wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:47 PM BST

PDB ID	:	5GAD
EMDB ID:	:	EMD-8000
Title	:	RNC-SRP-SR complex early state
Authors	:	Jomaa, A.; Boehringer, D.; Leibundgut, M.; Ban, N.
Deposited on	:	2015-11-24
Resolution	:	3.70 Å(reported)
Based on PDB ID	:	?

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

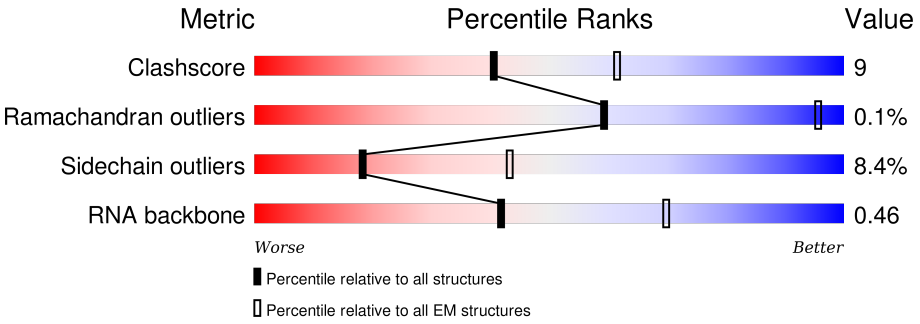
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.70 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 <=5%

Mol	Chain	Length	Quality of chain
1	1	113	12% 15% 11% • 62%
2	2	3	33% 33% 33%
3	A	2903	54% 37% 8% ••
4	B	120	73% 24% •
5	C	273	70% 26% ••
6	D	209	78% 21% •
7	E	201	78% 21% •
8	F	179	59% 35% ••

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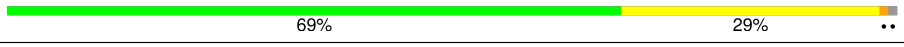
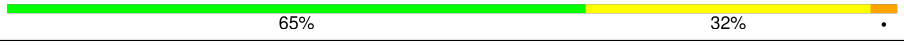
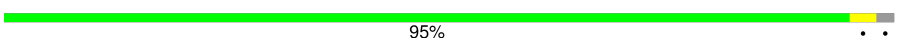
Mol	Chain	Length	Quality of chain
9	G	177	
10	H	149	
11	I	165	
12	J	142	
13	K	142	
14	L	123	
15	M	144	
16	N	136	
17	O	127	
18	P	117	
19	Q	115	
20	R	118	
21	S	103	
22	T	110	
23	U	100	
24	V	104	
25	W	94	
26	X	85	
27	Y	78	
28	Z	63	
29	a	59	
30	b	57	
31	c	55	
32	d	46	
33	e	65	

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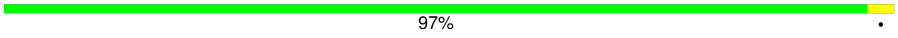
Mol	Chain	Length	Quality of chain
34	f	38	
35	i	450	
36	k	18	
37	l	497	

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 98006 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 ESRP 4.5S RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	43	926	413	174	296	43	0	0

- Molecule 2 is a RNA chain called tRNA CCAend.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	3	62	28	11	20	3	0	0

- Molecule 3 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	A	2883	61902	27613	11397	20009	2883	0	0

- Molecule 4 is a RNA chain called 5S rRNA.

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

- Molecule 5 is a protein called 50S ribosomal protein L2.

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

- Molecule 6 is a protein called 50S ribosomal protein L3.

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

- Molecule 7 is a protein called 50S ribosomal protein L4.

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

- Molecule 8 is a protein called 50S ribosomal protein L5.

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

- Molecule 9 is a protein called 50S ribosomal protein L6.

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

- Molecule 10 is a protein called 50S ribosomal protein L9.

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

- Molecule 11 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	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 12 is a protein called 50S ribosomal protein L11.

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

- Molecule 13 is a protein called 50S ribosomal protein L13.

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

- Molecule 14 is a protein called 50S ribosomal protein L14.

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

- Molecule 15 is a protein called 50S ribosomal protein L15.

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

- Molecule 16 is a protein called 50S ribosomal protein L16.

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

- Molecule 17 is a protein called 50S ribosomal protein L17.

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

- Molecule 18 is a protein called 50S ribosomal protein L18.

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

- Molecule 19 is a protein called 50S ribosomal protein L19.

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

- Molecule 20 is a protein called 50S ribosomal protein L20.

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

- Molecule 21 is a protein called 50S ribosomal protein L21.

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

- Molecule 22 is a protein called 50S ribosomal protein L22.

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

- Molecule 23 is a protein called 50S ribosomal protein L23.

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

- Molecule 24 is a protein called 50S ribosomal protein L24.

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

- Molecule 25 is a protein called 50S ribosomal protein L25.

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

- Molecule 26 is a protein called 50S ribosomal protein L27.

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

- Molecule 27 is a protein called 50S ribosomal protein L28.

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

- Molecule 28 is a protein called 50S ribosomal protein L29.

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

- Molecule 29 is a protein called 50S ribosomal protein L30.

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

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called 50S ribosomal protein L33.

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

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called Signal recognition particle protein Ffh.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	450	Total	C	N	O	S	0	0
			3337	2109	600	610	18		

- Molecule 36 is a protein called 1A9L SS.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	18	Total	C	N	O	S	0	0
			137	94	20	22	1		

- Molecule 37 is a protein called Signal recognition particle receptor FtsY.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	198	Total	C	N	O	S	0	0
			1492	944	266	277	5		

- Molecule 38 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
38	P	1	Total	Mg	0
			1	1	
38	i	1	Total	Mg	0
			1	1	
38	D	1	Total	Mg	0
			1	1	
38	E	1	Total	Mg	0
			1	1	
38	B	11	Total	Mg	0
			11	11	
38	b	1	Total	Mg	0
			1	1	
38	C	2	Total	Mg	0
			2	2	
38	A	412	Total	Mg	0
			412	412	
38	2	1	Total	Mg	0
			1	1	

