



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Nov 1, 2017 – 11:12 PM EDT

PDB ID : 5T6R  
EMDB ID: : EMD-8368  
Title : Nmd3 is a structural mimic of eIF5A, and activates the cpGTPase Lsg1 during  
60S ribosome biogenesis: 60S-Nmd3 Complex  
Authors : Malyutin, A.G.; Musalgaonkar, S.; Patchett, S.; Frank, J.; Johnson, A.W.  
Deposited on : unknown  
Resolution : 4.50 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](mailto: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.

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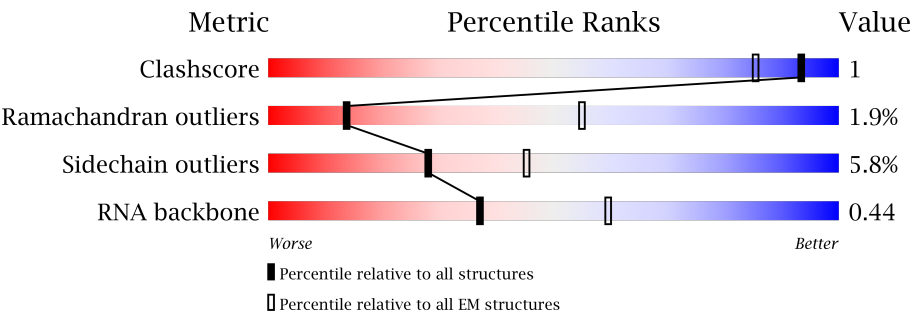
MolProbity : 4.02b-467  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

# 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 4.50 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.










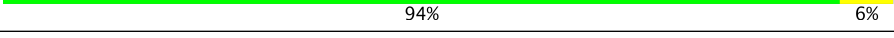
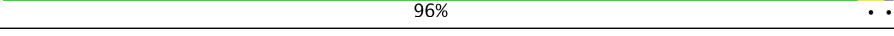
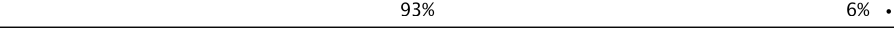
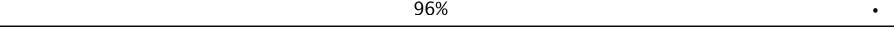
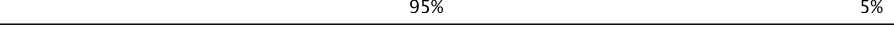
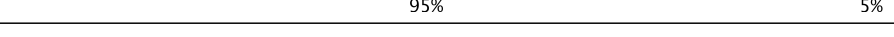
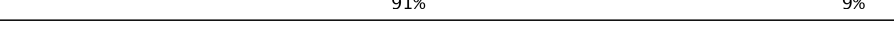

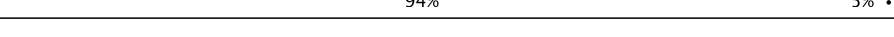
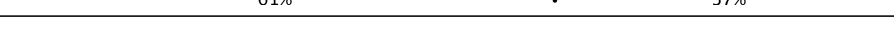

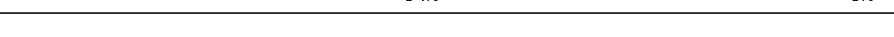






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

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  $\geq 3$ , 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	3396	<div><div>69%</div><div>23%</div><div>• 6%</div></div>
2	B	121	<div><div>81%</div><div>18%</div><div>•</div></div>
3	C	158	<div><div>75%</div><div>24%</div><div>•</div></div>
4	D	254	<div><div>95%</div><div>•</div><div>•</div></div>
5	E	387	<div><div>94%</div><div>6%</div></div>
6	F	362	<div><div>91%</div><div>9%</div></div>
7	G	297	<div><div>89%</div><div>10%</div><div>•</div></div>
8	H	176	<div><div>84%</div><div>5%</div><div>11%</div></div>





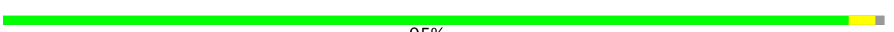







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Mol	Chain	Length	Quality of chain
9	I	244	
10	J	256	
11	K	191	
12	L	221	
13	M	174	
14	N	199	
15	O	138	
16	a	204	
17	b	199	
18	c	184	
19	d	186	
20	e	189	
21	f	172	
22	g	160	
23	h	121	
24	i	137	
25	j	155	
26	k	142	
27	l	127	
28	m	136	
29	n	149	
30	o	59	
31	p	105	
32	q	113	
33	r	130	

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Mol	Chain	Length	Quality of chain
34	s	107	 46% 53%
35	t	121	 89% 7%
36	u	120	 91% 8%
37	v	100	 91% 8%
38	w	88	 95%
39	x	78	 92% 6%
40	y	51	 96%
41	z	128	 37% 59%
42	Q	106	 88% 11%
43	R	92	 96%
44	S	210	 99%
45	V	917	 19% 6% 73%

## 2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 126616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 25S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	3204	Total	C	N	O	P	0	0
			68535	30613	12358	22360	3204		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 3 is a RNA chain called 5.8S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 4 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	252	Total	C	N	O	S	0	0
			1914	1191	388	334	1		

- Molecule 5 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 6 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	296	Total	C	N	O	S	0	0
			2375	1501	414	458	2		

- Molecule 8 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 9 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	222	Total	C	N	O	S	0	0
			1784	1151	324	308	1		

- Molecule 10 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	233	Total	C	N	O	S	0	0
			1804	1151	323	327	3		

- Molecule 11 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	191	Total	C	N	O	S	0	0
			1518	963	274	277	4		

- Molecule 12 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	211	Total	C	N	O	S	0	0
			1705	1083	322	294	6		

- Molecule 13 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	169	Total	C	N	O	S	0	0
			1353	847	253	249	4		

- Molecule 14 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	N	193	Total	C	N	O	0	0
			1543	962	315	266		

- Molecule 15 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	136	Total	C	N	O	S	0	0
			1053	675	199	177	2		

- Molecule 16 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	a	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 17 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	b	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 18 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	183	Total	C	N	O	0	0
			1420	882	281	257		

- Molecule 19 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	d	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 20 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	e	188	Total	C	N	O	0	0
			1521	935	326	260		

- Molecule 21 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	f	172	Total	C	N	O	S	0	0
			1445	930	267	244	4		

- Molecule 22 is a protein called 60S ribosomal protein L21-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 23 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	100	Total	C	N	O	S	0	0
			796	516	131	149			

- Molecule 24 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	136	Total	C	N	O	S	0	0
			1003	628	189	179	7		

- Molecule 25 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	j	98	Total	C	N	O	S	0	0
			699	443	137	118	1		

- Molecule 26 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	k	121	Total	C	N	O	S	0	0
			964	620	169	173	2		

- Molecule 27 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	l	126	Total	C	N	O	S	0	0
			993	625	192	176			

- Molecule 28 is a protein called 60S ribosomal protein L27-A.



Mol	Chain	Residues	Atoms				AltConf	Trace
28	m	135	Total	C	N	O	0	0
			1092	710	202	180		

- Molecule 29 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	n	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	o	58	Total	C	N	O	0	0
			462	289	100	73		

- Molecule 31 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	p	97	Total	C	N	O	S	0	0
			743	479	124	139	1		

- Molecule 32 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	q	109	Total	C	N	O	S	0	0
			876	556	167	152	1		

- Molecule 33 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	r	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 34 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	50	Total	C	N	O	0	0
			406	258	77	71		

- Molecule 35 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	t	112	Total	C	N	O	S	0	0
			880	545	179	152	4		

- Molecule 36 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	u	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 37 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	v	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 38 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	w	87	Total	C	N	O	S	0	0
			681	414	148	114	5		

- Molecule 39 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	x	77	Total	C	N	O	0	0
			612	391	115	106		

- Molecule 40 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	y	50	Total	C	N	O	S	0	0
			436	272	97	65	2		

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	z	52	Total	C	N	O	S	0	0
			417	259	86	67	5		

- Molecule 42 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Q	105	Total	C	N	O	S	0	0
			847	534	170	138	5		

- Molecule 43 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 44 is a protein called Ribosomal Protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	S	210	Total	C	N	O		0	0
			1050	630	210	210			

- Molecule 45 is a protein called Maltose binding protein, 60S ribosomal export protein Nmd3 fusion.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	V	251	Total	C	N	O	S	0	0
			1975	1263	333	372	7		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-396	ILE	THR	conflict	UNP A0A0F8NYV9
V	-15	HIS	-	linker	UNP A0A0F8NYV9
V	-14	HIS	-	linker	UNP A0A0F8NYV9
V	-13	HIS	-	linker	UNP A0A0F8NYV9
V	-12	HIS	-	linker	UNP A0A0F8NYV9
V	-11	HIS	-	linker	UNP A0A0F8NYV9
V	-10	HIS	-	linker	UNP A0A0F8NYV9
V	-9	HIS	-	linker	UNP A0A0F8NYV9
V	-8	HIS	-	linker	UNP A0A0F8NYV9
V	-7	HIS	-	linker	UNP A0A0F8NYV9
V	-6	HIS	-	linker	UNP A0A0F8NYV9
V	-5	GLU	-	linker	UNP A0A0F8NYV9
V	-4	ASN	-	linker	UNP A0A0F8NYV9
V	-3	LEU	-	linker	UNP A0A0F8NYV9
V	-2	TYR	-	linker	UNP A0A0F8NYV9
V	-1	PHE	-	linker	UNP A0A0F8NYV9
V	0	GLN	-	linker	UNP A0A0F8NYV9
V	1	GLY	-	linker	UNP A0A0F8NYV9

- Molecule 46 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	A	84	Total 84	Mg 84	0
46	C	1	Total 1	Mg 1	0
46	i	1	Total 1	Mg 1	0

- Molecule 47 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
47	A	3	Total 3	K 3	0

