



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:35 PM BST

PDB ID : 5GAE
EMDB ID: : EMD-8001
Title : RNC in complex with a translocating SecYEG
Authors : Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on : 2015-11-25
Resolution : 3.33 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

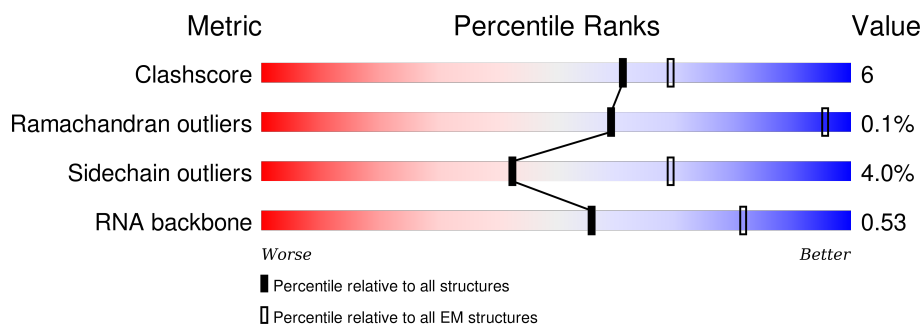
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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.











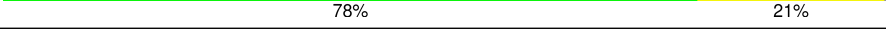

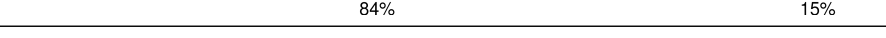
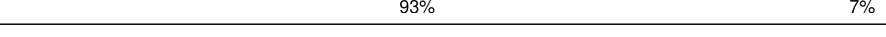

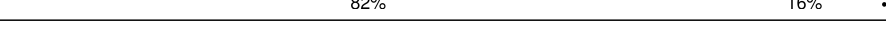


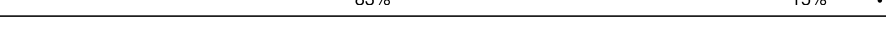

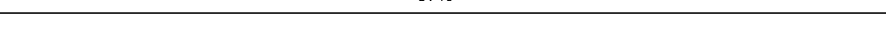






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

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	A	2903	68% 26% 5% .
2	B	120	68% 28% . .
3	C	273	80% 18% ..
4	D	209	85% 14%
5	E	201	87% 12% .
6	F	179	65% 32% . .
7	G	177	77% 22% ..
8	H	149	76% 22% .

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Mol	Chain	Length	Quality of chain
9	I	165	
10	J	142	
11	K	142	
12	L	123	
13	M	144	
14	N	136	
15	O	127	
16	P	117	
17	Q	115	
18	R	118	
19	S	103	
20	T	110	
21	U	100	
22	V	104	
23	W	94	
24	X	85	
25	Y	78	
26	Z	63	
27	a	59	
28	b	57	
29	c	55	
30	d	46	
31	e	65	
32	f	38	
33	g	443	

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Mol	Chain	Length	Quality of chain
34	h	127	<div><div></div><div>46%</div><div></div><div>54%</div></div>
35	i	25	<div><div></div><div>100%</div></div>
36	x	3	<div><div></div><div>67%</div><div></div><div>33%</div></div>

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 95192 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2884	Total	C	N	O	P	0	0
			61923	27622	11400	20017	2884		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			946	599	169	175	3		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	85	VAL	SER	conflict	UNP P0A7J3
I	86	THR	MET	conflict	UNP P0A7J3

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	70	Total	C	N	O	S	0	0
			502	309	92	98	3		

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	125	Total	C	N	O	S	0	0
			993	613	202	173	5		

- Molecule 16 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	117	Total	C	N	O	S	0	0
			900	557	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	95	Total	C	N	O	S	0	0
			756	479	141	135	1		

- Molecule 22 is a protein called 50S ribosomal protein L24.

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

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	76	Total	C	N	O	S	0	0
			580	359	117	103	1		

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L32.

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

- Molecule 29 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	51	Total	C	N	O	S	0	0
			414	266	76	72			

- Molecule 30 is a protein called 50S ribosomal protein L34.

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

- Molecule 31 is a protein called 50S ribosomal protein L35.

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

- Molecule 32 is a protein called 50S ribosomal protein L36.