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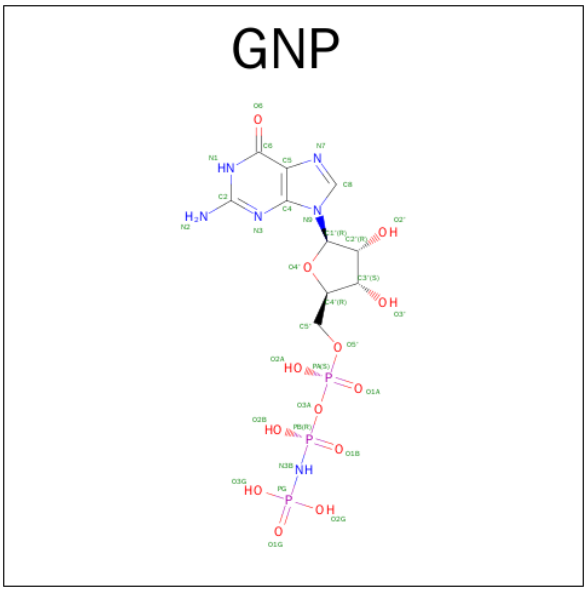
Mol	Chain	Residues	Atoms	AltConf
38	l	1	Total Mg 1 1	0
38	R	1	Total Mg 1 1	0

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 40 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



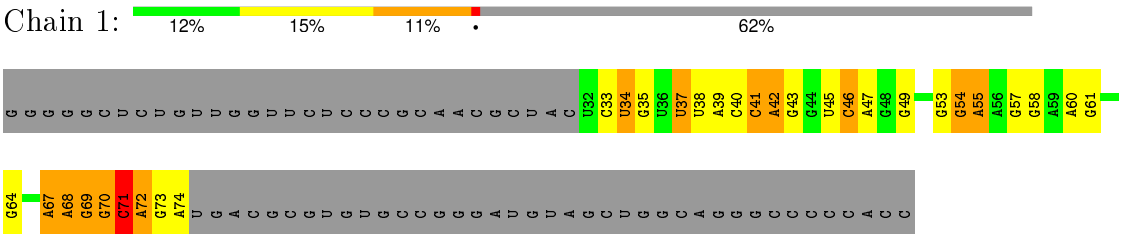
Mol	Chain	Residues	Atoms	AltConf
40	i	1	Total C N O P 32 10 6 13 3	0
40	l	1	Total C N O P 32 10 6 13 3	0

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.

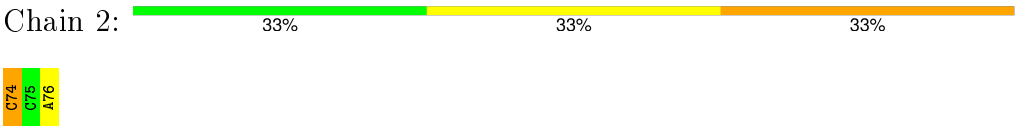
- Molecule 1: ESRP 4.5S RNA

Chain 1:



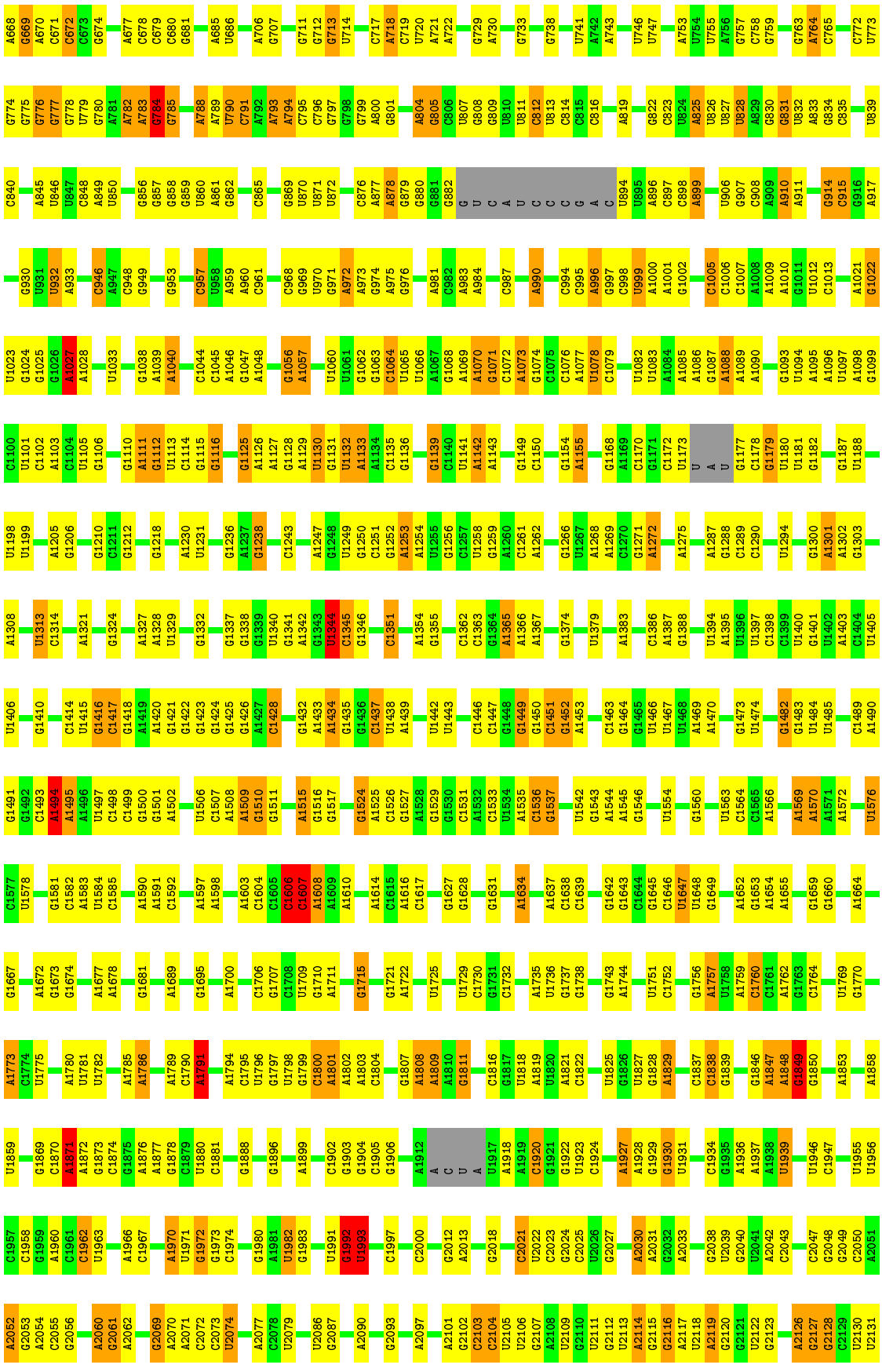
- Molecule 2: tRNA CCAend

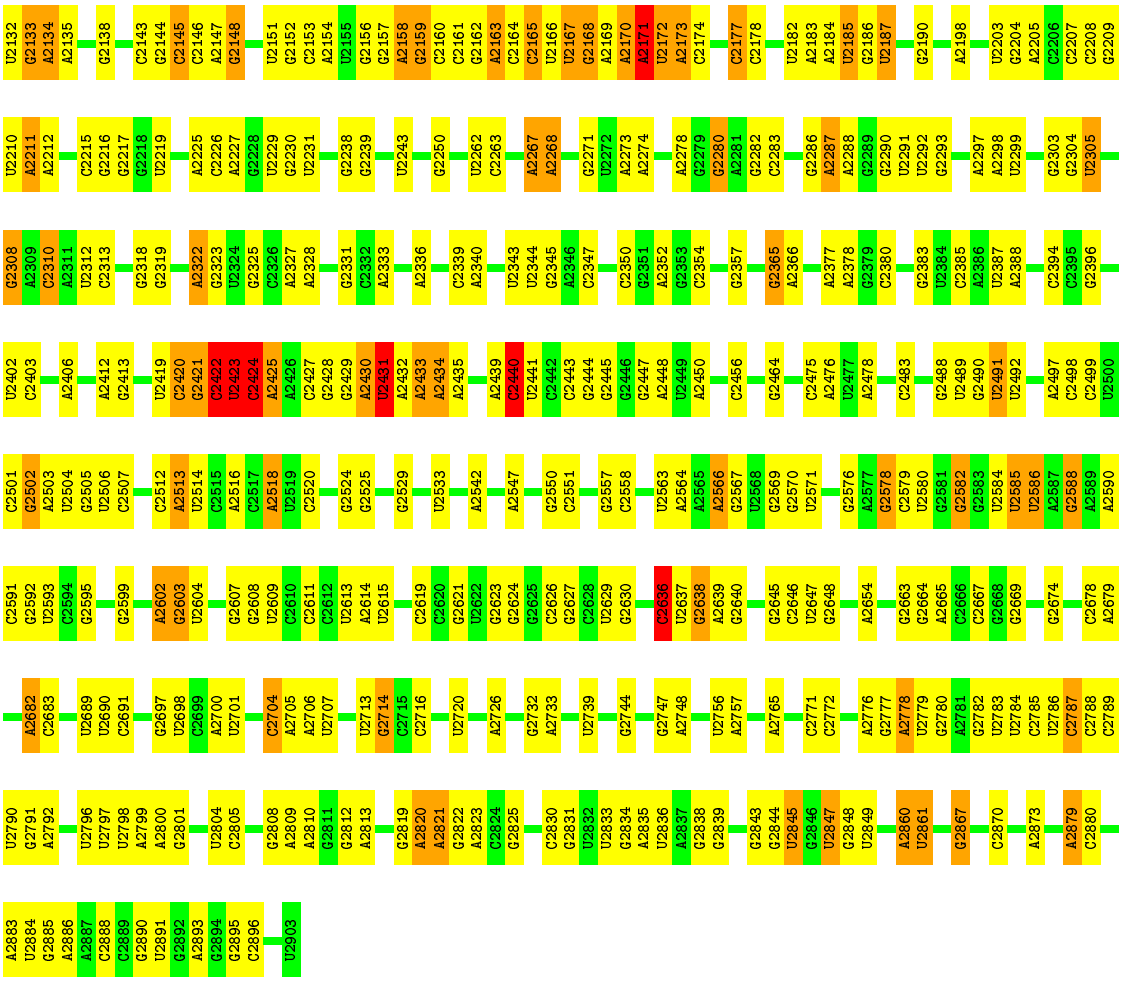
Chain 2:



- Molecule 3: 23S rRNA

Chain A:



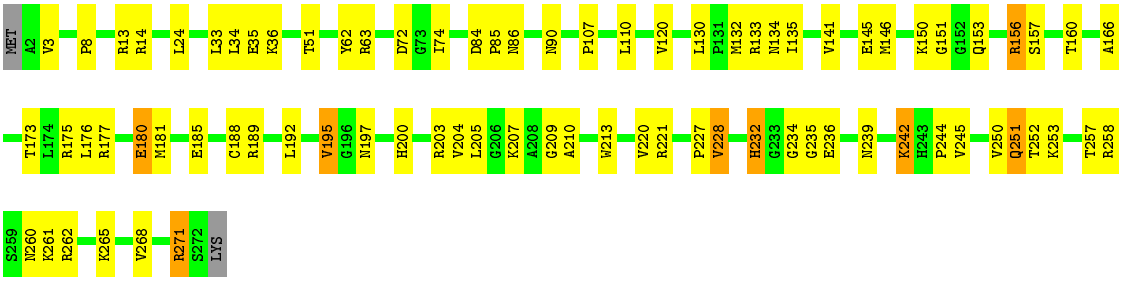


- Molecule 4: 5S rRNA

Chain B:

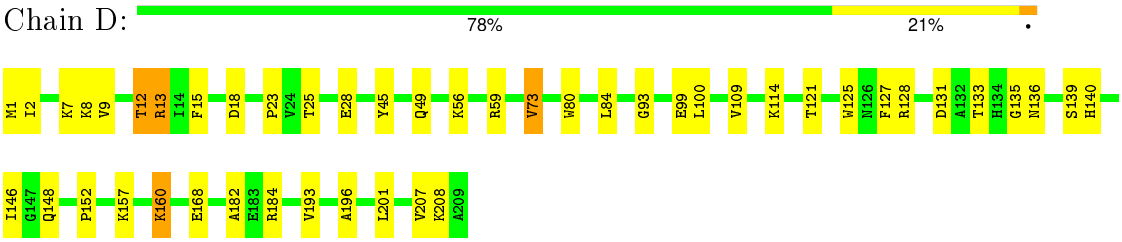
- Molecule 5: 50S ribosomal protein L2

Chain C:



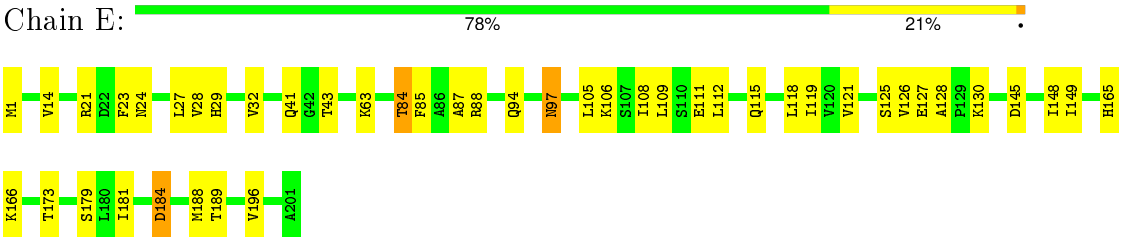
- Molecule 6: 50S ribosomal protein L3

Chain D:



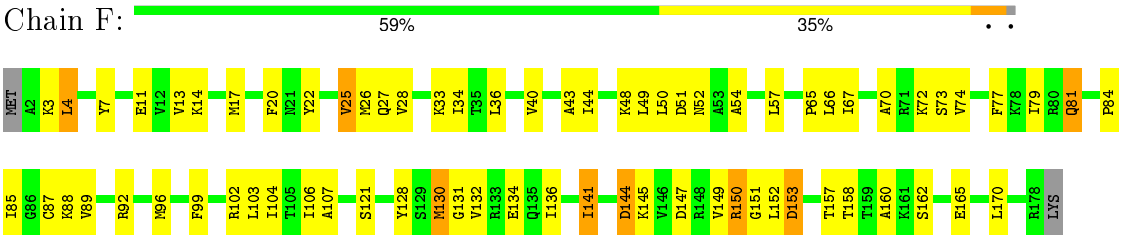
• Molecule 7: 50S ribosomal protein L4

Chain E:



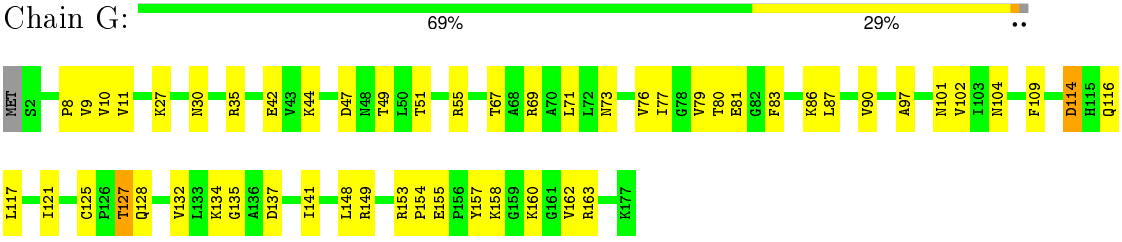
• Molecule 8: 50S ribosomal protein L5

Chain F:



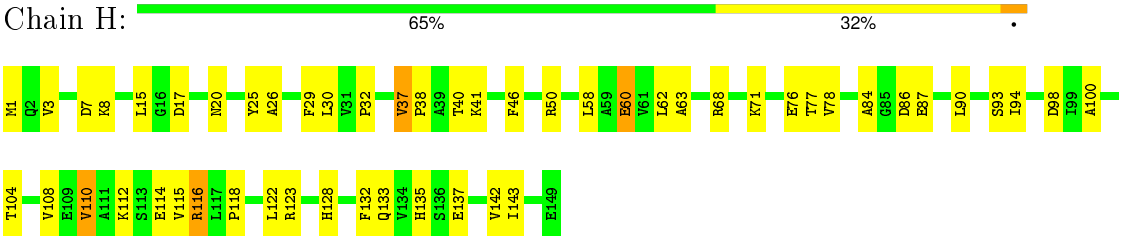
• Molecule 9: 50S ribosomal protein L6

Chain G:



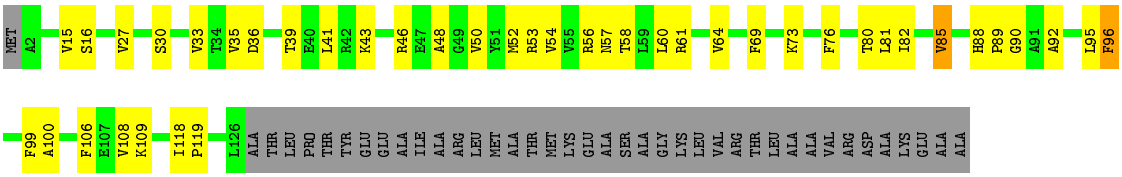
• Molecule 10: 50S ribosomal protein L9

Chain H:



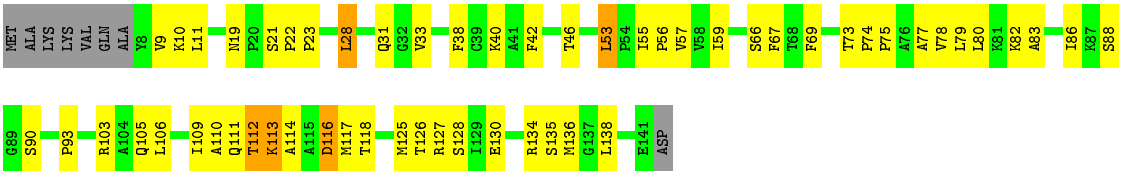
• Molecule 11: 50S ribosomal protein L10