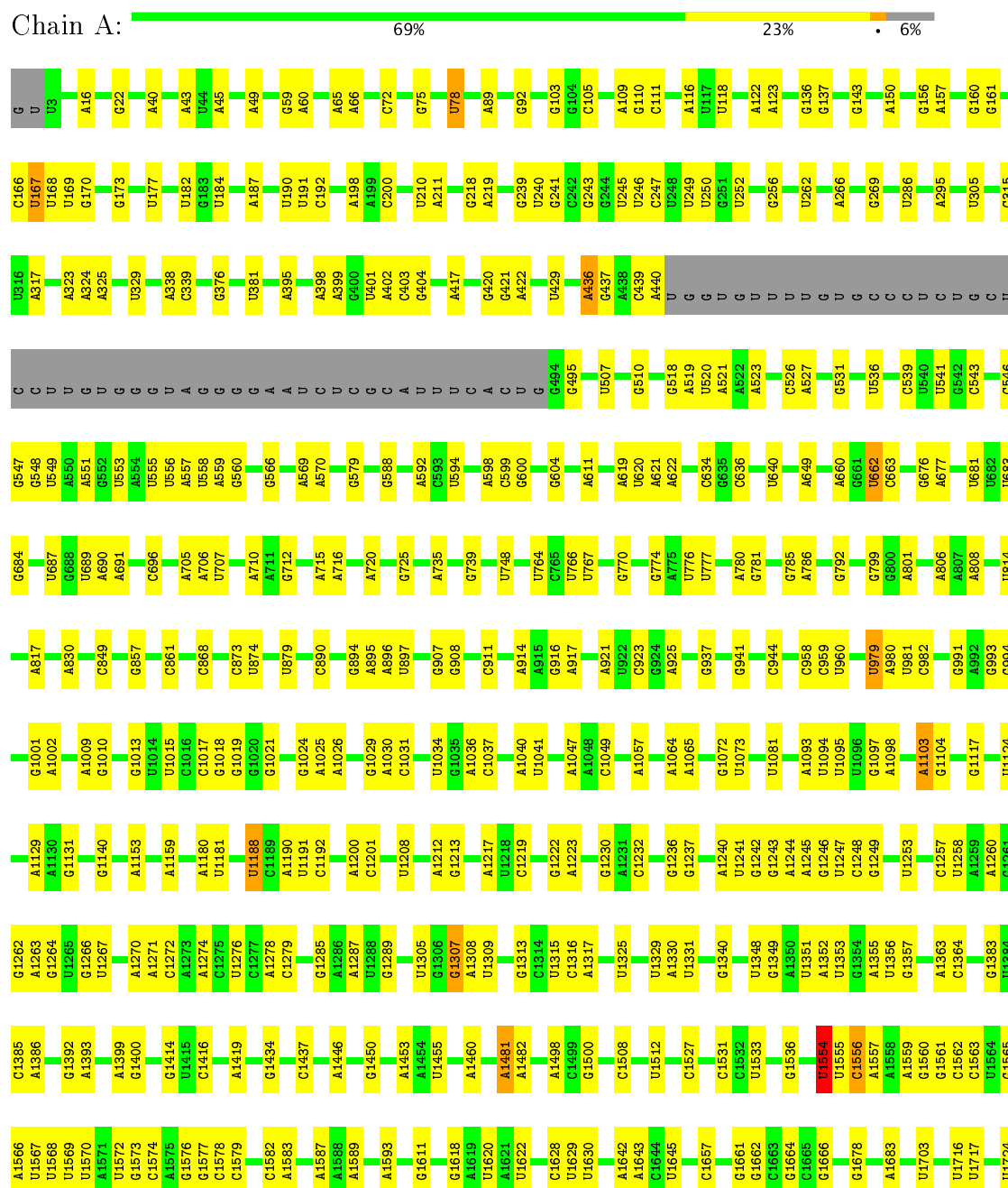
- Molecule 48 is water.

Mol	Chain	Residues	Atoms		AltConf
48	A	10	Total 10	O 10	0
48	c	1	Total 1	O 1	0
48	e	1	Total 1	O 1	0

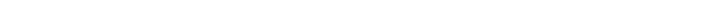
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

#### • Molecule 1: 25S Ribosomal RNA



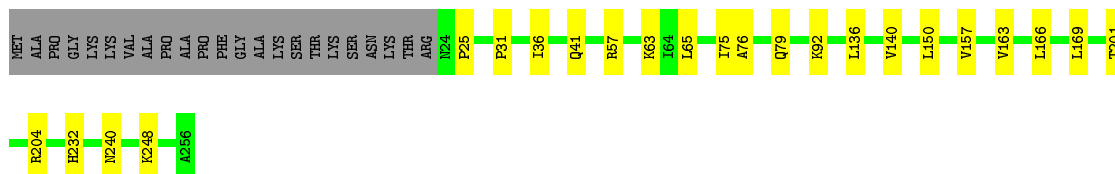


- Chain I:  85% 6% 9%



- Molecule 10: 60S ribosomal protein L8-A

Chain J: 82% 9% 9%



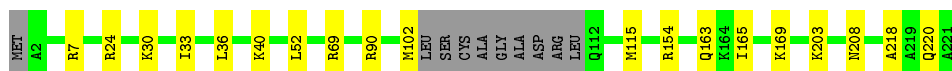
- Molecule 11: 60S ribosomal protein L9-A

Chain K: 91% 8% .



- Molecule 12: 60S ribosomal protein L10

Chain L: 87% 9% 5%



- Molecule 13: 60S ribosomal protein L11-A

Chain M: 87% 9% . .



- Molecule 14: 60S ribosomal protein L13-A

Chain N: 88% 9% .



- Molecule 15: 60S ribosomal protein L14-A

Chain O: 92% 7% .



- Molecule 16: 60S ribosomal protein L15-A

Chain a: 94% 6%





- Molecule 17: 60S ribosomal protein L16-A

Chain b: 96% ..



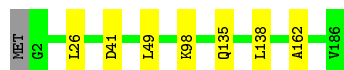
- Molecule 18: 60S ribosomal protein L17-A

Chain c: 93% 6% .



- Molecule 19: 60S ribosomal protein L18-A

Chain d: 96% ..



- Molecule 20: 60S ribosomal protein L19-A

Chain e: 95% 5% .



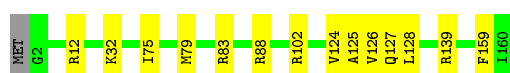
- Molecule 21: 60S ribosomal protein L20-A

Chain f: 95% 5%



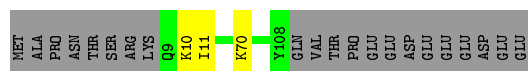
- Molecule 22: 60S ribosomal protein L21-A

Chain g: 91% 9% .



- Molecule 23: 60S ribosomal protein L22-A

Chain h: 80% 17%



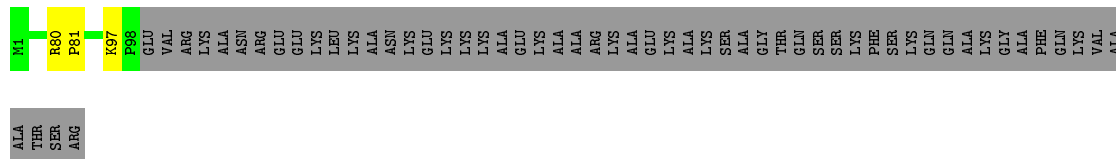
- Molecule 24: 60S ribosomal protein L23-A

Chain i:  94% 5% .




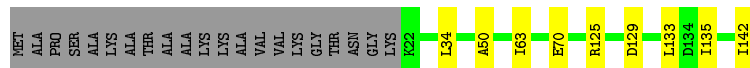
- Molecule 25: 60S ribosomal protein L24-A

Chain j:  61% . 37%



- Molecule 26: 60S ribosomal protein L25

Chain k:  79% 6% 15%



- Molecule 27: 60S ribosomal protein L26-A

Chain l:  94% 5% ..




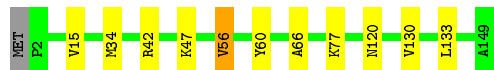
- Molecule 28: 60S ribosomal protein L27-A

Chain m:  93% 7% .



- Molecule 29: 60S ribosomal protein L28

Chain n:  92% 7% ..

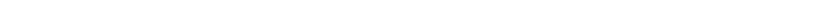


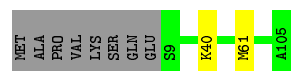
- Molecule 30: 60S ribosomal protein L29

Chain o:  88% 8% . .



- Molecule 31: 60S ribosomal protein L30

Chain p:  90% • 8%

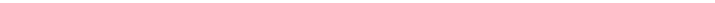


- Molecule 32: 60S ribosomal protein L31-A

Chain q:  90% 6% .



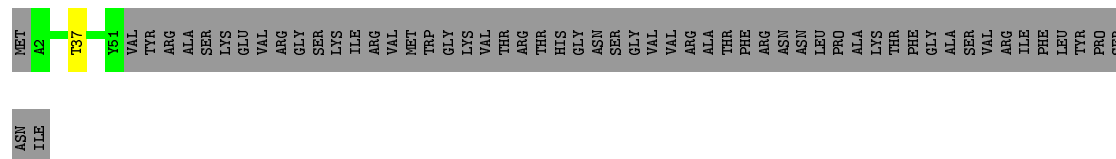
- Molecule 33: 60S ribosomal protein L32

Chain r:  90% 8% .

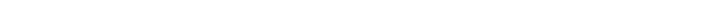


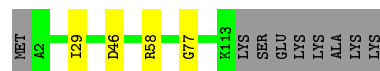
- Molecule 34: 60S ribosomal protein L33-A

Chain s:  46% . 53%



- Molecule 35: 60S ribosomal protein L34-A

Chain t:  89% 7%



- Molecule 36: 60S ribosomal protein L35-A

Chain u:  91% 8%



- Molecule 37: 60S ribosomal protein L36-A

Chain v:  91% 8%



- Molecule 38: 60S ribosomal protein L37-A

Chain w:  95% ..



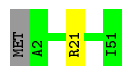
- Molecule 39: 60S ribosomal protein L38

Chain x:  92% 6% .



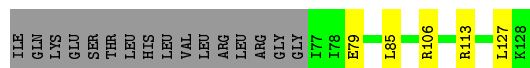
- Molecule 40: 60S ribosomal protein L39

Chain y:  96% ..




- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain z:  37% . 59%



- Molecule 42: 60S ribosomal protein L42-A

Chain Q:  88% 11% .



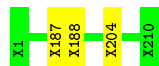
- Molecule 43: 60S ribosomal protein L43-A

Chain R:  96% ..

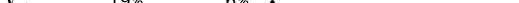


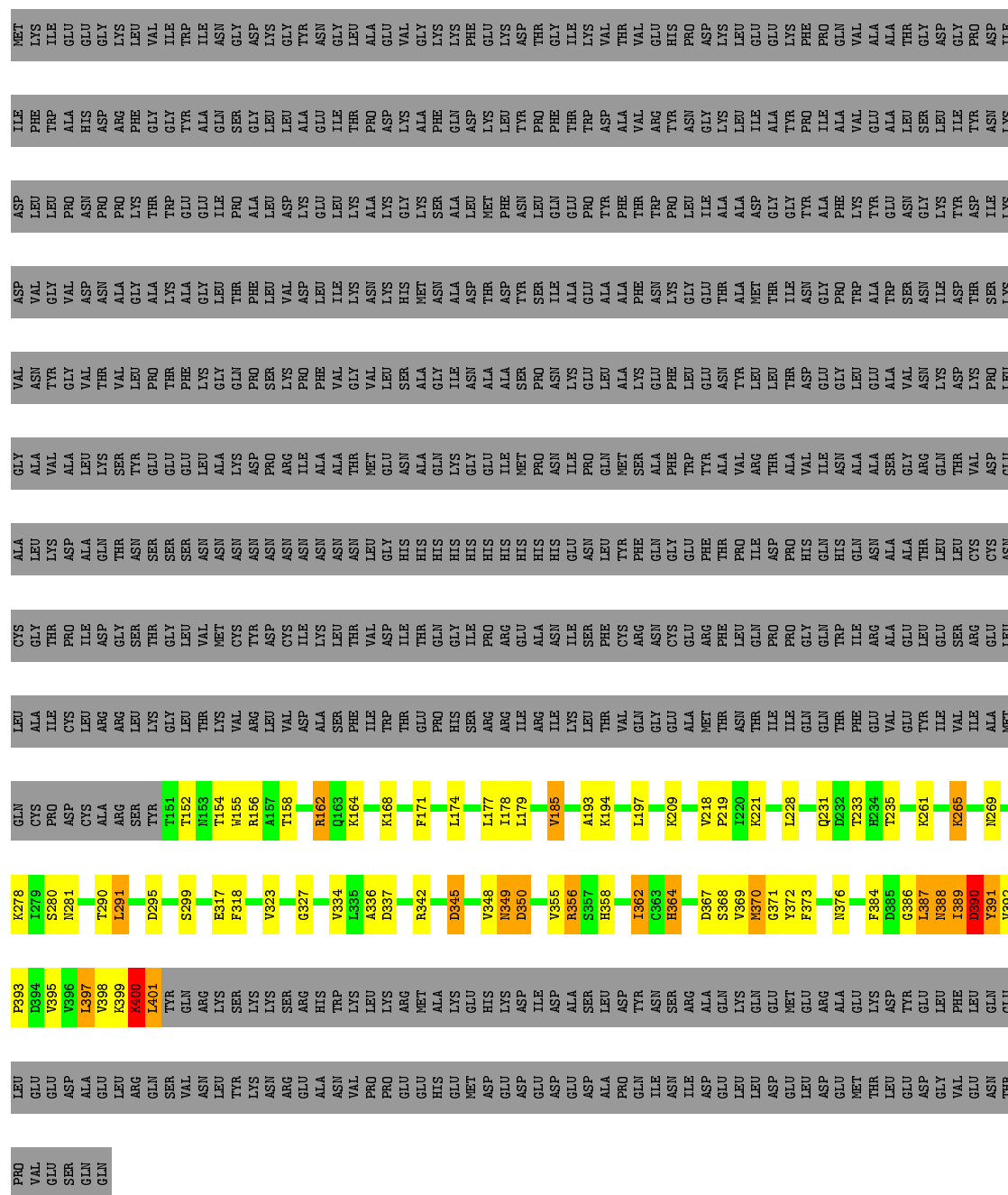
- Molecule 44: Ribosomal Protein uL1

Chain S:  99% .



