wwPDB EM Validation Summary Report (i)

Mar 6, 2025 – 06:22 pm GMT

PDB ID	:	8PEG
EMDB ID	:	EMD-17631
Title	:	Escherichia coli paused disome complex (queueing 70S non-rotated closed PRE state)
Authors	:	Fluegel, T.; Schacherl, M.
Deposited on	:	2023-06-13
Resolution	:	3.30 Å(reported)
Based on initial model	:	7N1P

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

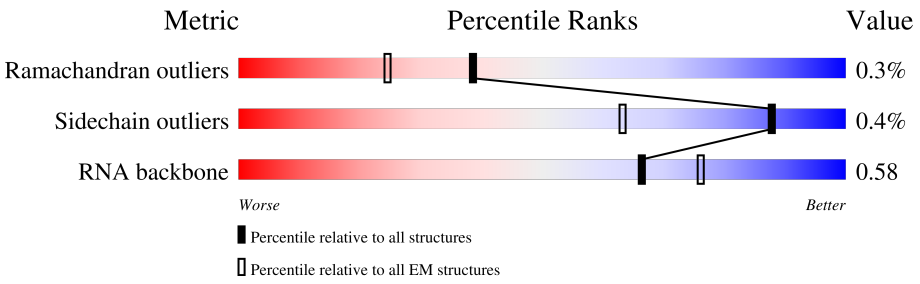
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 3.30 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	0	38	100%
2	1	78	96% • •
3	2	63	98% •
4	3	59	93% 5% •
5	4	70	94% • •
6	5	57	98% •
7	6	65	98% •
8	7	2903	81% 19% •
9	8	120	85% 13% •

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Mol	Chain	Length	Quality of chain
10	A	1542	81% 18%
11	B	241	93% 7%
12	C	233	90% 9%
13	D	206	99%
14	E	167	95% 5%
15	F	135	79% 21%
16	G	179	86% 13%
17	H	130	99%
18	I	130	98%
19	J	103	96%
20	K	129	88% 9%
21	L	124	99%
22	M	118	95%
23	N	101	99%
24	O	89	97%
25	P	82	99%
26	Q	84	95% 5%
27	R	75	96%
28	S	92	90% 10%
29	T	87	97%
30	U	71	99%
31	V	30	50% 50%
32	W	76	58% 33% 9%
33	X	78	63% 33%
34	Y	76	57% 37% 7%

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Mol	Chain	Length	Quality of chain
35	Z	557	31% 69%
36	a	234	57% 43%
37	b	273	99%
38	c	209	100%
39	d	201	100%
40	e	179	98%
41	f	177	98%
42	g	55	95% 5%
43	h	136	99%
44	i	149	99%
45	j	165	81% 18%
46	k	142	94% 6%
47	l	46	100%
48	m	142	100%
49	n	123	100%
50	o	144	100%
51	p	18	100%
52	q	127	94% 6%
53	r	117	97%
54	s	115	99%
55	t	118	99%
56	u	103	99%
57	v	110	99%
58	w	100	93% 7%
59	x	104	97%

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Mol	Chain	Length	Quality of chain
60	y	94	100%
61	z	85	99%

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 153284 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 L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	38	302	185	65	48	4	0	0

- Molecule 2 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	77	625	388	129	106	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	63	509	313	99	95	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	58	449	281	87	79	2	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	67	529	328	100	95	6	0	0

- Molecule 6 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	56	444	269	94	80	1	0	0

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	6	64	504	323	105	74	2	0	0

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	7	2903	62335	27815	11467	20150	2903	0	0

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	8	120	2569	1144	468	837	120	0	0

- Molecule 10 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
10	A	1542	33092	14767	6064	10719	1542	0	0

- Molecule 11 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	B	224	1751	1108	314	321	8	0	0

- Molecule 12 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	C	212	1658	1049	311	294	4	0	0

- Molecule 13 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	E	158	1166	725	220	215	6	0	0

- Molecule 15 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	F	106	862	545	156	154	7	0	0

- Molecule 16 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	G	155	1228	767	237	220	4	0	0

- Molecule 17 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 18 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 19 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	J	100	803	502	154	146	1	0	0

- Molecule 20 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	K	118	884	545	175	161	3	0	0

- Molecule 21 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 22 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	M	115	891	552	179	157	3	0	0

- Molecule 23 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 24 is a protein called 30S ribosomal protein S15.

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

- Molecule 25 is a protein called 30S ribosomal protein S16.

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

- Molecule 26 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 27 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	R	74	624	395	122	105	2	0	0

- Molecule 28 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	S	83	663	424	126	111	2	0	0

- Molecule 29 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	T	86	670	414	138	115	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	U	70	584	363	122	98	1	0	0

- Molecule 31 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
31	V	30	648	290	124	204	30	0	0

- Molecule 32 is a RNA chain called tRNA-Phe (P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
32	W	76	1632	731	289	534	76	2	0	0

- Molecule 33 is a RNA chain called tRNA-Ser (E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
33	X	78	1683	750	304	548	78	3	0	0

- Molecule 34 is a RNA chain called tRNA-Val (A-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
34	Y	76	1631	728	292	534	76	1	0	0

- Molecule 35 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
35	Z	170	1319	830	228	261	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	a	134	1026	645	186	193	2	0	0

- Molecule 37 is a protein called 50S ribosomal protein L2.

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

- Molecule 38 is a protein called 50S ribosomal protein L3.

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

- Molecule 39 is a protein called 50S ribosomal protein L4.

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

- Molecule 40 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	e	178	1420	905	251	258	6	0	0

- Molecule 41 is a protein called 50S ribosomal protein L6.

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

- Molecule 42 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	g	52	427	275	78	74	0	0

- Molecule 43 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	h	136	1085	692	209	178	6	1	0

- Molecule 44 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	i	149	1110	699	197	213	1	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	j	135	1023	648	179	192	4	0	0

- Molecule 46 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	k	134	979	619	169	185	6	0	0

- Molecule 47 is a protein called 50S ribosomal protein L34.

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

- Molecule 48 is a protein called 50S ribosomal protein L13.

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

- Molecule 49 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	n	123	946	593	181	166	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	o	144	1053	654	207	190	2	0	0

- Molecule 51 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
51	p	18	101	63	18	20	0	0

- Molecule 52 is a protein called 50S ribosomal protein L17.

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

- Molecule 53 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
53	r	116	891	552	178	161	0	0

- Molecule 54 is a protein called 50S ribosomal protein L19.

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

- Molecule 55 is a protein called 50S ribosomal protein L20.

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

- Molecule 56 is a protein called 50S ribosomal protein L21.

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

- Molecule 57 is a protein called 50S ribosomal protein L22.

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

- Molecule 58 is a protein called 50S ribosomal protein L23.

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

- Molecule 59 is a protein called 50S ribosomal protein L24.

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

- Molecule 60 is a protein called 50S ribosomal protein L25.

