11	Total	C	N	O	P	0	0
			234	105	41	77	11		

- Molecule 24 is a RNA chain called A/T-site Phe-tRNA^{Phe}.

Mol	Chain	Residues	Atoms					AltConf	Trace	
24	y	77	Total	C	N	O	P	S	0	0
			1643	740	291	534	76	2		

- Molecule 25 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	371	Total	C	N	O	S	1	0
			2881	1824	495	549	13		

- Molecule 26 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	2900	Total	C	N	O	P	0	0
			62276	27788	11460	20128	2900		

- Molecule 27 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
27	B	120	2572	1145	471	836	120	0	0

- Molecule 28 is a protein called 50S ribosomal protein L2.

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

- Molecule 29 is a protein called 50S ribosomal protein L3.

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

- Molecule 30 is a protein called 50S ribosomal protein L4.

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

- Molecule 31 is a protein called 50S ribosomal protein L5.

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

- Molecule 32 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	G	176	1323	832	243	246	2	0	0

- Molecule 33 is a protein called 50S ribosomal protein L9.

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

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	I	141	1032	651	179	196	6	0	0

- Molecule 35 is a protein called 50S ribosomal protein L13.

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

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

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

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	M	136	1074	686	205	177	6	0	0

- Molecule 39 is a protein called 50S ribosomal protein L17.

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

- Molecule 40 is a protein called 50S ribosomal protein L18.

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

- Molecule 41 is a protein called 50S ribosomal protein L19.

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

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Q	117	947	604	192	151		0	0

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	R	103	816	516	153	145	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L22.

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

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	T	93	738	466	139	131	2	0	0

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	U	102	779	492	146	141		0	0

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	V	94	753	479	137	134	3	0	0

- Molecule 48 is a protein called 50S ribosomal protein L27.

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

- Molecule 49 is a protein called 50S ribosomal protein L28.

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

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

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

- Molecule 51 is a protein called 50S ribosomal protein L30.

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

- Molecule 52 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	0	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 53 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 54 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 55 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 56 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 57 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 58 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

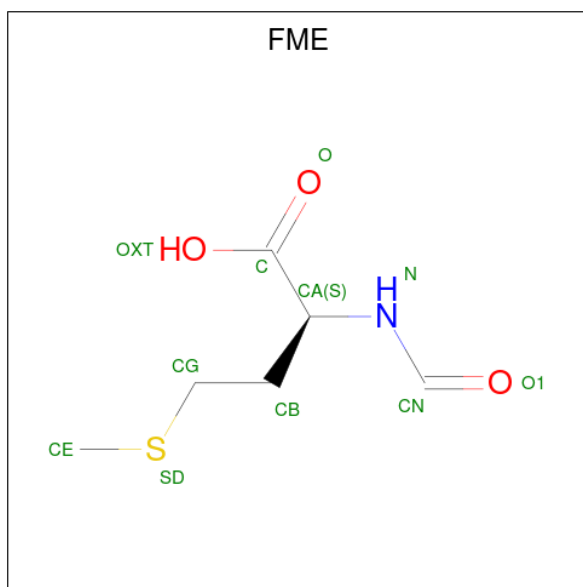
- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	a	83	Total	Mg	0
			83	83	
59	v	4	Total	Mg	0
			4	4	
59	z	1	Total	Mg	0
			1	1	
59	A	234	Total	Mg	0
			234	234	
59	B	7	Total	Mg	0
			7	7	
59	N	2	Total	Mg	0
			2	2	
59	0	1	Total	Mg	0
			1	1	
59	4	1	Total	Mg	0
			1	1	

- Molecule 60 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

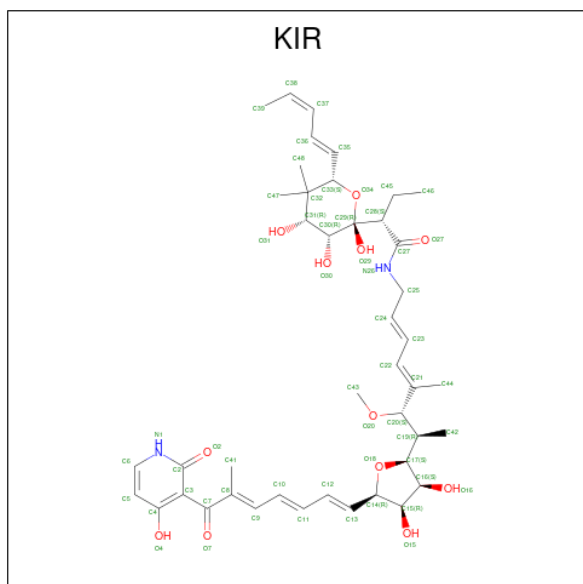
Mol	Chain	Residues	Atoms	AltConf
60	a	1	Total Cl 1 1	0
60	A	1	Total Cl 1 1	0

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



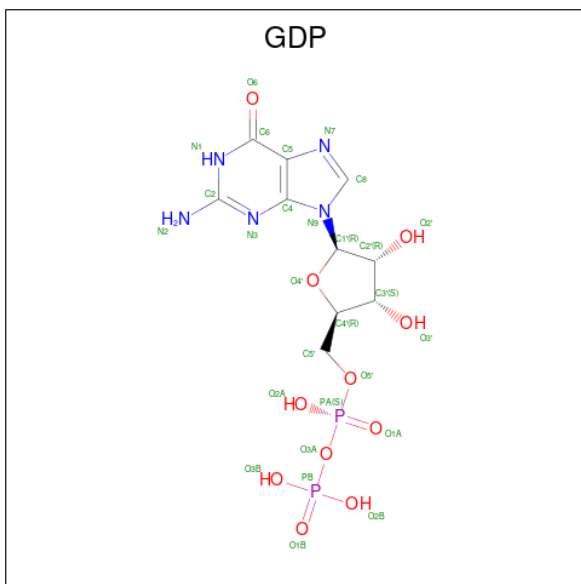
Mol	Chain	Residues	Atoms	AltConf
61	v	1	Total C N O S 10 6 1 2 1	0

- Molecule 62 is KIRROMYCIN (three-letter code: KIR) (formula: C₄₃H₆₀N₂O₁₂).



Mol	Chain	Residues	Atoms				AltConf
62	z	1	Total	C	N	O	0
			57	43	2	12	

- Molecule 63 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
63	z	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 64 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
64	A	1	Total	Na	0
			1	1	
64	B	1	Total	Na	0
			1	1	

- Molecule 65 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
65	4	1	Total	Zn	0
			1	1	
65	6	1	Total	Zn	0
			1	1	

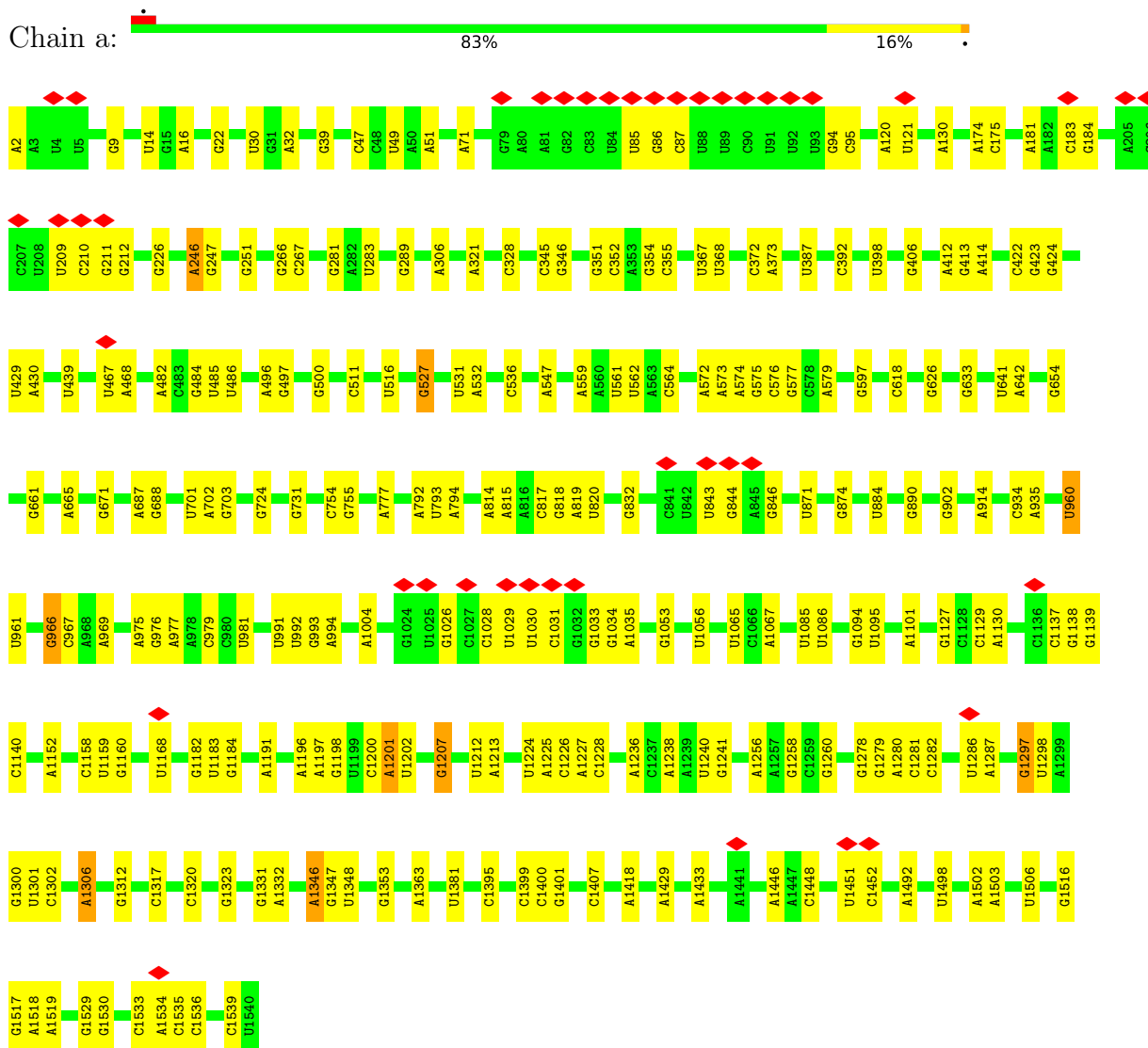
- Molecule 66 is water.

Mol	Chain	Residues	Atoms	AltConf
66	a	9	Total O 9 9	0
66	A	9	Total O 9 9	0
66	D	2	Total O 2 2	0
66	K	1	Total O 1 1	0

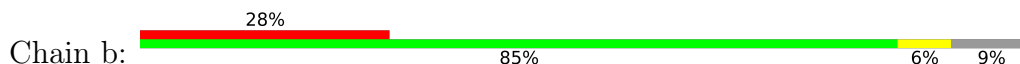
3 Residue-property plots

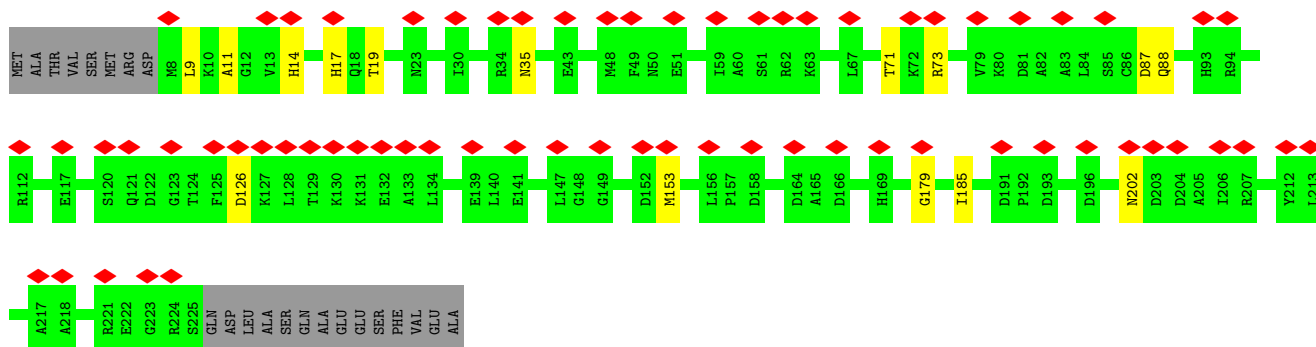
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: 16S ribosomal RNA

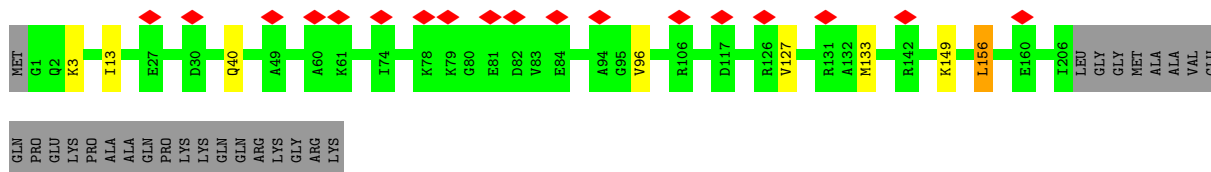
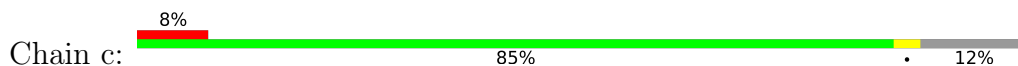


- Molecule 2: 30S ribosomal protein S2

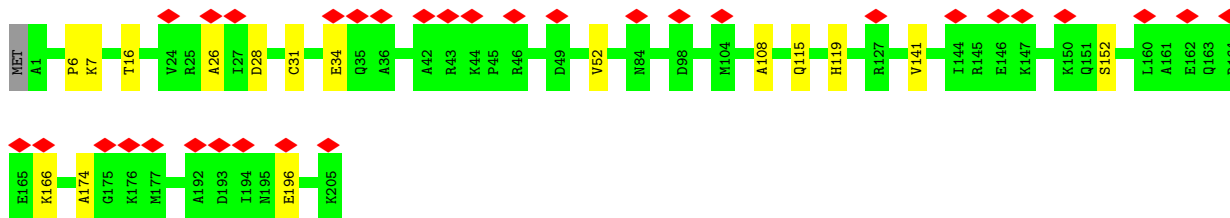




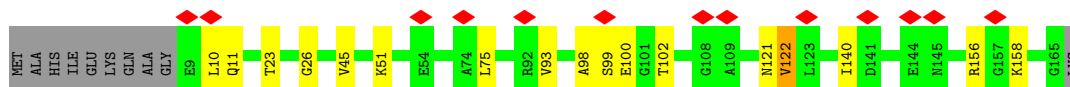
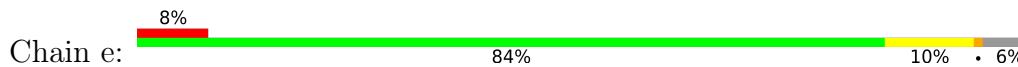
• Molecule 3: 30S ribosomal protein S3



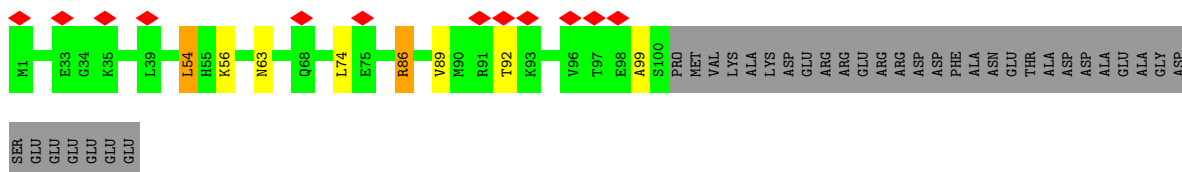
• Molecule 4: 30S ribosomal protein S4



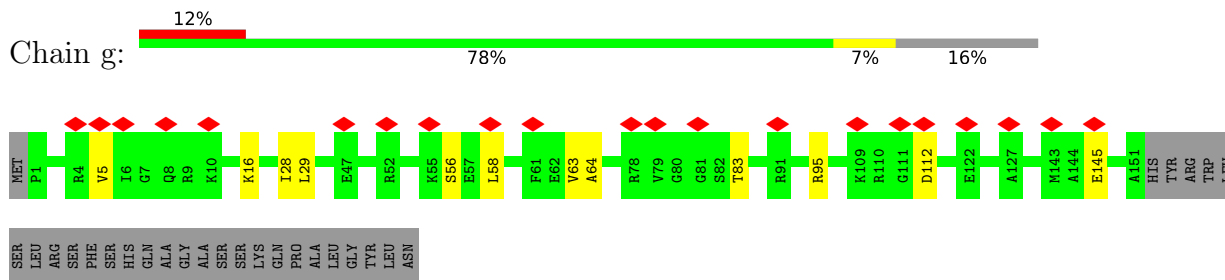
• Molecule 5: 30S ribosomal protein S5



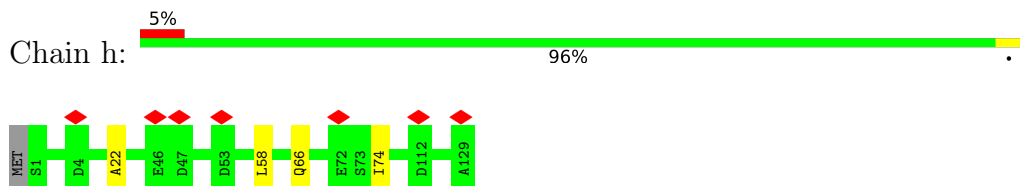
• Molecule 6: 30S ribosomal protein S6



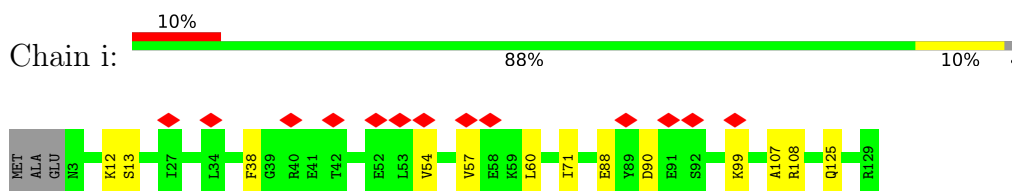
- Molecule 7: 30S ribosomal protein S7



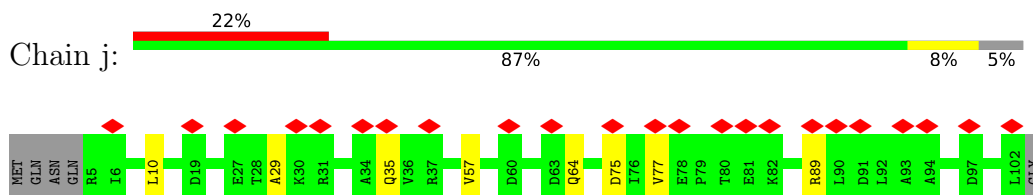
- Molecule 8: 30S ribosomal protein S8



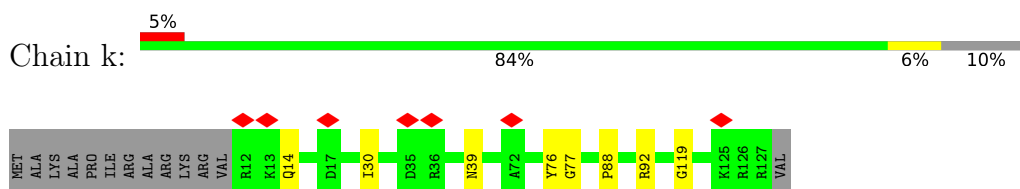
- Molecule 9: 30S ribosomal protein S9



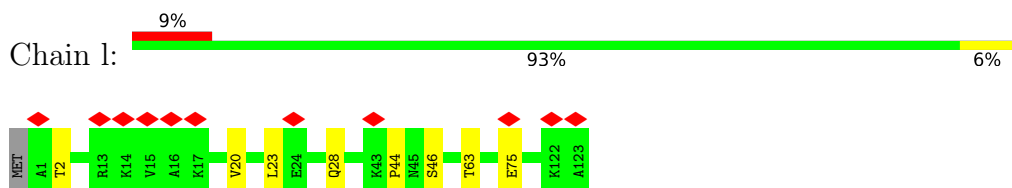
- Molecule 10: 30S ribosomal protein S10



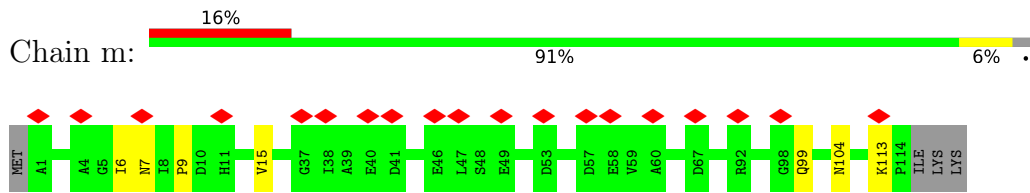
- Molecule 11: 30S ribosomal protein S11



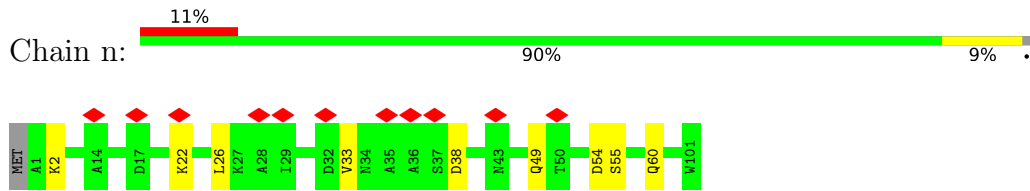
- Molecule 12: 30S ribosomal protein S12



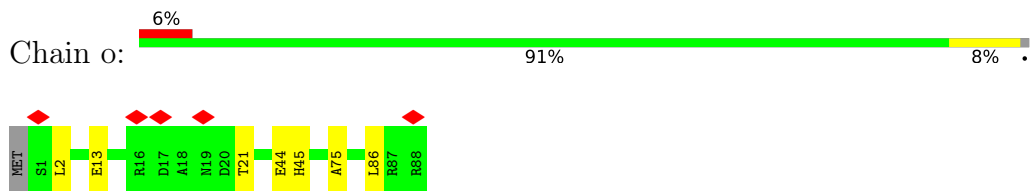
- Molecule 13: 30S ribosomal protein S13



