



wwPDB/EMDatabank EM Map/Model Validation Summary Report ⓘ

Dec 6, 2016 – 05:39 PM EST

PDB ID : 5JCS
EMDB ID: : EMD-3199
Title : CRYO-EM STRUCTURE OF THE RIX1-REA1 PRE-60S PARTICLE
Authors : Barrio-Garcia, C.; Thoms, M.; Flemming, D.; Kater, L.; Berninghausen, O.;
Bassler, J.; Beckmann, R.; Hurt, E.
Deposited on : 2016-04-15
Resolution : 9.50 Å(reported)

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

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

A user guide is available at

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

MolProbity : 4.02b-467
Mogul : 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) : rb-20028442

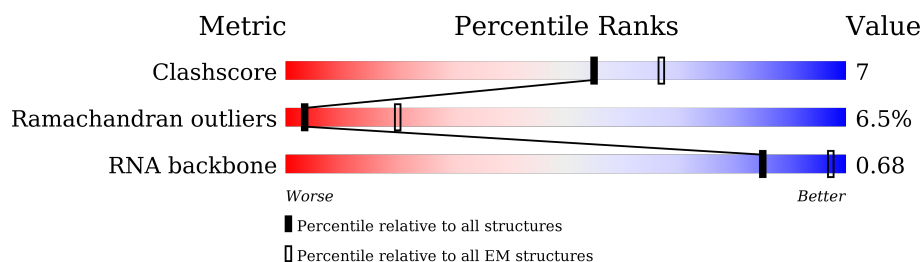
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.50 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.





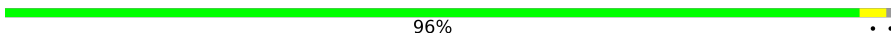


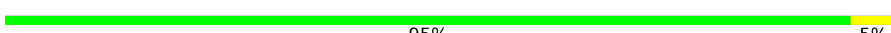










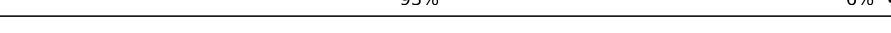
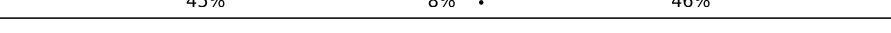
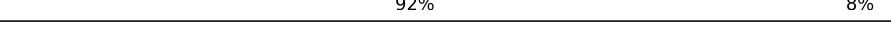
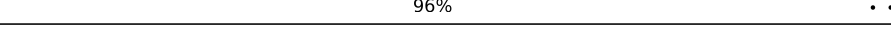

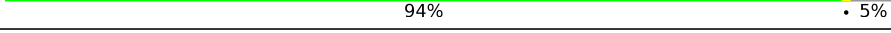


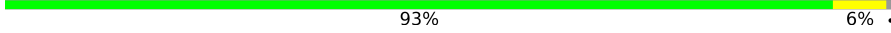
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
RNA backbone	3027	244

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	254	85% 13% ..
2	c	105	91% . 8%
3	B	387	92% 7%
4	d	113	93% . .
5	C	362	90% 9% .
6	e	130	96% ..
7	D	297	95% .
8	f	107	92% 6% ..
9	E	176	84% 5% 11%

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Mol	Chain	Length	Quality of chain
10	g	121	 88% 7%
11	F	244	 85% 6% 9%
12	h	120	 96% ..
13	G	256	 87% 9%
14	i	100	 93% 6%
15	H	191	 95% 5%
16	j	88	 91% 7% ..
17	I	217	 94% 6%
18	k	78	 97% ..
19	J	174	 75% 20% ..
20	l	51	 90% 8%
21	K	165	 66% 10% 23%
22	m	245	 88% 9%
23	L	199	 88% 8% ..
24	n	236	 87% 10%
25	M	138	 93% 6%
26	o	647	 45% 8% 46%
27	N	204	 92% 8%
28	p	92	 96% ..
29	O	199	 88% 11% ..
30	q	515	 94% 5%
31	P	184	 92% 7%
32	r	767	 34% 9% 57%
33	Q	186	 93% 6%
34	s	4910	 37% 59%

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Mol	Chain	Length	Quality of chain
35	R	189	88% 12% .
36	t	199	31% .. 68%
37	S	172	95% 5% .
38	u	593	61% . 37%
39	T	160	79% 18% ...
40	x	3396	87% 13%
41	U	121	76% 7% 17%
42	y	158	87% 13%
43	V	137	95% . .
44	z	121	94% 6%
45	X	142	80% 5% 15%
46	Y	127	92% 7% .
47	Z	136	93% 6% .
48	a	149	87% 10% ..