Chain I:



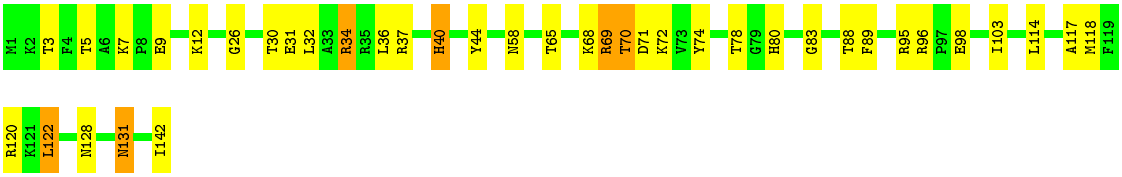
- Molecule 12: 50S ribosomal protein L11

Chain J:



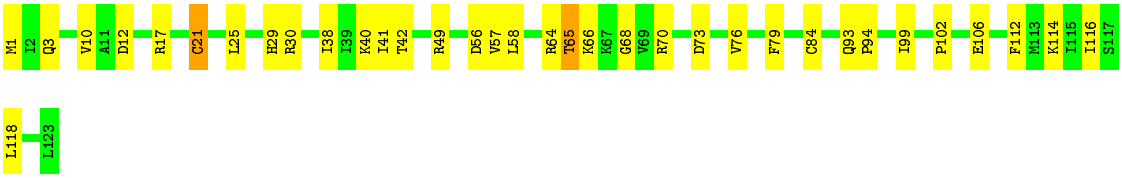
- Molecule 13: 50S ribosomal protein L13

Chain K:



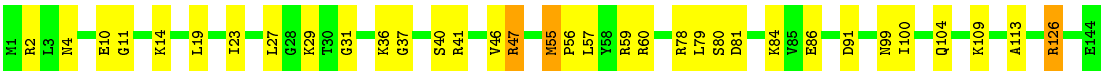
- Molecule 14: 50S ribosomal protein L14

Chain L:



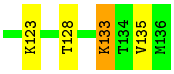
- Molecule 15: 50S ribosomal protein L15

Chain M:



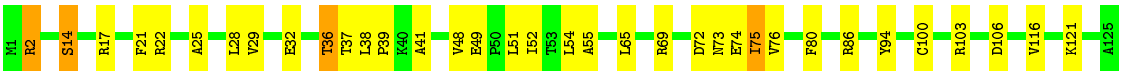
- Molecule 16: 50S ribosomal protein L16

Chain N:



• Molecule 17: 50S ribosomal protein L17

Chain O:



• Molecule 18: 50S ribosomal protein L18

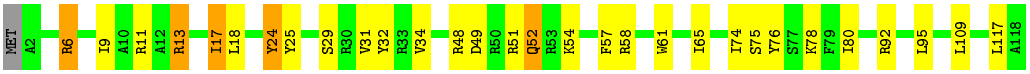
Chain P:

• Molecule 19: 50S ribosomal protein L19

Chain Q:

• Molecule 20: 50S ribosomal protein L20

Chain R:

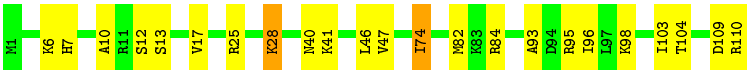


• Molecule 21: 50S ribosomal protein L21

Chain S:

• Molecule 22: 50S ribosomal protein L22

Chain T:

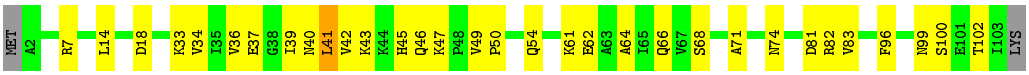


• Molecule 23: 50S ribosomal protein L23

Chain U:

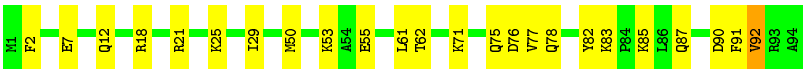
• Molecule 24: 50S ribosomal protein L24

Chain V:



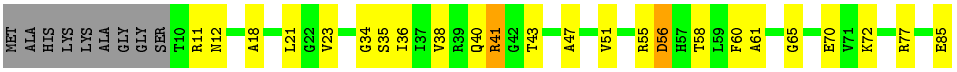
• Molecule 25: 50S ribosomal protein L25

Chain W:



• Molecule 26: 50S ribosomal protein L27

Chain X:

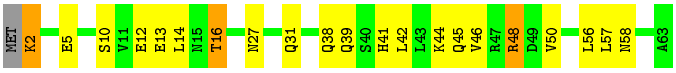


• Molecule 27: 50S ribosomal protein L28

Chain Y:

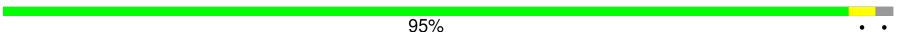
• Molecule 28: 50S ribosomal protein L29

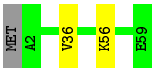
Chain Z:



• Molecule 29: 50S ribosomal protein L30

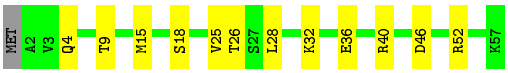
Chain a:





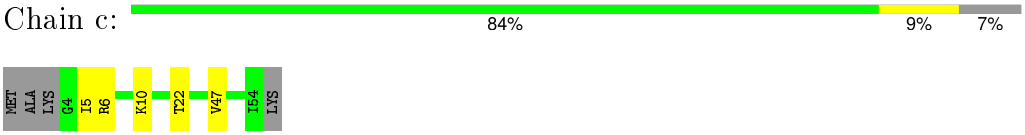
• Molecule 30: 50S ribosomal protein L32

Chain b:



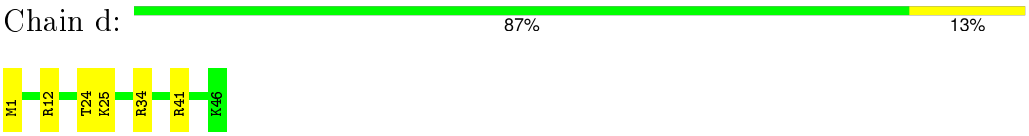
- Molecule 31: 50S ribosomal protein L33

