



Full wwPDB/EMDatabank EM Map/Model Validation 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 Full wwPDB/EMDatabank EM Map/Model Validation 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.

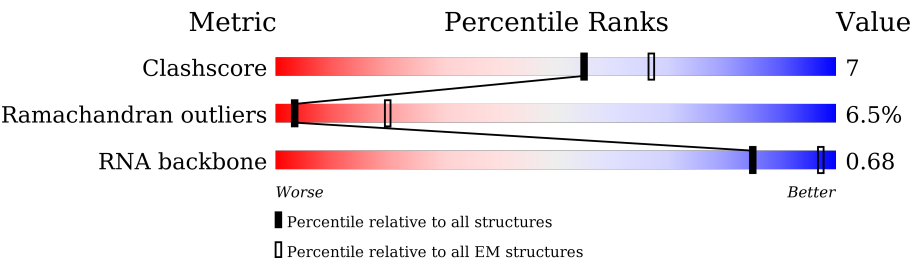
MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

1 Overall quality at a glance i

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.





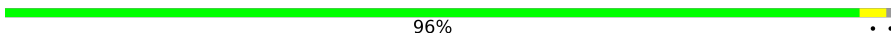


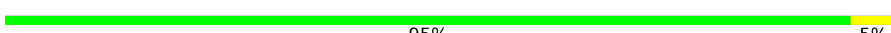










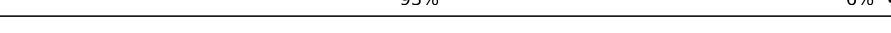
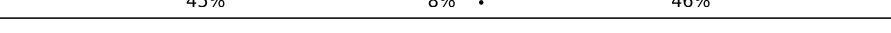
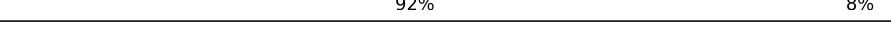
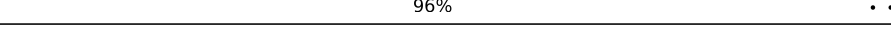

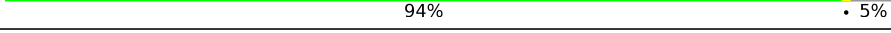


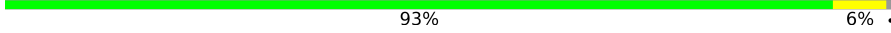
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
RNA backbone	3027	244

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		

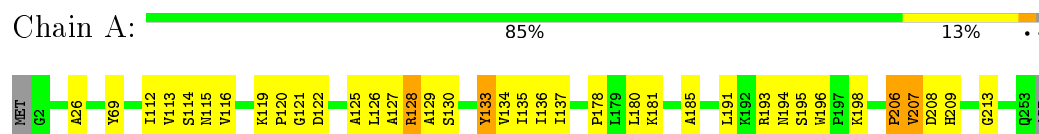
- Molecule 48 is a protein called 60S ribosomal protein L28.

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

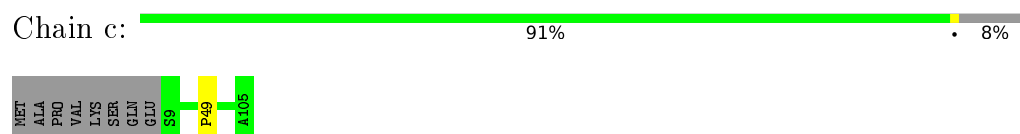
3 Residue-property plots

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.

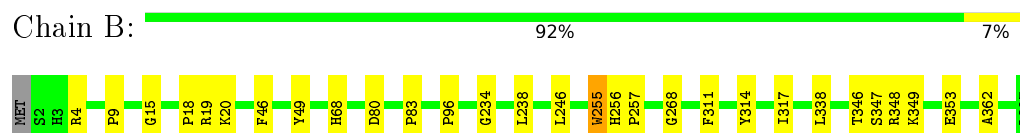
- Molecule 1: 60S ribosomal protein L2-A



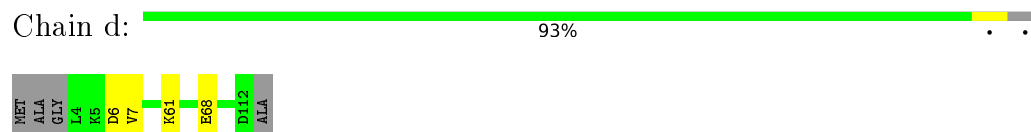
- Molecule 2: 60S ribosomal protein L30



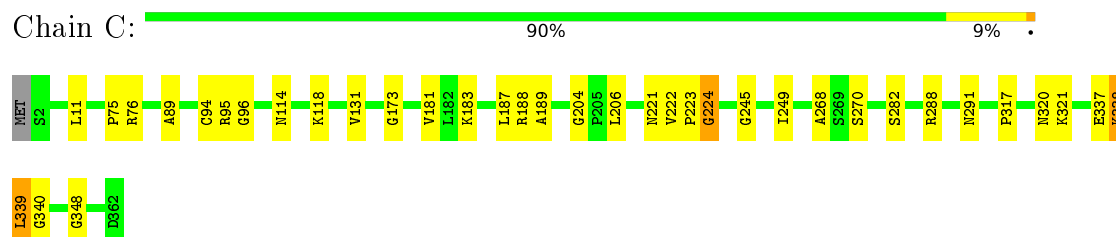
- Molecule 3: 60S ribosomal protein L3



- 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% .




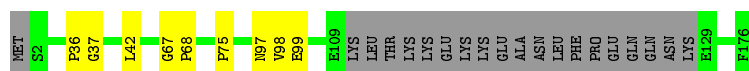
- Molecule 8: 60S ribosomal protein L33-A

Chain f:  92% 6% ..




- Molecule 9: 60S ribosomal protein L6-A

Chain E:  84% 5% 11%




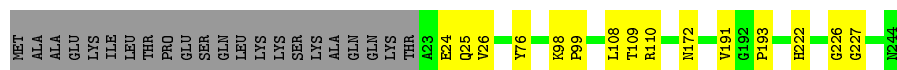
- Molecule 10: 60S ribosomal protein L34-A

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%



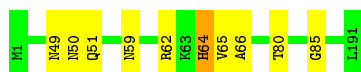
- Molecule 14: 60S ribosomal protein L36-A

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%



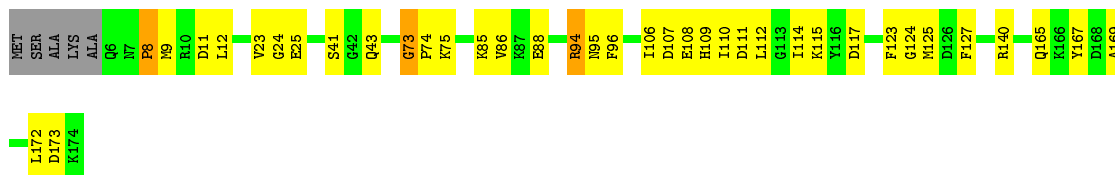
- Molecule 18: 60S ribosomal protein L38

Chain k: 97% ..



- Molecule 19: 60S ribosomal protein L11-A

Chain J: 75% 20% ..



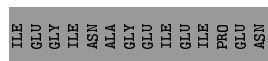
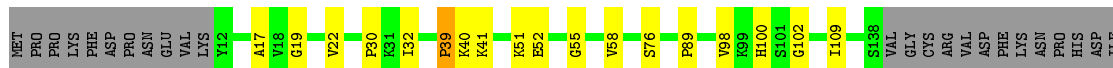
- Molecule 20: 60S ribosomal protein L39

Chain l: 90% 8% .



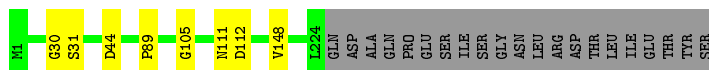
- Molecule 21: 60S ribosomal protein L12-A

Chain K: 66% 10% 23%



- Molecule 22: Eukaryotic translation initiation factor 6

Chain m: 88% 9%



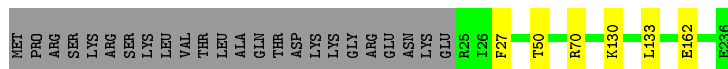
- Molecule 23: 60S ribosomal protein L13-A

Chain L: 88% 8% ..