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

- Molecule 61 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
61	z	84	634	391	129	113	1	0	0

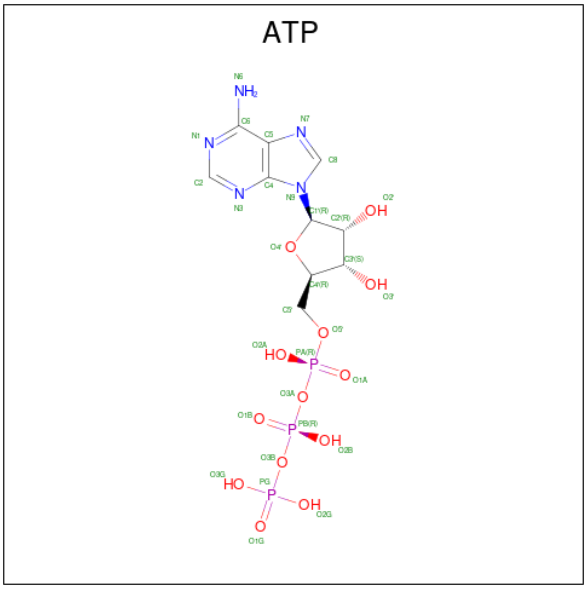
- Molecule 62 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
62	0	1	1	1	0
62	4	1	1	1	0

- Molecule 63 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
63	7	193	193	193	0
			Total	Mg	
63	A	63	63	63	0
			Total	Mg	
63	X	1	1	1	0
			Total	Mg	
63	Y	1	1	1	0
			Total	Mg	
63	b	1	1	1	0
			Total	Mg	
63	o	1	1	1	0

- Molecule 64 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

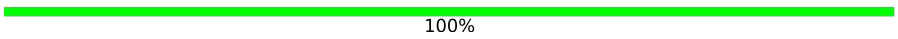


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
64	7	1	31	10	5	13	3	0
			Total	C	N	O	P	
64	7	1	31	10	5	13	3	0

3 Residue-property plots (i)

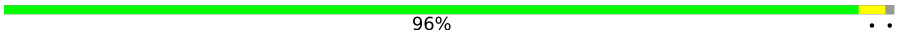
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 L36

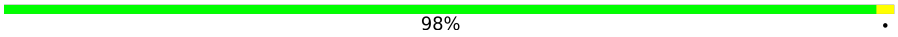
Chain 0: 

There are no outlier residues recorded for this chain.

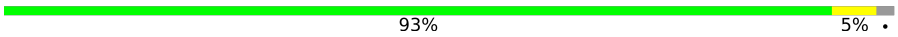
- Molecule 2: 50S ribosomal protein L28

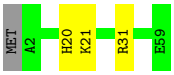
Chain 1: 

- Molecule 3: 50S ribosomal protein L29

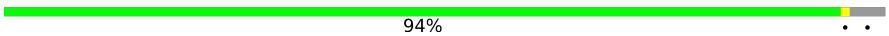
Chain 2: 

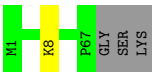
- Molecule 4: 50S ribosomal protein L30

Chain 3: 

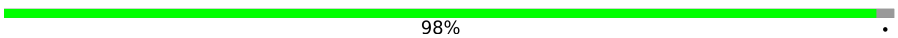


- Molecule 5: Large ribosomal subunit protein bL31A

Chain 4: 

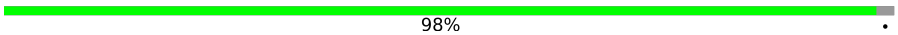


- Molecule 6: 50S ribosomal protein L32

Chain 5: 

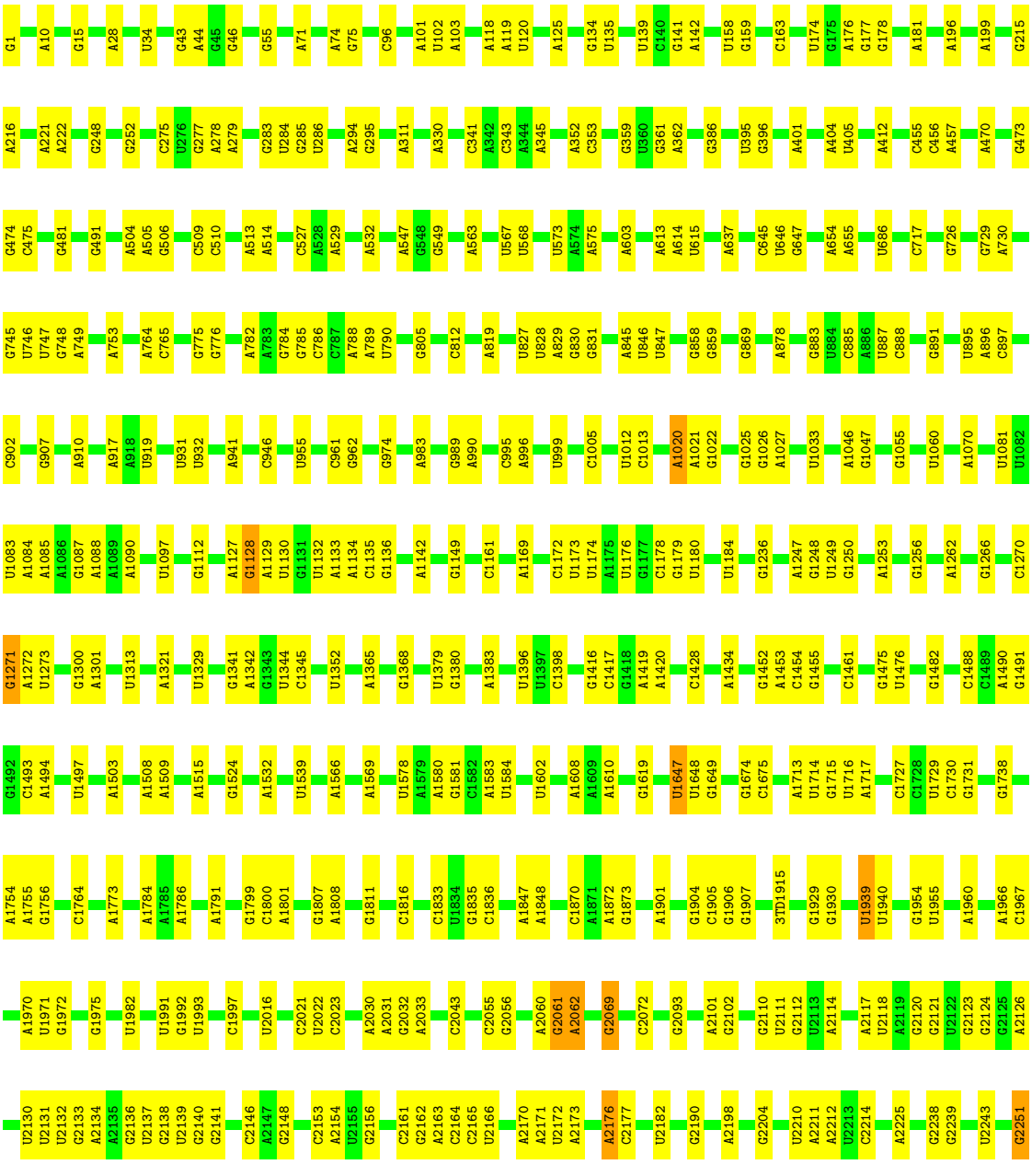
• Molecule 7: 50S ribosomal protein L35

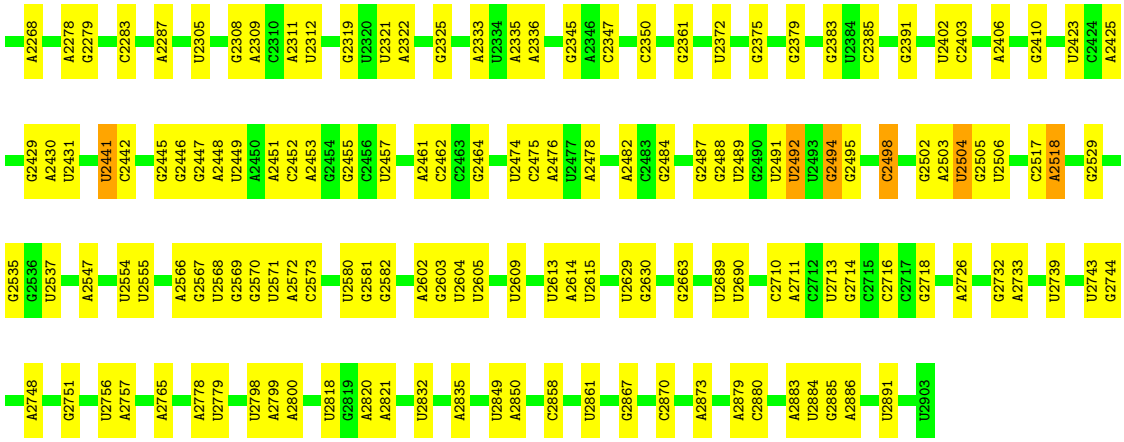
Chain 6:



• Molecule 8: 23S ribosomal RNA

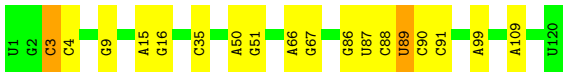
Chain 7:





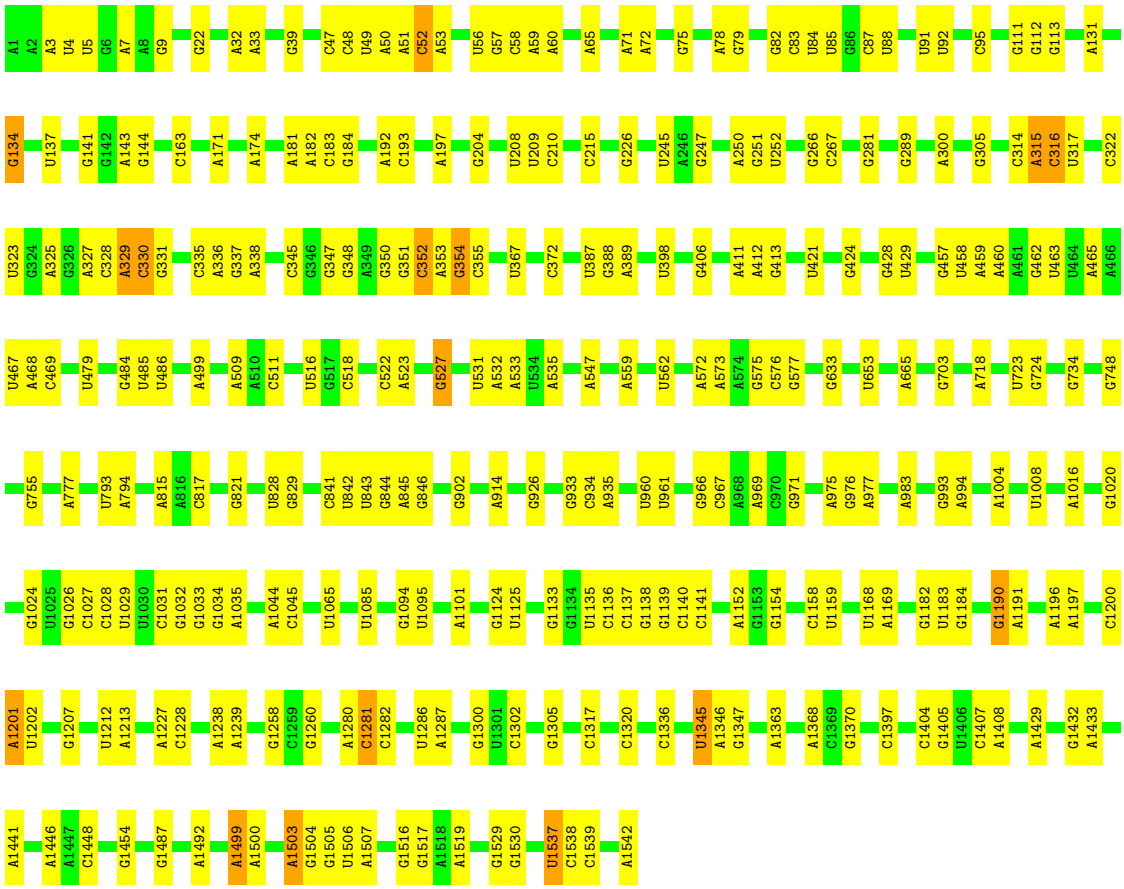
- Molecule 9: 5S ribosomal RNA

Chain 8: 85% 13% •



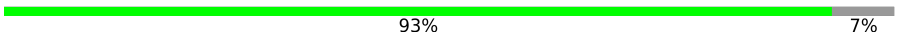
- Molecule 10: 16S ribosomal RNA

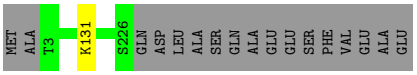
Chain A: 81% 18% •



- Molecule 11: Small ribosomal subunit protein uS2

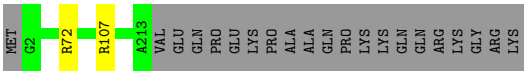
Chain B:





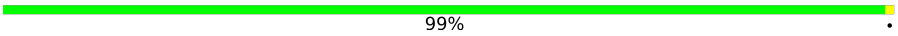
- Molecule 12: Small ribosomal subunit protein uS3

Chain C:



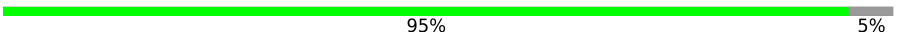
- Molecule 13: Small ribosomal subunit protein uS4

Chain D:



- Molecule 14: Small ribosomal subunit protein uS5

Chain E:

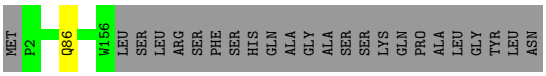


- Molecule 15: 30S ribosomal protein S6

Chain F:

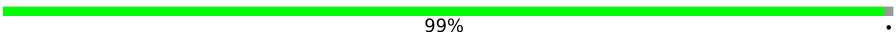
- Molecule 16: 30S ribosomal protein S7

Chain G:



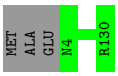
- Molecule 17: Small ribosomal subunit protein uS8

Chain H:



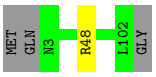
- Molecule 18: Small ribosomal subunit protein uS9

Chain I: 98%



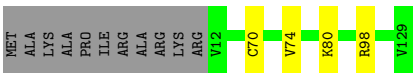
• Molecule 19: 30S ribosomal protein S10

Chain J: 96%



• Molecule 20: Small ribosomal subunit protein uS11

Chain K: 88% 9%

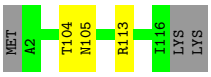


• Molecule 21: Small ribosomal subunit protein uS12

Chain L: 99%

• Molecule 22: Small ribosomal subunit protein uS13

Chain M: 95%



• Molecule 23: Small ribosomal subunit protein uS14

Chain N: 99%

• Molecule 24: 30S ribosomal protein S15

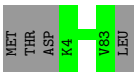
Chain O: 97%

• Molecule 25: 30S ribosomal protein S16

Chain P: 99%

• Molecule 26: Small ribosomal subunit protein uS17

Chain Q: 95% 5%



• Molecule 27: Small ribosomal subunit protein bS18

Chain R: 96%

• Molecule 28: Small ribosomal subunit protein uS19

Chain S: 90% 10%

• Molecule 29: Small ribosomal subunit protein bS20

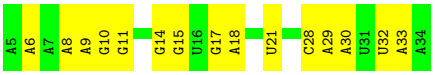
Chain T: 97%

• Molecule 30: 30S ribosomal protein S21

Chain U: 99%

• Molecule 31: mRNA

Chain V: 50% 50%



• Molecule 32: tRNA-Phe (P-site)

Chain W: 58% 33% 9%

G1 C2 C3 C4 U8 A9 G10 C11 G15 U16 U17 G18 G19 U20 A21 G22 U32 A35 A36 A37 A38 U39 C43 G44 U45 G46 U47 C48 C49 G52 G53 U54 U55 A58 C72 A73 C74 C75 A76

- Molecule 33: tRNA-Ser (E-site)

Chain X: 63% 33% •

G1 G2 U3 G7 U8 G9 G13 A16 G17 G18 C19 U20 G21 A22 C33 U34 A38 A46 U47 A63 U64 C65 C66 U72 A75 A76 U77 G82 C89 G90 A93

- Molecule 34: tRNA-Val (A-site)

Chain Y: 57% 37% 7%

G1 U7 U8 A9 G10 C11 C16 U17 G18 G19 G20 C32 U33 N34 A35 C36 A37 G46 U47 C48 G49 G53 U54 U55 C56 G57 A58 U59 C60 C61 C62 G63 U64 C65 C72 A73 C74 C75 A76

