



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Nov 10, 2016 – 11:46 AM EST

PDB ID : 3JCN
EMDB ID: : EMD-3285
Title : Structures of ribosome-bound initiation factor 2 reveal the mechanism of sub-unit association: Initiation Complex I
Authors : Sprink, T.; Ramrath, D.J.F.; Yamamoto, H.; Yamamoto, K.; Loerke, J.; Ismer, J.; Hildebrand, P.W.; Scheerer, P.; Buerger, J.; Mielke, T.; Spahn, C.M.T.
Deposited on : 2016-01-04
Resolution : 4.60 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
EM map analysis : **NOT EXECUTED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028320

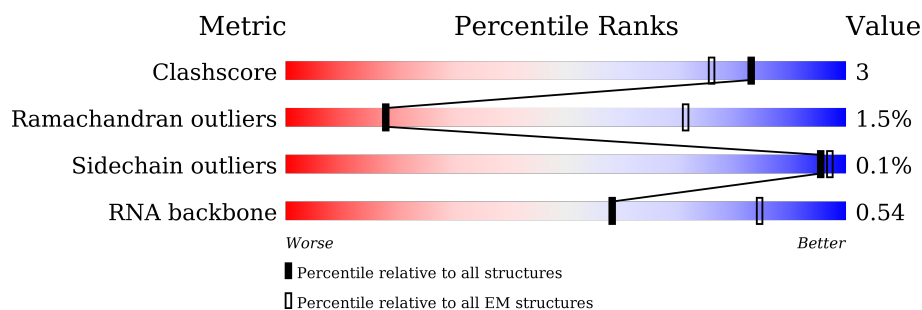
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.60 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.




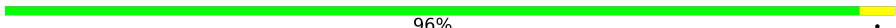

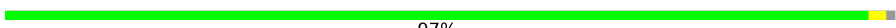









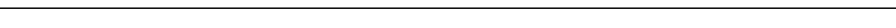

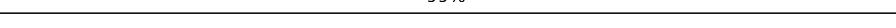
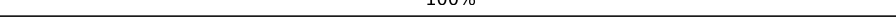


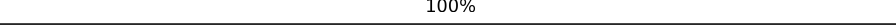


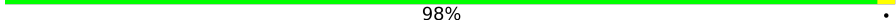
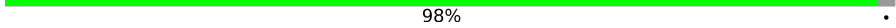

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	0	57	96% ..
2	1	55	87% . 9%
3	2	46	96% .
4	3	65	94% 5% .
5	4	38	97% .
6	A	2904	85% 14% .
7	B	120	87% 12% ..
8	C	273	94% 5% .




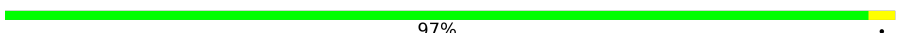











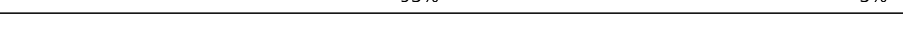
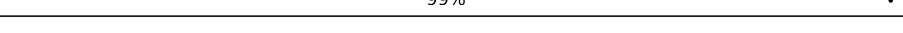




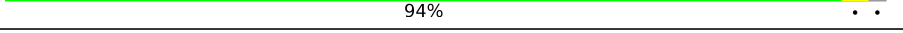
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Mol	Chain	Length	Quality of chain
9	D	209	 94% 6%
10	E	201	 96% .
11	F	179	 92% 7% .
12	G	177	 97% ..
13	H	149	 21% 7% . 70%
14	I	142	 92% 7% .
15	J	142	 93% 6% .
16	K	123	 90% 8% ..
17	L	144	 93% 6% .
18	M	136	 94% 6%
19	N	127	 91% . 6%
20	O	117	 92% 7% .
21	P	115	 97% ..
22	Q	118	 97% ..
23	R	103	 99% .
24	S	110	 100%
25	T	100	 88% 5% 7%
26	U	104	 92% 6% .
27	V	94	 100%
28	W	85	 86% . 11%
29	X	78	 90% 9% .
30	Y	63	 98% .
31	Z	59	 98% .
32	a	1542	 87% 13%
33	b	890	 57% . 43%

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Mol	Chain	Length	Quality of chain
34	c	233	 87% 12%
35	d	241	 88% 10%
36	f	159	 92% 6%
37	g	206	 97%
38	h	179	 84% 16%
39	i	135	 72% 26%
40	j	130	 95%
41	k	130	 98%
42	l	129	 89% 9%
43	m	102	 94%
44	n	118	 96%
45	o	124	 97%
46	p	89	 98%
47	q	101	 93% 5%
48	r	84	 93% 5%
49	s	82	 99%
50	t	92	 86% 14%
51	u	75	 71% 27%
52	v	77	 68% 26% 6%
53	w	71	 69% 28%
54	x	87	 94%
55	z	6	 83% 17%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 147293 atoms, of which 1 is hydrogen 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 L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	2897	Total	C	N	O	P	0	0
			62195	27745	11446	20107	2897		

- Molecule 7 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	119	Total	C	N	O	P	0	0
			2546	1135	466	827	118		

- Molecule 8 is a protein called 50S ribosomal protein L2.

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

- Molecule 9 is a protein called 50S ribosomal protein L3.

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

- Molecule 10 is a protein called 50S ribosomal protein L4.