- Molecule 24: Ribosome assembly factor MRT4

Chain n: 87% 10%



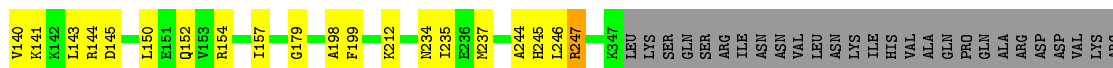
- Molecule 25: 60S ribosomal protein L14-A

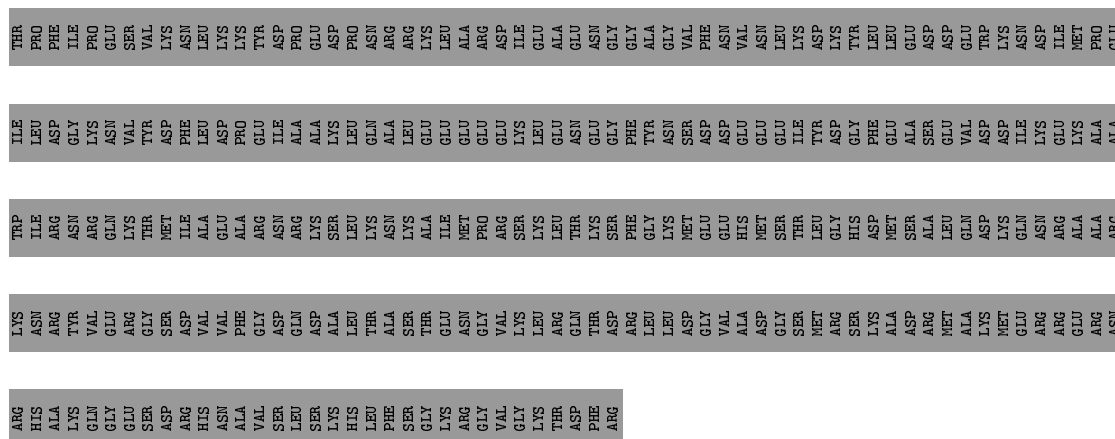
Chain M: 93% 6%



- Molecule 26: Nucleolar GTP-binding protein 1

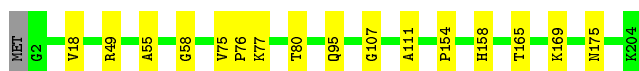
Chain o: 45% 8% 46%





- Molecule 27: 60S ribosomal protein L15-A

Chain N: 92% 8%

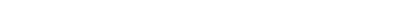


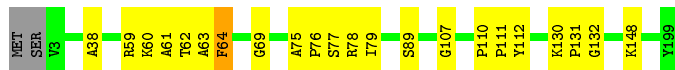
- Molecule 28: 60S ribosomal protein L43-A

Chain p: 96% .



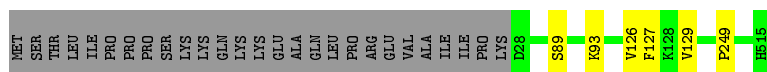
- Molecule 29: 60S ribosomal protein L16-A

Chain 0:  88% 11% ..



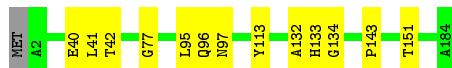
- Molecule 30: Ribosome assembly protein 4

Chain q: 94% • 5%



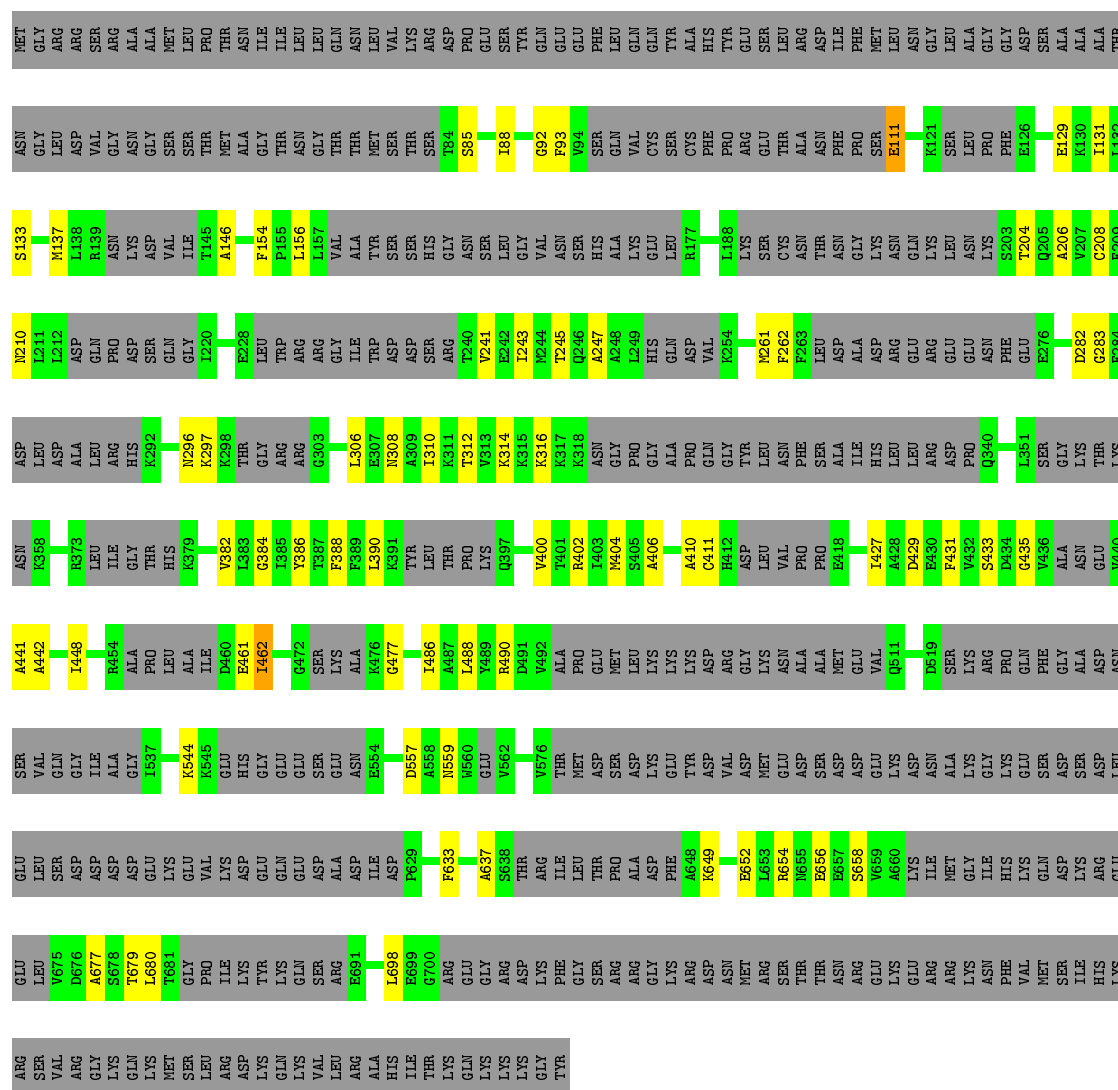
- Molecule 31: 60S ribosomal protein L17-A

Chain P: 92% 7%



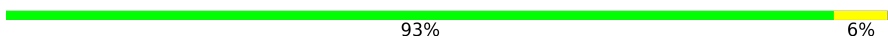
- Molecule 32: Protein SDA1

Chain r:



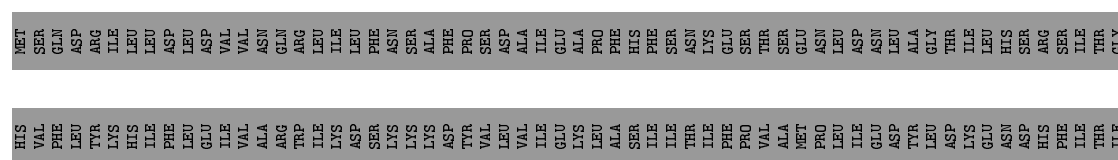
- Molecule 33: 60S ribosomal protein L18-A

Chain Q:



- Molecule 34: Midasin

Chain s:





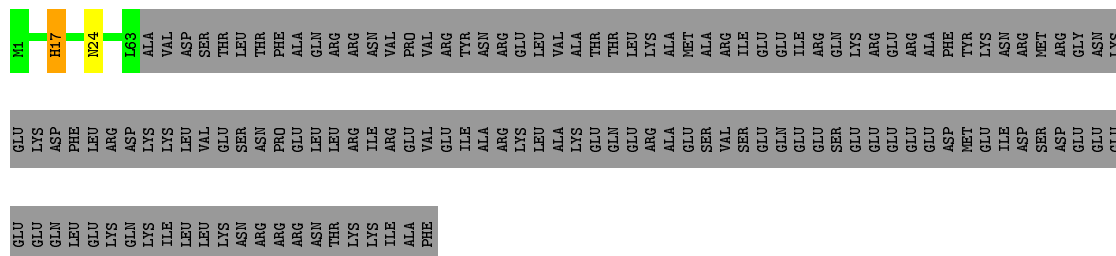

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM





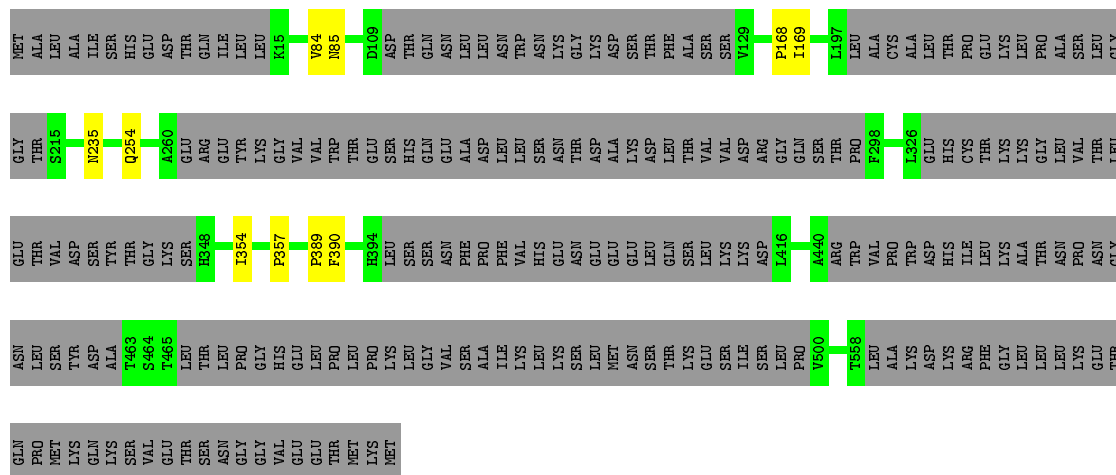
- Molecule 36: Ribosome biogenesis protein RLP24



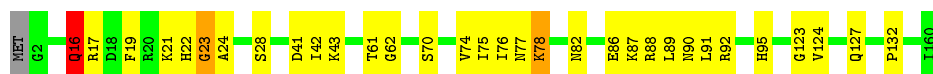
- Molecule 37: 60S ribosomal protein L20-A



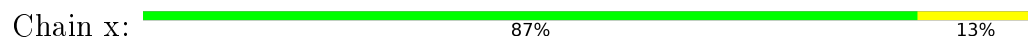
- Molecule 38: Probable metalloprotease ARX1



- Molecule 39: 60S ribosomal protein L21-A



- Molecule 40: 25S ribosomal RNA





- Molecule 43: 60S ribosomal protein L23-A

Chain V: 95%



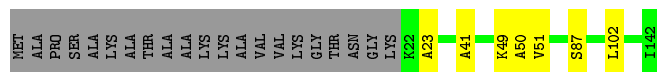
- Molecule 44: 5S ribosomal RNA

Chain z: 94%



- Molecule 45: 60S ribosomal protein L25

Chain X: 80%



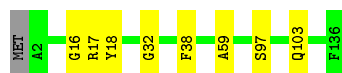
- Molecule 46: 60S ribosomal protein L26-A

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

All (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
8	f	100	ILE	C-N	7.04	1.50	1.34
34	s	2362	ALA	C-O	7.02	1.36	1.23
40	x	2781	U	O3'-P	-6.79	1.53	1.61
26	o	56	GLY	C-O	6.14	1.33	1.23
39	T	16	GLN	N-CA	6.11	1.58	1.46
40	x	443	G	O3'-P	5.87	1.68	1.61
26	o	44	ALA	CA-C	5.81	1.68	1.52
40	x	1025	A	C6-N6	5.56	1.38	1.33
40	x	1130	A	O3'-P	5.55	1.67	1.61
32	r	111	GLU	C-N	5.49	1.46	1.34
48	a	112	ILE	N-CA	-5.43	1.35	1.46
1	A	207	VAL	N-CA	5.27	1.56	1.46