- Molecule 35: 30S ribosomal protein S1

Chain Z: 31% 69%

MET T2 R171 ALA VAL ILE GLU SER GLU ASN SER ALA GLU ARG ASP GLN LEU LEU GLU ASN LEU GLN GLU GLY MET GLU VAL LYS GLY ILE VAL LYS ASN LEU THR ASP TYR GLY ALA PHE VAL ASP LEU GLY GLY VAL ASP GLY LEU LEU HIS ILE THR ASP MET ALA TRP LYS ARG

VAL LYS HIS PRO SER GLU ILE VAL ASN VAL GLY ASP GLU ILE THR VAL LYS VAL LEU LYS PHE ASP ARG GLU ARG THR ARG VAL SER LEU GLY LEU LYS GLN LEU GLY GLU ASP PRO TRP VAL ALA ILE ALA LYS ARG TYR PRO GLU GLY THR LYS LEU THR GLY ARG VAL THR ASN LEU

THR ASP TYR GLY CYS PHE VAL GLU ILE GLU GLU GLY VAL GLU GLY LEU VAL HIS VAL SER GLU MET ASP TRP THR ASN LYS ASN ILE HIS PRO SER LYS VAL VAL ASN VAL GLY ASP VAL VAL GLU VAL MET VAL LEU ASP ILE ASP GLU GLU ARG ARG ARG ILE SER LEU GLY LEU LYS

GLN CYS LYS ALA ASN PRO TRP GLN GLN PHE ALA GLU THR HIS ASN LYS GLY ASP ARG VAL GLU GLY LYS ILE LYS SER ILE THR ASP PHE GLY ILE PHE ILE GLY LEU ASP GLY GLY ILE ASP GLY LEU VAL HIS LEU SER ASP ILE SER TRP ASN VAL ALA GLY GLU GLU ALA VAL ARG

GLU TYR LYS LYS GLY ASP GLU ILE ALA ALA VAL VAL LEU GLN VAL ASP ALA GLU ARG GLU ARG ILE SER LEU GLY VAL LYS GLN LEU ALA GLU ASP PRO PHE ASN ASN TRP VAL ALA LEU ASN LYS LYS GLY ALA ILE VAL THR GLY LYS VAL THR ALA VAL ASP ALA LYS GLY ALA THR

VAL GLU LEU ALA ASP GLY VAL GLU GLY TYR LEU ARG ALA SER GLU ALA SER ARG ASP ARG VAL GLU ASP ALA THR LEU VAL LEU SER VAL GLY ASP GLU VAL GLU ALA LYS PHE THR GLY VAL ASP ARG LYS ASN ARG ALA ILE SER LEU SER VAL ARG ALA LYS ASP GLU ALA ASP GLU

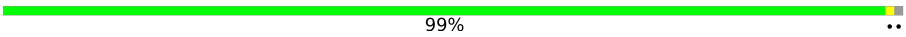
LYS ASP ALA ILE ALA THR VAL ASN LYS GLN GLU ASP ALA ASN PHE SER ASN ASN ALA MET ALA GLU ALA ALA PHE LYS ALA ALA LYS SER GLU GLU

- Molecule 36: Large ribosomal subunit protein uL1

Chain a: 57% 43%

MET ALA X3 T69 GLY ARG SER VAL ARG VAL ALA VAL PHE THR GLN GLY ALA ASN ALA GLU ALA ALA LYS ALA ALA GLY ALA GLU GLU LEU VAL GLY MET GLU ASP LEU ALA ASP GLN ILE LYS LYS GLY GLU MET ASN PHE ASP VAL VAL ILE ALA SER PRO ASP ALA MET ARG VAL VAL

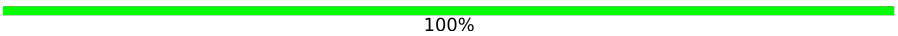
- Molecule 37: 50S ribosomal protein L2

Chain b: 

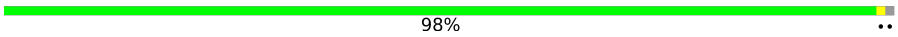
- Molecule 38: 50S ribosomal protein L3

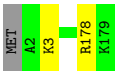
Chain c:

- Molecule 39: 50S ribosomal protein L4

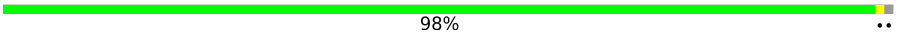
Chain d: 

- Molecule 40: 50S ribosomal protein L5

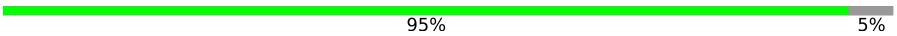
Chain e: 

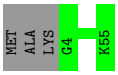


- Molecule 41: 50S ribosomal protein L6

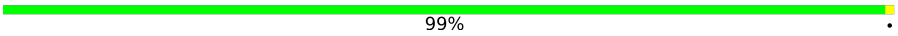
Chain f: 

- Molecule 42: 50S ribosomal protein L33

Chain g: 

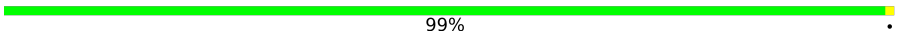


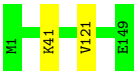
- Molecule 43: 50S ribosomal protein L16

Chain h: 

• Molecule 44: 50S ribosomal protein L9

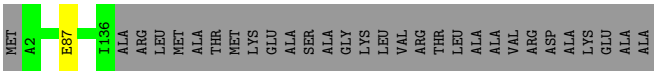
Chain i:





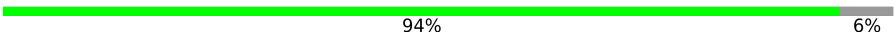
• Molecule 45: Large ribosomal subunit protein uL10

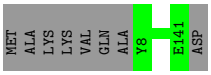
Chain j:



• Molecule 46: 50S ribosomal protein L11

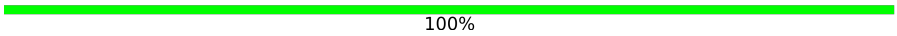
Chain k:





• Molecule 47: 50S ribosomal protein L34

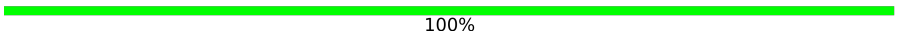
Chain l:



There are no outlier residues recorded for this chain.

• Molecule 48: 50S ribosomal protein L13

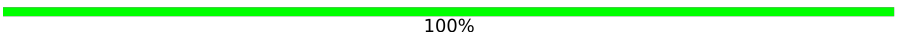
Chain m:



There are no outlier residues recorded for this chain.

• Molecule 49: 50S ribosomal protein L14

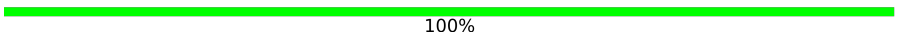
Chain n:



There are no outlier residues recorded for this chain.

• Molecule 50: 50S ribosomal protein L15

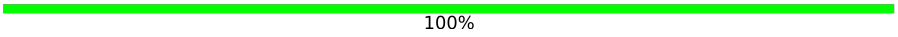
Chain o:



There are no outlier residues recorded for this chain.

• Molecule 51: Nascent chain

Chain p:



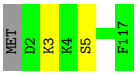
There are no outlier residues recorded for this chain.

- Molecule 52: 50S ribosomal protein L17

Chain q: 94% 6%

- Molecule 53: 50S ribosomal protein L18

Chain r: 97%



- Molecule 54: 50S ribosomal protein L19

Chain s: 99%

- Molecule 55: 50S ribosomal protein L20

Chain t: 99%

- Molecule 56: 50S ribosomal protein L21

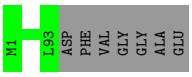
Chain u: 99%

- Molecule 57: 50S ribosomal protein L22

Chain v: 99%

- Molecule 58: 50S ribosomal protein L23

Chain w: 93% 7%



• Molecule 59: 50S ribosomal protein L24

Chain x: 97%

• Molecule 60: 50S ribosomal protein L25

Chain y: 100%

There are no outlier residues recorded for this chain.

