



wwPDB X-ray Structure Validation Summary Report

Sep 15, 2014 – 06:30 PM EDT

PDB ID : 1VXQ
Title : Crystal Structure of tRNA Proline (CGG) Bound to Codon CCC-G on the Ribosome
Authors : Maehigashi, T.; Dunkle, J.A.; Dunham, C.M.
Deposited on : 2013-07-23
Resolution : 3.14 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.

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

A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

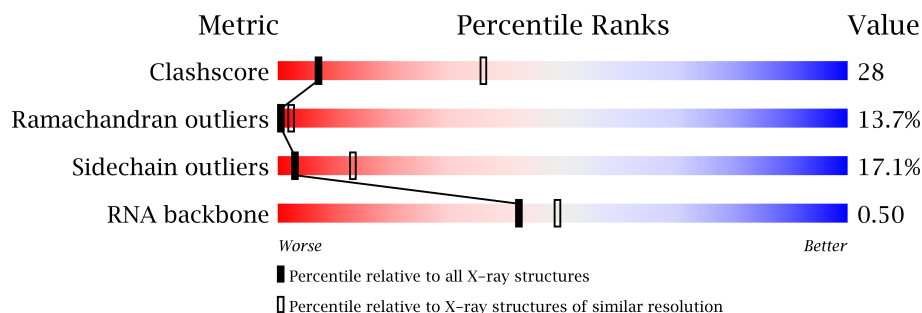
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23489

1 Overall quality at a glance

The reported resolution of this entry is 3.14 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	79885	1656 (3.20-3.08)
Ramachandran outliers	78287	1614 (3.20-3.08)
Sidechain outliers	78261	1613 (3.20-3.08)
RNA backbone	1838	1002 (3.66-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	2916	
2	B	122	
3	D	276	
4	E	206	
5	F	210	
6	G	182	
7	H	180	
8	I	148	
9	N	140	
10	O	122	
11	P	150	
12	Q	141	
13	R	118	
14	S	112	

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Mol	Chain	Length	Quality of chain
15	T	146	
16	U	118	
17	V	101	
18	W	113	
19	X	96	
20	Y	110	
21	Z	206	
22	0	85	
23	1	98	
24	2	72	
25	3	60	
26	4	71	
27	5	60	
28	6	54	
29	7	49	
30	8	65	
31	9	37	
32	a	3	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 92242 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2882	Total	C	N	O	P	0	0	0
			62071	27627	11611	19952	2881			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	P	0	0	0
			2573	1146	476	832	119			

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	272	Total	C	N	O	S	0	0	0
			2115	1335	420	357	3			

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	205	Total	C	N	O	S	0	0	0
			1568	991	300	271	6			

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	202	Total	C	N	O	S	0	0	0
			1585	1011	297	275	2			

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	181	Total	C	N	O	S	0	0	0
			1474	942	268	260	4			

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	170	Total	C	N	O	S	0	0	0
			1307	829	245	232	1			

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	146	Total	C	N	O	S	0	0	0
			1136	726	201	208	1			

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	N	138	Total	C	N	O	S	0	0	0
			1104	712	206	182	4			

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	O	122	Total	C	N	O	S	0	0	0
			933	588	171	170	4			

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	P	150	Total	C	N	O	S	0	0	0
			1145	712	232	198	3			

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	Q	141	Total	C	N	O	S	0	0	0
			1122	715	212	188	7			

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	118	Total	C	N	O	S	0	0	0
			968	604	203	160	1			

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
14	S	111	Total	C	N	O	0	0	0
			882	556	176	150			

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	T	137	Total	C	N	O	S	0	0	0
			1141	710	234	196	1			

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
16	U	117	Total	C	N	O	S	0	0	0
			964	610	202	151	1			

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
17	V	101	Total	C	N	O	S	0	0	0
			779	501	142	135	1			

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
18	W	113	Total	C	N	O	S	0	0	0
			900	566	177	155	2			

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
19	X	92	Total	C	N	O	0	0	0
			725	471	131	123			

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
20	Y	102	Total	C	N	O	S	0	0	0
			785	505	150	125	5			

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
21	Z	183	Total	C	N	O	S	0	0	0
			1461	933	260	265	3			

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
22	0	82	Total	C	N	O	S	0	0	0
			648	401	138	108	1			

