



Full wwPDB EM Validation Report ⓘ

Mar 19, 2025 – 01:05 pm GMT

PDB ID : 9F58
EMDB ID : EMD-50188
Title : Gen2 dimer bound to the 60S ribosomal subunit
Authors : Paternoga, H.; Dimitrova-Paternoga, L.; Wilson, D.N.
Deposited on : 2024-04-28
Resolution : 3.10 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

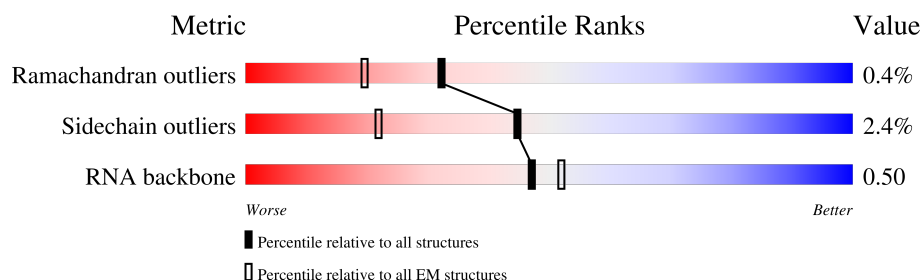
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



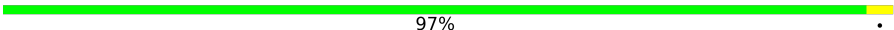









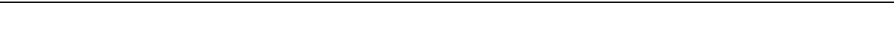

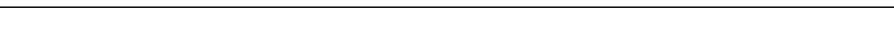
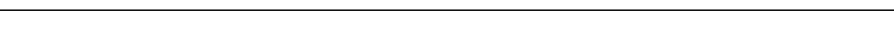
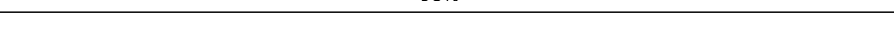


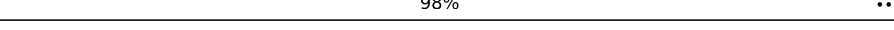

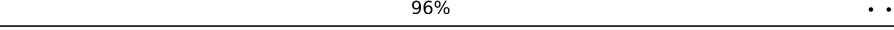


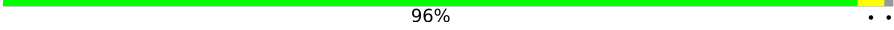

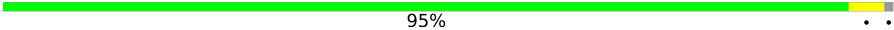
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	1659	
1	C	1659	
1	D	1659	
1	E	1659	
1	H	1659	
1	I	1659	
2	P	25	
3	4	158	
4	b	121	



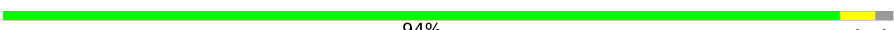
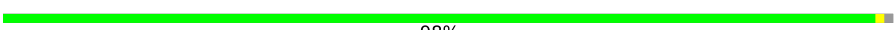








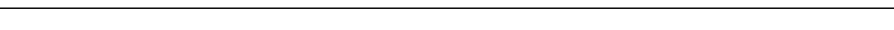
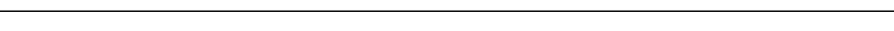
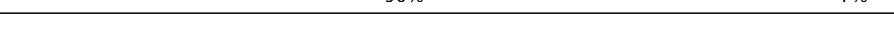
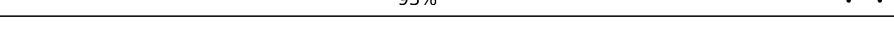
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Mol	Chain	Length	Quality of chain
5	d	387	 97%
6	e	297	 94%
7	f	176	 88% 11%
8	g	244	 88% 11%
9	h	256	 89% 9%
10	i	191	 96%
11	j	221	 93% 5%
12	k	174	 93% 5%
13	m	199	 93%
14	n	138	 98%
15	o	204	 99%
16	p	199	 97%
17	q	184	 95%
18	r	186	 98%
19	s	189	 81% 18%
20	t	172	 92% 7%
21	u	160	 98%
22	v	121	 80% 17%
23	w	137	 96%
24	y	155	 39% 59%
25	z	142	 83% 15%
26	J	127	 96%
27	K	136	 93% 5%
28	L	149	 95%
29	M	59	 95%

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Mol	Chain	Length	Quality of chain
30	N	105	 92% 8%
31	O	113	 94% . .
32	Q	130	 94% . .
33	R	107	 98% ..
34	T	120	 97% ..
35	U	100	 95% . .
36	V	88	 92% 6% ..
37	W	78	 95% . .
38	X	51	 94% . .
39	Y	128	 39% . 59%
40	Z	106	 95% . .
41	0	92	 93% 5% .
42	3	362	 94% . .
43	S	121	 90% . 7%
44	c	254	 93% . .
45	a	3396	 74% 17% . 8%

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 135896 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 eIF-2-alpha kinase GCN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	322	Total	C	N	O	S	0	0
			2590	1683	417	477	13		
1	H	104	Total	C	N	O	S	2	0
			845	531	150	160	4		
1	I	108	Total	C	N	O	S	0	0
			864	543	155	164	2		
1	C	259	Total	C	N	O	S	0	0
			2125	1358	366	392	9		
1	D	474	Total	C	N	O	S	0	0
			3796	2430	637	720	9		
1	E	473	Total	C	N	O	S	0	0
			3790	2429	634	718	9		

- Molecule 2 is a protein called Large ribosomal subunit protein eL41B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	P	15	Total	C	N	O	S	0	0
			144	89	38	16	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	158	Total	C	N	O	P	0	0
			3354	1500	586	1110	158		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	121	Total	C	N	O	P	0	0
			2580	1152	461	846	121		

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

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

- Molecule 6 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	e	291	Total	C	N	O	S	0	0
			2333	1474	407	450	2		

- Molecule 7 is a protein called 60S ribosomal protein L6-A.

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

- Molecule 8 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	g	218	Total	C	N	O	S	0	0
			1754	1133	319	301	1		

- Molecule 9 is a protein called 60S ribosomal protein L8-A.

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

- Molecule 10 is a protein called 60S ribosomal protein L9-A.

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

- Molecule 11 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	j	210	Total	C	N	O	S	0	0
			1700	1080	321	293	6		

- Molecule 12 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	k	166	Total	C	N	O	S	0	0
			1327	832	247	244	4		

- Molecule 13 is a protein called 60S ribosomal protein L13-A.

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

- Molecule 14 is a protein called 60S ribosomal protein L14-A.

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

- Molecule 15 is a protein called 60S ribosomal protein L15-A.

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

- Molecule 16 is a protein called 60S ribosomal protein L16-A.

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

- Molecule 17 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	183	Total	C	N	O	S	0	0
			1420	882	281	257			

- Molecule 18 is a protein called 60S ribosomal protein L18-A.

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

- Molecule 19 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	s	155	Total	C	N	O	0	0
			1249	776	264	209		

- Molecule 20 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	170	Total	C	N	O	S	0	0
			1432	922	265	242	3		

- Molecule 21 is a protein called 60S ribosomal protein L21-A.

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

- Molecule 22 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	v	100	Total	C	N	O	0	0
			796	516	131	149		

- Molecule 23 is a protein called 60S ribosomal protein L23-A.