• Molecule 61: 50S ribosomal protein L27

Chain z: 99%

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	32334	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	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: ZN, PSU, 3TD, 2MG, MA6, OMU, ATP, MIA, UR3, RSP, 12A, 6MZ, 5MU, 5MC, 2MA, 4OC, OMG, CM0, 1MG, G7M, 4SU, OMC, 7MG, MG, H2U

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	0	0.23	0/303	0.60	0/397
2	1	0.25	0/635	0.63	0/848
3	2	0.25	0/510	0.54	0/677
4	3	0.24	0/453	0.61	0/605
5	4	0.27	0/539	0.58	0/721
6	5	0.25	0/450	0.58	0/599
7	6	0.24	0/513	0.56	0/676
8	7	0.23	1/69284 (0.0%)	0.75	60/108082 (0.1%)
9	8	0.23	0/2872	0.76	6/4478 (0.1%)
10	A	0.23	0/36772	0.75	47/57358 (0.1%)
11	B	0.26	0/1782	0.53	0/2401
12	C	0.26	0/1685	0.57	0/2270
13	D	0.25	0/1665	0.56	0/2227
14	E	0.27	0/1179	0.55	0/1584
15	F	0.25	0/881	0.54	0/1189
16	G	0.27	0/1246	0.55	0/1672
17	H	0.26	0/989	0.57	0/1326
18	I	0.26	0/1034	0.60	0/1375
19	J	0.28	0/813	0.67	0/1100
20	K	0.26	0/900	0.59	0/1215
21	L	0.27	0/969	0.64	0/1300
22	M	0.31	0/900	0.64	0/1204
23	N	0.26	0/817	0.62	0/1088
24	O	0.24	0/722	0.63	0/964
25	P	0.26	0/659	0.62	0/884
26	Q	0.27	0/657	0.61	0/881
27	R	0.30	0/635	0.65	0/849
28	S	0.26	0/680	0.54	0/915
29	T	0.25	0/676	0.55	0/895
30	U	0.30	0/592	0.64	0/785
31	V	0.26	0/727	0.80	0/1132

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	W	0.34	1/1585 (0.1%)	0.86	4/2467 (0.2%)
33	X	0.35	1/1728 (0.1%)	0.91	1/2686 (0.0%)
34	Y	0.43	1/1672 (0.1%)	0.97	7/2599 (0.3%)
35	Z	0.25	0/1334	0.52	0/1799
36	a	0.24	0/1033	0.50	0/1387
37	b	0.26	0/2121	0.63	1/2852 (0.0%)
38	c	0.26	0/1586	0.56	0/2134
39	d	0.25	0/1571	0.53	0/2113
40	e	0.25	0/1444	0.55	0/1937
41	f	0.25	0/1343	0.55	0/1816
42	g	0.25	0/434	0.54	0/576
43	h	0.27	0/1104	0.60	0/1474
44	i	0.25	0/1121	0.54	0/1515
45	j	0.27	0/1037	0.55	0/1400
46	k	0.27	0/993	0.56	0/1341
47	l	0.29	0/380	0.65	0/498
48	m	0.25	0/1152	0.55	0/1551
49	n	0.27	0/955	0.63	0/1279
50	o	0.27	0/1062	0.62	0/1413
51	p	0.82	0/36	1.05	0/48
52	q	0.26	0/973	0.61	0/1301
53	r	0.25	0/901	0.61	0/1209
54	s	0.26	0/929	0.56	0/1242
55	t	0.25	0/960	0.53	0/1278
56	u	0.26	0/829	0.59	0/1107
57	v	0.24	0/864	0.57	0/1156
58	w	0.25	0/744	0.54	0/994
59	x	0.26	0/787	0.54	0/1051
60	y	0.26	0/766	0.54	0/1025
61	z	0.25	0/642	0.56	0/848
All	All	0.25	4/164625 (0.0%)	0.71	126/245793 (0.1%)

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	D	0	1
19	J	0	1
20	K	0	1
24	O	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
25	P	0	1
29	T	0	2
39	d	0	1
41	f	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	Y	1	G	OP3-P	-7.60	1.52	1.61
8	7	1	G	OP3-P	-7.55	1.52	1.61
32	W	1	G	OP3-P	-7.52	1.52	1.61
33	X	1	G	OP3-P	-7.50	1.52	1.61

The worst 5 of 126 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	7	1129	A	P-O3'-C3'	-12.54	104.65	119.70
8	7	2605	PSU	P-O3'-C3'	-11.15	106.32	119.70
10	A	1407	5MC	P-O3'-C3'	-10.99	106.51	119.70
8	7	2453	A	P-O3'-C3'	-10.77	106.78	119.70
10	A	1408	A	P-O3'-C3'	-10.70	106.86	119.70

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	D	104	ARG	Sidechain
19	J	48	ARG	Sidechain
20	K	98	ARG	Sidechain
24	O	84	ARG	Sidechain
25	P	51	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
2	1	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
3	2	61/63 (97%)	60 (98%)	0	1 (2%)	8	32
4	3	56/59 (95%)	49 (88%)	5 (9%)	2 (4%)	3	18
5	4	65/70 (93%)	49 (75%)	16 (25%)	0	100	100
6	5	54/57 (95%)	54 (100%)	0	0	100	100
7	6	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
11	B	222/241 (92%)	209 (94%)	12 (5%)	1 (0%)	25	56
12	C	210/233 (90%)	208 (99%)	2 (1%)	0	100	100
13	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
14	E	156/167 (93%)	151 (97%)	5 (3%)	0	100	100
15	F	104/135 (77%)	103 (99%)	1 (1%)	0	100	100
16	G	153/179 (86%)	149 (97%)	4 (3%)	0	100	100
17	H	127/130 (98%)	127 (100%)	0	0	100	100
18	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
19	J	98/103 (95%)	93 (95%)	5 (5%)	0	100	100
20	K	116/129 (90%)	102 (88%)	11 (10%)	3 (3%)	4	23
21	L	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
22	M	113/118 (96%)	106 (94%)	7 (6%)	0	100	100
23	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
24	O	86/89 (97%)	83 (96%)	2 (2%)	1 (1%)	11	38
25	P	80/82 (98%)	78 (98%)	2 (2%)	0	100	100
26	Q	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
27	R	72/75 (96%)	63 (88%)	7 (10%)	2 (3%)	4	22
28	S	81/92 (88%)	80 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	T	84/87 (97%)	84 (100%)	0	0	100	100
30	U	68/71 (96%)	61 (90%)	7 (10%)	0	100	100
35	Z	168/557 (30%)	161 (96%)	7 (4%)	0	100	100
36	a	130/234 (56%)	126 (97%)	4 (3%)	0	100	100
37	b	269/273 (98%)	262 (97%)	6 (2%)	1 (0%)	30	61
38	c	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
39	d	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
40	e	176/179 (98%)	171 (97%)	5 (3%)	0	100	100
41	f	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
42	g	50/55 (91%)	50 (100%)	0	0	100	100
43	h	135/136 (99%)	134 (99%)	1 (1%)	0	100	100
44	i	147/149 (99%)	132 (90%)	14 (10%)	1 (1%)	19	50
45	j	133/165 (81%)	122 (92%)	11 (8%)	0	100	100
46	k	132/142 (93%)	124 (94%)	8 (6%)	0	100	100
47	l	44/46 (96%)	44 (100%)	0	0	100	100
48	m	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
49	n	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
50	o	142/144 (99%)	137 (96%)	5 (4%)	0	100	100
51	p	4/18 (22%)	3 (75%)	1 (25%)	0	100	100
52	q	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
53	r	114/117 (97%)	105 (92%)	7 (6%)	2 (2%)	7	30
54	s	112/115 (97%)	107 (96%)	5 (4%)	0	100	100
55	t	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
56	u	101/103 (98%)	93 (92%)	7 (7%)	1 (1%)	13	42
57	v	108/110 (98%)	96 (89%)	11 (10%)	1 (1%)	14	44
58	w	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
59	x	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
60	y	92/94 (98%)	92 (100%)	0	0	100	100
61	z	82/85 (96%)	77 (94%)	5 (6%)	0	100	100
All	All	6208/7029 (88%)	5944 (96%)	248 (4%)	16 (0%)	38	66