- Molecule 45: Maltose binding protein, 60S ribosomal export protein Nmd3 fusion

Chain V:  19% 6% 73%



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	65650	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 2$	RMSZ	$\# Z  > 2$
1	A	0.24	1/76717 (0.0%)	0.69	8/119611 (0.0%)
10	J	0.37	0/1836	0.54	0/2481
11	K	0.36	0/1539	0.57	0/2073
12	L	0.38	0/1741	0.61	0/2335
13	M	0.38	0/1374	0.64	0/1842
14	N	0.39	0/1568	0.65	0/2106
15	O	0.36	0/1068	0.59	0/1438
16	a	0.38	0/1757	0.68	0/2354
17	b	0.37	0/1585	0.55	0/2128
18	c	0.36	0/1443	0.62	0/1944
19	d	0.37	0/1465	0.65	0/1965
2	B	0.24	0/2883	0.67	0/4491
20	e	0.36	0/1538	0.62	0/2050
21	f	0.36	0/1481	0.59	0/1990
22	g	0.36	0/1300	0.58	0/1743
23	h	0.39	0/812	0.51	0/1099
24	i	0.36	0/1018	0.59	0/1369
25	j	0.38	0/712	0.58	0/958
26	k	0.35	0/979	0.55	0/1321
27	l	0.36	0/1004	0.60	0/1341
28	m	0.37	0/1118	0.54	0/1497
29	n	0.35	0/1204	0.62	0/1612
3	C	0.23	0/3746	0.68	1/5832 (0.0%)
30	o	0.37	0/473	0.61	0/629
31	p	0.36	0/751	0.50	0/1008
32	q	0.35	0/890	0.60	0/1196
33	r	0.36	0/1041	0.60	0/1394
34	s	0.36	0/414	0.58	0/556
35	t	0.35	0/890	0.63	0/1189
36	u	0.37	0/978	0.60	0/1301
37	v	0.40	0/778	0.60	0/1034
38	w	0.39	0/696	0.66	0/923

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  > 2	RMSZ	# Z  > 2
39	x	0.35	0/618	0.56	0/826
4	D	0.35	0/1948	0.63	0/2617
40	y	0.39	0/443	0.64	0/588
41	z	0.38	0/423	0.61	0/562
42	Q	0.37	0/860	0.60	0/1136
43	R	0.37	0/701	0.65	0/934
45	V	0.39	0/2015	0.75	3/2738 (0.1%)
5	E	0.36	0/3146	0.62	0/4228
6	F	0.37	0/2800	0.58	0/3790
7	G	0.38	0/2425	0.60	1/3271 (0.0%)
8	H	0.37	0/1260	0.56	0/1694
9	I	0.38	0/1821	0.57	0/2451
All	All	0.30	1/135259 (0.0%)	0.66	13/199645 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
30	o	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2595	A	C5-C6	5.44	1.46	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	V	386	GLY	C-N-CA	14.40	157.70	121.70
45	V	386	GLY	O-C-N	-13.14	101.67	122.70
45	V	386	GLY	CA-C-N	9.55	138.20	117.20
1	A	2249	G	C2'-C3'-O3'	7.62	126.26	109.50
1	A	1307	G	C2'-C3'-O3'	7.11	125.14	109.50
1	A	1554	U	O4'-C1'-N1	5.87	112.89	108.20
1	A	3003	G	C2'-C3'-O3'	5.69	122.80	113.70
1	A	2434	U	N1-C1'-C2'	5.55	121.22	114.00
1	A	78	U	N3-C4-O4	-5.33	115.67	119.40
3	C	82	U	C2'-C3'-O3'	5.18	122.00	113.70
1	A	979	U	C2'-C3'-O3'	5.17	121.97	113.70
1	A	78	U	O4'-C1'-N1	5.08	112.26	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	131	LEU	CA-CB-CG	5.03	126.87	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
30	o	20	GLY	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	68535	0	34437	205	0
2	B	2579	0	1304	1	0
3	C	3353	0	1695	0	0
4	D	1914	0	1981	3	0
5	E	3075	0	3142	4	0
6	F	2748	0	2859	1	0
7	G	2375	0	2325	2	0
8	H	1239	0	1326	0	0
9	I	1784	0	1862	5	0
10	J	1804	0	1877	2	0
11	K	1518	0	1587	3	0
12	L	1705	0	1736	11	0
13	M	1353	0	1383	0	0
14	N	1543	0	1608	2	0
15	O	1053	0	1149	0	0
16	a	1720	0	1779	0	0
17	b	1555	0	1659	0	0
18	c	1420	0	1437	0	0
19	d	1441	0	1543	0	0
20	e	1521	0	1617	0	0
21	f	1445	0	1487	0	0
22	g	1276	0	1323	0	0
23	h	796	0	812	0	0
24	i	1003	0	1048	0	0
25	j	699	0	640	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	k	964	0	1025	0	0
27	l	993	0	1081	0	0
28	m	1092	0	1155	0	0
29	n	1173	0	1215	0	0
30	o	462	0	491	0	0
31	p	743	0	797	0	0
32	q	876	0	912	0	0
33	r	1020	0	1090	0	0
34	s	406	0	416	0	0
35	t	880	0	945	0	0
36	u	969	0	1078	0	0
37	v	771	0	849	0	0
38	w	681	0	687	0	0
39	x	612	0	682	0	0
40	y	436	0	475	0	0
41	z	417	0	459	0	0
42	Q	847	0	918	0	0
43	R	694	0	738	0	0
44	S	1050	0	247	2	0
45	V	1975	0	1984	70	0
46	A	84	0	0	0	0
46	C	1	0	0	0	0
46	i	1	0	0	0	0
47	A	3	0	0	0	0
48	A	10	0	0	2	0
48	c	1	0	0	0	0
48	e	1	0	0	0	0
All	All	126616	0	90860	286	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 1.

