



Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:52 PM EST

PDB ID : 7LV0
EMDB ID : EMD-23528
Title : Pre-translocation rotated ribosome +1-frameshifting(CCC-A) complex (Structure Irot-FS)
Authors : Demo, G.; Loveland, A.B.; Svidritskiy, E.; Gamper, H.B.; Hou, Y.M.; Korostelev, A.A.
Deposited on : 2021-02-23
Resolution : 3.20 Å(reported)
Based on initial models : 6ENJ, 4V7D, 5UYM, 4V9P

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

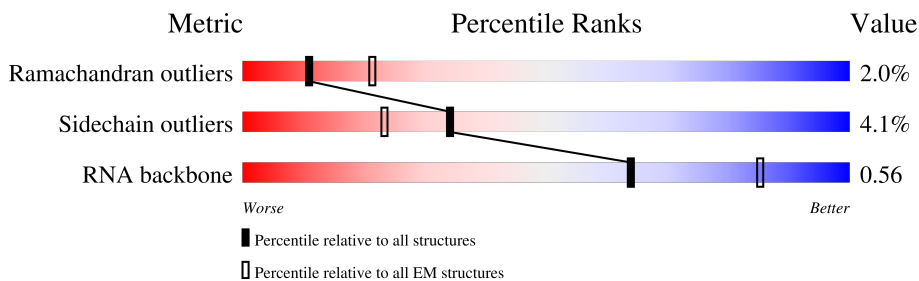
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.20 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.



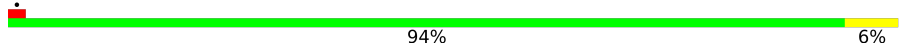

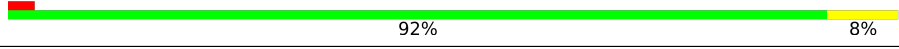

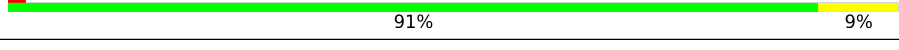
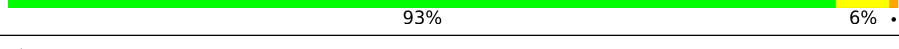
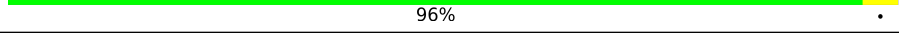
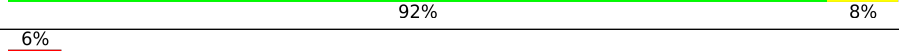
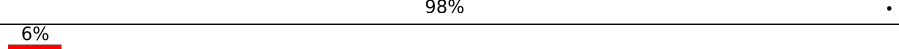
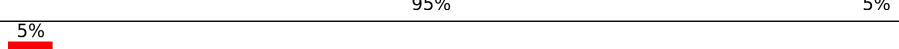
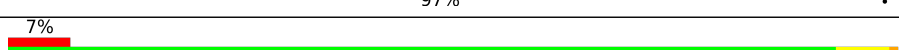
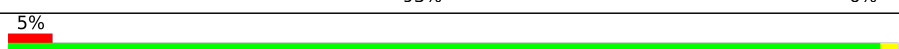
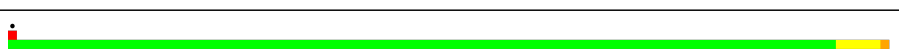
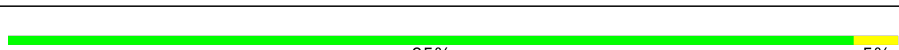
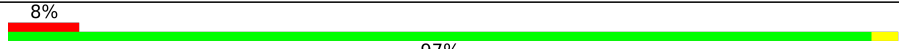


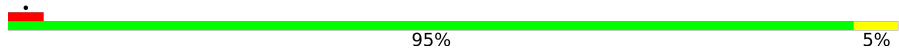
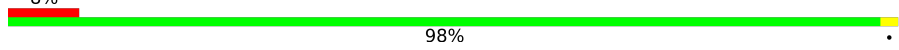
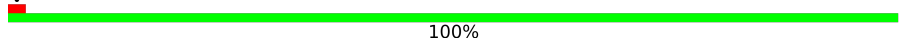
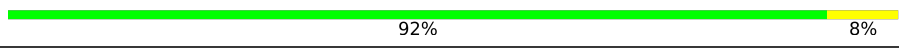
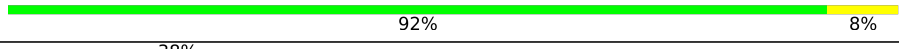
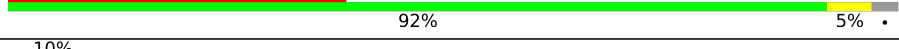
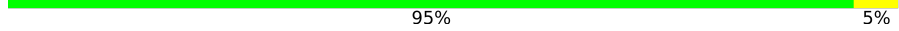

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	b	271	92% (Green), 8% (Yellow)
2	c	209	93% (Green), 7% (Yellow), 10% (Red)
3	d	201	95% (Green), 5% (Yellow), 10% (Red)
4	e	177	91% (Green), 9% (Yellow), 10% (Red)
5	f	176	94% (Green), 6% (Yellow), 5% (Red)
6	g	149	34% (Green), 62% (Grey), 11% (Red)
7	h	131	56% (Green), 40% (Grey), 10% (Yellow), 50% (Red)
8	i	141	42% (Green), 50% (Grey), 10% (Yellow), 40% (Red)

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Mol	Chain	Length	Quality of chain
9	j	142	 94% 6%
10	k	122	 86% 13%
11	l	143	 92% 8%
12	m	136	 84% 16%
13	n	120	 91% 9%
14	o	116	 93% 6%
15	p	114	 96%
16	q	117	 92% 8%
17	r	103	 98% 6%
18	s	110	 95% 5% 6%
19	t	93	 97% 5%
20	u	102	 93% 6% 7%
21	v	94	 98% 5%
22	w	75	 93% 5%
23	x	77	 95% 5%
24	y	63	 97% 8%
25	z	58	 91% 9%
26	A	66	 65% 6% 21% 29%
27	B	56	 95% 5%
28	C	50	 98% 8%
29	D	46	 100%
30	E	64	 92% 8%
31	F	38	 92% 8%
32	G	225	 92% 5% 38%
33	H	206	 95% 5% 10%

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Mol	Chain	Length	Quality of chain
34	I	205	13% 95% 5%
35	J	157	92% 8%
36	K	100	88% 12%
37	L	151	13% 92% 8%
38	M	129	95% 5%
39	N	127	20% 96% .
40	O	98	34% 90% 9% .
41	P	116	92% 8%
42	Q	123	92% 7% .
43	R	114	11% 94% 6%
44	S	100	92% 8%
45	T	88	93% 7%
46	U	82	9% 89% 11%
47	V	80	95% 5%
48	W	65	94% 6%
49	X	79	94% 6%
50	Y	85	5% 98% .
51	Z	65	15% 80% 17% .
52	a	223	37% 53% 6% 40% .
53	3	1539	84% 15% .
54	1	2903	80% 18% .
55	2	120	85% 14% .
56	5	77	9% 66% 31% .
57	6	77	73% 26% .
58	4	18	22% 72% 28%

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 147330 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	b	271	2083	1288	423	365	7	0	0

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	e	177	1411	899	249	257	6	0	0

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	g	57	440	281	79	79	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	h	79	593	369	109	111	4	0	0

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	i	71	511	313	93	102	3	0	0

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	k	122	939	587	180	166	6	0	0

- Molecule 11 is a protein called 50S ribosomal protein L15.

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

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	n	120	961	593	196	167	5	0	0

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	q	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	t	93	Total	C	N	O	S	0	0
			739	466	139	132	2		

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	102	Total	C	N	O	0	0
			780	492	146	142		

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

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

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	47	Total	C	N	O	S	0	0
			364	227	64	67	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	J	157	1157	719	218	214	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	K	100	818	515	148	149	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	L	151	1182	735	227	216	4	0	0

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	O	98	787	493	150	143	1	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	P	116	870	535	173	159	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
55	2	120	2568	1145	471	833	119	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 56 is a RNA chain called tRNAPro.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
56	5	77	1647	733	295	542	77	0	0

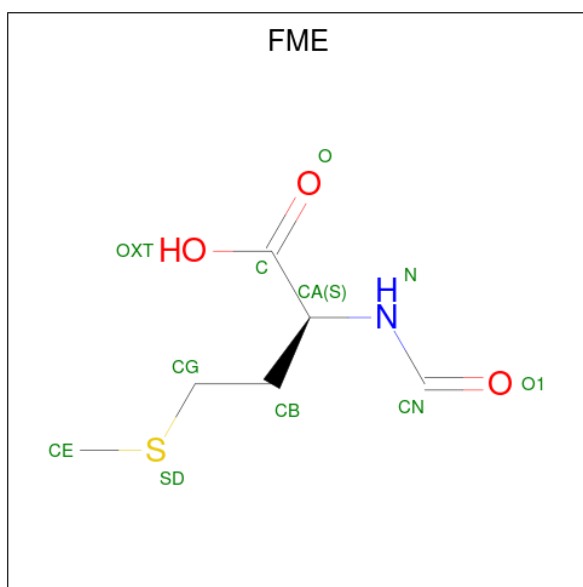
- Molecule 57 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
57	6	77	1640	732	297	535	76	0	0

- Molecule 58 is a RNA chain called mRNA.

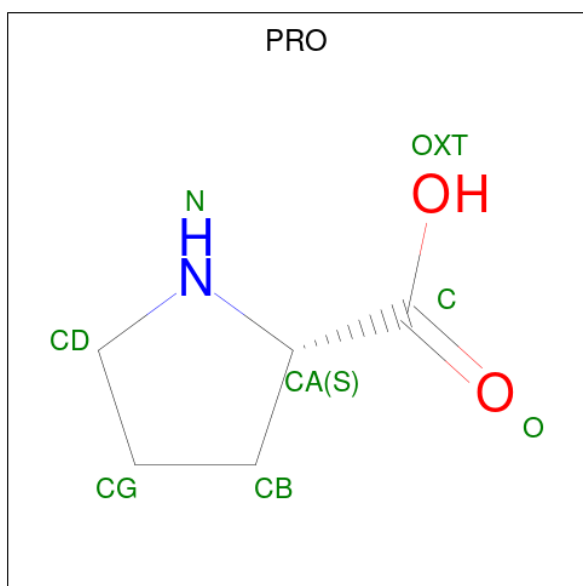
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
58	4	18	388	175	78	118	17	0	0

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
59	1	1	10	6	1	2	1	0

- Molecule 60 is PROLINE (three-letter code: PRO) (formula: C₅H₉NO₂) (labeled as "Ligand of Interest" by depositor).

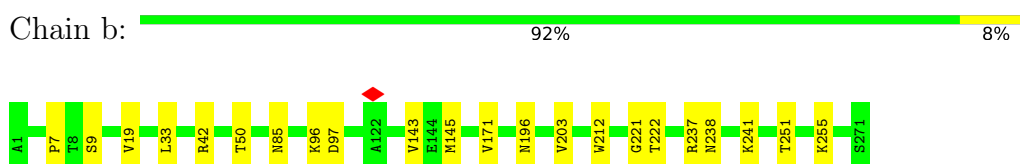


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	5	1	7	5	1	1	0

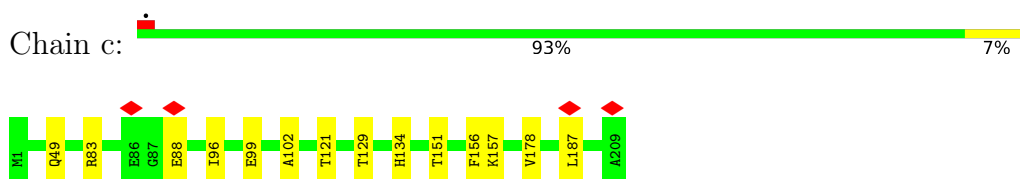
3 Residue-property plots [i](#)