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 118855 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 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	A	252	Total	C	N	O	0	0
			1007	504	252	251		

- Molecule 2 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	c	97	Total	C	N	O	0	0
			387	194	97	96		

- Molecule 3 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	B	386	Total	C	N	O	0	0
			1543	772	386	385		

- Molecule 4 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	d	109	Total	C	N	O	0	0
			435	218	109	108		

- Molecule 5 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	C	361	Total	C	N	O	0	0
			1443	722	361	360		

- Molecule 6 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	e	127	Total	C	N	O	0	0
			507	254	127	126		

- Molecule 7 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	D	296	Total	C	N	O	0	0
			1183	592	296	295		

- Molecule 8 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	f	106	Total	C	N	O	0	0
			423	212	106	105		

- Molecule 9 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	E	156	Total	C	N	O	0	0
			622	312	156	154		

- Molecule 10 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	g	112	Total	C	N	O	0	0
			447	224	112	111		

- Molecule 11 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	F	222	Total	C	N	O	0	0
			887	444	222	221		

- Molecule 12 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	h	119	Total	C	N	O	0	0
			475	238	119	118		

- Molecule 13 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	G	233	Total	C	N	O	0	0
			931	466	233	232		

- Molecule 14 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	i	99	Total	C	N	O	0	0
			395	198	99	98		

- Molecule 15 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	H	191	Total	C	N	O	0	0
			763	382	191	190		

- Molecule 16 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	j	87	Total	C	N	O	0	0
			347	174	87	86		

- Molecule 17 is a protein called 60S ribosomal protein L1-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	I	217	Total	C	N	O	0	0
			867	434	217	216		

- Molecule 18 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	k	77	Total	C	N	O	0	0
			307	154	77	76		

- Molecule 19 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	J	169	Total	C	N	O	0	0
			675	338	169	168		

- Molecule 20 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	l	50	Total	C	N	O	0	0
			199	100	50	49		

- Molecule 21 is a protein called 60S ribosomal protein L12-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	K	127	Total	C	N	O	0	0
			507	254	127	126		

- Molecule 22 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	m	224	Total	C	N	O	0	0
			895	448	224	223		

- Molecule 23 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	L	193	Total	C	N	O	0	0
			771	386	193	192		

- Molecule 24 is a protein called Ribosome assembly factor MRT4.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	n	212	Total	C	N	O	0	0
			847	424	212	211		

- Molecule 25 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	M	136	Total	C	N	O	0	0
			543	272	136	135		

- Molecule 26 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	o	347	Total	C	N	O	0	0
			1387	694	347	346		

- Molecule 27 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	N	203	Total	C	N	O	0	0
			811	406	203	202		

- Molecule 28 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	p	91	Total	C	N	O	0	0
			363	182	91	90		

- Molecule 29 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	O	197	Total	C	N	O	0	0
			787	394	197	196		

- Molecule 30 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	q	488	Total	C	N	O	0	0
			1951	976	488	487		

- Molecule 31 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	P	183	Total	C	N	O	0	0
			731	366	183	182		

- Molecule 32 is a protein called Protein SDA1.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	r	333	Total	C	N	O	0	0
			1304	666	333	305		

- Molecule 33 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Q	185	Total	C	N	O	0	0
			739	370	185	184		

- Molecule 34 is a protein called Midasin.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	2003	Total	C	N	O	0	0
			8007	4006	2003	1998		

- Molecule 35 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	R	188	Total	C	N	O	0	0
			751	376	188	187		

- Molecule 36 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	t	63	Total	C	N	O	0	0
			251	126	63	62		

- Molecule 37 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	S	172	Total	C	N	O	0	0
			687	344	172	171		

- Molecule 38 is a protein called Probable metalloprotease ARX1.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	u	373	Total	C	N	O	0	0
			1491	746	373	372		

- Molecule 39 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	T	159	Total	C	N	O	0	0
			635	318	159	158		

- Molecule 40 is a RNA chain called 25S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	x	3394	Total	C	N	O	P	0	0
			72570	32410	13042	23725	3393		

- Molecule 41 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	U	100	Total	C	N	O	0	0
			399	200	100	99		

- Molecule 42 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	y	158	Total	C	N	O	P	0	0
			3350	1500	586	1107	157		

- Molecule 43 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	V	136	Total	C	N	O	0	0
			543	272	136	135		

- Molecule 44 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z	121	Total	C	N	O	P	0	0
			2576	1152	461	843	120		

- Molecule 45 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	X	121	Total	C	N	O	0	0
			483	242	121	120		

- Molecule 46 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	Y	126	Total	C	N	O	0	0
			503	252	126	125		

- Molecule 47 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Z	135	Total	C	N	O	0	0
			539	270	135	134		

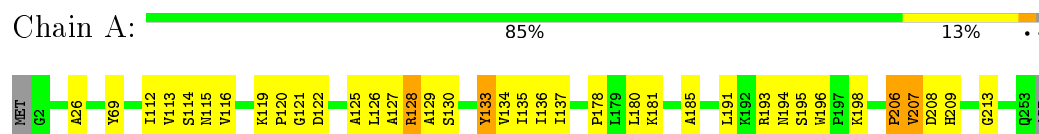
- Molecule 48 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	a	148	Total	C	N	O	0	0
			591	296	148	147		

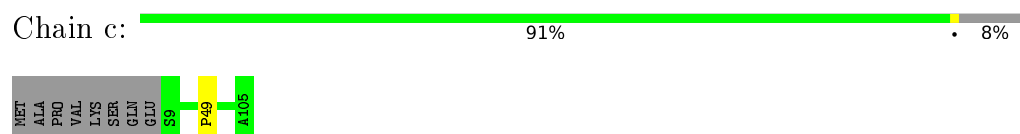
3 Residue-property plots

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.