Chain c:



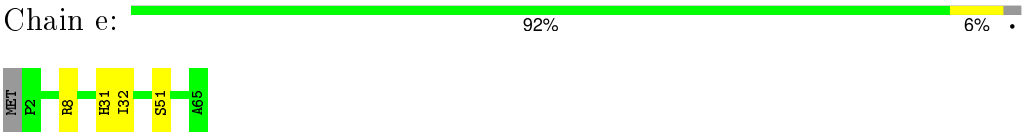
- Molecule 32: 50S ribosomal protein L34

Chain d:



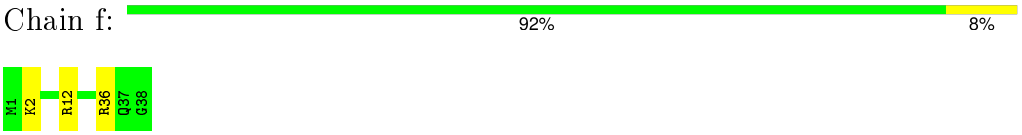
- Molecule 33: 50S ribosomal protein L35

Chain e:



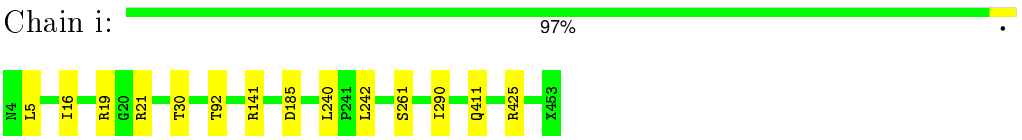
- Molecule 34: 50S ribosomal protein L36

Chain f:



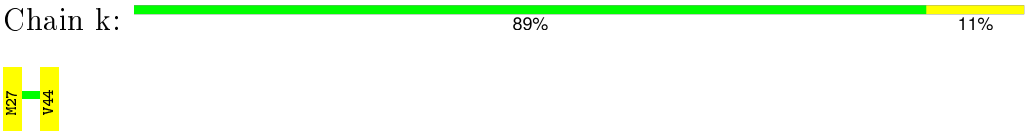
- Molecule 35: Signal recognition particle protein Ffh

Chain i:



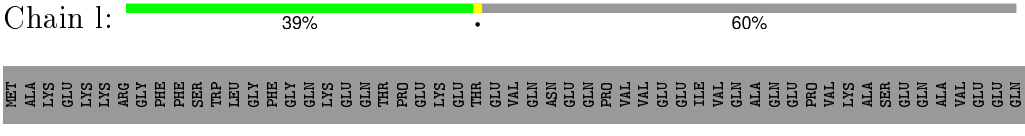
- Molecule 36: 1A9L SS

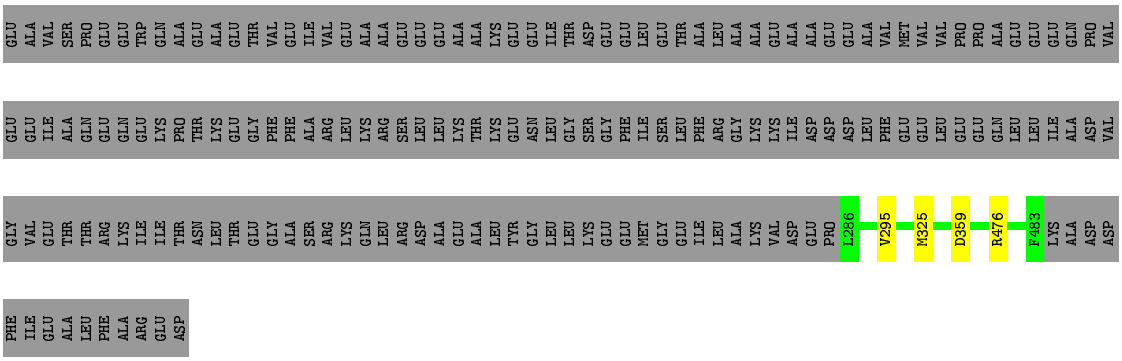
Chain k:



- Molecule 37: Signal recognition particle receptor FtsY

Chain l:




GLU ALA VAL SER PRO GLU GLU TRP GLN ALA GLU ALA GLU THR VAL GLU ILE VAL GLU ALA ALA GLU GLU GLU ALA ALA LYS GLU GLU ILE THR ASP GLU GLU LEU GLU THR ALA LEU ALA ALA GLU ALA ALA GLU GLU ALA VAL MET VAL VAL PRO PRO ALA GLU GLU GLN PRO VAL
GLU GLU ILE ALA GLN GLU GLN GLU LYS PRO THR LYS GLU GLY PHE PHE ALA ARG LEU LYS ARG SER LEU LEU LYS THR LYS GLU ASN LEU GLY SER GLY PHE ILE SER LEU PHE ARG GLY LYS LYS ILE ASP ASP LEU PHE GLU GLU LEU GLU GLU GLN LEU LEU ILE ALA ASP VAL
GLY VAL GLU THR THR ARG LYS ILE ILE THR ASN LEU THR GLU GLY ALA SER ARG LYS GLN LEU ARG ASP ALA GLU ALA LEU TYR GLY LEU LEU LYS GLU GLU MET GLY GLU ILE LEU ALA LYS VAL ASP GLU PRO L286 V295 M325 D359 R476 F483 LYS ALA ASP ASP
PHE ILE GLU ALA LEU PHE ALA ARG GLU ASP

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	81197	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 ($e^-/Å^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	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, GNP