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

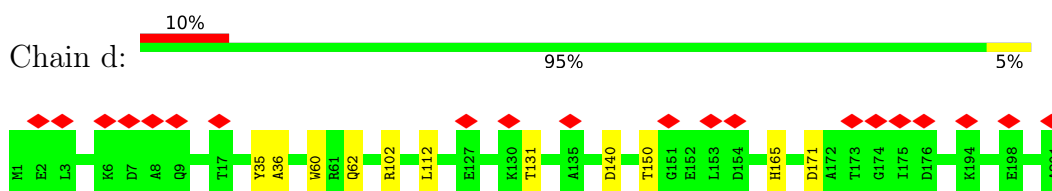
- Molecule 1: 50S ribosomal protein L2



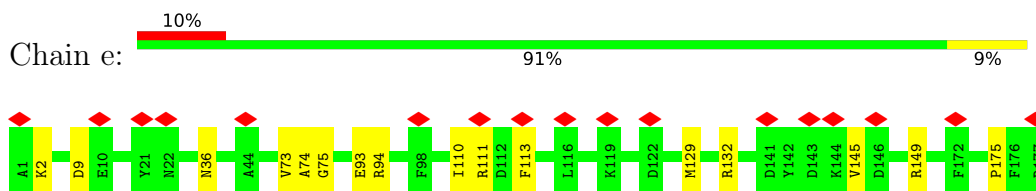
- Molecule 2: 50S ribosomal protein L3



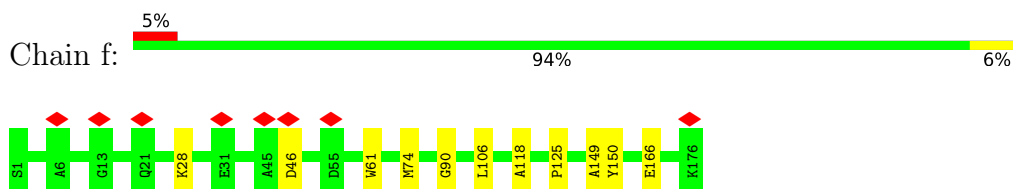
- Molecule 3: 50S ribosomal protein L4



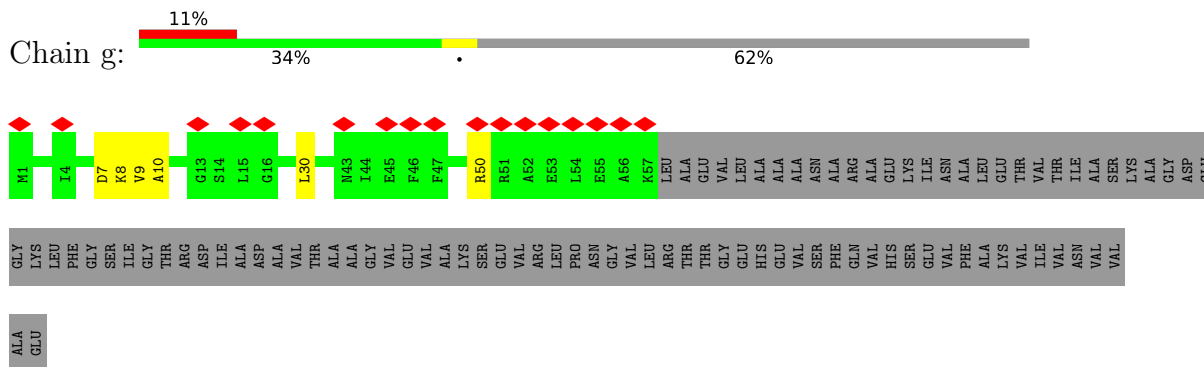
- Molecule 4: 50S ribosomal protein L5



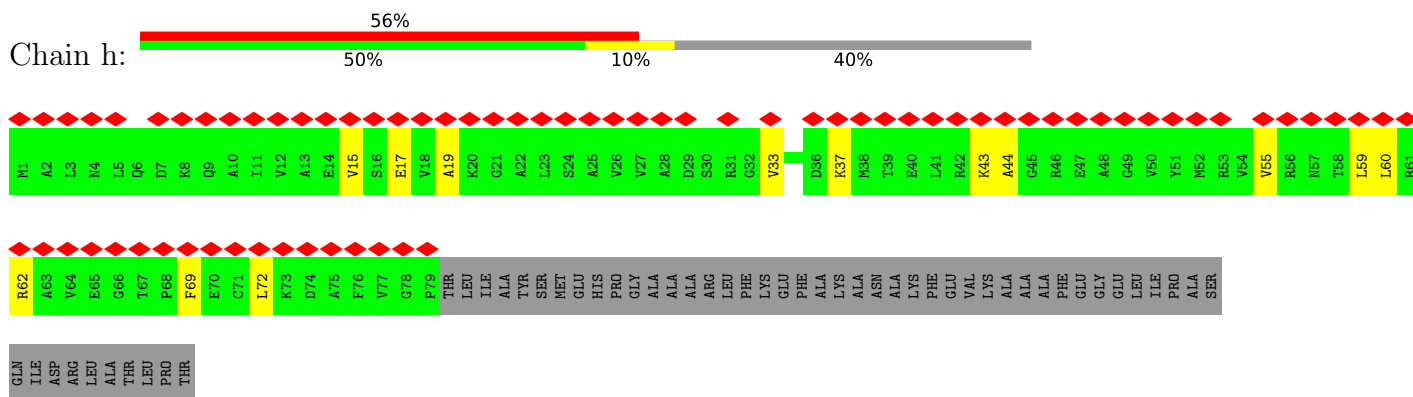
- Molecule 5: 50S ribosomal protein L6



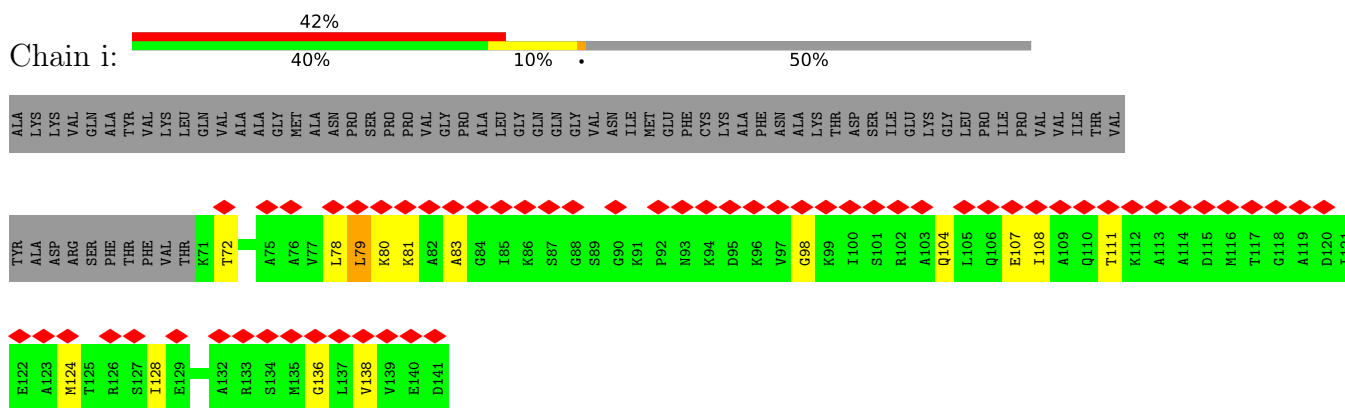
• Molecule 6: 50S ribosomal protein L9



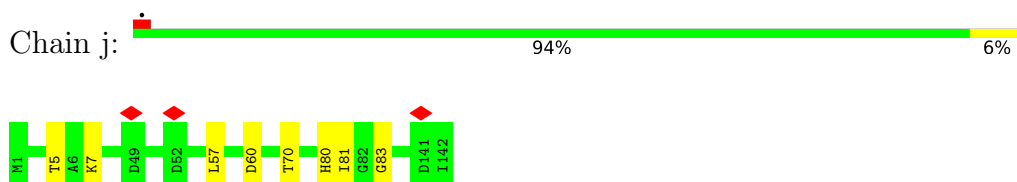
• Molecule 7: 50S ribosomal protein L10



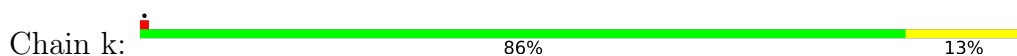
• Molecule 8: 50S ribosomal protein L11



• Molecule 9: 50S ribosomal protein L13

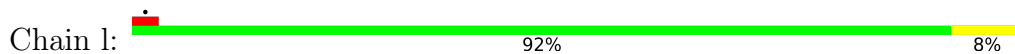


• Molecule 10: 50S ribosomal protein L14

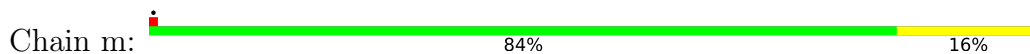




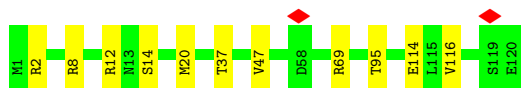
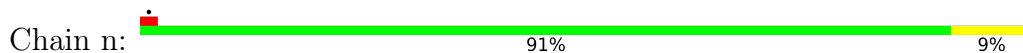
- Molecule 11: 50S ribosomal protein L15



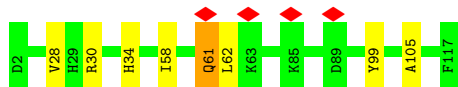
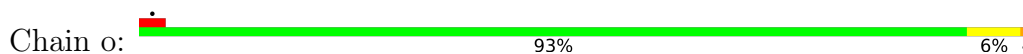
- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



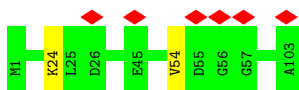
- Molecule 15: 50S ribosomal protein L19



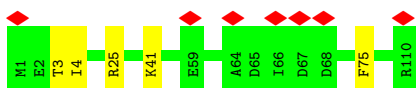
- Molecule 16: 50S ribosomal protein L20



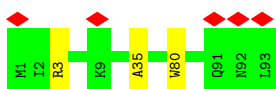
- Molecule 17: 50S ribosomal protein L21



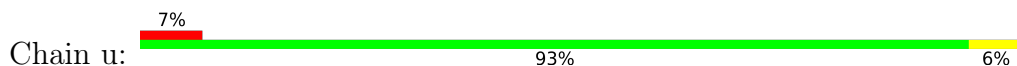
- Molecule 18: 50S ribosomal protein L22



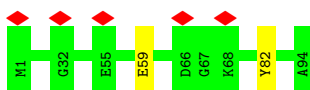
- Molecule 19: 50S ribosomal protein L23



- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



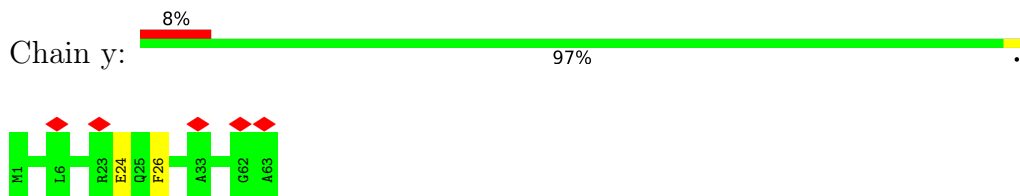
- Molecule 22: 50S ribosomal protein L27



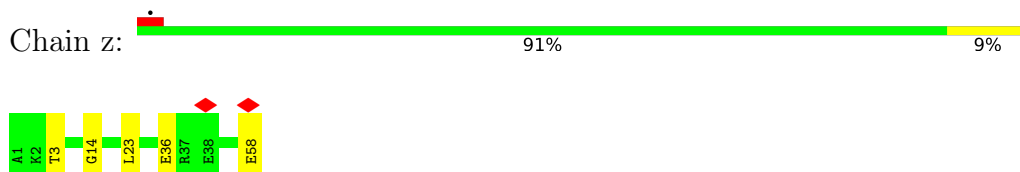
- Molecule 23: 50S ribosomal protein L28



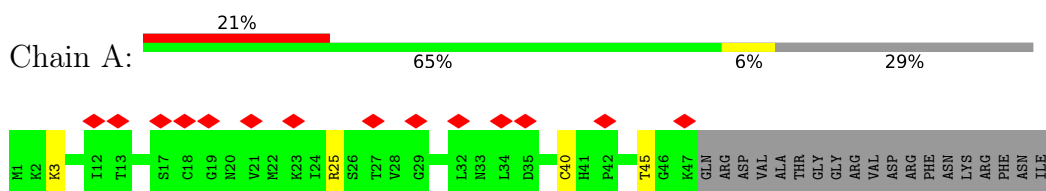
- Molecule 24: 50S ribosomal protein L29



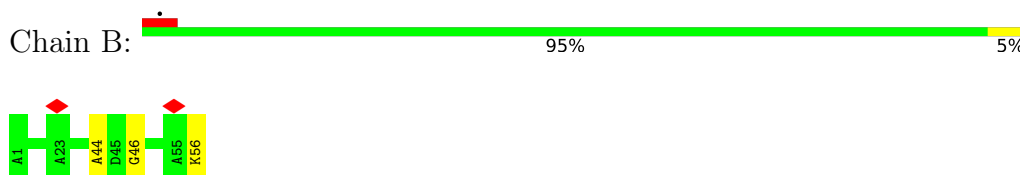
- Molecule 25: 50S ribosomal protein L30



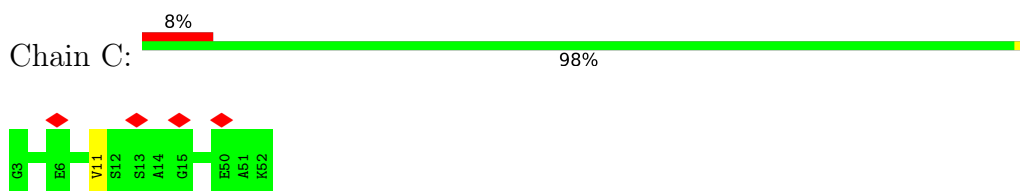
- Molecule 26: 50S ribosomal protein L31



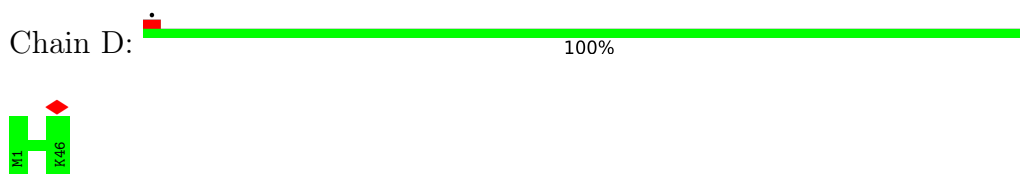
- Molecule 27: 50S ribosomal protein L32



- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34



- Molecule 30: 50S ribosomal protein L35





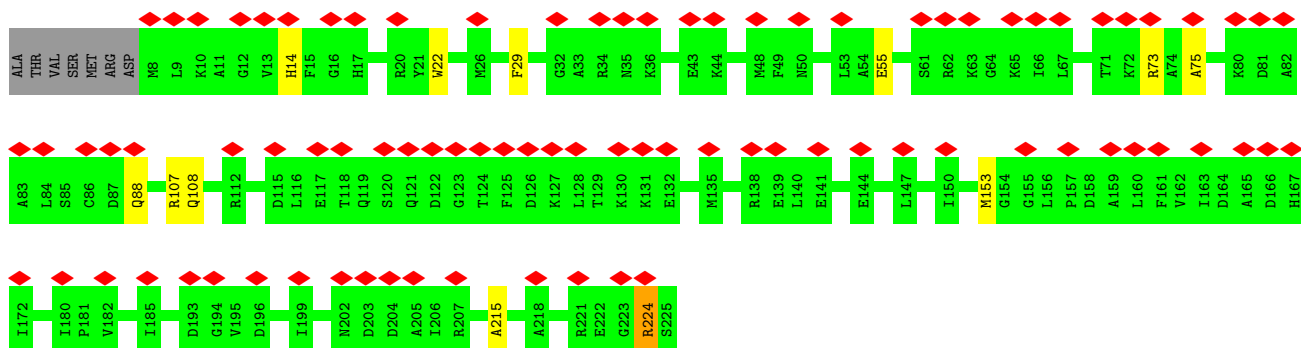
- Molecule 31: 50S ribosomal protein L36

Chain F: 92% 8%



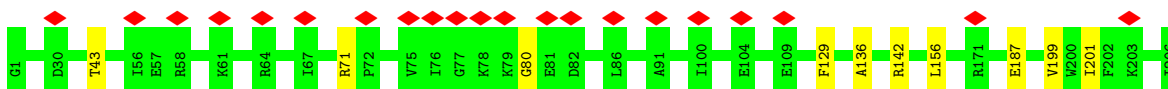
- Molecule 32: 30S ribosomal protein S2

Chain G: 38% 92% 5%



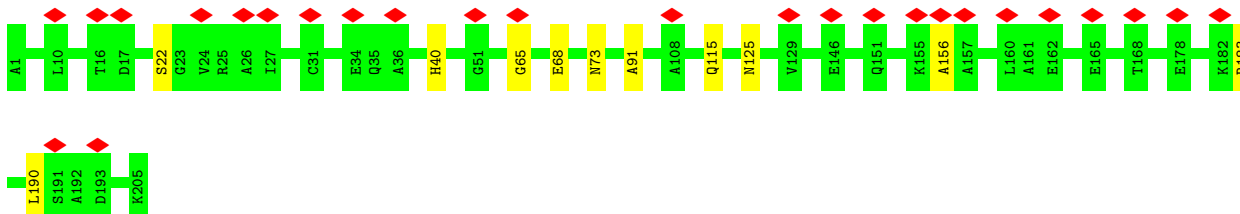
- Molecule 33: 30S ribosomal protein S3

Chain H: 10% 95% 5%



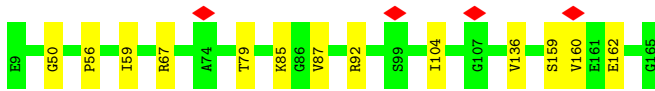
- Molecule 34: 30S ribosomal protein S4

Chain I: 13% 95% 5%

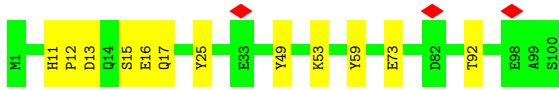
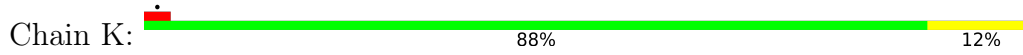


- Molecule 35: 30S ribosomal protein S5

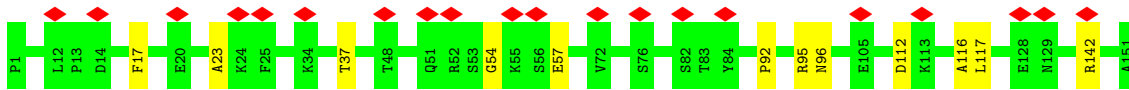
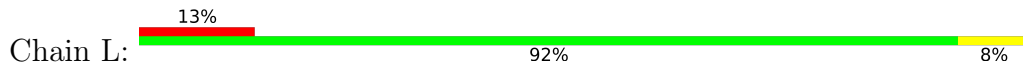
Chain J: 92% 8%



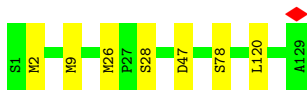
- Molecule 36: 30S ribosomal protein S6



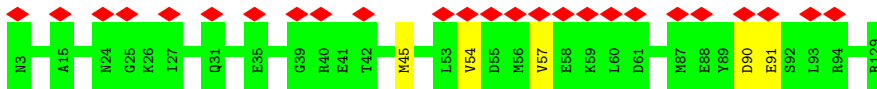
- Molecule 37: 30S ribosomal protein S7



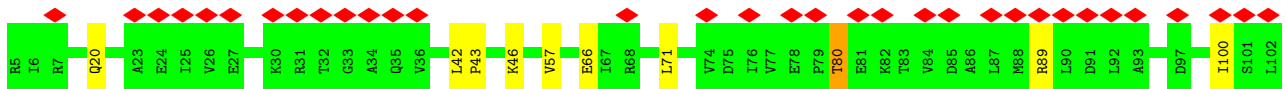
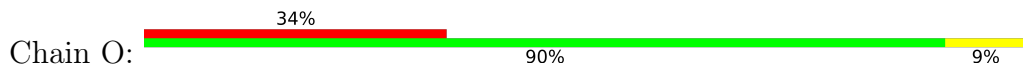
- Molecule 38: 30S ribosomal protein S8



- Molecule 39: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S10

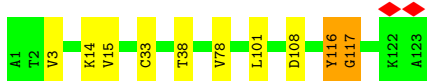


- Molecule 41: 30S ribosomal protein S11



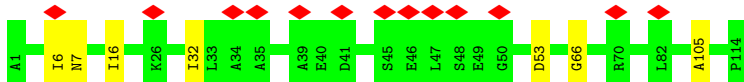
- Molecule 42: 30S ribosomal protein S12

Chain Q:  92% 7%




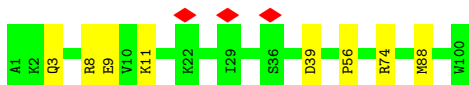
• Molecule 43: 30S ribosomal protein S13

Chain R:  11% 94% 6%



• Molecule 44: 30S ribosomal protein S14

Chain S:  92% 8%




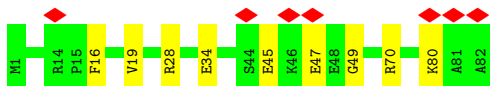
• Molecule 45: 30S ribosomal protein S15

Chain T:  93% 7%



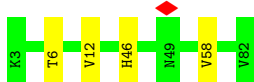
• Molecule 46: 30S ribosomal protein S16

Chain U:  9% 89% 11%



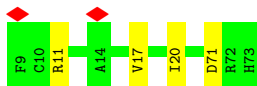
• Molecule 47: 30S ribosomal protein S17

Chain V:  95% 5%

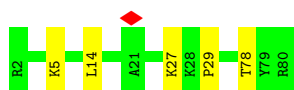


• Molecule 48: 30S ribosomal protein S18

Chain W:  94% 6%



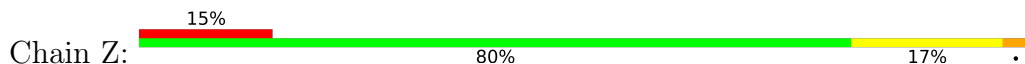
• Molecule 49: 30S ribosomal protein S19