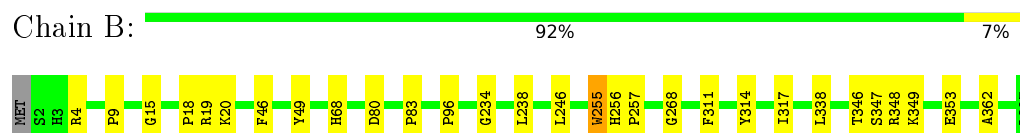
- Molecule 1: 60S ribosomal protein L2-A



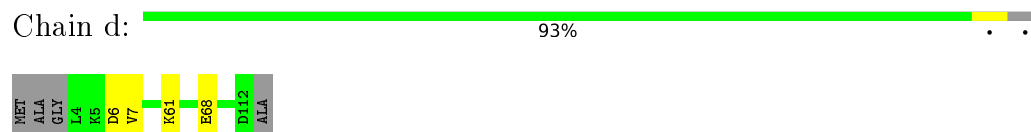
- Molecule 2: 60S ribosomal protein L30



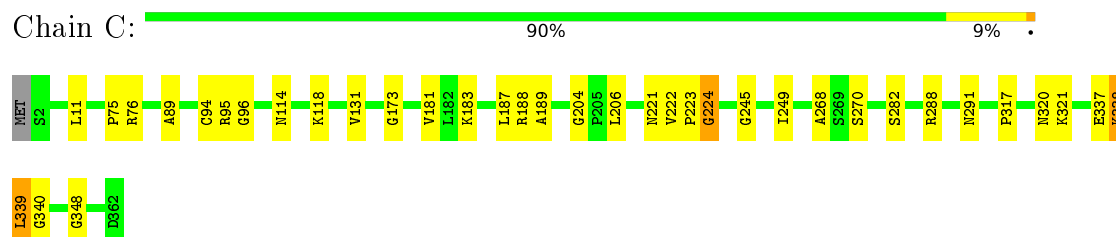
- Molecule 3: 60S ribosomal protein L3



- Molecule 4: 60S ribosomal protein L31-A



- Molecule 5: 60S ribosomal protein L4-A



- Molecule 6: 60S ribosomal protein L32

Chain e:  96% ..



- Molecule 7: 60S ribosomal protein L5

Chain D:  95% .




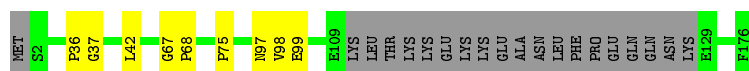
- Molecule 8: 60S ribosomal protein L33-A

Chain f:  92% 6% ..




- Molecule 9: 60S ribosomal protein L6-A

Chain E:  84% 5% 11%




- Molecule 10: 60S ribosomal protein L34-A

Chain g:  88% . 7%



- Molecule 11: 60S ribosomal protein L7-A

Chain F:  85% 6% 9%



- Molecule 12: 60S ribosomal protein L35-A

Chain h:  96% ..



- Molecule 13: 60S ribosomal protein L8-A

Chain G:  87% . 9%



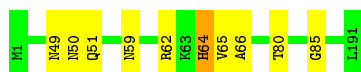
- Molecule 14: 60S ribosomal protein L36-A

Chain i: 93% 6% .



- Molecule 15: 60S ribosomal protein L9-A

Chain H: 95% 5% .



- Molecule 16: 60S ribosomal protein L37-A

Chain j: 91% 7% ..



- Molecule 17: 60S ribosomal protein L1-A

Chain I: 94% 6%



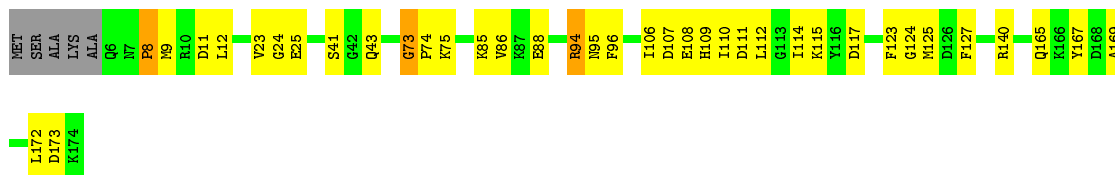
- Molecule 18: 60S ribosomal protein L38

Chain k: 97% ..



- Molecule 19: 60S ribosomal protein L11-A

Chain J: 75% 20% ..



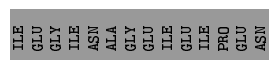
- Molecule 20: 60S ribosomal protein L39

Chain l: 90% 8% .



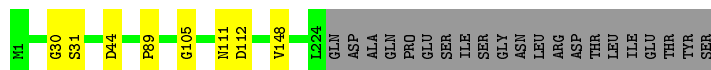
- Molecule 21: 60S ribosomal protein L12-A

Chain K: 66% 10% 23%



- Molecule 22: Eukaryotic translation initiation factor 6

Chain m: 88% 9%



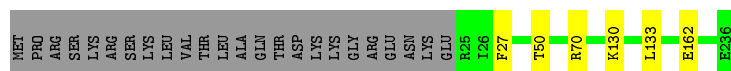
- Molecule 23: 60S ribosomal protein L13-A

Chain L: 88% 8% ..