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

- Molecule 33 is a protein called Protein translocase subunit SecY.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	399	Total	C	N	O	S	0	0
			3099	2056	508	520	15		

- Molecule 34 is a protein called Protein translocase subunit SecE.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	59	Total	C	N	O	S	0	0
			459	298	82	78	1		

- Molecule 35 is a protein called SecG.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	i	25	Total	C	N	O	0	0
			150	100	25	25		

- Molecule 36 is a RNA chain called tRNA CCA end (5'-R(P*CP*CP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
36	x	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	B	8	Total	Mg	0
			8	8	
37	A	313	Total	Mg	0
			313	313	
37	R	1	Total	Mg	0
			1	1	
37	b	1	Total	Mg	0
			1	1	

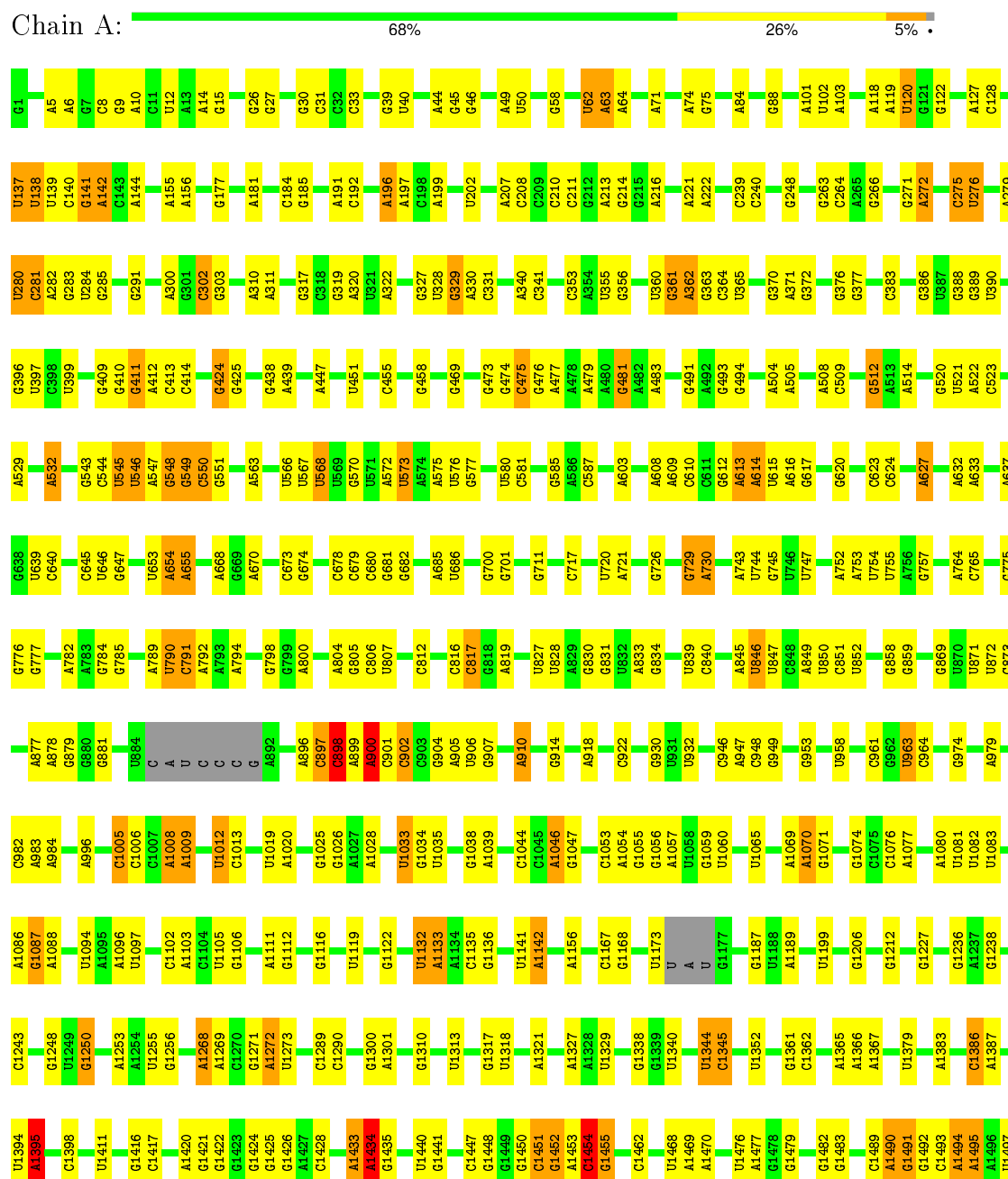
- Molecule 38 is ZINC ION (three-letter code: ZN) (formula: Zn).