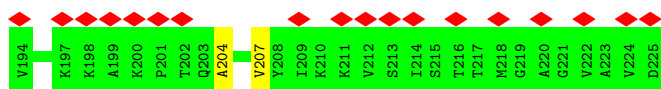
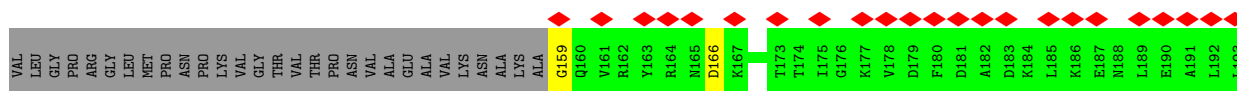
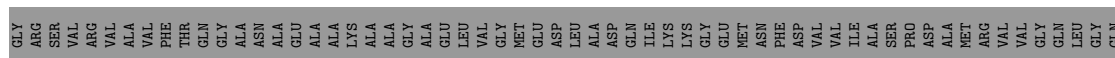
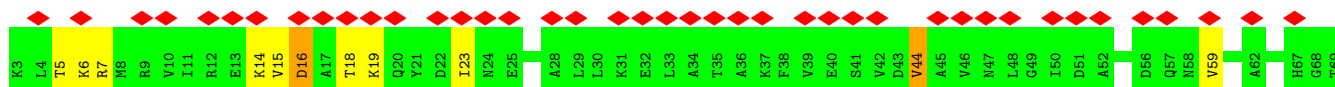
• Molecule 50: 30S ribosomal protein S20



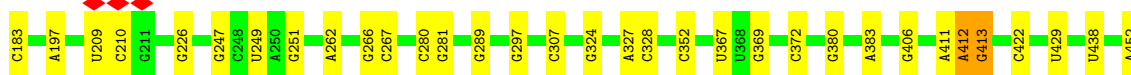
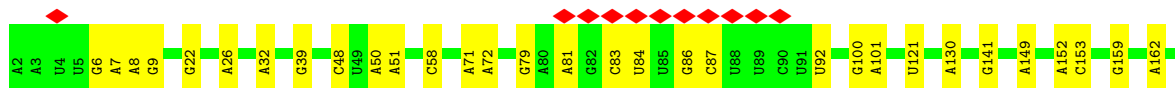
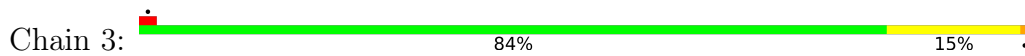
• Molecule 51: 30S ribosomal protein S21

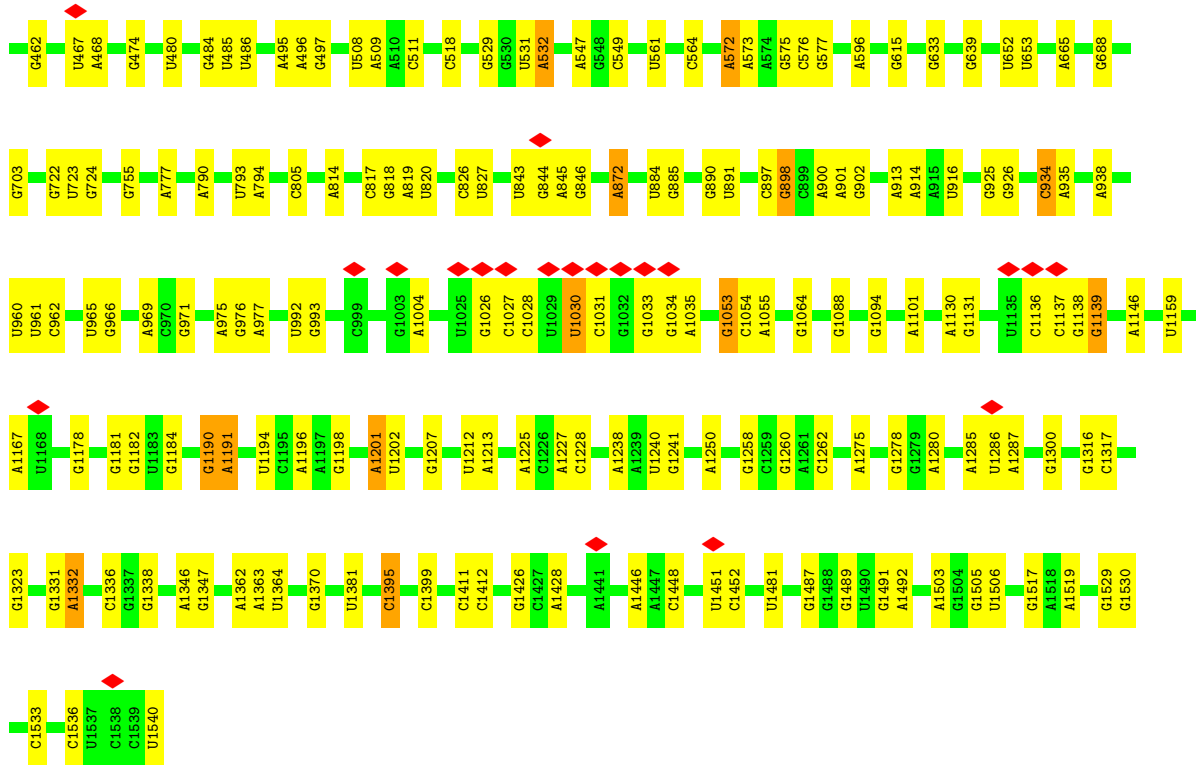


• Molecule 52: 50S ribosomal protein L1

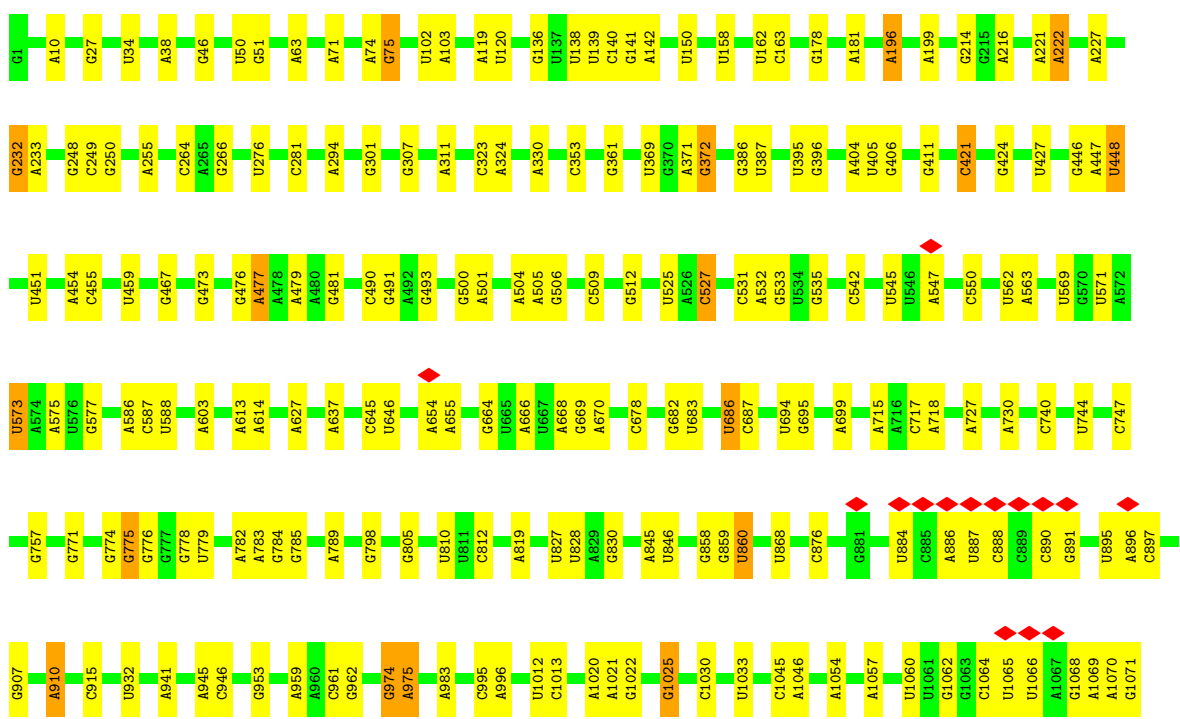
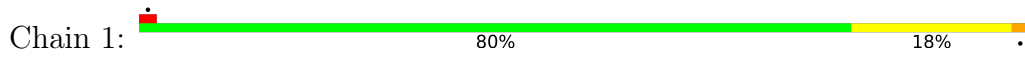


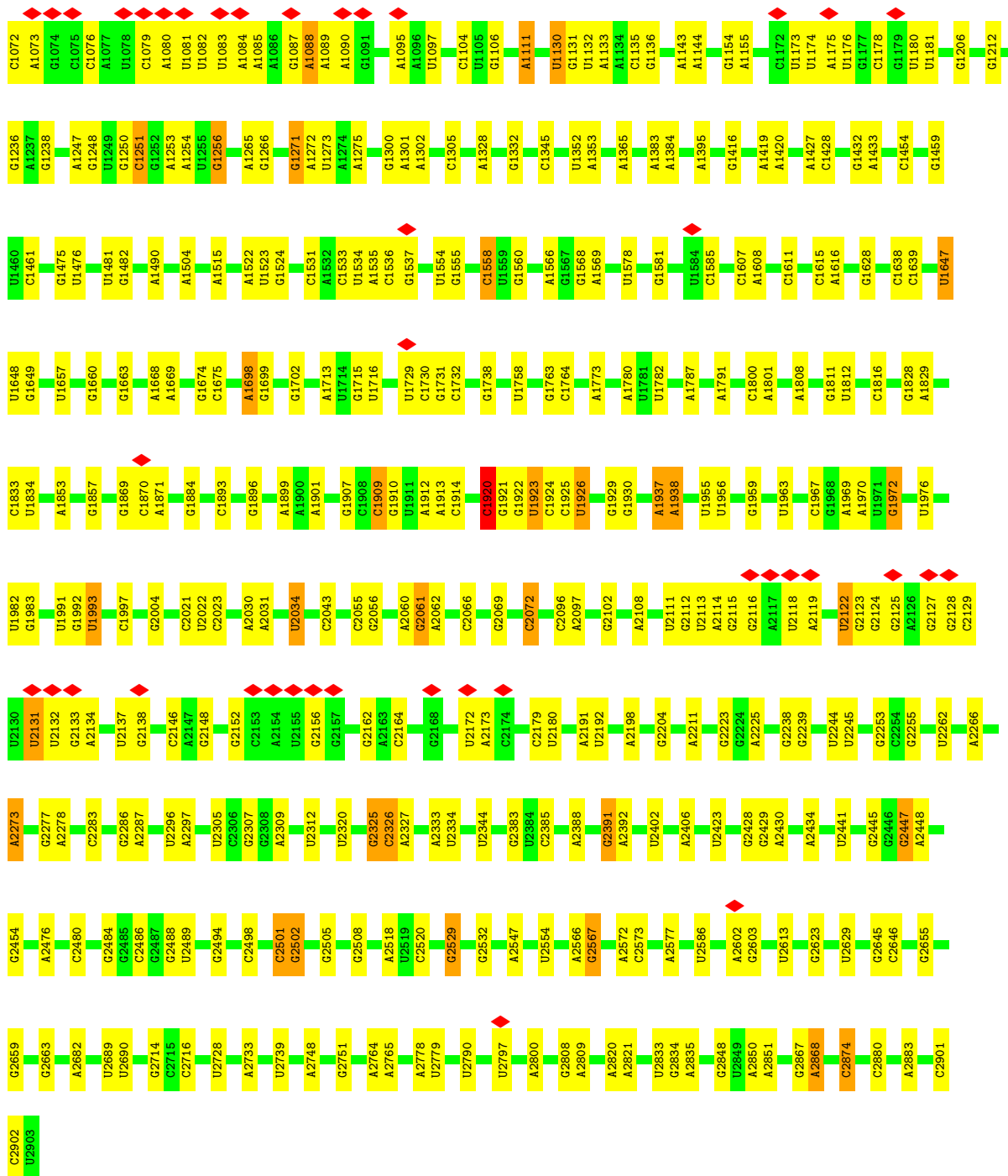
• Molecule 53: 16S ribosomal RNA



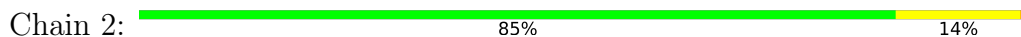


• Molecule 54: 23S ribosomal RNA





- Molecule 55: 5S ribosomal RNA

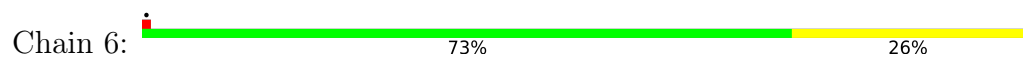


- Molecule 56: tRNAPro

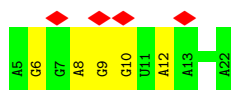




- Molecule 57: tRNAfMet



- Molecule 58: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3658	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	20.138	Depositor
Minimum map value	-7.423	Depositor
Average map value	0.007	Depositor
Map value standard deviation	1.205	Depositor
Recommended contour level	3.5	Depositor
Map size (Å)	424.96, 424.96, 424.96	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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

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	b	0.75	3/2122 (0.1%)	0.81	0/2852
2	c	0.79	2/1586 (0.1%)	0.79	0/2134
3	d	0.85	4/1571 (0.3%)	0.79	0/2113
4	e	0.93	8/1435 (0.6%)	0.84	1/1926 (0.1%)
5	f	0.81	3/1343 (0.2%)	0.81	1/1816 (0.1%)
6	g	0.95	2/445 (0.4%)	0.96	0/597
7	h	1.28	9/597 (1.5%)	1.03	1/803 (0.1%)
8	i	1.42	14/513 (2.7%)	1.07	2/684 (0.3%)
9	j	0.69	2/1152 (0.2%)	0.76	1/1551 (0.1%)
10	k	0.79	2/948 (0.2%)	0.94	3/1268 (0.2%)
11	l	0.76	1/1054 (0.1%)	0.83	0/1403
12	m	0.88	5/1093 (0.5%)	0.85	1/1460 (0.1%)
13	n	0.78	2/974 (0.2%)	0.72	0/1301
14	o	0.88	4/902 (0.4%)	0.79	1/1209 (0.1%)
15	p	0.63	0/929	0.70	0/1242
16	q	0.87	2/960 (0.2%)	0.79	1/1278 (0.1%)
17	r	0.68	0/829	0.77	0/1107
18	s	0.77	1/864 (0.1%)	0.78	0/1156
19	t	0.72	0/745	0.78	0/994
20	u	0.61	0/788	0.72	0/1051
21	v	0.71	0/766	0.74	0/1025
22	w	0.70	0/582	0.74	0/769
23	x	0.87	2/635 (0.3%)	0.81	0/848
24	y	0.73	1/510 (0.2%)	0.76	0/677
25	z	0.65	1/453 (0.2%)	0.75	0/605
26	A	0.78	1/371 (0.3%)	0.79	1/496 (0.2%)
27	B	0.62	0/450	0.73	0/599
28	C	0.71	0/417	0.67	0/554
29	D	0.75	0/380	0.78	0/498
30	E	0.80	0/513	0.80	0/676
31	F	0.76	1/303 (0.3%)	0.89	0/397
32	G	0.87	7/1736 (0.4%)	0.83	1/2338 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	H	0.87	4/1652 (0.2%)	0.77	0/2225
34	I	0.76	2/1665 (0.1%)	0.76	0/2227
35	J	0.82	3/1170 (0.3%)	0.86	3/1573 (0.2%)
36	K	1.01	7/836 (0.8%)	0.90	4/1128 (0.4%)
37	L	0.87	5/1196 (0.4%)	0.87	2/1602 (0.1%)
38	M	0.75	1/989 (0.1%)	0.81	0/1326
39	N	0.71	0/1034	0.71	0/1375
40	O	0.85	3/797 (0.4%)	0.89	0/1077
41	P	0.74	0/886	0.79	0/1195
42	Q	0.82	1/969 (0.1%)	0.84	1/1300 (0.1%)
43	R	0.87	5/893 (0.6%)	0.86	0/1193
44	S	0.80	1/817 (0.1%)	0.75	0/1088
45	T	0.80	2/722 (0.3%)	0.82	0/964
46	U	0.75	1/659 (0.2%)	0.67	0/884
47	V	0.62	0/658	0.73	0/881
48	W	0.71	0/545	0.79	0/731
49	X	0.73	0/653	0.77	0/877
50	Y	0.83	1/671 (0.1%)	0.73	0/888
51	Z	0.83	1/551 (0.2%)	0.95	1/728 (0.1%)
52	a	1.12	5/1034 (0.5%)	1.00	3/1387 (0.2%)
53	3	0.83	0/36963	0.71	6/57662 (0.0%)
54	1	0.83	9/69796 (0.0%)	0.72	29/108888 (0.0%)
55	2	0.64	2/2872 (0.1%)	0.71	0/4479
56	5	0.72	0/1840	0.77	2/2868 (0.1%)
57	6	0.55	0/1832	0.70	0/2855
58	4	0.66	0/436	0.69	0/679
All	All	0.82	130/160102 (0.1%)	0.74	65/239507 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	d	0	1
35	J	0	1
42	Q	0	1
53	3	0	42
54	1	0	113
55	2	0	4
56	5	0	4
57	6	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
58	4	0	1
All	All	0	169