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

- Molecule 11 is a protein called 50S ribosomal protein L5.

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

- Molecule 12 is a protein called 50S ribosomal protein L6.

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

- Molecule 13 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	44	Total	C	N	O	S	0	0
			328	210	59	58	1		

- Molecule 14 is a protein called 50S ribosomal protein L11.

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

- Molecule 15 is a protein called 50S ribosomal protein L13.

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

- Molecule 16 is a protein called 50S ribosomal protein L14.

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

- Molecule 17 is a protein called 50S ribosomal protein L15.

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

- Molecule 18 is a protein called 50S ribosomal protein L16.

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

- Molecule 19 is a protein called 50S ribosomal protein L17.

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

- Molecule 20 is a protein called 50S ribosomal protein L18.

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

- Molecule 21 is a protein called 50S ribosomal protein L19.

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

- Molecule 22 is a protein called 50S ribosomal protein L20.

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

- Molecule 23 is a protein called 50S ribosomal protein L21.

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

- Molecule 24 is a protein called 50S ribosomal protein L22.

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

- Molecule 25 is a protein called 50S ribosomal protein L23.

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

- Molecule 26 is a protein called 50S ribosomal protein L24.

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

- Molecule 27 is a protein called 50S ribosomal protein L25.

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

- Molecule 28 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	W	76	Total	C	N	O	S	0	0
			575	356	117	101	1		

- Molecule 29 is a protein called 50S ribosomal protein L28.

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

- Molecule 30 is a protein called 50S ribosomal protein L29.

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

- Molecule 31 is a protein called 50S ribosomal protein L30.

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

- Molecule 32 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	a	1539	Total	C	N	O	P	0	0
			33015	14725	6052	10699	1539		

- Molecule 33 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	b	509	Total	C	N	O	S	0	0
			3847	2409	675	748	15		

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S2.

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

- Molecule 36 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	f	150	Total	C	N	O	S	0	0
			1106	687	211	202	6		

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S7.

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

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

- Molecule 40 is a protein called 30S ribosomal protein S9.

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

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	l	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S12.

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

- Molecule 46 is a protein called 30S ribosomal protein S15.

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

- Molecule 47 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	96	Total	C	N	O	S	0	0
			774	483	160	128	3		

- Molecule 48 is a protein called 30S ribosomal protein S17.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

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

- Molecule 50 is a protein called 30S ribosomal protein S19.

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

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	u	55	Total	C	N	O	0	0
			455	288	86	81		

- Molecule 52 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace	
52	v	77	Total	C	N	O	P	S	0	0
			1643	733	297	535	77	1		

- Molecule 53 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	w	51	Total	C	N	O	S	0	0
			425	265	86	73	1		

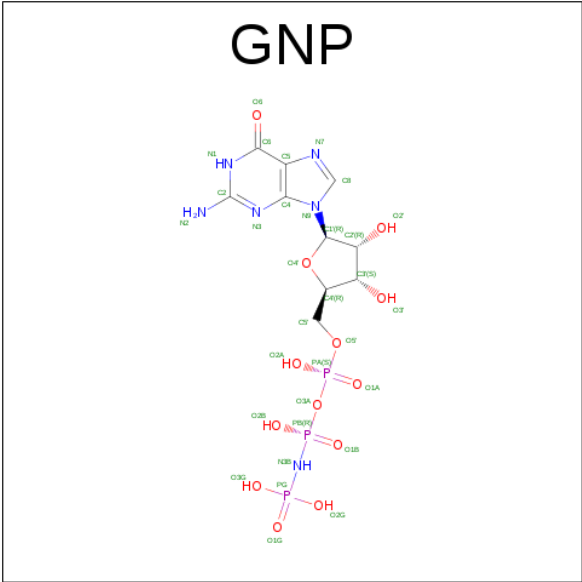
- Molecule 54 is a protein called 30S ribosomal protein S20.

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

- Molecule 55 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

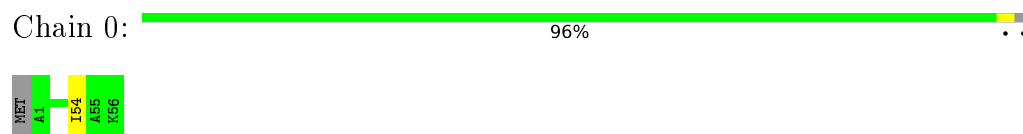
- Molecule 56 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



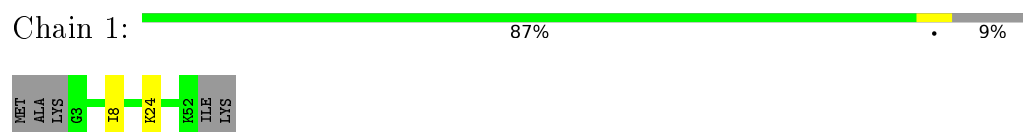
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

