



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 01:59 pm GMT

PDB ID : 8S1U
EMDB ID : EMD-19641
Title : YlmH bound to stalled 50S subunits with RqcH and PtRNA
Authors : Paternoga, H.; Wilson, D.N.
Deposited on : 2024-02-16
Resolution : 3.40 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**
Mogul : 1.8.4, CSD as541be (2020)
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

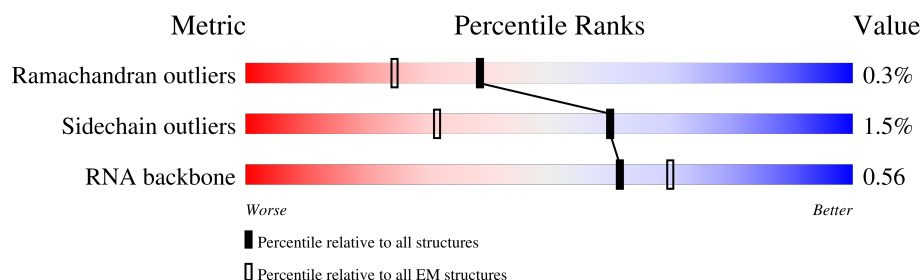
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



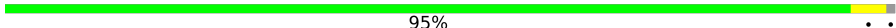
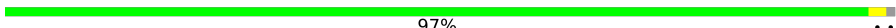
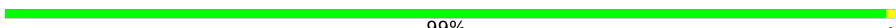
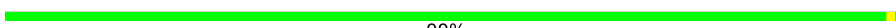
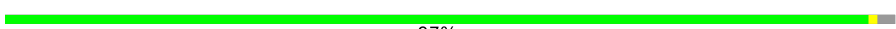







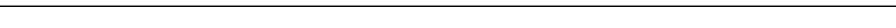


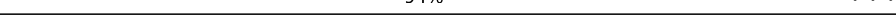
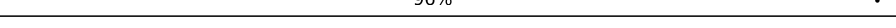
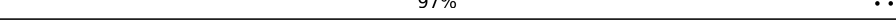



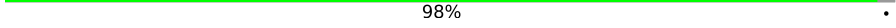
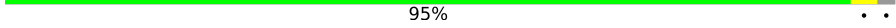

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	76	
1	c	76	
2	0	59	
3	1	49	
4	2	44	
5	3	66	
6	4	37	
7	6	66	
8	B	112	

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Mol	Chain	Length	Quality of chain
9	C	277	 95% ..
10	D	209	 97% ..
11	E	207	 99% .
12	F	179	 99% ..
13	G	179	 97% ..
14	J	145	 98% ..
15	K	122	 98% .
16	L	146	 99% .
17	M	144	 92% .. 6%
18	N	120	 97% ..
19	O	120	 100%
20	P	115	 95% ..
21	Q	119	 97% ..
22	R	102	 100%
23	S	113	 94% ...
24	T	95	 96% .
25	U	103	 97% ..
26	V	275	 89% . 9%
27	W	94	 84% . 15%
28	X	62	 95% ..
29	Y	66	 98% .
30	Z	59	 95% ..
31	H	570	 91% 9%
32	A	2928	 80% 15% 5%

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 93269 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 P-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	c	66	Total	C	N	O	P	0	0
			1413	628	254	465	66		
1	a	69	Total	C	N	O	P	0	0
			1477	657	268	483	69		

- Molecule 2 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	53	Total	C	N	O	S	0	0
			418	258	84	69	7		

- Molecule 3 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	49	Total	C	N	O	S	0	0
			411	250	82	75	4		

- Molecule 4 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 5 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	64	Total	C	N	O	S	0	0
			512	321	107	82	2		

- Molecule 6 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	46	Total	C	N	O	S	0	0
			356	222	63	66	5		

- Molecule 8 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 9 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	273	Total	C	N	O	S	0	0
			2094	1302	412	374	6		

- Molecule 10 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 11 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

- Molecule 12 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F	178	Total	C	N	O	S	0	0
			1405	893	245	260	7		

- Molecule 13 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 14 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	143	Total	C	N	O	S	0	0
			1131	714	207	205	5		

- Molecule 15 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 16 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 17 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 18 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 19 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 20 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	113	Total	C	N	O	S	0	0
			922	588	177	156	1		

- Molecule 21 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	118	Total	C	N	O	S	0	0
			950	597	191	158	4		

- Molecule 22 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	102	Total	C	N	O	S	0	0
			795	506	140	148	1		

- Molecule 23 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	110	Total	C	N	O	S	0	0
			850	530	165	151	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	91	Total	C	N	O	S	0	0
			733	458	135	137	3		

- Molecule 25 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	102	Total	C	N	O	S	0	0
			770	482	143	141	4		

- Molecule 26 is a protein called Putative RNA-binding protein YlmH.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	249	Total	C	N	O	S	0	0
			1988	1256	350	376	6		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	258	GLY	-	expression tag	UNP P71020
V	259	SER	-	expression tag	UNP P71020
V	260	GLY	-	expression tag	UNP P71020
V	261	SER	-	expression tag	UNP P71020
V	262	GLY	-	expression tag	UNP P71020
V	263	SER	-	expression tag	UNP P71020
V	264	GLY	-	expression tag	UNP P71020
V	265	SER	-	expression tag	UNP P71020
V	266	GLY	-	expression tag	UNP P71020
V	267	SER	-	expression tag	UNP P71020
V	268	ASP	-	expression tag	UNP P71020
V	269	TYR	-	expression tag	UNP P71020
V	270	LYS	-	expression tag	UNP P71020
V	271	ASP	-	expression tag	UNP P71020
V	272	ASP	-	expression tag	UNP P71020
V	273	ASP	-	expression tag	UNP P71020
V	274	ASP	-	expression tag	UNP P71020
V	275	LYS	-	expression tag	UNP P71020