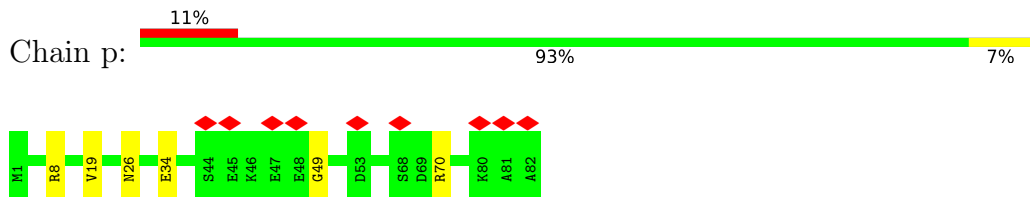
- Molecule 14: 30S ribosomal protein S14



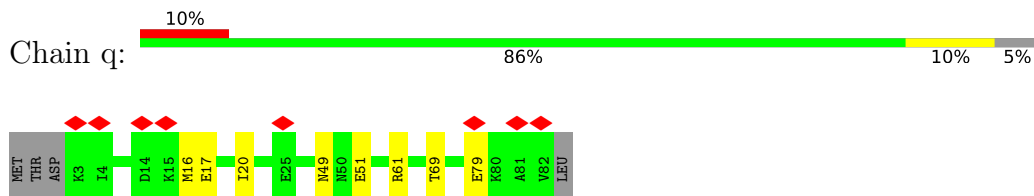
- Molecule 15: 30S ribosomal protein S15



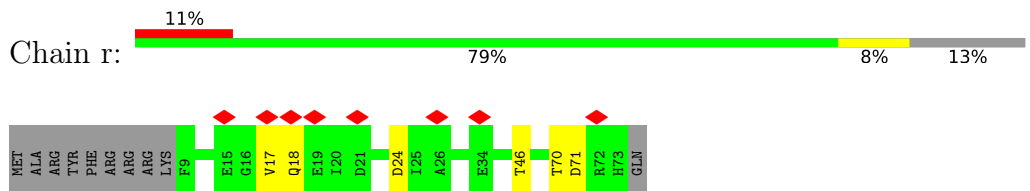
- Molecule 16: 30S ribosomal protein S16



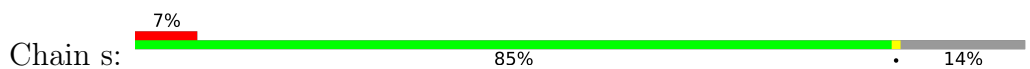
- Molecule 17: 30S ribosomal protein S17

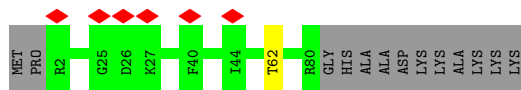


- Molecule 18: 30S ribosomal protein S18

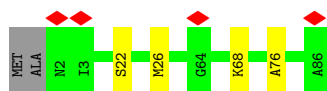
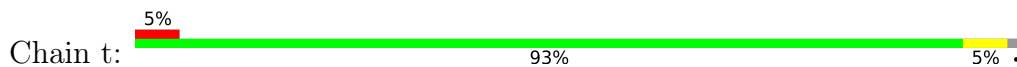


- Molecule 19: 30S ribosomal protein S19

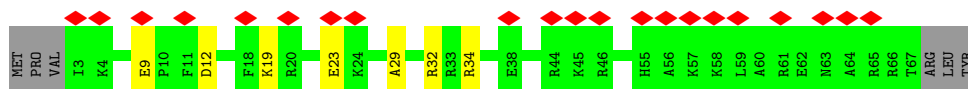
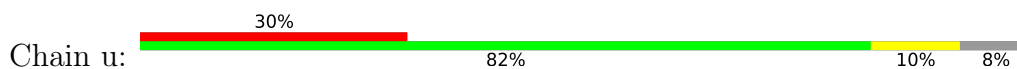




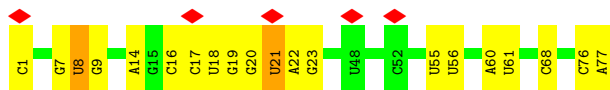
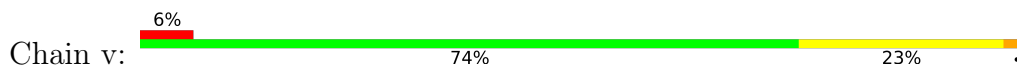
- Molecule 20: 30S ribosomal protein S20



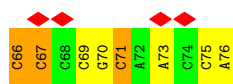
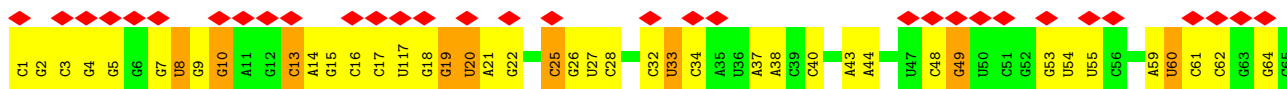
- Molecule 21: 30S ribosomal protein S21



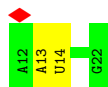
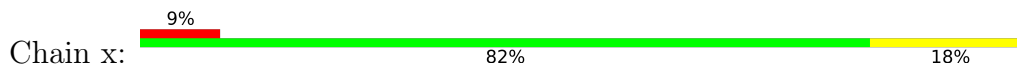
- Molecule 22: P-site fMet-tRNA^{fMet}



- Molecule 22: P-site fMet-tRNA^{fMet}

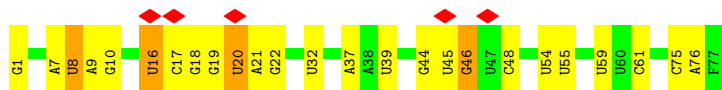


- Molecule 23: mRNA

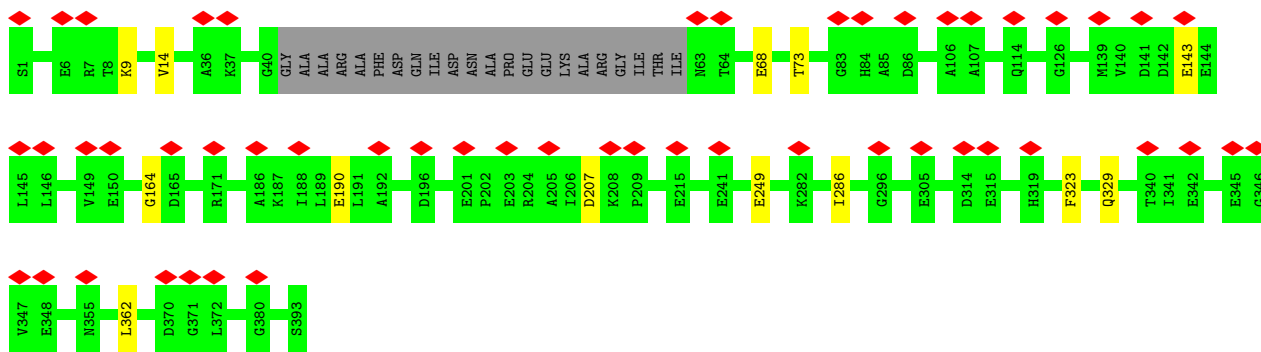
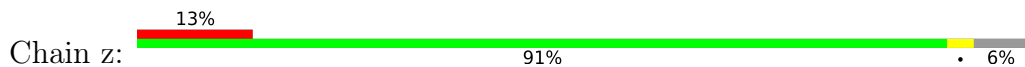


- Molecule 24: A/T-site Phe-tRNA^{Phe}

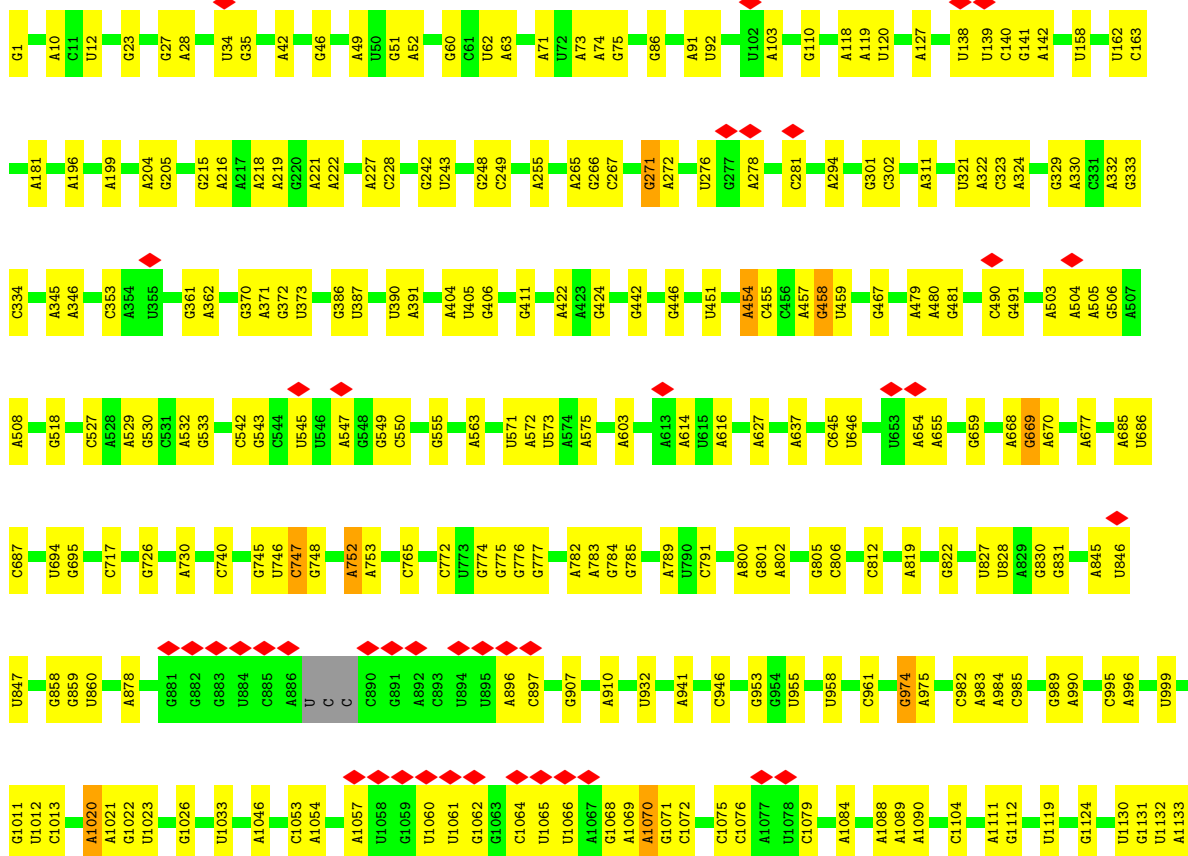
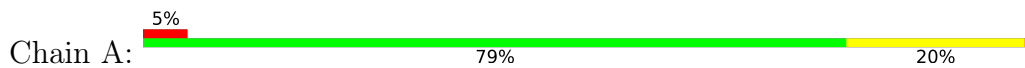


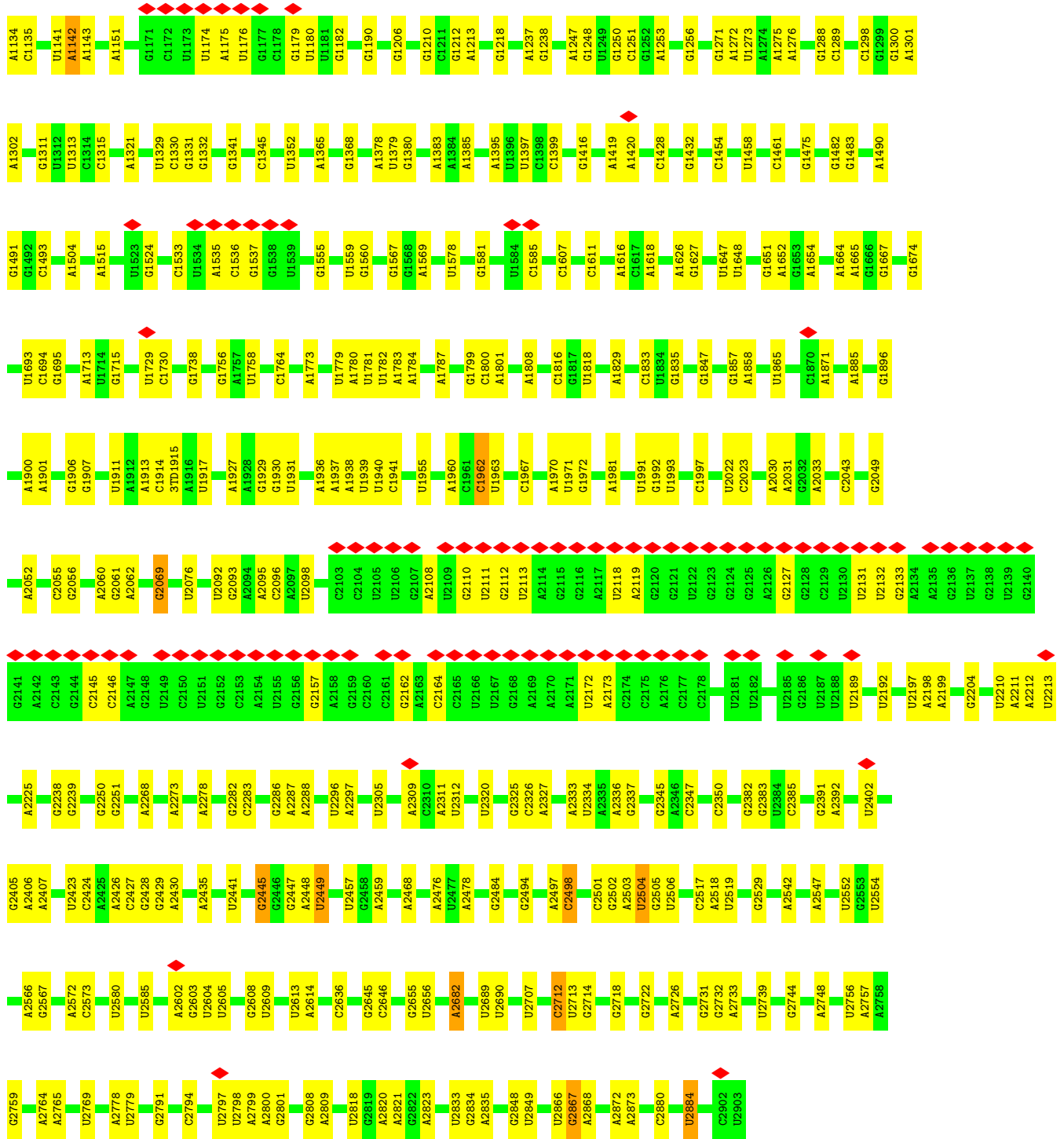


• Molecule 25: Elongation factor Tu 2

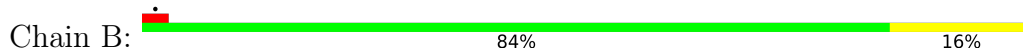


• Molecule 26: 23S ribosomal RNA



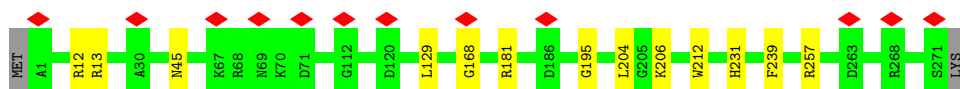


- Molecule 27: 5S ribosomal RNA



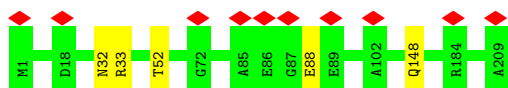
- Molecule 28: 50S ribosomal protein L2

Chain C:  95% 5%



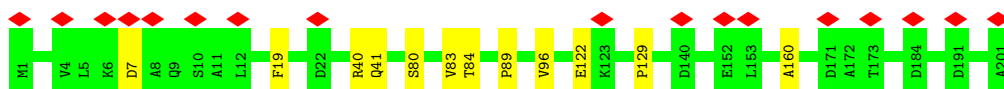
- Molecule 29: 50S ribosomal protein L3

Chain D:  5% 98%

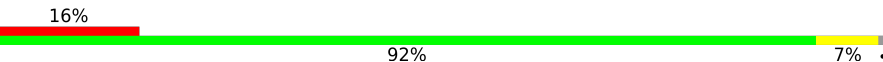


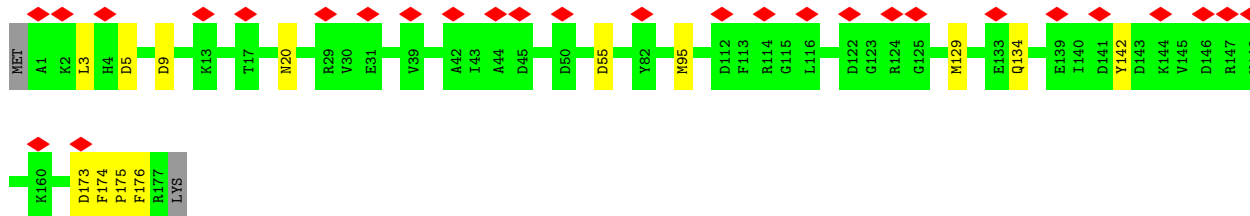
- Molecule 30: 50S ribosomal protein L4

Chain E:  8% 94% 6%



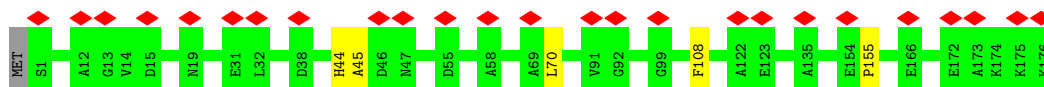
- Molecule 31: 50S ribosomal protein L5

Chain F:  16% 92% 7%

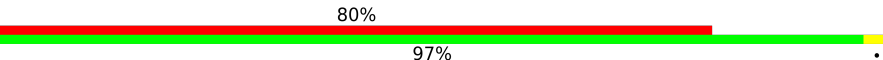


- Molecule 32: 50S ribosomal protein L6

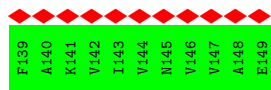
Chain G:  14% 97%



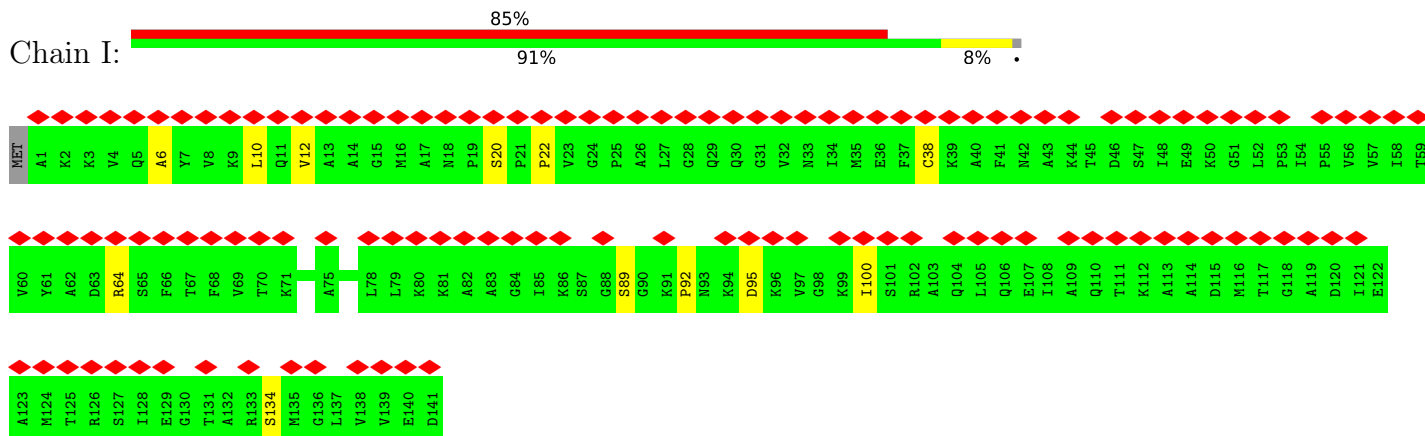
- Molecule 33: 50S ribosomal protein L9

Chain H:  80% 97%

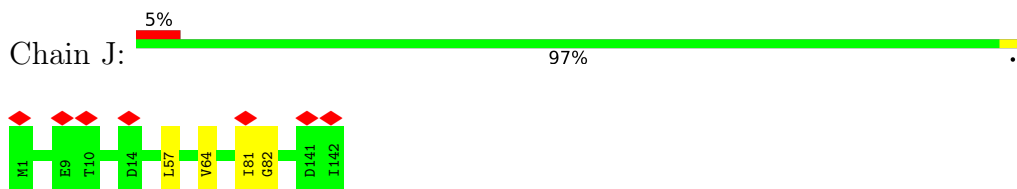




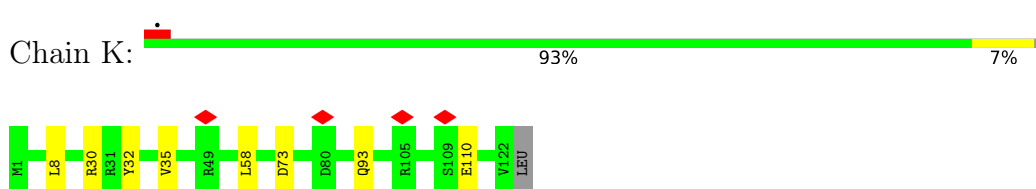
- Molecule 34: 50S ribosomal protein L11



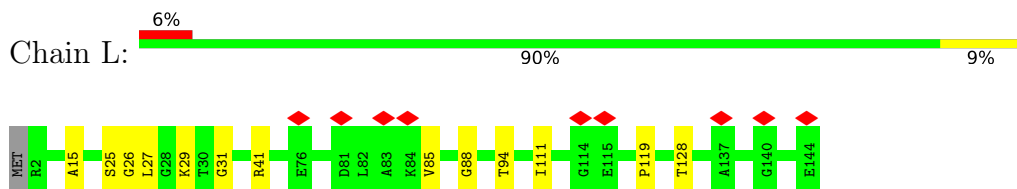
- Molecule 35: 50S ribosomal protein L13



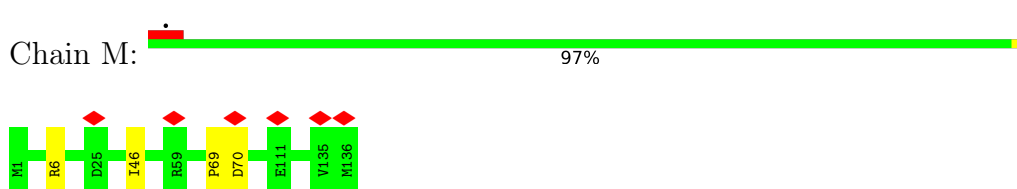
- Molecule 36: 50S ribosomal protein L14