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

- Molecule 24 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	63	Total	C	N	O	S	0	0
			521	336	102	82	1		

- Molecule 25 is a protein called 60S ribosomal protein L25.

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

- Molecule 26 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	J	126	Total	C	N	O	0	0
			993	625	192	176		

- Molecule 27 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	K	129	Total	C	N	O	0	0
			1046	684	193	169		

- Molecule 28 is a protein called 60S ribosomal protein L28.

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

- Molecule 29 is a protein called 60S ribosomal protein L29.

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

- Molecule 30 is a protein called 60S ribosomal protein L30.

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

- Molecule 31 is a protein called 60S ribosomal protein L31-A.

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

- Molecule 32 is a protein called 60S ribosomal protein L32.

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

- Molecule 33 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	R	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 34 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	T	117	Total	C	N	O	S	0	0
			960	610	184	165	1		

- Molecule 35 is a protein called 60S ribosomal protein L36-A.

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

- Molecule 36 is a protein called 60S ribosomal protein L37-A.

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

- Molecule 37 is a protein called 60S ribosomal protein L38.

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

- Molecule 38 is a protein called 60S ribosomal protein L39.

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

- Molecule 39 is a protein called Ubiquitin-60S ribosomal protein L40.

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

- Molecule 40 is a protein called 60S ribosomal protein L42-A.

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

- Molecule 41 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	0	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 42 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	3	356	Total	C	N	O	S	0	0
			2714	1710	516	485	3		

- Molecule 43 is a protein called 60S ribosomal protein L34-A.

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

- Molecule 44 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	c	246	Total	C	N	O	S	0	0
			1874	1168	380	325	1		

- Molecule 45 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	a	3134	Total	C	N	O	P	0	0
			67031	29941	12080	21876	3134		

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
46	V	1	Total	Zn	0
			1	1	
46	Y	1	Total	Zn	0
			1	1	
46	Z	1	Total	Zn	0
			1	1	

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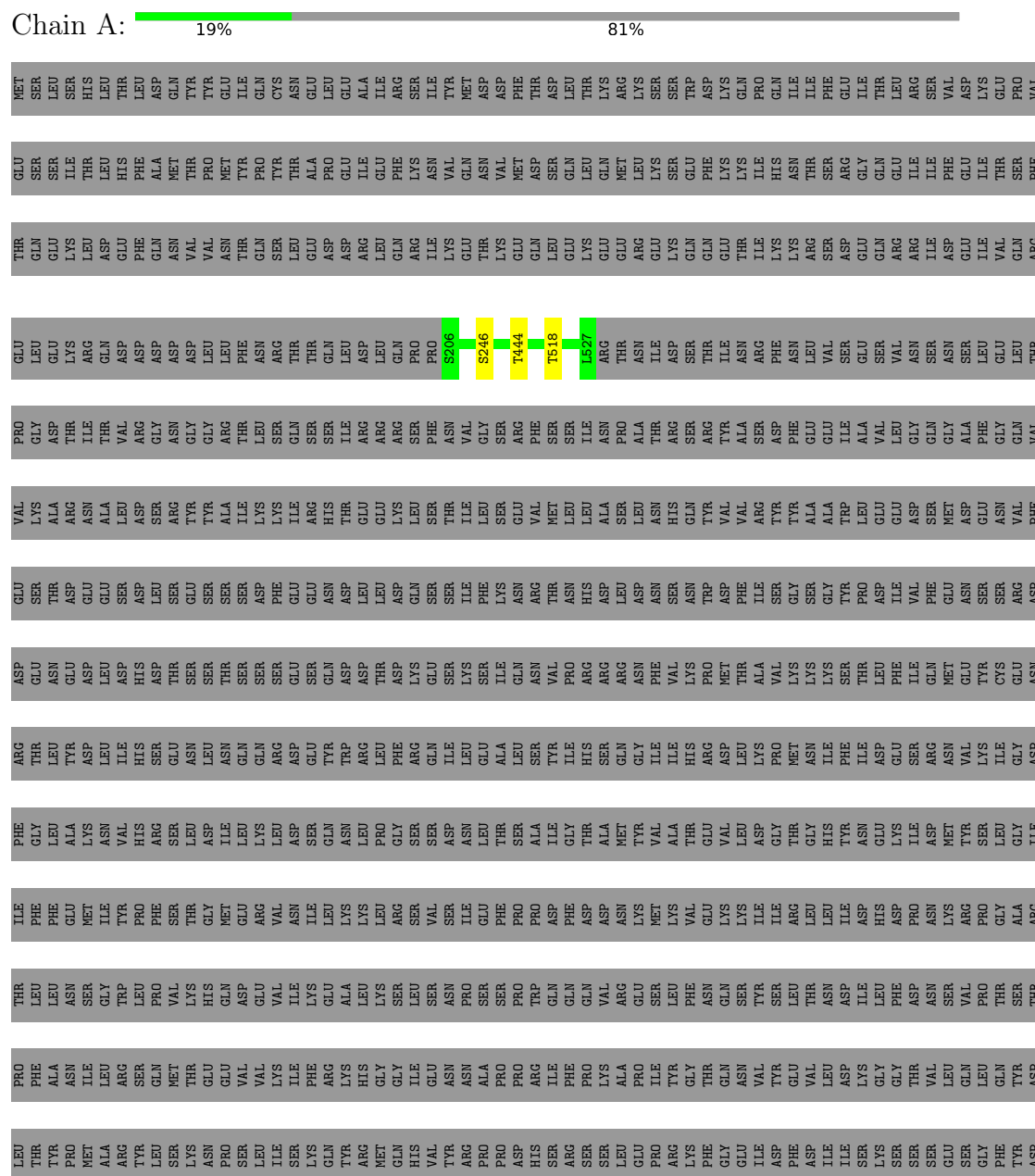
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Mol	Chain	Residues	Atoms		AltConf
46	0	1	Total 1	Zn 1	0
46	S	1	Total 1	Zn 1	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: eIF-2-alpha kinase GCN2



[illegible]

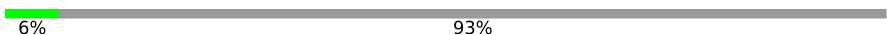
- Molecule 1: eIF-2-alpha kinase GCN2

Chain H: 6% 94%

[illegible]

- Molecule 1: eIF-2-alpha kinase GCN2

Chain I:



NET	SER	SER	LEU	SER	HIS	LEU	THR	LEU	LEU	ASP	GLN	TYR	TYR	GLU	GLN	CYS	ASN	LEU	GLU	GLU	ALA	ILE	ASP	ASP	PHE	THR	ASP	LEU	LYS	ARG	LYS	SER	SER	TRP	GLN	PRO	GLN	ILE	ILE	PHE	GLU	ILE	THR	LEU	ARG	SER	VAL	ASP	LYS	GLU	PRO	VAL
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----






- Molecule 2: Large ribosomal subunit protein eL41B

Chain P:  60% 40%


M1	R15	LYS
		ARG
		ARG
		LYS
		VAL
		ARG
		ALA
		ARG
		SER
		LYS

- Molecule 3: 5.8S rRNA

Chain 4:  78% 22%



- Molecule 4: 5S rRNA

Chain b:  87% 13%



- Molecule 5: 60S ribosomal protein L3

Chain d:  97%




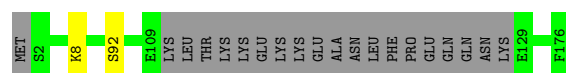
- Molecule 6: 60S ribosomal protein L5

Chain e:  94%




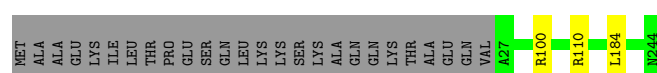
- Molecule 7: 60S ribosomal protein L6-A

Chain f:  88% 11%




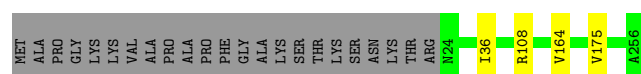
- Molecule 8: 60S ribosomal protein L7-A

Chain g:  88% 11%



- Molecule 9: 60S ribosomal protein L8-A

Chain h:  89% 9%



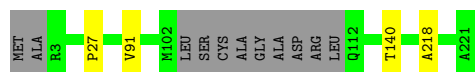
- Molecule 10: 60S ribosomal protein L9-A

Chain i:  96% .