- Molecule 27 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	W	80	Total	C	N	O	0	0
			611	378	119	114		

- Molecule 28 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	X	61	Total	C	N	O	S	0
			468	289	98	79	2	0

- Molecule 29 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	Y	65	Total	C	N	O	S	0
			530	328	102	98	2	0

- Molecule 30 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Z	58	Total	C	N	O	S	0
			456	281	89	85	1	0

- Molecule 31 is a protein called Rqc2 homolog RqcH.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	H	518	Total	C	N	O	0	0
			2567	1530	518	519		

- Molecule 32 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	A	2789	Total	C	N	O	P	0	0
			59910	26733	11076	19313	2788		

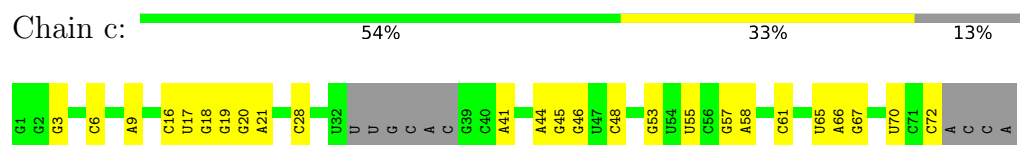
- Molecule 33 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
33	A	15	Total	K	0
			15	15	

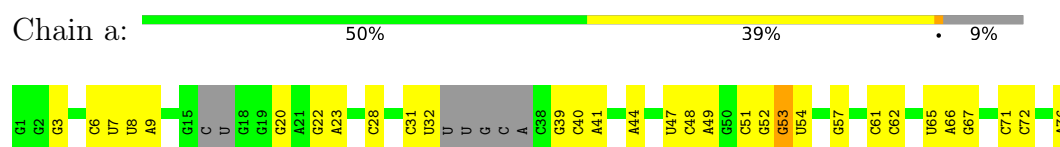
3 Residue-property plots [i](#)

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.

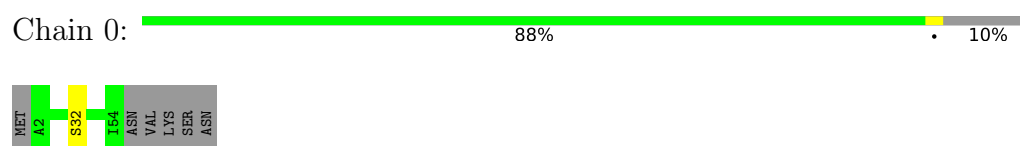
- Molecule 1: P-tRNA



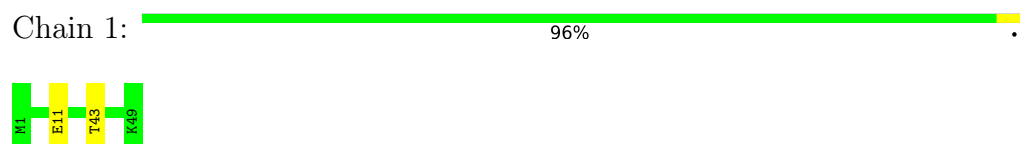
- Molecule 1: P-tRNA



- Molecule 2: 50S ribosomal protein L32



- Molecule 3: 50S ribosomal protein L33 1

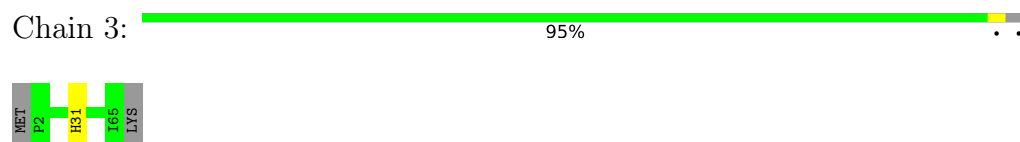


- Molecule 4: 50S ribosomal protein L34



There are no outlier residues recorded for this chain.

- Molecule 5: 50S ribosomal protein L35



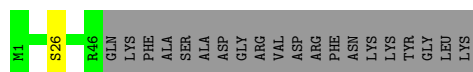
- Molecule 6: 50S ribosomal protein L36

Chain 4:  100%


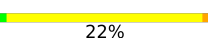
There are no outlier residues recorded for this chain.

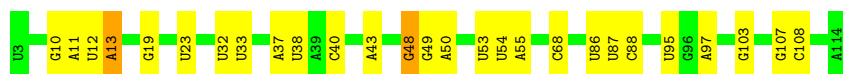
- Molecule 7: 50S ribosomal protein L31

Chain 6:  68%  30%



- Molecule 8: 5S rRNA

Chain B:  76%  22%



- Molecule 9: 50S ribosomal protein L2

Chain C:  95%



- Molecule 10: 50S ribosomal protein L3

Chain D:  97%



- Molecule 11: 50S ribosomal protein L4

Chain E:  99%

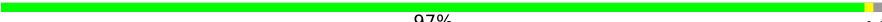


- Molecule 12: 50S ribosomal protein L5

Chain F:  99%



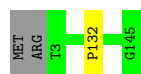
- Molecule 13: Large ribosomal subunit protein uL6

Chain G:  97% ..