All (130) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	73	VAL	C-O	12.13	1.46	1.23
36	K	13	ASP	C-O	11.45	1.45	1.23
52	a	159	GLY	C-O	11.04	1.41	1.23
7	h	44	ALA	C-O	10.91	1.44	1.23
14	o	58	ILE	C-O	9.75	1.41	1.23
8	i	107	GLU	C-O	8.89	1.40	1.23
8	i	138	VAL	C-O	8.80	1.40	1.23
37	L	92	PRO	C-O	8.35	1.40	1.23
36	K	17	GLN	N-CA	8.34	1.63	1.46
52	a	59	VAL	C-O	8.14	1.38	1.23
32	G	75	ALA	C-O	8.00	1.38	1.23
3	d	150	THR	C-O	7.93	1.38	1.23
36	K	59	TYR	C-O	7.84	1.38	1.23
8	i	136	GLY	C-O	7.68	1.35	1.23
52	a	44	VAL	C-O	7.56	1.37	1.23
2	c	157	LYS	C-O	7.51	1.37	1.23
52	a	19	LYS	N-CA	7.46	1.61	1.46
34	I	156	ALA	C-O	7.39	1.37	1.23
7	h	43	LYS	C-O	7.38	1.37	1.23
4	e	93	GLU	C-O	7.35	1.37	1.23
40	O	80	THR	C-O	7.33	1.37	1.23
43	R	66	GLY	C-O	7.29	1.35	1.23
45	T	6	ALA	C-O	7.26	1.37	1.23
37	L	96	ASN	N-CA	7.24	1.60	1.46
33	H	80	GLY	C-O	7.11	1.35	1.23
35	J	159	SER	C-O	7.06	1.36	1.23
4	e	9	ASP	C-O	6.99	1.36	1.23
7	h	33	VAL	C-O	6.97	1.36	1.23
43	R	7	ASN	C-O	6.90	1.36	1.23
33	H	43	THR	C-O	6.87	1.36	1.23
12	m	119	LEU	C-O	6.83	1.36	1.23
50	Y	60	GLN	C-O	6.83	1.36	1.23
54	1	1923	U	N1-C2	6.79	1.44	1.38
37	L	57	GLU	C-O	6.78	1.36	1.23
3	d	35	TYR	C-O	6.66	1.36	1.23
32	G	215	ALA	C-O	6.66	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	o	30	ARG	N-CA	6.57	1.59	1.46
7	h	15	VAL	C-O	6.49	1.35	1.23
1	b	9	SER	C-O	6.48	1.35	1.23
32	G	55	GLU	C-O	6.46	1.35	1.23
37	L	116	ALA	C-O	6.37	1.35	1.23
33	H	199	VAL	C-O	6.36	1.35	1.23
8	i	98	GLY	C-O	6.29	1.33	1.23
8	i	80	LYS	C-O	6.28	1.35	1.23
10	k	113	MET	N-CA	6.27	1.58	1.46
40	O	20	GLN	C-O	6.24	1.35	1.23
23	x	63	ILE	C-O	6.24	1.35	1.23
13	n	14	SER	C-O	6.21	1.35	1.23
5	f	90	GLY	C-O	6.20	1.33	1.23
32	G	14	HIS	C-O	6.20	1.35	1.23
3	d	112	LEU	C-O	6.18	1.35	1.23
40	O	46	LYS	N-CA	6.06	1.58	1.46
54	1	587	C	N1-C2	6.02	1.46	1.40
55	2	1	U	N3-C4	-6.02	1.33	1.38
54	1	1909	C	N1-C2	5.97	1.46	1.40
8	i	124	MET	C-O	5.96	1.34	1.23
44	S	39	ASP	C-O	5.94	1.34	1.23
51	Z	61	ARG	N-CA	5.91	1.58	1.46
34	I	91	ALA	C-O	5.89	1.34	1.23
18	s	41	LYS	N-CA	5.87	1.58	1.46
7	h	59	LEU	C-O	5.87	1.34	1.23
8	i	83	ALA	C-N	5.86	1.43	1.33
1	b	221	GLY	C-O	5.86	1.33	1.23
12	m	73	ILE	C-O	5.85	1.34	1.23
16	q	82	LEU	C-O	5.80	1.34	1.23
43	R	16	ILE	C-O	5.77	1.34	1.23
54	1	573	U	N1-C2	5.76	1.43	1.38
45	T	70	LYS	C-O	5.75	1.34	1.23
43	R	32	ILE	C-O	5.73	1.34	1.23
8	i	79	LEU	C-O	5.68	1.34	1.23
23	x	64	ASP	C-O	5.68	1.34	1.23
5	f	74	MET	C-O	5.66	1.34	1.23
12	m	88	ASN	C-O	5.65	1.34	1.23
4	e	132	ARG	C-O	5.65	1.34	1.23
4	e	36	ASN	N-CA	5.65	1.57	1.46
1	b	19	VAL	N-CA	5.64	1.57	1.46
54	1	1924	C	N1-C2	5.61	1.45	1.40
3	d	36	ALA	C-O	5.58	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	o	62	LEU	N-CA	5.58	1.57	1.46
36	K	12	PRO	C-O	5.57	1.34	1.23
7	h	37	LYS	N-CA	5.56	1.57	1.46
4	e	36	ASN	C-O	5.56	1.33	1.23
4	e	94	ARG	C-O	5.55	1.33	1.23
7	h	17	GLU	C-O	5.55	1.33	1.23
32	G	108	GLN	C-O	5.52	1.33	1.23
35	J	56	PRO	C-O	5.51	1.34	1.23
43	R	6	ILE	N-CA	5.51	1.57	1.46
4	e	110	ILE	C-O	5.50	1.33	1.23
33	H	136	ALA	C-O	5.47	1.33	1.23
8	i	111	THR	C-O	5.46	1.33	1.23
2	c	121	THR	C-O	5.45	1.33	1.23
13	n	47	VAL	C-O	5.44	1.33	1.23
26	A	45	THR	C-O	5.43	1.33	1.23
54	l	1920	C	N1-C2	5.43	1.45	1.40
32	G	107	ARG	C-O	5.43	1.33	1.23
5	f	150	TYR	N-CA	5.43	1.57	1.46
8	i	104	GLN	C-O	5.41	1.33	1.23
42	Q	116	TYR	C-O	5.40	1.33	1.23
11	l	130	GLY	C-O	5.39	1.32	1.23
8	i	78	LEU	C-O	5.38	1.33	1.23
36	K	25	TYR	C-O	5.34	1.33	1.23
12	m	100	LYS	N-CA	5.34	1.57	1.46
37	L	23	ALA	C-O	5.33	1.33	1.23
31	F	23	ILE	N-CA	5.33	1.57	1.46
25	z	23	LEU	C-O	5.31	1.33	1.23
52	a	23	ILE	C-O	5.30	1.33	1.23
32	G	73	ARG	C-O	-5.30	1.13	1.23
36	K	16	GLU	N-CA	5.26	1.56	1.46
35	J	160	VAL	C-O	5.26	1.33	1.23
12	m	75	GLU	C-O	5.25	1.33	1.23
8	i	111	THR	N-CA	5.24	1.56	1.46
10	k	91	SER	N-CA	5.20	1.56	1.46
46	U	49	GLY	C-O	5.20	1.31	1.23
16	q	97	ILE	C-O	5.20	1.33	1.23
36	K	73	GLU	C-O	5.20	1.33	1.23
54	l	2072	C	N1-C2	5.19	1.45	1.40
8	i	128	ILE	N-CA	5.18	1.56	1.46
55	2	1	U	C2-O2	-5.18	1.17	1.22
7	h	62	ARG	C-O	5.17	1.33	1.23
7	h	19	ALA	N-CA	5.16	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	26	PHE	C-O	5.15	1.33	1.23
9	j	81	ILE	N-CA	5.13	1.56	1.46
38	M	9	MET	C-O	5.12	1.33	1.23
6	g	7	ASP	N-CA	5.11	1.56	1.46
6	g	30	LEU	C-O	5.10	1.33	1.23
9	j	7	LYS	C-O	5.10	1.33	1.23
14	o	105	ALA	C-O	5.09	1.33	1.23
8	i	108	ILE	C-O	5.07	1.32	1.23
54	1	527	C	N1-C2	5.06	1.45	1.40
54	1	740	C	N1-C2	5.03	1.45	1.40

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1	974	G	N9-C1'-C2'	7.85	124.20	114.00
52	a	18	THR	C-N-CA	-7.72	102.39	121.70
35	J	85	LYS	C-N-CA	-7.53	106.50	122.30
54	1	2122	U	N1-C1'-C2'	7.50	123.74	114.00
10	k	112	PHE	C-N-CA	-7.39	103.22	121.70
26	A	40	CYS	C-N-CA	-7.25	103.58	121.70
54	1	2874	C	N1-C1'-C2'	7.23	123.40	114.00
54	1	2645	G	N9-C1'-C2'	7.09	123.22	114.00
37	L	95	ARG	C-N-CA	-6.74	104.85	121.70
16	q	72	GLY	N-CA-C	6.36	129.01	113.10
54	1	1459	G	N9-C1'-C2'	6.27	122.16	114.00
10	k	49	ARG	C-N-CA	-6.26	109.16	122.30
36	K	16	GLU	C-N-CA	-6.24	106.10	121.70
54	1	421	C	N1-C1'-C2'	6.22	122.09	114.00
54	1	477	A	N9-C1'-C2'	6.20	122.06	114.00
53	3	1201	A	C2'-C3'-O3'	6.15	123.54	113.70
54	1	2391	G	C2'-C3'-O3'	6.02	123.33	113.70
54	1	301	G	N9-C1'-C2'	6.02	121.82	114.00
32	G	75	ALA	C-N-CA	-5.94	106.85	121.70
51	Z	58	LYS	C-N-CA	-5.91	106.92	121.70
53	3	1190	G	C2'-C3'-O3'	5.84	123.04	113.70
36	K	13	ASP	CA-C-O	5.83	132.34	120.10
8	i	83	ALA	C-N-CA	-5.81	110.09	122.30
54	1	686	U	N1-C1'-C2'	5.72	121.44	114.00
53	3	572	A	N9-C1'-C2'	5.71	121.43	114.00
35	J	162	GLU	C-N-CA	-5.70	107.46	121.70
53	3	413	G	N9-C1'-C2'	5.69	121.40	114.00
56	5	69	G	N9-C1'-C2'	5.66	121.36	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	1	2501	C	N1-C1'-C2'	5.66	121.35	114.00
7	h	69	PHE	C-N-CA	-5.64	107.60	121.70
8	i	81	LYS	C-N-CA	-5.63	107.62	121.70
54	1	1081	U	N1-C1'-C2'	5.62	121.31	114.00
54	1	2326	C	C2'-C3'-O3'	5.61	122.68	113.70
53	3	1030	U	N1-C1'-C2'	5.59	121.27	114.00
36	K	13	ASP	O-C-N	-5.57	113.79	122.70
54	1	2131	U	N1-C1'-C2'	5.55	121.21	114.00
54	1	1266	G	N9-C1'-C2'	5.52	121.18	114.00
54	1	1669	A	N9-C1'-C2'	5.49	121.13	114.00
54	1	1060	U	N1-C1'-C2'	5.40	121.03	114.00
54	1	895	U	N1-C1'-C2'	5.39	121.01	114.00
54	1	2502	G	N9-C1'-C2'	5.35	120.96	114.00
56	5	43	U	N1-C1'-C2'	5.33	120.93	114.00
14	o	61	GLN	C-N-CA	-5.31	108.42	121.70
5	f	149	ALA	C-N-CA	-5.30	108.45	121.70
42	Q	117	GLY	N-CA-C	5.29	126.33	113.10
54	1	1909	C	N1-C1'-C2'	5.24	120.81	114.00
54	1	1395	A	C1'-O4'-C4'	-5.24	105.71	109.90
54	1	227	A	N9-C1'-C2'	5.23	120.80	114.00
12	m	45	GLN	C-N-CA	-5.22	108.65	121.70
54	1	1558	C	N1-C1'-C2'	5.22	120.78	114.00
54	1	1130	U	C2'-C3'-O3'	5.20	122.01	113.70
54	1	2447	G	N9-C1'-C2'	5.19	120.75	114.00
52	a	44	VAL	O-C-N	5.16	130.95	122.70
52	a	14	LYS	C-N-CA	-5.15	108.82	121.70
54	1	448	U	N1-C1'-C2'	5.13	120.67	114.00
36	K	15	SER	C-N-CA	-5.09	108.97	121.70
10	k	110	GLU	O-C-N	-5.08	114.57	122.70
54	1	2728	U	N1-C1'-C2'	5.08	120.61	114.00
37	L	92	PRO	O-C-N	-5.08	114.57	122.70
35	J	59	ILE	C-N-CA	-5.08	109.00	121.70
54	1	2180	U	N1-C1'-C2'	5.06	120.58	114.00
4	e	175	PRO	N-CA-C	5.06	125.26	112.10
53	3	1426	G	N9-C1'-C2'	5.04	120.55	114.00
54	1	372	G	C1'-O4'-C4'	-5.02	105.89	109.90
9	j	80	HIS	C-N-CA	-5.01	109.18	121.70

There are no chirality outliers.

All (169) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	1	1025	G	Sidechain
54	1	1062	G	Sidechain
54	1	1080	A	Sidechain
54	1	1088	A	Sidechain
54	1	1111	A	Sidechain
54	1	1154	G	Sidechain
54	1	1236	G	Sidechain
54	1	1251	C	Sidechain
54	1	1254	A	Sidechain
54	1	1256	G	Sidechain
54	1	1271	G	Sidechain
54	1	1328	A	Sidechain
54	1	1353	A	Sidechain
54	1	136	G	Sidechain
54	1	1432	G	Sidechain
54	1	1433	A	Sidechain
54	1	150	U	Sidechain
54	1	1554	U	Sidechain
54	1	1558	C	Sidechain
54	1	1568	G	Sidechain
54	1	1615	C	Sidechain
54	1	1628	G	Sidechain
54	1	1638	C	Sidechain
54	1	1647	U	Sidechain
54	1	1657	U	Sidechain
54	1	1663	G	Sidechain
54	1	1668	A	Sidechain
54	1	1698	A	Sidechain
54	1	1763	G	Sidechain
54	1	1828	G	Sidechain
54	1	1834	U	Sidechain
54	1	1853	A	Sidechain
54	1	1857	G	Sidechain
54	1	1893	C	Sidechain
54	1	1899	A	Sidechain
54	1	1909	C	Sidechain
54	1	1910	G	Sidechain
54	1	1920	C	Sidechain
54	1	1926	U	Sidechain
54	1	1929	G	Sidechain
54	1	1937	A	Sidechain
54	1	1938	A	Sidechain
54	1	1956	U	Sidechain

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Mol	Chain	Res	Type	Group
54	1	1959	G	Sidechain
54	1	196	A	Sidechain
54	1	1969	A	Sidechain
54	1	1972	G	Sidechain
54	1	1976	U	Sidechain
54	1	1993	U	Sidechain
54	1	2034	U	Sidechain
54	1	2061	G	Sidechain
54	1	2066	C	Sidechain
54	1	2114	A	Sidechain
54	1	214	G	Sidechain
54	1	222	A	Sidechain
54	1	2244	U	Sidechain
54	1	2245	U	Sidechain
54	1	2255	G	Sidechain
54	1	2262	U	Sidechain
54	1	2266	A	Sidechain
54	1	2273	A	Sidechain
54	1	232	G	Sidechain
54	1	2325	G	Sidechain
54	1	2447	G	Sidechain
54	1	2454	G	Sidechain
54	1	2486	C	Sidechain
54	1	2488	G	Sidechain
54	1	2489	U	Sidechain
54	1	250	G	Sidechain
54	1	2501	C	Sidechain
54	1	2508	G	Sidechain
54	1	2529	G	Sidechain
54	1	2532	G	Sidechain
54	1	2567	G	Sidechain
54	1	2577	A	Sidechain
54	1	2659	G	Sidechain
54	1	27	G	Sidechain
54	1	2834	G	Sidechain
54	1	2848	G	Sidechain
54	1	2868	A	Sidechain
54	1	307	G	Sidechain
54	1	395	U	Sidechain
54	1	427	U	Sidechain
54	1	446	G	Sidechain
54	1	454	A	Sidechain

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Mol	Chain	Res	Type	Group
54	1	476	G	Sidechain
54	1	477	A	Sidechain
54	1	493	G	Sidechain
54	1	500	G	Sidechain
54	1	501	A	Sidechain
54	1	506	G	Sidechain
54	1	512	G	Sidechain
54	1	525	U	Sidechain
54	1	562	U	Sidechain
54	1	571	U	Sidechain
54	1	577	G	Sidechain
54	1	666	A	Sidechain
54	1	682	G	Sidechain
54	1	683	U	Sidechain
54	1	727	A	Sidechain
54	1	744	U	Sidechain
54	1	75	G	Sidechain
54	1	757	G	Sidechain
54	1	775	G	Sidechain
54	1	778	G	Sidechain
54	1	798	G	Sidechain
54	1	810	U	Sidechain
54	1	860	U	Sidechain
54	1	868	U	Sidechain
54	1	884	U	Sidechain
54	1	910	A	Sidechain
54	1	974	G	Sidechain
54	1	975	A	Sidechain
55	2	1	U	Sidechain
55	2	119	A	Sidechain
55	2	24	G	Sidechain
55	2	59	A	Sidechain
53	3	1053	G	Sidechain
53	3	1064	G	Sidechain
53	3	1139	G	Sidechain
53	3	1167	A	Sidechain
53	3	1178	G	Sidechain
53	3	1191	A	Sidechain
53	3	1194	U	Sidechain
53	3	1285	A	Sidechain
53	3	1316	G	Sidechain
53	3	1332	A	Sidechain