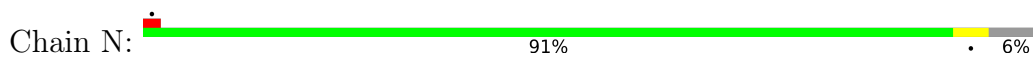
- Molecule 37: 50S ribosomal protein L15



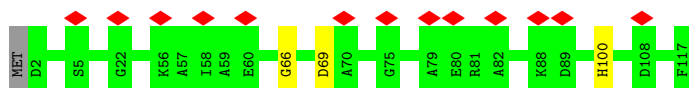
- Molecule 38: 50S ribosomal protein L16



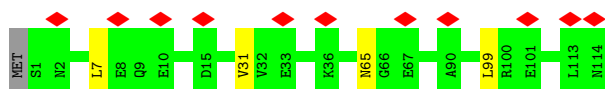
- Molecule 39: 50S ribosomal protein L17



- Molecule 40: 50S ribosomal protein L18



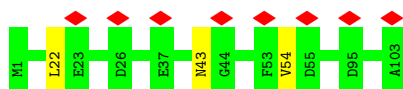
- Molecule 41: 50S ribosomal protein L19



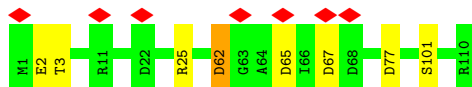
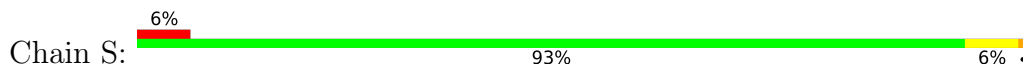
- Molecule 42: 50S ribosomal protein L20



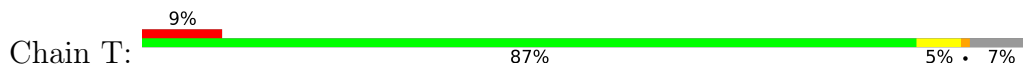
- Molecule 43: 50S ribosomal protein L21



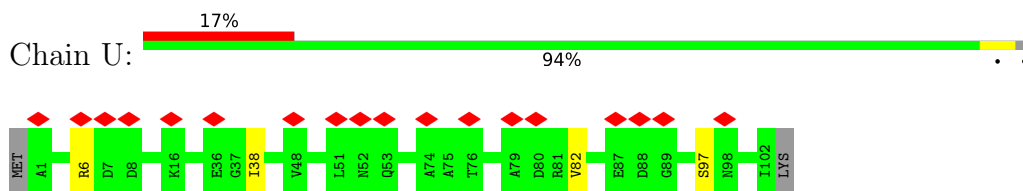
- Molecule 44: 50S ribosomal protein L22



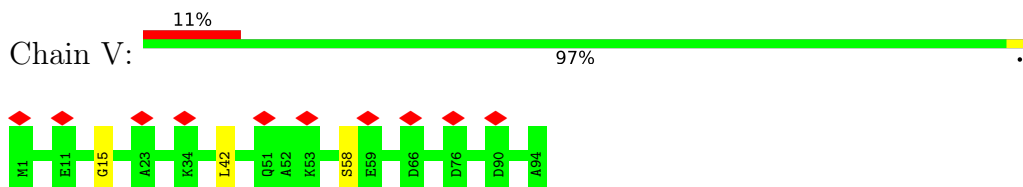
- Molecule 45: 50S ribosomal protein L23



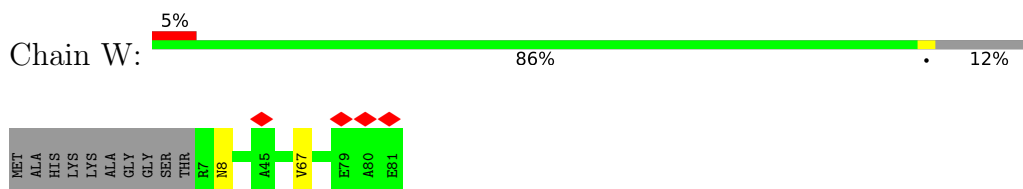
- Molecule 46: 50S ribosomal protein L24



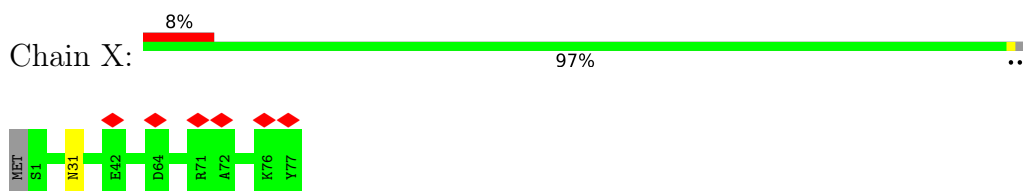
- Molecule 47: 50S ribosomal protein L25



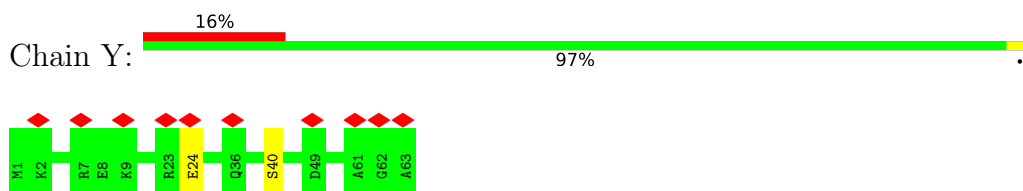
- Molecule 48: 50S ribosomal protein L27



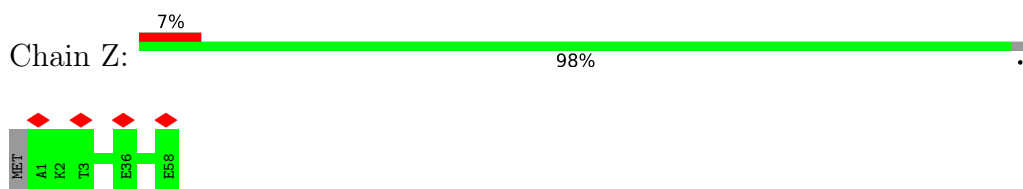
- Molecule 49: 50S ribosomal protein L28



- Molecule 50: 50S ribosomal protein L29

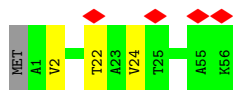


- Molecule 51: 50S ribosomal protein L30

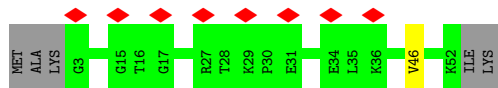
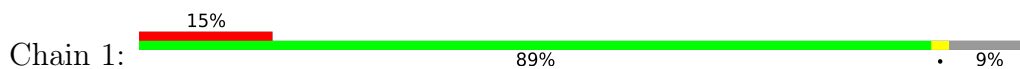


- Molecule 52: 50S ribosomal protein L32

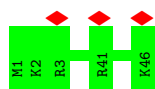




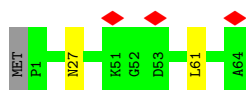
• Molecule 53: 50S ribosomal protein L33



• Molecule 54: 50S ribosomal protein L34



• Molecule 55: 50S ribosomal protein L35

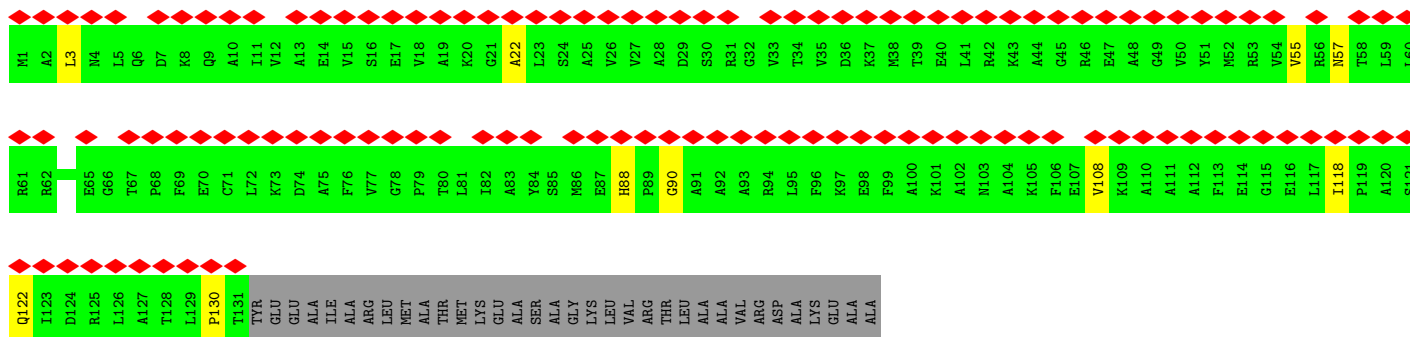


• Molecule 56: 50S ribosomal protein L36



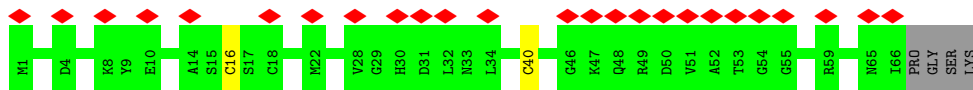
There are no outlier residues recorded for this chain.

• Molecule 57: 50S ribosomal protein L10



• Molecule 58: 50S ribosomal protein L31





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	417201	Depositor
Resolution determination method	Not provided	
CTF correction method	LOCAL CTF CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	192000	Depositor
Image detector	FEI FALCON I (4k x 4k)	Depositor
Maximum map value	4.711	Depositor
Minimum map value	-2.426	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.214	Depositor
Recommended contour level	0.43	Depositor
Map size (\AA)	317.205, 317.205, 317.205	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.75525, 0.75525, 0.75525	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FME, OMC, 7MG, PSU, GDP, 3TD, 2MA, ZN, CL, MG, H2U, 5MU, OMU, MA6, 5MC, 6MZ, UR3, OMG, 2MG, MIA, NA, 4OC, 1MG, 4SU, KIR

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.39	1/36701 (0.0%)	0.85	12/57246 (0.0%)
2	b	0.30	0/1735	0.44	0/2338
3	c	0.32	0/1651	0.46	0/2225
4	d	0.28	0/1665	0.44	0/2227
5	e	0.31	0/1154	0.46	0/1554
6	f	0.35	0/835	0.48	0/1128
7	g	0.36	0/1195	0.50	0/1602
8	h	0.27	0/989	0.45	0/1326
9	i	0.27	0/1034	0.45	0/1375
10	j	0.36	0/796	0.54	0/1077
11	k	0.28	0/885	0.48	0/1195
12	l	0.29	0/969	0.47	0/1300
13	m	0.36	0/892	0.50	0/1193
14	n	0.27	0/811	0.40	0/1081
15	o	0.32	0/722	0.44	0/964
16	p	0.33	0/659	0.45	0/884
17	q	0.27	0/657	0.46	0/881
18	r	0.28	0/511	0.43	0/689
19	s	0.28	0/652	0.44	0/877
20	t	0.38	0/671	0.48	0/888
21	u	0.29	0/500	0.42	0/668
22	v	0.41	1/1747 (0.1%)	0.82	0/2721
22	w	0.98	1/1747 (0.1%)	1.40	24/2721 (0.9%)
23	x	0.62	1/261 (0.4%)	0.85	0/404
24	y	0.39	1/1618 (0.1%)	0.81	0/2514
25	z	0.34	0/2935	0.47	0/3970
26	A	0.46	1/69174 (0.0%)	0.90	50/107910 (0.0%)
27	B	0.38	1/2876 (0.0%)	0.86	0/4483
28	C	0.31	0/2121	0.47	0/2852
29	D	0.35	0/1586	0.48	0/2134
30	E	0.26	0/1571	0.41	0/2113

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	F	0.30	0/1434	0.47	0/1926
32	G	0.35	0/1343	0.47	0/1816
33	H	0.23	0/1122	0.40	0/1515
34	I	0.23	0/1046	0.44	0/1410
35	J	0.29	0/1152	0.43	0/1551
36	K	0.28	0/947	0.41	0/1268
37	L	0.26	0/1054	0.45	0/1403
38	M	0.32	0/1093	0.46	0/1460
39	N	0.28	0/973	0.44	0/1301
40	O	0.33	0/902	0.44	0/1209
41	P	0.28	0/929	0.43	0/1242
42	Q	0.34	0/960	0.43	0/1278
43	R	0.34	0/829	0.52	0/1107
44	S	0.28	0/864	0.47	0/1156
45	T	0.29	0/744	0.45	0/994
46	U	0.35	0/787	0.44	0/1051
47	V	0.31	0/766	0.45	0/1025
48	W	0.33	0/582	0.47	0/769
49	X	0.28	0/635	0.40	0/848
50	Y	0.33	0/510	0.45	0/677
51	Z	0.25	0/453	0.41	0/605
52	0	0.26	0/450	0.41	0/599
53	1	0.26	0/416	0.41	0/554
54	2	0.29	0/380	0.44	0/498
55	3	0.27	0/513	0.43	0/676
56	4	0.28	0/303	0.40	0/397
57	5	0.25	0/1001	0.45	0/1350
58	6	0.33	0/531	0.54	0/709
All	All	0.41	7/164039 (0.0%)	0.80	86/244934 (0.0%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	w	1	C	OP3-P	-10.97	1.48	1.61
27	B	1	U	OP3-P	-10.59	1.48	1.61
26	A	1	G	OP3-P	-10.58	1.48	1.61
22	v	1	C	OP3-P	-10.56	1.48	1.61
1	a	2	A	OP3-P	-10.52	1.48	1.61
24	y	1	G	OP3-P	-10.48	1.48	1.61
23	x	14	U	C1'-N1	5.60	1.57	1.48

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	974	G	N1-C6-O6	9.46	125.57	119.90
26	A	1936	A	N1-C6-N6	9.14	124.09	118.60
22	w	13	C	C6-N1-C2	-8.20	117.02	120.30
22	w	62	C	C6-N1-C2	-8.13	117.05	120.30
22	w	62	C	C5-C6-N1	7.73	124.87	121.00
22	w	62	C	N1-C2-O2	7.54	123.42	118.90
22	w	62	C	C2-N1-C1'	7.33	126.86	118.80
26	A	1936	A	C2-N3-C4	-7.29	106.95	110.60
26	A	783	A	N7-C8-N9	7.27	117.44	113.80
1	a	1297	G	P-O3'-C3'	7.20	128.34	119.70
26	A	783	A	C5-N7-C8	-7.14	100.33	103.90
26	A	62	U	C2-N1-C1'	6.93	126.02	117.70
26	A	974	G	C6-C5-N7	-6.73	126.36	130.40
22	w	71	C	C5-C4-N4	-6.56	115.61	120.20
26	A	62	U	N1-C2-O2	6.55	127.38	122.80
22	w	66	C	C6-N1-C2	-6.54	117.68	120.30
26	A	783	A	N1-C6-N6	6.49	122.49	118.60
26	A	1779	U	C5-C6-N1	-6.44	119.48	122.70
26	A	2884	U	C2-N1-C1'	6.41	125.39	117.70
26	A	984	A	C2-N3-C4	-6.39	107.41	110.60
26	A	2884	U	N1-C2-O2	6.27	127.19	122.80
22	w	71	C	N3-C4-C5	6.12	124.35	121.90
26	A	2076	U	C2-N1-C1'	6.09	125.01	117.70
26	A	62	U	N3-C2-O2	-6.00	118.00	122.20
26	A	1313	U	C2-N1-C1'	5.95	124.83	117.70
22	w	71	C	C6-N1-C1'	-5.90	113.72	120.80
22	w	66	C	C5-C6-N1	5.88	123.94	121.00
22	w	71	C	C2-N1-C1'	5.81	125.19	118.80
22	w	49	G	C6-C5-N7	-5.74	126.96	130.40
1	a	1158	C	C2-N1-C1'	5.72	125.09	118.80
26	A	974	G	N7-C8-N9	5.71	115.95	113.10
22	w	61	C	N1-C2-O2	5.68	122.31	118.90
26	A	2682	A	C8-N9-C4	5.68	108.07	105.80
26	A	2501	C	C2-N1-C1'	-5.65	112.58	118.80
26	A	2884	U	N3-C2-O2	-5.63	118.26	122.20
26	A	2542	A	C8-N9-C4	5.62	108.05	105.80
22	w	33	U	C5-C6-N1	5.62	125.51	122.70
26	A	458	G	C4-N9-C1'	-5.58	119.24	126.50
22	w	4	G	N3-C4-N9	-5.58	122.65	126.00
22	w	49	G	C4-N9-C1'	5.58	133.75	126.50
22	w	25	C	N3-C4-C5	5.57	124.13	121.90
26	A	2867	G	N3-C4-N9	-5.56	122.66	126.00
1	a	246	A	P-O3'-C3'	5.55	126.36	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1399	C	P-O3'-C3'	5.54	126.35	119.70
26	A	2867	G	C6-C5-N7	5.50	133.70	130.40
26	A	669	G	C8-N9-C1'	-5.48	119.87	127.00
26	A	2867	G	C4-N9-C1'	-5.48	119.37	126.50
22	w	62	C	N3-C2-O2	-5.45	118.09	121.90
22	w	67	C	C5-C6-N1	5.42	123.71	121.00
26	A	974	G	C4-C5-N7	5.40	112.96	110.80
22	w	10	G	C5-C6-O6	-5.39	125.37	128.60
26	A	1142	A	OP1-P-O3'	5.38	117.04	105.20
26	A	783	A	C8-N9-C4	-5.38	103.65	105.80
26	A	783	A	C5-C6-N1	-5.37	115.02	117.70
22	w	60	U	N1-C2-O2	5.36	126.55	122.80
26	A	752	A	P-O3'-C3'	5.33	126.09	119.70
26	A	1936	A	C4-C5-N7	5.28	113.34	110.70
26	A	669	G	C4-N9-C1'	5.28	133.36	126.50
26	A	1936	A	C5-N7-C8	-5.25	101.27	103.90
26	A	2501	C	C5-C6-N1	-5.25	118.38	121.00
26	A	974	G	C5-C6-O6	-5.22	125.47	128.60
1	a	1306	A	N7-C8-N9	5.18	116.39	113.80
26	A	783	A	C2-N3-C4	-5.17	108.01	110.60
26	A	2712	C	P-O3'-C3'	5.17	125.90	119.70
26	A	1020	A	P-O3'-C3'	5.16	125.89	119.70
26	A	271	G	OP1-P-O3'	5.15	116.54	105.20
1	a	1201	A	P-O3'-C3'	5.14	125.87	119.70
26	A	1475	G	OP2-P-O3'	5.11	116.44	105.20
1	a	246	A	OP1-P-O3'	5.10	116.43	105.20
26	A	974	G	C5-C6-N1	-5.08	108.96	111.50
22	w	19	G	C4'-C3'-O3'	-5.08	98.72	109.40
1	a	16	A	C8-N9-C4	5.08	107.83	105.80
26	A	2759	G	N1-C2-N3	5.07	126.94	123.90
1	a	1158	C	N1-C2-O2	5.06	121.94	118.90
22	w	27	U	OP1-P-O3'	5.05	116.31	105.20
26	A	458	G	O4'-C1'-N9	5.05	112.24	108.20
26	A	1652	A	C8-N9-C4	5.04	107.82	105.80
26	A	451	U	C5-C6-N1	-5.03	120.19	122.70
1	a	754	C	C2-N1-C1'	5.03	124.33	118.80
1	a	960	U	P-O3'-C3'	5.02	125.73	119.70
22	w	13	C	C5-C6-N1	5.01	123.51	121.00
26	A	1936	A	C6-C5-N7	-5.01	128.79	132.30
26	A	454	A	OP2-P-O3'	5.01	116.23	105.20
26	A	2076	U	N1-C2-O2	5.01	126.31	122.80
26	A	1070	A	P-O3'-C3'	5.01	125.71	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1346	A	O4'-C1'-N9	5.00	112.20	108.20

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	
2	b	216/240 (90%)	183 (85%)	23 (11%)	10 (5%)	2	9
3	c	204/233 (88%)	184 (90%)	18 (9%)	2 (1%)	15	45
4	d	203/206 (98%)	172 (85%)	21 (10%)	10 (5%)	2	8
5	e	155/167 (93%)	130 (84%)	16 (10%)	9 (6%)	1	5
6	f	98/135 (73%)	81 (83%)	11 (11%)	6 (6%)	1	4
7	g	149/179 (83%)	124 (83%)	15 (10%)	10 (7%)	1	3
8	h	127/130 (98%)	110 (87%)	14 (11%)	3 (2%)	6	22
9	i	125/130 (96%)	98 (78%)	19 (15%)	8 (6%)	1	4
10	j	96/103 (93%)	74 (77%)	16 (17%)	6 (6%)	1	4
11	k	114/129 (88%)	92 (81%)	16 (14%)	6 (5%)	2	6
12	l	121/124 (98%)	96 (79%)	20 (16%)	5 (4%)	3	11
13	m	112/118 (95%)	99 (88%)	8 (7%)	5 (4%)	2	9
14	n	99/102 (97%)	82 (83%)	12 (12%)	5 (5%)	2	7
15	o	86/89 (97%)	71 (83%)	10 (12%)	5 (6%)	1	5
16	p	80/82 (98%)	67 (84%)	11 (14%)	2 (2%)	5	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	q	78/84 (93%)	65 (83%)	8 (10%)	5 (6%)	1	4
18	r	63/75 (84%)	53 (84%)	5 (8%)	5 (8%)	1	2
19	s	77/92 (84%)	66 (86%)	11 (14%)	0	100	100
20	t	83/87 (95%)	77 (93%)	4 (5%)	2 (2%)	6	22
21	u	63/71 (89%)	44 (70%)	14 (22%)	5 (8%)	1	2
25	z	368/393 (94%)	327 (89%)	35 (10%)	6 (2%)	9	32
28	C	269/273 (98%)	243 (90%)	21 (8%)	5 (2%)	8	28
29	D	207/209 (99%)	185 (89%)	20 (10%)	2 (1%)	15	45
30	E	199/201 (99%)	172 (86%)	20 (10%)	7 (4%)	3	14
31	F	175/179 (98%)	149 (85%)	20 (11%)	6 (3%)	3	15
32	G	174/177 (98%)	148 (85%)	21 (12%)	5 (3%)	4	18
33	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	5	19
34	I	139/142 (98%)	110 (79%)	20 (14%)	9 (6%)	1	3
35	J	140/142 (99%)	129 (92%)	9 (6%)	2 (1%)	11	36
36	K	120/123 (98%)	103 (86%)	14 (12%)	3 (2%)	5	21
37	L	141/144 (98%)	110 (78%)	20 (14%)	11 (8%)	1	2
38	M	134/136 (98%)	117 (87%)	14 (10%)	3 (2%)	6	24
39	N	118/127 (93%)	103 (87%)	12 (10%)	3 (2%)	5	21
40	O	114/117 (97%)	102 (90%)	11 (10%)	1 (1%)	17	48
41	P	112/115 (97%)	93 (83%)	18 (16%)	1 (1%)	17	48
42	Q	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
43	R	101/103 (98%)	82 (81%)	17 (17%)	2 (2%)	7	27
44	S	108/110 (98%)	90 (83%)	12 (11%)	6 (6%)	2	5
45	T	91/100 (91%)	77 (85%)	11 (12%)	3 (3%)	4	15
46	U	100/104 (96%)	80 (80%)	17 (17%)	3 (3%)	4	17
47	V	92/94 (98%)	78 (85%)	12 (13%)	2 (2%)	6	24
48	W	73/85 (86%)	66 (90%)	6 (8%)	1 (1%)	11	36
49	X	75/78 (96%)	69 (92%)	5 (7%)	1 (1%)	12	37
50	Y	61/63 (97%)	55 (90%)	5 (8%)	1 (2%)	9	32
51	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
52	0	54/57 (95%)	49 (91%)	4 (7%)	1 (2%)	8	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	1	48/55 (87%)	43 (90%)	5 (10%)	0	100	100
54	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
55	3	62/65 (95%)	54 (87%)	7 (11%)	1 (2%)	9	32
56	4	36/38 (95%)	28 (78%)	8 (22%)	0	100	100
57	5	129/165 (78%)	100 (78%)	22 (17%)	7 (5%)	2	6
58	6	64/70 (91%)	53 (83%)	10 (16%)	1 (2%)	9	32
All	All	6215/6613 (94%)	5318 (86%)	691 (11%)	206 (3%)	6	15