- Molecule 14: 50S ribosomal protein L13

Chain J:  98% ..



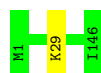
- Molecule 15: 50S ribosomal protein L14

Chain K:  98% .



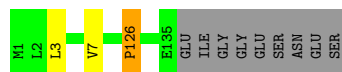
- Molecule 16: 50S ribosomal protein L15

Chain L:  99% .



- Molecule 17: 50S ribosomal protein L16

Chain M:  92% .. 6%



- Molecule 18: 50S ribosomal protein L17

Chain N:  97% ..



- Molecule 19: 50S ribosomal protein L18

Chain O:  100%

There are no outlier residues recorded for this chain.

- Molecule 20: 50S ribosomal protein L19

Chain P:  95% . .



- Molecule 21: Large ribosomal subunit protein bL20

Chain Q: 97% ..



- Molecule 22: 50S ribosomal protein L21

Chain R: 100%

There are no outlier residues recorded for this chain.

- Molecule 23: 50S ribosomal protein L22

Chain S: 94% ...



- Molecule 24: Large ribosomal subunit protein uL23

Chain T: 96% .



- Molecule 25: 50S ribosomal protein L24

Chain U: 97% ..



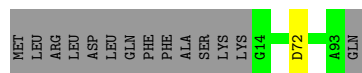
- Molecule 26: Putative RNA-binding protein YlmH

Chain V: 89% . 9%



- Molecule 27: Large ribosomal subunit protein bL27

Chain W: 84% . 15%



-
- A diagram of a protein structure with residues MET, A2, R3, V59, and V62 highlighted in different colors. MET is in a grey box, A2 is in a green box, R3 is in a yellow box, V59 is in a yellow box, and V62 is in a green box. The residues are connected by lines representing the protein backbone.

- M1 N65 LYS

-
- A diagram of a protein structure with residues MET, A2, S51, E58, and Q59 highlighted in different colors. MET is in a grey box, A2 is in a green box, S51 is in a yellow box, E58 is in a yellow box, and Q59 is in a green box. The residues are connected by lines representing the protein backbone.

- 5570 M338 LEU LYS LYS GLY ASP GLN GLU VAL ILE ASN ASP GLU SER PRO THR ILE THR PRO LEU ASN PRO ASN LYS THR P369 E428 GLY LYS LYS THR LEU ARG PRO LYS GLN GLN LYS GLY GLN LYS GLN LYS LYS PRO HIS ASN PRO VAL LEU E451

- [illegible]

A2794	C2503	G2311	A	C2084	A1877	U1595	A1473	G1182	G1068
A2807	C2504	C2312	G	G2085	U1899	U1602	C1474	A1188	A1072
C2823	A2505	U	C	A2089	A1900	C1607	U1489	C1216	U1079
G2824	G2531	A2316	U	G2090	A1901	A1614	A1490	U	U1091
U2833	A2532	U2334	G	G2098	C1911	A1617	A1499	C	A1092
A2844	U2533	A2338	U	G2099	C1934	U1626	U1500	G1220	G1093
A2860	G2539	A2339	G	G2122	G1935	U1632	U1506	A1260	A1096
C2886	A2547	A2340	G	A2123	G1936	A1631	U1507	A1293	G1102
G2892	C2558	U2341	A	A2124	G1939	G1632	C1508	G1296	A1103
G2897	U2559	C2342	G	U2127	U	G1637	C1514	U1104	G1105
A2908	C2563	G2347	C	U2128	A	C1652	G1525	U1107	U1106
G2918	G2566	C2348	A	A2132	A	A1653	C1527	U1108	G1108
C2925	U2576	A2349	U	C	U	A1654	C1528	G1109	C1110
C	G2577	U2351	G	A	A	A1691	U1529	U1111	U1112
A	G2582	C2352	U	C	C1949	U1692	G1530	A1113	G1114
U	U2583	G2363	G	G	G1958	C1693	U1535	A1115	A1116
	A2595	A2364	A	U	G1959	G1719	A1536	A1360	
	G2596	U2376	U	A	A1965	U1751	A1540	G1363	A1119
	C2602	C2379	C	A	A1966	G1752	U1543	C1364	
	G2603	G2382	U	G	A1967	U1757	C1544	G1367	A1123
	G2607	A2383	C	U	U1984	U1759	A1583	U1127	C1124
A2616	A2616	G2408	C	A	C1992	A1768	U	U1128	
A2631	G2632	G2412	U	G	G1993	A1776	A1585	U1129	U1130
G2638	U2638	G2413	G	U	C1994	G1792	A1556	C1389	A1131
U2642	U2643	C2414	C	A	A1995	G1793	G1557	C1390	
A2643	G2643	U2431	U	G	C1996	U1999	G1558	U1391	G1135
G2692	G2692	C2435	A	A	A1999	A1802	C1589	A1398	
C2710	C2710	C2453	C	C	G2001	U1807	G1563	G1139	G1140
U2718	A2718	A2454	U	U	U2020	G1810	C1564	A1141	A1141
C2720	G2719	G2457	G	G	G2021	C1811	U1565	A1142	U1143
G2743	C2720	A2459	C	A	U2022	A1820	G1566	U1143	A1144
U2755	G2743	A2464	A	A	A2052	A1829	C1577	A1157	G1158
A2762	C2747	C2470	C	C	A2060	G1830	A	G1158	U1159
C2763	G2475	G2267	G	C	G2061	A1831	A	U1159	G1160
G2764	G2476	G2268	G	G	U2062	A1845	A	A1174	
G2773	C2476	G2280	A	A	G2064	A1858	U	G1177	U1178
A2777	A2477	A2297	C	C	C2072	C2079	G	A1179	A1180
	U2486	G2308	C	C	A2080		A	C1465	C1181