All (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
40	x	440	A	P-O5'-C5'	14.20	143.62	120.90
40	x	494	G	P-O5'-C5'	13.60	142.66	120.90
40	x	2873	U	P-O5'-C5'	13.29	142.16	120.90
40	x	2873	U	C5'-C4'-C3'	13.19	137.10	116.00
40	x	1026	A	N1-C6-N6	12.33	126.00	118.60
40	x	2819	A	O5'-P-OP2	12.13	125.26	110.70
40	x	913	A	N1-C6-N6	12.08	125.85	118.60
40	x	2705	A	N1-C6-N6	11.74	125.64	118.60
40	x	2183	A	N1-C6-N6	11.71	125.62	118.60
40	x	2182	A	N1-C6-N6	11.69	125.62	118.60
40	x	1025	A	N1-C6-N6	11.68	125.61	118.60
40	x	494	G	C4'-C3'-O3'	11.52	136.04	113.00
40	x	2149	A	N1-C6-N6	11.40	125.44	118.60
40	x	2147	A	N1-C6-N6	11.30	125.38	118.60
40	x	2617	U	C4'-C3'-O3'	-11.24	85.79	109.40
40	x	2870	C	C4'-C3'-O3'	11.14	135.28	113.00
9	E	67	GLY	N-CA-C	-11.04	85.50	113.10
40	x	1218	U	P-O5'-C5'	10.86	138.28	120.90
40	x	1002	A	P-O5'-C5'	10.69	138.00	120.90
48	a	110	GLY	CA-C-O	-10.67	101.40	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	x	2873	U	P-O3'-C3'	10.64	132.47	119.70
40	x	2873	U	C2'-C3'-O3'	10.31	132.19	109.50
8	f	100	ILE	O-C-N	-10.18	106.41	122.70
34	s	1015	ARG	O-C-N	-10.16	106.44	122.70
40	x	2819	A	C4'-C3'-O3'	10.11	133.21	113.00
40	x	2867	C	C4'-C3'-O3'	10.09	133.17	113.00
40	x	313	A	P-O3'-C3'	-10.07	107.62	119.70
40	x	442	G	C4'-C3'-O3'	9.86	132.72	113.00
40	x	2874	G	O5'-C5'-C4'	9.59	129.91	111.70
40	x	2403	G	C4'-C3'-O3'	-9.56	89.32	109.40
40	x	2874	G	C4'-C3'-O3'	-9.40	89.67	109.40
40	x	1131	G	O4'-C4'-C3'	-9.31	94.69	104.00
40	x	2637	A	C4'-C3'-O3'	-9.07	90.34	109.40
40	x	2639	G	P-O5'-C5'	8.91	135.16	120.90
40	x	315	C	C5'-C4'-O4'	-8.89	98.43	109.10
40	x	2638	C	C4'-C3'-O3'	8.84	130.68	113.00
40	x	2869	U	C2'-C3'-O3'	8.74	128.73	109.50
40	x	2818	U	N1-C1'-C2'	-8.70	102.44	112.00
40	x	315	C	C2'-C3'-O3'	8.60	128.42	109.50
40	x	2818	U	O4'-C4'-C3'	-8.57	95.43	104.00
40	x	315	C	P-O5'-C5'	-8.50	107.30	120.90
40	x	1000	C	C4'-C3'-O3'	8.48	129.96	113.00
40	x	2259	A	C4'-C3'-O3'	8.42	129.84	113.00
40	x	2874	G	P-O5'-C5'	-8.35	107.54	120.90
40	x	1130	A	C4'-C3'-O3'	8.26	129.52	113.00
40	x	2403	G	P-O3'-C3'	8.26	129.61	119.70
26	o	247	ARG	N-CA-C	8.24	133.26	111.00
40	x	2319	U	C2'-C3'-O3'	-8.24	91.36	109.50
40	x	1001	G	C2'-C3'-O3'	-8.21	91.45	109.50
40	x	1001	G	C4'-C3'-O3'	8.18	129.37	113.00
40	x	2254	U	C4'-C3'-O3'	7.93	128.87	113.00
40	x	2181	C	O4'-C1'-N1	7.88	114.50	108.20
26	o	119	GLY	O-C-N	7.80	135.18	122.70
40	x	2818	U	O4'-C1'-N1	7.72	114.38	108.20
40	x	1003	A	N9-C1'-C2'	-7.71	103.52	112.00
40	x	2319	U	C4'-C3'-O3'	7.71	128.41	113.00
48	a	110	GLY	CA-C-N	7.64	134.01	117.20
40	x	2404	A	C5'-C4'-C3'	7.61	128.17	116.00
40	x	1554	U	P-O3'-C3'	7.58	128.79	119.70
40	x	1025	A	O4'-C1'-N9	7.45	114.16	108.20
48	a	110	GLY	C-N-CA	7.35	140.08	121.70
26	o	119	GLY	CA-C-N	-7.31	101.12	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	x	2319	U	C5'-C4'-O4'	7.24	117.78	109.10
40	x	2874	G	O4'-C1'-N9	7.22	113.97	108.20
40	x	2256	A	C2'-C3'-O3'	7.21	125.36	109.50
40	x	2818	U	OP2-P-O3'	-7.15	89.47	105.20
26	o	119	GLY	C-N-CA	7.14	139.56	121.70
40	x	2617	U	P-O5'-C5'	7.11	132.28	120.90
40	x	1130	A	O3'-P-O5'	7.03	117.35	104.00
38	u	389	PRO	N-CA-C	7.02	130.34	112.10
34	s	630	ASN	C-N-CA	-6.97	104.27	121.70
40	x	2146	C	P-O3'-C3'	-6.87	111.46	119.70
40	x	2640	A	P-O5'-C5'	-6.84	109.96	120.90
40	x	2617	U	C2'-C3'-O3'	6.83	124.63	113.70
40	x	2585	G	C4'-C3'-O3'	-6.79	95.13	109.40
40	x	983	A	C4'-C3'-O3'	-6.74	95.24	109.40
40	x	2585	G	P-O5'-C5'	6.72	131.66	120.90
40	x	2817	A	P-O3'-C3'	6.71	127.76	119.70
39	T	16	GLN	N-CA-C	6.70	129.08	111.00
40	x	2873	U	O4'-C1'-N1	6.69	113.55	108.20
40	x	2874	G	C5'-C4'-O4'	6.65	117.08	109.10
40	x	313	A	O3'-P-O5'	6.56	116.47	104.00
40	x	2705	A	C4-C5-C6	6.53	120.26	117.00
29	O	59	ARG	N-CA-C	6.44	128.39	111.00
26	o	44	ALA	N-CA-C	6.43	128.37	111.00
40	x	444	U	P-O5'-C5'	6.42	131.18	120.90
40	x	1025	A	C4-C5-C6	6.42	120.21	117.00
40	x	2639	G	O5'-C5'-C4'	-6.41	99.53	111.70
40	x	2183	A	C4-C5-C6	6.40	120.20	117.00
40	x	2182	A	O4'-C1'-N9	6.40	113.32	108.20
39	T	16	GLN	C-N-CA	6.40	137.69	121.70
40	x	1002	A	O5'-C5'-C4'	-6.39	99.56	111.70
40	x	2210	G	C4'-C3'-O3'	6.39	125.78	113.00
40	x	494	G	O5'-C5'-C4'	-6.37	99.60	111.70
40	x	440	A	O5'-C5'-C4'	-6.35	99.63	111.70
40	x	2586	G	C4'-C3'-O3'	6.35	125.69	113.00
40	x	1003	A	O3'-P-O5'	-6.21	92.20	104.00
40	x	1218	U	O5'-C5'-C4'	-6.21	99.90	111.70
16	j	38	GLY	O-C-N	-6.20	112.78	122.70
40	x	2258	U	O5'-P-OP2	-6.18	100.14	105.70
40	x	1554	U	C4'-C3'-O3'	6.14	125.29	113.00
40	x	913	A	C4-C5-C6	6.13	120.07	117.00
40	x	2868	U	O4'-C1'-N1	6.13	113.10	108.20
26	o	117	LYS	C-N-CA	6.10	136.96	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	E	67	GLY	C-N-CA	-6.08	96.46	122.00
40	x	2816	G	C2'-C3'-O3'	-6.08	96.14	109.50
40	x	2182	A	C4-C5-C6	6.05	120.03	117.00
40	x	1026	A	C4-C5-C6	5.97	119.98	117.00
9	E	68	PRO	CA-C-N	-5.96	104.08	117.20
40	x	1004	U	C5'-C4'-C3'	5.93	125.49	116.00
40	x	2316	G	C4'-C3'-O3'	5.92	124.83	113.00
40	x	2586	G	O4'-C1'-N9	-5.91	103.47	108.20
40	x	1026	A	C5-C6-N6	-5.91	118.98	123.70
40	x	1131	G	P-O5'-C5'	5.90	130.33	120.90
40	x	2318	U	O4'-C1'-N1	5.88	112.91	108.20
40	x	2147	A	O4'-C1'-N9	5.88	112.90	108.20
40	x	1556	C	O4'-C1'-N1	5.86	112.89	108.20
40	x	441	U	P-O3'-C3'	5.86	126.73	119.70
40	x	2587	U	C4'-C3'-O3'	-5.83	97.16	109.40
40	x	2183	A	O4'-C1'-N9	5.82	112.85	108.20
9	E	68	PRO	N-CA-C	-5.80	97.02	112.10
40	x	2616	C	C2'-C3'-O3'	5.78	122.95	113.70
40	x	1000	C	P-O3'-C3'	5.78	126.63	119.70
40	x	443	G	C4'-C3'-O3'	5.77	124.54	113.00
40	x	2319	U	P-O3'-C3'	5.76	126.62	119.70
40	x	1556	C	N1-C1'-C2'	5.76	121.49	114.00
40	x	493	G	O3'-P-O5'	5.75	114.93	104.00
40	x	2818	U	O5'-C5'-C4'	5.74	122.61	111.70
40	x	1025	A	C5-C6-N6	-5.74	119.11	123.70
40	x	1002	A	P-O3'-C3'	5.74	126.58	119.70
40	x	913	A	C5-C6-N6	-5.70	119.14	123.70
32	r	442	ALA	N-CA-C	-5.69	95.64	111.00
40	x	2825	C	C5'-C4'-C3'	5.69	125.10	116.00
40	x	2320	A	C5'-C4'-C3'	5.65	125.04	116.00
34	s	1479	LEU	O-C-N	-5.65	113.67	122.70
40	x	2147	A	C4-C5-C6	5.64	119.82	117.00
40	x	2818	U	O3'-P-O5'	5.63	114.70	104.00
34	s	630	ASN	N-CA-C	-5.62	95.82	111.00
40	x	2637	A	C2'-C3'-O3'	5.62	122.69	113.70
40	x	1131	G	O4'-C1'-N9	5.62	112.69	108.20
40	x	2617	U	N1-C1'-C2'	-5.62	105.82	112.00
40	x	2705	A	C5-C6-N1	-5.62	114.89	117.70
26	o	237	MET	N-CA-C	-5.61	95.86	111.00
40	x	2256	A	C4'-C3'-O3'	-5.58	97.69	109.40
40	x	2207	A	C4'-C3'-O3'	5.57	124.14	113.00
40	x	2181	C	N3-C4-N4	5.57	121.90	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	x	2586	G	C2'-C3'-O3'	5.56	122.59	113.70
40	x	2405	C	O5'-C5'-C4'	-5.55	101.15	111.70
40	x	2404	A	O5'-C5'-C4'	5.55	122.25	111.70
40	x	2403	G	N9-C1'-C2'	5.54	121.19	114.00
40	x	2149	A	C5-C6-N6	-5.53	119.28	123.70
40	x	2868	U	C5'-C4'-O4'	5.52	115.72	109.10
40	x	2616	C	P-O3'-C3'	5.51	126.31	119.70
40	x	913	A	O4'-C1'-N9	5.50	112.60	108.20
5	C	187	LEU	N-CA-C	-5.49	96.17	111.00
40	x	1220	U	O4'-C1'-N1	5.49	112.59	108.20
40	x	1220	U	P-O3'-C3'	-5.47	113.13	119.70
40	x	2873	U	O4'-C4'-C3'	-5.46	98.54	104.00
40	x	443	G	O3'-P-O5'	5.45	114.36	104.00
40	x	494	G	C2'-C3'-O3'	-5.43	97.55	109.50
40	x	2183	A	C5-C6-N6	-5.43	119.35	123.70
40	x	2182	A	C5-C6-N6	-5.42	119.36	123.70
40	x	2181	C	N3-C4-C5	-5.41	119.74	121.90
40	x	913	A	C5-C6-N1	-5.38	115.01	117.70
40	x	2873	U	C2-N1-C1'	5.38	124.15	117.70
40	x	2869	U	P-O5'-C5'	5.37	129.50	120.90
34	s	1409	PRO	CA-C-N	-5.37	105.39	117.20
40	x	2182	A	C5-C6-N1	-5.36	115.02	117.70
40	x	2183	A	C5-C6-N1	-5.36	115.02	117.70
40	x	1026	A	C5-C6-N1	-5.35	115.03	117.70
40	x	2615	G	C4'-C3'-O3'	5.35	123.69	113.00
40	x	2147	A	C5-C6-N1	-5.34	115.03	117.70
40	x	2585	G	P-O3'-C3'	5.34	126.10	119.70
34	s	578	ASP	N-CA-C	-5.33	96.60	111.00
32	r	306	LEU	N-CA-C	-5.33	96.60	111.00
40	x	2705	A	C5-C6-N6	-5.30	119.46	123.70
26	o	118	PHE	CA-C-N	5.29	126.79	116.20
32	r	88	ILE	N-CA-C	-5.29	96.72	111.00
40	x	2870	C	C2'-C3'-O3'	-5.26	97.94	109.50
40	x	2209	U	C5'-C4'-O4'	-5.25	102.81	109.10
40	x	2319	U	O4'-C4'-C3'	-5.24	98.76	104.00
40	x	2258	U	C4'-C3'-O3'	5.22	123.43	113.00
40	x	2817	A	C4'-C3'-O3'	-5.22	98.44	109.40
40	x	2871	G	P-O3'-C3'	-5.19	113.47	119.70
32	r	129	GLU	N-CA-C	-5.19	97.00	111.00
26	o	94	SER	N-CA-C	-5.17	97.04	111.00
40	x	2868	U	P-O5'-C5'	-5.17	112.63	120.90
40	x	2618	G	P-O5'-C5'	5.16	129.16	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	x	2147	A	C5-C6-N6	-5.14	119.59	123.70
40	x	2149	A	C4-C5-C6	5.13	119.57	117.00
40	x	441	U	O5'-C5'-C4'	-5.13	101.95	111.70
40	x	2862	U	P-O3'-C3'	-5.12	113.56	119.70
40	x	2269	U	P-O5'-C5'	5.10	129.06	120.90
40	x	1556	C	C5'-C4'-O4'	5.08	115.20	109.10
40	x	1555	U	C4'-C3'-O3'	5.07	123.14	113.00
40	x	2781	U	P-O3'-C3'	5.06	125.77	119.70
40	x	2618	G	O5'-C5'-C4'	-5.05	102.11	111.70
34	s	859	LYS	C-N-CA	-5.04	111.71	122.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
48	a	34	MET	CA