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Mol	Chain	Res	Type	Group
53	3	1395	C	Sidechain
53	3	1399	C	Sidechain
53	3	1412	C	Sidechain
53	3	1481	U	Sidechain
53	3	1489	G	Sidechain
53	3	1491	G	Sidechain
53	3	159	G	Sidechain
53	3	249	U	Sidechain
53	3	26	A	Sidechain
53	3	297	G	Sidechain
53	3	324	G	Sidechain
53	3	380	G	Sidechain
53	3	383	A	Sidechain
53	3	412	A	Sidechain
53	3	413	G	Sidechain
53	3	529	G	Sidechain
53	3	532	A	Sidechain
53	3	549	C	Sidechain
53	3	58	C	Sidechain
53	3	722	G	Sidechain
53	3	820	U	Sidechain
53	3	826	C	Sidechain
53	3	827	U	Sidechain
53	3	872	A	Sidechain
53	3	897	C	Sidechain
53	3	898	G	Sidechain
53	3	900	A	Sidechain
53	3	901	A	Sidechain
53	3	916	U	Sidechain
53	3	925	G	Sidechain
53	3	934	C	Sidechain
53	3	938	A	Sidechain
58	4	9	G	Sidechain
56	5	43	U	Sidechain
56	5	51	A	Sidechain
56	5	65	U	Sidechain
56	5	69	G	Sidechain
57	6	27	U	Sidechain
57	6	44	A	Sidechain
35	J	92	ARG	Mainchain
42	Q	14	LYS	Peptide
3	d	102	ARG	Mainchain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/271 (99%)	216 (80%)	50 (19%)	3 (1%)	14	51
2	c	207/209 (99%)	160 (77%)	43 (21%)	4 (2%)	8	39
3	d	199/201 (99%)	154 (77%)	43 (22%)	2 (1%)	15	54
4	e	175/177 (99%)	143 (82%)	29 (17%)	3 (2%)	9	42
5	f	174/176 (99%)	139 (80%)	30 (17%)	5 (3%)	4	28
6	g	55/149 (37%)	40 (73%)	11 (20%)	4 (7%)	1	7
7	h	77/131 (59%)	49 (64%)	26 (34%)	2 (3%)	5	31
8	i	69/141 (49%)	59 (86%)	9 (13%)	1 (1%)	11	46
9	j	140/142 (99%)	114 (81%)	24 (17%)	2 (1%)	11	46
10	k	120/122 (98%)	88 (73%)	28 (23%)	4 (3%)	4	25
11	l	141/143 (99%)	99 (70%)	37 (26%)	5 (4%)	3	24
12	m	134/136 (98%)	113 (84%)	17 (13%)	4 (3%)	4	28
13	n	118/120 (98%)	97 (82%)	20 (17%)	1 (1%)	19	58
14	o	114/116 (98%)	94 (82%)	18 (16%)	2 (2%)	8	41
15	p	112/114 (98%)	88 (79%)	23 (20%)	1 (1%)	17	56
16	q	115/117 (98%)	99 (86%)	14 (12%)	2 (2%)	9	42
17	r	101/103 (98%)	78 (77%)	22 (22%)	1 (1%)	15	54
18	s	108/110 (98%)	93 (86%)	14 (13%)	1 (1%)	17	56
19	t	91/93 (98%)	77 (85%)	12 (13%)	2 (2%)	6	35
20	u	100/102 (98%)	76 (76%)	21 (21%)	3 (3%)	4	28
21	v	92/94 (98%)	82 (89%)	10 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	w	73/75 (97%)	59 (81%)	12 (16%)	2 (3%)	5	30
23	x	75/77 (97%)	64 (85%)	10 (13%)	1 (1%)	12	47
24	y	61/63 (97%)	53 (87%)	7 (12%)	1 (2%)	9	43
25	z	56/58 (97%)	50 (89%)	5 (9%)	1 (2%)	8	41
26	A	45/66 (68%)	32 (71%)	12 (27%)	1 (2%)	6	35
27	B	54/56 (96%)	38 (70%)	14 (26%)	2 (4%)	3	22
28	C	48/50 (96%)	41 (85%)	7 (15%)	0	100	100
29	D	44/46 (96%)	35 (80%)	9 (20%)	0	100	100
30	E	62/64 (97%)	49 (79%)	12 (19%)	1 (2%)	9	43
31	F	36/38 (95%)	26 (72%)	9 (25%)	1 (3%)	5	29
32	G	216/225 (96%)	170 (79%)	43 (20%)	3 (1%)	11	46
33	H	204/206 (99%)	172 (84%)	32 (16%)	0	100	100
34	I	203/205 (99%)	154 (76%)	48 (24%)	1 (0%)	29	67
35	J	155/157 (99%)	117 (76%)	36 (23%)	2 (1%)	12	47
36	K	98/100 (98%)	73 (74%)	24 (24%)	1 (1%)	15	54
37	L	149/151 (99%)	117 (78%)	30 (20%)	2 (1%)	12	47
38	M	127/129 (98%)	114 (90%)	10 (8%)	3 (2%)	6	34
39	N	125/127 (98%)	88 (70%)	34 (27%)	3 (2%)	6	34
40	O	96/98 (98%)	75 (78%)	17 (18%)	4 (4%)	3	20
41	P	114/116 (98%)	86 (75%)	23 (20%)	5 (4%)	2	19
42	Q	121/123 (98%)	85 (70%)	31 (26%)	5 (4%)	3	21
43	R	112/114 (98%)	96 (86%)	15 (13%)	1 (1%)	17	56
44	S	98/100 (98%)	74 (76%)	22 (22%)	2 (2%)	7	38
45	T	86/88 (98%)	75 (87%)	11 (13%)	0	100	100
46	U	80/82 (98%)	61 (76%)	16 (20%)	3 (4%)	3	22
47	V	78/80 (98%)	59 (76%)	19 (24%)	0	100	100
48	W	63/65 (97%)	48 (76%)	12 (19%)	3 (5%)	2	17
49	X	77/79 (98%)	61 (79%)	15 (20%)	1 (1%)	12	47
50	Y	83/85 (98%)	73 (88%)	10 (12%)	0	100	100
51	Z	63/65 (97%)	36 (57%)	20 (32%)	7 (11%)	0	2
52	a	130/223 (58%)	100 (77%)	26 (20%)	4 (3%)	4	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	5743/6178 (93%)	4539 (79%)	1092 (19%)	112 (2%)	11	38

All (112) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	h	72	LEU
10	k	92	GLU
10	k	105	ARG
11	l	38	GLN
11	l	39	LYS
14	o	34	HIS
24	y	24	GLU
31	F	11	CYS
35	J	87	VAL
39	N	90	ASP
41	P	13	LYS
51	Z	8	ASN
51	Z	37	TYR
51	Z	62	GLU
3	d	131	THR
4	e	113	PHE
5	f	28	LYS
6	g	9	VAL
17	r	54	VAL
25	z	14	GLY
26	A	3	LYS
32	G	88	GLN
32	G	224	ARG
34	I	65	GLY
37	L	54	GLY
38	M	28	SER
38	M	47	ASP
38	M	78	SER
40	O	89	ARG
42	Q	15	VAL
42	Q	117	GLY
48	W	17	VAL
48	W	20	ILE
51	Z	34	ARG
51	Z	61	ARG
52	a	204	ALA
52	a	207	VAL

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Mol	Chain	Res	Type
5	f	118	ALA
12	m	27	SER
16	q	27	ARG
19	t	3	ARG
19	t	35	ALA
23	x	2	ARG
27	B	44	ALA
30	E	54	LEU
39	N	91	GLU
40	O	43	PRO
41	P	14	GLN
42	Q	101	LEU
43	R	105	ALA
44	S	3	GLN
46	U	45	GLU
51	Z	65	ARG
3	d	62	GLN
4	e	75	GLY
6	g	8	LYS
6	g	10	ALA
7	h	60	LEU
9	j	60	ASP
10	k	14	SER
11	l	36	LYS
12	m	42	THR
20	u	51	LEU
22	w	40	LYS
22	w	53	HIS
36	K	92	THR
39	N	57	VAL
41	P	39	ASN
46	U	47	GLU
46	U	80	LYS
48	W	71	ASP
52	a	6	LYS
52	a	16	ASP
1	b	7	PRO
1	b	96	LYS
2	c	99	GLU
2	c	102	ALA
2	c	129	THR
4	e	74	ALA

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Mol	Chain	Res	Type
5	f	46	ASP
5	f	61	TRP
6	g	50	ARG
8	i	72	THR
9	j	83	GLY
10	k	104	THR
11	l	107	PHE
12	m	121	ALA
16	q	49	ARG
18	s	25	ARG
32	G	153	MET
37	L	112	ASP
41	P	91	GLY
44	S	74	ARG
51	Z	15	LEU
1	b	255	LYS
2	c	134	HIS
14	o	99	TYR
35	J	50	GLY
40	O	42	LEU
40	O	57	VAL
42	Q	33	CYS
49	X	27	LYS
42	Q	3	VAL
5	f	125	PRO
11	l	56	PRO
12	m	69	PRO
13	n	116	VAL
15	p	53	GLY
27	B	46	GLY
41	P	47	GLY
20	u	55	GLY
20	u	54	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	200 (93%)	16 (7%)	13	46
2	c	164/164 (100%)	156 (95%)	8 (5%)	25	61
3	d	165/165 (100%)	161 (98%)	4 (2%)	49	77
4	e	148/148 (100%)	143 (97%)	5 (3%)	37	70
5	f	137/137 (100%)	135 (98%)	2 (2%)	65	85
6	g	45/114 (40%)	45 (100%)	0	100	100
7	h	62/100 (62%)	61 (98%)	1 (2%)	62	84
8	i	53/109 (49%)	52 (98%)	1 (2%)	57	81
9	j	116/116 (100%)	113 (97%)	3 (3%)	46	76
10	k	103/103 (100%)	94 (91%)	9 (9%)	10	37
11	l	102/102 (100%)	97 (95%)	5 (5%)	25	61
12	m	109/109 (100%)	97 (89%)	12 (11%)	6	26
13	n	100/100 (100%)	92 (92%)	8 (8%)	12	42
14	o	86/86 (100%)	84 (98%)	2 (2%)	50	78
15	p	99/99 (100%)	95 (96%)	4 (4%)	31	66
16	q	89/89 (100%)	85 (96%)	4 (4%)	27	63
17	r	84/84 (100%)	83 (99%)	1 (1%)	71	88
18	s	93/93 (100%)	90 (97%)	3 (3%)	39	71
19	t	80/80 (100%)	79 (99%)	1 (1%)	69	87
20	u	83/83 (100%)	78 (94%)	5 (6%)	19	54
21	v	78/78 (100%)	76 (97%)	2 (3%)	46	76
22	w	57/57 (100%)	53 (93%)	4 (7%)	15	48
23	x	67/67 (100%)	66 (98%)	1 (2%)	65	85
24	y	55/55 (100%)	55 (100%)	0	100	100
25	z	48/48 (100%)	45 (94%)	3 (6%)	18	52
26	A	43/59 (73%)	42 (98%)	1 (2%)	50	78
27	B	47/47 (100%)	46 (98%)	1 (2%)	53	79
28	C	45/45 (100%)	44 (98%)	1 (2%)	52	79
29	D	38/38 (100%)	38 (100%)	0	100	100
30	E	51/51 (100%)	47 (92%)	4 (8%)	12	43
31	F	34/34 (100%)	33 (97%)	1 (3%)	42	74
32	G	180/186 (97%)	177 (98%)	3 (2%)	60	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	H	170/170 (100%)	164 (96%)	6 (4%)	36	69
34	I	172/172 (100%)	164 (95%)	8 (5%)	26	62
35	J	119/119 (100%)	115 (97%)	4 (3%)	37	70
36	K	87/87 (100%)	84 (97%)	3 (3%)	37	70
37	L	124/124 (100%)	120 (97%)	4 (3%)	39	71
38	M	104/104 (100%)	101 (97%)	3 (3%)	42	74
39	N	105/105 (100%)	103 (98%)	2 (2%)	57	81
40	O	86/86 (100%)	82 (95%)	4 (5%)	26	62
41	P	89/89 (100%)	85 (96%)	4 (4%)	27	63
42	Q	103/103 (100%)	99 (96%)	4 (4%)	32	67
43	R	92/92 (100%)	91 (99%)	1 (1%)	73	88
44	S	83/83 (100%)	78 (94%)	5 (6%)	19	54
45	T	76/76 (100%)	72 (95%)	4 (5%)	22	58
46	U	65/65 (100%)	60 (92%)	5 (8%)	13	44
47	V	74/74 (100%)	70 (95%)	4 (5%)	22	58
48	W	56/56 (100%)	55 (98%)	1 (2%)	59	82
49	X	70/70 (100%)	66 (94%)	4 (6%)	20	56
50	Y	65/65 (100%)	64 (98%)	1 (2%)	65	85
51	Z	55/55 (100%)	49 (89%)	6 (11%)	6	26
52	a	110/174 (63%)	104 (94%)	6 (6%)	21	57
All	All	4782/5031 (95%)	4588 (96%)	194 (4%)	34	66

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	33	LEU
1	b	42	ARG
1	b	50	THR
1	b	85	ASN
1	b	97	ASP
1	b	143	VAL
1	b	145	MET
1	b	171	VAL
1	b	196	ASN
1	b	203	VAL

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Mol	Chain	Res	Type
1	b	212	TRP
1	b	222	THR
1	b	237	ARG
1	b	238	ASN
1	b	241	LYS
1	b	251	THR
2	c	49	GLN
2	c	83	ARG
2	c	88	GLU
2	c	96	ILE
2	c	151	THR
2	c	156	PHE
2	c	178	VAL
2	c	187	LEU
3	d	60	TRP
3	d	140	ASP
3	d	165	HIS
3	d	171	ASP
4	e	2	LYS
4	e	111	ARG
4	e	129	MET
4	e	145	VAL
4	e	149	ARG
5	f	106	LEU
5	f	166	GLU
7	h	55	VAL
8	i	79	LEU
9	j	5	THR
9	j	57	LEU
9	j	70	THR
10	k	13	ASN
10	k	32	TYR
10	k	40	LYS
10	k	54	LYS
10	k	58	LEU
10	k	61	VAL
10	k	76	VAL
10	k	79	PHE
10	k	92	GLU
11	l	2	ARG
11	l	19	LEU
11	l	46	VAL

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Mol	Chain	Res	Type
11	l	47	ARG
11	l	81	ASP
12	m	17	ASN
12	m	18	ARG
12	m	24	THR
12	m	44	ARG
12	m	90	GLU
12	m	91	TYR
12	m	95	LEU
12	m	110	GLU
12	m	111	GLU
12	m	124	LEU
12	m	125	PRO
12	m	126	ILE
13	n	2	ARG
13	n	8	ARG
13	n	12	ARG
13	n	20	MET
13	n	37	THR
13	n	69	ARG
13	n	95	THR
13	n	114	GLU
14	o	28	VAL
14	o	61	GLN
15	p	19	PHE
15	p	72	VAL
15	p	111	GLU
15	p	113	LEU
16	q	13	HIS
16	q	48	ASP
16	q	51	GLN
16	q	63	ARG
17	r	24	LYS
18	s	3	THR
18	s	4	ILE
18	s	75	PHE
19	t	80	TRP
20	u	36	GLU
20	u	39	ASN
20	u	51	LEU
20	u	61	GLU
20	u	73	ASN

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Mol	Chain	Res	Type
21	v	59	GLU
21	v	82	TYR
22	w	10	ARG
22	w	16	ARG
22	w	39	THR
22	w	40	LYS
23	x	16	ASN
25	z	3	THR
25	z	36	GLU
25	z	58	GLU
26	A	25	ARG
27	B	56	LYS
28	C	11	VAL
30	E	3	ILE
30	E	29	ARG
30	E	41	ARG
30	E	61	LEU
31	F	9	LYS
32	G	22	TRP
32	G	29	PHE
32	G	224	ARG
33	H	71	ARG
33	H	129	PHE
33	H	142	ARG
33	H	156	LEU
33	H	187	GLU
33	H	201	ILE
34	I	22	SER
34	I	40	HIS
34	I	68	GLU
34	I	73	ASN
34	I	115	GLN
34	I	125	ASN
34	I	183	ARG
34	I	190	LEU
35	J	67	ARG
35	J	79	THR
35	J	104	ILE
35	J	136	VAL
36	K	11	HIS
36	K	49	TYR
36	K	53	LYS