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
57	v	64	ALA
4	3	21	LYS
20	K	70	CYS
20	K	80	LYS
53	r	5	SER

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	34/34 (100%)	34 (100%)	0	100	100
2	1	67/68 (98%)	65 (97%)	2 (3%)	36	62
3	2	55/55 (100%)	55 (100%)	0	100	100
4	3	48/49 (98%)	47 (98%)	1 (2%)	48	70
5	4	60/62 (97%)	59 (98%)	1 (2%)	56	74
6	5	47/48 (98%)	47 (100%)	0	100	100
7	6	51/52 (98%)	51 (100%)	0	100	100
11	B	186/199 (94%)	186 (100%)	0	100	100
12	C	172/190 (90%)	170 (99%)	2 (1%)	67	80
13	D	172/173 (99%)	171 (99%)	1 (1%)	84	90
14	E	120/126 (95%)	120 (100%)	0	100	100
15	F	92/116 (79%)	92 (100%)	0	100	100
16	G	128/147 (87%)	127 (99%)	1 (1%)	79	87
17	H	104/105 (99%)	104 (100%)	0	100	100
18	I	105/107 (98%)	105 (100%)	0	100	100
19	J	88/90 (98%)	88 (100%)	0	100	100
20	K	91/99 (92%)	91 (100%)	0	100	100
21	L	103/104 (99%)	103 (100%)	0	100	100
22	M	93/96 (97%)	90 (97%)	3 (3%)	34	61
23	N	83/84 (99%)	83 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	O	76/77 (99%)	76 (100%)	0	100	100
25	P	65/65 (100%)	65 (100%)	0	100	100
26	Q	74/78 (95%)	74 (100%)	0	100	100
27	R	64/65 (98%)	64 (100%)	0	100	100
28	S	72/79 (91%)	72 (100%)	0	100	100
29	T	65/66 (98%)	65 (100%)	0	100	100
30	U	59/61 (97%)	59 (100%)	0	100	100
35	Z	143/461 (31%)	143 (100%)	0	100	100
36	a	110/181 (61%)	110 (100%)	0	100	100
37	b	216/218 (99%)	216 (100%)	0	100	100
38	c	164/164 (100%)	163 (99%)	1 (1%)	84	90
39	d	165/165 (100%)	165 (100%)	0	100	100
40	e	149/150 (99%)	147 (99%)	2 (1%)	65	79
41	f	137/138 (99%)	136 (99%)	1 (1%)	81	88
42	g	47/49 (96%)	47 (100%)	0	100	100
43	h	110/109 (101%)	109 (99%)	1 (1%)	75	85
44	i	114/114 (100%)	113 (99%)	1 (1%)	75	85
45	j	103/123 (84%)	102 (99%)	1 (1%)	73	84
46	k	104/110 (94%)	104 (100%)	0	100	100
47	l	38/38 (100%)	38 (100%)	0	100	100
48	m	116/116 (100%)	116 (100%)	0	100	100
49	n	104/104 (100%)	104 (100%)	0	100	100
50	o	103/103 (100%)	103 (100%)	0	100	100
51	p	4/4 (100%)	4 (100%)	0	100	100
52	q	100/103 (97%)	99 (99%)	1 (1%)	73	84
53	r	86/87 (99%)	86 (100%)	0	100	100
54	s	99/100 (99%)	99 (100%)	0	100	100
55	t	89/90 (99%)	89 (100%)	0	100	100
56	u	84/84 (100%)	84 (100%)	0	100	100
57	v	93/93 (100%)	93 (100%)	0	100	100
58	w	80/84 (95%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
59	x	83/85 (98%)	82 (99%)	1 (1%)	67 80
60	y	78/78 (100%)	78 (100%)	0	100 100
61	z	62/63 (98%)	62 (100%)	0	100 100
All	All	5155/5709 (90%)	5135 (100%)	20 (0%)	88 93

5 of 20 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	f	69	ARG
45	j	87	GLU
59	x	6	ARG
52	q	2	ARG
13	D	44	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
41	f	101	ASN
46	k	105	GLN
57	v	61	ASN
54	s	10	GLN
20	K	119	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	A	1538/1542 (99%)	248 (16%)	20 (1%)
31	V	29/30 (96%)	14 (48%)	3 (10%)
32	W	74/76 (97%)	23 (31%)	2 (2%)
33	X	74/78 (94%)	25 (33%)	4 (5%)
34	Y	73/76 (96%)	25 (34%)	7 (9%)
8	7	2898/2903 (99%)	485 (16%)	55 (1%)
9	8	119/120 (99%)	14 (11%)	1 (0%)
All	All	4805/4825 (99%)	834 (17%)	92 (1%)

5 of 834 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	7	10	A

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Mol	Chain	Res	Type
8	7	15	G
8	7	28	A
8	7	34	U
8	7	44	A

5 of 92 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
10	A	84	U
10	A	1201	A
10	A	181	A
10	A	522	C
10	A	1432	G