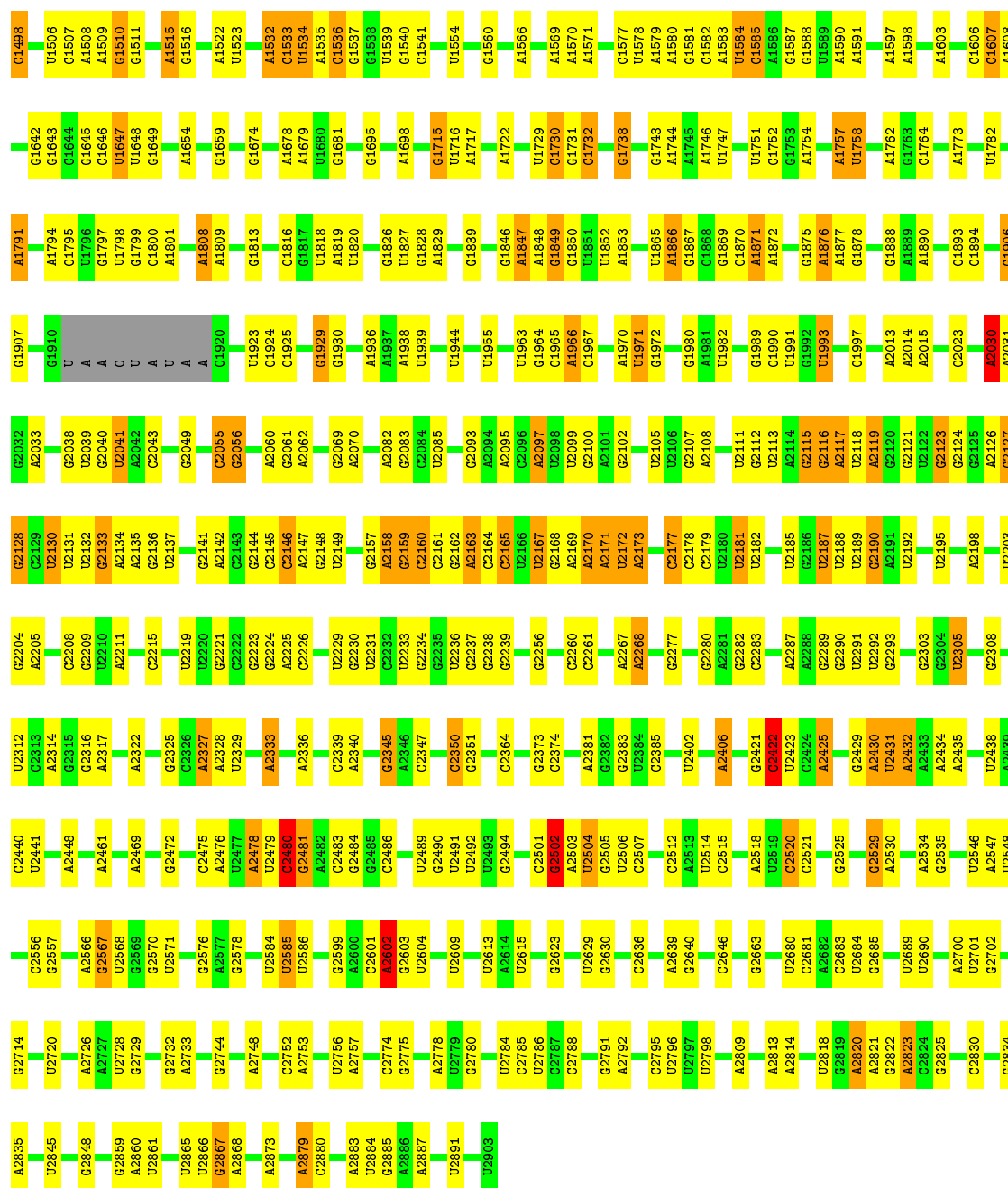
Mol	Chain	Residues	Atoms		AltConf
38	f	1	Total	Zn	0
			1	1	