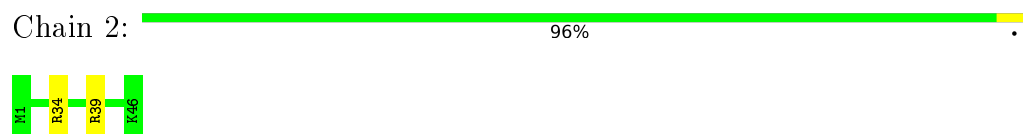
- Molecule 1: 50S ribosomal protein L32



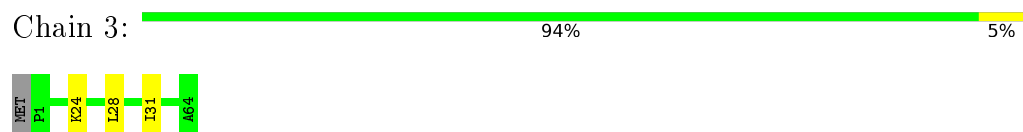
- Molecule 2: 50S ribosomal protein L33



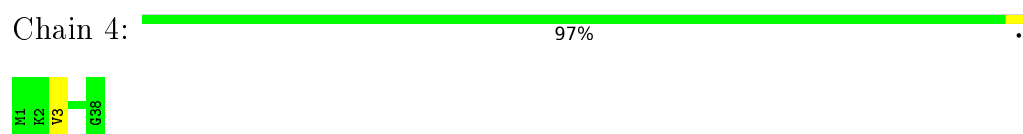
- Molecule 3: 50S ribosomal protein L34



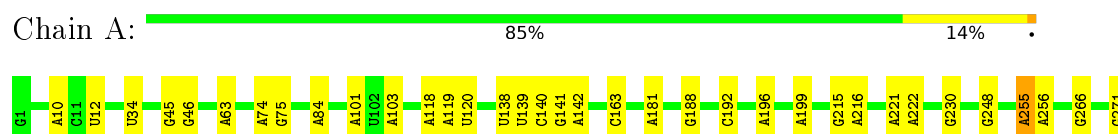
- Molecule 4: 50S ribosomal protein L35

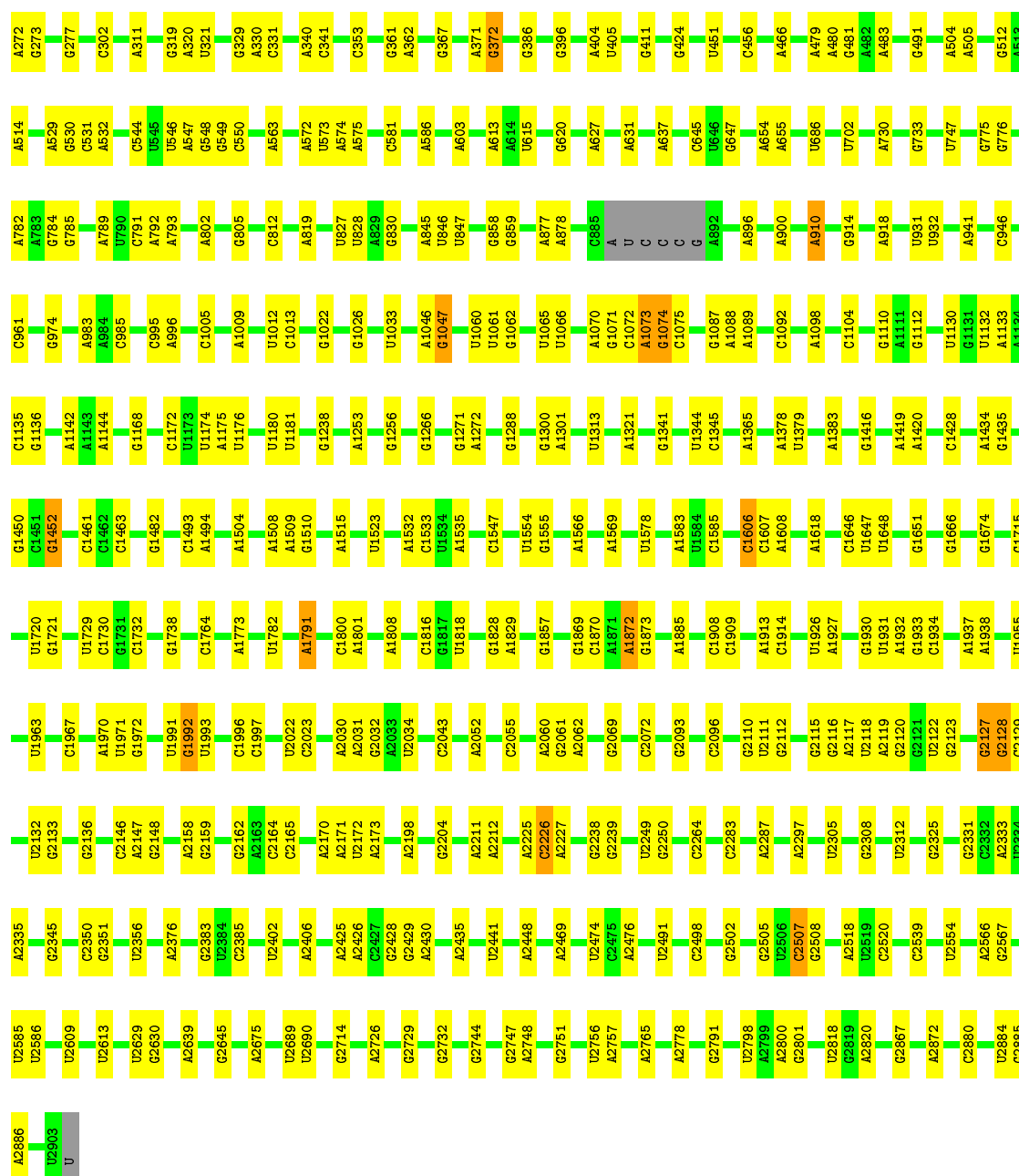


- Molecule 5: 50S ribosomal protein L36



- Molecule 6: 23S ribosomal RNA





• Molecule 7: 5S ribosomal RNA

Chain B: 87% 12% ..