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Mol	Chain	Res	Type
37	L	17	PHE
37	L	37	THR
37	L	117	LEU
37	L	142	ARG
38	M	2	MET
38	M	26	MET
38	M	120	LEU
39	N	45	MET
39	N	54	VAL
40	O	66	GLU
40	O	71	LEU
40	O	80	THR
40	O	100	ILE
41	P	27	ASN
41	P	28	ASN
41	P	56	LYS
41	P	124	LYS
42	Q	38	THR
42	Q	78	VAL
42	Q	108	ASP
42	Q	116	TYR
43	R	53	ASP
44	S	8	ARG
44	S	9	GLU
44	S	11	LYS
44	S	56	PRO
44	S	88	MET
45	T	13	GLU
45	T	62	ARG
45	T	66	LEU
45	T	84	LEU
46	U	16	PHE
46	U	19	VAL
46	U	28	ARG
46	U	34	GLU
46	U	70	ARG
47	V	6	THR
47	V	12	VAL
47	V	46	HIS
47	V	58	VAL
48	W	11	ARG
49	X	5	LYS

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Mol	Chain	Res	Type
49	X	14	LEU
49	X	29	PRO
49	X	78	THR
50	Y	52	GLU
51	Z	6	ARG
51	Z	11	PHE
51	Z	32	ARG
51	Z	57	LYS
51	Z	62	GLU
51	Z	66	ARG
52	a	5	THR
52	a	7	ARG
52	a	15	VAL
52	a	16	ASP
52	a	44	VAL
52	a	166	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	44	ASN
1	b	133	ASN
1	b	199	HIS
1	b	229	HIS
1	b	259	ASN
2	c	49	GLN
2	c	136	ASN
2	c	140	HIS
2	c	173	GLN
3	d	97	ASN
4	e	20	ASN
9	j	40	HIS
14	o	43	ASN
20	u	39	ASN
24	y	39	GLN
24	y	41	HIS
29	D	26	ASN
32	G	14	HIS
32	G	23	ASN
32	G	57	ASN
32	G	93	HIS
32	G	119	GLN

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Mol	Chain	Res	Type
32	G	202	ASN
33	H	99	GLN
33	H	184	ASN
35	J	60	GLN
35	J	76	ASN
36	K	17	GLN
37	L	147	ASN
39	N	109	GLN
40	O	56	HIS
41	P	27	ASN
41	P	37	GLN
42	Q	28	GLN
44	S	34	ASN
45	T	61	GLN
45	T	79	GLN
47	V	30	HIS
48	W	18	GLN
48	W	51	GLN
49	X	51	HIS
49	X	68	HIS
50	Y	2	ASN
50	Y	12	GLN
52	a	58	ASN
52	a	160	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	3	1538/1539 (99%)	207 (13%)	10 (0%)
54	1	2902/2903 (99%)	462 (15%)	27 (0%)
55	2	119/120 (99%)	14 (11%)	1 (0%)
56	5	76/77 (98%)	20 (26%)	2 (2%)
57	6	76/77 (98%)	20 (26%)	0
58	4	17/18 (94%)	4 (23%)	0
All	All	4728/4734 (99%)	727 (15%)	40 (0%)

All (727) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	3	6	G
53	3	7	A

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Mol	Chain	Res	Type
53	3	8	A
53	3	9	G
53	3	22	G
53	3	32	A
53	3	39	G
53	3	48	C
53	3	50	A
53	3	51	A
53	3	71	A
53	3	72	A
53	3	79	G
53	3	81	A
53	3	83	C
53	3	84	U
53	3	86	G
53	3	87	C
53	3	92	U
53	3	100	G
53	3	101	A
53	3	121	U
53	3	130	A
53	3	141	G
53	3	149	A
53	3	152	A
53	3	153	C
53	3	162	A
53	3	183	C
53	3	197	A
53	3	209	U
53	3	210	C
53	3	226	G
53	3	247	G
53	3	251	G
53	3	262	A
53	3	266	G
53	3	267	C
53	3	280	C
53	3	281	G
53	3	289	G
53	3	307	C
53	3	327	A
53	3	328	C

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Mol	Chain	Res	Type
53	3	352	C
53	3	367	U
53	3	369	G
53	3	372	C
53	3	406	G
53	3	411	A
53	3	412	A
53	3	422	C
53	3	429	U
53	3	438	U
53	3	452	A
53	3	462	G
53	3	467	U
53	3	468	A
53	3	474	G
53	3	480	U
53	3	484	G
53	3	485	U
53	3	486	U
53	3	495	A
53	3	496	A
53	3	497	G
53	3	508	U
53	3	509	A
53	3	511	C
53	3	518	C
53	3	531	U
53	3	532	A
53	3	547	A
53	3	561	U
53	3	564	C
53	3	572	A
53	3	573	A
53	3	575	G
53	3	576	C
53	3	577	G
53	3	596	A
53	3	615	G
53	3	633	G
53	3	639	G
53	3	652	U
53	3	653	U

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Mol	Chain	Res	Type
53	3	665	A
53	3	688	G
53	3	703	G
53	3	723	U
53	3	724	G
53	3	755	G
53	3	777	A
53	3	790	A
53	3	793	U
53	3	794	A
53	3	805	C
53	3	814	A
53	3	817	C
53	3	818	G
53	3	819	A
53	3	843	U
53	3	844	G
53	3	846	G
53	3	872	A
53	3	885	G
53	3	890	G
53	3	891	U
53	3	898	G
53	3	902	G
53	3	913	A
53	3	914	A
53	3	926	G
53	3	934	C
53	3	935	A
53	3	960	U
53	3	961	U
53	3	962	C
53	3	965	U
53	3	966	G
53	3	969	A
53	3	971	G
53	3	975	A
53	3	976	G
53	3	977	A
53	3	992	U
53	3	993	G
53	3	1004	A

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Mol	Chain	Res	Type
53	3	1026	G
53	3	1027	C
53	3	1028	C
53	3	1030	U
53	3	1031	C
53	3	1033	G
53	3	1034	G
53	3	1035	A
53	3	1053	G
53	3	1054	C
53	3	1055	A
53	3	1088	G
53	3	1094	G
53	3	1101	A
53	3	1130	A
53	3	1131	G
53	3	1136	C
53	3	1137	C
53	3	1138	G
53	3	1139	G
53	3	1146	A
53	3	1159	U
53	3	1182	G
53	3	1184	G
53	3	1191	A
53	3	1196	A
53	3	1198	G
53	3	1201	A
53	3	1202	U
53	3	1207	G
53	3	1212	U
53	3	1213	A
53	3	1225	A
53	3	1227	A
53	3	1228	C
53	3	1238	A
53	3	1240	U
53	3	1241	G
53	3	1250	A
53	3	1258	G
53	3	1260	G
53	3	1262	C

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Mol	Chain	Res	Type
53	3	1275	A
53	3	1278	G
53	3	1280	A
53	3	1286	U
53	3	1287	A
53	3	1300	G
53	3	1317	C
53	3	1323	G
53	3	1332	A
53	3	1336	C
53	3	1338	G
53	3	1346	A
53	3	1347	G
53	3	1362	A
53	3	1363	A
53	3	1364	U
53	3	1370	G
53	3	1381	U
53	3	1395	C
53	3	1411	C
53	3	1428	A
53	3	1446	A
53	3	1448	C
53	3	1451	U
53	3	1452	C
53	3	1487	G
53	3	1492	A
53	3	1503	A
53	3	1505	G
53	3	1506	U
53	3	1517	G
53	3	1519	A
53	3	1529	G
53	3	1530	G
53	3	1533	C
53	3	1536	C
53	3	1540	U
54	1	10	A
54	1	34	U
54	1	38	A
54	1	46	G
54	1	50	U

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Mol	Chain	Res	Type
54	1	51	G
54	1	63	A
54	1	71	A
54	1	74	A
54	1	75	G
54	1	102	U
54	1	103	A
54	1	119	A
54	1	120	U
54	1	138	U
54	1	139	U
54	1	140	C
54	1	141	G
54	1	142	A
54	1	158	U
54	1	162	U
54	1	163	C
54	1	178	G
54	1	181	A
54	1	196	A
54	1	199	A
54	1	216	A
54	1	221	A
54	1	222	A
54	1	232	G
54	1	233	A
54	1	248	G
54	1	249	C
54	1	255	A
54	1	264	C
54	1	266	G
54	1	276	U
54	1	281	C
54	1	294	A
54	1	311	A
54	1	323	C
54	1	324	A
54	1	330	A
54	1	353	C
54	1	361	G
54	1	369	U
54	1	371	A

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Mol	Chain	Res	Type
54	1	372	G
54	1	386	G
54	1	387	U
54	1	396	G
54	1	404	A
54	1	405	U
54	1	406	G
54	1	411	G
54	1	421	C
54	1	424	G
54	1	447	A
54	1	448	U
54	1	451	U
54	1	455	C
54	1	459	U
54	1	467	G
54	1	473	G
54	1	479	A
54	1	481	G
54	1	490	C
54	1	491	G
54	1	504	A
54	1	505	A
54	1	509	C
54	1	527	C
54	1	531	C
54	1	532	A
54	1	533	G
54	1	535	G
54	1	542	C
54	1	545	U
54	1	547	A
54	1	550	C
54	1	563	A
54	1	569	U
54	1	573	U
54	1	575	A
54	1	586	A
54	1	588	U
54	1	603	A
54	1	613	A
54	1	614	A

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Mol	Chain	Res	Type
54	1	627	A
54	1	637	A
54	1	645	C
54	1	646	U
54	1	654	A
54	1	655	A
54	1	664	G
54	1	668	A
54	1	669	G
54	1	670	A
54	1	678	C
54	1	686	U
54	1	687	C
54	1	694	U
54	1	695	G
54	1	699	A
54	1	715	A
54	1	717	C
54	1	718	A
54	1	730	A
54	1	747	C
54	1	771	G
54	1	775	G
54	1	776	G
54	1	779	U
54	1	782	A
54	1	783	A
54	1	784	G
54	1	785	G
54	1	789	A
54	1	805	G
54	1	812	C
54	1	819	A
54	1	827	U
54	1	828	U
54	1	830	G
54	1	845	A
54	1	846	U
54	1	858	G
54	1	859	G
54	1	860	U
54	1	876	C

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Mol	Chain	Res	Type
54	1	886	A
54	1	887	U
54	1	888	C
54	1	890	C
54	1	891	G
54	1	896	A
54	1	897	C
54	1	907	G
54	1	910	A
54	1	915	C
54	1	932	U
54	1	941	A
54	1	945	A
54	1	946	C
54	1	953	G
54	1	959	A
54	1	961	C
54	1	962	G
54	1	975	A
54	1	983	A
54	1	995	C
54	1	996	A
54	1	1012	U
54	1	1013	C
54	1	1021	A
54	1	1022	G
54	1	1025	G
54	1	1030	C
54	1	1033	U
54	1	1045	C
54	1	1046	A
54	1	1054	A
54	1	1057	A
54	1	1064	C
54	1	1065	U
54	1	1066	U
54	1	1068	G
54	1	1069	A
54	1	1070	A
54	1	1071	G
54	1	1072	C
54	1	1073	A

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Mol	Chain	Res	Type
54	1	1076	C
54	1	1079	C
54	1	1082	U
54	1	1083	U
54	1	1084	A
54	1	1085	A
54	1	1087	G
54	1	1088	A
54	1	1089	A
54	1	1090	A
54	1	1095	A
54	1	1097	U
54	1	1104	C
54	1	1106	G
54	1	1111	A
54	1	1130	U
54	1	1131	G
54	1	1132	U
54	1	1133	A
54	1	1135	C
54	1	1136	G
54	1	1144	A
54	1	1155	A
54	1	1173	U
54	1	1174	U
54	1	1175	A
54	1	1176	U
54	1	1178	C
54	1	1180	U
54	1	1181	U
54	1	1206	G
54	1	1212	G
54	1	1238	G
54	1	1247	A
54	1	1248	G
54	1	1250	G
54	1	1251	C
54	1	1253	A
54	1	1256	G
54	1	1265	A
54	1	1271	G
54	1	1272	A

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Mol	Chain	Res	Type
54	1	1273	U
54	1	1275	A
54	1	1300	G
54	1	1301	A
54	1	1302	A
54	1	1305	C
54	1	1332	G
54	1	1345	C
54	1	1352	U
54	1	1365	A
54	1	1383	A
54	1	1384	A
54	1	1416	G
54	1	1419	A
54	1	1420	A
54	1	1427	A
54	1	1428	C
54	1	1454	C
54	1	1461	C
54	1	1476	U
54	1	1481	U
54	1	1482	G
54	1	1490	A
54	1	1504	A
54	1	1515	A
54	1	1522	A
54	1	1523	U
54	1	1524	G
54	1	1531	C
54	1	1533	C
54	1	1534	U
54	1	1535	A
54	1	1536	C
54	1	1537	G
54	1	1555	G
54	1	1560	G
54	1	1566	A
54	1	1569	A
54	1	1578	U
54	1	1581	G
54	1	1585	C
54	1	1607	C

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Mol	Chain	Res	Type
54	1	1608	A
54	1	1611	C
54	1	1616	A
54	1	1639	C
54	1	1647	U
54	1	1648	U
54	1	1649	G
54	1	1660	G
54	1	1674	G
54	1	1675	C
54	1	1698	A
54	1	1699	G
54	1	1702	G
54	1	1713	A
54	1	1715	G
54	1	1716	U
54	1	1729	U
54	1	1730	C
54	1	1731	G
54	1	1732	C
54	1	1738	G
54	1	1758	U
54	1	1764	C
54	1	1773	A
54	1	1780	A
54	1	1782	U
54	1	1787	A
54	1	1791	A
54	1	1800	C
54	1	1801	A
54	1	1808	A
54	1	1811	G
54	1	1812	U
54	1	1816	C
54	1	1829	A
54	1	1833	C
54	1	1869	G
54	1	1870	C
54	1	1871	A
54	1	1884	G
54	1	1896	G
54	1	1901	A

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Mol	Chain	Res	Type
54	1	1907	G
54	1	1912	A
54	1	1913	A
54	1	1914	C
54	1	1920	C
54	1	1921	G
54	1	1922	G
54	1	1923	U
54	1	1926	U
54	1	1930	G
54	1	1937	A
54	1	1938	A
54	1	1955	U
54	1	1963	U
54	1	1967	C
54	1	1970	A
54	1	1972	G
54	1	1982	U
54	1	1983	G
54	1	1991	U
54	1	1992	G
54	1	1993	U
54	1	1997	C
54	1	2004	G
54	1	2021	C
54	1	2022	U
54	1	2023	C
54	1	2030	A
54	1	2031	A
54	1	2034	U
54	1	2043	C
54	1	2055	C
54	1	2056	G
54	1	2060	A
54	1	2061	G
54	1	2062	A
54	1	2069	G
54	1	2072	C
54	1	2096	C
54	1	2097	A
54	1	2102	G
54	1	2108	A

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Mol	Chain	Res	Type
54	1	2111	U
54	1	2112	G
54	1	2113	U
54	1	2115	G
54	1	2116	G
54	1	2118	U
54	1	2119	A
54	1	2122	U
54	1	2123	G
54	1	2124	G
54	1	2125	G
54	1	2127	G
54	1	2129	C
54	1	2131	U
54	1	2132	U
54	1	2133	G
54	1	2134	A
54	1	2137	U
54	1	2138	G
54	1	2146	C
54	1	2148	G
54	1	2152	G
54	1	2156	G
54	1	2162	G
54	1	2164	C
54	1	2172	U
54	1	2173	A
54	1	2179	C
54	1	2191	A
54	1	2192	U
54	1	2198	A
54	1	2204	G
54	1	2211	A
54	1	2223	G
54	1	2225	A
54	1	2238	G
54	1	2239	G
54	1	2253	G
54	1	2273	A
54	1	2278	A
54	1	2283	C
54	1	2287	A

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Mol	Chain	Res	Type
54	1	2297	A
54	1	2305	U
54	1	2307	G
54	1	2309	A
54	1	2312	U
54	1	2320	U
54	1	2325	G
54	1	2327	A
54	1	2334	U
54	1	2344	U
54	1	2383	G
54	1	2385	C
54	1	2388	A
54	1	2392	A
54	1	2402	U
54	1	2406	A
54	1	2423	U
54	1	2428	G
54	1	2429	G
54	1	2430	A
54	1	2434	A
54	1	2441	U
54	1	2445	G
54	1	2448	A
54	1	2476	A
54	1	2480	C
54	1	2484	G
54	1	2494	G
54	1	2498	C
54	1	2502	G
54	1	2505	G
54	1	2518	A
54	1	2520	C
54	1	2529	G
54	1	2547	A
54	1	2554	U
54	1	2566	A
54	1	2567	G
54	1	2572	A
54	1	2573	C
54	1	2586	U
54	1	2602	A

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Mol	Chain	Res	Type
54	1	2603	G
54	1	2613	U
54	1	2623	G
54	1	2629	U
54	1	2646	C
54	1	2655	G
54	1	2663	G
54	1	2682	A
54	1	2689	U
54	1	2690	U
54	1	2714	G
54	1	2716	C
54	1	2733	A
54	1	2739	U
54	1	2748	A
54	1	2751	G
54	1	2764	A
54	1	2765	A
54	1	2778	A
54	1	2779	U
54	1	2797	U
54	1	2800	A
54	1	2808	G
54	1	2809	A
54	1	2820	A
54	1	2821	A
54	1	2833	U
54	1	2835	A
54	1	2850	A
54	1	2851	A
54	1	2867	G
54	1	2868	A
54	1	2874	C
54	1	2880	C
54	1	2883	A
54	1	2901	C
54	1	2902	C
55	2	4	C
55	2	13	G
55	2	15	A
55	2	35	C
55	2	44	G

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Mol	Chain	Res	Type
55	2	51	G
55	2	66	A
55	2	67	G
55	2	86	G
55	2	88	C
55	2	89	U
55	2	90	C
55	2	108	A
55	2	109	A
56	5	3	G
56	5	4	C
56	5	5	G
56	5	6	A
56	5	9	A
56	5	10	G
56	5	14	A
56	5	18	G
56	5	19	G
56	5	20	U
56	5	25	C
56	5	27	A
56	5	30	G
56	5	41	A
56	5	42	G
56	5	47	U
56	5	52	G
56	5	73	A
56	5	74	C
56	5	76	A
57	6	4	G
57	6	8	U
57	6	9	G
57	6	14	A
57	6	17	C
57	6	18	G
57	6	19	G
57	6	21	A
57	6	22	G
57	6	27	U
57	6	43	A
57	6	46	G
57	6	47	U

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Mol	Chain	Res	Type
57	6	48	C
57	6	49	G
57	6	56	C
57	6	57	A
57	6	61	C
57	6	70	G
57	6	73	A
58	4	6	G
58	4	8	A
58	4	10	G
58	4	12	A

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	3	86	G
53	3	485	U
53	3	845	A
53	3	884	U
53	3	890	G
53	3	1138	G
53	3	1181	G
53	3	1190	G
53	3	1201	A
53	3	1331	G
54	1	490	C
54	1	686	U
54	1	774	G
54	1	858	G
54	1	859	G
54	1	1020	A
54	1	1130	U
54	1	1132	U
54	1	1143	A
54	1	1332	G
54	1	1475	G
54	1	1715	G
54	1	1730	C
54	1	1801	A
54	1	1912	A
54	1	1920	C
54	1	1925	C

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Mol	Chain	Res	Type
54	1	2128	G
54	1	2238	G
54	1	2277	G
54	1	2286	G
54	1	2296	U
54	1	2326	C
54	1	2333	A
54	1	2391	G
54	1	2790	U
54	1	2808	G
55	2	88	C
56	5	2	G
56	5	40	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 ligands 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	$\# Z > 2$
59	FME	1	3001	60	8,9,10	0.64	0	7,9,11	0.96	0
60	PRO	5	101	59,56	5,7,8	0.54	0	7,8,10	1.27	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	1	3001	60	-	2/7/9/11	-
60	PRO	5	101	59,56	-	0/0/9/11	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
60	5	101	PRO	O-C-CA	-2.63	117.89	124.78

There are no chirality outliers.