- Molecule 11: 60S ribosomal protein L10

Chain j:  93% . 5%



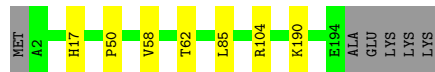
- Molecule 12: 60S ribosomal protein L11-A

Chain k:  93% . 5%



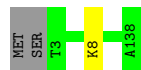
- Molecule 13: 60S ribosomal protein L13-A

Chain m:  93% . .



- Molecule 14: 60S ribosomal protein L14-A

Chain n:  98% ..



- Molecule 15: 60S ribosomal protein L15-A

Chain o:  99% .



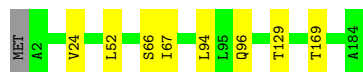
- Molecule 16: 60S ribosomal protein L16-A

Chain p:  97% ..



- Molecule 17: 60S ribosomal protein L17-A

Chain q:  95% ..




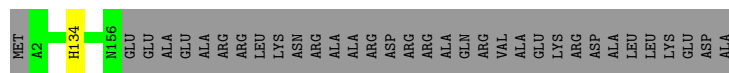
- Molecule 18: 60S ribosomal protein L18-A

Chain r:  98% ..



- Molecule 19: 60S ribosomal protein L19-A

Chain s:  81% 18% ..



- Molecule 20: 60S ribosomal protein L20-A

Chain t:  92% 7% ..




- Molecule 21: 60S ribosomal protein L21-A

Chain u:  98% ..



- Molecule 22: 60S ribosomal protein L22-A

Chain v:  80% 17% ..



- Molecule 23: 60S ribosomal protein L23-A

Chain w:  96% ..



- Molecule 24: 60S ribosomal protein L24-A

- Molecule 31: 60S ribosomal protein L31-A

Chain O:  94% ..



- Molecule 32: 60S ribosomal protein L32

Chain Q:  94% ..



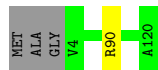
- Molecule 33: 60S ribosomal protein L33-A

Chain R:  98% ..



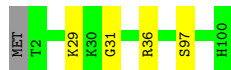
- Molecule 34: 60S ribosomal protein L35-A

Chain T:  97% ..



- Molecule 35: 60S ribosomal protein L36-A

Chain U:  95% ..



- Molecule 36: 60S ribosomal protein L37-A

Chain V:  92% 6% ..



- Molecule 37: 60S ribosomal protein L38

Chain W:  95% ..



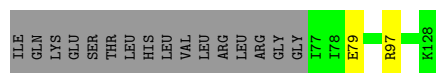
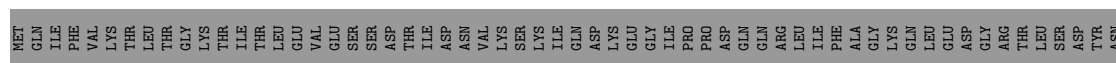
- Molecule 38: 60S ribosomal protein L39

Chain X:  94%



- Molecule 39: Ubiquitin-60S ribosomal protein L40

Chain Y:  39%



- Molecule 40: 60S ribosomal protein L42-A

Chain Z:  95%



- Molecule 41: 60S ribosomal protein L43-A

Chain 0:  93%




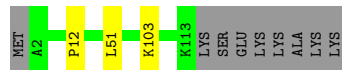
- Molecule 42: 60S ribosomal protein L4-A

Chain 3:  94%



- Molecule 43: 60S ribosomal protein L34-A

Chain S:  90%



- Molecule 44: 60S ribosomal protein L2-A

Chain c:  93%



Chain a: 74% 17% 8%



G3208	A3209	A3012	A2802	G2614	C	U2411
A3209	A3213	A3048	A2803	G2618	U	U2418
A3213	A3217	A3049	C2810	G2619	A	A2419
C3217	A3218	U3056	G2816	G2620	C	G2435
A3218	G3219	U3057	A2817	G2621	U	G2440
G3219	A3227	U3058	C2821	A2626	U	A2441
A3227	C3228	G3059	U2842	U2629	A	G2442
C3228	G3229	A3073	U2843	U2652	U	A2443
G3229	C3235	G3074	C2844	U2656	G	C2444
C3235	G3239	U3078	A2845	A2656	U	A
A3243	A3244	U3079	A2846	G2661	U2505	U
A3244	A3245	G3080	A2847	A2674	U2506	A
G3245	G3246	C3082	C2867	G2677	U2513	G
U3259	G3260	U3104	A2871	U2681	U2514	A
G3260	G3263	U3107	A2872	G2677	A2515	G
G3263	G3264	U3119	U2875	A2689	G2522	G
G3264	G3265	A3122	C2876	G2690	A2523	U
G3265	A3268	G3128	A2887	A2691	U2531	U
A3268	U3269	A3129	G2898	A2694	U2532	A
U3269	C3272	A3130	C2899	A2696	G2533	G
C3272	A3273	U3131	U2918	A2704	U2538	A
A3273	A3274	G3142	U2923	C2726	A2539	A
U3275	G3276	C3143	C2928	A2727	U2540	U
G3276	U3277	G3154	U2935	G2728	U2541	A
U3277	C3278	U3155	A2936	U2729	U2542	G
C3278	A3279	U3156	G2939	U2735	U2549	U
A3279	U3281	G3164	A2940	A2740	G2552	G
U3281	U3287	A3165	A2941	A2748	U2553	A
U3287	G3288	G3173	C2942	U2752	A2554	G
G3288	G3289	A3174	G2947	G2753	U2561	U
G3289	A3294	G3176	G2950	G2761	A2569	C
A3294	U3304	U3179	G2977	A2762	U2570	U
U3304	U3313	A3180	U2978	C2772	U2571	C
U3313	A3316	C3181	U2979	G2777	C2572	G
A3316	U3317	A3187	C2983	G2778	G2573	C
U3317	G3318	U3196	G2990	G2796	G2576	C
G3318	U3319	G3197	U2996	A2800	G2585	A
U3319	U3341	U3198	G2997	A2801	U2589	U
U3341	A3342	U3207			A2593	A
A3342					C2594	A
					U2600	U
					G2606	A
					G2607	C
						A

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14552	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (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:
ZN