All (286) 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)
1:A:2434:U:O4	1:A:2595:A:N1	1.60	1.33
12:L:102:MET:CG	45:V:152:THR:HA	1.58	1.32
12:L:102:MET:HG3	45:V:152:THR:CA	1.63	1.28
45:V:388:ASN:O	45:V:390:ASP:N	1.73	1.21
1:A:2410:U:O4	1:A:2801:A:N1	1.87	1.06
1:A:2461:A:C4	1:A:2485:A:C2	2.45	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2490:C:C2	1:A:2491:A:N6	2.28	1.02
1:A:1453:A:H61	1:A:1840:U:H3	1.07	1.02
1:A:2469:G:C6	1:A:2470:C:N4	2.32	0.97
1:A:2449:A:N1	1:A:2498:U:O2	1.97	0.97
1:A:2482:U:O4	1:A:2486:A:N6	1.98	0.96
1:A:2434:U:O4	1:A:2595:A:C2	2.19	0.95
1:A:2440:G:N2	1:A:2508:U:O2	2.00	0.95
1:A:78:U:H3	1:A:325:A:H61	1.08	0.95
1:A:2463:G:N2	1:A:2493:U:N3	2.15	0.95
1:A:2448:G:O6	1:A:2498:U:C2	2.20	0.94
1:A:2490:C:O2	1:A:2491:A:N7	2.01	0.94
1:A:2922:G:O6	45:V:235:THR:OG1	1.85	0.94
1:A:2636:A:H61	1:A:2641:U:H3	1.05	0.94
1:A:2448:G:C2	1:A:2499:U:O2	2.21	0.93
1:A:1190:A:H61	1:A:1315:U:H3	1.15	0.93
45:V:389:ILE:HG22	45:V:389:ILE:O	1.67	0.92
1:A:2461:A:C5	1:A:2485:A:C2	2.58	0.92
1:A:2448:G:O6	1:A:2498:U:O2	1.91	0.89
45:V:337:ASP:OD2	45:V:356:ARG:HG3	1.70	0.89
1:A:3077:A:N6	48:A:3501:HOH:O	2.04	0.89
1:A:1554:U:H3	1:A:1559:A:H61	1.14	0.89
12:L:102:MET:HG3	45:V:152:THR:HA	0.87	0.87
1:A:2450:G:N1	1:A:2497:U:N3	2.21	0.87
1:A:2450:G:H1	1:A:2497:U:H3	1.23	0.85
1:A:2658:G:N2	1:A:2713:U:O2	2.08	0.85
1:A:2507:C:H6	1:A:2507:C:H5''	1.43	0.83
1:A:2463:G:N2	1:A:2493:U:C4	2.47	0.82
1:A:2636:A:N6	1:A:2641:U:H3	1.79	0.80
12:L:102:MET:CB	45:V:152:THR:HA	2.10	0.80
45:V:367:ASP:CG	45:V:400:LYS:NZ	2.35	0.79
1:A:2449:A:C2	1:A:2498:U:O2	2.36	0.79
1:A:2636:A:N1	1:A:2641:U:O4	2.16	0.79
45:V:367:ASP:CG	45:V:400:LYS:HZ2	1.85	0.78
45:V:372:TYR:CE1	45:V:398:VAL:HG21	2.20	0.77
1:A:78:U:O4	1:A:324:A:N1	2.18	0.77
45:V:372:TYR:CE1	45:V:398:VAL:CG2	2.68	0.77
1:A:2445:A:N3	1:A:2502:A:C2	2.53	0.77
1:A:2469:G:C5	1:A:2470:C:N4	2.52	0.77
1:A:1554:U:H3	1:A:1559:A:N6	1.82	0.76
1:A:2876:C:H4'	45:V:233:THR:HB	1.67	0.76
1:A:1190:A:N1	1:A:1315:U:O4	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1453:A:N6	1:A:1840:U:H3	1.84	0.75
1:A:2448:G:N1	1:A:2499:U:C2	2.54	0.75
1:A:2449:A:C6	1:A:2498:U:O2	2.39	0.75
1:A:2469:G:N1	1:A:2470:C:N4	2.33	0.75
1:A:2249:G:C8	1:A:2272:G:C8	2.74	0.75
1:A:2437:G:C6	1:A:2438:A:C6	2.73	0.75
1:A:1481:A:O2'	1:A:1858:A:H1'	1.87	0.75
45:V:367:ASP:OD2	45:V:400:LYS:NZ	2.19	0.75
1:A:2439:A:C2	1:A:2440:G:C5	2.75	0.74
1:A:2451:G:H21	1:A:2495:C:N4	1.85	0.74
1:A:2463:G:N2	1:A:2493:U:H3	1.83	0.74
1:A:2493:U:C4	1:A:2494:A:C4	2.75	0.74
1:A:1188:U:O4	1:A:1317:A:N1	2.21	0.74
1:A:2410:U:O4	1:A:2801:A:C2	2.40	0.74
1:A:2490:C:H1'	1:A:2491:A:N7	2.03	0.74
1:A:78:U:H3	1:A:325:A:N6	1.84	0.74
1:A:2488:A:OP2	1:A:2490:C:N4	2.21	0.73
1:A:2253:G:O6	1:A:2263:C:N4	2.22	0.73
1:A:3064:U:O4	48:A:3501:HOH:O	2.07	0.73
1:A:2463:G:C2	1:A:2493:U:O4	2.43	0.72
45:V:368:SER:O	45:V:401:LEU:C	2.28	0.71
45:V:372:TYR:HE1	45:V:398:VAL:CG2	2.03	0.71
1:A:1190:A:N6	1:A:1315:U:H3	1.86	0.71
1:A:1453:A:N1	1:A:1840:U:O4	2.25	0.70
1:A:2461:A:C5	1:A:2485:A:N1	2.60	0.69
1:A:2410:U:H3	1:A:2801:A:H61	1.39	0.69
1:A:2470:C:H1'	1:A:2489:C:O4'	1.92	0.68
1:A:2482:U:C4	1:A:2486:A:N6	2.59	0.68
45:V:323:VAL:HG13	45:V:336:ALA:HB1	1.76	0.68
1:A:2447:A:N1	1:A:2499:U:O4	2.27	0.68
1:A:2447:A:C2	1:A:2500:A:C2	2.82	0.68
1:A:2469:G:C2	1:A:2470:C:N4	2.62	0.67
1:A:2440:G:C2	1:A:2508:U:O2	2.47	0.66
1:A:78:U:O4	1:A:325:A:N1	2.28	0.66
1:A:2450:G:N2	1:A:2497:U:C2	2.62	0.66
45:V:261:LYS:O	45:V:265:LYS:HG3	1.96	0.66
45:V:401:LEU:HD13	45:V:401:LEU:O	1.96	0.66
1:A:2624:G:OP1	45:V:162:ARG:HD3	1.96	0.66
45:V:389:ILE:CG2	45:V:389:ILE:O	2.40	0.66
45:V:350:ASP:OD2	45:V:350:ASP:N	2.27	0.65
45:V:401:LEU:HD22	45:V:401:LEU:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2490:C:N3	1:A:2491:A:N6	2.42	0.65
45:V:231:GLN:O	45:V:231:GLN:HG3	1.97	0.64
12:L:102:MET:HG3	45:V:152:THR:N	2.12	0.64
1:A:2437:G:C6	1:A:2438:A:C5	2.86	0.64
1:A:2448:G:N1	1:A:2499:U:O2	2.30	0.63
1:A:2249:G:N7	1:A:2272:G:C4	2.67	0.63
1:A:2469:G:H2'	1:A:2470:C:C6	2.35	0.62
45:V:373:PHE:HD1	45:V:395:VAL:HG22	1.64	0.62
45:V:342:ARG:HB2	45:V:345:ASP:HB2	1.80	0.62
45:V:369:VAL:HG12	45:V:400:LYS:HA	1.81	0.62
5:E:67:PHE:CE1	9:I:88:ARG:HB2	111.24	0.62
1:A:2493:U:C5	1:A:2494:A:C8	2.89	0.61
45:V:362:ILE:HG13	45:V:362:ILE:O	2.00	0.61
45:V:392:VAL:HG13	45:V:393:PRO:HD2	1.82	0.61
1:A:2452:G:N2	1:A:2462:A:C8	2.68	0.60
45:V:348:VAL:O	45:V:349:ASN:CB	2.49	0.60
1:A:2469:G:H2'	1:A:2470:C:C5	2.36	0.60
1:A:2445:A:C2	1:A:2502:A:N1	2.69	0.60
1:A:2463:G:N2	1:A:2464:U:C2	2.70	0.60
1:A:2461:A:C4	1:A:2485:A:H2	2.17	0.59
1:A:640:U:OP1	14:N:21:ARG:NH2	43.38	0.59
1:A:2439:A:C2	1:A:2440:G:C4	2.91	0.59
1:A:2656:A:N1	1:A:2713:U:O4	2.36	0.59
1:A:2450:G:N1	1:A:2497:U:C4	2.70	0.59
1:A:78:U:H3	1:A:324:A:N6	2.01	0.59
1:A:2449:A:N1	1:A:2498:U:C2	2.71	0.59
45:V:387:LEU:HD13	45:V:392:VAL:HG22	1.85	0.59
1:A:167:U:O2	1:A:256:G:N2	2.36	0.58
45:V:291:LEU:HD11	45:V:358:HIS:CB	2.34	0.58
1:A:2492:C:H2'	1:A:2493:U:C5	2.38	0.58
1:A:324:A:C6	1:A:325:A:N6	2.72	0.58
1:A:2445:A:C4	1:A:2502:A:N1	2.72	0.58
1:A:2451:G:N2	1:A:2495:C:N4	2.50	0.58
45:V:392:VAL:CG1	45:V:393:PRO:HD2	2.34	0.57
1:A:1661:G:H2'	1:A:1662:G:C8	2.39	0.57
1:A:2507:C:H6	1:A:2507:C:C5'	2.13	0.57
1:A:2445:A:C2	1:A:2502:A:C2	2.92	0.57
1:A:2253:G:C2	1:A:2264:U:C2	2.93	0.56
1:A:2482:U:H3	1:A:2486:A:H61	1.52	0.56
1:A:2446:U:H2'	1:A:2447:A:C8	2.40	0.56
1:A:2448:G:C6	1:A:2499:U:C2	2.94	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2437:G:C5	1:A:2438:A:C5	2.94	0.56
1:A:2448:G:N2	1:A:2499:U:O2	2.39	0.56
1:A:103:G:OP1	14:N:70:ARG:NH2	2.39	0.56
45:V:162:ARG:NH2	45:V:193:ALA:HB3	2.21	0.55
1:A:2437:G:O6	1:A:2438:A:C6	2.59	0.55
1:A:2445:A:N3	1:A:2502:A:N1	2.55	0.55
1:A:2457:G:N2	1:A:2486:A:C2	2.74	0.55
45:V:318:PHE:CE2	45:V:342:ARG:HG2	2.41	0.55
45:V:388:ASN:HB3	45:V:391:TYR:HB2	1.88	0.55
1:A:2490:C:O2	1:A:2491:A:C5	2.59	0.54
1:A:324:A:N6	1:A:325:A:N6	2.55	0.54
45:V:372:TYR:HE1	45:V:398:VAL:HG21	1.62	0.54
1:A:1820:U:O2	1:A:1820:U:O4'	2.25	0.54
1:A:2469:G:C4	1:A:2470:C:N4	2.75	0.54
1:A:2499:U:C4	1:A:2500:A:C5	2.96	0.54
1:A:2469:G:C2	1:A:2470:C:C4	2.96	0.54
1:A:662:U:H2'	1:A:663:C:C6	2.43	0.54
1:A:2249:G:H2'	1:A:2250:G:H8	1.73	0.53
1:A:160:G:N2	1:A:262:U:O2	2.41	0.53
1:A:2271:A:N7	1:A:2272:G:C6	2.76	0.53
1:A:78:U:N3	1:A:324:A:N6	2.57	0.53
12:L:102:MET:CG	45:V:152:THR:CA	2.43	0.53
1:A:1556:C:O4'	1:A:1556:C:O2	2.25	0.53
1:A:2493:U:H3'	1:A:2494:A:O4'	2.09	0.53
45:V:261:LYS:NZ	45:V:265:LYS:HD3	2.23	0.53
45:V:401:LEU:HD22	45:V:401:LEU:C	2.29	0.53
1:A:2499:U:O4	1:A:2500:A:C6	2.62	0.53
1:A:2507:C:C6	1:A:2507:C:H5''	2.34	0.53
2:B:121:U:O4'	2:B:121:U:O2	2.27	0.53
45:V:348:VAL:O	45:V:349:ASN:HB3	2.09	0.53
1:A:2456:A:H2'	1:A:2457:G:O4'	2.09	0.53
1:A:2445:A:C2	1:A:2502:A:C6	2.97	0.53
1:A:3217:C:O2	1:A:3217:C:C2'	2.57	0.52
1:A:2449:A:C6	1:A:2498:U:C2	2.98	0.52
1:A:2490:C:C1'	1:A:2491:A:N7	2.72	0.52
1:A:2410:U:C4	1:A:2801:A:N1	2.72	0.52
1:A:2470:C:C4	1:A:2471:U:O4	2.62	0.52
1:A:3153:U:O2	1:A:3153:U:O4'	2.28	0.52
1:A:2438:A:H2'	1:A:2439:A:H8	1.76	0.51
12:L:102:MET:HB2	45:V:152:THR:HA	1.91	0.51