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	1	0.30	0/1037	0.99	2/1616 (0.1%)
10	H	0.42	0/1121	0.57	0/1515
11	I	0.48	0/958	0.62	1/1292 (0.1%)
12	J	0.58	0/993	0.69	1/1341 (0.1%)
13	K	0.46	0/1152	0.57	0/1551
14	L	0.45	0/955	0.63	0/1279
15	M	0.47	0/1062	0.64	0/1413
16	N	0.48	0/1093	0.59	0/1460
17	O	0.47	0/1006	0.67	0/1345
18	P	0.41	0/910	0.56	0/1219
19	Q	0.48	0/929	0.60	0/1242
2	2	0.56	0/68	1.26	1/103 (1.0%)
20	R	0.56	0/960	0.59	0/1278
21	S	0.46	0/829	0.62	0/1107
22	T	0.52	0/864	0.71	0/1156
23	U	0.64	3/763 (0.4%)	0.73	1/1021 (0.1%)
24	V	0.38	0/787	0.54	0/1051
25	W	0.40	0/766	0.57	0/1025
26	X	0.50	0/587	0.60	0/776
27	Y	0.48	0/635	0.61	0/848
28	Z	0.33	0/500	0.47	0/661
29	a	0.38	0/453	0.56	0/605
3	A	0.68	13/69329 (0.0%)	1.17	188/108152 (0.2%)
30	b	0.43	0/450	0.62	0/599
31	c	0.44	0/421	0.61	0/561
32	d	0.51	0/380	0.66	0/498
33	e	0.47	0/513	0.62	0/676
34	f	0.49	0/303	0.58	0/397
35	i	0.31	0/2942	0.51	0/3950
36	k	0.32	0/137	0.58	0/186
37	l	0.37	0/1511	1.08	3/2040 (0.1%)
4	B	0.51	0/2872	1.04	1/4478 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >2	RMSZ	#|Z| >2
5	C	0.48	0/2121	0.65	0/2852
6	D	0.47	0/1586	0.63	0/2134
7	E	0.44	0/1571	0.61	1/2113 (0.0%)
8	F	0.39	0/1434	0.56	0/1926
9	G	0.39	0/1343	0.58	0/1816
All	All	0.61	16/105341 (0.0%)	1.04	199/157282 (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
12	J	0	1
35	i	0	1
5	C	0	1
9	G	0	1
All	All	0	4

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2542	A	N9-C4	-6.88	1.33	1.37
23	U	89	GLU	N-CA	6.84	1.60	1.46
3	A	1254	A	N9-C4	-6.35	1.34	1.37
3	A	2114	A	N9-C4	6.24	1.41	1.37
3	A	1321	A	N9-C4	6.01	1.41	1.37

The worst 5 of 199 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	l	476	ARG	NE-CZ-NH2	-25.15	107.72	120.30
37	l	476	ARG	NE-CZ-NH1	-25.05	107.78	120.30
37	l	476	ARG	NH1-CZ-NH2	22.82	144.50	119.40
3	A	2423	U	C6-N1-C2	-12.22	113.67	121.00
3	A	1838	C	C6-N1-C2	9.47	124.09	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	C	232	HIS	Peptide
9	G	47	ASP	Peptide
12	J	19	ASN	Peptide
35	i	240	LEU	Peptide

5.2 Too-close contacts (i)

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	1	926	0	467	26	0
2	2	62	0	34	1	0
3	A	61902	0	31133	685	0
4	B	2569	0	1301	20	0
5	C	2082	0	2154	51	0
6	D	1565	0	1616	35	0
7	E	1552	0	1619	24	0
8	F	1410	0	1444	43	0
9	G	1323	0	1371	32	0
10	H	1110	0	1148	25	0
11	I	946	0	978	31	0
12	J	979	0	1028	38	0
13	K	1129	0	1162	24	0
14	L	946	0	1023	19	0
15	M	1053	0	1129	26	0
16	N	1074	0	1157	23	0
17	O	993	0	1034	25	0
18	P	900	0	935	20	0
19	Q	917	0	962	18	0
20	R	947	0	1019	23	0
21	S	816	0	839	20	0
22	T	857	0	922	13	0
23	U	756	0	817	21	0
24	V	779	0	831	18	0
25	W	753	0	780	14	0
26	X	580	0	594	16	0
27	Y	625	0	652	17	0
28	Z	501	0	529	16	0
29	a	449	0	488	0	0
30	b	444	0	458	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	c	414	0	442	0	0
32	d	377	0	418	0	0
33	e	504	0	572	0	0
34	f	302	0	340	0	0
35	i	3337	0	3457	0	0
36	k	137	0	168	0	0
37	l	1492	0	1544	0	0
38	2	1	0	0	0	0
38	A	412	0	0	0	0
38	B	11	0	0	0	0
38	C	2	0	0	0	0
38	D	1	0	0	0	0
38	E	1	0	0	0	0
38	P	1	0	0	0	0
38	R	1	0	0	0	0
38	b	1	0	0	0	0
38	i	1	0	0	0	0
38	l	1	0	0	0	0
39	f	1	0	0	0	0
40	i	32	0	13	0	0
40	l	32	0	13	0	0
All	All	98006	0	66591	1182	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 9.

The worst 5 of 1182 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)
3:A:1818:U:OP2	5:C:156:ARG:NH1	2.00	0.95
3:A:1168:G:H1	3:A:1181:U:H3	1.20	0.90
23:U:53:VAL:HG21	23:U:93:LEU:HD11	1.53	0.89
3:A:276:U:O2	3:A:278:A:N6	2.07	0.87
10:H:3:VAL:HG12	10:H:38:PRO:HA	1.57	0.86