3 Residue-property plots

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: 23S rRNA





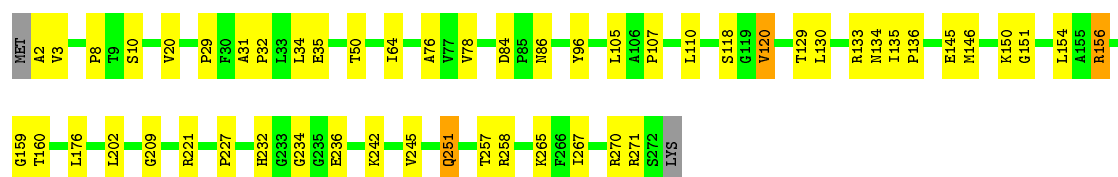
- Molecule 2: 5S rRNA

Chain B: 68% 28%



- Molecule 3: 50S ribosomal protein L2

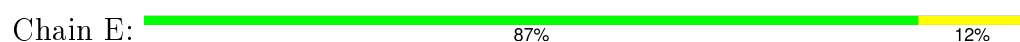
Chain C: 80% 18%



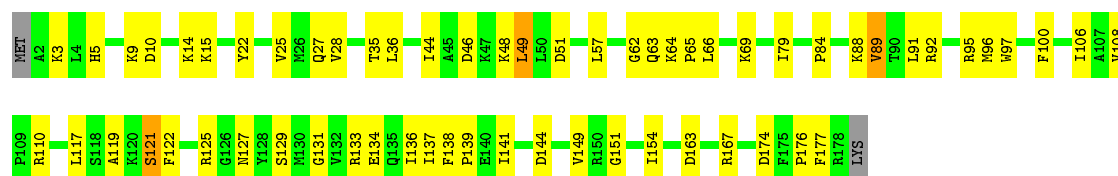
- Molecule 4: 50S ribosomal protein L3



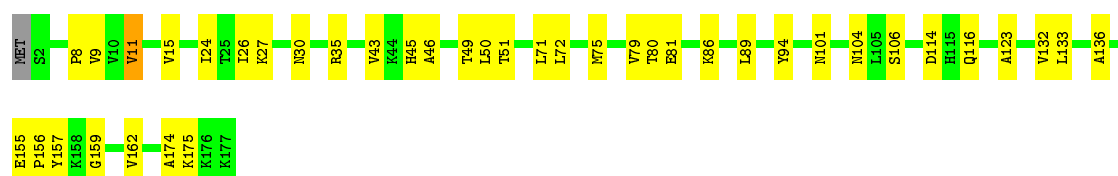
- Molecule 5: 50S ribosomal protein L4



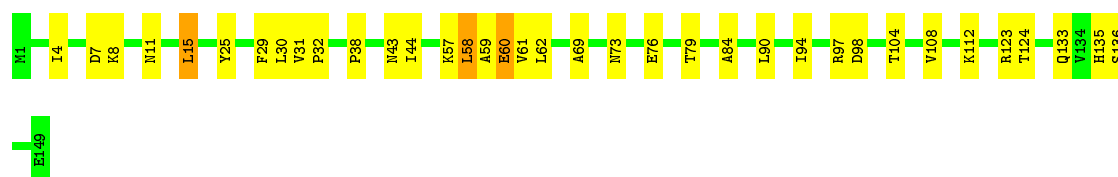
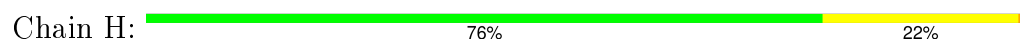
- Molecule 6: 50S ribosomal protein L5