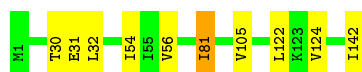


• Molecule 8: 50S ribosomal protein L2

Chain C: 94% 5% •



- Chain J: 93% 6%



- Molecule 16: 50S ribosomal protein L14

Chain K: 90% 8% ..



- Molecule 17: 50S ribosomal protein L15

Chain L: 93% 6% .



- Molecule 18: 50S ribosomal protein L16

Chain M: 94% 6%



- Molecule 19: 50S ribosomal protein L17

Chain N: 91% . 6%



- Molecule 20: 50S ribosomal protein L18

Chain O: 92% 7% .



- Molecule 21: 50S ribosomal protein L19

Chain P: 97% ..



- Molecule 22: 50S ribosomal protein L20

Chain Q: 97% ..



- Molecule 23: 50S ribosomal protein L21

Chain R:  99%




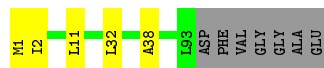
- Molecule 24: 50S ribosomal protein L22

Chain S:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L23

Chain T:  88% 5% 7%



- Molecule 26: 50S ribosomal protein L24

Chain U:  92% 6%



- Molecule 27: 50S ribosomal protein L25

Chain V:  100%


There are no outlier residues recorded for this chain.

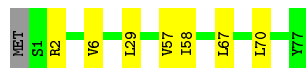
- Molecule 28: 50S ribosomal protein L27

Chain W:  86% 11%



- Molecule 29: 50S ribosomal protein L28

Chain X:  90% 9%



- Molecule 30: 50S ribosomal protein L29

Chain Y:  98%



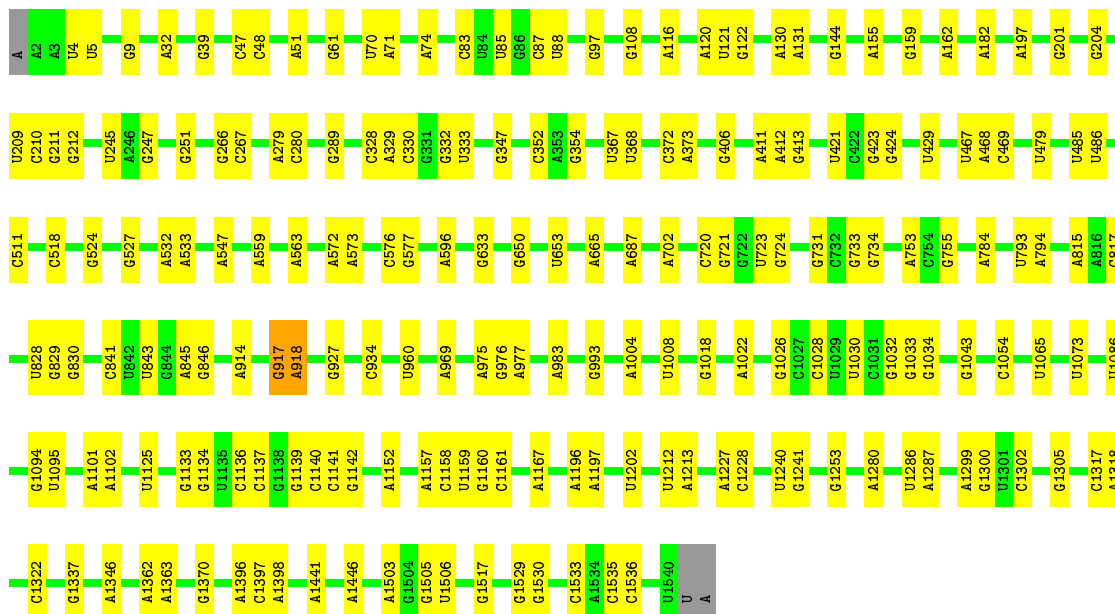
- Molecule 31: 50S ribosomal protein L30