- Molecule 24: Ribosome assembly factor MRT4

Chain n: 87% 10%



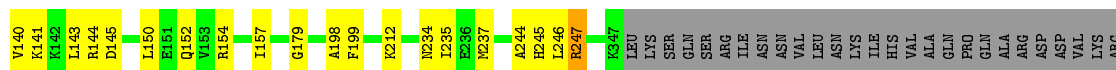
- Molecule 25: 60S ribosomal protein L14-A

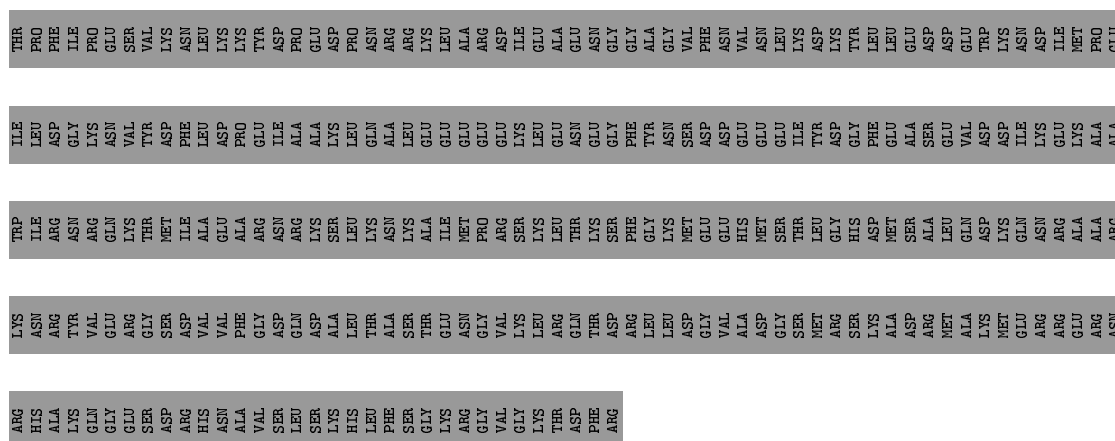
Chain M: 93% 6%



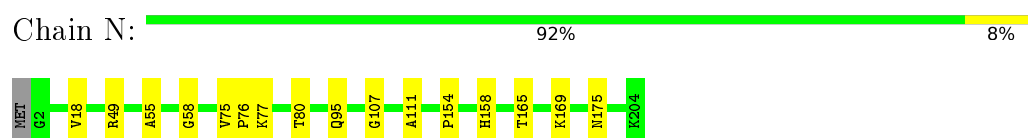
- Molecule 26: Nucleolar GTP-binding protein 1

Chain o: 45% 8% 46%

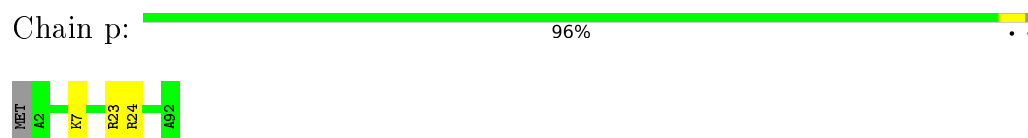




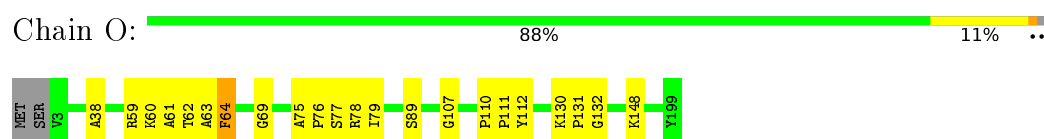
- Molecule 27: 60S ribosomal protein L15-A



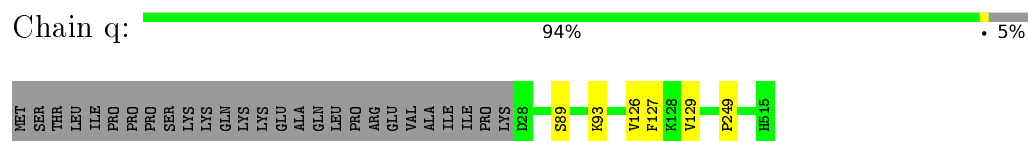
- Molecule 28: 60S ribosomal protein L43-A



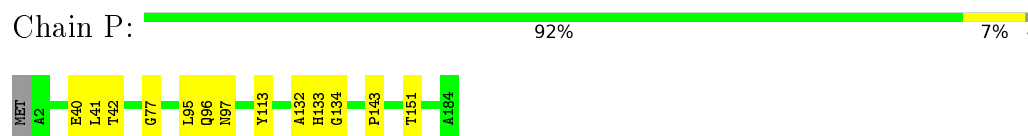
- Molecule 29: 60S ribosomal protein L16-A