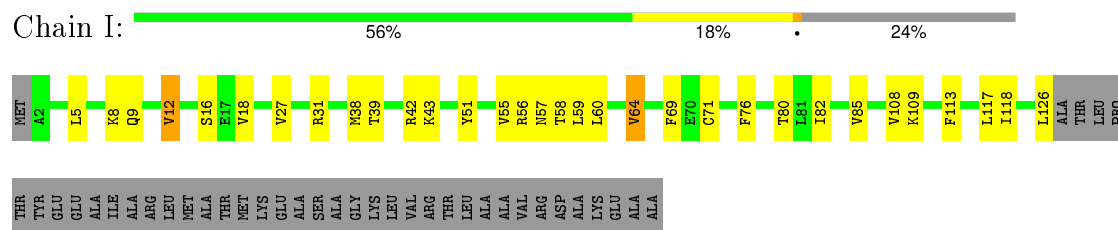
- Molecule 7: 50S ribosomal protein L6



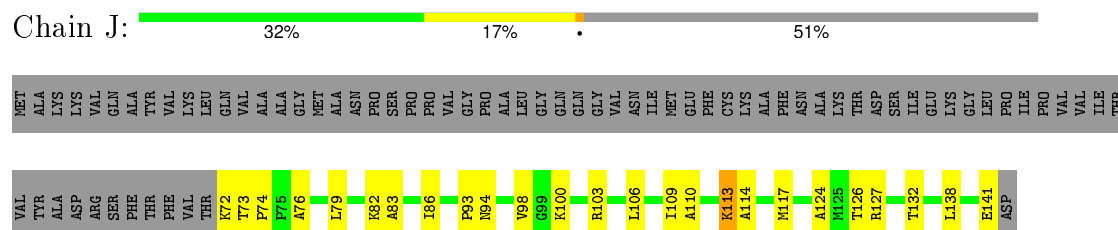
- Molecule 8: 50S ribosomal protein L9



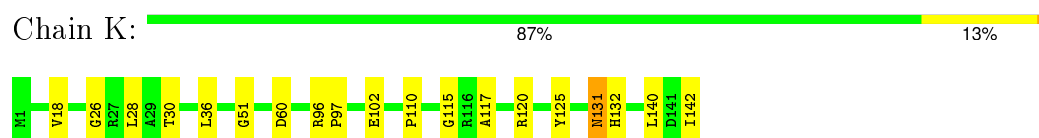
- Molecule 9: 50S ribosomal protein L10



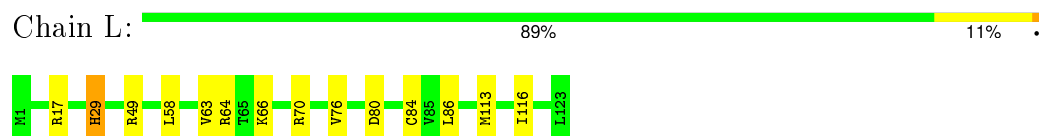
- Molecule 10: 50S ribosomal protein L11



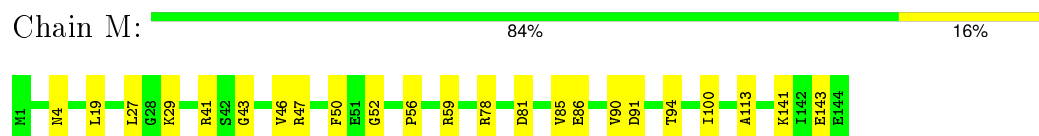
- Molecule 11: 50S ribosomal protein L13



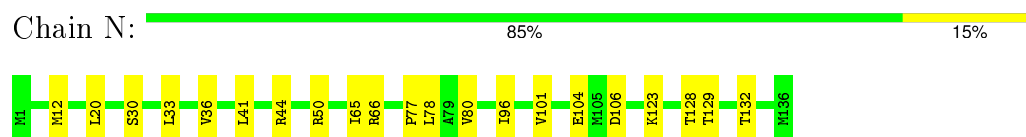
- Molecule 12: 50S ribosomal protein L14



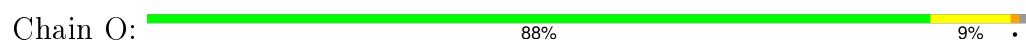
- Molecule 13: 50S ribosomal protein L15



- Molecule 14: 50S ribosomal protein L16



- Molecule 15: 50S ribosomal protein L17





- Molecule 16: 50S ribosomal protein L18

Chain P: 90% 9%



- Molecule 17: 50S ribosomal protein L19

Chain Q: 78% 21%



- Molecule 18: 50S ribosomal protein L20

Chain R: 84% 15%



- Molecule 19: 50S ribosomal protein L21

Chain S: 84% 15%



- Molecule 20: 50S ribosomal protein L22

Chain T: 93% 7%



- Molecule 21: 50S ribosomal protein L23

Chain U: 79% 16% 5%

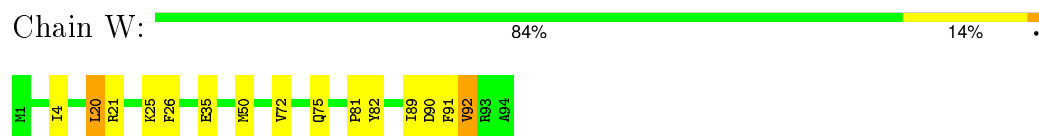


- Molecule 22: 50S ribosomal protein L24

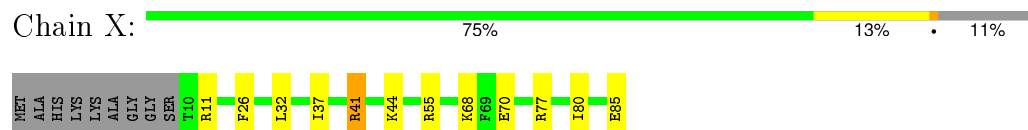
Chain V: 82% 16%



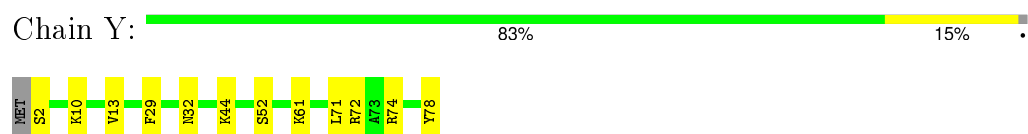
- Molecule 23: 50S ribosomal protein L25