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

55 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	$\#\|Z\| > 2$
32	H2U	W	16	32	18,21,22	3.08	5 (27%)	21,30,33	2.03	5 (23%)
8	3TD	7	1915	8	19,22,23	0.83	1 (5%)	21,32,35	0.59	0
34	PSU	Y	55	34	18,21,22	0.88	1 (5%)	22,30,33	0.58	0
8	2MG	7	1835	8	18,26,27	1.03	2 (11%)	16,38,41	0.79	0
34	5MU	Y	54	34	19,22,23	0.24	0	28,32,35	0.21	0
33	5MU	X	71	33	19,22,23	0.25	0	28,32,35	0.27	0
8	PSU	7	2605	8	18,21,22	0.86	1 (5%)	22,30,33	0.54	0
32	5MU	W	54	32	19,22,23	0.25	0	28,32,35	0.37	0
8	OMU	7	2552	8	19,22,23	0.21	0	26,31,34	0.50	0
8	2MG	7	2445	8	18,26,27	1.02	2 (11%)	16,38,41	0.76	0
33	RSP	X	33	33	17,21,22	4.18	7 (41%)	22,30,33	0.72	0
34	6MZ	Y	37	34	18,25,26	0.66	0	16,36,39	0.58	1 (6%)
33	4SU	X	8	33	18,21,22	3.81	7 (38%)	26,30,33	2.26	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	PSU	A	516	10,63	18,21,22	0.89	1 (5%)	22,30,33	1.14	3 (13%)
10	5MC	A	967	10	18,22,23	4.04	7 (38%)	26,32,35	1.01	2 (7%)
10	5MC	A	1407	10	18,22,23	0.33	0	26,32,35	0.58	0
8	PSU	7	2504	8	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
8	PSU	7	746	63,8	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
8	PSU	7	955	8	18,21,22	0.86	1 (5%)	22,30,33	0.59	0
34	4SU	Y	7	34	18,21,22	0.37	0	26,30,33	1.35	3 (11%)
32	PSU	W	32	32	18,21,22	4.66	8 (44%)	22,30,33	1.82	5 (22%)
33	PSU	X	72	33	18,21,22	0.87	1 (5%)	22,30,33	0.61	0
10	4OC	A	1402	10	20,23,24	0.38	0	26,32,35	0.41	0
32	MIA	W	37	32	24,31,32	2.36	3 (12%)	26,44,47	2.55	7 (26%)
33	H2U	X	20	33	18,21,22	3.07	5 (27%)	21,30,33	2.05	4 (19%)
10	UR3	A	1498	10	19,22,23	0.30	0	26,32,35	0.67	0
32	PSU	W	55	32	18,21,22	0.90	1 (5%)	22,30,33	0.70	0
34	CM0	Y	34	34	23,26,27	1.11	1 (4%)	27,37,40	0.56	0
10	MA6	A	1518	10	18,26,27	0.73	0	19,38,41	0.54	0
8	5MC	7	1962	8	18,22,23	0.33	0	26,32,35	0.52	0
34	7MG	Y	46	34	22,26,27	3.88	10 (45%)	29,39,42	2.08	9 (31%)
10	2MG	A	1516	10	18,26,27	1.04	2 (11%)	16,38,41	0.73	0
8	5MU	7	1939	63,8	19,22,23	0.27	0	28,32,35	0.40	0
8	OMG	7	2251	32,8	18,26,27	1.02	2 (11%)	19,38,41	0.69	0
8	5MU	7	747	8	19,22,23	0.23	0	28,32,35	0.33	0
8	PSU	7	2580	8	18,21,22	0.85	1 (5%)	22,30,33	0.97	1 (4%)
8	2MA	7	2503	8	19,25,26	0.88	0	21,37,40	2.04	5 (23%)
8	G7M	7	2069	8	20,26,27	1.12	3 (15%)	17,39,42	0.53	0
8	6MZ	7	2030	8	18,25,26	0.73	0	16,36,39	1.02	2 (12%)
10	G7M	A	527	10	20,26,27	1.13	3 (15%)	17,39,42	0.39	0
8	6MZ	7	1618	8	18,25,26	0.68	0	16,36,39	0.83	0
8	OMC	7	2498	63,8	19,22,23	0.30	0	26,31,34	0.34	0
32	PSU	W	39	32	18,21,22	4.65	8 (44%)	22,30,33	1.89	5 (22%)
10	MA6	A	1519	10	18,26,27	0.75	1 (5%)	19,38,41	0.42	0
8	PSU	7	2457	8	18,21,22	0.85	1 (5%)	22,30,33	0.78	1 (4%)
8	H2U	7	2449	8	18,21,22	4.41	14 (77%)	21,30,33	2.21	5 (23%)
33	12A	X	38	10,33	29,36,37	4.79	16 (55%)	34,52,55	3.02	9 (26%)
32	H2U	W	20	32	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
32	G7M	W	46	32	20,26,27	2.81	7 (35%)	17,39,42	1.13	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
10	2MG	A	966	10	18,26,27	2.83	7 (38%)	16,38,41	1.43	4 (25%)
32	4SU	W	8	32	18,21,22	3.79	7 (38%)	26,30,33	2.23	5 (19%)
10	2MG	A	1207	10	18,26,27	1.01	3 (16%)	16,38,41	0.88	1 (6%)
8	PSU	7	2604	8	18,21,22	0.87	1 (5%)	22,30,33	0.67	0
32	H2U	W	17	32	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
8	1MG	7	745	8	18,26,27	0.97	1 (5%)	19,39,42	0.71	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	H2U	W	16	32	-	1/7/38/39	0/2/2/2
8	3TD	7	1915	8	-	0/7/25/26	0/2/2/2
34	PSU	Y	55	34	-	4/7/25/26	0/2/2/2
8	2MG	7	1835	8	-	1/5/27/28	0/3/3/3
34	5MU	Y	54	34	-	0/7/25/26	0/2/2/2
33	5MU	X	71	33	-	0/7/25/26	0/2/2/2
8	PSU	7	2605	8	-	0/7/25/26	0/2/2/2
32	5MU	W	54	32	-	4/7/25/26	0/2/2/2
8	OMU	7	2552	8	-	0/9/27/28	0/2/2/2
8	2MG	7	2445	8	-	2/5/27/28	0/3/3/3
33	RSP	X	33	33	-	1/7/25/26	0/2/2/2
34	6MZ	Y	37	34	-	0/5/27/28	0/3/3/3
33	4SU	X	8	33	-	2/7/25/26	0/2/2/2
10	PSU	A	516	10,63	-	0/7/25/26	0/2/2/2
10	5MC	A	967	10	-	0/7/25/26	0/2/2/2
10	5MC	A	1407	10	-	0/7/25/26	0/2/2/2
8	PSU	7	2504	8	-	0/7/25/26	0/2/2/2
8	PSU	7	746	63,8	-	6/7/25/26	0/2/2/2
8	PSU	7	955	8	-	0/7/25/26	0/2/2/2
34	4SU	Y	7	34	-	0/7/25/26	0/2/2/2
32	PSU	W	32	32	-	0/7/25/26	0/2/2/2
33	PSU	X	72	33	-	0/7/25/26	0/2/2/2
10	4OC	A	1402	10	-	0/9/29/30	0/2/2/2
32	MIA	W	37	32	-	4/11/33/34	0/3/3/3
33	H2U	X	20	33	-	5/7/38/39	0/2/2/2
10	UR3	A	1498	10	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	W	55	32	-	0/7/25/26	0/2/2/2
34	CM0	Y	34	34	-	2/12/30/31	0/2/2/2
10	MA6	A	1518	10	-	0/7/29/30	0/3/3/3
8	5MC	7	1962	8	-	4/7/25/26	0/2/2/2
34	7MG	Y	46	34	-	1/7/37/38	0/3/3/3
10	2MG	A	1516	10	-	1/5/27/28	0/3/3/3
8	5MU	7	1939	63,8	-	0/7/25/26	0/2/2/2
8	OMG	7	2251	32,8	-	3/5/27/28	0/3/3/3
8	5MU	7	747	8	-	0/7/25/26	0/2/2/2
8	PSU	7	2580	8	-	0/7/25/26	0/2/2/2
8	2MA	7	2503	8	-	0/3/25/26	0/3/3/3
8	G7M	7	2069	8	-	1/3/25/26	0/3/3/3
8	6MZ	7	2030	8	-	1/5/27/28	0/3/3/3
10	G7M	A	527	10	-	2/3/25/26	0/3/3/3
8	6MZ	7	1618	8	-	2/5/27/28	0/3/3/3
8	OMC	7	2498	63,8	-	2/9/27/28	0/2/2/2
32	PSU	W	39	32	-	0/7/25/26	0/2/2/2
10	MA6	A	1519	10	-	4/7/29/30	0/3/3/3
8	PSU	7	2457	8	-	0/7/25/26	0/2/2/2
8	H2U	7	2449	8	-	0/7/38/39	0/2/2/2
33	12A	X	38	10,33	-	10/21/43/44	0/3/3/3
32	H2U	W	20	32	-	3/7/38/39	0/2/2/2
32	G7M	W	46	32	-	3/3/25/26	0/3/3/3
10	2MG	A	966	10	-	0/5/27/28	0/3/3/3
32	4SU	W	8	32	-	2/7/25/26	0/2/2/2
10	2MG	A	1207	10	-	0/5/27/28	0/3/3/3
8	PSU	7	2604	8	-	0/7/25/26	0/2/2/2
32	H2U	W	17	32	-	6/7/38/39	0/2/2/2
8	1MG	7	745	8	-	0/3/25/26	0/3/3/3

The worst 5 of 153 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	X	38	12A	C2-S2	14.59	1.88	1.75
32	W	32	PSU	C6-C5	12.17	1.49	1.35
32	W	39	PSU	C6-C5	12.14	1.49	1.35
33	X	33	RSP	C2-N3	11.88	1.49	1.36
33	X	38	12A	C2'-C3'	-10.51	1.24	1.53

The worst 5 of 92 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	X	38	12A	N6-C6-N1	-11.23	98.72	118.84
32	W	37	MIA	C11-S10-C2	9.96	109.70	102.27
33	X	38	12A	C2M-S2-C2	9.30	109.21	102.27
33	X	8	4SU	C4-N3-C2	-7.94	119.63	127.34
32	W	8	4SU	C4-N3-C2	-7.83	119.74	127.34