- Molecule 30: Ribosome assembly protein 4

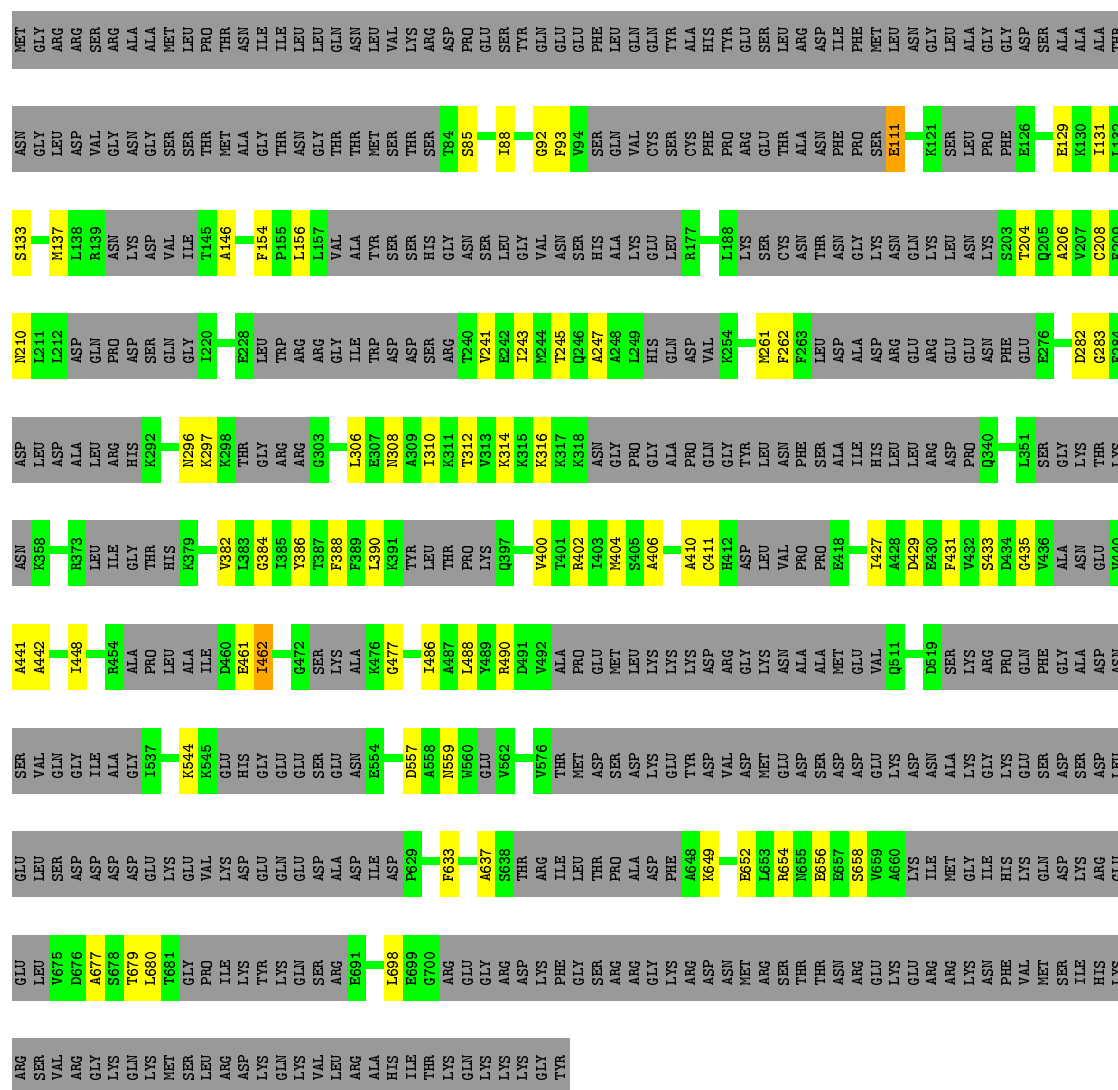


- Molecule 31: 60S ribosomal protein L17-A



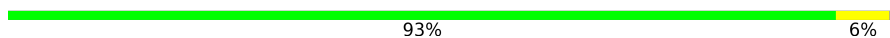
- Molecule 32: Protein SDA1

Chain r:



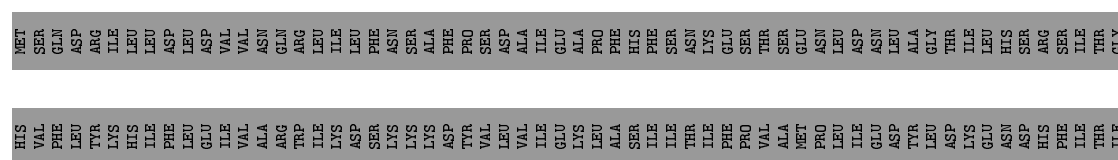
- Molecule 33: 60S ribosomal protein L18-A

Chain Q:



- Molecule 34: Midasin

Chain s:



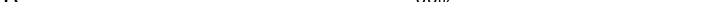
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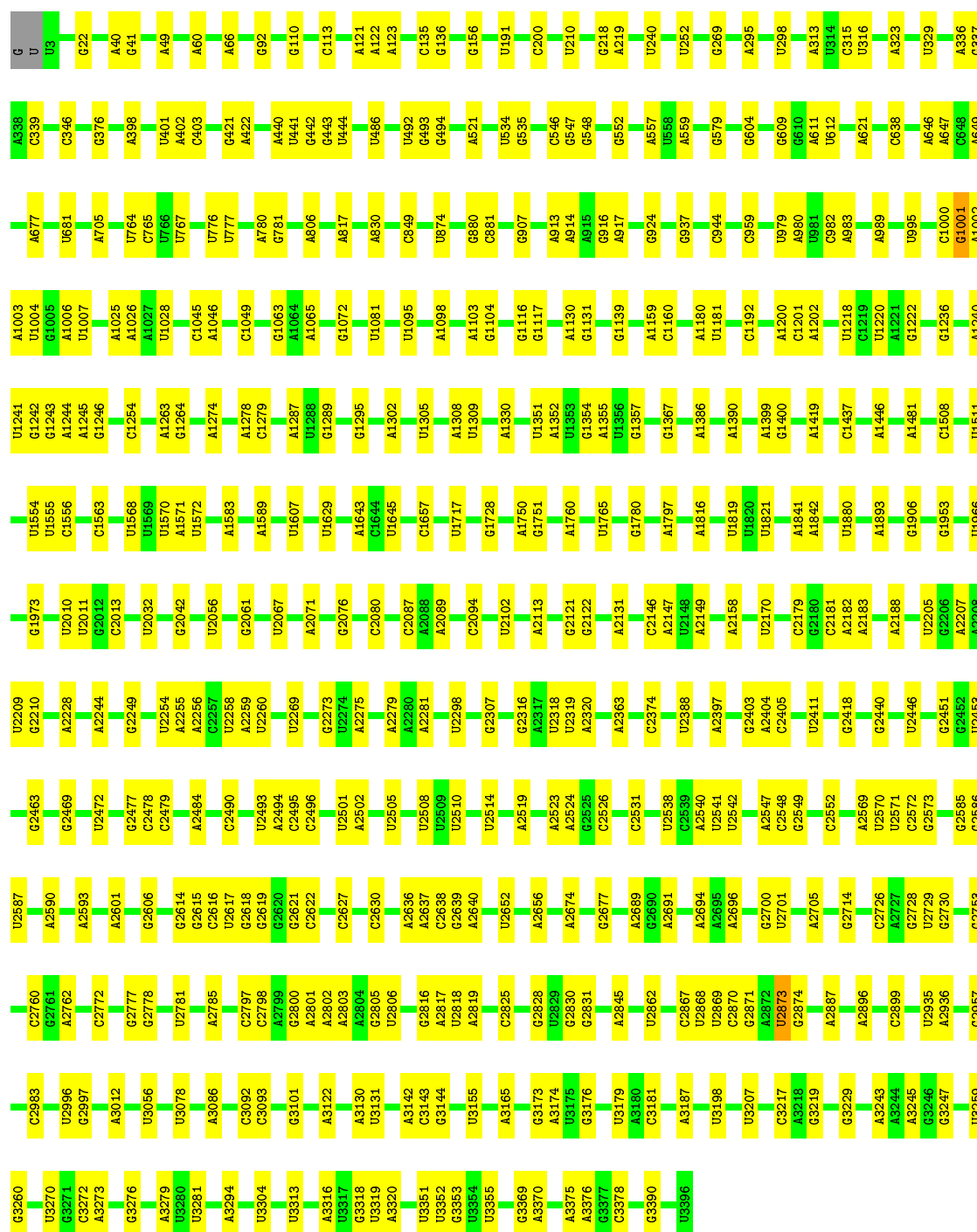
WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM

[illegible]

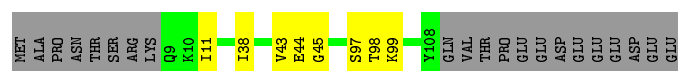
- Molecule 35: 60S ribosomal protein L19-A

Chain R:  88% 12%



- Molecule 41: 60S ribosomal protein L22-A

Chain U:



- Molecule 42: 5.8S ribosomal RNA

Chain y:



- Molecule 43: 60S ribosomal protein L23-A

Chain V:  95%




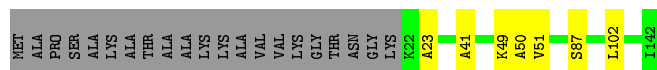
- Molecule 44: 5S ribosomal RNA

Chain z:  94%



- Molecule 45: 60S ribosomal protein L25

Chain X:  80%



- Molecule 46: 60S ribosomal protein L26-A

Chain Y:  92%




- Molecule 47: 60S ribosomal protein L27-A

Chain Z:  93%



- Molecule 48: 60S ribosomal protein L28

Chain a:  87%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	15749	Depositor
Resolution determination method	FSC 0.5 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)	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 ⓘ