Chain Z: 98%



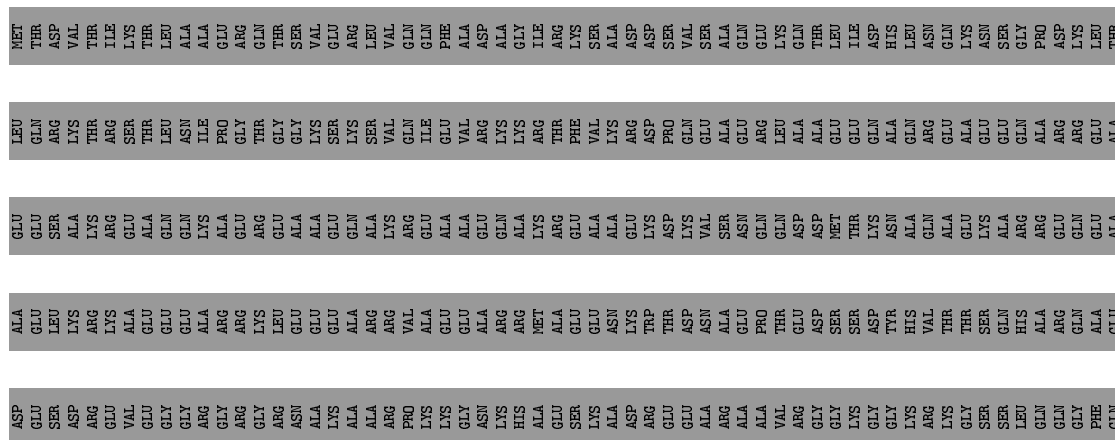
- Molecule 32: 16S ribosomal RNA

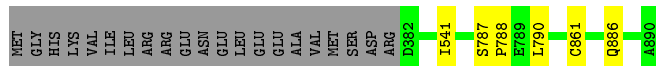
Chain a: 87% 13%



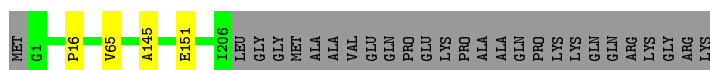
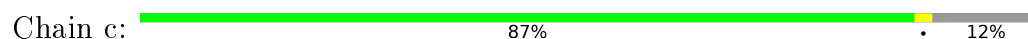
- Molecule 33: Translation initiation factor IF-2

Chain b:  57% . 43%

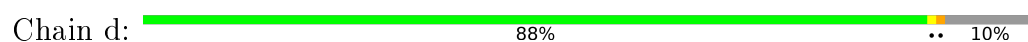




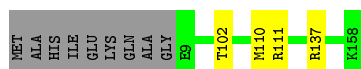
- Molecule 34: 30S ribosomal protein S3



- Molecule 35: 30S ribosomal protein S2



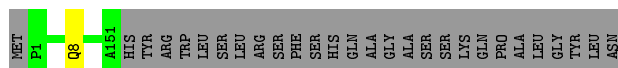
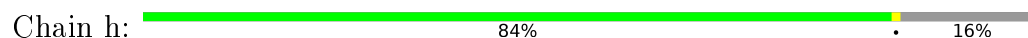
- Molecule 36: 30S ribosomal protein S5



- Molecule 37: 30S ribosomal protein S4



- Molecule 38: 30S ribosomal protein S7



- Molecule 39: 30S ribosomal protein S6



- Molecule 40: 30S ribosomal protein S9





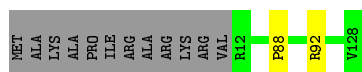
- Molecule 41: 30S ribosomal protein S8

Chain k: 98% ..



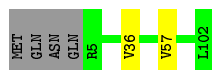
- Molecule 42: 30S ribosomal protein S11

Chain l: 89% • 9%



- Molecule 43: 30S ribosomal protein S10

Chain m: 94% • •



- Molecule 44: 30S ribosomal protein S13

Chain n: 96% • •



- Molecule 45: 30S ribosomal protein S12

Chain o: 97% • •



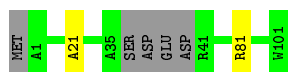
- Molecule 46: 30S ribosomal protein S15

Chain p: 98% • •



- Molecule 47: 30S ribosomal protein S14

Chain q: 93% • 5%



- Molecule 48: 30S ribosomal protein S17

Chain r:  93% 5%




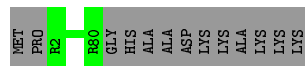
- Molecule 49: 30S ribosomal protein S16

Chain s:  99%



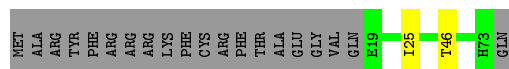
- Molecule 50: 30S ribosomal protein S19

Chain t:  86% 14%



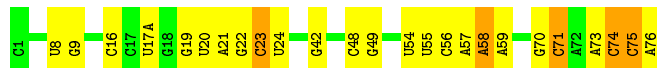
- Molecule 51: 30S ribosomal protein S18

Chain u:  71% 27%



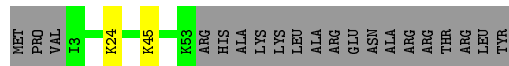
- Molecule 52: tRNA

Chain v:  68% 26% 6%



- Molecule 53: 30S ribosomal protein S21

Chain w:  69% 28%




- Molecule 54: 30S ribosomal protein S20

Chain x:  94%



- Molecule 55: messenger RNA

Chain z:  83% 17%

A13
A14
U15
A16
U17
G18

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	14872	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300, FEI POLARA 300	Depositor
Voltage (kV)	300, 300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20, 20	Depositor
Minimum defocus (nm)	640, 190	Depositor
Maximum defocus (nm)	7180, 7570	Depositor
Magnification	39000, 39000	Depositor
Image detector	GATAN K2 Summit (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, GNP, FME, H2U, 4SU, PSU