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3770	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: G7M, PSU, H2U, K, 2MA, 2MG, OMG, 5MU

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	0.62	0/1648	1.10	3/2564 (0.1%)
1	c	0.62	0/1577	1.03	1/2456 (0.0%)
2	0	0.43	0/425	0.75	0/563
3	1	0.42	0/416	0.83	0/551
4	2	0.51	0/371	0.84	0/483
5	3	0.44	0/519	0.76	0/680
6	4	0.42	0/300	0.77	0/393
7	6	0.40	0/363	0.56	0/485
8	B	0.57	0/2675	1.04	4/4170 (0.1%)
9	C	0.42	0/2131	0.77	0/2859
10	D	0.42	0/1597	0.76	0/2140
11	E	0.36	0/1586	0.70	0/2139
12	F	0.38	0/1424	0.64	0/1910
13	G	0.39	0/1360	0.66	0/1832
14	J	0.45	0/1154	0.72	0/1552
15	K	0.41	0/928	0.76	0/1245
16	L	0.41	0/1094	0.70	0/1457
17	M	0.41	0/1099	0.78	1/1468 (0.1%)
18	N	0.38	0/961	0.73	0/1284
19	O	0.38	0/922	0.71	0/1236
20	P	0.38	0/935	0.73	0/1251
21	Q	0.41	0/962	0.77	1/1277 (0.1%)
22	R	0.39	0/806	0.71	0/1080
23	S	0.39	0/859	0.75	1/1156 (0.1%)
24	T	0.42	0/739	0.78	0/985
25	U	0.38	0/780	0.68	0/1043
26	V	0.39	0/2016	0.67	0/2709
27	W	0.45	0/619	0.77	0/824
28	X	0.39	0/472	0.71	0/627
29	Y	0.35	0/531	0.71	0/707
30	Z	0.38	0/458	0.77	0/613
31	H	0.34	0/2564	0.50	0/3569

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	A	0.61	0/66810	1.00	34/104210 (0.0%)
All	All	0.56	0/101101	0.94	45/151518 (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
9	C	0	1
20	P	0	1
23	S	0	1
All	All	0	3

There are no bond length outliers.

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	1177	G	O3'-P-O5'	-6.51	91.62	104.00
32	A	207	A	O3'-P-O5'	-6.28	92.08	104.00
1	a	51	C	C2'-C3'-O3'	6.24	123.69	113.70
32	A	795	G	C1'-O4'-C4'	-6.07	105.04	109.90
32	A	2080	A	O3'-P-O5'	-6.01	92.58	104.00
32	A	1398	A	O3'-P-O5'	-5.91	92.77	104.00
32	A	2347	G	O3'-P-O5'	-5.91	92.78	104.00
8	B	86	U	O3'-P-O5'	-5.89	92.81	104.00
32	A	721	G	O3'-P-O5'	-5.83	92.92	104.00
32	A	1417	A	O3'-P-O5'	-5.81	92.95	104.00
1	a	71	C	O3'-P-O5'	-5.71	93.16	104.00
23	S	11	ARG	CG-CD-NE	-5.69	99.85	111.80
32	A	2476	G	OP1-P-O3'	5.68	117.69	105.20
32	A	1810	G	O3'-P-O5'	-5.66	93.25	104.00
32	A	786	A	O3'-P-O5'	-5.65	93.27	104.00
32	A	2090	G	O3'-P-O5'	-5.57	93.41	104.00
32	A	988	G	OP2-P-O3'	5.55	117.42	105.20
32	A	1363	G	O3'-P-O5'	-5.55	93.46	104.00
32	A	2643	A	O3'-P-O5'	-5.52	93.51	104.00
32	A	2710	C	O3'-P-O5'	-5.48	93.58	104.00
32	A	2382	G	O3'-P-O5'	-5.45	93.64	104.00
32	A	1965	A	C1'-O4'-C4'	-5.43	105.56	109.90
8	B	48	G	C2'-C3'-O3'	5.43	122.38	113.70
32	A	2079	C	O3'-P-O5'	-5.42	93.70	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	2616	A	OP2-P-O3'	5.41	117.11	105.20
32	A	872	C	OP1-P-O3'	5.34	116.96	105.20
32	A	2340	A	O3'-P-O5'	-5.33	93.87	104.00
32	A	834	C	O5'-P-OP1	5.32	117.08	110.70
17	M	126	PRO	N-CA-CB	-5.29	96.78	102.60
1	a	53	G	O3'-P-O5'	-5.28	93.98	104.00
1	c	58	A	O3'-P-O5'	-5.21	94.10	104.00
32	A	2844	A	O3'-P-O5'	-5.21	94.10	104.00
8	B	68	C	O3'-P-O5'	-5.18	94.15	104.00
32	A	72	U	C3'-C2'-C1'	-5.18	97.36	101.50
32	A	1807	U	O3'-P-O5'	-5.16	94.20	104.00
32	A	2383	A	O3'-P-O5'	-5.15	94.21	104.00
32	A	498	U	C1'-O4'-C4'	-5.11	105.81	109.90
32	A	723	A	O3'-P-O5'	-5.11	94.30	104.00
21	Q	94	MET	CG-SD-CE	5.10	108.36	100.20
32	A	558	G	O4'-C1'-N9	5.10	112.28	108.20
32	A	1367	G	O3'-P-O5'	-5.09	94.33	104.00
8	B	13	A	C3'-C2'-C1'	-5.05	97.46	101.50
32	A	1934	C	O3'-P-O5'	-5.05	94.41	104.00
32	A	1525	G	C2'-C3'-O3'	5.03	121.74	113.70
32	A	505	G	C3'-C2'-C1'	-5.00	97.50	101.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	C	80	THR	Peptide
20	P	26	LEU	Peptide
23	S	11	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	0	51/59 (86%)	44 (86%)	6 (12%)	1 (2%)	6	25
3	1	47/49 (96%)	42 (89%)	4 (8%)	1 (2%)	5	24
4	2	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
5	3	62/66 (94%)	56 (90%)	6 (10%)	0	100	100
6	4	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
7	6	44/66 (67%)	44 (100%)	0	0	100	100
9	C	271/277 (98%)	254 (94%)	16 (6%)	1 (0%)	30	60
10	D	205/209 (98%)	187 (91%)	17 (8%)	1 (0%)	25	54
11	E	204/207 (99%)	193 (95%)	11 (5%)	0	100	100
12	F	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
13	G	173/179 (97%)	168 (97%)	5 (3%)	0	100	100
14	J	141/145 (97%)	139 (99%)	2 (1%)	0	100	100
15	K	120/122 (98%)	106 (88%)	13 (11%)	1 (1%)	16	44
16	L	144/146 (99%)	133 (92%)	10 (7%)	1 (1%)	19	47
17	M	133/144 (92%)	120 (90%)	13 (10%)	0	100	100
18	N	117/120 (98%)	108 (92%)	9 (8%)	0	100	100
19	O	118/120 (98%)	113 (96%)	5 (4%)	0	100	100
20	P	111/115 (96%)	104 (94%)	7 (6%)	0	100	100
21	Q	116/119 (98%)	108 (93%)	8 (7%)	0	100	100
22	R	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
23	S	108/113 (96%)	105 (97%)	3 (3%)	0	100	100
24	T	89/95 (94%)	85 (96%)	4 (4%)	0	100	100
25	U	100/103 (97%)	91 (91%)	9 (9%)	0	100	100
26	V	243/275 (88%)	225 (93%)	14 (6%)	4 (2%)	8	29
27	W	78/94 (83%)	73 (94%)	5 (6%)	0	100	100
28	X	59/62 (95%)	54 (92%)	3 (5%)	2 (3%)	3	17
29	Y	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
30	Z	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
31	H	512/570 (90%)	502 (98%)	10 (2%)	0	100	100
All	All	3718/3942 (94%)	3513 (94%)	193 (5%)	12 (0%)	38	66