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
23	1	97	Total	C	N	O	S	0	0	0
			763	481	150	131	1			

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
24	2	69	Total	C	N	O	S	0	0	0
			581	358	118	104	1			

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
25	3	59	Total	C	N	O	0	0	0
			469	298	90	81			

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
26	4	71	Total	C	N	O	S	0	0	0
			581	364	108	104	5			

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
27	5	59	Total	C	N	O	S	0	0	0
			459	288	90	76	5			

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
28	6	49	Total	C	N	O	S	0	0	0
			424	264	87	69	4			

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
29	7	49	Total	C	N	O	S	0	0	0
			430	263	108	57	2			

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
30	8	64	Total	C	N	O	S	0	0	0
			517	331	102	82	2			

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
31	9	37	Total	C	N	O	S	0	0	0
			307	188	68	47	4			

- Molecule 32 is a RNA chain called tRNA acceptor end mimic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
32	a	3	Total	C	N	O	P	0	0	0
			74	40	13	19	2			

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	P	1	Total	Mg	0	0
			1	1		
33	0	1	Total	Mg	0	0
			1	1		
33	D	1	Total	Mg	0	0
			1	1		
33	E	2	Total	Mg	0	0
			2	2		
33	B	2	Total	Mg	0	0
			2	2		
33	A	240	Total	Mg	0	0
			240	240		

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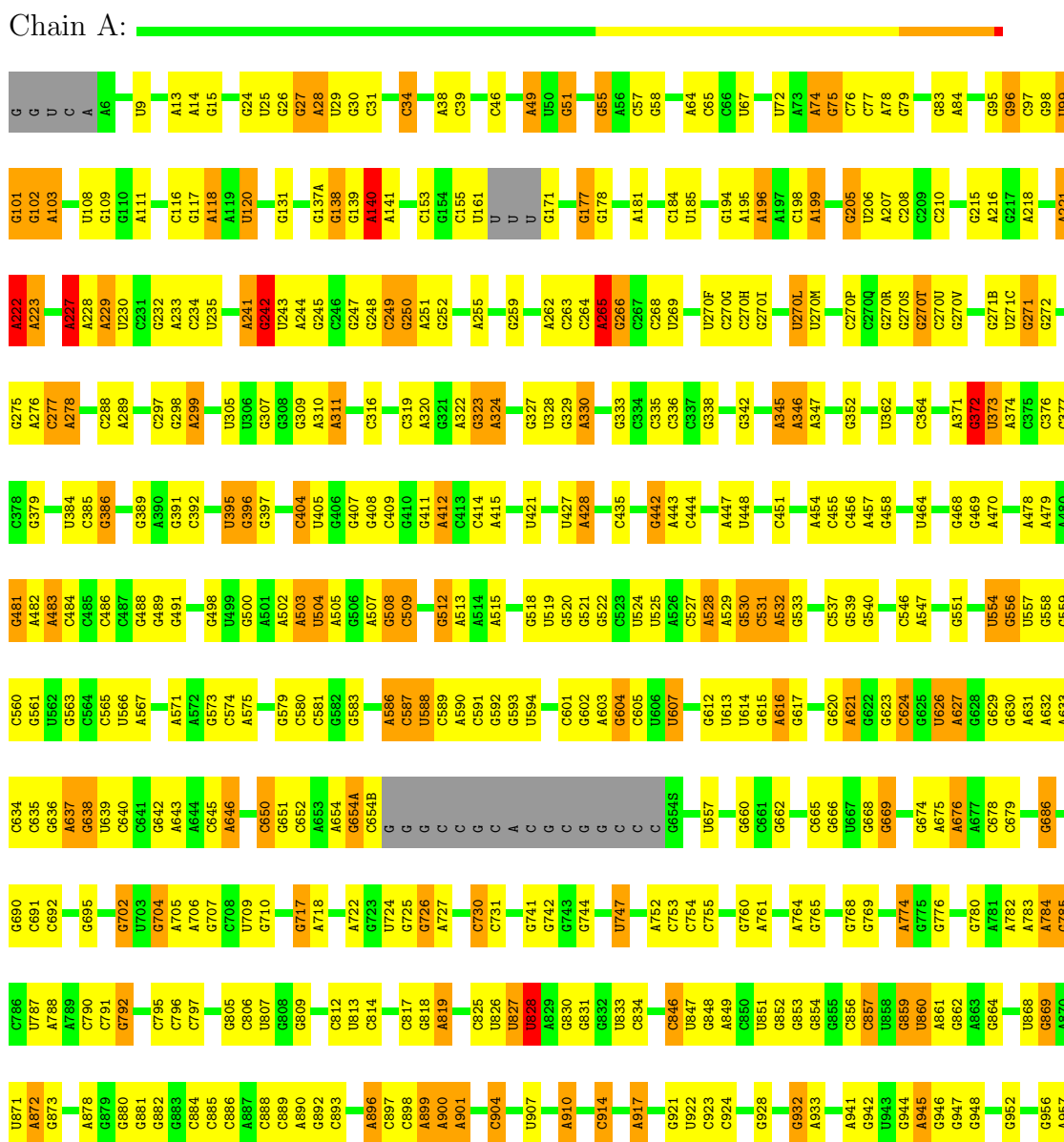
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
33	5	1	Total 1	Mg 1	0	0
33	R	2	Total 2	Mg 2	0	0
33	F	1	Total 1	Mg 1	0	0