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	0.35	1/1006 (0.1%)	0.47	0/1256
10	g	0.18	0/446	0.32	0/556
11	F	0.18	0/886	0.32	0/1106
12	h	0.17	0/474	0.29	0/591
13	G	0.18	0/930	0.32	0/1161
14	i	0.18	0/394	0.31	0/491
15	H	0.17	0/762	0.30	0/951
16	j	0.57	1/346 (0.3%)	0.57	1/431 (0.2%)
17	I	0.18	0/866	0.31	0/1081
18	k	0.17	0/306	0.29	0/381
19	J	0.54	0/674	0.78	0/841
2	c	0.17	0/386	0.27	0/481
20	l	0.17	0/198	0.36	0/246
21	K	0.18	0/506	0.34	0/631
22	m	0.18	0/894	0.30	0/1116
23	L	0.18	0/770	0.35	0/961
24	n	0.18	0/846	0.31	0/1056
25	M	0.17	0/542	0.30	0/676
26	o	0.59	2/1386 (0.1%)	0.85	9/1731 (0.5%)
27	N	0.19	0/810	0.38	0/1011
28	p	0.18	0/362	0.30	0/451
29	O	0.20	0/786	0.47	1/981 (0.1%)
3	B	0.19	0/1542	0.36	0/1926
30	q	0.92	0/1950	0.88	0/2436
31	P	0.17	0/730	0.33	0/911
32	r	0.55	1/1276 (0.1%)	0.90	4/1553 (0.3%)
33	Q	0.17	0/738	0.30	0/921
34	s	0.29	1/8001 (0.0%)	0.49	8/9992 (0.1%)
35	R	0.20	0/750	0.41	0/936
36	t	0.34	0/250	0.52	0/311
37	S	0.16	0/686	0.32	0/856
38	u	0.92	0/1483	0.86	1/1840 (0.1%)
39	T	0.44	1/634 (0.2%)	0.64	2/791 (0.3%)
4	d	0.18	0/434	0.31	0/541

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
40	x	0.20	5/81221 (0.0%)	0.74	168/126638 (0.1%)
41	U	0.18	0/398	0.31	0/496
42	y	0.13	0/3743	0.64	0/5828
43	V	0.22	0/542	0.35	0/676
44	z	0.13	0/2880	0.64	0/4487
45	X	0.17	0/482	0.29	0/601
46	Y	0.17	0/502	0.30	0/626
47	Z	0.18	0/538	0.31	0/671
48	a	0.80	3/590 (0.5%)	0.71	3/736 (0.4%)
5	C	0.19	0/1442	0.37	1/1801 (0.1%)
6	e	0.17	0/506	0.32	0/631
7	D	0.18	0/1182	0.32	0/1476
8	f	0.49	1/422 (0.2%)	0.71	1/526 (0.2%)
9	E	0.55	1/620 (0.2%)	0.70	4/772 (0.5%)
All	All	0.28	17/128118 (0.0%)	0.68	203/187166 (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
1	A	0	1
19	J	0	1
26	o	0	1
3	B	0	2
32	r	0	3
34	s	0	11
36	t	0	1
39	T	0	3
48	a	1	1
8	f	0	2
9	E	0	1
All	All	1	27

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	a	111	LYS	N-CA	14.13	1.74	1.46
48	a	110	GLY	C-N	10.00	1.57	1.34
9	E	67	GLY	CA-C	-9.76	1.36	1.51
16	j	39	TYR	C-O	-8.62	1.06	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	x	2638	C	O3'-P	-7.47	1.52	1.61

The worst 5 of 203 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	s	858	GLU	O-C-N	-21.28	88.65	122.70
40	x	440	A	O5'-P-OP1	-19.65	87.12	110.70
40	x	440	A	O5'-P-OP2	17.48	131.68	110.70
40	x	2638	C	P-O3'-C3'	-16.82	99.52	119.70
40	x	2873	U	C5'-C4'-O4'	-15.31	90.73	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
48	a	34	MET	CA

5 of 27 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	198	LYS	Peptide
3	B	255	TRP	Peptide
3	B	256	HIS	Peptide
8	f	100	ILE	Mainchain
8	f	103	TYR	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	1007	0	310	18	0
2	c	387	0	113	0	0
3	B	1543	0	433	4	0
4	d	435	0	114	0	0
5	C	1443	0	399	7	0
6	e	507	0	135	0	0
7	D	1183	0	325	1	0
8	f	423	0	117	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	E	622	0	160	1	0
10	g	447	0	121	0	0
11	F	887	0	241	3	0
12	h	475	0	118	0	0
13	G	931	0	242	1	0
14	i	395	0	109	0	0
15	H	763	0	215	3	0
16	j	347	0	104	0	0
17	I	867	0	230	2	0
18	k	307	0	79	0	0
19	J	675	0	191	11	0
20	l	199	0	47	0	0
21	K	507	0	140	1	0
22	m	895	0	257	0	0
23	L	771	0	199	4	0
24	n	847	0	224	0	0
25	M	543	0	145	2	0
26	o	1387	0	358	0	0
27	N	811	0	221	3	0
28	p	363	0	108	0	0
29	O	787	0	214	5	0
30	q	1951	0	540	0	0
31	P	731	0	197	4	0
32	r	1304	0	332	0	0
33	Q	739	0	205	1	0
34	s	8007	0	2136	0	0
35	R	751	0	203	14	0
36	t	251	0	68	0	0
37	S	687	0	175	3	0
38	u	1491	0	399	0	0
39	T	635	0	174	14	0
40	x	72570	0	36462	0	0
41	U	399	0	109	2	0
42	y	3350	0	1696	0	0
43	V	543	0	162	2	0
44	z	2576	0	1304	0	0
45	X	483	0	121	1	0
46	Y	503	0	134	1	0
47	Z	539	0	144	1	0
48	a	591	0	176	0	0
All	All	118855	0	50406	109	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 7.