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	222	GLY
10	D	73	GLU
26	V	37	PHE
26	V	65	ARG
2	0	32	SER
26	V	67	GLU
3	1	11	GLU
16	L	29	LYS
28	X	3	ARG
15	K	91	LYS
26	V	75	PRO
28	X	59	VAL

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	
2	0	47/53 (89%)	47 (100%)	0	100	100
3	1	47/47 (100%)	46 (98%)	1 (2%)	48	69
4	2	39/39 (100%)	39 (100%)	0	100	100
5	3	54/56 (96%)	53 (98%)	1 (2%)	52	71
6	4	35/35 (100%)	35 (100%)	0	100	100
7	6	39/55 (71%)	38 (97%)	1 (3%)	41	64
9	C	221/225 (98%)	213 (96%)	8 (4%)	30	56
10	D	168/170 (99%)	165 (98%)	3 (2%)	54	73
11	E	169/170 (99%)	167 (99%)	2 (1%)	67	80
12	F	153/154 (99%)	152 (99%)	1 (1%)	81	88
13	G	148/151 (98%)	146 (99%)	2 (1%)	62	77
14	J	121/123 (98%)	120 (99%)	1 (1%)	79	87
15	K	101/101 (100%)	99 (98%)	2 (2%)	50	70
16	L	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	M	109/116 (94%)	106 (97%)	3 (3%)	38	62
18	N	99/100 (99%)	96 (97%)	3 (3%)	36	61
19	O	93/93 (100%)	93 (100%)	0	100	100
20	P	98/100 (98%)	95 (97%)	3 (3%)	35	60
21	Q	97/98 (99%)	95 (98%)	2 (2%)	48	69
22	R	84/84 (100%)	84 (100%)	0	100	100
23	S	91/93 (98%)	88 (97%)	3 (3%)	33	58
24	T	82/85 (96%)	82 (100%)	0	100	100
25	U	86/87 (99%)	84 (98%)	2 (2%)	45	67
26	V	215/234 (92%)	215 (100%)	0	100	100
27	W	61/74 (82%)	60 (98%)	1 (2%)	58	75
28	X	49/50 (98%)	49 (100%)	0	100	100
29	Y	56/57 (98%)	56 (100%)	0	100	100
30	Z	52/53 (98%)	50 (96%)	2 (4%)	28	54
All	All	2724/2813 (97%)	2683 (98%)	41 (2%)	60	76

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1	43	THR
5	3	31	HIS
7	6	26	SER
9	C	8	PRO
9	C	10	SER
9	C	18	THR
9	C	61	GLN
9	C	87	ARG
9	C	199	GLN
9	C	211	SER
9	C	214	LYS
10	D	129	SER
10	D	143	PRO
10	D	191	ASN
11	E	55	SER
11	E	116	SER
12	F	79	LEU
13	G	19	LEU