1:A:2624:G:OP1	45:V:162:ARG:CD	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2507:C:C6	1:A:2507:C:C5'	2.93	0.50
1:A:2438:A:H2'	1:A:2439:A:C8	2.47	0.50
1:A:2440:G:N2	1:A:2508:U:C2	2.78	0.50
1:A:1573:G:H2'	1:A:1573:G:N3	2.27	0.50
11:K:22:SER:OG	11:K:23:ARG:N	2.42	0.50
1:A:2463:G:C2	1:A:2493:U:C4	2.97	0.50
5:E:67:PHE:CE2	9:I:88:ARG:HD3	108.85	0.50
1:A:2470:C:O4'	1:A:2489:C:H1'	2.12	0.50
1:A:3354:U:O2	1:A:3354:U:O4'	2.29	0.50
5:E:67:PHE:CD2	9:I:88:ARG:HD3	108.41	0.50
1:A:2481:G:H2'	1:A:2482:U:C4	2.48	0.49
1:A:2270:A:N6	1:A:2271:A:C6	2.81	0.49
1:A:2481:G:H2'	1:A:2482:U:C5	2.48	0.49
7:G:148:ILE:HG13	7:G:159:VAL:HG11	1.95	0.49
1:A:2505:U:H1'	1:A:2506:U:N3	2.28	0.48
1:A:2463:G:N2	1:A:2493:U:O4	2.45	0.48
1:A:324:A:C6	1:A:325:A:C6	3.02	0.48
12:L:102:MET:O	45:V:154:THR:CG2	2.62	0.48
45:V:355:VAL:HG21	45:V:395:VAL:O	2.12	0.48
1:A:2448:G:C6	1:A:2499:U:N3	2.82	0.48
1:A:2461:A:N9	1:A:2485:A:H2	2.11	0.48
1:A:2469:G:C4	1:A:2470:C:C5	3.02	0.47
1:A:2267:C:H2'	1:A:2268:U:C6	2.49	0.47
1:A:2505:U:H1'	1:A:2506:U:H3	1.79	0.47
1:A:2506:U:C3'	1:A:2506:U:C6	2.97	0.47
1:A:2439:A:N1	1:A:2440:G:C6	2.82	0.47
7:G:30:TYR:HB3	7:G:38:THR:HG22	10.94	0.47
5:E:67:PHE:CZ	9:I:88:ARG:HB2	111.02	0.47
45:V:174:LEU:O	45:V:178:ILE:HG22	2.15	0.47
1:A:2249:G:C4	1:A:2250:G:C8	3.03	0.47
12:L:102:MET:C	45:V:154:THR:HG23	2.36	0.46
45:V:218:VAL:HG22	45:V:219:PRO:HD2	1.96	0.46
45:V:387:LEU:HD13	45:V:392:VAL:CG2	2.46	0.46
1:A:2493:U:C4	1:A:2494:A:C5	3.03	0.46
1:A:3018:C:H2'	1:A:3019:U:C6	2.50	0.46
45:V:399:LYS:O	45:V:400:LYS:O	2.33	0.46
44:S:187:UNK:O	44:S:188:UNK:CB	2.63	0.46
1:A:2476:C:H2'	1:A:2477:G:H4'	1.98	0.45
1:A:1103:A:N6	1:A:1363:A:O2'	2.49	0.45
1:A:2467:G:H8	1:A:2467:G:O5'	1.99	0.45
1:A:2253:G:N1	1:A:2264:U:C4	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:V:162:ARG:HH22	45:V:193:ALA:HB3	1.82	0.45
1:A:2506:U:H3'	1:A:2507:C:H5''	1.98	0.45
45:V:323:VAL:CG1	45:V:336:ALA:HB1	2.46	0.45
1:A:2236:G:O2'	45:V:269:ASN:HB2	2.17	0.45
1:A:2437:G:H2'	1:A:2438:A:C8	2.52	0.45
45:V:364:HIS:CB	45:V:367:ASP:OD2	2.64	0.45
1:A:2249:G:C5	1:A:2250:G:N7	2.85	0.44
1:A:2689:A:N3	1:A:2689:A:H2'	2.32	0.44
45:V:280:SER:OG	45:V:281:ASN:N	2.49	0.44
1:A:2253:G:C6	1:A:2264:U:C4	3.05	0.44
1:A:2493:U:O4	1:A:2494:A:C5	2.70	0.44
11:K:41:ILE:HD11	11:K:67:ALA:HB1	1.99	0.44
1:A:2270:A:C5	1:A:2271:A:C5	3.06	0.44
1:A:2270:A:C6	1:A:2271:A:C6	3.05	0.44
1:A:2452:G:O2'	1:A:2462:A:OP2	2.31	0.44
1:A:2180:G:H2'	1:A:2181:C:C6	2.52	0.44
1:A:2922:G:C6	45:V:235:THR:OG1	2.55	0.44
45:V:261:LYS:HZ1	45:V:265:LYS:HD3	1.81	0.44
1:A:2439:A:C8	1:A:2439:A:O5'	2.71	0.44
4:D:112:ILE:HG23	4:D:133:TYR:HB2	1.99	0.44
1:A:2461:A:N9	1:A:2485:A:C2	2.81	0.43
1:A:3214:U:O4'	1:A:3214:U:O2	2.33	0.43
1:A:2838:A:N6	1:A:2850:G:O2'	2.50	0.43
6:F:181:VAL:HG11	6:F:224:GLY:HA3	2.00	0.43
1:A:1913:A:N3	1:A:2120:A:H2'	2.32	0.43
9:I:98:LYS:HB3	9:I:99:PRO:HD3	2.01	0.43
1:A:2506:U:H6	1:A:2506:U:H3'	1.84	0.43
1:A:3277:U:O2	1:A:3277:U:O4'	2.34	0.43
1:A:706:A:H2'	1:A:707:U:O4'	2.17	0.43
45:V:291:LEU:HD23	45:V:334:VAL:HG11	1.51	0.43
1:A:2439:A:N1	1:A:2440:G:C5	2.87	0.43
1:A:2606:G:N3	1:A:2606:G:H2'	2.34	0.43
1:A:2469:G:O6	1:A:2474:G:N1	2.51	0.42
1:A:2459:A:N1	1:A:2487:U:C2	2.87	0.42
12:L:36:LEU:HD11	12:L:69:ARG:HD3	2.00	0.42
45:V:371:GLY:HA3	45:V:397:LEU:HA	2.01	0.42
45:V:155:TRP:CZ3	45:V:158:THR:OG1	2.72	0.42
1:A:2270:A:N6	1:A:2271:A:N1	2.68	0.42
1:A:2470:C:N4	1:A:2474:G:H22	2.18	0.42
45:V:290:THR:O	45:V:291:LEU:C	2.57	0.42
1:A:2439:A:H8	1:A:2439:A:O5'	2.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2446:U:H2'	1:A:2447:A:H8	1.84	0.42
1:A:2493:U:H2'	1:A:2494:A:O4'	2.19	0.42
1:A:1554:U:O4	1:A:1559:A:N1	2.52	0.42
1:A:2499:U:C5	1:A:2500:A:N7	2.88	0.42
10:J:140:VAL:HG22	10:J:166:LEU:HD21	2.01	0.42
1:A:2213:A:H2'	1:A:2214:A:C8	2.55	0.42
1:A:2437:G:C5	1:A:2438:A:N7	2.89	0.41
1:A:2461:A:N7	1:A:2485:A:N1	2.67	0.41
10:J:75:ILE:O	10:J:76:ALA:HB3	2.20	0.41
1:A:78:U:C4	1:A:325:A:N1	2.88	0.41
1:A:436:A:H2'	1:A:437:G:O4'	2.20	0.41
45:V:384:PHE:O	45:V:387:LEU:HB2	2.20	0.41
1:A:1188:U:C4	1:A:1317:A:N1	2.89	0.41
1:A:3017:A:C6	1:A:3018:C:C4	3.08	0.41
1:A:2424:A:N1	4:D:230:VAL:HG11	2.36	0.41
12:L:102:MET:C	45:V:154:THR:CG2	2.89	0.41
45:V:355:VAL:HG22	45:V:356:ARG:O	2.20	0.41
1:A:2410:U:H3	1:A:2801:A:N6	2.11	0.41
1:A:2456:A:O2'	1:A:2457:G:C4'	2.69	0.41
1:A:1793:C:C4	4:D:179:LEU:HD11	2.55	0.41
11:K:112:ILE:HD13	11:K:161:LEU:HD12	2.03	0.41
45:V:265:LYS:HE3	45:V:265:LYS:HB3	1.72	0.41
45:V:291:LEU:HD11	45:V:358:HIS:HB2	2.01	0.41
1:A:2493:U:C3'	1:A:2494:A:O4'	2.69	0.41
45:V:367:ASP:CB	45:V:400:LYS:NZ	2.84	0.41
1:A:2249:G:C8	1:A:2272:G:N7	2.90	0.40
1:A:2191:U:H2'	1:A:2192:C:O4'	2.21	0.40
1:A:2490:C:OP1	44:S:204:UNK:O	2.38	0.40
1:A:2469:G:C4	1:A:2470:C:C4	3.10	0.40
1:A:2485:A:O5'	1:A:2485:A:H8	2.05	0.40
1:A:2594:C:C5	1:A:2595:A:C2	3.09	0.40
1:A:527:A:N6	1:A:566:G:C6	2.90	0.40
45:V:218:VAL:HG22	45:V:219:PRO:CD	2.52	0.40
45:V:317:GLU:HA	45:V:370:MET:HE3	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	
4	D	250/254 (98%)	228 (91%)	20 (8%)	2 (1%)	22	66
5	E	384/387 (99%)	343 (89%)	34 (9%)	7 (2%)	10	50
6	F	359/362 (99%)	311 (87%)	32 (9%)	16 (4%)	3	30
7	G	294/297 (99%)	267 (91%)	19 (6%)	8 (3%)	6	42
8	H	152/176 (86%)	137 (90%)	12 (8%)	3 (2%)	9	48
9	I	220/244 (90%)	203 (92%)	14 (6%)	3 (1%)	13	54
10	J	231/256 (90%)	202 (87%)	24 (10%)	5 (2%)	8	46
11	K	189/191 (99%)	173 (92%)	16 (8%)	0	100	100
12	L	207/221 (94%)	187 (90%)	17 (8%)	3 (1%)	13	54
13	M	167/174 (96%)	145 (87%)	15 (9%)	7 (4%)	3	32
14	N	191/199 (96%)	170 (89%)	19 (10%)	2 (1%)	18	61
15	O	134/138 (97%)	125 (93%)	5 (4%)	4 (3%)	5	39
16	a	201/204 (98%)	189 (94%)	9 (4%)	3 (2%)	12	54
17	b	195/199 (98%)	187 (96%)	7 (4%)	1 (0%)	32	74
18	c	181/184 (98%)	161 (89%)	20 (11%)	0	100	100
19	d	183/186 (98%)	169 (92%)	11 (6%)	3 (2%)	11	53
20	e	186/189 (98%)	175 (94%)	7 (4%)	4 (2%)	8	46
21	f	170/172 (99%)	158 (93%)	10 (6%)	2 (1%)	15	58
22	g	157/160 (98%)	142 (90%)	12 (8%)	3 (2%)	9	49
23	h	98/121 (81%)	84 (86%)	13 (13%)	1 (1%)	18	61
24	i	134/137 (98%)	126 (94%)	7 (5%)	1 (1%)	25	68
25	j	96/155 (62%)	83 (86%)	10 (10%)	3 (3%)	5	39
26	k	119/142 (84%)	111 (93%)	7 (6%)	1 (1%)	22	66
27	l	124/127 (98%)	115 (93%)	7 (6%)	2 (2%)	11	53
28	m	133/136 (98%)	113 (85%)	18 (14%)	2 (2%)	12	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	n	146/149 (98%)	125 (86%)	16 (11%)	5 (3%)	4	37
30	o	56/59 (95%)	48 (86%)	5 (9%)	3 (5%)	2	27
31	p	95/105 (90%)	89 (94%)	6 (6%)	0	100	100
32	q	107/113 (95%)	98 (92%)	7 (6%)	2 (2%)	9	49
33	r	125/130 (96%)	115 (92%)	8 (6%)	2 (2%)	11	53
34	s	48/107 (45%)	46 (96%)	2 (4%)	0	100	100
35	t	110/121 (91%)	105 (96%)	3 (3%)	2 (2%)	10	50
36	u	117/120 (98%)	108 (92%)	6 (5%)	3 (3%)	6	42
37	v	97/100 (97%)	88 (91%)	7 (7%)	2 (2%)	8	47
38	w	85/88 (97%)	76 (89%)	9 (11%)	0	100	100
39	x	75/78 (96%)	68 (91%)	4 (5%)	3 (4%)	3	33
40	y	48/51 (94%)	44 (92%)	4 (8%)	0	100	100
41	z	50/128 (39%)	48 (96%)	1 (2%)	1 (2%)	9	48
42	Q	103/106 (97%)	88 (85%)	11 (11%)	4 (4%)	3	33
43	R	89/92 (97%)	84 (94%)	5 (6%)	0	100	100
45	V	249/917 (27%)	222 (89%)	20 (8%)	7 (3%)	6	41
All	All	6355/7475 (85%)	5756 (91%)	479 (8%)	120 (2%)	14	49