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	c	156	LEU
5	e	122	VAL
6	f	63	ASN
9	i	12	LYS
9	i	71	ILE
10	j	57	VAL
10	j	75	ASP
10	j	89	ARG
16	p	8	ARG
17	q	79	GLU
18	r	17	VAL
28	C	204	LEU
31	F	175	PRO
32	G	108	PHE
35	J	81	ILE
36	K	93	GLN
37	L	15	ALA
37	L	85	VAL
37	L	128	THR
44	S	67	ASP
46	U	6	ARG
46	U	97	SER
49	X	31	ASN
55	3	27	ASN
2	b	17	HIS
2	b	19	THR
2	b	179	GLY
3	c	13	ILE
4	d	26	ALA

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Mol	Chain	Res	Type
4	d	108	ALA
5	e	23	THR
5	e	93	VAL
7	g	16	LYS
7	g	56	SER
7	g	63	VAL
7	g	112	ASP
7	g	145	GLU
8	h	66	GLN
9	i	57	VAL
10	j	29	ALA
10	j	77	VAL
11	k	76	TYR
11	k	77	GLY
11	k	88	PRO
12	l	75	GLU
13	m	104	ASN
14	n	54	ASP
15	o	21	THR
15	o	45	HIS
17	q	17	GLU
17	q	49	ASN
18	r	46	THR
20	t	68	LYS
21	u	12	ASP
28	C	195	GLY
28	C	231	HIS
33	H	9	VAL
34	I	64	ARG
34	I	89	SER
34	I	92	PRO
36	K	35	VAL
36	K	110	GLU
37	L	29	LYS
37	L	31	GLY
37	L	111	ILE
38	M	70	ASP
40	O	66	GLY
41	P	65	ASN
43	R	43	ASN
43	R	54	VAL
44	S	2	GLU

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Mol	Chain	Res	Type
44	S	3	THR
45	T	37	ASP
45	T	38	ALA
45	T	71	GLY
50	Y	24	GLU
57	5	55	VAL
2	b	73	ARG
2	b	87	ASP
2	b	153	MET
4	d	7	LYS
4	d	31	CYS
4	d	152	SER
4	d	166	LYS
4	d	174	ALA
5	e	98	ALA
5	e	99	SER
5	e	121	ASN
6	f	54	LEU
6	f	92	THR
7	g	64	ALA
7	g	95	ARG
8	h	74	ILE
9	i	90	ASP
9	i	107	ALA
9	i	125	GLN
10	j	35	GLN
11	k	14	GLN
12	l	2	THR
12	l	46	SER
13	m	6	ILE
13	m	7	ASN
13	m	113	LYS
14	n	22	LYS
14	n	38	ASP
14	n	55	SER
15	o	2	LEU
15	o	13	GLU
16	p	49	GLY
17	q	16	MET
20	t	76	ALA
21	u	29	ALA
21	u	32	ARG

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Mol	Chain	Res	Type
21	u	34	ARG
28	C	239	PHE
30	E	89	PRO
30	E	122	GLU
32	G	44	HIS
32	G	45	ALA
33	H	15	LEU
34	I	12	VAL
37	L	88	GLY
38	M	6	ARG
39	N	59	SER
44	S	62	ASP
57	5	88	HIS
57	5	118	ILE
58	6	40	CYS
2	b	11	ALA
2	b	88	GLN
2	b	126	ASP
5	e	100	GLU
5	e	102	THR
6	f	56	LYS
6	f	86	ARG
6	f	99	ALA
7	g	29	LEU
8	h	22	ALA
9	i	99	LYS
11	k	92	ARG
12	l	23	LEU
14	n	2	LYS
15	o	75	ALA
18	r	18	GLN
18	r	71	ASP
25	z	9	LYS
29	D	32	ASN
30	E	80	SER
30	E	160	ALA
31	F	20	ASN
31	F	142	TYR
31	F	173	ASP
31	F	176	PHE
33	H	2	GLN
34	I	6	ALA

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Mol	Chain	Res	Type
34	I	20	SER
37	L	25	SER
39	N	117	ASP
44	S	65	ASP
47	V	58	SER
48	W	8	ASN
52	0	2	VAL
57	5	22	ALA
57	5	90	GLY
57	5	130	PRO
2	b	14	HIS
4	d	34	GLU
18	r	70	THR
25	z	164	GLY
25	z	207	ASP
25	z	249	GLU
30	E	84	THR
31	F	174	PHE
32	G	70	LEU
33	H	3	VAL
34	I	22	PRO
34	I	100	ILE
35	J	82	GLY
37	L	94	THR
4	d	6	PRO
4	d	28	ASP
9	i	13	SER
25	z	14	VAL
29	D	148	GLN
30	E	83	VAL
34	I	38	CYS
37	L	119	PRO
44	S	101	SER
11	k	119	GLY
12	l	44	PRO
28	C	168	GLY
37	L	26	GLY
38	M	69	PRO
39	N	116	VAL
17	q	20	ILE
21	u	9	GLU
46	U	38	ILE

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Mol	Chain	Res	Type
7	g	5	VAL
25	z	286	ILE
47	V	15	GLY
57	5	108	VAL
7	g	28	ILE
30	E	129	PRO
5	e	26	GLY
13	m	9	PRO
32	G	155	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	180/198 (91%)	175 (97%)	5 (3%)	43	76
3	c	170/190 (90%)	163 (96%)	7 (4%)	30	64
4	d	172/173 (99%)	166 (96%)	6 (4%)	36	70
5	e	114/126 (90%)	105 (92%)	9 (8%)	12	34
6	f	87/116 (75%)	83 (95%)	4 (5%)	27	60
7	g	124/147 (84%)	122 (98%)	2 (2%)	62	86
8	h	104/105 (99%)	103 (99%)	1 (1%)	76	92
9	i	105/107 (98%)	100 (95%)	5 (5%)	25	58
10	j	86/90 (96%)	84 (98%)	2 (2%)	50	80
11	k	89/99 (90%)	87 (98%)	2 (2%)	52	81
12	l	103/104 (99%)	100 (97%)	3 (3%)	42	76
13	m	92/96 (96%)	90 (98%)	2 (2%)	52	81
14	n	79/84 (94%)	75 (95%)	4 (5%)	24	56
15	o	76/77 (99%)	74 (97%)	2 (3%)	46	77
16	p	65/65 (100%)	61 (94%)	4 (6%)	18	47
17	q	74/78 (95%)	71 (96%)	3 (4%)	30	64
18	r	48/65 (74%)	47 (98%)	1 (2%)	53	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	s	70/79 (89%)	69 (99%)	1 (1%)	67	89
20	t	65/66 (98%)	63 (97%)	2 (3%)	40	74
21	u	44/61 (72%)	42 (96%)	2 (4%)	27	61
25	z	311/326 (95%)	304 (98%)	7 (2%)	50	80
28	C	216/218 (99%)	208 (96%)	8 (4%)	34	68
29	D	164/164 (100%)	161 (98%)	3 (2%)	59	85
30	E	165/165 (100%)	160 (97%)	5 (3%)	41	75
31	F	148/150 (99%)	141 (95%)	7 (5%)	26	59
32	G	137/138 (99%)	137 (100%)	0	100	100
33	H	114/114 (100%)	114 (100%)	0	100	100
34	I	109/110 (99%)	106 (97%)	3 (3%)	43	76
35	J	116/116 (100%)	114 (98%)	2 (2%)	60	86
36	K	103/104 (99%)	98 (95%)	5 (5%)	25	57
37	L	102/103 (99%)	100 (98%)	2 (2%)	55	82
38	M	109/109 (100%)	108 (99%)	1 (1%)	78	93
39	N	100/103 (97%)	98 (98%)	2 (2%)	55	82
40	O	86/87 (99%)	84 (98%)	2 (2%)	50	80
41	P	99/100 (99%)	96 (97%)	3 (3%)	41	75
42	Q	89/90 (99%)	87 (98%)	2 (2%)	52	81
43	R	84/84 (100%)	83 (99%)	1 (1%)	71	91
44	S	93/93 (100%)	90 (97%)	3 (3%)	39	73
45	T	80/84 (95%)	76 (95%)	4 (5%)	24	57
46	U	83/85 (98%)	82 (99%)	1 (1%)	71	91
47	V	78/78 (100%)	77 (99%)	1 (1%)	69	90
48	W	57/63 (90%)	56 (98%)	1 (2%)	59	85
49	X	67/68 (98%)	67 (100%)	0	100	100
50	Y	55/55 (100%)	54 (98%)	1 (2%)	59	85
51	Z	48/49 (98%)	48 (100%)	0	100	100
52	0	47/48 (98%)	45 (96%)	2 (4%)	29	62
53	1	45/49 (92%)	44 (98%)	1 (2%)	52	81
54	2	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
55	3	51/52 (98%)	50 (98%)	1 (2%)	55	82
56	4	34/34 (100%)	34 (100%)	0	100	100
57	5	100/123 (81%)	97 (97%)	3 (3%)	41	75
58	6	59/62 (95%)	58 (98%)	1 (2%)	60	86
All	All	5134/5388 (95%)	4995 (97%)	139 (3%)	48	77

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	9	LEU
2	b	35	ASN
2	b	71	THR
2	b	185	ILE
2	b	202	ASN
3	c	3	LYS
3	c	40	GLN
3	c	96	VAL
3	c	127	VAL
3	c	133	MET
3	c	149	LYS
3	c	156	LEU
4	d	16	THR
4	d	52	VAL
4	d	115	GLN
4	d	119	HIS
4	d	141	VAL
4	d	196	GLU
5	e	10	LEU
5	e	11	GLN
5	e	45	VAL
5	e	51	LYS
5	e	75	LEU
5	e	122	VAL
5	e	140	ILE
5	e	156	ARG
5	e	158	LYS
6	f	54	LEU
6	f	74	LEU
6	f	86	ARG
6	f	89	VAL
7	g	58	LEU

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Mol	Chain	Res	Type
7	g	83	THR
8	h	58	LEU
9	i	38	PHE
9	i	54	VAL
9	i	60	LEU
9	i	88	GLU
9	i	108	ARG
10	j	10	LEU
10	j	64	GLN
11	k	30	ILE
11	k	39	ASN
12	l	20	VAL
12	l	28	GLN
12	l	63	THR
13	m	15	VAL
13	m	99	GLN
14	n	26	LEU
14	n	33	VAL
14	n	49	GLN
14	n	60	GLN
15	o	44	GLU
15	o	86	LEU
16	p	19	VAL
16	p	26	ASN
16	p	34	GLU
16	p	70	ARG
17	q	51	GLU
17	q	61	ARG
17	q	69	THR
18	r	24	ASP
19	s	62	THR
20	t	22	SER
20	t	26	MET
21	u	19	LYS
21	u	23	GLU
25	z	68	GLU
25	z	73	THR
25	z	143	GLU
25	z	190	GLU
25	z	323	PHE
25	z	329	GLN
25	z	362	LEU

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Mol	Chain	Res	Type
28	C	12	ARG
28	C	13	ARG
28	C	45	ASN
28	C	129	LEU
28	C	181	ARG
28	C	206	LYS
28	C	212	TRP
28	C	257	ARG
29	D	33	ARG
29	D	52	THR
29	D	88	GLU
30	E	7	ASP
30	E	19	PHE
30	E	40	ARG
30	E	41	GLN
30	E	96	VAL
31	F	3	LEU
31	F	5	ASP
31	F	9	ASP
31	F	55	ASP
31	F	95	MET
31	F	129	MET
31	F	134	GLN
34	I	10	LEU
34	I	95	ASP
34	I	134	SER
35	J	57	LEU
35	J	64	VAL
36	K	8	LEU
36	K	30	ARG
36	K	32	TYR
36	K	58	LEU
36	K	73	ASP
37	L	27	LEU
37	L	41	ARG
38	M	46	ILE
39	N	15	SER
39	N	113	ILE
40	O	69	ASP
40	O	100	HIS
41	P	7	LEU
41	P	31	VAL

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Mol	Chain	Res	Type
41	P	99	LEU
42	Q	48	ASP
42	Q	94	LEU
43	R	22	LEU
44	S	25	ARG
44	S	62	ASP
44	S	77	ASP
45	T	32	LEU
45	T	37	ASP
45	T	59	ASN
45	T	60	THR
46	U	82	VAL
47	V	42	LEU
48	W	67	VAL
50	Y	40	SER
52	0	22	THR
52	0	24	VAL
53	1	46	VAL
55	3	61	LEU
57	5	3	LEU
57	5	57	ASN
57	5	122	GLN
58	6	16	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	202	ASN
3	c	40	GLN
4	d	70	GLN
4	d	119	HIS
4	d	135	GLN
6	f	11	HIS
7	g	141	HIS
10	j	70	HIS
11	k	39	ASN
13	m	90	HIS
14	n	49	GLN
15	o	45	HIS
16	p	26	ASN
17	q	30	HIS
18	r	51	GLN

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Mol	Chain	Res	Type
19	s	51	HIS
19	s	56	HIS
25	z	19	HIS
25	z	78	HIS
25	z	135	ASN
25	z	329	GLN
28	C	196	ASN
29	D	49	GLN
29	D	149	ASN
31	F	134	GLN
32	G	103	ASN
32	G	138	GLN
34	I	11	GLN
35	J	40	HIS
42	Q	71	ASN
44	S	61	ASN
46	U	65	GLN
50	Y	41	HIS
52	0	5	ASN
58	6	65	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1535/1539 (99%)	242 (15%)	0
22	v	76/77 (98%)	17 (22%)	0
22	w	76/77 (98%)	43 (56%)	0
23	x	10/11 (90%)	1 (10%)	0
24	y	74/77 (96%)	19 (25%)	0
26	A	2894/2903 (99%)	542 (18%)	90 (3%)
27	B	119/120 (99%)	17 (14%)	4 (3%)
All	All	4784/4804 (99%)	881 (18%)	94 (1%)

All (881) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	9	G
1	a	14	U
1	a	22	G
1	a	30	U
1	a	32	A

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Mol	Chain	Res	Type
1	a	39	G
1	a	47	C
1	a	49	U
1	a	51	A
1	a	71	A
1	a	85	U
1	a	86	G
1	a	87	C
1	a	94	G
1	a	95	C
1	a	120	A
1	a	121	U
1	a	130	A
1	a	174	A
1	a	175	C
1	a	181	A
1	a	183	C
1	a	184	G
1	a	209	U
1	a	210	C
1	a	211	G
1	a	212	G
1	a	226	G
1	a	246	A
1	a	247	G
1	a	251	G
1	a	266	G
1	a	267	C
1	a	281	G
1	a	283	U
1	a	289	G
1	a	306	A
1	a	321	A
1	a	328	C
1	a	345	C
1	a	346	G
1	a	351	G
1	a	352	C
1	a	354	G
1	a	355	C
1	a	367	U
1	a	368	U

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Mol	Chain	Res	Type
1	a	372	C
1	a	373	A
1	a	387	U
1	a	392	C
1	a	398	U
1	a	406	G
1	a	412	A
1	a	413	G
1	a	414	A
1	a	422	C
1	a	423	G
1	a	424	G
1	a	429	U
1	a	430	A
1	a	439	U
1	a	467	U
1	a	468	A
1	a	482	A
1	a	484	G
1	a	485	U
1	a	486	U
1	a	496	A
1	a	497	G
1	a	500	G
1	a	511	C
1	a	527	7MG
1	a	531	U
1	a	532	A
1	a	536	C
1	a	547	A
1	a	559	A
1	a	561	U
1	a	562	U
1	a	564	C
1	a	572	A
1	a	573	A
1	a	574	A
1	a	575	G
1	a	576	C
1	a	577	G
1	a	579	A
1	a	597	G

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Mol	Chain	Res	Type
1	a	618	C
1	a	626	G
1	a	633	G
1	a	641	U
1	a	642	A
1	a	654	G
1	a	661	G
1	a	665	A
1	a	671	G
1	a	687	A
1	a	688	G
1	a	701	U
1	a	702	A
1	a	703	G
1	a	724	G
1	a	731	G
1	a	755	G
1	a	777	A
1	a	792	A
1	a	793	U
1	a	794	A
1	a	814	A
1	a	815	A
1	a	817	C
1	a	818	G
1	a	819	A
1	a	820	U
1	a	832	G
1	a	843	U
1	a	844	G
1	a	846	G
1	a	871	U
1	a	874	G
1	a	884	U
1	a	890	G
1	a	902	G
1	a	914	A
1	a	934	C
1	a	935	A
1	a	960	U
1	a	961	U
1	a	966	2MG

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Mol	Chain	Res	Type
1	a	969	A
1	a	975	A
1	a	976	G
1	a	977	A
1	a	979	C
1	a	981	U
1	a	991	U
1	a	992	U
1	a	993	G
1	a	994	A
1	a	1004	A
1	a	1026	G
1	a	1028	C
1	a	1029	U
1	a	1030	U
1	a	1031	C
1	a	1033	G
1	a	1034	G
1	a	1035	A
1	a	1053	G
1	a	1056	U
1	a	1065	U
1	a	1067	A
1	a	1085	U
1	a	1086	U
1	a	1094	G
1	a	1095	U
1	a	1101	A
1	a	1127	G
1	a	1129	C
1	a	1130	A
1	a	1137	C
1	a	1138	G
1	a	1139	G
1	a	1140	C
1	a	1152	A
1	a	1159	U
1	a	1160	G
1	a	1168	U
1	a	1182	G
1	a	1183	U
1	a	1184	G

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Mol	Chain	Res	Type
1	a	1191	A
1	a	1196	A
1	a	1197	A
1	a	1198	G
1	a	1200	C
1	a	1201	A
1	a	1202	U
1	a	1207	2MG
1	a	1212	U
1	a	1213	A
1	a	1224	U
1	a	1225	A
1	a	1226	C
1	a	1227	A
1	a	1228	C
1	a	1236	A
1	a	1238	A
1	a	1240	U
1	a	1241	G
1	a	1256	A
1	a	1258	G
1	a	1260	G
1	a	1278	G
1	a	1279	G
1	a	1280	A
1	a	1281	C
1	a	1282	C
1	a	1286	U
1	a	1287	A
1	a	1297	G
1	a	1298	U
1	a	1300	G
1	a	1301	U
1	a	1302	C
1	a	1306	A
1	a	1312	G
1	a	1317	C
1	a	1320	C
1	a	1323	G
1	a	1331	G
1	a	1332	A
1	a	1346	A

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Mol	Chain	Res	Type
1	a	1347	G
1	a	1348	U
1	a	1353	G
1	a	1363	A
1	a	1381	U
1	a	1395	C
1	a	1400	C
1	a	1401	G
1	a	1418	A
1	a	1429	A
1	a	1433	A
1	a	1446	A
1	a	1448	C
1	a	1451	U
1	a	1452	C
1	a	1492	A
1	a	1502	A
1	a	1503	A
1	a	1506	U
1	a	1517	G
1	a	1529	G
1	a	1530	G
1	a	1533	C
1	a	1534	A
1	a	1535	C
1	a	1536	C
1	a	1539	C
22	v	7	G
22	v	8	4SU
22	v	9	G
22	v	14	A
22	v	16	C
22	v	17	C
22	v	18	U
22	v	19	G
22	v	20	G
22	v	21	H2U
22	v	22	A
22	v	23	G
22	v	60	A
22	v	61	U
22	v	68	C

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Mol	Chain	Res	Type
22	v	76	C
22	v	77	A
22	w	2	G
22	w	3	C
22	w	5	G
22	w	7	G
22	w	8	4SU
22	w	9	G
22	w	10	G
22	w	13	C
22	w	14	A
22	w	15	G
22	w	16	C
22	w	17	C
22	w	117	U
22	w	18	G
22	w	19	G
22	w	20	H2U
22	w	21	A
22	w	22	G
22	w	25	C
22	w	26	G
22	w	28	C
22	w	32	C
22	w	33	U
22	w	34	C
22	w	37	A
22	w	38	A
22	w	40	C
22	w	43	A
22	w	44	A
22	w	48	C
22	w	49	G
22	w	53	G
22	w	59	A
22	w	60	U
22	w	64	G
22	w	66	C
22	w	67	C
22	w	69	C
22	w	70	G
22	w	71	C