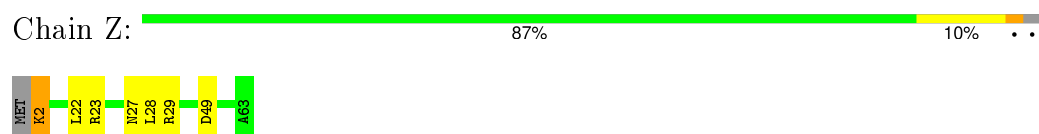
- Molecule 24: 50S ribosomal protein L27



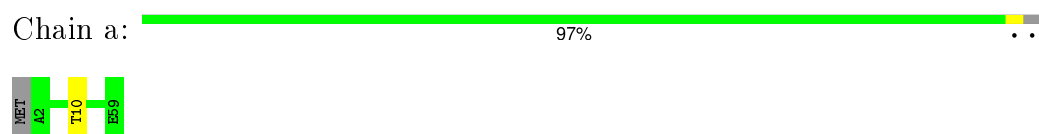
- Molecule 25: 50S ribosomal protein L28



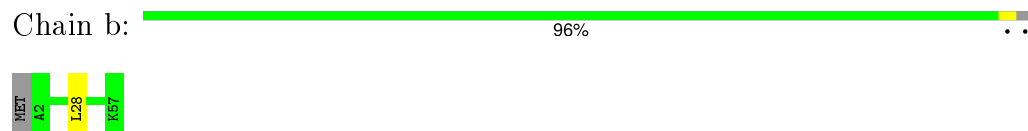
- Molecule 26: 50S ribosomal protein L29



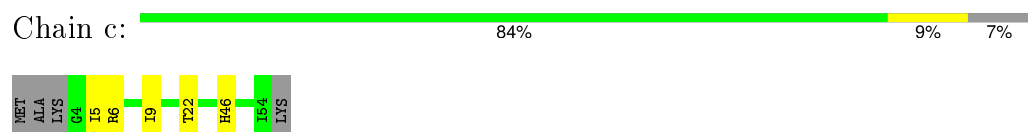
- Molecule 27: 50S ribosomal protein L30



- Molecule 28: 50S ribosomal protein L32



- Molecule 29: 50S ribosomal protein L33



- Molecule 30: 50S ribosomal protein L34





- Molecule 31: 50S ribosomal protein L35

Chain e: 92% 6%



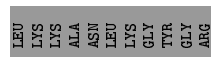
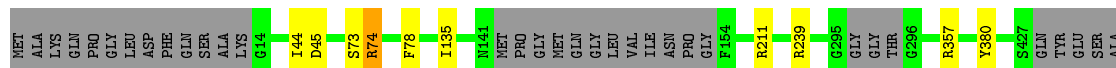
- Molecule 32: 50S ribosomal protein L36

Chain f: 95% 5%



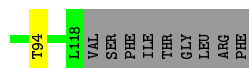
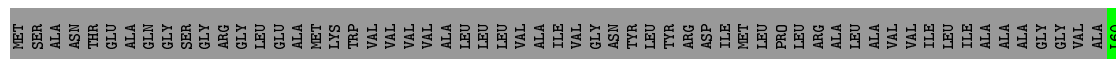
- Molecule 33: Protein translocase subunit SecY

Chain g: 88% 10%



- Molecule 34: Protein translocase subunit SecE

Chain h: 46% 54%



- Molecule 35: SecG

Chain i: 100%

There are no outlier residues recorded for this chain.