The worst 5 of 109 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)
39:T:62:GLY:N	39:T:75:ILE:H	1.51	1.07
39:T:43:LYS:O	39:T:95:HIS:CA	2.03	1.06
35:R:158:GLU:O	35:R:162:ARG:N	1.90	1.03
39:T:62:GLY:CA	39:T:75:ILE:H	1.72	1.03
39:T:62:GLY:HA3	39:T:75:ILE:N	1.80	0.96

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	
1	A	250/254 (98%)	156 (62%)	70 (28%)	24 (10%)	1	15
2	c	95/105 (90%)	84 (88%)	10 (10%)	1 (1%)	17	63
3	B	384/387 (99%)	294 (77%)	70 (18%)	20 (5%)	2	30
4	d	107/113 (95%)	88 (82%)	15 (14%)	4 (4%)	4	38
5	C	359/362 (99%)	254 (71%)	80 (22%)	25 (7%)	1	22
6	e	125/130 (96%)	99 (79%)	24 (19%)	2 (2%)	12	56
7	D	294/297 (99%)	229 (78%)	53 (18%)	12 (4%)	3	35
8	f	104/107 (97%)	78 (75%)	19 (18%)	7 (7%)	1	24
9	E	152/176 (86%)	113 (74%)	35 (23%)	4 (3%)	7	45
10	g	110/121 (91%)	78 (71%)	27 (24%)	5 (4%)	3	33
11	F	220/244 (90%)	181 (82%)	30 (14%)	9 (4%)	3	35
12	h	117/120 (98%)	92 (79%)	21 (18%)	4 (3%)	5	40
13	G	231/256 (90%)	180 (78%)	42 (18%)	9 (4%)	4	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	i	97/100 (97%)	78 (80%)	13 (13%)	6 (6%)	2	26
15	H	189/191 (99%)	147 (78%)	37 (20%)	5 (3%)	7	45
16	j	85/88 (97%)	53 (62%)	26 (31%)	6 (7%)	1	22
17	I	215/217 (99%)	159 (74%)	48 (22%)	8 (4%)	4	38
18	k	75/78 (96%)	66 (88%)	8 (11%)	1 (1%)	15	60
19	J	167/174 (96%)	116 (70%)	29 (17%)	22 (13%)	0	7
20	l	48/51 (94%)	33 (69%)	11 (23%)	4 (8%)	1	18
21	K	125/165 (76%)	81 (65%)	27 (22%)	17 (14%)	0	7
22	m	222/245 (91%)	170 (77%)	44 (20%)	8 (4%)	4	38
23	L	191/199 (96%)	141 (74%)	39 (20%)	11 (6%)	2	27
24	n	210/236 (89%)	156 (74%)	48 (23%)	6 (3%)	6	43
25	M	134/138 (97%)	106 (79%)	22 (16%)	6 (4%)	3	33
26	o	345/647 (53%)	223 (65%)	72 (21%)	50 (14%)	0	6
27	N	201/204 (98%)	147 (73%)	44 (22%)	10 (5%)	3	31
28	p	89/92 (97%)	72 (81%)	14 (16%)	3 (3%)	5	40
29	O	195/199 (98%)	143 (73%)	39 (20%)	13 (7%)	1	24
30	q	486/515 (94%)	458 (94%)	22 (4%)	6 (1%)	16	61
31	P	181/184 (98%)	141 (78%)	35 (19%)	5 (3%)	6	44
32	r	277/767 (36%)	155 (56%)	57 (21%)	65 (24%)	0	2
33	Q	183/186 (98%)	143 (78%)	30 (16%)	10 (6%)	2	29
34	s	1991/4910 (40%)	1585 (80%)	229 (12%)	177 (9%)	1	17
35	R	186/189 (98%)	136 (73%)	44 (24%)	6 (3%)	5	41
36	t	61/199 (31%)	52 (85%)	7 (12%)	2 (3%)	5	40
37	S	170/172 (99%)	133 (78%)	31 (18%)	6 (4%)	4	39
38	u	357/593 (60%)	342 (96%)	6 (2%)	9 (2%)	7	46
39	T	157/160 (98%)	90 (57%)	46 (29%)	21 (13%)	0	7
41	U	98/121 (81%)	77 (79%)	17 (17%)	4 (4%)	3	35
43	V	134/137 (98%)	95 (71%)	37 (28%)	2 (2%)	13	57
45	X	119/142 (84%)	91 (76%)	23 (19%)	5 (4%)	3	34
46	Y	124/127 (98%)	91 (73%)	26 (21%)	7 (6%)	2	28
47	Z	133/136 (98%)	97 (73%)	30 (23%)	6 (4%)	3	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
48	a	146/149 (98%)	89 (61%)	40 (27%)	17 (12%)	0	9
All	All	9939/14383 (69%)	7592 (76%)	1697 (17%)	650 (6%)	3	25

5 of 650 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ASP
1	A	128	ARG
1	A	133	TYR
1	A	135	ILE
1	A	137	ILE

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
40	x	3393/3396 (99%)	376 (11%)	0
42	y	157/158 (99%)	20 (12%)	0
44	z	120/121 (99%)	7 (5%)	0
All	All	3670/3675 (99%)	403 (10%)	0

5 of 403 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
40	x	22	G
40	x	40	A
40	x	41	G
40	x	49	A
40	x	60	A

There are no RNA pucker outliers to report.

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

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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.