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	527	G7M	O4'-C4'-C5'-O5'
10	A	527	G7M	C3'-C4'-C5'-O5'
10	A	1516	2MG	N3-C2-N2-CM2
10	A	1519	MA6	C5-C6-N6-C10
8	7	746	PSU	C2'-C1'-C5-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 264 ligands modelled in this entry, 262 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
64	ATP	7	3194	-	26,33,33	3.46	10 (38%)	31,52,52	2.19	7 (22%)
64	ATP	7	3193	-	26,33,33	3.48	10 (38%)	31,52,52	2.24	7 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
64	ATP	7	3194	-	-	4/18/38/38	0/3/3/3
64	ATP	7	3193	-	-	6/18/38/38	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
64	7	3194	ATP	C2'-C3'	-10.66	1.24	1.53
64	7	3193	ATP	C2'-C3'	-10.60	1.24	1.53
64	7	3194	ATP	O4'-C1'	7.46	1.51	1.41
64	7	3193	ATP	O4'-C1'	7.46	1.51	1.41
64	7	3193	ATP	O4'-C4'	-6.45	1.30	1.45

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
64	7	3193	ATP	C5-C6-N6	6.65	130.46	120.35
64	7	3194	ATP	C5-C6-N6	6.60	130.39	120.35
64	7	3194	ATP	N3-C2-N1	-5.50	120.08	128.68
64	7	3193	ATP	N3-C2-N1	-5.46	120.14	128.68
64	7	3193	ATP	C1'-N9-C4	4.93	135.31	126.64

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
64	7	3193	ATP	C5'-O5'-PA-O1A
64	7	3194	ATP	C5'-O5'-PA-O3A
64	7	3193	ATP	C3'-C4'-C5'-O5'
64	7	3193	ATP	C5'-O5'-PA-O3A
64	7	3193	ATP	C5'-O5'-PA-O2A

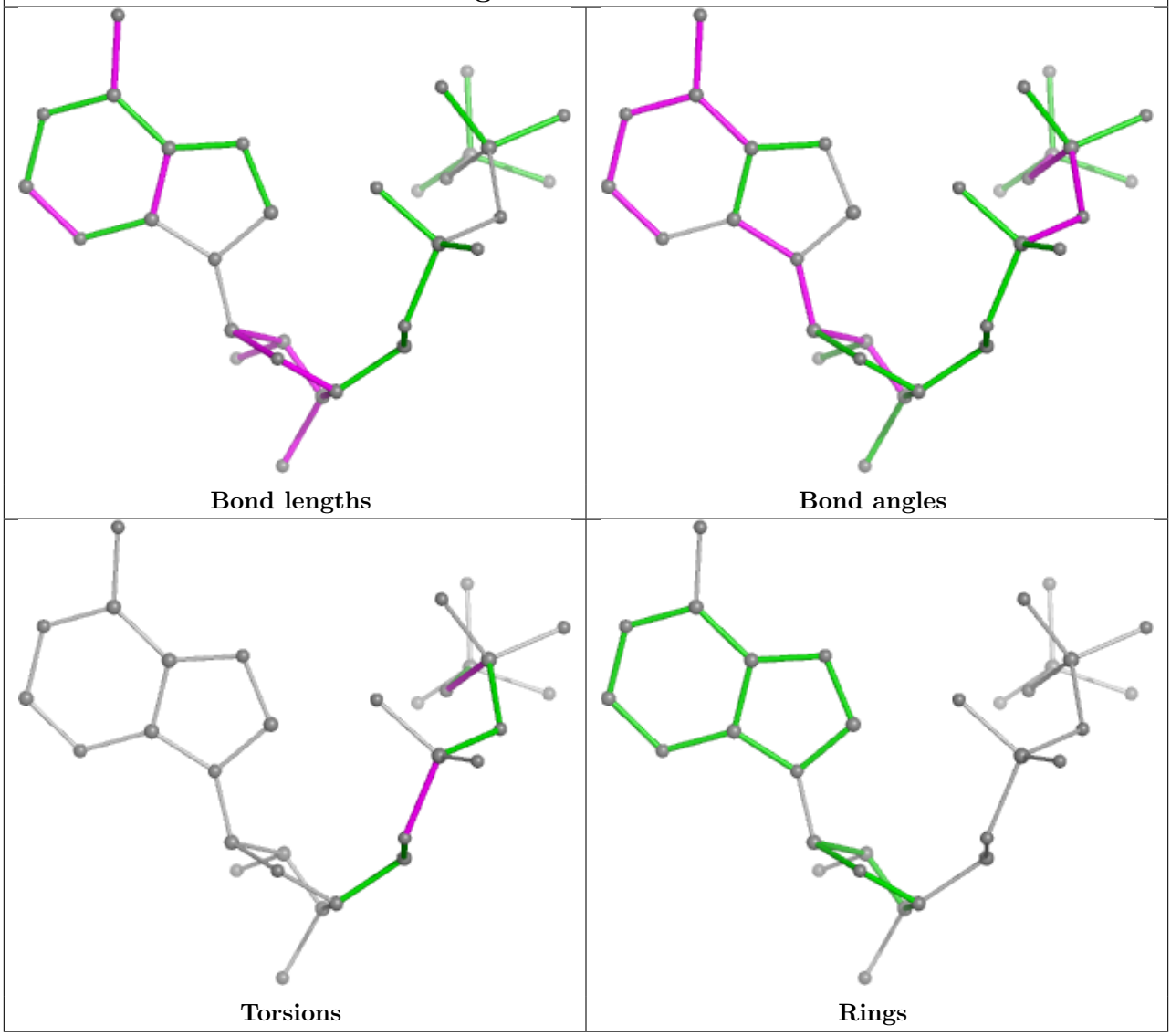
There are no ring outliers.

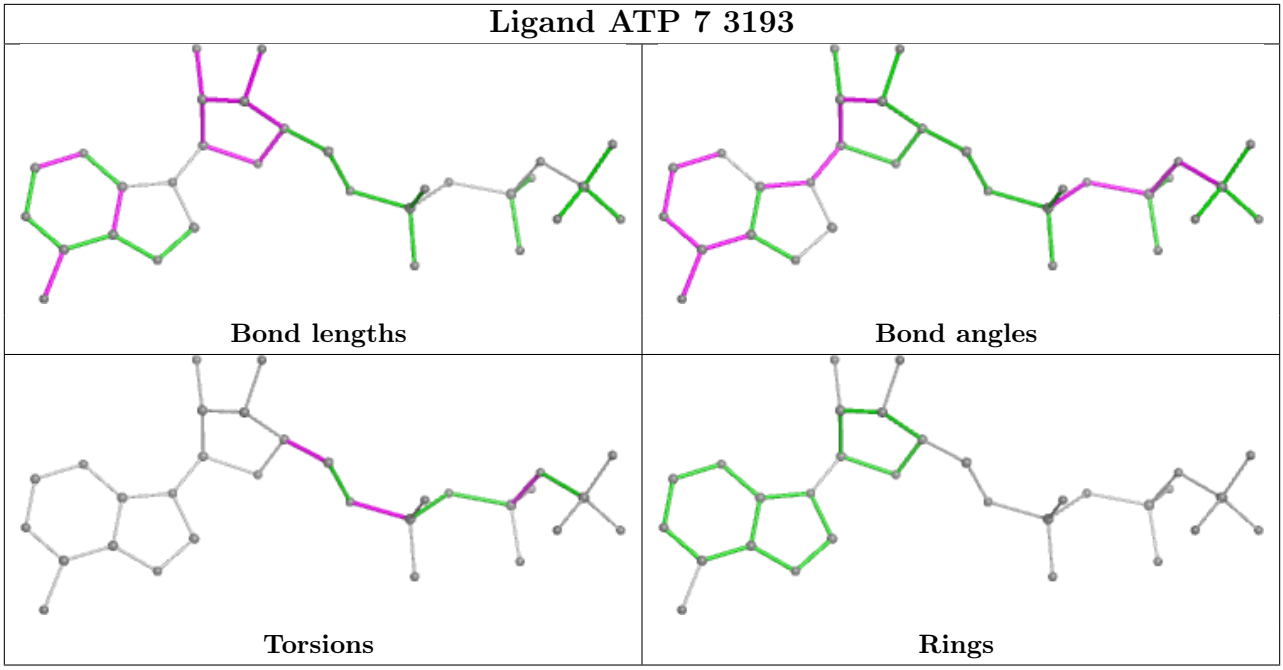
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ATP 7 3194





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	X	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	47:U	O3'	63:A	P	17.15