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	0	0.44	0/450	0.71	0/599
10	E	0.45	0/1571	0.63	0/2113
11	F	0.49	0/1434	0.69	0/1926
12	G	0.46	0/1343	0.62	0/1816
13	H	0.54	0/331	0.77	0/446
14	I	0.50	0/1046	0.67	0/1410
15	J	0.45	0/1152	0.63	0/1551
16	K	0.45	0/947	0.71	0/1268
17	L	0.47	0/1054	0.72	0/1403
18	M	0.44	0/1093	0.66	0/1460
19	N	0.48	0/973	0.70	0/1301
2	1	0.45	0/416	0.62	0/554
20	O	0.47	0/902	0.72	1/1209 (0.1%)
21	P	0.46	0/929	0.68	0/1242
22	Q	0.48	0/960	0.70	0/1278
23	R	0.43	0/829	0.61	0/1107
24	S	0.43	0/864	0.67	0/1156
25	T	0.44	0/744	0.65	0/994
26	U	0.46	0/787	0.68	0/1051
27	V	0.44	0/766	0.60	0/1025
28	W	0.43	0/582	0.63	0/769
29	X	0.45	0/635	0.64	0/848
3	2	0.46	0/380	0.85	0/498
30	Y	0.47	0/510	0.73	0/677
31	Z	0.44	0/453	0.67	0/605
32	a	0.22	0/36966	0.67	2/57666 (0.0%)
33	b	0.25	0/3895	0.46	1/5264 (0.0%)
34	c	0.47	0/1651	0.66	0/2225
35	d	0.51	0/1735	0.69	0/2338
36	f	0.48	0/1119	0.70	1/1504 (0.1%)
37	g	0.49	0/1665	0.70	0/2227
38	h	0.48	0/1195	0.68	0/1602

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
39	i	0.50	0/835	0.72	0/1128
4	3	0.44	0/513	0.69	0/676
40	j	0.51	0/1034	0.81	0/1375
41	k	0.44	0/989	0.64	0/1326
42	l	0.47	0/893	0.65	0/1205
43	m	0.48	0/797	0.72	0/1077
44	n	0.48	0/892	0.73	0/1193
45	o	0.46	0/969	0.72	0/1300
46	p	0.47	0/722	0.69	0/964
47	q	0.49	0/785	0.78	0/1043
48	r	0.49	0/657	0.72	0/881
49	s	0.47	0/659	0.71	0/884
5	4	0.42	0/303	0.74	0/397
50	t	0.48	0/652	0.67	0/877
51	u	0.51	0/462	0.73	0/621
52	v	0.24	0/1746	0.89	7/2721 (0.3%)
53	w	0.54	0/430	0.77	0/570
54	x	0.46	0/671	0.66	0/888
55	z	1.38	2/144 (1.4%)	3.79	20/222 (9.0%)
6	A	0.21	0/69659	0.67	2/108672 (0.0%)
7	B	0.21	0/2847	0.67	0/4440
8	C	0.46	0/2121	0.71	0/2852
9	D	0.45	0/1586	0.63	0/2134
All	All	0.31	2/159743 (0.0%)	0.68	34/238578 (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
13	H	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	z	17	U	O3'-P	-8.60	1.50	1.61
55	z	14	A	O3'-P	-5.66	1.54	1.61

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	z	15	U	O5'-P-OP2	-31.31	73.13	110.70
55	z	15	U	O5'-P-OP1	25.32	141.08	110.70
55	z	15	U	OP1-P-OP2	-13.41	99.49	119.60
55	z	14	A	P-O3'-C3'	-11.88	105.44	119.70
55	z	14	A	C2'-C3'-O3'	11.04	133.78	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	H	11	ASN	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	444	0	461	0	0
2	1	409	0	440	1	0
3	2	377	0	418	2	0
4	3	504	0	574	2	0
5	4	302	0	343	1	0
6	A	62195	0	31280	39	0
7	B	2546	0	1292	3	0
8	C	2082	0	2157	5	0
9	D	1565	0	1616	8	0
10	E	1552	0	1619	7	0
11	F	1410	0	1447	7	0
12	G	1323	0	1374	6	0
13	H	328	0	357	3	0
14	I	1032	0	1088	4	0
15	J	1129	0	1162	6	0
16	K	938	0	1012	7	0
17	L	1045	0	1117	3	0
18	M	1074	0	1157	3	0
19	N	960	0	1000	2	0
20	O	892	0	923	4	0
21	P	917	0	965	2	0
22	Q	947	0	1022	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	R	816	0	839	0	0
24	S	857	0	922	0	0
25	T	738	0	807	2	0
26	U	779	0	834	2	0
27	V	753	0	780	0	0
28	W	575	0	589	2	0
29	X	625	0	655	4	0
30	Y	509	0	543	0	0
31	Z	449	0	491	0	0
32	a	33015	0	16617	0	0
33	b	3847	0	3909	0	0
34	c	1624	0	1699	0	0
35	d	1704	0	1732	0	0
36	f	1106	0	1148	0	0
37	g	1643	0	1710	0	0
38	h	1181	0	1240	0	0
39	i	817	0	808	0	0
40	j	1022	0	1070	0	0
41	k	979	0	1034	0	0
42	l	877	0	887	0	0
43	m	787	0	828	0	0
44	n	883	0	944	0	0
45	o	955	0	1019	0	0
46	p	714	0	737	0	0
47	q	774	0	827	0	0
48	r	648	0	691	0	0
49	s	649	0	666	0	0
50	t	637	0	665	0	0
51	u	455	0	478	0	0
52	v	1643	0	835	0	0
53	w	425	0	449	0	0
54	x	665	0	714	0	0
55	z	129	0	65	0	0
56	b	32	0	13	0	0
57	v	9	1	10	0	0
All	All	147292	1	100079	111	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 111 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:G:176:LYS:HD3	12:G:176:LYS:OXT	1.48	1.14
12:G:176:LYS:CD	12:G:176:LYS:OXT	2.30	0.77
11:F:11:VAL:HG22	11:F:171:ALA:HB1	1.72	0.70
12:G:176:LYS:C	12:G:176:LYS:HD3	2.12	0.70
6:A:574:A:N6	6:A:2034:U:OP1	2.33	0.62