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	F	292	SER
9	I	178	ILE
10	J	31	PRO
10	J	157	VAL
14	N	47	ALA
16	a	94	TYR
20	e	131	ALA
22	g	124	VAL
25	j	81	PRO
42	Q	30	ALA
45	V	185	VAL
45	V	389	ILE
45	V	400	LYS
4	D	144	ASN
5	E	347	SER

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Mol	Chain	Res	Type
5	E	348	ARG
5	E	351	LEU
6	F	130	ALA
6	F	131	VAL
6	F	182	LEU
6	F	293	SER
7	G	87	GLY
8	H	98	VAL
9	I	159	GLN
10	J	36	ILE
10	J	79	GLN
13	M	10	ARG
13	M	95	ASN
15	O	8	LYS
19	d	41	ASP
25	j	97	LYS
27	l	84	LYS
29	n	77	LYS
45	V	390	ASP
5	E	187	SER
6	F	140	HIS
6	F	173	GLY
6	F	233	LEU
6	F	268	ALA
6	F	269	SER
7	G	258	LYS
7	G	259	LYS
7	G	260	PHE
8	H	5	LYS
10	J	25	PRO
12	L	24	ARG
13	M	114	ILE
15	O	9	ALA
15	O	29	ALA
17	b	187	GLU
19	d	98	LYS
21	f	24	LEU
22	g	159	PHE
26	k	50	ALA
28	m	17	ARG
29	n	66	ALA
30	o	25	LYS

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Mol	Chain	Res	Type
33	r	40	SER
35	t	46	ASP
36	u	84	LYS
39	x	18	ALA
39	x	33	LYS
42	Q	34	SER
45	V	194	LYS
6	F	338	LYS
7	G	21	ARG
12	L	218	ALA
13	M	8	PRO
13	M	9	MET
13	M	117	ASP
14	N	166	ALA
19	d	162	ALA
20	e	53	LYS
20	e	178	ALA
21	f	167	ARG
28	m	59	ALA
32	q	82	GLU
33	r	12	LYS
37	v	3	VAL
39	x	34	ALA
41	z	79	GLU
42	Q	17	CYS
42	Q	60	LYS
45	V	349	ASN
5	E	155	ALA
6	F	82	THR
6	F	232	SER
6	F	311	HIS
7	G	251	PRO
7	G	253	PHE
12	L	220	GLN
13	M	108	GLU
23	h	11	ILE
27	l	126	LEU
30	o	29	TYR
36	u	39	PRO
36	u	75	TYR
4	D	125	ALA
6	F	189	ALA

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Mol	Chain	Res	Type
7	G	125	VAL
16	a	81	TYR
16	a	184	LYS
20	e	129	GLY
22	g	125	ALA
29	n	15	VAL
29	n	47	LYS
32	q	7	VAL
24	i	3	GLY
29	n	56	VAL
45	V	327	GLY
5	E	317	ILE
35	t	77	GLY
37	v	21	THR
6	F	317	PRO
15	O	6	ILE
25	j	80	ARG
30	o	21	ILE
9	I	191	VAL
5	E	90	VAL
8	H	6	ALA

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	193/196 (98%)	187 (97%)	6 (3%)	45	72
5	E	318/323 (98%)	304 (96%)	14 (4%)	33	65
6	F	288/289 (100%)	275 (96%)	13 (4%)	32	64
7	G	244/245 (100%)	224 (92%)	20 (8%)	13	46
8	H	134/153 (88%)	128 (96%)	6 (4%)	32	64
9	I	186/205 (91%)	176 (95%)	10 (5%)	26	60
10	J	187/208 (90%)	173 (92%)	14 (8%)	16	49
11	K	171/171 (100%)	158 (92%)	13 (8%)	15	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	L	177/187 (95%)	164 (93%)	13 (7%)	16	50
13	M	147/150 (98%)	136 (92%)	11 (8%)	16	49
14	N	154/159 (97%)	141 (92%)	13 (8%)	13	45
15	O	107/109 (98%)	102 (95%)	5 (5%)	30	63
16	a	175/176 (99%)	166 (95%)	9 (5%)	28	61
17	b	160/162 (99%)	155 (97%)	5 (3%)	45	72
18	c	140/146 (96%)	129 (92%)	11 (8%)	14	48
19	d	150/151 (99%)	146 (97%)	4 (3%)	50	75
20	e	153/154 (99%)	148 (97%)	5 (3%)	43	71
21	f	156/156 (100%)	149 (96%)	7 (4%)	32	64
22	g	136/137 (99%)	125 (92%)	11 (8%)	14	47
23	h	87/107 (81%)	85 (98%)	2 (2%)	56	79
24	i	104/105 (99%)	98 (94%)	6 (6%)	23	57
25	j	57/129 (44%)	57 (100%)	0	100	100
26	k	104/118 (88%)	96 (92%)	8 (8%)	15	49
27	l	109/110 (99%)	103 (94%)	6 (6%)	25	59
28	m	115/116 (99%)	108 (94%)	7 (6%)	22	56
29	n	118/119 (99%)	111 (94%)	7 (6%)	23	57
30	o	46/47 (98%)	43 (94%)	3 (6%)	20	54
31	p	81/88 (92%)	79 (98%)	2 (2%)	53	77
32	q	92/97 (95%)	87 (95%)	5 (5%)	26	60
33	r	109/111 (98%)	101 (93%)	8 (7%)	16	50
34	s	43/91 (47%)	42 (98%)	1 (2%)	56	79
35	t	95/103 (92%)	93 (98%)	2 (2%)	59	80
36	u	104/105 (99%)	97 (93%)	7 (7%)	19	53
37	v	81/82 (99%)	75 (93%)	6 (7%)	16	50
38	w	70/71 (99%)	67 (96%)	3 (4%)	33	65
39	x	68/69 (99%)	66 (97%)	2 (3%)	48	73
40	y	45/46 (98%)	44 (98%)	1 (2%)	57	79
41	z	47/116 (40%)	43 (92%)	4 (8%)	12	45
42	Q	90/91 (99%)	82 (91%)	8 (9%)	11	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
43	R	71/72 (99%)	68 (96%)	3 (4%)	34 66
45	V	224/791 (28%)	193 (86%)	31 (14%)	4 25
All	All	5336/6261 (85%)	5024 (94%)	312 (6%)	28 57

All (312) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	17	THR
4	D	116	VAL
4	D	122	ASP
4	D	207	VAL
4	D	227	ARG
4	D	230	VAL
5	E	10	ARG
5	E	19	ARG
5	E	25	ILE
5	E	85	VAL
5	E	159	ARG
5	E	169	THR
5	E	188	ILE
5	E	232	ARG
5	E	246	LEU
5	E	252	ILE
5	E	296	THR
5	E	332	ARG
5	E	339	ARG
5	E	364	LYS
6	F	52	VAL
6	F	67	THR
6	F	73	ARG
6	F	74	ILE
6	F	99	MET
6	F	112	LYS
6	F	114	ASN
6	F	150	LEU
6	F	154	THR
6	F	179	LEU
6	F	246	ARG
6	F	307	GLN
6	F	361	HIS
7	G	13	SER

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Mol	Chain	Res	Type
7	G	15	ARG
7	G	18	THR
7	G	22	ARG
7	G	23	ARG
7	G	24	ARG
7	G	41	LYS
7	G	75	LEU
7	G	92	LEU
7	G	95	TRP
7	G	105	ILE
7	G	115	LEU
7	G	131	LEU
7	G	151	GLN
7	G	193	GLU
7	G	211	LEU
7	G	259	LYS
7	G	264	GLN
7	G	273	ARG
7	G	279	LYS
8	H	34	LEU
8	H	46	ARG
8	H	64	LEU
8	H	65	ILE
8	H	134	ARG
8	H	137	ASP
9	I	24	GLU
9	I	82	LYS
9	I	88	ARG
9	I	92	ILE
9	I	124	LEU
9	I	125	GLU
9	I	145	ARG
9	I	179	LEU
9	I	218	ARG
9	I	239	LEU
10	J	41	GLN
10	J	57	ARG
10	J	63	LYS
10	J	65	LEU
10	J	92	LYS
10	J	136	LEU
10	J	150	LEU

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Mol	Chain	Res	Type
10	J	163	VAL
10	J	169	LEU
10	J	201	THR
10	J	204	ARG
10	J	232	HIS
10	J	240	ASN
10	J	248	LYS
11	K	5	GLN
11	K	23	ARG
11	K	41	ILE
11	K	49	ASN
11	K	52	LEU
11	K	69	ARG
11	K	118	LEU
11	K	120	ASP
11	K	135	GLU
11	K	139	ASN
11	K	164	ILE
11	K	166	ARG
11	K	177	ASP
12	L	7	ARG
12	L	30	LYS
12	L	33	ILE
12	L	40	LYS
12	L	52	LEU
12	L	90	ARG
12	L	115	MET
12	L	154	ARG
12	L	163	GLN
12	L	165	ILE
12	L	169	LYS
12	L	203	LYS
12	L	208	ASN
13	M	10	ARG
13	M	11	ASP
13	M	12	LEU
13	M	13	LYS
13	M	40	LEU
13	M	80	LEU
13	M	81	GLU
13	M	94	ARG
13	M	107	ASP

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Mol	Chain	Res	Type
13	M	130	VAL
13	M	140	ARG
14	N	24	VAL
14	N	36	ARG
14	N	49	ARG
14	N	67	ARG
14	N	85	LEU
14	N	101	ARG
14	N	104	ARG
14	N	124	ILE
14	N	131	LYS
14	N	136	GLU
14	N	168	ARG
14	N	176	GLU
14	N	190	LYS
15	O	12	TRP
15	O	20	VAL
15	O	28	SER
15	O	72	LEU
15	O	108	ARG
16	a	22	LEU
16	a	27	VAL
16	a	50	ARG
16	a	133	ILE
16	a	138	GLN
16	a	174	ILE
16	a	180	PHE
16	a	183	THR
16	a	201	ARG
17	b	34	VAL
17	b	78	ARG
17	b	124	LEU
17	b	125	ARG
17	b	155	LYS
18	c	24	VAL
18	c	49	GLU
18	c	52	LEU
18	c	53	ASP
18	c	96	GLN
18	c	120	ASN
18	c	125	GLN
18	c	126	ARG

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Mol	Chain	Res	Type
18	c	127	ARG
18	c	168	LEU
18	c	180	LYS
19	d	26	LEU
19	d	49	LEU
19	d	135	GLN
19	d	138	LEU
20	e	17	VAL
20	e	25	ASP
20	e	74	ARG
20	e	103	ARG
20	e	138	LEU
21	f	12	ARG
21	f	45	LEU
21	f	61	ILE
21	f	71	LYS
21	f	115	ARG
21	f	137	ARG
21	f	172	TYR
22	g	12	ARG
22	g	32	LYS
22	g	75	ILE
22	g	79	MET
22	g	83	ARG
22	g	88	ARG
22	g	102	ARG
22	g	126	VAL
22	g	127	GLN
22	g	128	LEU
22	g	139	ARG
23	h	10	LYS
23	h	70	LYS
24	i	32	ARG
24	i	33	ASN
24	i	34	LEU
24	i	40	LYS
24	i	83	LYS
24	i	132	ASN
26	k	34	LEU
26	k	63	ILE
26	k	70	GLU
26	k	125	ARG

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Mol	Chain	Res	Type
26	k	129	ASP
26	k	133	LEU
26	k	135	ILE
26	k	142	ILE
27	l	13	ARG
27	l	37	LYS
27	l	50	ILE
27	l	56	VAL
27	l	74	TYR
27	l	126	LEU
28	m	3	LYS
28	m	14	VAL
28	m	24	VAL
28	m	34	LYS
28	m	120	GLU
28	m	121	ARG
28	m	126	LYS
29	n	34	MET
29	n	42	ARG
29	n	56	VAL
29	n	60	TYR
29	n	120	ASN
29	n	130	VAL
29	n	133	LEU
30	o	22	LYS
30	o	25	LYS
30	o	59	LYS
31	p	40	LYS
31	p	61	MET
32	q	16	LEU
32	q	50	ARG
32	q	55	LEU
32	q	79	ARG
32	q	86	LYS
33	r	19	ARG
33	r	27	ARG
33	r	33	ARG
33	r	44	ARG
33	r	47	ARG
33	r	87	MET
33	r	125	ARG
33	r	128	LEU