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	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	0/2649	0.56	0/3588
1	C	0.42	0/2165	0.64	0/2916
1	D	0.41	0/3873	0.62	0/5234
1	E	0.42	0/3868	0.60	0/5228
1	H	0.38	0/858	0.62	0/1157
1	I	0.37	0/880	0.60	0/1190
2	P	0.39	0/145	0.77	0/186
3	4	0.62	1/3747 (0.0%)	0.99	3/5832 (0.1%)
4	b	0.62	1/2884 (0.0%)	1.01	3/4491 (0.1%)
5	d	0.45	0/3146	0.71	1/4228 (0.0%)
6	e	0.39	0/2382	0.67	0/3214
7	f	0.40	0/1260	0.68	0/1694
8	g	0.43	0/1791	0.67	0/2410
9	h	0.37	0/1836	0.66	0/2481
10	i	0.39	0/1539	0.69	0/2073
11	j	0.40	0/1736	0.69	0/2328
12	k	0.37	0/1348	0.69	0/1807
13	m	0.40	0/1568	0.71	0/2106
14	n	0.37	0/1068	0.64	0/1438
15	o	0.43	0/1757	0.76	0/2354
16	p	0.43	0/1585	0.72	0/2128
17	q	0.42	0/1443	0.70	0/1944
18	r	0.42	0/1465	0.71	0/1965
19	s	0.40	0/1266	0.71	0/1690
20	t	0.43	0/1468	0.72	0/1973
21	u	0.42	0/1300	0.69	0/1743
22	v	0.37	0/812	0.65	0/1099
23	w	0.44	0/1018	0.74	1/1369 (0.1%)
24	y	0.45	0/533	0.68	0/707
25	z	0.40	0/979	0.68	0/1321
26	J	0.41	0/1004	0.71	0/1341
27	K	0.40	0/1070	0.67	0/1432

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	L	0.45	0/1204	0.69	0/1612
29	M	0.43	0/473	0.70	0/629
30	N	0.41	0/751	0.63	0/1008
31	O	0.38	0/890	0.71	0/1196
32	Q	0.42	0/1041	0.71	0/1394
33	R	0.42	0/868	0.68	0/1168
34	T	0.40	0/969	0.69	0/1289
35	U	0.42	0/778	0.69	0/1034
36	V	0.48	0/696	0.83	1/923 (0.1%)
37	W	0.39	0/618	0.71	0/826
38	X	0.39	0/443	0.80	0/588
39	Y	0.42	0/423	0.74	0/562
40	Z	0.41	0/860	0.67	0/1136
41	0	0.43	0/701	0.76	0/934
42	3	0.42	0/2765	0.72	2/3740 (0.1%)
43	S	0.43	0/890	0.74	0/1189
44	c	0.46	0/1908	0.74	0/2564
45	a	0.66	0/75028	1.04	94/116969 (0.1%)
All	All	0.56	2/145749 (0.0%)	0.91	105/213428 (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
5	d	0	1
14	n	0	1
15	o	0	1
16	p	0	1
20	t	0	1
35	U	0	1
45	a	0	2
All	All	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	1	G	OP3-P	-7.63	1.51	1.61
3	4	1	A	OP3-P	-7.10	1.52	1.61

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	a	2513	U	C3'-C2'-C1'	-9.69	93.75	101.50
45	a	420	G	O3'-P-O5'	-7.91	88.97	104.00
45	a	2403	G	O5'-P-OP2	-7.65	98.82	105.70
45	a	2939	G	O5'-P-OP2	-7.14	99.27	105.70
45	a	2313	A	O3'-P-O5'	-6.89	90.91	104.00
45	a	1417	G	O3'-P-O5'	-6.87	90.94	104.00
45	a	361	A	O3'-P-O5'	-6.82	91.04	104.00
3	4	110	C	O3'-P-O5'	-6.77	91.14	104.00
45	a	406	G	O4'-C1'-N9	6.75	113.60	108.20
45	a	2273	G	C3'-C2'-C1'	-6.68	96.16	101.50
36	V	40	PRO	N-CA-CB	-6.65	95.29	102.60
45	a	2661	G	OP1-P-O3'	6.63	119.79	105.20
45	a	1398	U	O3'-P-O5'	-6.59	91.48	104.00
45	a	1324	U	O3'-P-O5'	-6.57	91.52	104.00
45	a	110	G	O3'-P-O5'	-6.55	91.55	104.00
45	a	2728	G	C1'-O4'-C4'	-6.41	104.77	109.90
42	3	98	ARG	CG-CD-NE	-6.39	98.39	111.80
45	a	1483	G	C1'-O4'-C4'	-6.34	104.83	109.90
45	a	817	A	O3'-P-O5'	-6.24	92.15	104.00
45	a	2940	A	O5'-P-OP2	6.17	118.11	110.70
45	a	2100	A	O3'-P-O5'	-6.14	92.34	104.00
45	a	3362	A	C1'-O4'-C4'	-6.10	105.02	109.90
45	a	3228	C	P-O3'-C3'	6.04	126.94	119.70
45	a	1097	G	P-O3'-C3'	5.97	126.86	119.70
45	a	659	G	OP2-P-O3'	5.91	118.21	105.20
45	a	3107	U	O3'-P-O5'	-5.90	92.78	104.00
45	a	2871	G	O5'-P-OP1	-5.86	100.42	105.70
45	a	1496	C	OP2-P-O3'	5.79	117.94	105.20
45	a	2941	A	OP1-P-O3'	5.75	117.85	105.20
45	a	366	A	O5'-P-OP2	-5.72	100.55	105.70
4	b	76	A	O3'-P-O5'	-5.71	93.15	104.00
45	a	2147	A	O3'-P-O5'	-5.70	93.17	104.00
45	a	609	G	O5'-P-OP2	-5.70	100.58	105.70
45	a	2197	C	C3'-C2'-C1'	-5.67	96.96	101.50
45	a	2867	C	O3'-P-O5'	-5.66	93.24	104.00
45	a	1838	G	O3'-P-O5'	-5.65	93.26	104.00
45	a	637	C	C3'-C2'-C1'	-5.63	97.00	101.50
45	a	74	G	O3'-P-O5'	-5.62	93.32	104.00
45	a	599	C	O3'-P-O5'	-5.60	93.36	104.00
45	a	666	A	O3'-P-O5'	-5.58	93.40	104.00
42	3	317	PRO	N-CA-C	-5.53	97.73	112.10
45	a	941	G	OP1-P-O3'	5.52	117.35	105.20
45	a	2748	A	O3'-P-O5'	-5.52	93.51	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	a	1352	A	P-O3'-C3'	5.52	126.32	119.70
4	b	77	G	C3'-C2'-C1'	-5.50	97.10	101.50
45	a	406	G	C1'-O4'-C4'	-5.50	105.50	109.90
45	a	3375	A	O3'-P-O5'	-5.50	93.56	104.00
45	a	2761	G	O3'-P-O5'	-5.48	93.58	104.00
45	a	3359	A	O3'-P-O5'	-5.47	93.61	104.00
45	a	2867	C	O5'-P-OP1	-5.47	100.78	105.70
45	a	3048	A	C1'-O4'-C4'	-5.46	105.53	109.90
45	a	110	G	O5'-P-OP2	-5.45	100.80	105.70
45	a	1418	A	O3'-P-O5'	-5.45	93.64	104.00
45	a	2395	G	OP2-P-O3'	5.45	117.19	105.20
45	a	2351	U	O5'-P-OP2	5.44	117.23	110.70
45	a	1880	U	O3'-P-O5'	-5.41	93.73	104.00
45	a	1618	G	O3'-P-O5'	-5.37	93.80	104.00
5	d	10	ARG	CG-CD-NE	-5.36	100.55	111.80
45	a	913	A	O3'-P-O5'	-5.36	93.81	104.00
45	a	303	G	OP1-P-O3'	5.36	116.99	105.20
45	a	1907	C	O3'-P-O5'	-5.36	93.82	104.00
3	4	89	A	O3'-P-O5'	-5.34	93.86	104.00
45	a	1604	G	O3'-P-O5'	-5.33	93.86	104.00
45	a	2593	A	O3'-P-O5'	-5.33	93.87	104.00
45	a	1830	G	OP1-P-O3'	5.33	116.93	105.20
45	a	2621	G	O5'-P-OP2	-5.33	100.91	105.70
45	a	1482	A	P-O3'-C3'	5.32	126.08	119.70
45	a	2918	G	OP1-P-O3'	5.31	116.88	105.20
3	4	128	U	O5'-P-OP2	-5.30	100.93	105.70
45	a	2244	A	O5'-P-OP1	5.29	117.05	110.70
45	a	3317	U	P-O3'-C3'	5.29	126.05	119.70
45	a	1481	A	O3'-P-O5'	-5.29	93.96	104.00
45	a	960	U	C1'-O4'-C4'	-5.27	105.69	109.90
45	a	374	A	O3'-P-O5'	-5.26	94.00	104.00
45	a	2898	G	O3'-P-O5'	-5.26	94.00	104.00
23	w	88	ARG	CG-CD-NE	5.25	122.83	111.80
45	a	2192	C	O3'-P-O5'	-5.25	94.03	104.00
45	a	2400	G	OP2-P-O3'	5.24	116.72	105.20
45	a	1305	U	C3'-C2'-C1'	-5.22	97.32	101.50
45	a	1303	A	O3'-P-O5'	-5.21	94.11	104.00
45	a	2147	A	OP1-P-O3'	5.20	116.63	105.20
45	a	43	A	OP2-P-O3'	5.16	116.55	105.20
45	a	352	A	O3'-P-O5'	-5.16	94.20	104.00
45	a	51	A	OP2-P-O3'	5.15	116.52	105.20
45	a	399	A	O5'-P-OP1	-5.14	101.07	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	a	2374	C	OP2-P-O3'	5.14	116.51	105.20
45	a	1595	U	C3'-C2'-C1'	-5.13	97.39	101.50
45	a	3092	C	C1'-O4'-C4'	-5.13	105.80	109.90
45	a	505	G	OP1-P-O3'	5.12	116.47	105.20
45	a	2979	U	C1'-O4'-C4'	-5.12	105.81	109.90
45	a	1723	A	OP2-P-O3'	5.10	116.43	105.20
45	a	1888	U	O3'-P-O5'	-5.10	94.30	104.00
45	a	2222	A	O3'-P-O5'	-5.10	94.31	104.00
45	a	398	A	C1'-O4'-C4'	-5.09	105.83	109.90
45	a	1446	A	O3'-P-O5'	-5.09	94.33	104.00
45	a	91	G	O3'-P-O5'	-5.08	94.34	104.00
45	a	386	A	O3'-P-O5'	-5.08	94.35	104.00
4	b	120	C	O3'-P-O5'	-5.08	94.36	104.00
45	a	860	G	O3'-P-O5'	-5.06	94.38	104.00
45	a	90	C	OP1-P-O3'	5.06	116.33	105.20
45	a	1931	U	C3'-C2'-C1'	-5.06	97.45	101.50
45	a	2735	U	O3'-P-O5'	-5.05	94.40	104.00
45	a	870	G	O3'-P-O5'	-5.03	94.44	104.00
45	a	2978	U	C3'-C2'-C1'	-5.01	97.49	101.50
45	a	3119	U	O3'-P-O5'	-5.00	94.50	104.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
35	U	31	GLY	Peptide
45	a	2281	A	Sidechain
45	a	2950	G	Sidechain
5	d	253	GLY	Peptide
14	n	8	LYS	Peptide
15	o	127	TYR	Peptide
16	p	74	ARG	Sidechain
20	t	153	PRO	Peptide