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Mol	Chain	Res	Type
22	w	73	A
22	w	75	C
22	w	76	A
23	x	13	A
24	y	7	A
24	y	8	4SU
24	y	9	A
24	y	10	G
24	y	16	H2U
24	y	17	C
24	y	18	G
24	y	19	G
24	y	20	H2U
24	y	21	A
24	y	22	G
24	y	44	G
24	y	45	U
24	y	46	7MG
24	y	48	C
24	y	59	U
24	y	61	C
24	y	75	C
24	y	76	A
26	A	10	A
26	A	12	U
26	A	23	G
26	A	27	G
26	A	28	A
26	A	34	U
26	A	35	G
26	A	42	A
26	A	46	G
26	A	49	A
26	A	51	G
26	A	52	A
26	A	60	G
26	A	63	A
26	A	71	A
26	A	73	A
26	A	74	A
26	A	75	G
26	A	91	A

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Mol	Chain	Res	Type
26	A	92	U
26	A	103	A
26	A	110	G
26	A	118	A
26	A	119	A
26	A	120	U
26	A	127	A
26	A	138	U
26	A	139	U
26	A	140	C
26	A	141	G
26	A	142	A
26	A	158	U
26	A	162	U
26	A	163	C
26	A	181	A
26	A	196	A
26	A	199	A
26	A	204	A
26	A	205	G
26	A	215	G
26	A	216	A
26	A	218	A
26	A	219	A
26	A	221	A
26	A	222	A
26	A	227	A
26	A	228	C
26	A	242	G
26	A	243	U
26	A	248	G
26	A	249	C
26	A	255	A
26	A	265	A
26	A	266	G
26	A	267	C
26	A	272	A
26	A	276	U
26	A	278	A
26	A	281	C
26	A	294	A
26	A	301	G

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Mol	Chain	Res	Type
26	A	302	C
26	A	311	A
26	A	321	U
26	A	322	A
26	A	323	C
26	A	324	A
26	A	329	G
26	A	330	A
26	A	333	G
26	A	334	C
26	A	346	A
26	A	353	C
26	A	361	G
26	A	362	A
26	A	370	G
26	A	371	A
26	A	372	G
26	A	373	U
26	A	386	G
26	A	387	U
26	A	390	U
26	A	391	A
26	A	404	A
26	A	405	U
26	A	406	G
26	A	411	G
26	A	422	A
26	A	424	G
26	A	442	G
26	A	446	G
26	A	454	A
26	A	455	C
26	A	457	A
26	A	458	G
26	A	459	U
26	A	467	G
26	A	480	A
26	A	481	G
26	A	490	C
26	A	491	G
26	A	504	A
26	A	505	A

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Mol	Chain	Res	Type
26	A	506	G
26	A	508	A
26	A	518	G
26	A	527	C
26	A	529	A
26	A	530	G
26	A	532	A
26	A	533	G
26	A	542	C
26	A	543	G
26	A	545	U
26	A	547	A
26	A	550	C
26	A	555	G
26	A	563	A
26	A	572	A
26	A	573	U
26	A	575	A
26	A	603	A
26	A	614	A
26	A	616	A
26	A	627	A
26	A	637	A
26	A	645	C
26	A	646	U
26	A	654	A
26	A	655	A
26	A	659	G
26	A	668	A
26	A	669	G
26	A	670	A
26	A	677	A
26	A	685	A
26	A	686	U
26	A	687	C
26	A	694	U
26	A	695	G
26	A	717	C
26	A	726	G
26	A	730	A
26	A	740	C
26	A	747	5MC

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Mol	Chain	Res	Type
26	A	748	G
26	A	752	A
26	A	753	A
26	A	765	C
26	A	772	C
26	A	775	G
26	A	776	G
26	A	777	G
26	A	782	A
26	A	784	G
26	A	785	G
26	A	789	A
26	A	791	C
26	A	801	G
26	A	802	A
26	A	805	G
26	A	806	C
26	A	812	C
26	A	819	A
26	A	822	G
26	A	827	U
26	A	828	U
26	A	830	G
26	A	831	G
26	A	845	A
26	A	846	U
26	A	847	U
26	A	858	G
26	A	859	G
26	A	860	U
26	A	878	A
26	A	896	A
26	A	897	C
26	A	907	G
26	A	910	A
26	A	932	U
26	A	941	A
26	A	946	C
26	A	953	G
26	A	958	U
26	A	961	C
26	A	974	G

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Mol	Chain	Res	Type
26	A	975	A
26	A	982	C
26	A	983	A
26	A	985	C
26	A	989	G
26	A	990	A
26	A	995	C
26	A	996	A
26	A	999	U
26	A	1011	G
26	A	1012	U
26	A	1013	C
26	A	1021	A
26	A	1022	G
26	A	1023	U
26	A	1026	G
26	A	1033	U
26	A	1046	A
26	A	1053	C
26	A	1054	A
26	A	1057	A
26	A	1060	U
26	A	1061	U
26	A	1062	G
26	A	1064	C
26	A	1065	U
26	A	1066	U
26	A	1068	G
26	A	1069	A
26	A	1070	A
26	A	1071	G
26	A	1072	C
26	A	1075	C
26	A	1076	C
26	A	1079	C
26	A	1084	A
26	A	1088	A
26	A	1089	A
26	A	1090	A
26	A	1104	C
26	A	1111	A
26	A	1112	G

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Mol	Chain	Res	Type
26	A	1119	U
26	A	1130	U
26	A	1131	G
26	A	1132	U
26	A	1134	A
26	A	1135	C
26	A	1142	A
26	A	1143	A
26	A	1151	A
26	A	1174	U
26	A	1175	A
26	A	1176	U
26	A	1179	G
26	A	1180	U
26	A	1206	G
26	A	1212	G
26	A	1213	A
26	A	1218	G
26	A	1237	A
26	A	1238	G
26	A	1247	A
26	A	1248	G
26	A	1250	G
26	A	1251	C
26	A	1253	A
26	A	1256	G
26	A	1271	G
26	A	1272	A
26	A	1273	U
26	A	1276	A
26	A	1289	C
26	A	1298	C
26	A	1300	G
26	A	1301	A
26	A	1302	A
26	A	1311	G
26	A	1315	C
26	A	1321	A
26	A	1329	U
26	A	1330	C
26	A	1332	G
26	A	1341	G

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Mol	Chain	Res	Type
26	A	1345	C
26	A	1352	U
26	A	1365	A
26	A	1368	G
26	A	1378	A
26	A	1379	U
26	A	1380	G
26	A	1383	A
26	A	1385	A
26	A	1395	A
26	A	1397	U
26	A	1416	G
26	A	1419	A
26	A	1420	A
26	A	1428	C
26	A	1454	C
26	A	1458	U
26	A	1461	C
26	A	1482	G
26	A	1483	G
26	A	1490	A
26	A	1491	G
26	A	1493	C
26	A	1504	A
26	A	1515	A
26	A	1524	G
26	A	1533	C
26	A	1535	A
26	A	1536	C
26	A	1537	G
26	A	1555	G
26	A	1559	U
26	A	1560	G
26	A	1567	G
26	A	1569	A
26	A	1578	U
26	A	1581	G
26	A	1585	C
26	A	1607	C
26	A	1611	C
26	A	1616	A
26	A	1627	G

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Mol	Chain	Res	Type
26	A	1647	U
26	A	1648	U
26	A	1651	G
26	A	1654	A
26	A	1664	A
26	A	1665	A
26	A	1667	G
26	A	1674	G
26	A	1694	C
26	A	1695	G
26	A	1715	G
26	A	1729	U
26	A	1730	C
26	A	1738	G
26	A	1756	G
26	A	1758	U
26	A	1764	C
26	A	1773	A
26	A	1780	A
26	A	1781	U
26	A	1782	U
26	A	1784	A
26	A	1787	A
26	A	1800	C
26	A	1801	A
26	A	1808	A
26	A	1816	C
26	A	1818	U
26	A	1829	A
26	A	1833	C
26	A	1847	G
26	A	1858	A
26	A	1865	U
26	A	1871	A
26	A	1885	A
26	A	1896	G
26	A	1900	A
26	A	1901	A
26	A	1906	G
26	A	1907	G
26	A	1913	A
26	A	1914	C

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Mol	Chain	Res	Type
26	A	1927	A
26	A	1929	G
26	A	1930	G
26	A	1931	U
26	A	1937	A
26	A	1938	A
26	A	1940	U
26	A	1941	C
26	A	1955	U
26	A	1960	A
26	A	1962	5MC
26	A	1963	U
26	A	1967	C
26	A	1970	A
26	A	1971	U
26	A	1972	G
26	A	1981	A
26	A	1991	U
26	A	1992	G
26	A	1993	U
26	A	1997	C
26	A	2022	U
26	A	2023	C
26	A	2031	A
26	A	2033	A
26	A	2043	C
26	A	2049	G
26	A	2052	A
26	A	2055	C
26	A	2056	G
26	A	2060	A
26	A	2061	G
26	A	2062	A
26	A	2069	7MG
26	A	2093	G
26	A	2095	A
26	A	2096	C
26	A	2098	U
26	A	2108	A
26	A	2110	G
26	A	2111	U
26	A	2112	G

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Mol	Chain	Res	Type
26	A	2113	U
26	A	2118	U
26	A	2119	A
26	A	2127	G
26	A	2131	U
26	A	2132	U
26	A	2133	G
26	A	2145	C
26	A	2146	C
26	A	2157	G
26	A	2162	G
26	A	2164	C
26	A	2172	U
26	A	2173	A
26	A	2189	U
26	A	2192	U
26	A	2198	A
26	A	2199	A
26	A	2204	G
26	A	2211	A
26	A	2212	A
26	A	2213	U
26	A	2225	A
26	A	2238	G
26	A	2239	G
26	A	2250	G
26	A	2268	A
26	A	2273	A
26	A	2278	A
26	A	2283	C
26	A	2287	A
26	A	2288	A
26	A	2297	A
26	A	2305	U
26	A	2309	A
26	A	2311	A
26	A	2312	U
26	A	2320	U
26	A	2325	G
26	A	2327	A
26	A	2334	U
26	A	2336	A

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Mol	Chain	Res	Type
26	A	2337	G
26	A	2345	G
26	A	2347	C
26	A	2350	C
26	A	2382	G
26	A	2383	G
26	A	2385	C
26	A	2391	G
26	A	2392	A
26	A	2402	U
26	A	2406	A
26	A	2407	A
26	A	2423	U
26	A	2424	C
26	A	2426	A
26	A	2427	C
26	A	2428	G
26	A	2429	G
26	A	2430	A
26	A	2435	A
26	A	2441	U
26	A	2445	2MG
26	A	2447	G
26	A	2448	A
26	A	2449	H2U
26	A	2459	A
26	A	2468	A
26	A	2476	A
26	A	2478	A
26	A	2484	G
26	A	2494	G
26	A	2497	A
26	A	2498	OMC
26	A	2502	G
26	A	2504	PSU
26	A	2505	G
26	A	2506	U
26	A	2517	C
26	A	2518	A
26	A	2519	U
26	A	2529	G
26	A	2547	A

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Mol	Chain	Res	Type
26	A	2554	U
26	A	2567	G
26	A	2572	A
26	A	2573	C
26	A	2585	U
26	A	2602	A
26	A	2603	G
26	A	2608	G
26	A	2609	U
26	A	2613	U
26	A	2614	A
26	A	2636	C
26	A	2645	G
26	A	2646	C
26	A	2655	G
26	A	2656	U
26	A	2682	A
26	A	2689	U
26	A	2690	U
26	A	2707	U
26	A	2712	C
26	A	2713	U
26	A	2714	G
26	A	2718	G
26	A	2722	G
26	A	2726	A
26	A	2731	G
26	A	2732	G
26	A	2733	A
26	A	2739	U
26	A	2744	G
26	A	2748	A
26	A	2757	A
26	A	2764	A
26	A	2765	A
26	A	2769	U
26	A	2778	A
26	A	2779	U
26	A	2791	G
26	A	2794	C
26	A	2797	U
26	A	2799	A

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Mol	Chain	Res	Type
26	A	2800	A
26	A	2801	G
26	A	2808	G
26	A	2809	A
26	A	2818	U
26	A	2820	A
26	A	2821	A
26	A	2823	A
26	A	2833	U
26	A	2834	G
26	A	2835	A
26	A	2848	G
26	A	2849	U
26	A	2867	G
26	A	2868	A
26	A	2872	A
26	A	2873	A
26	A	2880	C
26	A	2884	U
27	B	4	C
27	B	12	C
27	B	13	G
27	B	24	G
27	B	25	U
27	B	35	C
27	B	40	U
27	B	44	G
27	B	45	A
27	B	56	G
27	B	67	G
27	B	88	C
27	B	89	U
27	B	91	C
27	B	108	A
27	B	109	A
27	B	116	G

All (94) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
26	A	51	G
26	A	86	G

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Mol	Chain	Res	Type
26	A	204	A
26	A	227	A
26	A	242	G
26	A	265	A
26	A	271	G
26	A	301	G
26	A	311	A
26	A	321	U
26	A	332	A
26	A	345	A
26	A	372	G
26	A	386	G
26	A	390	U
26	A	446	G
26	A	454	A
26	A	458	G
26	A	479	A
26	A	480	A
26	A	490	C
26	A	503	A
26	A	549	G
26	A	571	U
26	A	637	A
26	A	685	A
26	A	686	U
26	A	747	5MC
26	A	752	A
26	A	774	G
26	A	776	G
26	A	800	A
26	A	830	G
26	A	858	G
26	A	859	G
26	A	974	G
26	A	1012	U
26	A	1020	A
26	A	1022	G
26	A	1070	A
26	A	1089	A
26	A	1111	A
26	A	1124	G
26	A	1130	U

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Mol	Chain	Res	Type
26	A	1133	A
26	A	1134	A
26	A	1141	U
26	A	1142	A
26	A	1182	G
26	A	1190	G
26	A	1210	G
26	A	1212	G
26	A	1275	A
26	A	1288	G
26	A	1300	G
26	A	1331	G
26	A	1378	A
26	A	1399	C
26	A	1432	G
26	A	1626	A
26	A	1693	U
26	A	1713	A
26	A	1783	A
26	A	1799	G
26	A	1857	G
26	A	1930	G
26	A	1940	U
26	A	2060	A
26	A	2092	U
26	A	2197	U
26	A	2210	U
26	A	2282	G
26	A	2286	G
26	A	2296	U
26	A	2326	C
26	A	2333	A
26	A	2391	G
26	A	2405	G
26	A	2406	A
26	A	2517	C
26	A	2518	A
26	A	2566	A
26	A	2614	A
26	A	2655	G
26	A	2712	C
26	A	2756	U

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Mol	Chain	Res	Type
26	A	2798	U
26	A	2808	G
26	A	2820	A
26	A	2866	U
27	B	24	G
27	B	56	G
27	B	66	A
27	B	88	C

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

52 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
22	H2U	v	21	22	18,21,22	0.92	2 (11%)	21,30,33	1.57	2 (9%)
22	5MU	v	55	22	19,22,23	1.38	4 (21%)	28,32,35	2.23	5 (17%)
1	MA6	a	1519	1	19,26,27	0.97	1 (5%)	18,38,41	1.94	6 (33%)
26	2MG	A	1835	26	18,26,27	1.01	1 (5%)	16,38,41	1.25	3 (18%)
1	5MC	a	1407	1	18,22,23	0.95	2 (11%)	26,32,35	1.16	3 (11%)
26	2MG	A	2445	26	18,26,27	1.01	1 (5%)	16,38,41	1.14	2 (12%)
26	5MC	A	747	26	18,22,23	0.96	2 (11%)	26,32,35	1.38	3 (11%)
1	MA6	a	1518	1	19,26,27	1.13	2 (10%)	18,38,41	1.94	4 (22%)
1	UR3	a	1498	1	19,22,23	0.93	0	26,32,35	1.59	3 (11%)
26	PSU	A	955	26	18,21,22	1.42	4 (22%)	22,30,33	2.00	4 (18%)
26	PSU	A	2580	26	18,21,22	1.43	2 (11%)	22,30,33	2.02	4 (18%)
22	4SU	v	8	22	18,21,22	1.68	4 (22%)	26,30,33	2.28	5 (19%)
26	PSU	A	1911	26	18,21,22	1.33	2 (11%)	22,30,33	1.96	4 (18%)
24	H2U	y	20	24	18,21,22	0.95	2 (11%)	21,30,33	2.23	1 (4%)
26	6MZ	A	2030	26	18,25,26	0.92	1 (5%)	16,36,39	2.49	4 (25%)
1	2MG	a	1516	1	18,26,27	0.87	1 (5%)	16,38,41	1.12	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	6MZ	A	1618	26	18,25,26	0.98	1 (5%)	16,36,39	2.26	4 (25%)
26	PSU	A	2604	26	18,21,22	1.37	3 (16%)	22,30,33	1.90	4 (18%)
1	PSU	a	516	59,1	18,21,22	1.45	4 (22%)	22,30,33	2.13	5 (22%)
22	5MU	w	54	22	19,22,23	1.27	3 (15%)	28,32,35	2.32	10 (35%)
24	PSU	y	39	24	18,21,22	1.32	2 (11%)	22,30,33	1.89	4 (18%)
26	5MU	A	1939	26	19,22,23	1.37	4 (21%)	28,32,35	2.26	6 (21%)
24	PSU	y	32	24	18,21,22	1.33	2 (11%)	22,30,33	1.88	3 (13%)
22	4SU	w	8	22	18,21,22	1.79	4 (22%)	26,30,33	2.33	4 (15%)
26	1MG	A	745	26	18,26,27	0.80	0	19,39,42	1.07	1 (5%)
1	4OC	a	1402	1	20,23,24	0.77	0	26,32,35	0.91	0
24	MIA	y	37	24	24,31,32	2.26	3 (12%)	26,44,47	2.83	9 (34%)
24	PSU	y	55	24	18,21,22	1.37	2 (11%)	22,30,33	1.85	3 (13%)
26	3TD	A	1915	26	18,22,23	1.22	2 (11%)	22,32,35	1.92	3 (13%)
26	PSU	A	2504	26	18,21,22	1.34	2 (11%)	22,30,33	1.82	3 (13%)
22	H2U	w	20	22	18,21,22	1.33	3 (16%)	21,30,33	2.54	4 (19%)
26	PSU	A	746	59,26	18,21,22	1.33	2 (11%)	22,30,33	1.84	4 (18%)
26	OMG	A	2251	26,22	18,26,27	1.03	1 (5%)	19,38,41	1.01	1 (5%)
26	2MA	A	2503	59,26	17,25,26	1.00	1 (5%)	17,37,40	0.98	2 (11%)
24	4SU	y	8	24	18,21,22	1.76	4 (22%)	26,30,33	2.37	5 (19%)
26	OMU	A	2552	26	19,22,23	1.22	3 (15%)	26,31,34	2.17	7 (26%)
26	H2U	A	2449	26	18,21,22	0.91	2 (11%)	21,30,33	1.67	3 (14%)
26	PSU	A	2457	26	18,21,22	1.35	2 (11%)	22,30,33	2.06	4 (18%)
26	7MG	A	2069	26	22,26,27	1.40	4 (18%)	29,39,42	2.50	7 (24%)
1	5MC	a	967	1	18,22,23	0.98	1 (5%)	26,32,35	1.08	2 (7%)
26	OMC	A	2498	59,26	19,22,23	0.83	1 (5%)	26,31,34	0.87	0
26	PSU	A	2605	26	18,21,22	1.41	3 (16%)	22,30,33	1.82	4 (18%)
1	2MG	a	1207	1	18,26,27	0.96	1 (5%)	16,38,41	1.15	2 (12%)
26	PSU	A	1917	26	18,21,22	1.36	2 (11%)	22,30,33	1.85	3 (13%)
26	5MC	A	1962	26	18,22,23	0.98	2 (11%)	26,32,35	1.10	2 (7%)
22	PSU	w	55	22	18,21,22	1.49	3 (16%)	22,30,33	2.14	5 (22%)
1	2MG	a	966	1	18,26,27	0.88	1 (5%)	16,38,41	1.17	2 (12%)
22	PSU	v	56	22	18,21,22	1.35	2 (11%)	22,30,33	1.85	3 (13%)
24	5MU	y	54	24	19,22,23	1.39	5 (26%)	28,32,35	2.22	7 (25%)
1	7MG	a	527	1	22,26,27	1.37	4 (18%)	29,39,42	2.45	7 (24%)
24	7MG	y	46	24	22,26,27	1.32	4 (18%)	29,39,42	2.53	7 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	H2U	y	16	24	18,21,22	0.97	2 (11%)	21,30,33	1.45	2 (9%)

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
22	H2U	v	21	22	-	1/7/38/39	0/2/2/2
22	5MU	v	55	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	2/7/29/30	0/3/3/3
26	2MG	A	1835	26	-	0/5/27/28	0/3/3/3
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
26	2MG	A	2445	26	-	2/5/27/28	0/3/3/3
26	5MC	A	747	26	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	4/7/29/30	0/3/3/3
1	UR3	a	1498	1	-	2/7/25/26	0/2/2/2
26	PSU	A	955	26	-	0/7/25/26	0/2/2/2
26	PSU	A	2580	26	-	0/7/25/26	0/2/2/2
22	4SU	v	8	22	-	0/7/25/26	0/2/2/2
26	PSU	A	1911	26	-	0/7/25/26	0/2/2/2
24	H2U	y	20	24	-	5/7/38/39	0/2/2/2
26	6MZ	A	2030	26	-	2/5/27/28	0/3/3/3
1	2MG	a	1516	1	-	0/5/27/28	0/3/3/3
26	6MZ	A	1618	26	-	0/5/27/28	0/3/3/3
26	PSU	A	2604	26	-	0/7/25/26	0/2/2/2
1	PSU	a	516	59,1	-	2/7/25/26	0/2/2/2
22	5MU	w	54	22	-	2/7/25/26	0/2/2/2
24	PSU	y	39	24	-	0/7/25/26	0/2/2/2
26	5MU	A	1939	26	-	0/7/25/26	0/2/2/2
24	PSU	y	32	24	-	0/7/25/26	0/2/2/2
22	4SU	w	8	22	-	6/7/25/26	0/2/2/2
26	1MG	A	745	26	-	0/3/25/26	0/3/3/3
1	4OC	a	1402	1	-	0/9/29/30	0/2/2/2
24	MIA	y	37	24	-	3/11/33/34	0/3/3/3
24	PSU	y	55	24	-	0/7/25/26	0/2/2/2
26	3TD	A	1915	26	-	3/7/25/26	0/2/2/2
26	PSU	A	2504	26	-	2/7/25/26	0/2/2/2
22	H2U	w	20	22	-	2/7/38/39	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PSU	A	746	59,26	-	1/7/25/26	0/2/2/2
26	OMG	A	2251	26,22	-	0/5/27/28	0/3/3/3
26	2MA	A	2503	59,26	-	1/3/25/26	0/3/3/3
24	4SU	y	8	24	-	1/7/25/26	0/2/2/2
26	OMU	A	2552	26	-	2/9/27/28	0/2/2/2
26	H2U	A	2449	26	-	0/7/38/39	0/2/2/2
26	PSU	A	2457	26	-	0/7/25/26	0/2/2/2
26	7MG	A	2069	26	-	1/7/37/38	0/3/3/3
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
26	OMC	A	2498	59,26	-	1/9/27/28	0/2/2/2
26	PSU	A	2605	26	-	0/7/25/26	0/2/2/2
1	2MG	a	1207	1	-	2/5/27/28	0/3/3/3
26	PSU	A	1917	26	-	0/7/25/26	0/2/2/2
26	5MC	A	1962	26	-	1/7/25/26	0/2/2/2
22	PSU	w	55	22	-	2/7/25/26	0/2/2/2
1	2MG	a	966	1	-	2/5/27/28	0/3/3/3
22	PSU	v	56	22	-	2/7/25/26	0/2/2/2
24	5MU	y	54	24	-	0/7/25/26	0/2/2/2
1	7MG	a	527	1	-	3/7/37/38	0/3/3/3
24	7MG	y	46	24	-	3/7/37/38	0/3/3/3
24	H2U	y	16	24	-	0/7/38/39	0/2/2/2