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Mol	Chain	Res	Type
34	s	37	THR
35	t	29	ILE
35	t	58	ARG
36	u	20	GLN
36	u	21	LEU
36	u	49	LYS
36	u	71	LYS
36	u	107	LYS
36	u	115	LYS
36	u	119	LYS
37	v	26	ILE
37	v	45	ARG
37	v	57	LEU
37	v	58	ILE
37	v	75	LYS
37	v	76	ARG
38	w	17	THR
38	w	24	ARG
38	w	25	ARG
39	x	67	GLN
39	x	77	ARG
40	y	21	ARG
41	z	85	LEU
41	z	106	ARG
41	z	113	ARG
41	z	127	LEU
42	Q	35	LEU
42	Q	38	GLN
42	Q	45	ARG
42	Q	71	ARG
42	Q	78	LYS
42	Q	83	LEU
42	Q	99	GLN
42	Q	100	LYS
43	R	45	LYS
43	R	49	ARG
43	R	60	CYS
45	V	156	ARG
45	V	162	ARG
45	V	164	LYS
45	V	168	LYS
45	V	171	PHE

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Mol	Chain	Res	Type
45	V	177	LEU
45	V	179	LEU
45	V	185	VAL
45	V	197	LEU
45	V	209	LYS
45	V	221	LYS
45	V	228	LEU
45	V	265	LYS
45	V	278	LYS
45	V	291	LEU
45	V	295	ASP
45	V	299	SER
45	V	345	ASP
45	V	350	ASP
45	V	356	ARG
45	V	362	ILE
45	V	364	HIS
45	V	370	MET
45	V	376	ASN
45	V	387	LEU
45	V	388	ASN
45	V	390	ASP
45	V	391	TYR
45	V	397	LEU
45	V	400	LYS
45	V	401	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	48	GLN
6	F	114	ASN
6	F	221	ASN
8	H	167	ASN
9	I	225	GLN
11	K	8	GLN
12	L	12	GLN
12	L	14	ASN
16	a	87	GLN
16	a	182	ASN
19	d	73	GLN
29	n	74	ASN

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Mol	Chain	Res	Type
32	q	87	ASN
33	r	104	ASN
42	Q	82	GLN
45	V	160	GLN
45	V	163	GLN
45	V	231	GLN
45	V	388	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	3201/3396 (94%)	770 (24%)	77 (2%)
2	B	120/121 (99%)	22 (18%)	2 (1%)
3	C	157/158 (99%)	38 (24%)	3 (1%)
All	All	3478/3675 (94%)	830 (23%)	82 (2%)

All (830) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	16	A
1	A	22	G
1	A	40	A
1	A	43	A
1	A	45	A
1	A	49	A
1	A	59	G
1	A	60	A
1	A	65	A
1	A	66	A
1	A	72	C
1	A	75	G
1	A	89	A
1	A	92	G
1	A	105	C
1	A	109	A
1	A	110	G
1	A	111	C
1	A	116	A
1	A	118	U
1	A	122	A
1	A	123	A

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Mol	Chain	Res	Type
1	A	136	G
1	A	137	G
1	A	143	G
1	A	150	A
1	A	156	G
1	A	157	A
1	A	161	G
1	A	166	C
1	A	167	U
1	A	168	U
1	A	170	G
1	A	173	G
1	A	177	U
1	A	182	U
1	A	184	U
1	A	187	A
1	A	190	U
1	A	191	U
1	A	192	C
1	A	198	A
1	A	200	C
1	A	210	U
1	A	211	A
1	A	218	G
1	A	219	A
1	A	240	U
1	A	241	G
1	A	243	G
1	A	245	U
1	A	246	U
1	A	247	C
1	A	249	U
1	A	250	U
1	A	252	U
1	A	266	A
1	A	269	G
1	A	286	U
1	A	295	A
1	A	305	U
1	A	315	C
1	A	317	A
1	A	323	A

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Mol	Chain	Res	Type
1	A	329	U
1	A	338	A
1	A	339	C
1	A	376	G
1	A	381	U
1	A	395	A
1	A	398	A
1	A	399	A
1	A	401	U
1	A	402	A
1	A	403	C
1	A	404	G
1	A	417	A
1	A	420	G
1	A	421	G
1	A	422	A
1	A	429	U
1	A	436	A
1	A	439	C
1	A	440	A
1	A	495	G
1	A	507	U
1	A	510	G
1	A	518	G
1	A	519	A
1	A	520	U
1	A	521	A
1	A	523	A
1	A	526	C
1	A	531	G
1	A	536	U
1	A	539	C
1	A	541	U
1	A	543	C
1	A	546	C
1	A	547	G
1	A	548	G
1	A	549	U
1	A	551	A
1	A	553	U
1	A	555	U
1	A	556	U

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Mol	Chain	Res	Type
1	A	557	A
1	A	559	A
1	A	560	G
1	A	569	A
1	A	570	A
1	A	579	G
1	A	592	A
1	A	598	A
1	A	600	G
1	A	604	G
1	A	611	A
1	A	619	A
1	A	620	U
1	A	621	A
1	A	622	A
1	A	634	C
1	A	636	C
1	A	649	A
1	A	660	A
1	A	662	U
1	A	676	G
1	A	677	A
1	A	681	U
1	A	683	U
1	A	684	G
1	A	687	U
1	A	689	U
1	A	690	A
1	A	691	A
1	A	696	C
1	A	705	A
1	A	710	A
1	A	712	G
1	A	715	A
1	A	716	A
1	A	720	A
1	A	725	G
1	A	735	A
1	A	739	G
1	A	748	U
1	A	764	U
1	A	766	U

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Mol	Chain	Res	Type
1	A	767	U
1	A	774	G
1	A	776	U
1	A	777	U
1	A	780	A
1	A	781	G
1	A	785	G
1	A	786	A
1	A	792	G
1	A	799	G
1	A	801	A
1	A	806	A
1	A	808	A
1	A	814	U
1	A	817	A
1	A	830	A
1	A	849	C
1	A	857	G
1	A	861	C
1	A	868	C
1	A	874	U
1	A	879	U
1	A	890	C
1	A	894	G
1	A	895	A
1	A	896	A
1	A	897	U
1	A	907	G
1	A	908	G
1	A	911	C
1	A	914	A
1	A	916	G
1	A	917	A
1	A	921	A
1	A	923	C
1	A	925	A
1	A	937	G
1	A	941	G
1	A	944	C
1	A	958	C
1	A	959	C
1	A	960	U

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Mol	Chain	Res	Type
1	A	979	U
1	A	980	A
1	A	981	U
1	A	982	C
1	A	991	G
1	A	994	G
1	A	1001	G
1	A	1002	A
1	A	1009	A
1	A	1010	G
1	A	1013	G
1	A	1015	U
1	A	1017	C
1	A	1018	G
1	A	1019	G
1	A	1021	G
1	A	1024	G
1	A	1025	A
1	A	1026	A
1	A	1029	G
1	A	1030	A
1	A	1031	C
1	A	1034	U
1	A	1036	A
1	A	1037	C
1	A	1040	A
1	A	1041	U
1	A	1047	A
1	A	1049	C
1	A	1057	A
1	A	1064	A
1	A	1065	A
1	A	1072	G
1	A	1073	U
1	A	1081	U
1	A	1093	A
1	A	1094	U
1	A	1095	U
1	A	1098	A
1	A	1103	A
1	A	1104	G
1	A	1117	G

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Mol	Chain	Res	Type
1	A	1124	U
1	A	1129	A
1	A	1131	G
1	A	1140	G
1	A	1153	A
1	A	1159	A
1	A	1180	A
1	A	1181	U
1	A	1188	U
1	A	1191	U
1	A	1192	C
1	A	1200	A
1	A	1201	C
1	A	1208	U
1	A	1212	A
1	A	1213	G
1	A	1217	A
1	A	1219	C
1	A	1222	G
1	A	1223	A
1	A	1230	G
1	A	1232	C
1	A	1236	G
1	A	1237	G
1	A	1240	A
1	A	1241	U
1	A	1242	G
1	A	1243	G
1	A	1244	A
1	A	1245	A
1	A	1246	G
1	A	1247	U
1	A	1248	C
1	A	1249	G
1	A	1253	U
1	A	1257	C
1	A	1258	U
1	A	1260	A
1	A	1262	G
1	A	1263	A
1	A	1264	G
1	A	1266	G

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Mol	Chain	Res	Type
1	A	1267	U
1	A	1270	A
1	A	1271	A
1	A	1272	C
1	A	1274	A
1	A	1276	U
1	A	1278	A
1	A	1279	C
1	A	1285	G
1	A	1287	A
1	A	1289	G
1	A	1305	U
1	A	1307	G
1	A	1308	A
1	A	1309	U
1	A	1313	G
1	A	1316	C
1	A	1325	U
1	A	1329	U
1	A	1330	A
1	A	1331	U
1	A	1340	G
1	A	1348	U
1	A	1349	G
1	A	1351	U
1	A	1352	A
1	A	1353	U
1	A	1356	U
1	A	1357	G
1	A	1364	C
1	A	1383	G
1	A	1385	C
1	A	1386	A
1	A	1392	G
1	A	1393	A
1	A	1399	A
1	A	1400	G
1	A	1414	G
1	A	1416	C
1	A	1419	A
1	A	1434	G
1	A	1437	C

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Mol	Chain	Res	Type
1	A	1446	A
1	A	1450	G
1	A	1455	U
1	A	1460	A
1	A	1481	A
1	A	1482	A
1	A	1498	A
1	A	1500	G
1	A	1508	C
1	A	1512	U
1	A	1527	C
1	A	1531	C
1	A	1533	U
1	A	1536	G
1	A	1555	U
1	A	1556	C
1	A	1557	A
1	A	1560	G
1	A	1561	G
1	A	1562	C
1	A	1563	C
1	A	1565	G
1	A	1566	A
1	A	1567	U
1	A	1568	U
1	A	1569	U
1	A	1570	U
1	A	1572	U
1	A	1574	C
1	A	1576	G
1	A	1577	G
1	A	1578	C
1	A	1579	C
1	A	1582	C
1	A	1583	A
1	A	1587	A
1	A	1589	A
1	A	1593	A
1	A	1611	G
1	A	1618	G
1	A	1620	U
1	A	1622	U

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Mol	Chain	Res	Type
1	A	1628	C
1	A	1629	U
1	A	1630	U
1	A	1642	A
1	A	1643	A
1	A	1645	U
1	A	1657	C
1	A	1664	G
1	A	1666	G
1	A	1678	G
1	A	1683	A
1	A	1703	U
1	A	1716	U
1	A	1717	U
1	A	1724	U
1	A	1725	C
1	A	1741	A
1	A	1742	U
1	A	1749	A
1	A	1750	A
1	A	1751	G
1	A	1760	A
1	A	1761	C
1	A	1762	C
1	A	1765	U
1	A	1766	G
1	A	1770	G
1	A	1775	G
1	A	1779	C
1	A	1780	G
1	A	1797	A
1	A	1798	A
1	A	1808	G
1	A	1812	G
1	A	1813	A
1	A	1814	A
1	A	1815	U
1	A	1816	A
1	A	1817	G
1	A	1820	U
1	A	1821	U
1	A	1839	A