5.2 Too-close contacts

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
1	A	320/1659 (19%)	314 (98%)	6 (2%)	0	100	100
1	C	253/1659 (15%)	245 (97%)	7 (3%)	1 (0%)	30	63
1	D	468/1659 (28%)	440 (94%)	26 (6%)	2 (0%)	30	63
1	E	467/1659 (28%)	459 (98%)	8 (2%)	0	100	100
1	H	100/1659 (6%)	100 (100%)	0	0	100	100
1	I	104/1659 (6%)	104 (100%)	0	0	100	100
2	P	13/25 (52%)	13 (100%)	0	0	100	100
5	d	384/387 (99%)	362 (94%)	21 (6%)	1 (0%)	37	68
6	e	289/297 (97%)	273 (94%)	14 (5%)	2 (1%)	19	51
7	f	152/176 (86%)	143 (94%)	9 (6%)	0	100	100
8	g	216/244 (88%)	210 (97%)	6 (3%)	0	100	100
9	h	231/256 (90%)	219 (95%)	12 (5%)	0	100	100
10	i	189/191 (99%)	180 (95%)	9 (5%)	0	100	100
11	j	206/221 (93%)	193 (94%)	12 (6%)	1 (0%)	25	58
12	k	164/174 (94%)	155 (94%)	7 (4%)	2 (1%)	11	38
13	m	191/199 (96%)	178 (93%)	13 (7%)	0	100	100
14	n	134/138 (97%)	126 (94%)	8 (6%)	0	100	100
15	o	201/204 (98%)	188 (94%)	13 (6%)	0	100	100
16	p	195/199 (98%)	187 (96%)	8 (4%)	0	100	100
17	q	181/184 (98%)	166 (92%)	14 (8%)	1 (1%)	22	53
18	r	183/186 (98%)	170 (93%)	12 (7%)	1 (0%)	25	58
19	s	153/189 (81%)	148 (97%)	5 (3%)	0	100	100
20	t	168/172 (98%)	156 (93%)	11 (6%)	1 (1%)	22	53
21	u	157/160 (98%)	147 (94%)	9 (6%)	1 (1%)	22	53
22	v	98/121 (81%)	88 (90%)	10 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	w	134/137 (98%)	129 (96%)	5 (4%)	0	100	100
24	y	61/155 (39%)	60 (98%)	1 (2%)	0	100	100
25	z	119/142 (84%)	111 (93%)	7 (6%)	1 (1%)	16	48
26	J	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
27	K	125/136 (92%)	118 (94%)	6 (5%)	1 (1%)	16	48
28	L	146/149 (98%)	135 (92%)	11 (8%)	0	100	100
29	M	56/59 (95%)	51 (91%)	5 (9%)	0	100	100
30	N	95/105 (90%)	91 (96%)	4 (4%)	0	100	100
31	O	107/113 (95%)	100 (94%)	7 (6%)	0	100	100
32	Q	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
33	R	104/107 (97%)	99 (95%)	5 (5%)	0	100	100
34	T	115/120 (96%)	109 (95%)	6 (5%)	0	100	100
35	U	97/100 (97%)	87 (90%)	9 (9%)	1 (1%)	13	42
36	V	85/88 (97%)	78 (92%)	6 (7%)	1 (1%)	11	38
37	W	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
38	X	48/51 (94%)	44 (92%)	3 (6%)	1 (2%)	5	25
39	Y	50/128 (39%)	47 (94%)	2 (4%)	1 (2%)	6	26
40	Z	103/106 (97%)	92 (89%)	8 (8%)	3 (3%)	3	20
41	0	89/92 (97%)	81 (91%)	5 (6%)	3 (3%)	3	17
42	3	352/362 (97%)	324 (92%)	24 (7%)	4 (1%)	12	39
43	S	110/121 (91%)	106 (96%)	4 (4%)	0	100	100
44	c	244/254 (96%)	224 (92%)	17 (7%)	3 (1%)	11	38
All	All	7781/16537 (47%)	7361 (95%)	388 (5%)	32 (0%)	32	63

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	e	202	GLY
18	r	171	LYS
36	V	85	LYS
12	k	55	ARG
17	q	66	SER
20	t	154	HIS
41	0	18	TYR