All (116) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	37	MIA	C2-S10	-7.22	1.69	1.75
24	y	37	MIA	C13-C14	7.20	1.53	1.32
24	y	8	4SU	C4-S4	-4.75	1.59	1.68
22	w	8	4SU	C4-S4	-4.60	1.59	1.68
22	v	8	4SU	C4-S4	-4.42	1.60	1.68
26	A	2069	7MG	C4-N9	-3.83	1.33	1.37
1	a	527	7MG	C4-N9	-3.68	1.33	1.37
24	y	55	PSU	C6-C5	3.41	1.39	1.35
22	w	20	H2U	C2-N3	-3.40	1.31	1.38
26	A	1915	3TD	C10-N3	3.36	1.53	1.47
22	w	8	4SU	C4-N3	-3.32	1.34	1.37
22	v	56	PSU	C6-C5	3.29	1.39	1.35
26	A	1835	2MG	C6-N1	-3.21	1.33	1.37
26	A	1911	PSU	C6-C5	3.20	1.39	1.35
26	A	2251	OMG	C6-N1	-3.19	1.33	1.37
26	A	1618	6MZ	C5-C4	3.17	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	516	PSU	C4-N3	-3.11	1.33	1.38
26	A	955	PSU	C4-N3	-3.11	1.33	1.38
26	A	2580	PSU	C4-N3	-3.10	1.33	1.38
26	A	2605	PSU	C6-C5	3.05	1.38	1.35
26	A	1917	PSU	C6-C5	3.05	1.38	1.35
24	y	39	PSU	C6-C5	3.01	1.38	1.35
22	w	8	4SU	C5-C4	-3.01	1.38	1.42
22	w	55	PSU	C4-N3	-2.99	1.33	1.38
24	y	32	PSU	C6-C5	2.98	1.38	1.35
22	v	8	4SU	C4-N3	-2.98	1.34	1.37
26	A	2605	PSU	C4-N3	-2.97	1.33	1.38
1	a	967	5MC	C6-C5	2.96	1.39	1.34
24	y	46	7MG	C5-C4	2.96	1.47	1.38
24	y	8	4SU	C5-C4	-2.95	1.38	1.42
26	A	1939	5MU	C4-N3	-2.94	1.33	1.38
26	A	2604	PSU	C4-N3	-2.93	1.33	1.38
26	A	1939	5MU	C6-N1	-2.91	1.33	1.38
22	w	20	H2U	C2-N1	-2.90	1.31	1.35
26	A	2030	6MZ	C5-C4	2.88	1.48	1.40
24	y	8	4SU	C4-N3	-2.84	1.34	1.37
24	y	54	5MU	C4-N3	-2.84	1.33	1.38
26	A	2069	7MG	C5-N7	-2.83	1.32	1.35
24	y	46	7MG	C4-N9	-2.82	1.34	1.37
26	A	746	PSU	C4-N3	-2.81	1.33	1.38
22	w	55	PSU	C2-N1	-2.80	1.32	1.36
1	a	1518	MA6	C5-C4	2.77	1.48	1.40
26	A	746	PSU	C6-C5	2.76	1.38	1.35
26	A	2504	PSU	C4-N3	-2.75	1.33	1.38
26	A	2457	PSU	C4-N3	-2.74	1.33	1.38
26	A	1962	5MC	C6-N1	-2.73	1.33	1.38
1	a	527	7MG	C5-C4	2.72	1.47	1.38
22	v	55	5MU	C6-C5	2.72	1.39	1.34
22	w	55	PSU	C6-C5	2.72	1.38	1.35
26	A	2445	2MG	C6-N1	-2.71	1.33	1.37
24	y	32	PSU	C4-N3	-2.70	1.33	1.38
22	v	56	PSU	C4-N3	-2.68	1.33	1.38
1	a	1407	5MC	C6-N1	-2.67	1.33	1.38
22	w	54	5MU	C6-N1	-2.64	1.33	1.38
26	A	1917	PSU	C4-N3	-2.64	1.33	1.38
26	A	2504	PSU	C6-C5	2.63	1.38	1.35
24	y	39	PSU	C4-N3	-2.61	1.34	1.38
22	v	55	5MU	C4-N3	-2.58	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	516	PSU	C6-C5	2.57	1.38	1.35
26	A	2605	PSU	C2-N3	-2.57	1.33	1.37
26	A	747	5MC	C6-C5	2.56	1.38	1.34
26	A	2604	PSU	C2-N3	-2.55	1.33	1.37
26	A	2604	PSU	C6-C5	2.54	1.38	1.35
24	y	55	PSU	C4-N3	-2.52	1.34	1.38
26	A	2552	OMU	C4-N3	-2.51	1.34	1.38
1	a	966	2MG	C6-N1	-2.50	1.34	1.37
26	A	2069	7MG	C5-C4	2.49	1.46	1.38
26	A	2457	PSU	C6-C5	2.47	1.38	1.35
24	y	54	5MU	C6-N1	-2.46	1.33	1.38
24	y	20	H2U	C2-N3	-2.46	1.33	1.38
26	A	747	5MC	C6-N1	-2.46	1.33	1.38
26	A	2449	H2U	C2-N3	-2.45	1.33	1.38
26	A	1939	5MU	C6-C5	2.45	1.38	1.34
26	A	1939	5MU	C2-N3	-2.45	1.33	1.38
26	A	1915	3TD	C4-N3	-2.43	1.35	1.40
24	y	16	H2U	C2-N3	-2.43	1.33	1.38
22	v	55	5MU	C2-N1	2.42	1.42	1.38
22	w	54	5MU	C4-N3	-2.42	1.34	1.38
22	v	21	H2U	C2-N3	-2.42	1.33	1.38
26	A	1911	PSU	C4-N3	-2.42	1.34	1.38
1	a	1207	2MG	C6-N1	-2.42	1.34	1.37
22	w	20	H2U	C4-N3	-2.42	1.33	1.37
1	a	527	7MG	C6-N1	-2.41	1.34	1.38
24	y	54	5MU	C2-N3	-2.39	1.33	1.38
1	a	1407	5MC	C6-C5	2.37	1.38	1.34
26	A	2580	PSU	C6-C5	2.36	1.38	1.35
22	v	8	4SU	C5-C4	-2.35	1.39	1.42
22	w	8	4SU	C2-N3	-2.35	1.33	1.38
1	a	516	PSU	C2-N3	-2.33	1.33	1.37
26	A	955	PSU	C2-N3	-2.33	1.33	1.37
22	v	21	H2U	C4-N3	-2.30	1.33	1.37
1	a	1518	MA6	C6-N1	2.30	1.36	1.33
26	A	1962	5MC	C6-C5	2.30	1.38	1.34
26	A	2449	H2U	C4-N3	-2.29	1.33	1.37
24	y	37	MIA	C5-C4	2.28	1.47	1.40
24	y	54	5MU	C6-C5	2.28	1.38	1.34
26	A	955	PSU	C2-N1	-2.27	1.33	1.36
22	v	8	4SU	C2-N1	2.27	1.42	1.38
24	y	54	5MU	C4-C5	2.26	1.48	1.44
26	A	2503	2MA	C2-N3	2.26	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	20	H2U	C4-N3	-2.24	1.33	1.37
24	y	16	H2U	C4-N3	-2.24	1.33	1.37
26	A	2069	7MG	C6-N1	-2.23	1.34	1.38
1	a	527	7MG	C5-N7	-2.22	1.33	1.35
22	v	55	5MU	C6-N1	-2.20	1.34	1.38
24	y	46	7MG	C6-N1	-2.20	1.34	1.38
1	a	1519	MA6	C5-C4	2.20	1.46	1.40
24	y	8	4SU	C2-N3	-2.18	1.34	1.38
1	a	516	PSU	O4'-C1'	-2.18	1.40	1.43
22	w	54	5MU	C4-C5	2.14	1.48	1.44
26	A	2552	OMU	C2-N3	-2.11	1.34	1.38
26	A	955	PSU	C6-C5	2.11	1.37	1.35
26	A	2552	OMU	C2-N1	2.09	1.41	1.38
26	A	2498	OMC	C6-N1	-2.08	1.33	1.38
1	a	1516	2MG	C6-N1	-2.06	1.34	1.37
24	y	46	7MG	C8-N9	2.03	1.47	1.46

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	20	H2U	C4-N3-C2	-9.51	117.91	125.79
24	y	37	MIA	C12-C13-C14	-9.25	109.14	127.14
24	y	46	7MG	N9-C4-N3	8.84	138.69	125.47
22	w	20	H2U	C4-N3-C2	-8.60	118.66	125.79
26	A	2069	7MG	N9-C4-N3	8.59	138.32	125.47
1	a	527	7MG	N9-C4-N3	8.55	138.26	125.47
26	A	2030	6MZ	C2-N1-C6	7.18	122.75	116.59
22	w	8	4SU	C4-N3-C2	-7.00	120.54	127.34
22	v	8	4SU	C4-N3-C2	-6.86	120.68	127.34
1	a	516	PSU	N1-C2-N3	6.78	122.81	115.13
24	y	8	4SU	C4-N3-C2	-6.67	120.86	127.34
24	y	8	4SU	C5-C4-N3	6.65	120.86	114.69
22	w	55	PSU	N1-C2-N3	6.55	122.55	115.13
26	A	2580	PSU	N1-C2-N3	6.49	122.48	115.13
26	A	1915	3TD	N1-C2-N3	6.47	121.25	116.14
26	A	2457	PSU	N1-C2-N3	6.38	122.36	115.13
26	A	955	PSU	N1-C2-N3	6.24	122.20	115.13
26	A	1911	PSU	N1-C2-N3	6.08	122.01	115.13
26	A	1618	6MZ	C2-N1-C6	6.02	121.75	116.59
22	w	8	4SU	C5-C4-N3	6.01	120.27	114.69
26	A	2449	H2U	C4-N3-C2	-6.01	120.80	125.79
1	a	1498	UR3	C4-N3-C2	-6.01	118.90	124.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1917	PSU	N1-C2-N3	5.98	121.90	115.13
24	y	32	PSU	N1-C2-N3	5.88	121.79	115.13
24	y	55	PSU	N1-C2-N3	5.87	121.78	115.13
26	A	2504	PSU	N1-C2-N3	5.85	121.76	115.13
24	y	39	PSU	N1-C2-N3	5.84	121.74	115.13
26	A	2069	7MG	N9-C8-N7	-5.83	95.05	103.38
26	A	2604	PSU	N1-C2-N3	5.82	121.72	115.13
26	A	2605	PSU	N1-C2-N3	5.77	121.66	115.13
22	v	56	PSU	N1-C2-N3	5.75	121.65	115.13
22	v	8	4SU	C5-C4-N3	5.74	120.02	114.69
26	A	1939	5MU	C4-N3-C2	-5.73	119.94	127.35
22	v	21	H2U	C4-N3-C2	-5.70	121.06	125.79
26	A	746	PSU	N1-C2-N3	5.68	121.56	115.13
24	y	54	5MU	C4-N3-C2	-5.61	120.09	127.35
22	v	55	5MU	C4-N3-C2	-5.42	120.34	127.35
24	y	46	7MG	C5-C4-N3	-5.40	117.84	128.13
22	v	55	5MU	O4-C4-C5	-5.40	118.64	124.90
1	a	527	7MG	N9-C8-N7	-5.39	95.67	103.38
24	y	46	7MG	N9-C8-N7	-5.20	95.94	103.38
24	y	16	H2U	C4-N3-C2	-5.20	121.48	125.79
24	y	37	MIA	C11-S10-C2	-5.16	98.42	102.27
24	y	54	5MU	C5-C4-N3	5.15	119.70	115.31
26	A	2552	OMU	C4-N3-C2	-5.13	119.81	126.58
22	w	55	PSU	O2-C2-N1	-5.07	117.20	122.79
22	v	55	5MU	C5-C4-N3	5.05	119.62	115.31
26	A	1618	6MZ	C9-N6-C6	-5.04	118.53	122.87
26	A	1939	5MU	C5-C4-N3	4.99	119.57	115.31
22	w	54	5MU	C4-N3-C2	-4.98	120.90	127.35
26	A	1939	5MU	N3-C2-N1	4.97	121.49	114.89
1	a	527	7MG	C5-C4-N3	-4.93	118.73	128.13
24	y	8	4SU	C5-C4-S4	-4.93	118.12	124.47
26	A	2030	6MZ	C9-N6-C6	-4.87	118.67	122.87
26	A	2069	7MG	C5-C4-N3	-4.87	118.85	128.13
24	y	54	5MU	N3-C2-N1	4.84	121.31	114.89
22	v	55	5MU	N3-C2-N1	4.82	121.29	114.89
26	A	2552	OMU	N3-C2-N1	4.74	121.18	114.89
26	A	2552	OMU	C1'-N1-C2	4.62	125.94	117.57
22	w	8	4SU	C5-C4-S4	-4.61	118.52	124.47
26	A	1939	5MU	C5-C6-N1	-4.60	118.60	123.34
1	a	516	PSU	C4-N3-C2	-4.49	119.87	126.34
26	A	1939	5MU	O4-C4-C5	-4.47	119.72	124.90
1	a	1518	MA6	C10-N6-C6	-4.45	106.03	119.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	46	7MG	C2-N3-C4	4.40	120.14	112.30
22	w	20	H2U	C5-C4-N3	4.40	121.59	116.65
22	w	54	5MU	C5-C4-N3	4.38	119.05	115.31
22	w	54	5MU	N3-C2-N1	4.37	120.69	114.89
26	A	955	PSU	C4-N3-C2	-4.37	120.05	126.34
24	y	54	5MU	C5-C6-N1	-4.35	118.87	123.34
26	A	2604	PSU	C4-N3-C2	-4.33	120.10	126.34
22	w	8	4SU	N3-C2-N1	4.31	120.61	114.89
22	v	8	4SU	N3-C2-N1	4.28	120.57	114.89
22	v	8	4SU	C5-C4-S4	-4.26	118.98	124.47
26	A	2457	PSU	C4-N3-C2	-4.25	120.22	126.34
26	A	1911	PSU	C4-N3-C2	-4.22	120.26	126.34
24	y	37	MIA	C16-C14-C13	-4.18	110.56	122.65
26	A	2457	PSU	O2-C2-N1	-4.18	118.19	122.79
24	y	37	MIA	C5-C6-N1	-4.18	117.34	120.81
26	A	1915	3TD	C4-N3-C2	-4.15	120.11	124.61
22	w	20	H2U	C5-C6-N1	-4.13	98.00	111.61
22	w	54	5MU	O4-C4-C5	-4.09	120.17	124.90
26	A	746	PSU	C4-N3-C2	-4.07	120.47	126.34
22	w	55	PSU	C4-N3-C2	-4.07	120.47	126.34
24	y	39	PSU	C4-N3-C2	-4.06	120.48	126.34
24	y	37	MIA	C2-N3-C4	4.06	120.92	115.32
24	y	32	PSU	C4-N3-C2	-4.04	120.51	126.34
26	A	2069	7MG	C2-N3-C4	4.00	119.43	112.30
26	A	2552	OMU	C5-C4-N3	4.00	120.82	114.84
1	a	1519	MA6	N3-C2-N1	-3.99	122.45	128.68
24	y	54	5MU	O4-C4-C5	-3.96	120.31	124.90
22	w	54	5MU	C5M-C5-C4	3.89	123.05	118.77
26	A	955	PSU	O2-C2-N1	-3.87	118.53	122.79
1	a	527	7MG	C2-N3-C4	3.84	119.15	112.30
22	w	54	5MU	C1'-N1-C6	-3.84	114.73	121.12
24	y	37	MIA	C15-C14-C13	-3.82	111.60	122.65
22	v	55	5MU	C5-C6-N1	-3.81	119.41	123.34
22	w	54	5MU	C1'-N1-C2	3.80	124.45	117.57
26	A	2580	PSU	C4-N3-C2	-3.80	120.86	126.34
24	y	55	PSU	C4-N3-C2	-3.80	120.87	126.34
22	v	56	PSU	C4-N3-C2	-3.79	120.88	126.34
22	w	20	H2U	N3-C2-N1	-3.76	112.68	116.65
1	a	516	PSU	O2-C2-N1	-3.73	118.69	122.79
26	A	1917	PSU	C4-N3-C2	-3.67	121.05	126.34
26	A	2504	PSU	O2-C2-N1	-3.65	118.77	122.79
26	A	2504	PSU	C4-N3-C2	-3.63	121.11	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	1939	5MU	O2-C2-N1	-3.62	117.97	122.79
26	A	2605	PSU	C4-N3-C2	-3.61	121.13	126.34
1	a	1518	MA6	N1-C6-N6	3.61	120.85	117.06
26	A	2580	PSU	O2-C2-N1	-3.54	118.90	122.79
1	a	1518	MA6	N3-C2-N1	-3.53	123.16	128.68
1	a	1407	5MC	C5-C6-N1	-3.51	119.73	123.34
24	y	55	PSU	O2-C2-N1	-3.48	118.96	122.79
26	A	747	5MC	C5-C6-N1	-3.48	119.76	123.34
1	a	1519	MA6	C10-N6-C6	-3.45	109.07	119.51
26	A	1911	PSU	O2-C2-N1	-3.44	119.00	122.79
1	a	1519	MA6	C9-N6-C6	-3.39	109.25	119.51
24	y	8	4SU	N3-C2-N1	3.38	119.38	114.89
26	A	1917	PSU	O2-C2-N1	-3.29	119.17	122.79
26	A	2552	OMU	O4-C4-C5	-3.29	119.38	125.16
26	A	746	PSU	O2-C2-N1	-3.26	119.20	122.79
24	y	32	PSU	O2-C2-N1	-3.21	119.26	122.79
24	y	39	PSU	O2-C2-N1	-3.21	119.26	122.79
24	y	37	MIA	C4-C5-N7	-3.14	106.12	109.40
1	a	1518	MA6	C9-N6-C6	-3.09	110.17	119.51
1	a	1498	UR3	C1'-N1-C2	3.06	122.16	116.99
26	A	1618	6MZ	N3-C2-N1	-3.04	123.92	128.68
22	v	56	PSU	O2-C2-N1	-3.04	119.45	122.79
1	a	1519	MA6	N1-C6-N6	3.01	120.22	117.06
26	A	2030	6MZ	C4-C5-N7	-2.97	106.30	109.40
22	w	54	5MU	C5M-C5-C6	-2.96	118.89	122.85
26	A	1962	5MC	C5-C4-N3	-2.94	118.50	121.67
26	A	2030	6MZ	N3-C2-N1	-2.89	124.16	128.68
1	a	1519	MA6	C10-N6-C9	-2.88	106.86	116.12
1	a	967	5MC	C5-C6-N1	-2.87	120.38	123.34
24	y	8	4SU	C1'-N1-C2	2.84	122.71	117.57
26	A	1915	3TD	C10-N3-C4	2.83	122.02	117.69
24	y	46	7MG	C5-C6-N1	2.81	115.94	110.99
24	y	37	MIA	C2-N1-C6	2.79	122.18	117.19
26	A	1962	5MC	C5-C6-N1	-2.78	120.48	123.34
26	A	1835	2MG	C5-C6-N1	2.77	118.84	113.95
26	A	2069	7MG	C5-C4-N9	-2.72	102.81	106.35
22	w	54	5MU	C5-C6-N1	-2.70	120.56	123.34
26	A	2552	OMU	C1'-N1-C6	-2.67	115.01	120.84
26	A	745	1MG	C8-N7-C5	2.63	108.00	102.99
24	y	54	5MU	O2-C2-N1	-2.60	119.34	122.79
1	a	527	7MG	C5-C4-N9	-2.58	103.00	106.35
1	a	1407	5MC	C5-C4-N3	-2.56	118.91	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	2604	PSU	C5-C6-N1	-2.56	118.28	122.11
1	a	966	2MG	C5-C6-N1	2.54	118.44	113.95
1	a	1519	MA6	C4-C5-N7	-2.53	106.76	109.40
26	A	747	5MC	C5-C4-N3	-2.53	118.95	121.67
1	a	527	7MG	C5-C6-N1	2.51	115.42	110.99
26	A	2503	2MA	C8-N7-C5	2.50	107.75	102.99
26	A	1618	6MZ	C4-C5-N7	-2.48	106.82	109.40
26	A	2580	PSU	C5-C6-N1	-2.47	118.41	122.11
26	A	2604	PSU	O2-C2-N1	-2.44	120.11	122.79
1	a	1207	2MG	C5-C6-N1	2.38	118.16	113.95
1	a	967	5MC	C5-C4-N3	-2.38	119.11	121.67
26	A	2457	PSU	C5-C6-N1	-2.36	118.57	122.11
26	A	2069	7MG	O6-C6-C5	-2.35	121.78	127.54
26	A	2605	PSU	O2-C2-N1	-2.34	120.22	122.79
26	A	2445	2MG	O6-C6-C5	-2.33	119.82	124.37
1	a	966	2MG	C8-N7-C5	2.31	107.39	102.99
26	A	2449	H2U	O4-C4-N3	2.31	123.94	120.28
22	v	8	4SU	C1'-N1-C2	2.30	121.73	117.57
22	w	55	PSU	O4'-C1'-C2'	2.30	108.38	105.14
1	a	516	PSU	O4'-C1'-C2'	2.30	108.38	105.14
26	A	2605	PSU	C6-C5-C4	-2.29	116.60	118.20
26	A	2069	7MG	C5-C6-N1	2.27	115.00	110.99
1	a	527	7MG	O6-C6-C5	-2.27	121.97	127.54
24	y	39	PSU	C5-C6-N1	-2.26	118.72	122.11
26	A	2503	2MA	C5-C6-N1	2.25	117.90	114.02
26	A	1835	2MG	O6-C6-C5	-2.25	119.99	124.37
26	A	1835	2MG	C8-N7-C5	2.24	107.26	102.99
26	A	2449	H2U	C5-C6-N1	-2.23	104.26	111.61
24	y	54	5MU	C5M-C5-C4	2.22	121.21	118.77
24	y	46	7MG	C5-C4-N9	-2.22	103.46	106.35
22	w	54	5MU	O2-C2-N1	-2.19	119.87	122.79
26	A	746	PSU	C5-C6-N1	-2.19	118.83	122.11
1	a	1516	2MG	C5-C6-N1	2.19	117.81	113.95
1	a	516	PSU	C5-C6-N1	-2.18	118.83	122.11
24	y	16	H2U	C5-C6-N1	-2.16	104.49	111.61
26	A	2251	OMG	C8-N7-C5	2.16	107.11	102.99
22	w	55	PSU	C5-C6-N1	-2.13	118.91	122.11
1	a	1516	2MG	O6-C6-C5	-2.13	120.21	124.37
26	A	2445	2MG	C5-C6-N1	2.11	117.68	113.95
26	A	955	PSU	C5-C6-N1	-2.11	118.95	122.11
24	y	37	MIA	N3-C2-N1	-2.10	123.11	126.98
26	A	1911	PSU	C5-C6-N1	-2.09	118.98	122.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1207	2MG	C8-N7-C5	2.08	106.96	102.99
22	v	21	H2U	N3-C2-N1	2.07	118.85	116.65
24	y	46	7MG	O6-C6-C5	-2.05	122.52	127.54
26	A	747	5MC	C3'-C2'-C1'	2.04	105.31	101.43
1	a	1407	5MC	O2-C2-N3	-2.01	119.06	122.33
1	a	1498	UR3	C3U-N3-C2	2.01	120.83	117.31
26	A	2552	OMU	O2-C2-N3	-2.01	117.76	121.50