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Mol	Chain	Res	Type
13	G	172	ARG
14	J	132	PRO
15	K	89	ASP
15	K	90	ASP
17	M	3	LEU
17	M	7	VAL
17	M	126	PRO
18	N	35	THR
18	N	78	ASP
18	N	104	LEU
20	P	24	ASP
20	P	80	LYS
20	P	102	GLU
21	Q	15	LYS
21	Q	34	VAL
23	S	77	ASP
23	S	82	LEU
23	S	102	HIS
25	U	16	ASP
25	U	31	ASP
27	W	72	ASP
30	Z	51	SER
30	Z	58	GLU

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

Mol	Chain	Res	Type
2	0	40	HIS
5	3	31	HIS
5	3	35	ASN
5	3	60	GLN
9	C	194	GLN
10	D	126	HIS
11	E	49	HIS
14	J	136	GLN
15	K	3	GLN
15	K	4	GLN
15	K	110	ASN
23	S	73	GLN
24	T	58	ASN
25	U	99	GLN
26	V	7	HIS

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Mol	Chain	Res	Type
26	V	52	GLN
26	V	204	ASN
28	X	17	ASN
28	X	23	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	66/76 (86%)	29 (43%)	0
1	c	64/76 (84%)	24 (37%)	0
32	A	2778/2928 (94%)	372 (13%)	53 (1%)
8	B	111/112 (99%)	24 (21%)	5 (4%)
All	All	3019/3192 (94%)	449 (14%)	58 (1%)

All (449) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	c	3	G
1	c	6	C
1	c	9	A
1	c	16	C
1	c	17	U
1	c	18	G
1	c	19	G
1	c	20	G
1	c	21	A
1	c	28	C
1	c	41	A
1	c	44	A
1	c	45	G
1	c	46	G
1	c	48	C
1	c	53	G
1	c	55	U
1	c	57	G
1	c	61	C
1	c	65	U
1	c	66	A
1	c	67	G
1	c	70	U
1	c	72	C

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Mol	Chain	Res	Type
8	B	10	G
8	B	11	A
8	B	12	U
8	B	13	A
8	B	19	G
8	B	23	U
8	B	32	U
8	B	33	U
8	B	38	U
8	B	40	C
8	B	43	A
8	B	48	G
8	B	49	G
8	B	50	A
8	B	53	U
8	B	54	U
8	B	55	A
8	B	87	U
8	B	88	C
8	B	95	U
8	B	97	A
8	B	103	G
8	B	107	G
8	B	108	C
1	a	3	G
1	a	6	C
1	a	7	U
1	a	8	U
1	a	9	A
1	a	20	G
1	a	22	G
1	a	23	A
1	a	28	C
1	a	31	C
1	a	32	U
1	a	39	G
1	a	40	C
1	a	41	A
1	a	44	A
1	a	47	U
1	a	48	C
1	a	49	A

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Mol	Chain	Res	Type
1	a	52	G
1	a	53	G
1	a	54	U
1	a	57	G
1	a	61	C
1	a	62	C
1	a	65	U
1	a	66	A
1	a	67	G
1	a	72	C
1	a	76	A
32	A	12	A
32	A	13	A
32	A	15	G
32	A	34	U
32	A	45	G
32	A	46	C
32	A	60	G
32	A	63	G
32	A	71	A
32	A	74	U
32	A	75	G
32	A	89	U
32	A	90	A
32	A	93	C
32	A	117	A
32	A	118	A
32	A	119	U
32	A	164	U
32	A	166	A
32	A	175	G
32	A	176	A
32	A	177	G
32	A	183	A
32	A	184	G
32	A	199	A
32	A	202	A
32	A	203	U
32	A	216	A
32	A	219	A
32	A	224	A
32	A	225	A

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Mol	Chain	Res	Type
32	A	232	U
32	A	233	G
32	A	236	A
32	A	248	G
32	A	251	G
32	A	258	A
32	A	283	G
32	A	284	C
32	A	285	U
32	A	286	U
32	A	300	G
32	A	301	U
32	A	302	A
32	A	307	A
32	A	309	U
32	A	310	C
32	A	314	A
32	A	321	U
32	A	324	A
32	A	346	G
32	A	355	A
32	A	360	C
32	A	368	G
32	A	373	A
32	A	374	A
32	A	405	U
32	A	410	G
32	A	411	G
32	A	412	A
32	A	418	A
32	A	419	G
32	A	430	C
32	A	433	G
32	A	458	G
32	A	459	A
32	A	467	C
32	A	471	G
32	A	487	G
32	A	498	U
32	A	503	C
32	A	504	A
32	A	528	G

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Mol	Chain	Res	Type
32	A	540	G
32	A	551	A
32	A	568	G
32	A	576	G
32	A	577	U
32	A	578	A
32	A	579	G
32	A	584	A
32	A	595	G
32	A	600	A
32	A	607	G
32	A	617	G
32	A	619	A
32	A	630	A
32	A	631	G
32	A	647	A
32	A	658	A
32	A	659	A
32	A	673	A
32	A	680	G
32	A	683	A
32	A	691	U
32	A	692	A
32	A	733	U
32	A	777	C
32	A	794	5MU
32	A	811	A
32	A	812	G
32	A	822	G
32	A	829	A
32	A	831	U
32	A	832	G
32	A	837	U
32	A	838	C
32	A	852	G
32	A	859	C
32	A	874	U
32	A	875	U
32	A	892	U
32	A	906	G
32	A	913	A
32	A	943	A