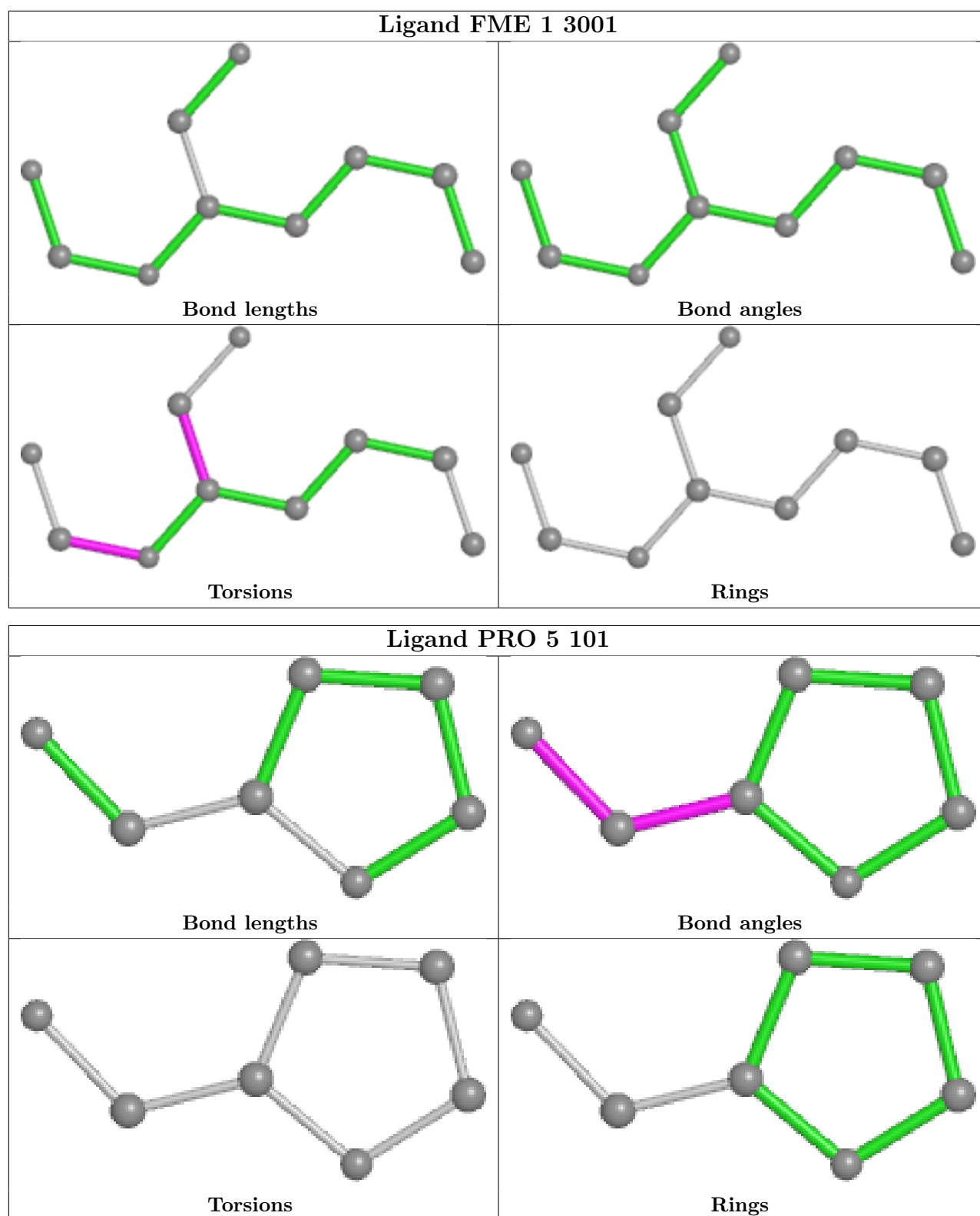
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	1	3001	FME	O1-CN-N-CA
59	1	3001	FME	O-C-CA-CB

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

There are no chain breaks in this entry.

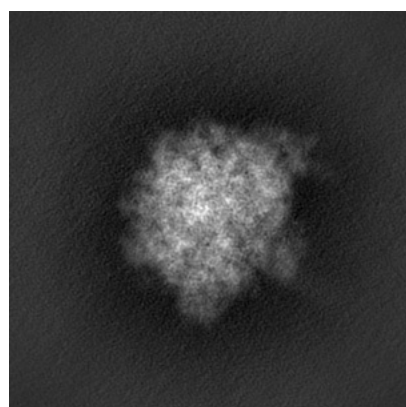
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23528. These allow visual inspection of the internal detail of the map and identification of artifacts.

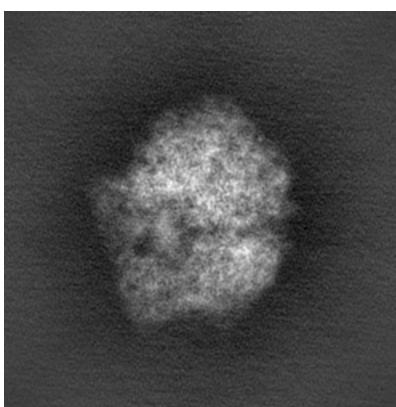
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

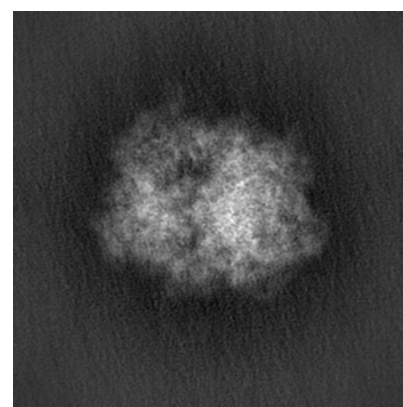
6.1.1 Primary map



X



Y

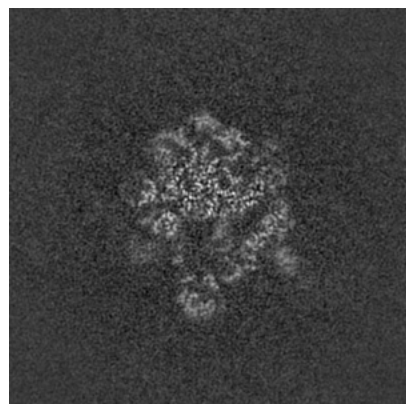


Z

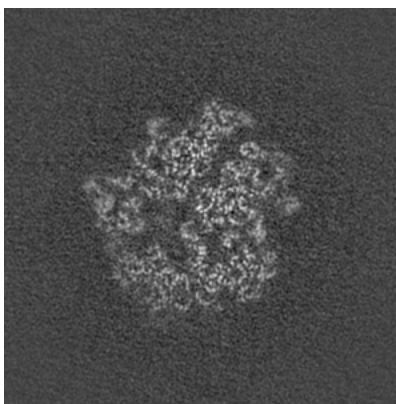
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

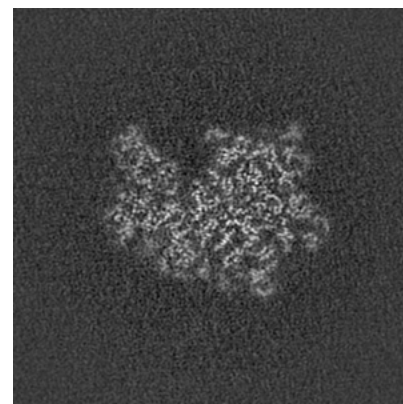
6.2.1 Primary map



X Index: 256



Y Index: 256

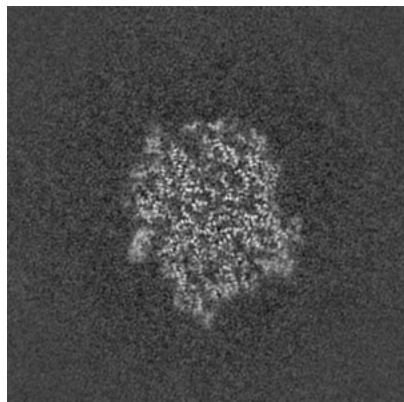


Z Index: 256

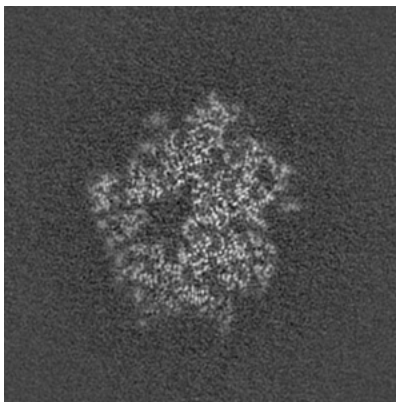
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

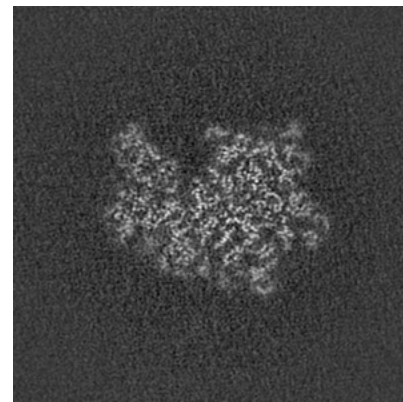
6.3.1 Primary map



X Index: 284



Y Index: 247



Z Index: 256

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 3.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

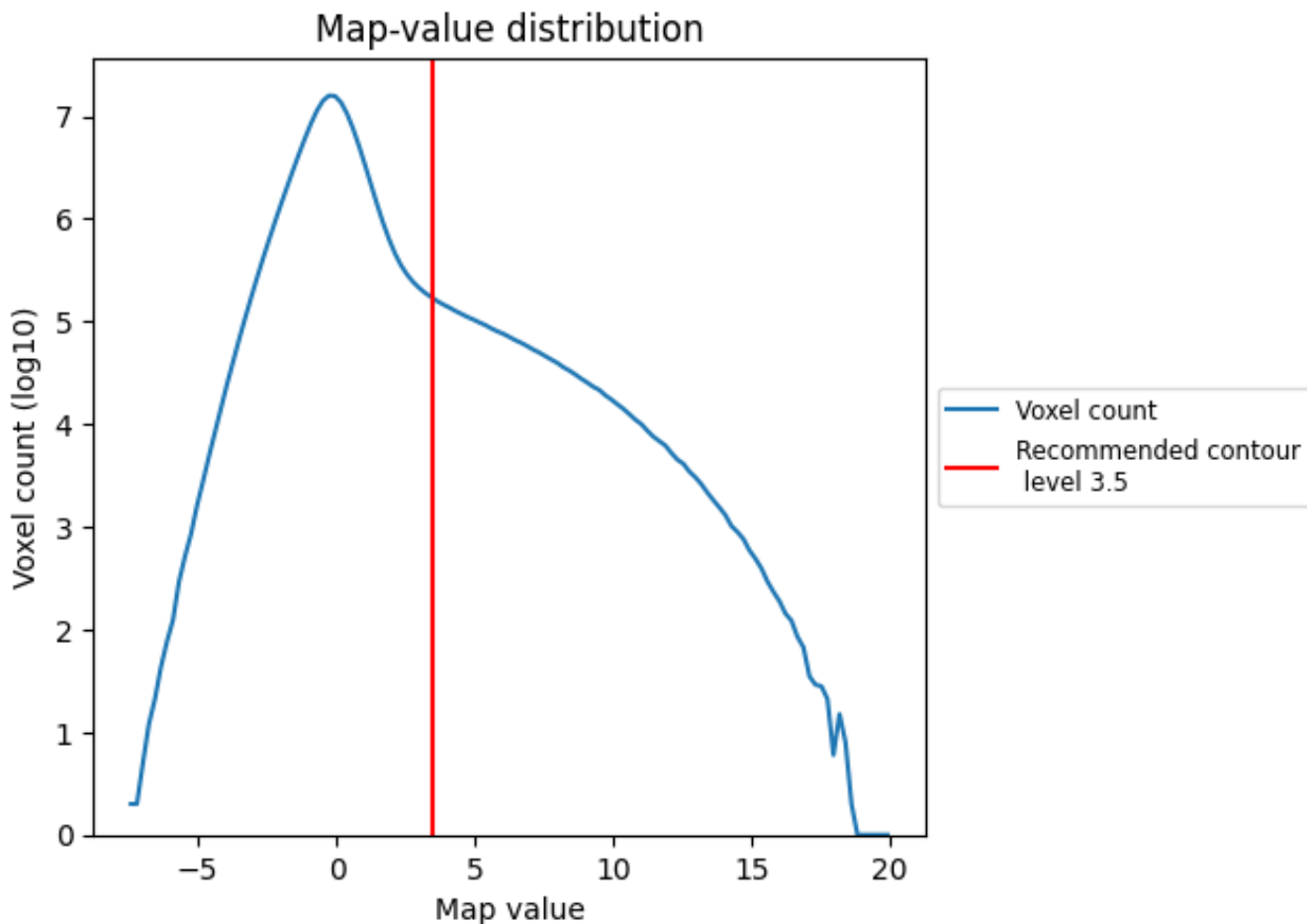
6.5 Mask visualisation

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

7 Map analysis [i](#)

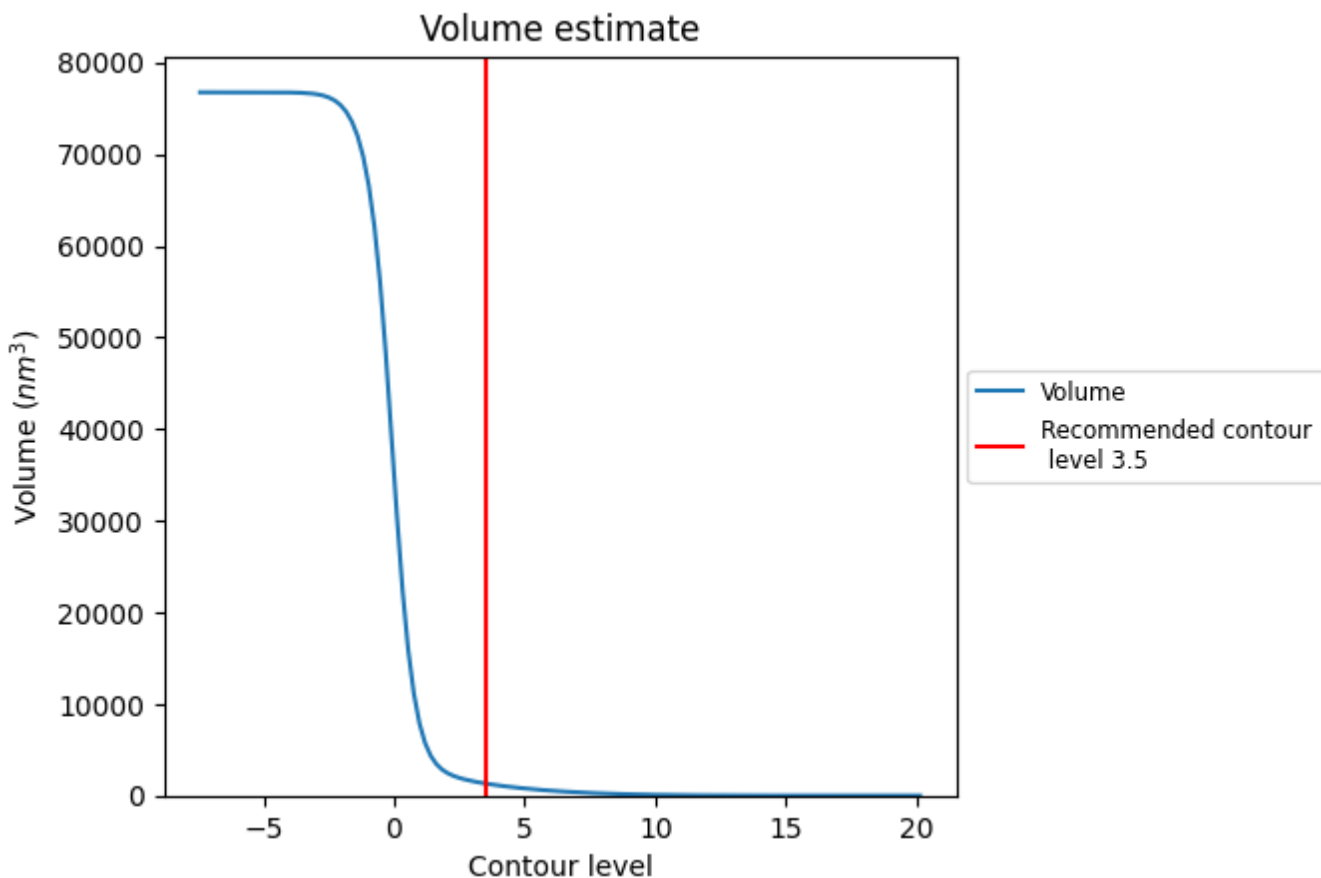
This section contains the results of statistical analysis of the map.