All (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
9	E	42	LEU	Mainchain
19	J	8	PRO	Peptide
39	T	16	GLN	Mainchain
39	T	23	GLY	Peptide
39	T	86	GLU	Peptide
48	a	111	LYS	Peptide
8	f	100	ILE	Mainchain
8	f	103	TYR	Peptide
26	o	43	ARG	Mainchain
32	r	111	GLU	Mainchain
32	r	461	GLU	Peptide
32	r	462	ILE	Peptide
34	s	1015	ARG	Mainchain
34	s	1018	ASN	Peptide
34	s	1466	ASP	Peptide
34	s	1479	LEU	Mainchain
34	s	576	SER	Mainchain,Peptide
34	s	578	ASP	Peptide
34	s	628	PHE	Peptide
34	s	858	GLU	Mainchain

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Mol	Chain	Res	Type	Group
34	s	859	LYS	Peptide
34	s	903	SER	Peptide
36	t	17	HIS	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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.

All (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
39:T:41:ASP:O	39:T:43:LYS:N	2.00	0.93
1:A:114:SER:CA	1:A:134:VAL:H	1.81	0.89
1:A:206:PRO:O	1:A:208:ASP:N	2.06	0.88
35:R:158:GLU:O	35:R:161:ALA:N	2.08	0.86
1:A:119:LYS:O	1:A:121:GLY:N	2.12	0.82
1:A:115:ASN:CA	1:A:133:TYR:CA	2.58	0.81
39:T:62:GLY:CA	39:T:75:ILE:N	2.42	0.81
1:A:115:ASN:N	1:A:133:TYR:CA	2.45	0.80
19:J:106:ILE:O	19:J:125:MET:N	2.14	0.79
35:R:157:GLU:O	35:R:161:ALA:N	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:N	1:A:134:VAL:C	2.39	0.73
19:J:94:ARG:O	19:J:96:PHE:N	2.22	0.71
39:T:74:VAL:O	39:T:89:LEU:N	2.25	0.69
35:R:173:ARG:O	35:R:177:VAL:N	2.24	0.68
39:T:62:GLY:H	39:T:75:ILE:H	1.42	0.68
1:A:114:SER:C	1:A:133:TYR:CA	2.63	0.67
1:A:113:VAL:N	1:A:134:VAL:O	2.26	0.66
19:J:85:LYS:O	19:J:88:GLU:N	2.28	0.66
1:A:206:PRO:C	1:A:208:ASP:H	1.98	0.65
23:L:99:HIS:O	23:L:101:ARG:N	2.28	0.63
35:R:158:GLU:O	35:R:159:ALA:C	2.36	0.63
39:T:62:GLY:N	39:T:75:ILE:N	2.36	0.62
39:T:76:ILE:O	39:T:78:LYS:N	2.34	0.60
3:B:238:LEU:N	3:B:246:LEU:O	2.36	0.59
35:R:81:ARG:O	35:R:83:GLY:N	2.35	0.59
1:A:134:VAL:O	1:A:136:ILE:N	2.35	0.59
29:O:62:THR:O	29:O:64:PHE:N	2.29	0.58
35:R:79:GLY:O	35:R:81:ARG:N	2.36	0.58
13:G:35:GLY:O	13:G:37:GLY:N	2.37	0.58
1:A:125:ALA:O	1:A:127:ALA:N	2.37	0.58
35:R:158:GLU:O	35:R:161:ALA:CA	2.52	0.57
1:A:114:SER:C	1:A:134:VAL:H	2.07	0.56
19:J:94:ARG:C	19:J:96:PHE:H	2.09	0.56
31:P:95:LEU:O	31:P:97:ASN:N	2.38	0.55
1:A:125:ALA:C	1:A:127:ALA:H	2.10	0.54
39:T:61:THR:CA	39:T:75:ILE:O	2.55	0.54
29:O:110:PRO:O	29:O:112:TYR:N	2.41	0.54
39:T:43:LYS:C	39:T:95:HIS:CA	2.75	0.54
43:V:46:LEU:O	43:V:48:ARG:N	2.41	0.53
27:N:107:GLY:O	27:N:111:ALA:N	2.41	0.53
35:R:150:GLN:O	35:R:154:ALA:N	2.40	0.53
39:T:61:THR:C	39:T:75:ILE:O	2.46	0.53
1:A:114:SER:CA	1:A:134:VAL:N	2.64	0.52
1:A:114:SER:C	1:A:134:VAL:N	2.63	0.52
5:C:94:CYS:O	5:C:96:GLY:N	2.42	0.52
27:N:75:VAL:O	27:N:77:LYS:N	2.43	0.52
37:S:132:THR:O	37:S:134:ASP:N	2.43	0.52
31:P:40:GLU:O	31:P:42:THR:N	2.42	0.52
39:T:74:VAL:O	39:T:88:ARG:CA	2.58	0.51
1:A:112:ILE:CA	1:A:134:VAL:O	2.59	0.51
1:A:125:ALA:C	1:A:127:ALA:N	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:I:39:LYS:N	17:I:205:VAL:O	2.41	0.50
27:N:165:THR:O	27:N:169:LYS:N	2.28	0.50
3:B:46:PHE:O	3:B:338:LEU:N	2.45	0.50
3:B:346:THR:O	3:B:348:ARG:N	2.45	0.49
7:D:257:GLU:O	7:D:259:LYS:N	2.44	0.49
31:P:132:ALA:O	31:P:134:GLY:N	2.45	0.49
19:J:23:VAL:O	19:J:25:GLU:N	2.39	0.49
19:J:73:GLY:O	19:J:75:LYS:N	2.46	0.49
5:C:181:VAL:O	5:C:183:LYS:N	2.43	0.49
23:L:164:GLU:O	23:L:166:ALA:N	2.45	0.49
25:M:34:ALA:O	25:M:47:ASP:N	2.46	0.48
15:H:80:THR:O	15:H:85:GLY:N	2.47	0.48
3:B:49:TYR:O	3:B:80:ASP:N	2.46	0.48
37:S:79:VAL:N	37:S:90:MET:O	2.45	0.48
5:C:337:GLU:O	5:C:339:LEU:N	2.48	0.47
46:Y:115:ARG:O	46:Y:117:ALA:N	2.48	0.47
1:A:128:ARG:C	1:A:130:SER:H	2.17	0.47
21:K:39:PRO:O	21:K:41:LYS:N	2.47	0.47
35:R:81:ARG:C	35:R:83:GLY:H	2.18	0.47
35:R:85:ARG:O	35:R:89:LEU:N	2.47	0.47
11:F:108:LEU:O	11:F:110:ARG:N	2.48	0.46
47:Z:16:GLY:O	47:Z:18:TYR:N	2.48	0.46
23:L:27:ASP:O	23:L:29:ALA:N	2.49	0.46
5:C:114:ASN:O	5:C:118:LYS:N	2.42	0.46
23:L:165:SER:O	23:L:167:PHE:N	2.47	0.46
35:R:66:HIS:O	35:R:70:LYS:N	2.41	0.45
5:C:206:LEU:O	5:C:249:ILE:N	2.39	0.45
11:F:24:GLU:O	11:F:26:VAL:N	2.50	0.45
19:J:109:HIS:N	19:J:123:PHE:O	2.49	0.44
5:C:338:LYS:O	5:C:340:GLY:N	2.50	0.44
37:S:79:VAL:O	37:S:90:MET:N	2.49	0.44
45:X:49:LYS:O	45:X:51:VAL:N	2.51	0.44
11:F:222:HIS:O	11:F:227:GLY:N	2.51	0.44
33:Q:170:ARG:O	33:Q:172:PHE:N	2.51	0.43
5:C:222:VAL:O	5:C:224:GLY:N	2.52	0.43
15:H:49:ASN:O	15:H:51:GLN:N	2.51	0.43
17:I:73:ASP:O	17:I:75:ASP:N	2.51	0.43
19:J:110:ILE:C	19:J:112:LEU:H	2.21	0.43
41:U:97:SER:O	41:U:99:LYS:N	2.52	0.43
41:U:43:VAL:O	41:U:45:GLY:N	2.52	0.43
43:V:23:MET:O	43:V:34:LEU:N	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:H:64:HIS:O	15:H:66:ALA:N	2.52	0.42
35:R:158:GLU:C	35:R:161:ALA:H	2.22	0.42
19:J:107:ASP:CA	19:J:124:GLY:HA2	2.50	0.42
31:P:113:TYR:O	31:P:151:THR:N	2.48	0.42
29:O:130:LYS:O	29:O:132:GLY:N	2.53	0.42
9:E:97:ASN:O	9:E:99:GLU:N	2.53	0.41
19:J:41:SER:C	19:J:43:GLN:H	2.24	0.41
29:O:38:ALA:H	29:O:107:GLY:HA2	1.85	0.41
25:M:34:ALA:N	25:M:47:ASP:O	2.52	0.41
19:J:110:ILE:O	19:J:112:LEU:N	2.53	0.40
29:O:62:THR:N	29:O:69:GLY:HA2	2.36	0.40
35:R:158:GLU:O	35:R:161:ALA:C	2.54	0.40