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Mol	Chain	Res	Type
42	3	90	PHE
1	D	1478	ASP
5	d	139	GLN
11	j	218	ALA
12	k	167	TYR
25	z	50	ALA
38	X	3	ALA
1	D	1474	ASN
27	K	103	GLN
35	U	97	SER
40	Z	94	GLY
41	0	51	ALA
42	3	132	ALA
44	c	125	ALA
44	c	143	GLU
44	c	180	LEU
6	e	292	ALA
39	Y	79	GLU
40	Z	96	GLU
42	3	5	GLN
21	u	125	ALA
40	Z	17	CYS
1	C	940	ILE
42	3	192	GLY
41	0	12	GLY

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	
1	A	294/1520 (19%)	291 (99%)	3 (1%)	73	86
1	C	232/1520 (15%)	230 (99%)	2 (1%)	75	88
1	D	429/1520 (28%)	425 (99%)	4 (1%)	75	88
1	E	428/1520 (28%)	427 (100%)	1 (0%)	92	96
1	H	94/1520 (6%)	90 (96%)	4 (4%)	25	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	96/1520 (6%)	89 (93%)	7 (7%)	11	37
2	P	14/23 (61%)	14 (100%)	0	100	100
5	d	320/323 (99%)	313 (98%)	7 (2%)	47	71
6	e	240/245 (98%)	231 (96%)	9 (4%)	28	59
7	f	134/153 (88%)	132 (98%)	2 (2%)	60	80
8	g	183/205 (89%)	180 (98%)	3 (2%)	58	79
9	h	187/208 (90%)	183 (98%)	4 (2%)	48	72
10	i	171/171 (100%)	163 (95%)	8 (5%)	22	52
11	j	177/187 (95%)	174 (98%)	3 (2%)	56	78
12	k	144/150 (96%)	141 (98%)	3 (2%)	48	72
13	m	154/159 (97%)	147 (96%)	7 (4%)	23	53
14	n	107/109 (98%)	107 (100%)	0	100	100
15	o	175/176 (99%)	174 (99%)	1 (1%)	84	91
16	p	160/162 (99%)	157 (98%)	3 (2%)	52	75
17	q	140/146 (96%)	133 (95%)	7 (5%)	20	50
18	r	150/151 (99%)	149 (99%)	1 (1%)	81	90
19	s	128/154 (83%)	127 (99%)	1 (1%)	79	89
20	t	155/156 (99%)	145 (94%)	10 (6%)	14	41
21	u	136/137 (99%)	135 (99%)	1 (1%)	81	90
22	v	87/107 (81%)	84 (97%)	3 (3%)	32	62
23	w	104/105 (99%)	101 (97%)	3 (3%)	37	65
24	y	55/129 (43%)	53 (96%)	2 (4%)	30	60
25	z	104/118 (88%)	102 (98%)	2 (2%)	52	75
26	J	109/110 (99%)	105 (96%)	4 (4%)	29	59
27	K	110/116 (95%)	109 (99%)	1 (1%)	75	88
28	L	118/119 (99%)	112 (95%)	6 (5%)	20	49
29	M	46/47 (98%)	44 (96%)	2 (4%)	25	55
30	N	81/88 (92%)	81 (100%)	0	100	100
31	O	92/97 (95%)	89 (97%)	3 (3%)	33	62
32	Q	109/111 (98%)	104 (95%)	5 (5%)	23	52
33	R	90/91 (99%)	89 (99%)	1 (1%)	70	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	T	104/105 (99%)	103 (99%)	1 (1%)	73	86
35	U	81/82 (99%)	79 (98%)	2 (2%)	42	69
36	V	70/71 (99%)	65 (93%)	5 (7%)	12	39
37	W	68/69 (99%)	65 (96%)	3 (4%)	24	54
38	X	45/46 (98%)	44 (98%)	1 (2%)	47	71
39	Y	47/116 (40%)	46 (98%)	1 (2%)	48	72
40	Z	90/91 (99%)	89 (99%)	1 (1%)	70	84
41	0	71/72 (99%)	69 (97%)	2 (3%)	38	66
42	3	285/289 (99%)	275 (96%)	10 (4%)	31	61
43	S	95/103 (92%)	92 (97%)	3 (3%)	34	63
44	c	189/196 (96%)	183 (97%)	6 (3%)	34	63
All	All	6698/14613 (46%)	6540 (98%)	158 (2%)	45	70

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	246	SER
1	A	444	THR
1	A	518	THR
1	H	1547	MET
1	H	1572	MET
1	H	1574	LEU
1	H	1595	ILE
1	I	1538	ASN
1	I	1564	ASP
1	I	1573	ILE
1	I	1577	LEU
1	I	1593	LEU
1	I	1594	GLU
1	I	1652	SER
1	C	812	TYR
1	C	881	LEU
1	D	1001	SER
1	D	1431	VAL
1	D	1482	ASP
1	D	1491	GLU
1	E	1001	SER
5	d	85	VAL

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Mol	Chain	Res	Type
5	d	146	ARG
5	d	169	THR
5	d	205	VAL
5	d	238	LEU
5	d	276	THR
5	d	332	ARG
6	e	34	LYS
6	e	38	THR
6	e	81	HIS
6	e	95	TRP
6	e	152	ARG
6	e	155	THR
6	e	177	GLU
6	e	245	GLU
6	e	293	LEU
7	f	8	LYS
7	f	92	SER
8	g	100	ARG
8	g	110	ARG
8	g	184	LEU
9	h	36	ILE
9	h	108	ARG
9	h	164	VAL
9	h	175	VAL
10	i	12	VAL
10	i	16	VAL
10	i	23	ARG
10	i	41	ILE
10	i	70	THR
10	i	82	VAL
10	i	92	TYR
10	i	93	VAL
11	j	27	PRO
11	j	91	VAL
11	j	140	THR
12	k	15	GLU
12	k	115	LYS
12	k	137	ARG
13	m	17	HIS
13	m	50	PRO
13	m	58	VAL
13	m	62	THR

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Mol	Chain	Res	Type
13	m	85	LEU
13	m	104	ARG
13	m	190	LYS
15	o	117	ASN
16	p	117	ARG
16	p	121	PRO
16	p	124	LEU
17	q	24	VAL
17	q	52	LEU
17	q	67	ILE
17	q	94	LEU
17	q	96	GLN
17	q	129	THR
17	q	169	THR
18	r	32	LEU
19	s	134	HIS
20	t	3	HIS
20	t	12	ARG
20	t	13	ARG
20	t	23	LYS
20	t	55	SER
20	t	71	LYS
20	t	96	ASP
20	t	134	ASP
20	t	160	THR
20	t	172	TYR
21	u	104	GLU
22	v	64	THR
22	v	91	ASP
22	v	92	TRP
23	w	54	LEU
23	w	81	GLN
23	w	135	VAL
24	y	43	ARG
24	y	46	PRO
25	z	71	THR
25	z	87	SER
26	J	51	ARG
26	J	56	VAL
26	J	74	TYR
26	J	85	VAL
27	K	93	LYS