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	7MG	C3'-C4'-C5'-O5'
1	a	1207	2MG	O4'-C4'-C5'-O5'
1	a	1207	2MG	C3'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1518	MA6	C5-C6-N6-C10
1	a	1518	MA6	N1-C6-N6-C9
1	a	1518	MA6	N1-C6-N6-C10
1	a	1519	MA6	C5-C6-N6-C9
22	v	56	PSU	O4'-C1'-C5-C4
22	v	56	PSU	O4'-C1'-C5-C6
22	w	8	4SU	O4'-C4'-C5'-O5'
22	w	55	PSU	O4'-C1'-C5-C4
22	w	55	PSU	O4'-C1'-C5-C6
24	y	20	H2U	O4'-C1'-N1-C2
24	y	20	H2U	O4'-C1'-N1-C6
24	y	37	MIA	C5-C6-N6-C12
24	y	37	MIA	C12-C13-C14-C15
26	A	1915	3TD	C2'-C1'-C5-C4
26	A	1915	3TD	O4'-C1'-C5-C4
26	A	1915	3TD	O4'-C1'-C5-C6
26	A	2030	6MZ	O4'-C4'-C5'-O5'
26	A	2445	2MG	O4'-C4'-C5'-O5'
26	A	2445	2MG	C3'-C4'-C5'-O5'
26	A	2552	OMU	O4'-C1'-N1-C2
26	A	2552	OMU	O4'-C1'-N1-C6
1	a	1498	UR3	O4'-C1'-N1-C2
22	w	8	4SU	C3'-C4'-C5'-O5'
24	y	20	H2U	O4'-C4'-C5'-O5'
26	A	2504	PSU	O4'-C4'-C5'-O5'
1	a	966	2MG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
24	y	20	H2U	C3'-C4'-C5'-O5'
26	A	2030	6MZ	C3'-C4'-C5'-O5'
26	A	2504	PSU	C3'-C4'-C5'-O5'
24	y	46	7MG	C2'-C1'-N9-C8
1	a	1498	UR3	O4'-C1'-N1-C6
1	a	966	2MG	C3'-C4'-C5'-O5'
24	y	37	MIA	N1-C6-N6-C12
1	a	527	7MG	O4'-C4'-C5'-O5'
1	a	1519	MA6	N1-C6-N6-C9
26	A	2503	2MA	O4'-C4'-C5'-O5'
26	A	1962	5MC	C4'-C5'-O5'-P
22	v	21	H2U	C4'-C5'-O5'-P
22	w	20	H2U	C4'-C5'-O5'-P
22	w	54	5MU	O4'-C4'-C5'-O5'
22	w	8	4SU	C2'-C1'-N1-C6
1	a	527	7MG	C4'-C5'-O5'-P
24	y	20	H2U	C4'-C5'-O5'-P
24	y	46	7MG	O4'-C4'-C5'-O5'
22	w	8	4SU	O4'-C1'-N1-C6
1	a	516	PSU	O4'-C1'-C5-C4
22	w	8	4SU	O4'-C1'-N1-C2
24	y	46	7MG	O4'-C1'-N9-C8
22	w	54	5MU	C3'-C4'-C5'-O5'
1	a	516	PSU	O4'-C1'-C5-C6
22	w	20	H2U	C2'-C1'-N1-C2
26	A	746	PSU	O4'-C1'-C5-C6
24	y	8	4SU	O4'-C4'-C5'-O5'
26	A	2069	7MG	O4'-C4'-C5'-O5'
22	w	8	4SU	C2'-C1'-N1-C2
26	A	2498	OMC	C4'-C5'-O5'-P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 342 ligands modelled in this entry, 339 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
63	GDP	z	402	59	24,30,30	0.90	1 (4%)	30,47,47	1.45	4 (13%)
61	FME	v	105	-	8,9,10	0.92	1 (12%)	7,9,11	1.50	1 (14%)
62	KIR	z	401	-	56,59,59	0.64	1 (1%)	62,84,84	1.76	14 (22%)

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
63	GDP	z	402	59	-	1/12/32/32	0/3/3/3
61	FME	v	105	-	-	3/7/9/11	-
62	KIR	z	401	-	-	23/54/98/98	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GDP	C6-N1	-2.27	1.34	1.37
62	z	401	KIR	C3-C2	2.14	1.49	1.43
61	v	105	FME	CA-N	2.11	1.49	1.46

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	z	401	KIR	C23-C22-C21	-6.01	118.50	127.32
62	z	401	KIR	C15-C14-C13	-4.56	107.29	114.64
63	z	402	GDP	PA-O3A-PB	-3.96	119.23	132.83
62	z	401	KIR	C44-C21-C22	-3.63	119.55	124.03
62	z	401	KIR	C5-C4-C3	-3.55	117.84	120.66
62	z	401	KIR	C16-C15-C14	3.50	106.04	101.87
62	z	401	KIR	C44-C21-C20	2.90	120.70	115.68
62	z	401	KIR	C36-C37-C38	-2.80	119.39	124.69
62	z	401	KIR	C39-C38-C37	-2.77	118.60	125.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GDP	C3'-C2'-C1'	2.76	105.13	100.98
62	z	401	KIR	O27-C27-C28	-2.51	118.76	122.25
63	z	402	GDP	C8-N7-C5	2.48	107.72	102.99
61	v	105	FME	CA-N-CN	-2.46	119.04	122.82
62	z	401	KIR	C6-N1-C2	2.43	122.25	116.43
63	z	402	GDP	C5-C6-N1	2.43	118.25	113.95
62	z	401	KIR	C10-C9-C8	-2.28	119.90	126.61
62	z	401	KIR	C15-C16-C17	2.08	105.45	102.45
62	z	401	KIR	C41-C8-C7	2.06	119.31	115.53
62	z	401	KIR	C12-C11-C10	-2.03	120.29	124.81

There are no chirality outliers.

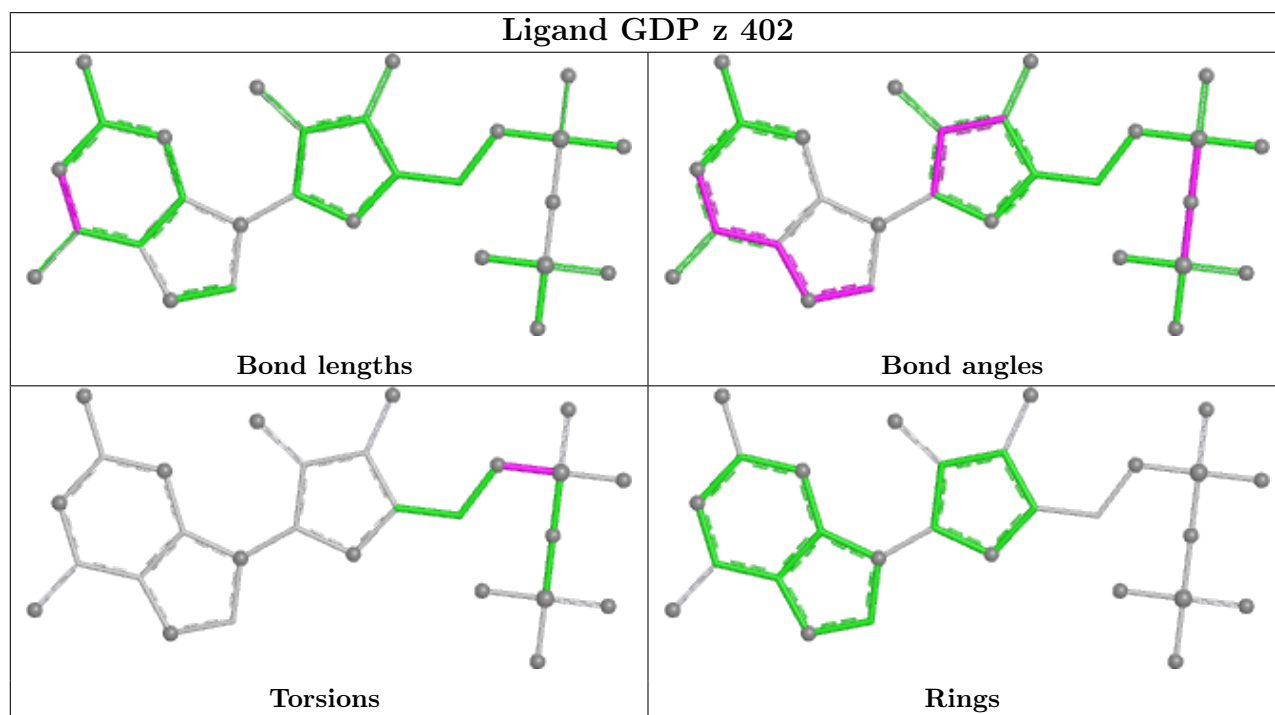
All (27) torsion outliers are listed below:

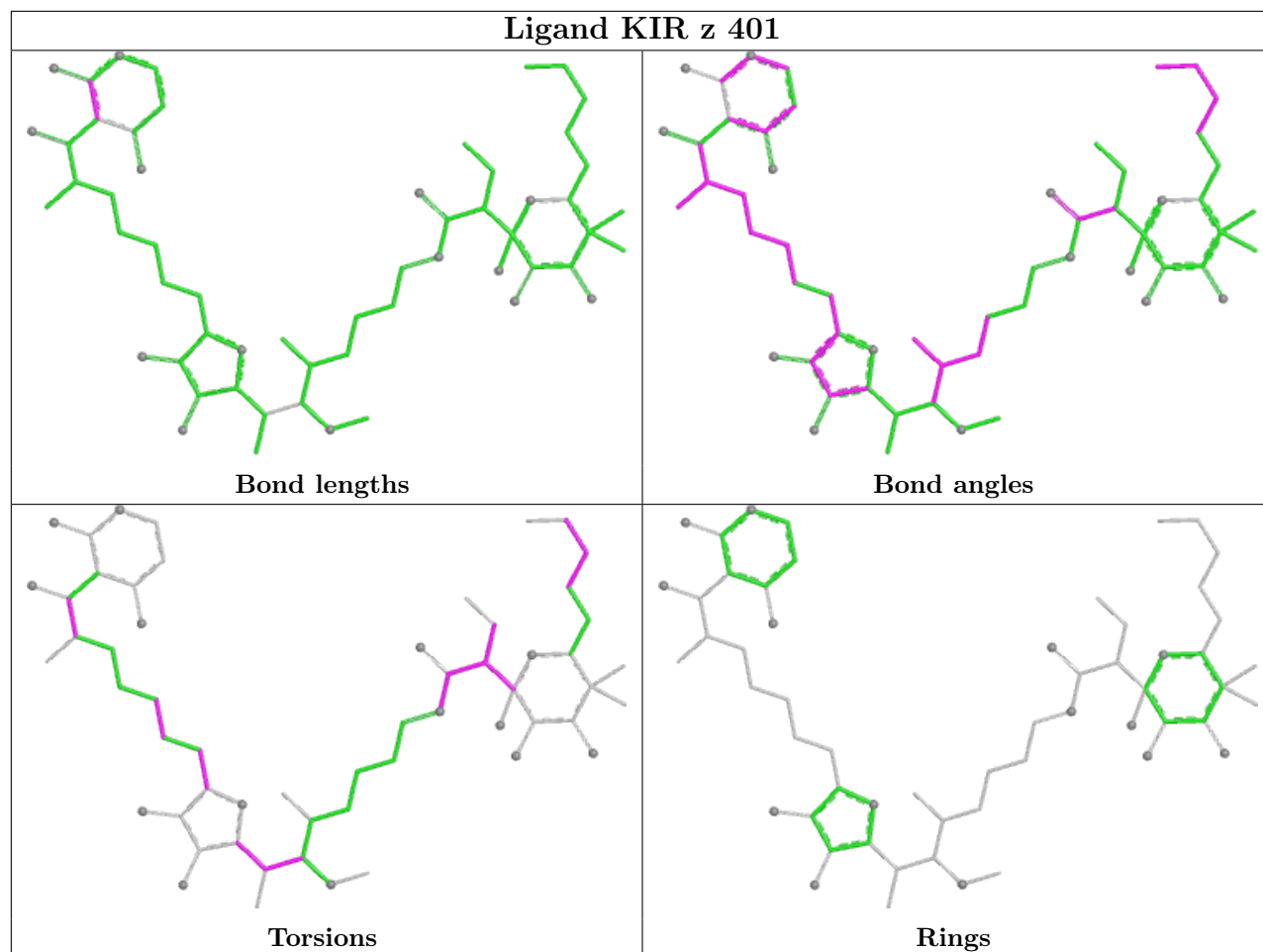
Mol	Chain	Res	Type	Atoms
61	v	105	FME	O1-CN-N-CA
62	z	401	KIR	C17-C19-C20-C21
62	z	401	KIR	C42-C19-C20-C21
62	z	401	KIR	C17-C19-C20-O20
62	z	401	KIR	C42-C19-C20-O20
62	z	401	KIR	C12-C13-C14-C15
62	z	401	KIR	C16-C17-C19-C20
62	z	401	KIR	C16-C17-C19-C42
62	z	401	KIR	O18-C17-C19-C20
62	z	401	KIR	O18-C17-C19-C42
62	z	401	KIR	C45-C28-C29-O29
62	z	401	KIR	C45-C28-C29-O34
63	z	402	GDP	C5'-O5'-PA-O1A
62	z	401	KIR	O27-C27-N26-C25
62	z	401	KIR	C36-C37-C38-C39
61	v	105	FME	CB-CG-SD-CE
62	z	401	KIR	C35-C36-C37-C38
62	z	401	KIR	C28-C27-N26-C25
62	z	401	KIR	C12-C13-C14-O18
62	z	401	KIR	O27-C27-C28-C29
62	z	401	KIR	C27-C28-C45-C46
62	z	401	KIR	N26-C27-C28-C29
62	z	401	KIR	N26-C27-C28-C45
61	v	105	FME	C-CA-CB-CG
62	z	401	KIR	C3-C7-C8-C41
62	z	401	KIR	C10-C11-C12-C13
62	z	401	KIR	O27-C27-C28-C45

There are no ring outliers.

No monomer is involved in short contacts.

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

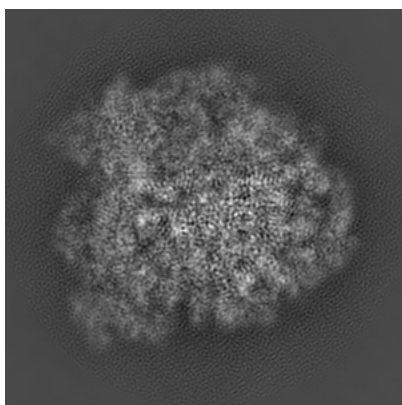
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2847. These allow visual inspection of the internal detail of the map and identification of artifacts.

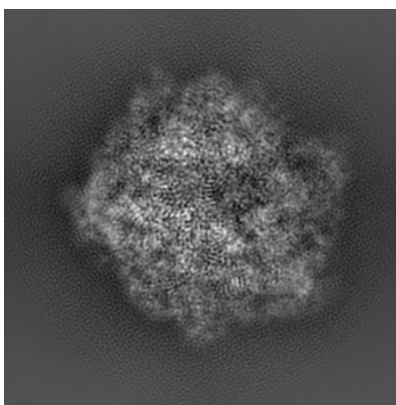
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

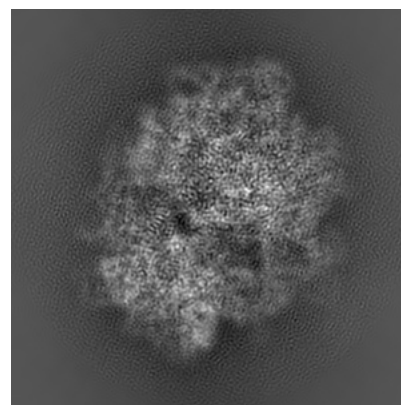
6.1.1 Primary map



X



Y

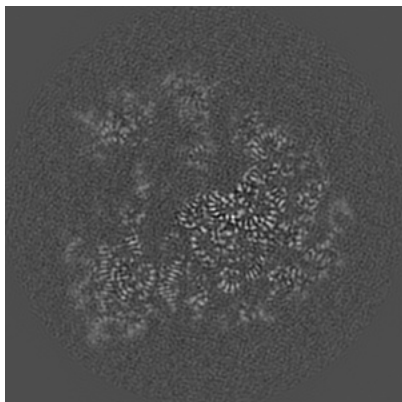


Z

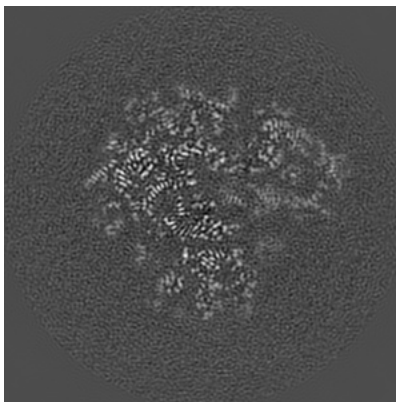
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

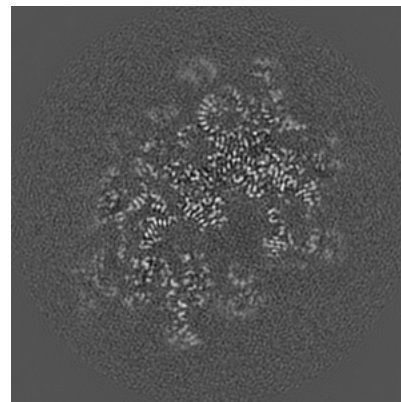
6.2.1 Primary map



X Index: 210



Y Index: 210

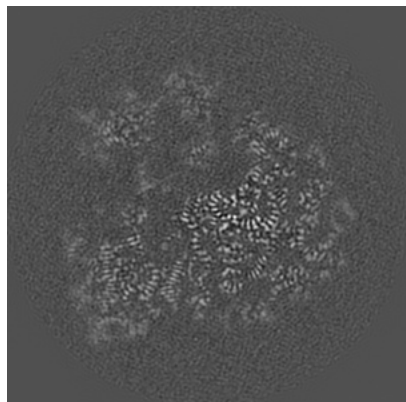


Z Index: 210

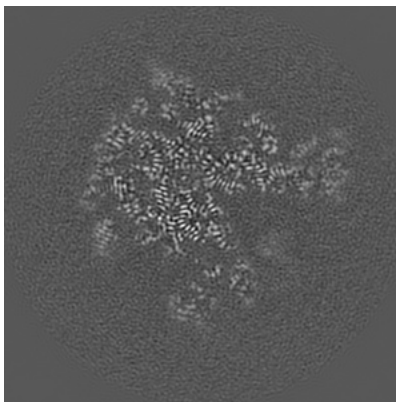
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

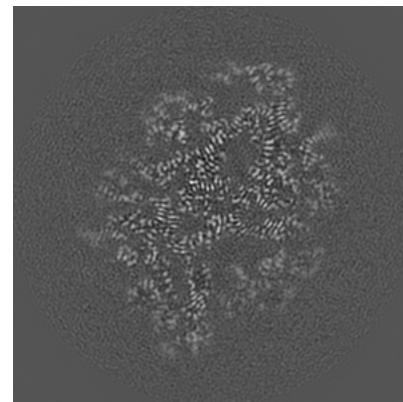
6.3.1 Primary map



X Index: 209



Y Index: 228

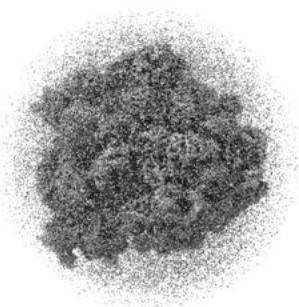


Z Index: 189

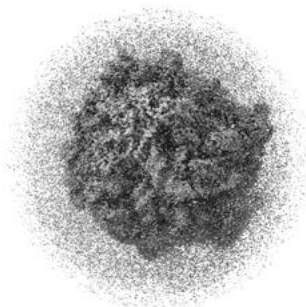
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

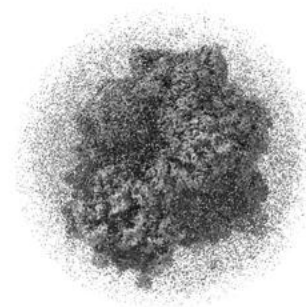
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