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

All (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
1	A	196	TRP
1	A	206	PRO
1	A	207	VAL
5	C	95	ARG
5	C	188	ARG
5	C	317	PRO
8	f	103	TYR
8	f	104	PRO
11	F	99	PRO
16	j	5	THR
19	J	8	PRO
19	J	11	ASP
19	J	12	LEU
19	J	74	PRO
19	J	94	ARG
19	J	127	PHE
19	J	165	GLN
20	l	22	PRO
21	K	30	PRO
21	K	58	VAL
23	L	100	ARG
25	M	49	PRO
26	o	13	PRO
26	o	18	LEU
26	o	30	PRO
26	o	31	THR
26	o	32	VAL

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Mol	Chain	Res	Type
26	o	55	GLU
26	o	59	GLU
26	o	61	PHE
26	o	88	LYS
26	o	98	ILE
26	o	100	ARG
26	o	108	VAL
26	o	110	ARG
26	o	112	TYR
26	o	114	ARG
26	o	116	LEU
26	o	139	ILE
26	o	143	LEU
26	o	145	ASP
26	o	157	ILE
26	o	234	ASN
26	o	245	HIS
26	o	246	LEU
26	o	247	ARG
29	O	63	ALA
29	O	75	ALA
29	O	76	PRO
29	O	79	ILE
30	q	249	PRO
31	P	143	PRO
32	r	131	ILE
32	r	137	MET
32	r	154	PHE
32	r	156	LEU
32	r	243	ILE
32	r	382	VAL
32	r	390	LEU
32	r	400	VAL
32	r	402	ARG
32	r	404	MET
32	r	406	ALA
32	r	410	ALA
32	r	441	ALA
32	r	486	ILE
32	r	490	ARG
32	r	559	ASN
32	r	649	LYS

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Mol	Chain	Res	Type
32	r	654	ARG
32	r	679	THR
34	s	368	ARG
34	s	428	VAL
34	s	442	ILE
34	s	443	TYR
34	s	452	ILE
34	s	474	PHE
34	s	475	PRO
34	s	513	SER
34	s	737	TRP
34	s	738	LYS
34	s	754	ILE
34	s	759	ASN
34	s	762	ASN
34	s	773	ARG
34	s	777	HIS
34	s	808	VAL
34	s	809	PHE
34	s	853	SER
34	s	854	ILE
34	s	859	LYS
34	s	866	LYS
34	s	869	PRO
34	s	877	MET
34	s	929	VAL
34	s	1019	VAL
34	s	1076	ARG
34	s	1157	THR
34	s	1285	TYR
34	s	1361	LYS
34	s	1362	GLU
34	s	1409	PRO
34	s	1432	ASN
34	s	1434	GLN
34	s	1467	SER
34	s	1468	LEU
34	s	1500	SER
34	s	1501	VAL
34	s	1517	LEU
34	s	1539	MET
34	s	1613	SER

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Mol	Chain	Res	Type
34	s	1774	SER
34	s	1791	ARG
34	s	1905	PRO
34	s	1933	SER
34	s	2030	LEU
34	s	2047	ASN
34	s	2048	TRP
34	s	2055	PRO
34	s	2060	LYS
34	s	2089	ILE
34	s	2099	THR
34	s	2126	ASN
34	s	2146	THR
34	s	2147	PRO
34	s	2167	HIS
34	s	2184	ILE
34	s	2186	LYS
34	s	2190	VAL
34	s	2192	PHE
34	s	2201	LYS
34	s	2239	GLU
34	s	2244	ASP
34	s	2248	ARG
34	s	2250	LEU
34	s	2303	GLU
34	s	2327	PRO
34	s	2328	LEU
34	s	2356	PRO
34	s	2364	VAL
34	s	2367	ILE
34	s	2375	LYS
34	s	2405	MET
35	R	80	LYS
35	R	144	GLN
38	u	84	VAL
38	u	168	PRO
38	u	235	ASN
38	u	254	GLN
38	u	354	ILE
39	T	17	ARG
39	T	42	ILE
39	T	70	SER

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Mol	Chain	Res	Type
39	T	77	ASN
39	T	87	LYS
39	T	90	ASN
39	T	91	LEU
39	T	92	ARG
39	T	132	PRO
48	a	112	ILE
48	a	119	PRO
1	A	116	VAL
1	A	126	LEU
1	A	185	ALA
1	A	194	ASN
2	c	49	PRO
3	B	4	ARG
3	B	18	PRO
3	B	19	ARG
3	B	20	LYS
3	B	96	PRO
4	d	68	GLU
5	C	76	ARG
5	C	189	ALA
5	C	224	GLY
5	C	270	SER
5	C	282	SER
5	C	338	LYS
7	D	56	THR
7	D	259	LYS
7	D	261	THR
11	F	25	GLN
11	F	109	THR
12	h	112	PRO
13	G	65	LEU
13	G	163	VAL
14	i	22	PRO
14	i	24	PRO
15	H	65	VAL
17	I	98	LYS
19	J	9	MET
19	J	73	GLY
19	J	86	VAL
19	J	115	LYS
19	J	167	TYR

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Mol	Chain	Res	Type
20	l	24	PRO
22	m	30	GLY
22	m	89	PRO
23	L	28	GLN
24	n	27	PHE
25	M	8	LYS
26	o	44	ALA
26	o	57	PHE
26	o	69	PRO
26	o	73	ASP
26	o	89	ASN
26	o	94	SER
26	o	118	PHE
26	o	141	LYS
26	o	144	ARG
26	o	152	GLN
26	o	154	ARG
27	N	18	VAL
27	N	76	PRO
29	O	60	LYS
29	O	61	ALA
29	O	64	PHE
29	O	77	SER
29	O	78	ARG
29	O	111	PRO
29	O	148	LYS
30	q	126	VAL
30	q	127	PHE
32	r	85	SER
32	r	93	PHE
32	r	206	ALA
32	r	208	CYS
32	r	210	ASN
32	r	241	VAL
32	r	245	THR
32	r	261	MET
32	r	262	PHE
32	r	282	ASP
32	r	283	GLY
32	r	296	ASN
32	r	297	LYS
32	r	310	ILE

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Mol	Chain	Res	Type
32	r	312	THR
32	r	386	TYR
32	r	388	PHE
32	r	427	ILE
32	r	429	ASP
32	r	431	PHE
32	r	433	SER
32	r	448	ILE
32	r	477	GLY
32	r	488	LEU
32	r	557	ASP
32	r	633	PHE
32	r	656	GLU
32	r	658	SER
33	Q	19	PRO
33	Q	97	PRO
33	Q	171	LYS
33	Q	173	GLU
34	s	440	ASN
34	s	482	PRO
34	s	483	LYS
34	s	594	THR
34	s	725	HIS
34	s	763	GLU
34	s	768	LYS
34	s	799	GLN
34	s	942	LYS
34	s	960	SER
34	s	992	PHE
34	s	1057	ILE
34	s	1134	GLU
34	s	1139	GLU
34	s	1417	GLN
34	s	1452	ASN
34	s	1465	ARG
34	s	1579	ARG
34	s	1740	HIS
34	s	1950	ASN
34	s	1951	GLN
34	s	2031	GLU
34	s	2056	SER
34	s	2148	GLU

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Mol	Chain	Res	Type
34	s	2185	THR
34	s	2226	ASN
34	s	2246	GLN
34	s	2249	VAL
34	s	2285	LEU
34	s	2305	ILE
34	s	2333	PRO
34	s	2354	GLU
34	s	2359	GLU
34	s	2376	TRP
35	R	82	LYS
36	t	17	HIS
36	t	24	ASN
37	S	22	PRO
37	S	50	LYS
38	u	169	ILE
38	u	390	PHE
39	T	16	GLN
39	T	19	PHE
39	T	21	LYS
39	T	24	ALA
39	T	78	LYS
39	T	124	VAL
41	U	44	GLU
41	U	98	THR
45	X	50	ALA
45	X	87	SER
45	X	102	LEU
46	Y	116	LYS
46	Y	126	LEU
47	Z	17	ARG
48	a	17	ALA
48	a	41	HIS
48	a	104	THR
1	A	120	PRO
1	A	181	LYS
1	A	191	LEU
1	A	193	ARG
1	A	195	SER
3	B	68	HIS
3	B	255	TRP
3	B	257	PRO