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.

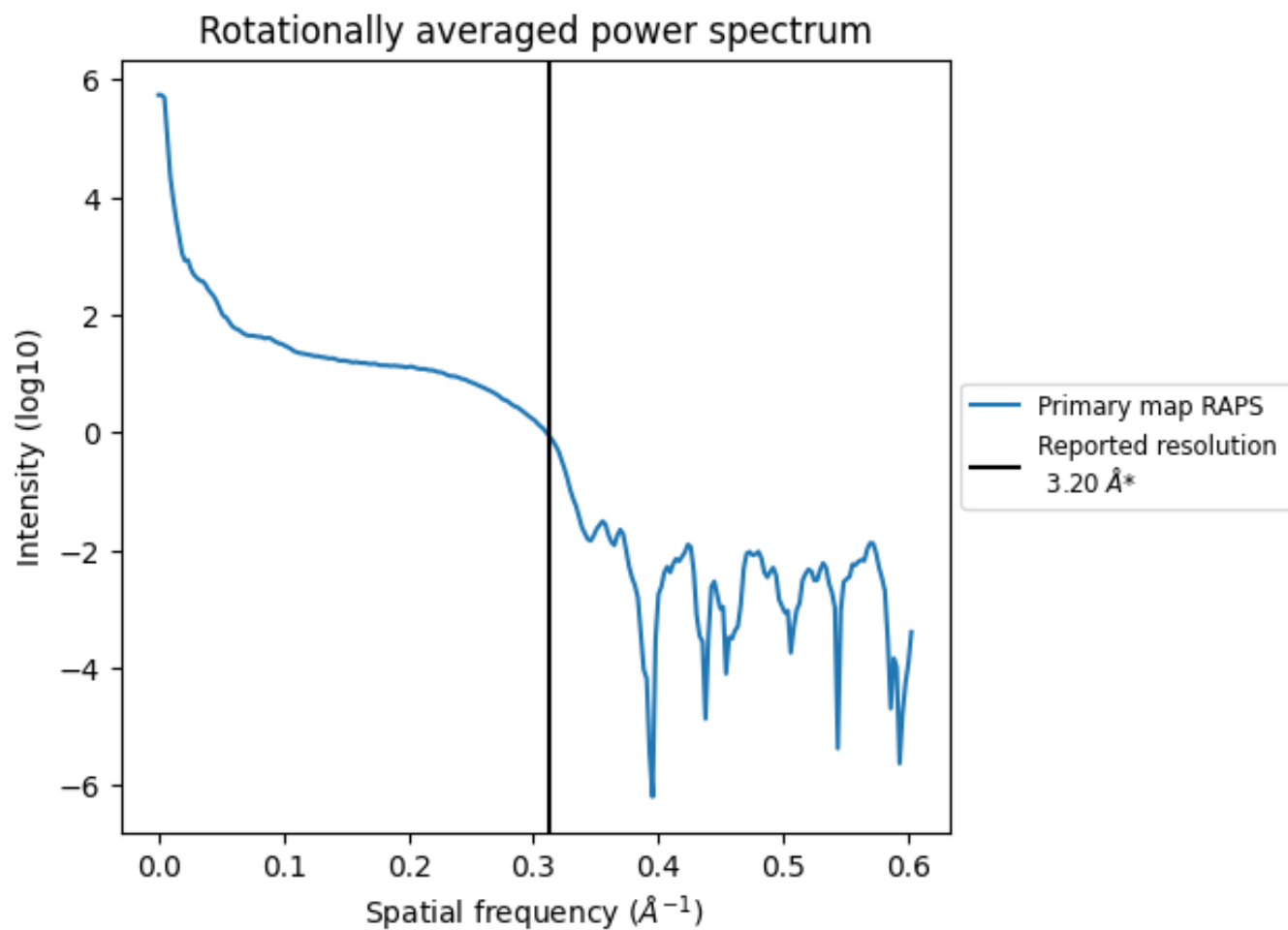
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1314 nm³; this corresponds to an approximate mass of 1187 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 0.312\AA^{-1}

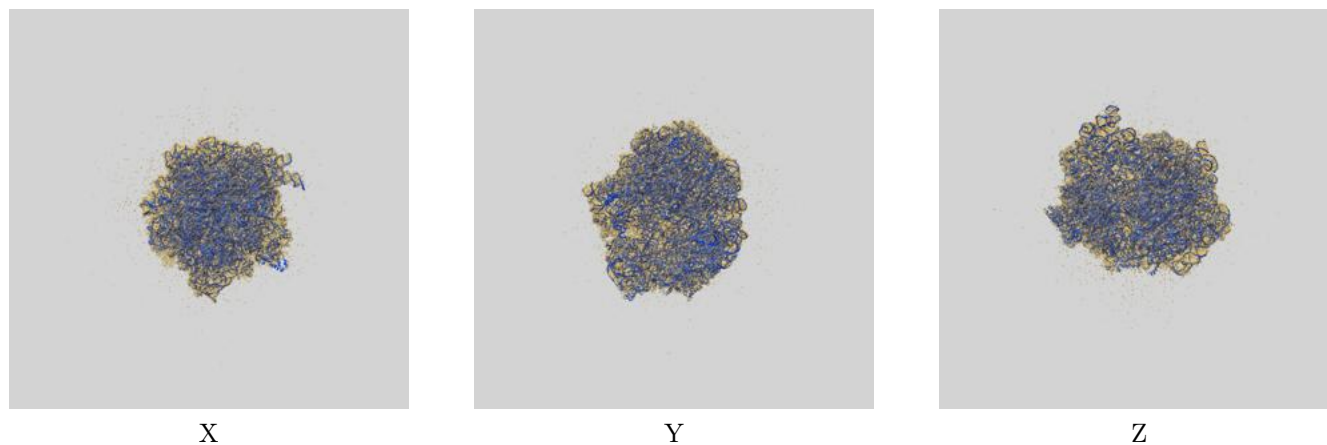
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

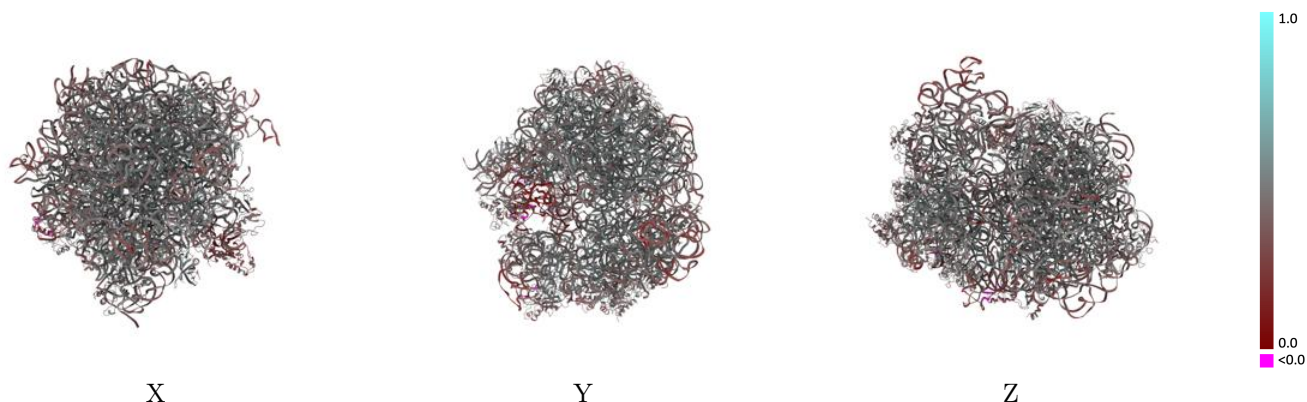
This section contains information regarding the fit between EMDB map EMD-23528 and PDB model 7LV0. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



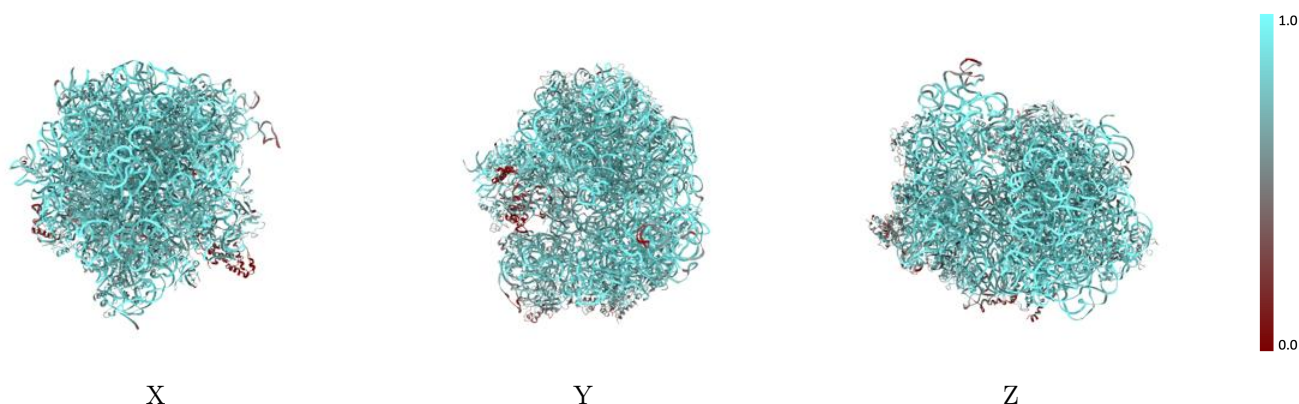
The images above show the 3D surface view of the map at the recommended contour level 3.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



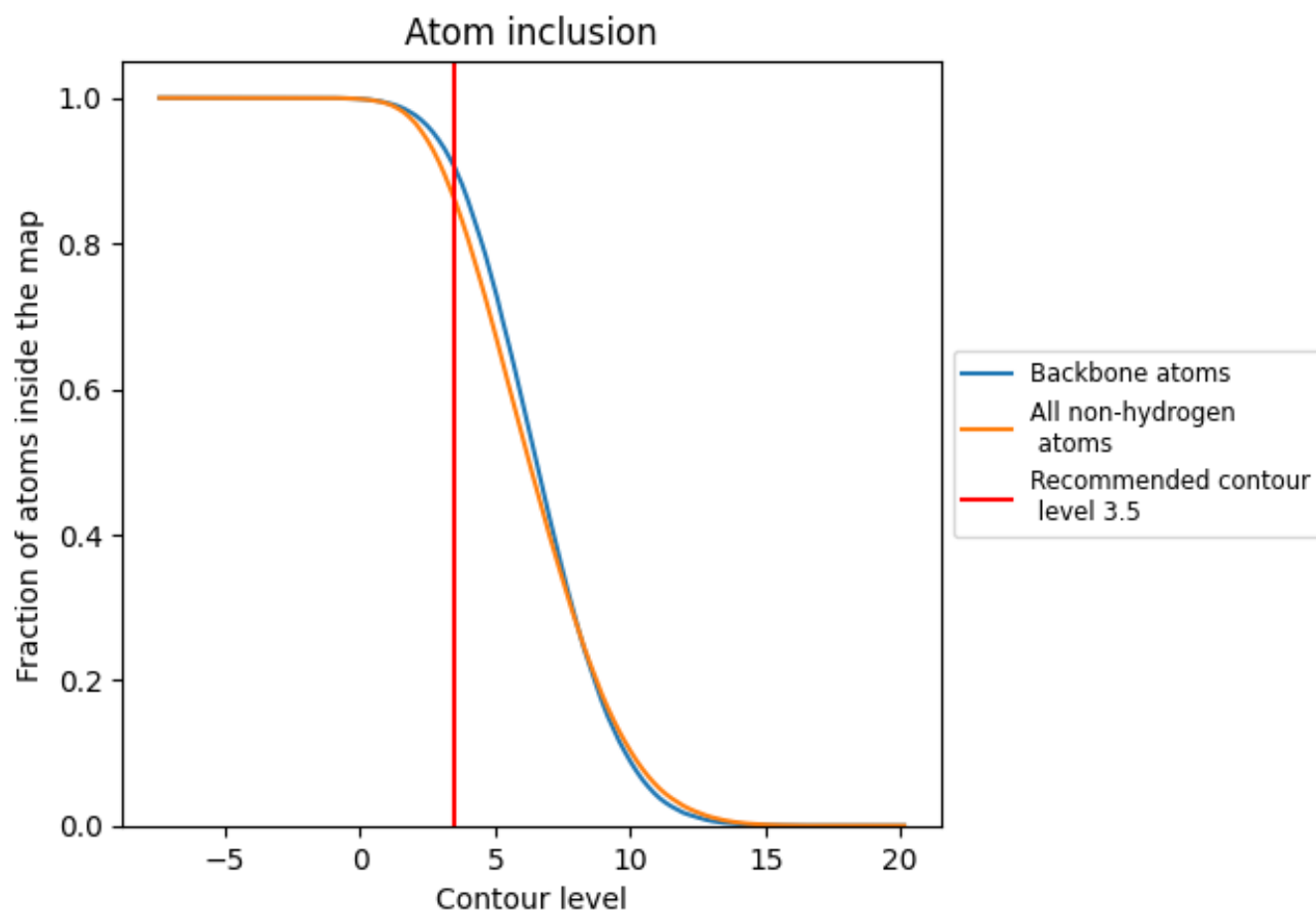
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 86% 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 (3.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8597	 0.4370
1	 0.9273	 0.4380
2	 0.9085	 0.4150
3	 0.9023	 0.4310
4	 0.6572	 0.3070
5	 0.7050	 0.2740
6	 0.9055	 0.3510
A	 0.5706	 0.3670
B	 0.8388	 0.4880
C	 0.7090	 0.4790
D	 0.8901	 0.5110
E	 0.8982	 0.5100
F	 0.8562	 0.5040
G	 0.4845	 0.3990
H	 0.6846	 0.4550
I	 0.6818	 0.4320
J	 0.8026	 0.4770
K	 0.7629	 0.4250
L	 0.6201	 0.4110
M	 0.7917	 0.4840
N	 0.6537	 0.4230
O	 0.5315	 0.4210
P	 0.8475	 0.4650
Q	 0.8654	 0.4790
R	 0.7007	 0.4140
S	 0.7390	 0.4500
T	 0.8551	 0.4610
U	 0.7751	 0.4500
V	 0.8246	 0.4710
W	 0.7922	 0.4580
X	 0.7588	 0.4320
Y	 0.7385	 0.4260
Z	 0.6718	 0.4040
a	 0.3455	 0.2710
b	 0.9172	 0.5150



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Chain	Atom inclusion	Q-score
c	 0.8095	 0.4900
d	 0.7276	 0.4600
e	 0.7140	 0.4080
f	 0.7402	 0.4240
g	 0.5704	 0.4120
h	 0.1073	 0.2860
i	 0.1703	 0.2860
j	 0.8345	 0.4880
k	 0.8403	 0.4870
l	 0.8356	 0.4790
m	 0.8484	 0.4850
n	 0.8440	 0.4870
o	 0.7648	 0.4520
p	 0.8108	 0.4760
q	 0.8458	 0.4830
r	 0.7365	 0.4740
s	 0.7895	 0.4820
t	 0.7884	 0.4660
u	 0.7057	 0.4460
v	 0.7981	 0.4610
w	 0.8497	 0.5050
x	 0.8885	 0.4880
y	 0.7203	 0.4110
z	 0.8032	 0.4840