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Mol	Chain	Res	Type
32	A	944	C
32	A	947	A
32	A	952	A
32	A	957	A
32	A	961	C
32	A	962	C
32	A	964	A
32	A	973	G
32	A	987	A
32	A	991	A
32	A	992	G
32	A	1004	U
32	A	1005	A
32	A	1007	G
32	A	1020	A
32	A	1029	A
32	A	1030	G
32	A	1031	C
32	A	1042	A
32	A	1058	U
32	A	1059	A
32	A	1068	G
32	A	1072	A
32	A	1079	U
32	A	1091	U
32	A	1092	A
32	A	1093	G
32	A	1096	A
32	A	1102	G
32	A	1104	U
32	A	1105	G
32	A	1107	U
32	A	1108	G
32	A	1110	C
32	A	1112	U
32	A	1113	A
32	A	1114	G
32	A	1115	A
32	A	1116	A
32	A	1119	A
32	A	1123	A
32	A	1124	C

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Mol	Chain	Res	Type
32	A	1127	U
32	A	1128	U
32	A	1129	U
32	A	1131	A
32	A	1135	G
32	A	1139	G
32	A	1140	U
32	A	1141	A
32	A	1142	A
32	A	1143	U
32	A	1144	A
32	A	1157	A
32	A	1158	G
32	A	1159	U
32	A	1160	G
32	A	1174	A
32	A	1178	U
32	A	1179	A
32	A	1180	C
32	A	1181	C
32	A	1182	G
32	A	1188	A
32	A	1260	A
32	A	1293	A
32	A	1296	G
32	A	1311	G
32	A	1312	A
32	A	1315	G
32	A	1339	A
32	A	1340	A
32	A	1341	U
32	A	1342	G
32	A	1360	A
32	A	1364	C
32	A	1377	G
32	A	1388	A
32	A	1389	C
32	A	1391	U
32	A	1404	A
32	A	1418	U
32	A	1423	A
32	A	1435	U

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Mol	Chain	Res	Type
32	A	1450	C
32	A	1457	U
32	A	1458	U
32	A	1459	U
32	A	1460	G
32	A	1465	A
32	A	1473	A
32	A	1474	C
32	A	1489	U
32	A	1490	A
32	A	1499	A
32	A	1500	U
32	A	1505	U
32	A	1507	U
32	A	1508	C
32	A	1514	C
32	A	1525	G
32	A	1526	G
32	A	1527	C
32	A	1528	U
32	A	1529	G
32	A	1531	G
32	A	1536	A
32	A	1540	A
32	A	1544	C
32	A	1556	A
32	A	1557	G
32	A	1558	G
32	A	1559	C
32	A	1560	U
32	A	1563	G
32	A	1566	G
32	A	1595	U
32	A	1607	C
32	A	1614	A
32	A	1617	A
32	A	1626	U
32	A	1631	A
32	A	1632	G
32	A	1637	G
32	A	1653	A
32	A	1654	A

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Mol	Chain	Res	Type
32	A	1691	A
32	A	1693	C
32	A	1719	G
32	A	1752	G
32	A	1757	G
32	A	1768	A
32	A	1776	A
32	A	1792	G
32	A	1793	G
32	A	1802	A
32	A	1811	C
32	A	1820	A
32	A	1829	C
32	A	1830	G
32	A	1831	A
32	A	1845	A
32	A	1858	A
32	A	1867	C
32	A	1877	A
32	A	1899	U
32	A	1900	A
32	A	1901	A
32	A	1911	C
32	A	1935	G
32	A	1936	G
32	A	1958	G
32	A	1959	G
32	A	1966	A
32	A	1967	A
32	A	1984	U
32	A	1992	C
32	A	1994	C
32	A	1996	C
32	A	1999	A
32	A	2000	A
32	A	2001	G
32	A	2020	U
32	A	2022	U
32	A	2052	A
32	A	2060	A
32	A	2061	G
32	A	2062	A

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Mol	Chain	Res	Type
32	A	2072	C
32	A	2084	C
32	A	2085	G
32	A	2089	A
32	A	2090	G
32	A	2098	G
32	A	2099	G
32	A	2122	G
32	A	2124	A
32	A	2128	U
32	A	2132	A
32	A	2227	A
32	A	2232	G
32	A	2233	C
32	A	2240	U
32	A	2241	A
32	A	2254	A
32	A	2267	G
32	A	2268	G
32	A	2297	A
32	A	2308	G
32	A	2312	C
32	A	2316	A
32	A	2334	U
32	A	2338	A
32	A	2341	U
32	A	2342	C
32	A	2348	C
32	A	2349	A
32	A	2350	G
32	A	2351	A
32	A	2356	A
32	A	2362	A
32	A	2363	C
32	A	2364	A
32	A	2376	C
32	A	2379	C
32	A	2408	G
32	A	2412	G
32	A	2414	C
32	A	2431	U
32	A	2435	C

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Mol	Chain	Res	Type
32	A	2453	C
32	A	2454	A
32	A	2457	G
32	A	2458	G
32	A	2459	A
32	A	2464	A
32	A	2470	C
32	A	2477	A
32	A	2503	C
32	A	2505	A
32	A	2531	G
32	A	2534	G
32	A	2547	A
32	A	2558	G
32	A	2559	U
32	A	2563	C
32	A	2577	G
32	A	2583	U
32	A	2595	A
32	A	2596	G
32	A	2602	C
32	A	2607	G
32	A	2631	A
32	A	2632	G
32	A	2638	U
32	A	2642	U
32	A	2692	G
32	A	2718	U
32	A	2720	C
32	A	2743	G
32	A	2755	U
32	A	2762	A
32	A	2763	C
32	A	2764	G
32	A	2773	G
32	A	2777	A
32	A	2794	A
32	A	2807	A
32	A	2823	C
32	A	2824	G
32	A	2833	U
32	A	2860	A