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Mol	Chain	Res	Type
1	A	1840	U
1	A	1841	A
1	A	1842	A
1	A	1847	A
1	A	1849	C
1	A	1850	A
1	A	1855	U
1	A	1866	C
1	A	1880	U
1	A	1886	A
1	A	1893	A
1	A	1906	G
1	A	1908	A
1	A	1910	A
1	A	1936	A
1	A	1951	C
1	A	1952	G
1	A	1953	G
1	A	1954	G
1	A	2095	G
1	A	2099	A
1	A	2101	C
1	A	2102	U
1	A	2111	G
1	A	2112	U
1	A	2113	A
1	A	2114	C
1	A	2115	G
1	A	2120	A
1	A	2121	G
1	A	2122	G
1	A	2131	A
1	A	2134	G
1	A	2140	U
1	A	2158	A
1	A	2169	G
1	A	2180	G
1	A	2185	G
1	A	2192	C
1	A	2193	U
1	A	2198	A
1	A	2204	C

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Mol	Chain	Res	Type
1	A	2205	U
1	A	2210	G
1	A	2211	U
1	A	2228	A
1	A	2239	G
1	A	2244	A
1	A	2245	C
1	A	2246	G
1	A	2250	G
1	A	2252	A
1	A	2253	G
1	A	2255	A
1	A	2256	A
1	A	2257	C
1	A	2258	U
1	A	2270	A
1	A	2273	G
1	A	2274	U
1	A	2276	G
1	A	2279	A
1	A	2281	A
1	A	2282	U
1	A	2285	C
1	A	2288	G
1	A	2298	U
1	A	2307	G
1	A	2308	C
1	A	2310	U
1	A	2313	A
1	A	2314	U
1	A	2315	G
1	A	2327	U
1	A	2334	U
1	A	2335	G
1	A	2336	U
1	A	2337	C
1	A	2357	A
1	A	2372	A
1	A	2373	A
1	A	2374	C
1	A	2375	G
1	A	2385	G

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Mol	Chain	Res	Type
1	A	2388	U
1	A	2393	G
1	A	2397	A
1	A	2402	A
1	A	2403	G
1	A	2404	A
1	A	2411	U
1	A	2418	G
1	A	2419	A
1	A	2421	U
1	A	2422	C
1	A	2425	G
1	A	2437	G
1	A	2438	A
1	A	2440	G
1	A	2442	G
1	A	2443	A
1	A	2444	C
1	A	2445	A
1	A	2446	U
1	A	2448	G
1	A	2449	A
1	A	2450	G
1	A	2451	G
1	A	2452	G
1	A	2453	U
1	A	2454	G
1	A	2455	U
1	A	2456	A
1	A	2457	G
1	A	2458	A
1	A	2459	A
1	A	2461	A
1	A	2462	A
1	A	2463	G
1	A	2465	G
1	A	2472	U
1	A	2473	C
1	A	2474	G
1	A	2475	G
1	A	2477	G
1	A	2481	G

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Mol	Chain	Res	Type
1	A	2484	A
1	A	2487	U
1	A	2488	A
1	A	2491	A
1	A	2492	C
1	A	2494	A
1	A	2495	C
1	A	2496	C
1	A	2497	U
1	A	2498	U
1	A	2499	U
1	A	2501	U
1	A	2502	A
1	A	2503	G
1	A	2505	U
1	A	2506	U
1	A	2507	C
1	A	2508	U
1	A	2513	U
1	A	2514	U
1	A	2515	A
1	A	2522	G
1	A	2530	G
1	A	2531	C
1	A	2532	U
1	A	2533	G
1	A	2537	U
1	A	2538	U
1	A	2539	C
1	A	2540	A
1	A	2541	U
1	A	2542	U
1	A	2543	U
1	A	2544	U
1	A	2547	A
1	A	2548	C
1	A	2549	G
1	A	2550	U
1	A	2552	C
1	A	2554	A
1	A	2555	G
1	A	2558	U

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Mol	Chain	Res	Type
1	A	2561	A
1	A	2562	A
1	A	2565	U
1	A	2566	C
1	A	2568	C
1	A	2569	A
1	A	2570	U
1	A	2571	U
1	A	2572	C
1	A	2573	G
1	A	2575	G
1	A	2576	G
1	A	2582	C
1	A	2585	G
1	A	2586	G
1	A	2593	A
1	A	2594	C
1	A	2602	G
1	A	2606	G
1	A	2607	G
1	A	2614	G
1	A	2621	G
1	A	2626	A
1	A	2652	U
1	A	2655	U
1	A	2656	A
1	A	2657	A
1	A	2665	U
1	A	2674	A
1	A	2677	G
1	A	2681	U
1	A	2689	A
1	A	2691	A
1	A	2692	A
1	A	2694	A
1	A	2696	A
1	A	2703	A
1	A	2704	A
1	A	2713	U
1	A	2719	U
1	A	2726	C
1	A	2728	G

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Mol	Chain	Res	Type
1	A	2729	U
1	A	2737	C
1	A	2752	U
1	A	2753	G
1	A	2754	G
1	A	2762	A
1	A	2772	C
1	A	2777	G
1	A	2778	G
1	A	2800	G
1	A	2801	A
1	A	2803	A
1	A	2810	C
1	A	2814	G
1	A	2816	G
1	A	2817	A
1	A	2821	C
1	A	2841	G
1	A	2842	U
1	A	2843	U
1	A	2844	C
1	A	2845	A
1	A	2847	A
1	A	2849	C
1	A	2850	G
1	A	2861	U
1	A	2867	C
1	A	2871	G
1	A	2872	A
1	A	2887	A
1	A	2898	G
1	A	2899	C
1	A	2904	U
1	A	2907	G
1	A	2914	G
1	A	2921	U
1	A	2923	U
1	A	2935	U
1	A	2936	A
1	A	2938	G
1	A	2941	A
1	A	2942	C

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Mol	Chain	Res	Type
1	A	2947	G
1	A	2971	A
1	A	2975	U
1	A	2983	C
1	A	2996	U
1	A	2997	G
1	A	3004	C
1	A	3011	A
1	A	3012	A
1	A	3014	U
1	A	3028	G
1	A	3049	A
1	A	3056	U
1	A	3057	U
1	A	3058	U
1	A	3059	G
1	A	3078	U
1	A	3079	U
1	A	3086	A
1	A	3092	C
1	A	3102	G
1	A	3109	G
1	A	3110	C
1	A	3114	A
1	A	3115	C
1	A	3117	C
1	A	3122	A
1	A	3124	G
1	A	3128	G
1	A	3129	A
1	A	3130	A
1	A	3131	U
1	A	3142	A
1	A	3143	C
1	A	3153	U
1	A	3154	C
1	A	3155	U
1	A	3156	U
1	A	3157	U
1	A	3163	A
1	A	3164	C
1	A	3165	A

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Mol	Chain	Res	Type
1	A	3170	A
1	A	3173	G
1	A	3174	A
1	A	3176	G
1	A	3179	U
1	A	3181	C
1	A	3187	A
1	A	3196	U
1	A	3197	G
1	A	3200	G
1	A	3202	G
1	A	3207	U
1	A	3208	G
1	A	3212	C
1	A	3213	A
1	A	3217	C
1	A	3218	A
1	A	3219	G
1	A	3228	C
1	A	3229	G
1	A	3232	G
1	A	3234	A
1	A	3243	A
1	A	3244	A
1	A	3245	A
1	A	3246	G
1	A	3247	G
1	A	3249	C
1	A	3259	U
1	A	3260	G
1	A	3261	C
1	A	3263	G
1	A	3270	U
1	A	3271	G
1	A	3275	U
1	A	3276	G
1	A	3279	A
1	A	3280	U
1	A	3283	U
1	A	3284	G
1	A	3286	G
1	A	3289	G

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Mol	Chain	Res	Type
1	A	3294	A
1	A	3295	A
1	A	3304	U
1	A	3308	C
1	A	3313	U
1	A	3316	A
1	A	3317	U
1	A	3318	G
1	A	3319	U
1	A	3320	A
1	A	3324	C
1	A	3325	G
1	A	3342	A
1	A	3345	G
1	A	3349	C
1	A	3350	C
1	A	3351	U
1	A	3352	U
1	A	3353	G
1	A	3354	U
1	A	3355	U
1	A	3356	G
1	A	3357	U
1	A	3363	U
1	A	3366	G
1	A	3368	U
1	A	3369	G
1	A	3375	A
1	A	3378	C
1	A	3382	U
1	A	3383	G
1	A	3386	G
1	A	3390	G
1	A	3396	U
2	B	10	C
2	B	19	C
2	B	22	A
2	B	42	A
2	B	49	G
2	B	52	G
2	B	53	U
2	B	54	U

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Mol	Chain	Res	Type
2	B	55	A
2	B	56	A
2	B	60	G
2	B	65	G
2	B	71	G
2	B	73	C
2	B	91	G
2	B	99	G
2	B	101	G
2	B	102	A
2	B	112	G
2	B	114	U
2	B	120	C
2	B	121	U
3	C	2	A
3	C	23	U
3	C	24	G
3	C	34	U
3	C	35	C
3	C	50	C
3	C	52	A
3	C	53	A
3	C	57	C
3	C	59	A
3	C	62	C
3	C	63	G
3	C	80	A
3	C	81	U
3	C	82	U
3	C	83	C
3	C	84	C
3	C	86	U
3	C	87	G
3	C	90	U
3	C	91	C
3	C	95	G
3	C	104	A
3	C	106	C
3	C	108	C
3	C	111	A
3	C	113	U
3	C	125	U

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Mol	Chain	Res	Type
3	C	126	A
3	C	129	C
3	C	136	G
3	C	138	A
3	C	146	U
3	C	148	G
3	C	151	C
3	C	152	G
3	C	155	A
3	C	158	U

All (82) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	65	A
1	A	169	U
1	A	239	G
1	A	518	G
1	A	547	G
1	A	558	U
1	A	588	G
1	A	594	U
1	A	599	C
1	A	619	A
1	A	770	G
1	A	873	C
1	A	896	A
1	A	916	G
1	A	959	C
1	A	960	U
1	A	979	U
1	A	993	G
1	A	1064	A
1	A	1097	G
1	A	1103	A
1	A	1263	A
1	A	1307	G
1	A	1329	U
1	A	1352	A
1	A	1355	A
1	A	1482	A
1	A	1554	U

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Mol	Chain	Res	Type
1	A	1556	C
1	A	1562	C
1	A	1576	G
1	A	1716	U
1	A	1778	G
1	A	1814	A
1	A	1815	U
1	A	1816	A
1	A	1820	U
1	A	1841	A
1	A	1846	C
1	A	1858	A
1	A	2101	C
1	A	2112	U
1	A	2144	A
1	A	2209	U
1	A	2249	G
1	A	2269	U
1	A	2281	A
1	A	2418	G
1	A	2434	U
1	A	2453	U
1	A	2495	C
1	A	2496	C
1	A	2501	U
1	A	2506	U
1	A	2513	U
1	A	2537	U
1	A	2541	U
1	A	2585	G
1	A	2593	A
1	A	2754	G
1	A	2801	A
1	A	2983	C
1	A	3003	G
1	A	3048	A
1	A	3055	U
1	A	3056	U
1	A	3057	U
1	A	3078	U
1	A	3195	U
1	A	3218	A

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Mol	Chain	Res	Type
1	A	3228	C
1	A	3242	G
1	A	3269	U
1	A	3317	U
1	A	3350	C
1	A	3351	U
1	A	3353	G
2	B	52	G
2	B	111	U
3	C	80	A
3	C	82	U
3	C	85	G

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 89 ligands modelled in this entry, 89 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.