3 Residue-property plots

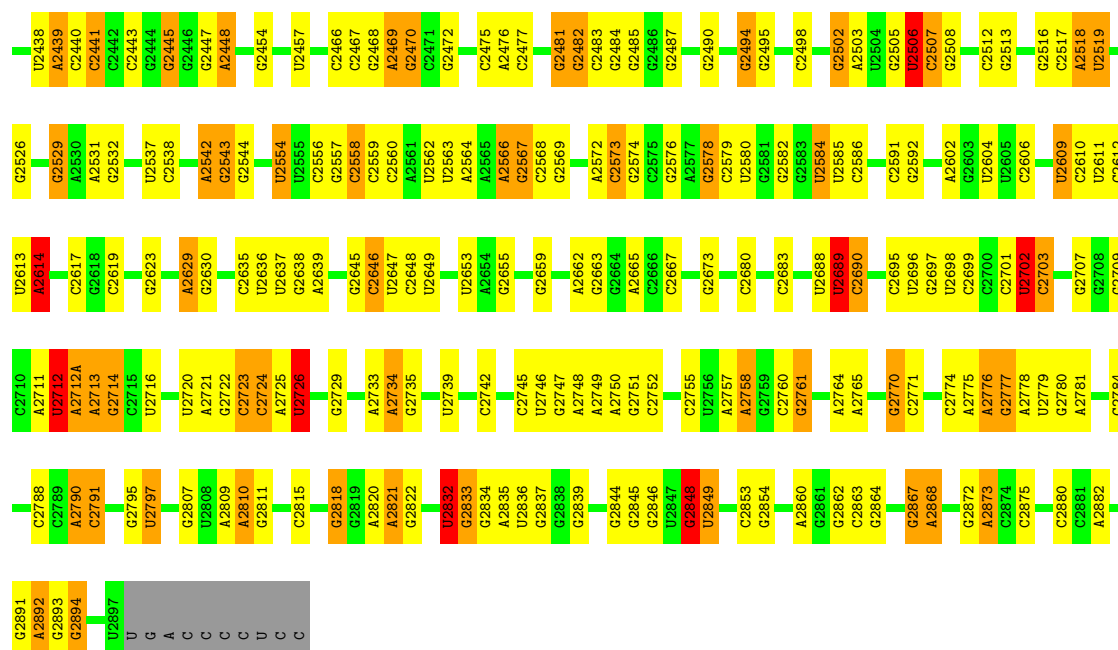
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

Note EDS was not executed.