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Mol	Chain	Res	Type
3	B	311	PHE
3	B	347	SER
4	d	6	ASP
4	d	61	LYS
5	C	11	LEU
5	C	223	PRO
5	C	268	ALA
5	C	320	ASN
5	C	321	LYS
5	C	339	LEU
6	e	12	LYS
7	D	151	GLN
8	f	20	LYS
8	f	91	ALA
9	E	37	GLY
9	E	98	VAL
10	g	48	GLY
10	g	60	ARG
10	g	78	GLY
11	F	98	LYS
11	F	193	PRO
11	F	226	GLY
14	i	16	LYS
15	H	50	ASN
16	j	10	LYS
16	j	39	TYR
16	j	72	ARG
16	j	77	GLY
17	I	18	LYS
17	I	74	VAL
17	I	136	THR
18	k	18	ALA
19	J	140	ARG
19	J	169	ALA
19	J	173	ASP
20	l	36	ARG
21	K	17	ALA
21	K	39	PRO
21	K	40	LYS
21	K	76	SER
21	K	89	PRO
21	K	98	VAL

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Mol	Chain	Res	Type
21	K	102	GLY
23	L	61	PRO
23	L	62	THR
23	L	165	SER
23	L	166	ALA
24	n	50	THR
26	o	34	ARG
26	o	53	THR
26	o	91	TYR
26	o	96	ALA
26	o	150	LEU
26	o	199	PHE
26	o	244	ALA
27	N	80	THR
27	N	158	HIS
27	N	175	ASN
28	p	23	ARG
28	p	24	ARG
29	O	89	SER
30	q	89	SER
30	q	93	LYS
30	q	129	VAL
31	P	41	LEU
31	P	96	GLN
31	P	133	HIS
32	r	133	SER
32	r	204	THR
32	r	247	ALA
32	r	314	LYS
32	r	316	LYS
32	r	637	ALA
32	r	652	GLU
32	r	698	LEU
33	Q	73	GLN
34	s	308	SER
34	s	362	PRO
34	s	459	GLU
34	s	765	GLU
34	s	787	ALA
34	s	851	SER
34	s	905	GLU
34	s	1063	LYS

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Mol	Chain	Res	Type
34	s	1194	GLN
34	s	1233	GLU
34	s	1469	ASN
34	s	1512	GLU
34	s	1515	LEU
34	s	1523	SER
34	s	1723	ALA
34	s	1752	GLY
34	s	1820	ALA
34	s	1888	THR
34	s	1923	CYS
34	s	2029	PRO
34	s	2098	LEU
34	s	2168	PRO
34	s	2188	ALA
35	R	16	GLY
35	R	136	ARG
35	R	139	VAL
37	S	133	ALA
37	S	154	HIS
38	u	85	ASN
39	T	22	HIS
45	X	41	ALA
46	Y	5	SER
46	Y	89	LYS
47	Z	59	ALA
48	a	32	ARG
48	a	46	ASP
48	a	47	LYS
48	a	52	TYR
48	a	58	MET
48	a	97	GLU
48	a	132	LYS
1	A	69	TYR
1	A	180	LEU
3	B	9	PRO
3	B	15	GLY
3	B	234	GLY
3	B	314	TYR
3	B	353	GLU
3	B	362	ALA
5	C	89	ALA

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Mol	Chain	Res	Type
5	C	288	ARG
5	C	291	ASN
7	D	87	GLY
7	D	256	THR
7	D	258	LYS
8	f	105	SER
9	E	75	PRO
10	g	73	SER
11	F	76	TYR
11	F	172	ASN
12	h	81	ARG
13	G	36	ILE
13	G	196	ALA
15	H	62	ARG
15	H	64	HIS
16	j	15	SER
19	J	95	ASN
19	J	108	GLU
19	J	114	ILE
19	J	117	ASP
21	K	19	GLY
21	K	51	LYS
21	K	52	GLU
21	K	55	GLY
22	m	31	SER
22	m	111	ASN
23	L	152	THR
24	n	133	LEU
24	n	162	GLU
25	M	9	ALA
26	o	87	GLU
26	o	179	GLY
26	o	198	ALA
26	o	212	LYS
26	o	235	ILE
27	N	95	GLN
32	r	92	GLY
32	r	146	ALA
32	r	544	LYS
32	r	677	ALA
33	Q	154	GLY
33	Q	166	LEU

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Mol	Chain	Res	Type
34	s	797	GLU
34	s	1180	GLU
34	s	1389	LEU
34	s	1413	ARG
34	s	1484	ARG
34	s	1564	PRO
34	s	1783	PHE
34	s	1816	GLU
34	s	1949	LEU
34	s	1956	GLU
34	s	2057	ASN
34	s	2097	ASP
37	S	32	SER
38	u	357	PRO
39	T	82	ASN
48	a	78	LEU
1	A	26	ALA
1	A	129	ALA
1	A	209	HIS
1	A	213	GLY
3	B	317	ILE
3	B	349	LYS
5	C	75	PRO
5	C	131	VAL
5	C	221	ASN
6	e	48	GLY
7	D	125	VAL
7	D	260	PHE
8	f	62	SER
11	F	191	VAL
12	h	79	ASP
13	G	50	VAL
13	G	68	ARG
14	i	3	VAL
15	H	59	ASN
17	I	151	VAL
17	I	168	ALA
19	J	24	GLY
19	J	111	ASP
19	J	172	LEU
20	l	5	LYS
21	K	32	ILE

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Mol	Chain	Res	Type
21	K	100	HIS
21	K	109	ILE
22	m	112	ASP
23	L	84	GLY
23	L	94	GLY
23	L	136	GLU
24	n	130	LYS
25	M	6	ILE
25	M	82	SER
25	M	90	VAL
27	N	49	ARG
27	N	55	ALA
27	N	58	GLY
28	p	7	LYS
29	O	131	PRO
32	r	308	ASN
32	r	680	LEU
33	Q	9	GLN
33	Q	38	ARG
34	s	530	ASN
34	s	803	ILE
34	s	1176	PRO
34	s	1238	ALA
34	s	1302	THR
34	s	1447	LYS
34	s	1449	ASP
34	s	1799	ASP
34	s	2080	MET
34	s	2199	LEU
34	s	2213	ASN
34	s	2219	PRO
34	s	2331	TYR
34	s	2347	ASP
34	s	2411	ILE
39	T	28	SER
39	T	127	GLN
41	U	11	ILE
41	U	38	ILE
45	X	23	ALA
46	Y	34	PRO
47	Z	32	GLY
47	Z	38	PHE

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Mol	Chain	Res	Type
47	Z	97	SER
3	B	83	PRO
4	d	7	VAL
7	D	19	PRO
8	f	90	PRO
9	E	36	PRO
13	G	157	VAL
14	i	33	ALA
17	I	104	SER
22	m	44	ASP
23	L	32	LYS
24	n	70	ARG
26	o	121	SER
26	o	140	VAL
32	r	384	GLY
32	r	411	CYS
33	Q	175	ALA
34	s	593	PRO
34	s	602	ILE
34	s	646	THR
34	s	764	ASN
34	s	953	SER
34	s	1170	ASN
34	s	2150	PHE
34	s	2217	CYS
34	s	2330	HIS
37	S	132	THR
43	V	3	GLY
5	C	173	GLY
10	g	104	VAL
12	h	47	VAL
13	G	30	THR
34	s	289	VAL
34	s	604	ILE
34	s	956	LYS
47	Z	103	GLN
21	K	22	VAL
26	o	29	THR
31	P	77	GLY
32	r	462	ILE
34	s	2096	VAL
39	T	23	GLY

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Mol	Chain	Res	Type
39	T	123	GLY
1	A	178	PRO
5	C	204	GLY
5	C	245	GLY
5	C	348	GLY
7	D	181	PRO
34	s	1186	PRO
34	s	1627	VAL
34	s	2338	ARG
46	Y	96	PRO
48	a	57	GLY
13	G	75	ILE
14	i	7	ILE
22	m	105	GLY
22	m	148	VAL
34	s	2365	ILE
46	Y	123	GLY
48	a	72	VAL
3	B	268	GLY
7	D	139	PRO
17	I	125	GLY
27	N	154	PRO
32	r	435	GLY
34	s	693	LYS
34	s	1005	LYS
34	s	2254	PRO
34	s	2355	GLU
43	V	107	GLY
48	a	36	GLY
48	a	110	GLY