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Mol	Chain	Res	Type
32	A	2886	C
32	A	2892	G
32	A	2897	G
32	A	2908	A
32	A	2918	G

All (58) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	B	32	U
8	B	37	A
8	B	48	G
8	B	49	G
8	B	107	G
32	A	12	A
32	A	92	G
32	A	118	A
32	A	175	G
32	A	183	A
32	A	202	A
32	A	224	A
32	A	389	A
32	A	558	G
32	A	599	G
32	A	615	U
32	A	691	U
32	A	702	A
32	A	732	A
32	A	811	A
32	A	831	U
32	A	837	U
32	A	913	A
32	A	990	C
32	A	1004	U
32	A	1030	G
32	A	1111	U
32	A	1179	A
32	A	1339	A
32	A	1364	C
32	A	1507	U
32	A	1525	G
32	A	1527	C

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Mol	Chain	Res	Type
32	A	1530	G
32	A	1535	U
32	A	1536	A
32	A	1543	U
32	A	1558	G
32	A	1565	U
32	A	1602	U
32	A	1631	A
32	A	1652	C
32	A	1653	A
32	A	1692	U
32	A	1751	U
32	A	2064	G
32	A	2127	U
32	A	2311	G
32	A	2316	A
32	A	2348	C
32	A	2349	A
32	A	2362	A
32	A	2459	A
32	A	2558	G
32	A	2576	U
32	A	2631	A
32	A	2823	C
32	A	2892	G

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

12 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	PSU	A	1001	32	18,21,22	0.83	1 (5%)	22,30,33	0.72	0
32	5MU	A	794	32	19,22,23	0.28	0	28,32,35	0.33	0
32	OMG	A	2582	32	18,26,27	1.04	3 (16%)	19,38,41	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	5MU	A	620	33,32	19,22,23	0.36	0	28,32,35	0.66	2 (7%)
32	2MG	A	2474	32	18,26,27	1.17	3 (16%)	16,38,41	0.77	0
32	PSU	A	2533	33,32	18,21,22	1.00	1 (5%)	22,30,33	0.75	0
32	5MU	A	1968	32	19,22,23	0.49	0	28,32,35	0.47	0
32	2MA	A	2532	33,32	19,25,26	1.28	2 (10%)	21,37,40	1.93	4 (19%)
32	G7M	A	2603	32	20,26,27	0.99	1 (5%)	17,39,42	0.44	0
32	H2U	A	2478	32	18,21,22	0.66	0	21,30,33	0.74	0
32	OMG	A	2280	1,33,32	18,26,27	1.14	3 (16%)	19,38,41	0.80	0
32	PSU	A	2486	32	18,21,22	0.97	1 (5%)	22,30,33	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PSU	A	1001	32	-	0/7/25/26	0/2/2/2
32	5MU	A	794	32	-	0/7/25/26	0/2/2/2
32	OMG	A	2582	32	-	0/5/27/28	0/3/3/3
32	5MU	A	620	33,32	-	0/7/25/26	0/2/2/2
32	2MG	A	2474	32	-	0/5/27/28	0/3/3/3
32	PSU	A	2533	33,32	-	0/7/25/26	0/2/2/2
32	5MU	A	1968	32	-	0/7/25/26	0/2/2/2
32	2MA	A	2532	33,32	-	2/3/25/26	0/3/3/3
32	G7M	A	2603	32	-	0/3/25/26	0/3/3/3
32	H2U	A	2478	32	-	0/7/38/39	0/2/2/2
32	OMG	A	2280	1,33,32	-	0/5/27/28	0/3/3/3
32	PSU	A	2486	32	-	0/7/25/26	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	2533	PSU	C6-C5	3.82	1.39	1.35
32	A	2486	PSU	C6-C5	3.74	1.39	1.35
32	A	2532	2MA	C2-N1	3.27	1.39	1.34
32	A	2603	G7M	C8-N9	3.13	1.38	1.33
32	A	1001	PSU	C6-C5	3.11	1.38	1.35
32	A	2280	OMG	C5-C6	-3.04	1.41	1.47
32	A	2474	2MG	C5-C6	-2.77	1.41	1.47
32	A	2582	OMG	C5-C6	-2.72	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	2532	2MA	C6-N1	2.63	1.38	1.33
32	A	2280	OMG	C8-N7	-2.42	1.30	1.35
32	A	2474	2MG	C5-C4	-2.40	1.37	1.43
32	A	2474	2MG	C8-N7	-2.17	1.31	1.35
32	A	2582	OMG	C8-N7	-2.13	1.31	1.35
32	A	2280	OMG	C5-C4	-2.09	1.37	1.43
32	A	2582	OMG	C5-C4	-2.01	1.38	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	2532	2MA	C5-C6-N1	-5.92	117.12	121.01
32	A	2532	2MA	C5-C6-N6	4.05	126.50	120.35
32	A	2532	2MA	CM2-C2-N1	3.45	122.54	117.15
32	A	2532	2MA	N3-C2-N1	-2.60	120.98	125.73
32	A	620	5MU	O3'-C3'-C4'	-2.33	104.30	111.05
32	A	620	5MU	O3'-C3'-C2'	2.05	118.44	111.82

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	A	2532	2MA	C4'-C5'-O5'-P
32	A	2532	2MA	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 15 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.