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	
5	C	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
6	D	207/209 (99%)	201 (97%)	6 (3%)	0	100	100
7	E	199/201 (99%)	190 (96%)	9 (4%)	0	100	100
8	F	175/179 (98%)	166 (95%)	9 (5%)	0	100	100
9	G	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
10	H	147/149 (99%)	137 (93%)	9 (6%)	1 (1%)	26	72
11	I	123/165 (74%)	113 (92%)	9 (7%)	1 (1%)	24	70
12	J	132/142 (93%)	126 (96%)	6 (4%)	0	100	100
13	K	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
14	L	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
15	M	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
16	N	134/136 (98%)	131 (98%)	3 (2%)	0	100	100
17	O	123/127 (97%)	118 (96%)	5 (4%)	0	100	100
18	P	115/117 (98%)	112 (97%)	3 (3%)	0	100	100
19	Q	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
20	R	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
21	S	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
22	T	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
23	U	93/100 (93%)	89 (96%)	3 (3%)	1 (1%)	17	65
24	V	100/104 (96%)	99 (99%)	1 (1%)	0	100	100
25	W	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
26	X	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
27	Y	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
28	Z	56/63 (89%)	54 (96%)	2 (4%)	0	100	100
29	a	56/59 (95%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
30	b	54/57 (95%)	50 (93%)	4 (7%)	0	100 100
31	c	49/55 (89%)	48 (98%)	1 (2%)	0	100 100
32	d	44/46 (96%)	43 (98%)	1 (2%)	0	100 100
33	e	62/65 (95%)	59 (95%)	3 (5%)	0	100 100
34	f	36/38 (95%)	36 (100%)	0	0	100 100
35	i	378/450 (84%)	361 (96%)	17 (4%)	0	100 100
36	k	16/18 (89%)	11 (69%)	5 (31%)	0	100 100
37	l	196/497 (39%)	189 (96%)	7 (4%)	0	100 100
All	All	4018/4539 (88%)	3876 (96%)	139 (4%)	3 (0%)	59 90

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	U	89	GLU
10	H	118	PRO
11	I	108	VAL

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
5	C	216/218 (99%)	192 (89%)	24 (11%)	8 39
6	D	164/164 (100%)	154 (94%)	10 (6%)	23 65
7	E	165/165 (100%)	152 (92%)	13 (8%)	15 55
8	F	148/150 (99%)	130 (88%)	18 (12%)	6 34
9	G	137/138 (99%)	129 (94%)	8 (6%)	25 67
10	H	114/114 (100%)	100 (88%)	14 (12%)	6 34
11	I	95/123 (77%)	89 (94%)	6 (6%)	22 64
12	J	104/110 (94%)	93 (89%)	11 (11%)	8 42
13	K	116/116 (100%)	105 (90%)	11 (10%)	11 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
14	L	104/104 (100%)	94 (90%)	10 (10%)	10 46
15	M	103/103 (100%)	94 (91%)	9 (9%)	13 51
16	N	109/109 (100%)	100 (92%)	9 (8%)	14 53
17	O	102/103 (99%)	95 (93%)	7 (7%)	19 61
18	P	87/87 (100%)	75 (86%)	12 (14%)	4 30
19	Q	99/100 (99%)	90 (91%)	9 (9%)	12 49
20	R	89/90 (99%)	82 (92%)	7 (8%)	15 55
21	S	84/84 (100%)	76 (90%)	8 (10%)	11 47
22	T	93/93 (100%)	88 (95%)	5 (5%)	27 69
23	U	82/84 (98%)	76 (93%)	6 (7%)	17 59
24	V	83/85 (98%)	76 (92%)	7 (8%)	14 53
25	W	78/78 (100%)	72 (92%)	6 (8%)	16 56
26	X	57/63 (90%)	51 (90%)	6 (10%)	8 42
27	Y	67/68 (98%)	63 (94%)	4 (6%)	24 66
28	Z	54/55 (98%)	48 (89%)	6 (11%)	8 39
29	a	48/49 (98%)	46 (96%)	2 (4%)	36 75
30	b	47/48 (98%)	35 (74%)	12 (26%)	1 6
31	c	45/49 (92%)	40 (89%)	5 (11%)	8 39
32	d	38/38 (100%)	32 (84%)	6 (16%)	3 23
33	e	51/52 (98%)	47 (92%)	4 (8%)	16 56
34	f	34/34 (100%)	31 (91%)	3 (9%)	12 51
35	i	311/313 (99%)	298 (96%)	13 (4%)	36 75
36	k	17/17 (100%)	15 (88%)	2 (12%)	6 36
37	l	156/405 (38%)	153 (98%)	3 (2%)	65 88
All	All	3297/3609 (91%)	3021 (92%)	276 (8%)	18 53

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
14	L	116	ILE
18	P	31	THR
34	f	2	LYS
15	M	47	ARG
16	N	115	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
15	M	104	GLN
19	Q	66	ASN
35	i	196	HIS
16	N	3	GLN
18	P	100	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	42/113 (37%)	18 (42%)	1 (2%)
2	2	2/3 (66%)	1 (50%)	0
3	A	2878/2903 (99%)	521 (18%)	19 (0%)
4	B	119/120 (99%)	13 (10%)	0
All	All	3041/3139 (96%)	553 (18%)	20 (0%)

5 of 553 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	33	C
1	1	34	U
1	1	37	U
1	1	39	A
1	1	41	C

5 of 20 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	A	1344	U
3	A	1494	A
3	A	2424	C
3	A	830	G
3	A	1110	G

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 436 ligands modelled in this entry, 434 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	$\#\|Z\| > 2$
40	GNP	i	1400	38	29,34,34	2.18	8 (27%)	29,54,54	2.66	12 (41%)
40	GNP	l	1400	38	29,34,34	1.98	8 (27%)	29,54,54	2.54	11 (37%)

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
40	GNP	i	1400	38	-	0/13/38/38	0/3/3/3
40	GNP	l	1400	38	-	0/13/38/38	0/3/3/3

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	i	1400	GNP	PG-O3G	-3.01	1.48	1.56
40	i	1400	GNP	PB-O2B	-3.00	1.48	1.56
40	l	1400	GNP	PG-O3G	-2.58	1.49	1.56
40	i	1400	GNP	PG-O2G	-2.54	1.49	1.56
40	l	1400	GNP	PG-O2G	-2.45	1.50	1.56

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	i	1400	GNP	C6-C5-C4	-5.55	114.51	120.86
40	l	1400	GNP	C6-C5-C4	-5.21	114.91	120.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	i	1400	GNP	N3-C2-N1	-4.57	121.34	127.56
40	i	1400	GNP	O3'-C3'-C4'	-4.18	98.54	111.01
40	l	1400	GNP	N3-C2-N1	-3.80	122.39	127.56

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

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	Z	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	15:ASN	C	16:THR	N	3.07
1	Z	40:SER	C	41:HIS	N	2.90