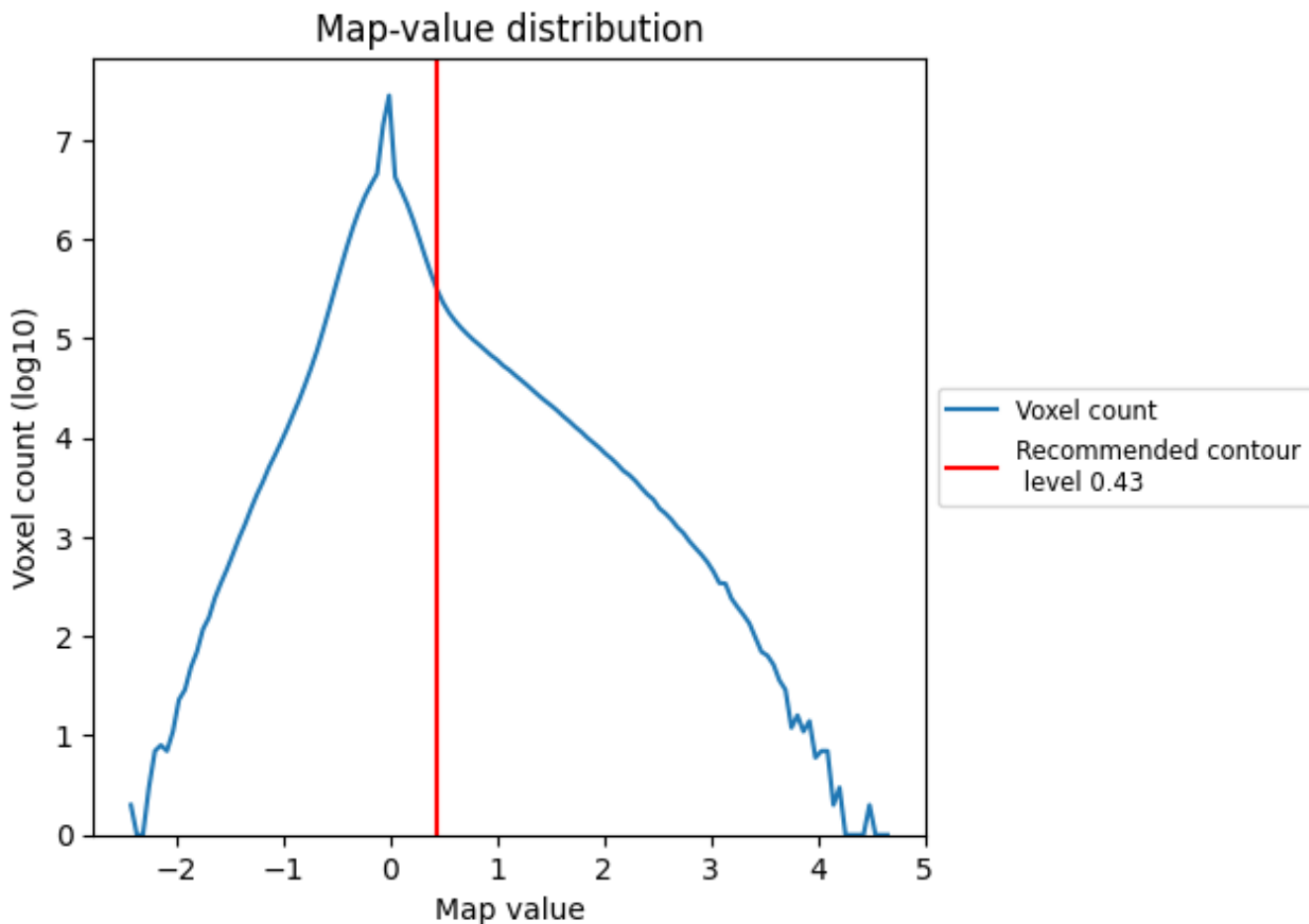
6.5 Mask visualisation

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

7 Map analysis [i](#)

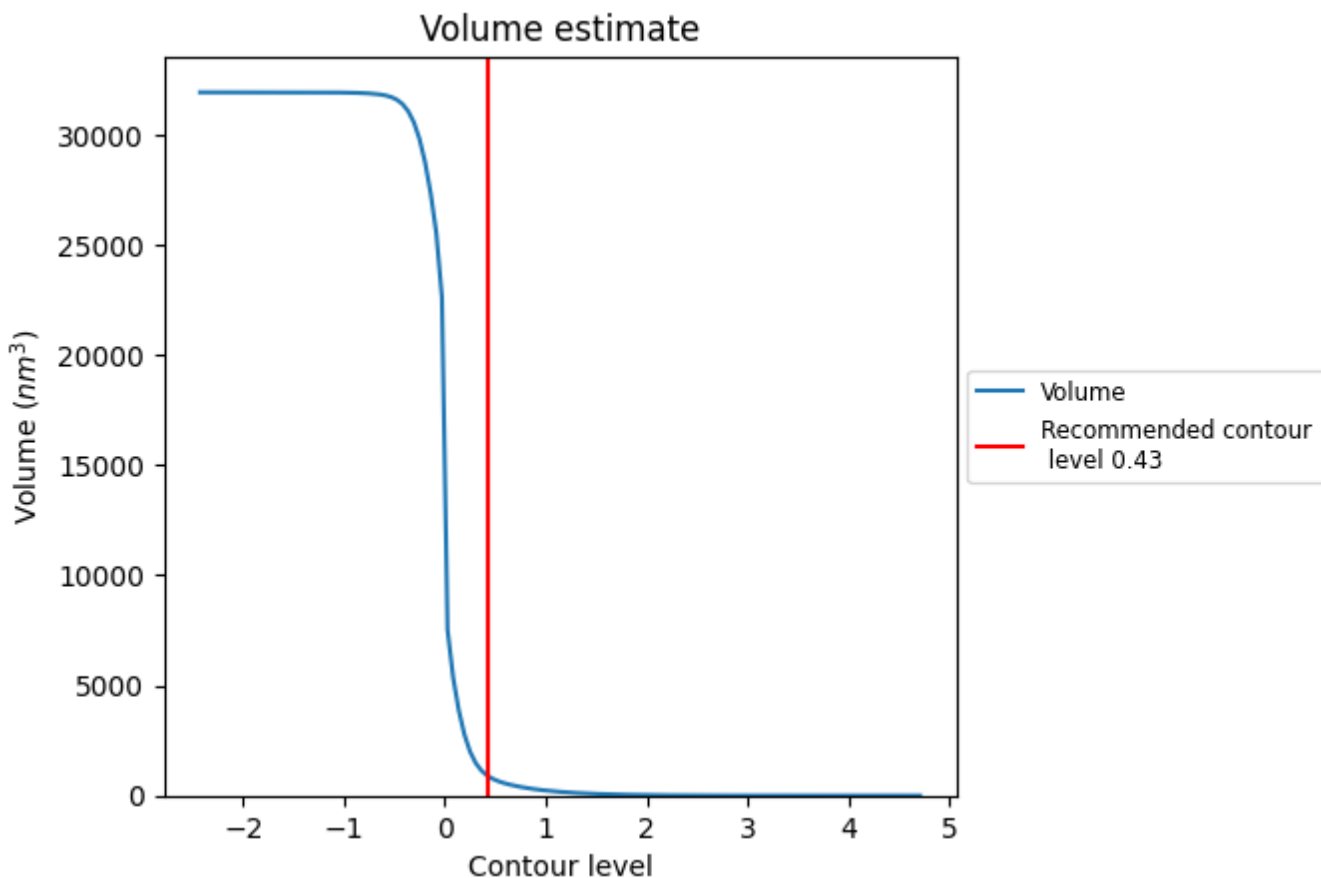
This section contains the results of statistical analysis of the map.

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.

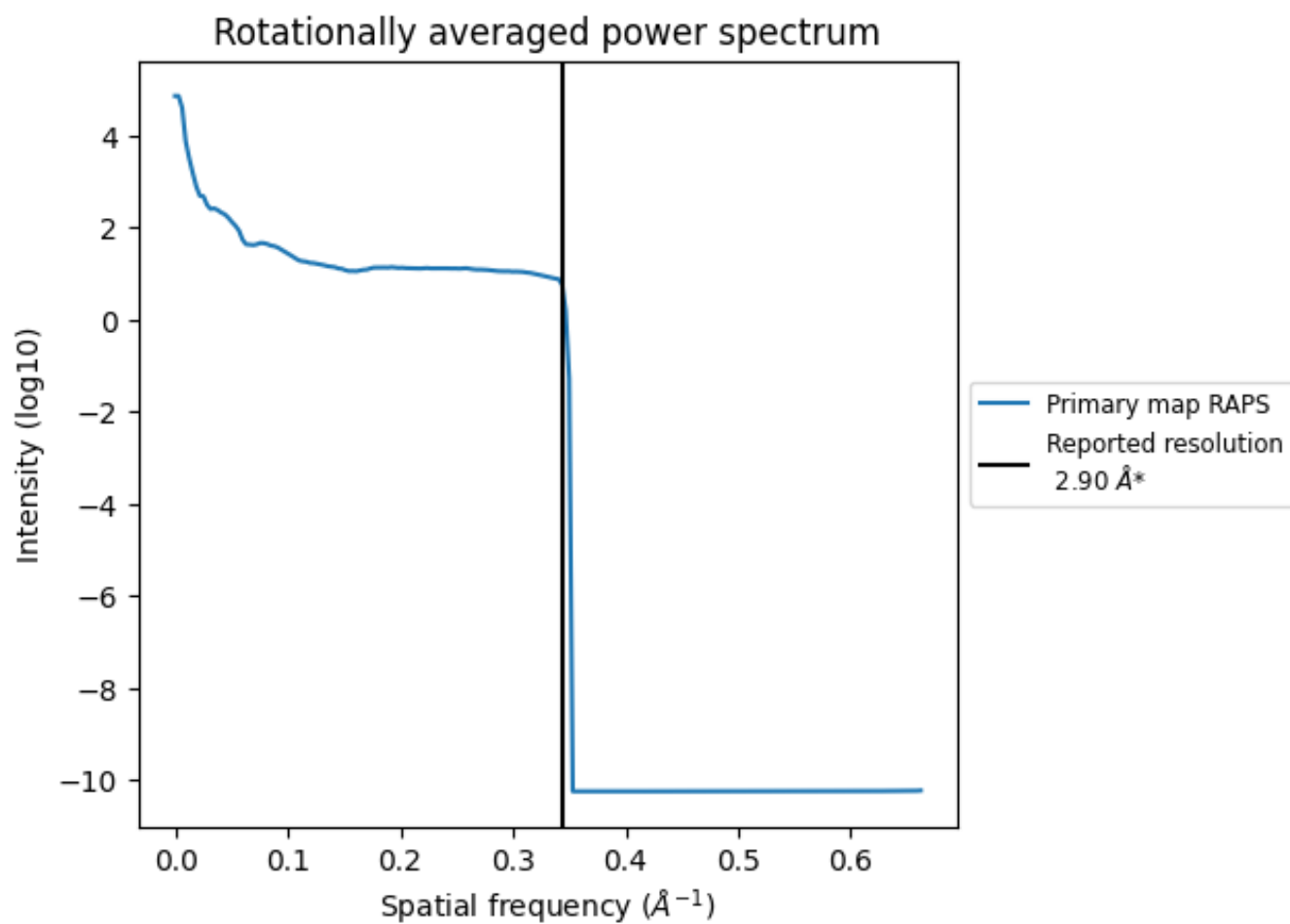
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 882 nm^3 ; this corresponds to an approximate mass of 797 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [\(i\)](#)



*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

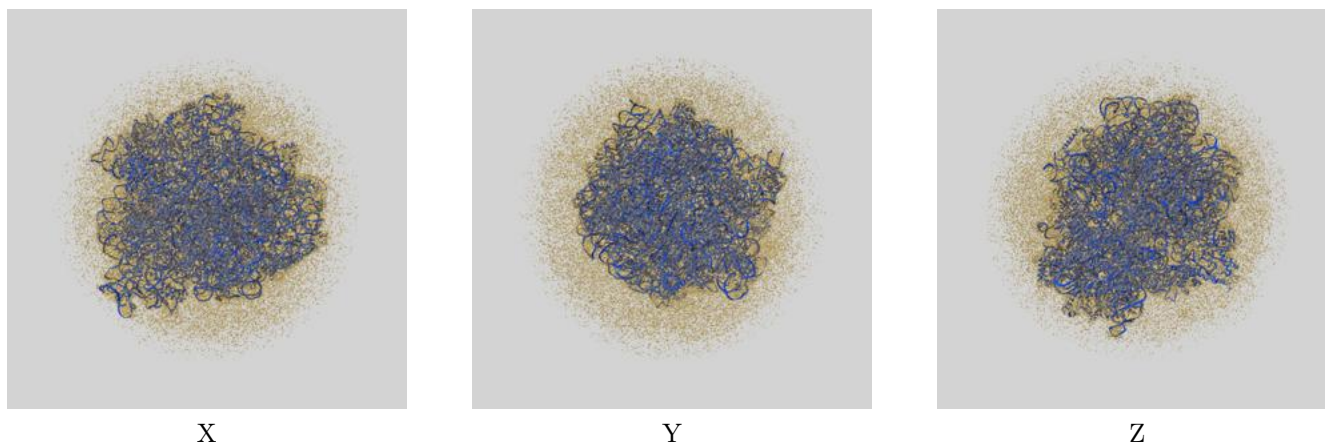
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

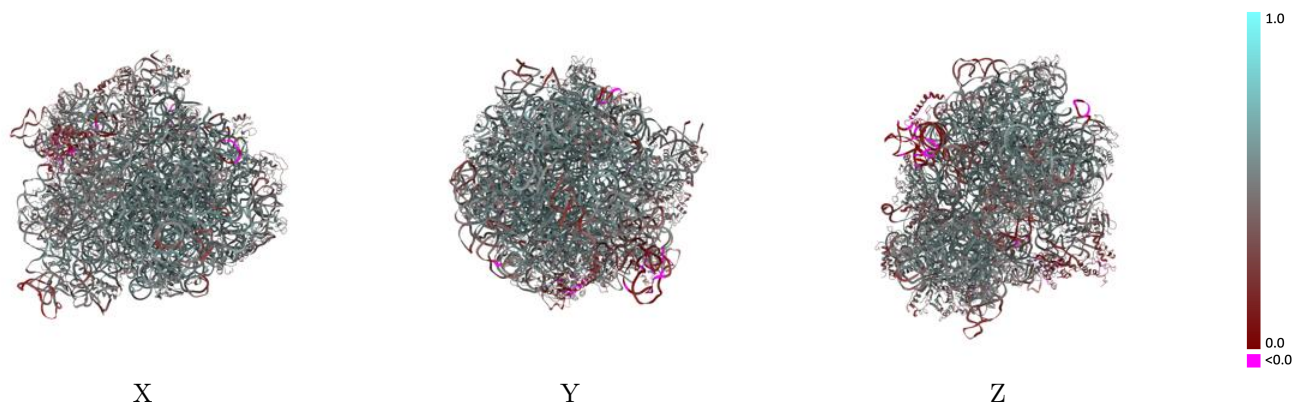
This section contains information regarding the fit between EMDB map EMD-2847 and PDB model 5AFI. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



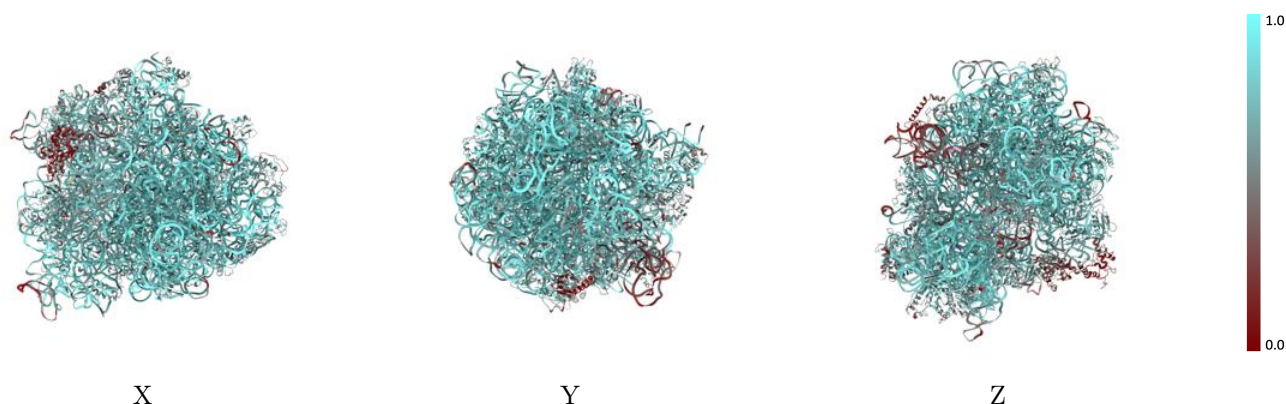
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



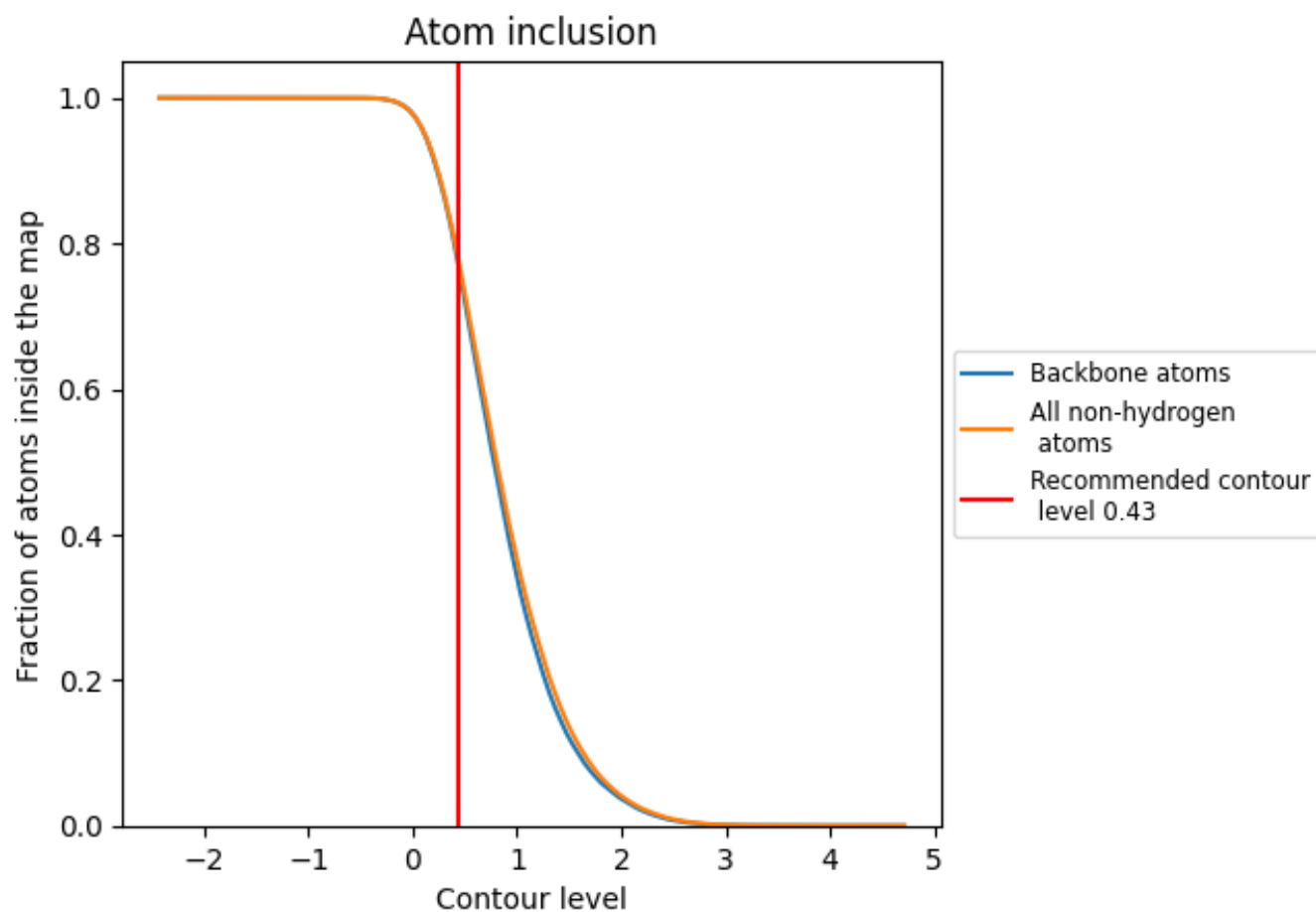
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.43).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 78% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7833	 0.4980
0	 0.7529	 0.5130
1	 0.6359	 0.4690
2	 0.8056	 0.5360
3	 0.7902	 0.5620
4	 0.7619	 0.5050
5	 0.1591	 0.1980
6	 0.4512	 0.3410
A	 0.8601	 0.5270
B	 0.8252	 0.4790
C	 0.7708	 0.5200
D	 0.7484	 0.5180
E	 0.6730	 0.4760
F	 0.5921	 0.4100
G	 0.6114	 0.4260
H	 0.2153	 0.1780
I	 0.2045	 0.2050
J	 0.7473	 0.5070
K	 0.7404	 0.5320
L	 0.7165	 0.4870
M	 0.7390	 0.5040
N	 0.7738	 0.5320
O	 0.6559	 0.4530
P	 0.7061	 0.4940
Q	 0.7775	 0.5360
R	 0.7127	 0.4760
S	 0.7392	 0.5170
T	 0.6842	 0.4660
U	 0.6206	 0.4460
V	 0.6734	 0.4530
W	 0.7460	 0.5280
X	 0.7188	 0.4930
Y	 0.6298	 0.4170
Z	 0.7071	 0.4910
a	 0.8649	 0.5260



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Chain	Atom inclusion	Q-score
b	 0.4973	 0.3890
c	 0.6730	 0.4720
d	 0.6465	 0.4540
e	 0.7337	 0.4940
f	 0.6394	 0.3820
g	 0.6320	 0.4330
h	 0.7177	 0.4990
i	 0.6568	 0.4350
j	 0.5900	 0.4150
k	 0.7337	 0.4820
l	 0.7448	 0.5170
m	 0.6381	 0.4230
n	 0.6862	 0.4650
o	 0.7304	 0.4770
p	 0.6794	 0.4660
q	 0.6804	 0.4650
r	 0.7299	 0.4930
s	 0.6602	 0.4580
t	 0.6723	 0.4770
u	 0.5294	 0.3610
v	 0.7684	 0.4980
w	 0.4294	 0.3010
x	 0.7607	 0.4850
y	 0.7626	 0.4810
z	 0.6081	 0.4350