- Molecule 36: tRNA CCA end (5'-R(P*CP*CP*A)-3')

Chain x: 67% 33%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	216907	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	59000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG

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	A	0.56	0/69352	0.96	54/108188 (0.0%)
10	J	0.45	0/504	0.54	0/673
11	K	0.37	0/1152	0.50	0/1551
12	L	0.38	0/955	0.55	0/1279
13	M	0.36	0/1062	0.55	0/1413
14	N	0.39	0/1093	0.52	0/1460
15	O	0.39	0/1006	0.56	0/1345
16	P	0.31	0/910	0.47	0/1219
17	Q	0.39	0/929	0.54	0/1242
18	R	0.48	0/960	0.55	0/1278
19	S	0.38	0/829	0.53	0/1107
2	B	0.44	0/2872	0.89	2/4478 (0.0%)
20	T	0.38	0/864	0.58	0/1156
21	U	0.35	0/763	0.51	0/1021
22	V	0.32	0/787	0.47	0/1051
23	W	0.31	0/766	0.50	0/1025
24	X	0.42	0/587	0.53	0/776
25	Y	0.38	0/635	0.52	0/848
26	Z	0.30	0/502	0.41	0/667
27	a	0.34	0/453	0.51	0/605
28	b	0.37	0/450	0.54	0/599
29	c	0.32	0/421	0.48	0/561
3	C	0.36	0/2121	0.54	0/2852
30	d	0.41	0/380	0.57	0/498
31	e	0.37	0/513	0.55	0/676
32	f	0.31	0/303	0.48	0/397
33	g	0.45	0/3169	0.53	0/4299
34	h	0.48	0/465	0.47	0/633
36	x	0.32	0/68	0.99	0/103
4	D	0.38	0/1586	0.55	0/2134
5	E	0.37	0/1571	0.50	0/2113
6	F	0.36	0/1434	0.50	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
7	G	0.30	0/1343	0.48	0/1816
8	H	0.34	0/1121	0.48	0/1515
9	I	0.45	0/958	0.52	0/1292
All	All	0.51	0/102884	0.86	56/153796 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	C	0	1
33	g	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 56 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1607	C	N1-C2-O2	8.21	123.82	118.90
1	A	550	C	C2-N1-C1'	7.67	127.24	118.80
1	A	1607	C	N3-C2-O2	-7.58	116.59	121.90
1	A	280	U	C6-N1-C2	-7.38	116.57	121.00
1	A	1584	U	C2-N1-C1'	7.33	126.50	117.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	232	HIS	Peptide
33	g	74	ARG	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	A	61923	0	31144	436	0
2	B	2569	0	1301	24	0
3	C	2082	0	2154	35	0
4	D	1565	0	1616	20	0
5	E	1552	0	1619	17	0
6	F	1410	0	1444	36	0
7	G	1323	0	1371	24	0
8	H	1110	0	1148	21	0
9	I	946	0	978	19	0
10	J	502	0	540	17	0
11	K	1129	0	1162	13	0
12	L	946	0	1023	8	0
13	M	1053	0	1129	15	0
14	N	1074	0	1157	12	0
15	O	993	0	1034	7	0
16	P	900	0	935	9	0
17	Q	917	0	962	13	0
18	R	947	0	1019	12	0
19	S	816	0	839	6	0
20	T	857	0	922	4	0
21	U	756	0	817	9	0
22	V	779	0	831	9	0
23	W	753	0	780	10	0
24	X	580	0	594	9	0
25	Y	625	0	652	6	0
26	Z	501	0	531	5	0
27	a	449	0	488	0	0
28	b	444	0	458	0	0
29	c	414	0	442	0	0
30	d	377	0	418	0	0
31	e	504	0	572	0	0
32	f	302	0	341	0	0
33	g	3099	0	3246	0	0
34	h	459	0	503	0	0
35	i	150	0	153	0	0
36	x	62	0	34	0	0
37	A	313	0	0	0	0
37	B	8	0	0	0	0
37	R	1	0	0	0	0
37	b	1	0	0	0	0
38	f	1	0	0	0	0
All	All	95192	0	64357	700	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 6.