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Mol	Chain	Res	Type
28	L	58	MET
28	L	60	TYR
28	L	77	LYS
28	L	89	GLN
28	L	92	LYS
28	L	133	LEU
29	M	14	ARG
29	M	22	LYS
31	O	16	LEU
31	O	50	ARG
31	O	64	VAL
32	Q	19	ARG
32	Q	36	LYS
32	Q	47	ARG
32	Q	68	PRO
32	Q	86	THR
33	R	58	GLU
34	T	90	ARG
35	U	29	LYS
35	U	36	ARG
36	V	5	THR
36	V	24	ARG
36	V	34	CYS
36	V	40	PRO
36	V	68	LYS
37	W	10	GLN
37	W	36	LYS
37	W	53	THR
38	X	45	ARG
39	Y	97	ARG
40	Z	21	THR
41	0	60	CYS
41	0	88	GLU
42	3	54	GLU
42	3	60	THR
42	3	99	MET
42	3	120	TYR
42	3	133	SER
42	3	138	ARG
42	3	156	LEU
42	3	177	ASP
42	3	230	VAL

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Mol	Chain	Res	Type
42	3	339	LEU
43	S	12	PRO
43	S	51	LEU
43	S	103	LYS
44	c	29	LEU
44	c	47	GLN
44	c	62	VAL
44	c	157	VAL
44	c	176	ASP
44	c	207	VAL

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

Mol	Chain	Res	Type
1	C	818	GLN
1	D	1015	GLN
1	E	1015	GLN
1	E	1227	ASN
1	E	1439	GLN
1	E	1474	ASN
5	d	293	ASN
9	h	38	GLN
9	h	59	GLN
9	h	145	ASN
15	o	194	GLN
16	p	50	ASN
23	w	98	ASN
28	L	64	GLN
33	R	42	GLN
36	V	79	GLN
38	X	33	ASN
39	Y	109	ASN
44	c	47	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	4	157/158 (99%)	30 (19%)	4 (2%)
4	b	120/121 (99%)	12 (10%)	0
45	a	3128/3396 (92%)	558 (17%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3405/3675 (92%)	600 (17%)	4 (0%)

All (600) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	4	21	C
3	4	23	U
3	4	34	U
3	4	35	C
3	4	50	C
3	4	53	A
3	4	59	A
3	4	62	C
3	4	63	G
3	4	80	A
3	4	81	U
3	4	82	U
3	4	84	C
3	4	85	G
3	4	86	U
3	4	87	G
3	4	90	U
3	4	95	G
3	4	104	A
3	4	105	A
3	4	106	C
3	4	111	A
3	4	113	U
3	4	125	U
3	4	126	A
3	4	138	A
3	4	144	G
3	4	151	C
3	4	152	G
3	4	158	U
4	b	11	A
4	b	13	A
4	b	22	A
4	b	51	A
4	b	54	U
4	b	60	G
4	b	65	G

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Mol	Chain	Res	Type
4	b	74	C
4	b	91	G
4	b	102	A
4	b	112	G
4	b	121	U
45	a	16	A
45	a	26	A
45	a	40	A
45	a	43	A
45	a	44	U
45	a	49	A
45	a	59	G
45	a	60	A
45	a	65	A
45	a	66	A
45	a	74	G
45	a	76	G
45	a	83	U
45	a	92	G
45	a	95	A
45	a	99	A
45	a	105	C
45	a	109	A
45	a	110	G
45	a	116	A
45	a	121	A
45	a	122	A
45	a	133	U
45	a	135	C
45	a	136	G
45	a	142	C
45	a	156	G
45	a	157	A
45	a	161	G
45	a	166	C
45	a	170	G
45	a	172	G
45	a	182	U
45	a	187	A
45	a	190	U
45	a	191	U
45	a	213	A

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Mol	Chain	Res	Type
45	a	218	G
45	a	219	A
45	a	240	U
45	a	241	G
45	a	243	G
45	a	252	U
45	a	269	G
45	a	271	C
45	a	283	G
45	a	284	A
45	a	286	U
45	a	295	A
45	a	305	U
45	a	307	A
45	a	315	C
45	a	316	U
45	a	323	A
45	a	329	U
45	a	339	C
45	a	350	C
45	a	370	U
45	a	376	G
45	a	392	G
45	a	398	A
45	a	399	A
45	a	401	U
45	a	402	A
45	a	403	C
45	a	421	G
45	a	422	A
45	a	439	C
45	a	440	A
45	a	495	G
45	a	507	U
45	a	521	A
45	a	525	C
45	a	531	G
45	a	532	A
45	a	535	G
45	a	536	U
45	a	546	C
45	a	547	G

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Mol	Chain	Res	Type
45	a	548	G
45	a	552	G
45	a	555	U
45	a	556	U
45	a	557	A
45	a	558	U
45	a	559	A
45	a	569	A
45	a	579	G
45	a	592	A
45	a	594	U
45	a	595	G
45	a	609	G
45	a	611	A
45	a	619	A
45	a	620	U
45	a	621	A
45	a	636	C
45	a	649	A
45	a	660	A
45	a	675	C
45	a	677	A
45	a	681	U
45	a	691	A
45	a	705	A
45	a	710	A
45	a	712	G
45	a	715	A
45	a	716	A
45	a	765	C
45	a	767	U
45	a	774	G
45	a	776	U
45	a	777	U
45	a	780	A
45	a	781	G
45	a	785	G
45	a	786	A
45	a	805	G
45	a	806	A
45	a	816	A
45	a	817	A

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Mol	Chain	Res	Type
45	a	830	A
45	a	833	G
45	a	849	C
45	a	861	C
45	a	874	U
45	a	879	U
45	a	890	C
45	a	896	A
45	a	897	U
45	a	907	G
45	a	908	G
45	a	909	G
45	a	914	A
45	a	916	G
45	a	917	A
45	a	923	C
45	a	937	G
45	a	944	C
45	a	959	C
45	a	960	U
45	a	979	U
45	a	980	A
45	a	981	U
45	a	993	G
45	a	994	G
45	a	995	U
45	a	1001	G
45	a	1002	A
45	a	1003	A
45	a	1010	G
45	a	1015	U
45	a	1017	C
45	a	1018	G
45	a	1019	G
45	a	1021	G
45	a	1022	U
45	a	1033	U
45	a	1036	A
45	a	1037	C
45	a	1041	U
45	a	1047	A
45	a	1049	C

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Mol	Chain	Res	Type
45	a	1064	A
45	a	1065	A
45	a	1072	G
45	a	1081	U
45	a	1083	G
45	a	1087	G
45	a	1093	A
45	a	1094	U
45	a	1095	U
45	a	1096	U
45	a	1098	A
45	a	1103	A
45	a	1104	G
45	a	1117	G
45	a	1126	G
45	a	1131	G
45	a	1153	A
45	a	1159	A
45	a	1163	A
45	a	1170	A
45	a	1180	A
45	a	1181	U
45	a	1182	A
45	a	1186	G
45	a	1190	A
45	a	1191	U
45	a	1192	C
45	a	1196	C
45	a	1201	C
45	a	1208	U
45	a	1209	G
45	a	1212	A
45	a	1221	A
45	a	1222	G
45	a	1232	C
45	a	1235	U
45	a	1236	G
45	a	1237	G
45	a	1239	C
45	a	1242	G
45	a	1244	A
45	a	1245	A

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Mol	Chain	Res	Type
45	a	1246	G
45	a	1258	U
45	a	1262	G
45	a	1263	A
45	a	1265	U
45	a	1270	A
45	a	1271	A
45	a	1272	C
45	a	1273	A
45	a	1285	G
45	a	1286	A
45	a	1287	A
45	a	1307	G
45	a	1309	U
45	a	1313	G
45	a	1330	A
45	a	1331	U
45	a	1348	U
45	a	1349	G
45	a	1351	U
45	a	1352	A
45	a	1353	U
45	a	1355	A
45	a	1356	U
45	a	1357	G
45	a	1386	A
45	a	1399	A
45	a	1400	G
45	a	1418	A
45	a	1419	A
45	a	1434	G
45	a	1437	C
45	a	1450	G
45	a	1460	A
45	a	1481	A
45	a	1482	A
45	a	1483	G
45	a	1503	A
45	a	1508	C
45	a	1527	C
45	a	1533	U
45	a	1536	G