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	51 (94%)	2 (4%)	1 (2%)	10	53
2	1	48/55 (87%)	44 (92%)	4 (8%)	0	100	100
3	2	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
4	3	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
5	4	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
8	C	269/273 (98%)	248 (92%)	17 (6%)	4 (2%)	13	58
9	D	207/209 (99%)	189 (91%)	15 (7%)	3 (1%)	14	59
10	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
11	F	175/179 (98%)	161 (92%)	12 (7%)	2 (1%)	17	64
12	G	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
13	H	42/149 (28%)	29 (69%)	6 (14%)	7 (17%)	0	5
14	I	139/142 (98%)	113 (81%)	21 (15%)	5 (4%)	4	40
15	J	140/142 (99%)	136 (97%)	3 (2%)	1 (1%)	26	71
16	K	120/123 (98%)	112 (93%)	6 (5%)	2 (2%)	11	56
17	L	141/144 (98%)	118 (84%)	19 (14%)	4 (3%)	6	46
18	M	134/136 (98%)	125 (93%)	7 (5%)	2 (2%)	13	58

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	N	118/127 (93%)	110 (93%)	7 (6%)	1 (1%)	24	69
20	O	114/117 (97%)	106 (93%)	7 (6%)	1 (1%)	21	67
21	P	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
22	Q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
23	R	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	19	65
24	S	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
25	T	91/100 (91%)	84 (92%)	6 (7%)	1 (1%)	17	64
26	U	100/104 (96%)	90 (90%)	7 (7%)	3 (3%)	5	44
27	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
28	W	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
29	X	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
30	Y	61/63 (97%)	52 (85%)	8 (13%)	1 (2%)	12	57
31	Z	56/59 (95%)	56 (100%)	0	0	100	100
33	b	507/890 (57%)	488 (96%)	17 (3%)	2 (0%)	39	80
34	c	204/233 (88%)	181 (89%)	20 (10%)	3 (2%)	13	58
35	d	216/241 (90%)	189 (88%)	22 (10%)	5 (2%)	8	50
36	f	148/159 (93%)	127 (86%)	18 (12%)	3 (2%)	9	53
37	g	203/206 (98%)	186 (92%)	11 (5%)	6 (3%)	5	44
38	h	149/179 (83%)	138 (93%)	10 (7%)	1 (1%)	26	71
39	i	98/135 (73%)	82 (84%)	13 (13%)	3 (3%)	5	44
40	j	125/130 (96%)	107 (86%)	14 (11%)	4 (3%)	5	43
41	k	127/130 (98%)	117 (92%)	8 (6%)	2 (2%)	12	57
42	l	115/129 (89%)	101 (88%)	12 (10%)	2 (2%)	11	56
43	m	96/102 (94%)	85 (88%)	9 (9%)	2 (2%)	9	52
44	n	112/118 (95%)	106 (95%)	5 (4%)	1 (1%)	21	67
45	o	121/124 (98%)	106 (88%)	12 (10%)	3 (2%)	7	48
46	p	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	16	62
47	q	92/101 (91%)	75 (82%)	15 (16%)	2 (2%)	8	51
48	r	78/84 (93%)	66 (85%)	10 (13%)	2 (3%)	7	47
49	s	80/82 (98%)	71 (89%)	8 (10%)	1 (1%)	15	60
50	t	77/92 (84%)	70 (91%)	7 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	u	53/75 (71%)	50 (94%)	1 (2%)	2 (4%)	4	38
53	w	49/71 (69%)	40 (82%)	7 (14%)	2 (4%)	3	36
54	x	83/87 (95%)	79 (95%)	1 (1%)	3 (4%)	4	40
All	All	6020/6866 (88%)	5514 (92%)	417 (7%)	89 (2%)	18	58