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

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3670/3675 (99%)	403 (10%)	0

All (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
40	x	66	A
40	x	92	G
40	x	110	G
40	x	113	C
40	x	121	A
40	x	122	A
40	x	123	A
40	x	135	C
40	x	136	G
40	x	156	G
40	x	191	U
40	x	200	C
40	x	210	U
40	x	218	G
40	x	219	A
40	x	240	U
40	x	252	U
40	x	269	G
40	x	295	A
40	x	298	U
40	x	316	U
40	x	323	A
40	x	329	U
40	x	336	A
40	x	337	G
40	x	339	C
40	x	346	C
40	x	376	G
40	x	398	A
40	x	401	U
40	x	402	A
40	x	403	C

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Mol	Chain	Res	Type
40	x	421	G
40	x	422	A
40	x	486	U
40	x	492	U
40	x	521	A
40	x	534	U
40	x	535	G
40	x	546	C
40	x	547	G
40	x	548	G
40	x	552	G
40	x	557	A
40	x	559	A
40	x	579	G
40	x	604	G
40	x	609	G
40	x	611	A
40	x	612	U
40	x	621	A
40	x	638	C
40	x	646	A
40	x	647	A
40	x	649	A
40	x	677	A
40	x	681	U
40	x	705	A
40	x	764	U
40	x	765	C
40	x	767	U
40	x	776	U
40	x	777	U
40	x	780	A
40	x	781	G
40	x	806	A
40	x	817	A
40	x	830	A
40	x	849	C
40	x	874	U
40	x	880	G
40	x	881	C
40	x	907	G
40	x	914	A

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Mol	Chain	Res	Type
40	x	916	G
40	x	917	A
40	x	924	G
40	x	937	G
40	x	944	C
40	x	959	C
40	x	979	U
40	x	980	A
40	x	982	C
40	x	989	A
40	x	995	U
40	x	1001	G
40	x	1006	A
40	x	1007	U
40	x	1028	U
40	x	1045	C
40	x	1046	A
40	x	1049	C
40	x	1063	G
40	x	1065	A
40	x	1072	G
40	x	1081	U
40	x	1095	U
40	x	1098	A
40	x	1103	A
40	x	1104	G
40	x	1116	G
40	x	1117	G
40	x	1139	G
40	x	1159	A
40	x	1160	C
40	x	1180	A
40	x	1181	U
40	x	1192	C
40	x	1200	A
40	x	1201	C
40	x	1202	A
40	x	1222	G
40	x	1236	G
40	x	1240	A
40	x	1241	U
40	x	1242	G

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Mol	Chain	Res	Type
40	x	1243	G
40	x	1244	A
40	x	1245	A
40	x	1246	G
40	x	1254	C
40	x	1263	A
40	x	1264	G
40	x	1274	A
40	x	1278	A
40	x	1279	C
40	x	1287	A
40	x	1289	G
40	x	1295	G
40	x	1302	A
40	x	1305	U
40	x	1308	A
40	x	1309	U
40	x	1330	A
40	x	1351	U
40	x	1352	A
40	x	1354	G
40	x	1355	A
40	x	1357	G
40	x	1367	G
40	x	1386	A
40	x	1390	A
40	x	1399	A
40	x	1400	G
40	x	1419	A
40	x	1437	C
40	x	1446	A
40	x	1481	A
40	x	1508	C
40	x	1511	U
40	x	1563	C
40	x	1568	U
40	x	1570	U
40	x	1571	A
40	x	1572	U
40	x	1583	A
40	x	1589	A
40	x	1607	U

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Mol	Chain	Res	Type
40	x	1629	U
40	x	1643	A
40	x	1645	U
40	x	1657	C
40	x	1717	U
40	x	1728	G
40	x	1750	A
40	x	1751	G
40	x	1760	A
40	x	1765	U
40	x	1780	G
40	x	1797	A
40	x	1816	A
40	x	1819	U
40	x	1821	U
40	x	1841	A
40	x	1842	A
40	x	1880	U
40	x	1893	A
40	x	1906	G
40	x	1953	G
40	x	1966	U
40	x	1973	G
40	x	2010	U
40	x	2011	U
40	x	2013	C
40	x	2032	U
40	x	2042	G
40	x	2056	U
40	x	2061	G
40	x	2067	U
40	x	2071	A
40	x	2076	G
40	x	2080	C
40	x	2087	C
40	x	2089	A
40	x	2094	C
40	x	2102	U
40	x	2113	A
40	x	2121	G
40	x	2122	G
40	x	2131	A

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Mol	Chain	Res	Type
40	x	2158	A
40	x	2170	U
40	x	2179	C
40	x	2188	A
40	x	2205	U
40	x	2228	A
40	x	2244	A
40	x	2249	G
40	x	2255	A
40	x	2260	U
40	x	2273	G
40	x	2275	A
40	x	2279	A
40	x	2281	A
40	x	2298	U
40	x	2307	G
40	x	2363	A
40	x	2374	C
40	x	2388	U
40	x	2397	A
40	x	2411	U
40	x	2418	G
40	x	2440	G
40	x	2446	U
40	x	2451	G
40	x	2453	U
40	x	2463	G
40	x	2469	G
40	x	2472	U
40	x	2477	G
40	x	2478	C
40	x	2479	C
40	x	2484	A
40	x	2490	C
40	x	2493	U
40	x	2494	A
40	x	2495	C
40	x	2496	C
40	x	2501	U
40	x	2502	A
40	x	2505	U
40	x	2508	U

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Mol	Chain	Res	Type
40	x	2510	U
40	x	2514	U
40	x	2519	A
40	x	2523	A
40	x	2524	A
40	x	2526	C
40	x	2531	C
40	x	2538	U
40	x	2540	A
40	x	2541	U
40	x	2542	U
40	x	2547	A
40	x	2548	C
40	x	2549	G
40	x	2552	C
40	x	2569	A
40	x	2570	U
40	x	2571	U
40	x	2572	C
40	x	2573	G
40	x	2590	A
40	x	2593	A
40	x	2601	A
40	x	2606	G
40	x	2614	G
40	x	2619	G
40	x	2621	G
40	x	2622	C
40	x	2627	C
40	x	2630	C
40	x	2636	A
40	x	2652	U
40	x	2656	A
40	x	2674	A
40	x	2677	G
40	x	2689	A
40	x	2691	A
40	x	2694	A
40	x	2696	A
40	x	2700	G
40	x	2701	U
40	x	2714	G

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Mol	Chain	Res	Type
40	x	2726	C
40	x	2728	G
40	x	2729	U
40	x	2730	G
40	x	2753	G
40	x	2760	C
40	x	2762	A
40	x	2772	C
40	x	2777	G
40	x	2778	G
40	x	2785	A
40	x	2797	C
40	x	2798	C
40	x	2800	G
40	x	2801	A
40	x	2802	A
40	x	2803	A
40	x	2805	G
40	x	2806	U
40	x	2828	G
40	x	2830	G
40	x	2831	G
40	x	2845	A
40	x	2873	U
40	x	2887	A
40	x	2896	A
40	x	2899	C
40	x	2935	U
40	x	2936	A
40	x	2957	G
40	x	2983	C
40	x	2996	U
40	x	2997	G
40	x	3012	A
40	x	3056	U
40	x	3078	U
40	x	3086	A
40	x	3092	C
40	x	3093	C
40	x	3101	G
40	x	3122	A
40	x	3130	A

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Mol	Chain	Res	Type
40	x	3131	U
40	x	3142	A
40	x	3143	C
40	x	3144	G
40	x	3155	U
40	x	3165	A
40	x	3173	G
40	x	3174	A
40	x	3176	G
40	x	3179	U
40	x	3181	C
40	x	3187	A
40	x	3198	U
40	x	3207	U
40	x	3217	C
40	x	3219	G
40	x	3229	G
40	x	3243	A
40	x	3245	A
40	x	3247	G
40	x	3259	U
40	x	3260	G
40	x	3270	U
40	x	3272	C
40	x	3273	A
40	x	3276	G
40	x	3279	A
40	x	3281	U
40	x	3294	A
40	x	3304	U
40	x	3313	U
40	x	3316	A
40	x	3318	G
40	x	3319	U
40	x	3320	A
40	x	3351	U
40	x	3352	U
40	x	3353	G
40	x	3355	U
40	x	3369	G
40	x	3370	A
40	x	3375	A

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Mol	Chain	Res	Type
40	x	3376	A
40	x	3378	C
40	x	3390	G
42	y	17	A
42	y	34	U
42	y	35	C
42	y	37	A
42	y	39	G
42	y	52	A
42	y	59	A
42	y	62	C
42	y	63	G
42	y	72	A
42	y	80	A
42	y	86	U
42	y	90	U
42	y	95	G
42	y	104	A
42	y	106	C
42	y	111	A
42	y	113	U
42	y	125	U
42	y	126	A
44	z	13	A
44	z	53	U
44	z	54	U
44	z	65	G
44	z	87	G
44	z	102	A
44	z	112	G

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.