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Mol	Chain	Res	Type
45	a	1555	U
45	a	1556	C
45	a	1557	A
45	a	1560	G
45	a	1562	C
45	a	1563	C
45	a	1564	U
45	a	1567	U
45	a	1568	U
45	a	1569	U
45	a	1575	A
45	a	1576	G
45	a	1578	C
45	a	1580	A
45	a	1581	C
45	a	1583	A
45	a	1587	A
45	a	1589	A
45	a	1596	C
45	a	1618	G
45	a	1620	U
45	a	1629	U
45	a	1639	C
45	a	1642	A
45	a	1643	A
45	a	1657	C
45	a	1675	G
45	a	1687	U
45	a	1718	G
45	a	1724	U
45	a	1725	C
45	a	1741	A
45	a	1742	U
45	a	1750	A
45	a	1751	G
45	a	1759	C
45	a	1760	A
45	a	1765	U
45	a	1766	G
45	a	1770	G
45	a	1775	G
45	a	1780	G

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Mol	Chain	Res	Type
45	a	1794	G
45	a	1797	A
45	a	1814	A
45	a	1815	U
45	a	1816	A
45	a	1817	G
45	a	1819	U
45	a	1820	U
45	a	1821	U
45	a	1839	A
45	a	1842	A
45	a	1846	C
45	a	1847	A
45	a	1849	C
45	a	1850	A
45	a	1878	G
45	a	1880	U
45	a	1884	A
45	a	1886	A
45	a	1893	A
45	a	1904	C
45	a	1906	G
45	a	1908	A
45	a	1920	U
45	a	1951	C
45	a	1952	G
45	a	2094	C
45	a	2096	A
45	a	2097	U
45	a	2098	C
45	a	2101	C
45	a	2102	U
45	a	2112	U
45	a	2113	A
45	a	2121	G
45	a	2122	G
45	a	2131	A
45	a	2138	A
45	a	2140	U
45	a	2158	A
45	a	2159	U
45	a	2169	G

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Mol	Chain	Res	Type
45	a	2171	G
45	a	2181	C
45	a	2192	C
45	a	2205	U
45	a	2206	G
45	a	2209	U
45	a	2210	G
45	a	2223	A
45	a	2225	U
45	a	2244	A
45	a	2246	G
45	a	2249	G
45	a	2251	G
45	a	2252	A
45	a	2255	A
45	a	2256	A
45	a	2257	C
45	a	2258	U
45	a	2261	G
45	a	2262	A
45	a	2270	A
45	a	2273	G
45	a	2279	A
45	a	2281	A
45	a	2282	U
45	a	2288	G
45	a	2307	G
45	a	2308	C
45	a	2310	U
45	a	2313	A
45	a	2314	U
45	a	2315	G
45	a	2319	U
45	a	2334	U
45	a	2335	G
45	a	2336	U
45	a	2337	C
45	a	2374	C
45	a	2375	G
45	a	2388	U
45	a	2393	G
45	a	2397	A

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Mol	Chain	Res	Type
45	a	2402	A
45	a	2403	G
45	a	2404	A
45	a	2411	U
45	a	2418	G
45	a	2419	A
45	a	2435	G
45	a	2440	G
45	a	2442	G
45	a	2443	A
45	a	2506	U
45	a	2513	U
45	a	2514	U
45	a	2515	A
45	a	2522	G
45	a	2523	A
45	a	2531	C
45	a	2532	U
45	a	2533	G
45	a	2538	U
45	a	2539	C
45	a	2540	A
45	a	2541	U
45	a	2542	U
45	a	2549	G
45	a	2552	C
45	a	2554	A
45	a	2561	A
45	a	2569	A
45	a	2570	U
45	a	2571	U
45	a	2572	C
45	a	2573	G
45	a	2576	G
45	a	2585	G
45	a	2589	G
45	a	2593	A
45	a	2594	C
45	a	2600	C
45	a	2606	G
45	a	2607	G
45	a	2614	G

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Mol	Chain	Res	Type
45	a	2618	G
45	a	2619	G
45	a	2626	A
45	a	2629	U
45	a	2652	U
45	a	2656	A
45	a	2674	A
45	a	2677	G
45	a	2681	U
45	a	2689	A
45	a	2690	G
45	a	2691	A
45	a	2694	A
45	a	2695	A
45	a	2696	A
45	a	2704	A
45	a	2726	C
45	a	2728	G
45	a	2729	U
45	a	2740	A
45	a	2752	U
45	a	2753	G
45	a	2762	A
45	a	2772	C
45	a	2777	G
45	a	2778	G
45	a	2796	G
45	a	2800	G
45	a	2801	A
45	a	2802	A
45	a	2803	A
45	a	2810	C
45	a	2816	G
45	a	2817	A
45	a	2821	C
45	a	2842	U
45	a	2843	U
45	a	2845	A
45	a	2847	A
45	a	2867	C
45	a	2871	G
45	a	2872	A

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Mol	Chain	Res	Type
45	a	2875	U
45	a	2876	C
45	a	2887	A
45	a	2899	C
45	a	2911	A
45	a	2923	U
45	a	2928	C
45	a	2935	U
45	a	2936	A
45	a	2941	A
45	a	2942	C
45	a	2947	G
45	a	2977	G
45	a	2983	C
45	a	2990	G
45	a	2996	U
45	a	2997	G
45	a	3012	A
45	a	3049	A
45	a	3056	U
45	a	3057	U
45	a	3058	U
45	a	3059	G
45	a	3073	A
45	a	3074	G
45	a	3078	U
45	a	3079	U
45	a	3080	G
45	a	3092	C
45	a	3104	U
45	a	3122	A
45	a	3128	G
45	a	3129	A
45	a	3131	U
45	a	3142	A
45	a	3143	C
45	a	3154	C
45	a	3155	U
45	a	3156	U
45	a	3157	U
45	a	3164	C
45	a	3165	A

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Mol	Chain	Res	Type
45	a	3173	G
45	a	3174	A
45	a	3176	G
45	a	3179	U
45	a	3181	C
45	a	3187	A
45	a	3196	U
45	a	3198	U
45	a	3207	U
45	a	3209	A
45	a	3213	A
45	a	3217	C
45	a	3218	A
45	a	3219	G
45	a	3227	A
45	a	3229	G
45	a	3235	C
45	a	3239	G
45	a	3243	A
45	a	3244	A
45	a	3245	A
45	a	3246	G
45	a	3259	U
45	a	3260	G
45	a	3263	G
45	a	3265	C
45	a	3268	A
45	a	3269	U
45	a	3272	C
45	a	3273	A
45	a	3275	U
45	a	3276	G
45	a	3277	U
45	a	3279	A
45	a	3281	U
45	a	3287	U
45	a	3289	G
45	a	3294	A
45	a	3304	U
45	a	3313	U
45	a	3316	A
45	a	3318	G

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Mol	Chain	Res	Type
45	a	3319	U
45	a	3341	U
45	a	3342	A
45	a	3345	G
45	a	3352	U
45	a	3353	G
45	a	3355	U
45	a	3356	G
45	a	3359	A
45	a	3360	C
45	a	3363	U
45	a	3369	G
45	a	3375	A
45	a	3378	C
45	a	3386	G
45	a	3389	U
45	a	3396	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	4	84	C
3	4	85	G
3	4	90	U
3	4	105	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 5 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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.