5 of 89 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	C	121	ALA
9	D	151	THR
11	F	173	ASP
13	H	31	VAL
13	H	33	GLN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	45 (100%)	0	100	100
3	2	38/38 (100%)	38 (100%)	0	100	100
4	3	51/52 (98%)	51 (100%)	0	100	100
5	4	34/34 (100%)	34 (100%)	0	100	100
8	C	216/218 (99%)	216 (100%)	0	100	100
9	D	164/164 (100%)	164 (100%)	0	100	100
10	E	165/165 (100%)	165 (100%)	0	100	100
11	F	148/150 (99%)	148 (100%)	0	100	100
12	G	137/138 (99%)	137 (100%)	0	100	100
13	H	35/114 (31%)	35 (100%)	0	100	100
14	I	109/110 (99%)	109 (100%)	0	100	100
15	J	116/116 (100%)	115 (99%)	1 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	K	103/104 (99%)	103 (100%)	0	100	100
17	L	102/103 (99%)	102 (100%)	0	100	100
18	M	109/109 (100%)	109 (100%)	0	100	100
19	N	100/103 (97%)	100 (100%)	0	100	100
20	O	86/87 (99%)	86 (100%)	0	100	100
21	P	99/100 (99%)	99 (100%)	0	100	100
22	Q	89/90 (99%)	89 (100%)	0	100	100
23	R	84/84 (100%)	84 (100%)	0	100	100
24	S	93/93 (100%)	93 (100%)	0	100	100
25	T	80/84 (95%)	80 (100%)	0	100	100
26	U	83/85 (98%)	83 (100%)	0	100	100
27	V	78/78 (100%)	78 (100%)	0	100	100
28	W	56/63 (89%)	56 (100%)	0	100	100
29	X	67/68 (98%)	67 (100%)	0	100	100
30	Y	55/55 (100%)	55 (100%)	0	100	100
31	Z	48/49 (98%)	48 (100%)	0	100	100
33	b	409/713 (57%)	406 (99%)	3 (1%)	88	94
34	c	170/190 (90%)	169 (99%)	1 (1%)	90	95
35	d	180/199 (90%)	178 (99%)	2 (1%)	80	91
36	f	113/119 (95%)	113 (100%)	0	100	100
37	g	172/173 (99%)	172 (100%)	0	100	100
38	h	124/147 (84%)	124 (100%)	0	100	100
39	i	87/116 (75%)	87 (100%)	0	100	100
40	j	105/107 (98%)	105 (100%)	0	100	100
41	k	104/105 (99%)	104 (100%)	0	100	100
42	l	90/99 (91%)	90 (100%)	0	100	100
43	m	86/90 (96%)	86 (100%)	0	100	100
44	n	92/96 (96%)	92 (100%)	0	100	100
45	o	103/104 (99%)	103 (100%)	0	100	100
46	p	76/77 (99%)	76 (100%)	0	100	100
47	q	79/84 (94%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
48	r	74/78 (95%)	74 (100%)	0	100	100
49	s	65/65 (100%)	65 (100%)	0	100	100
50	t	70/79 (89%)	70 (100%)	0	100	100
51	u	48/65 (74%)	48 (100%)	0	100	100
53	w	44/61 (72%)	44 (100%)	0	100	100
54	x	65/66 (98%)	65 (100%)	0	100	100
All	All	4993/5584 (89%)	4986 (100%)	7 (0%)	95	97

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
33	b	861	CYS
35	d	219	THR
34	c	151	GLU
33	b	541	ILE
35	d	19	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
33	b	399	HIS
33	b	448	HIS
44	n	104	ASN
33	b	426	GLN
10	E	90	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
32	a	1538/1542 (99%)	197 (12%)	0
52	v	76/77 (98%)	25 (32%)	0
55	z	5/6 (83%)	2 (40%)	0
6	A	2895/2904 (99%)	365 (12%)	20 (0%)
7	B	118/120 (98%)	11 (9%)	0
All	All	4632/4649 (99%)	600 (12%)	20 (0%)

5 of 600 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	10	A
6	A	12	U
6	A	34	U
6	A	45	G
6	A	46	G

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1180	U
6	A	1288	G
6	A	2127	G
6	A	995	C
6	A	1061	U

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

4 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	$\# Z > 2$
52	H2U	v	20	52	17,21,22	0.80	0	23,30,33	1.33	5 (21%)
52	5MU	v	54	52	13,22,23	0.77	0	16,32,35	2.62	2 (12%)
52	PSU	v	55	52	15,21,22	1.39	1 (6%)	16,30,33	2.38	5 (31%)
52	4SU	v	8	52	12,21,22	1.14	2 (16%)	15,30,33	1.88	6 (40%)

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
52	H2U	v	20	52	-	0/7/38/39	0/2/2/2
52	5MU	v	54	52	-	0/3/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
52	PSU	v	55	52	-	0/7/25/26	0/2/2/2
52	4SU	v	8	52	-	0/3/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	v	55	PSU	C5-C1'	-4.41	1.48	1.52
52	v	8	4SU	C2-N3	-2.17	1.33	1.38
52	v	8	4SU	O4'-C1'	2.56	1.44	1.41

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	v	54	5MU	C5-C4-N3	-7.47	119.08	125.35
52	v	55	PSU	C5-C6-N1	-3.74	119.16	124.38
52	v	8	4SU	C5-C4-N3	-3.41	119.94	123.56
52	v	55	PSU	C5-C1'-C2'	-3.21	109.99	115.44
52	v	20	H2U	C4-N3-C2	-2.64	123.38	125.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates 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
56	GNP	b	901	-	29,34,34	4.63	11 (37%)	28,54,54	1.38	4 (14%)
57	FME	v	101	52	8,8,10	0.40	0	8,8,11	1.48	2 (25%)

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
56	GNP	b	901	-	-	0/16/38/38	0/3/3/3
57	FME	v	101	52	-	0/7/7/11	0/0/0/0

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	b	901	GNP	C4-N9	-10.36	1.33	1.47
56	b	901	GNP	C8-N9	-3.77	1.35	1.47
56	b	901	GNP	PB-O2B	-3.11	1.48	1.56
56	b	901	GNP	PG-O3G	-3.08	1.48	1.56
56	b	901	GNP	C5-C6	-2.41	1.48	1.53

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	b	901	GNP	PA-O3A-PB	-3.41	120.33	132.71
57	v	101	FME	CA-N-CN	-2.67	120.67	124.12
57	v	101	FME	O1-CN-N	-2.64	120.75	124.80
56	b	901	GNP	C3'-C2'-C1'	2.25	105.96	101.44
56	b	901	GNP	C4-C5-N7	2.47	106.52	102.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.