The worst 5 of 700 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)
6:F:106:ILE:HD12	6:F:139:PRO:HG2	1.54	0.85
1:A:1852:U:O2	1:A:1890:A:N6	2.09	0.85
1:A:1865:U:O2	1:A:1876:A:N6	2.11	0.83
3:C:154:LEU:HD13	3:C:176:LEU:HD21	1.63	0.81
13:M:56:PRO:HG2	13:M:59:ARG:HG3	1.62	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
4	D	207/209 (99%)	203 (98%)	4 (2%)	0	100	100
5	E	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
6	F	175/179 (98%)	170 (97%)	5 (3%)	0	100	100
7	G	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
8	H	147/149 (99%)	137 (93%)	10 (7%)	0	100	100
9	I	123/165 (74%)	114 (93%)	8 (6%)	1 (1%)	24	64
10	J	68/142 (48%)	64 (94%)	4 (6%)	0	100	100
11	K	140/142 (99%)	137 (98%)	3 (2%)	0	100	100
12	L	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
13	M	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
14	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
15	O	123/127 (97%)	120 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
17	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
18	R	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
19	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
20	T	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
21	U	93/100 (93%)	89 (96%)	4 (4%)	0	100	100
22	V	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
23	W	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
24	X	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
25	Y	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
26	Z	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
27	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
28	b	54/57 (95%)	54 (100%)	0	0	100	100
29	c	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
30	d	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
31	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
32	f	36/38 (95%)	36 (100%)	0	0	100	100
33	g	393/443 (89%)	370 (94%)	22 (6%)	1 (0%)	46	81
34	h	57/127 (45%)	55 (96%)	2 (4%)	0	100	100
All	All	3818/4144 (92%)	3700 (97%)	116 (3%)	2 (0%)	59	89

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
33	g	135	ILE
9	I	108	VAL

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	
3	C	216/218 (99%)	207 (96%)	9 (4%)	36	73
4	D	164/164 (100%)	160 (98%)	4 (2%)	57	84
5	E	165/165 (100%)	162 (98%)	3 (2%)	66	86
6	F	148/150 (99%)	135 (91%)	13 (9%)	12	43
7	G	137/138 (99%)	133 (97%)	4 (3%)	50	81
8	H	114/114 (100%)	108 (95%)	6 (5%)	28	66
9	I	95/123 (77%)	88 (93%)	7 (7%)	17	53
10	J	52/110 (47%)	50 (96%)	2 (4%)	40	76
11	K	116/116 (100%)	115 (99%)	1 (1%)	84	93
12	L	104/104 (100%)	98 (94%)	6 (6%)	25	64
13	M	103/103 (100%)	101 (98%)	2 (2%)	65	86
14	N	109/109 (100%)	106 (97%)	3 (3%)	51	82
15	O	102/103 (99%)	98 (96%)	4 (4%)	39	75
16	P	87/87 (100%)	86 (99%)	1 (1%)	80	91
17	Q	99/100 (99%)	94 (95%)	5 (5%)	29	68
18	R	89/90 (99%)	85 (96%)	4 (4%)	34	72
19	S	84/84 (100%)	77 (92%)	7 (8%)	14	47
20	T	93/93 (100%)	92 (99%)	1 (1%)	80	91
21	U	82/84 (98%)	79 (96%)	3 (4%)	41	76
22	V	83/85 (98%)	79 (95%)	4 (5%)	31	70
23	W	78/78 (100%)	75 (96%)	3 (4%)	40	76
24	X	57/63 (90%)	54 (95%)	3 (5%)	28	66
25	Y	67/68 (98%)	65 (97%)	2 (3%)	48	80
26	Z	54/55 (98%)	53 (98%)	1 (2%)	65	86
27	a	48/49 (98%)	47 (98%)	1 (2%)	61	85
28	b	47/48 (98%)	46 (98%)	1 (2%)	61	85
29	c	45/49 (92%)	40 (89%)	5 (11%)	8	30
30	d	38/38 (100%)	35 (92%)	3 (8%)	15	50
31	e	51/52 (98%)	47 (92%)	4 (8%)	16	50
32	f	34/34 (100%)	32 (94%)	2 (6%)	24	63
33	g	327/359 (91%)	318 (97%)	9 (3%)	51	82
34	h	49/99 (50%)	48 (98%)	1 (2%)	63	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3137/3332 (94%)	3013 (96%)	124 (4%)	42 74

5 of 124 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	M	86	GLU
17	Q	92	VAL
33	g	44	ILE
14	N	12	MET
15	O	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	43	ASN
14	N	13	HIS
26	Z	27	ASN
12	L	29	HIS
6	F	27	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2903 (99%)	438 (15%)	14 (0%)
2	B	119/120 (99%)	17 (14%)	1 (0%)
36	x	2/3 (66%)	1 (50%)	0
All	All	3000/3026 (99%)	456 (15%)	15 (0%)

5 of 456 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U
1	A	14	A
1	A	15	G
1	A	46	G

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1344	U
1	A	1454	C
1	A	2601	C
1	A	901	C
1	A	2158	A

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 324 ligands modelled in this entry, 324 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
33	g	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	g	398:PRO	C	399:PHE	N	5.57
1	A	2789:C	O3'	2790:U	P	3.00