• Molecule 1: 23S rRNA

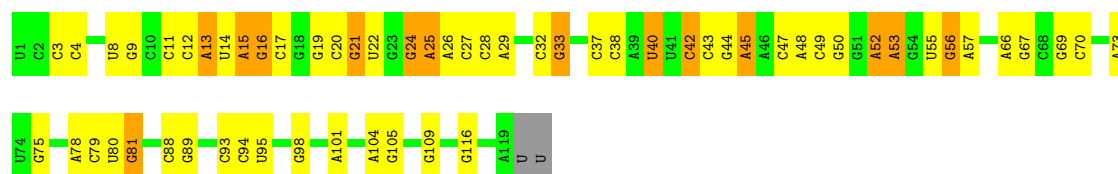






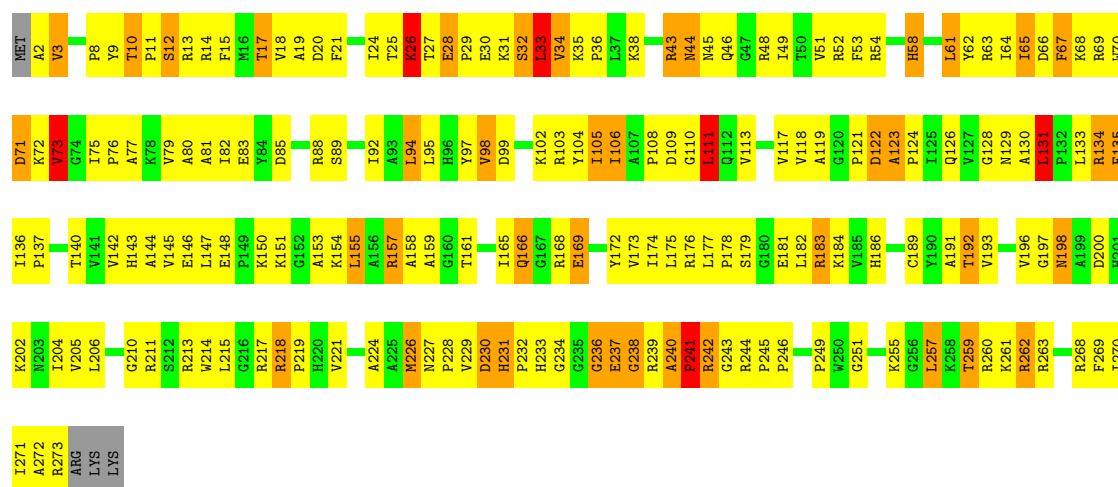
- Molecule 2: 5S rRNA

Chain B:



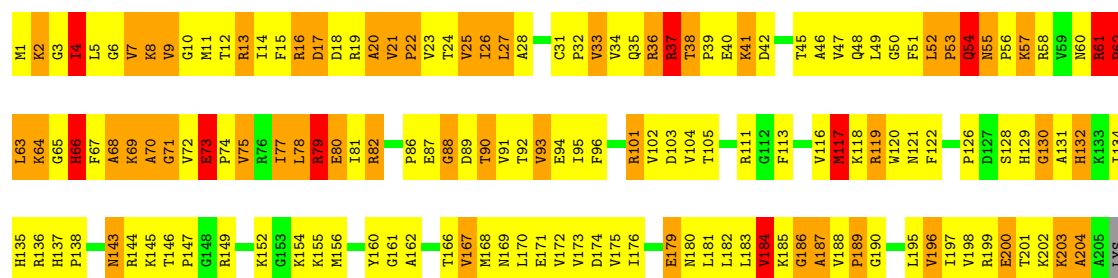
- Molecule 3: 50S ribosomal protein L2

Chain D:



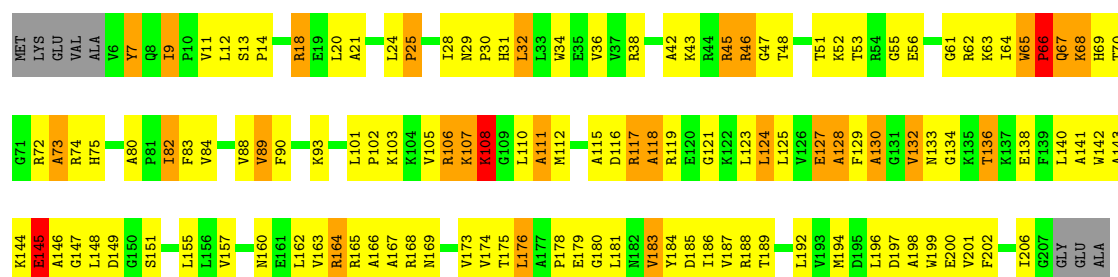
- Molecule 4: 50S ribosomal protein L3

Chain E:



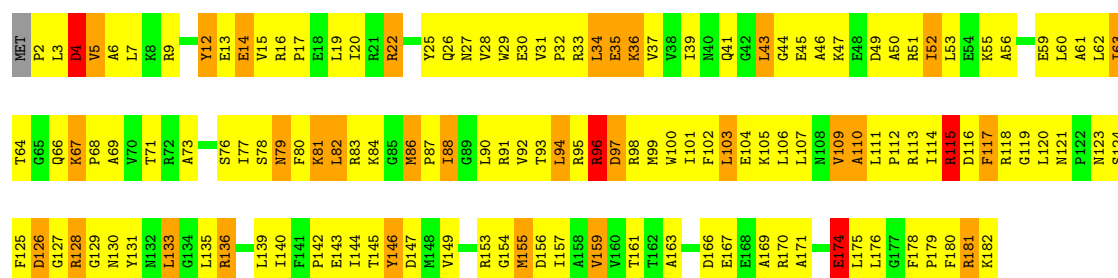
• Molecule 5: 50S ribosomal protein L4

Chain F:



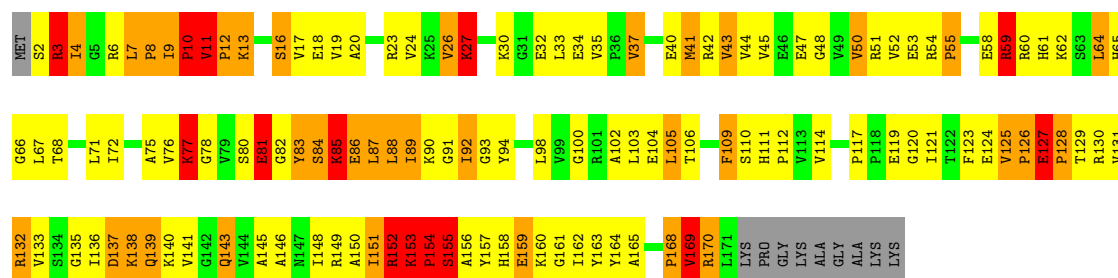
• Molecule 6: 50S ribosomal protein L5

Chain G:



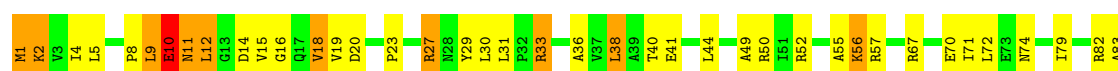
• Molecule 7: 50S ribosomal protein L6

Chain H:



• Molecule 8: 50S ribosomal protein L9

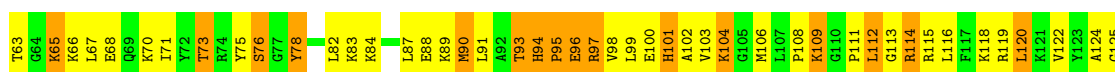
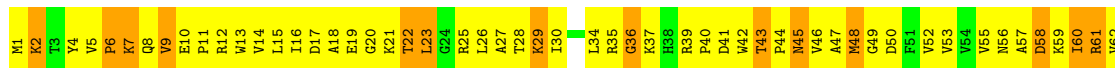
Chain I:





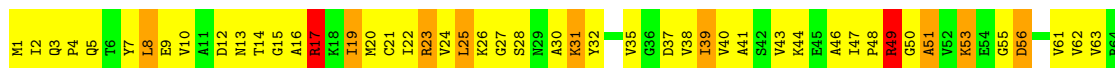
• Molecule 9: 50S ribosomal protein L11

Chain N:



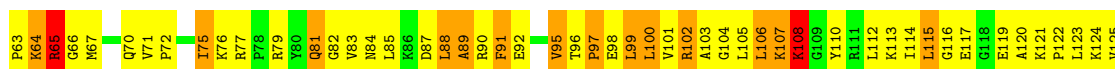
• Molecule 10: 50S ribosomal protein L13

Chain O:



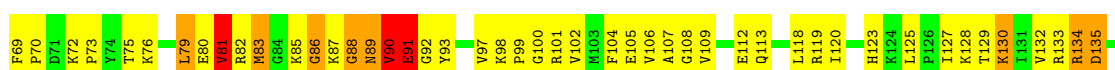
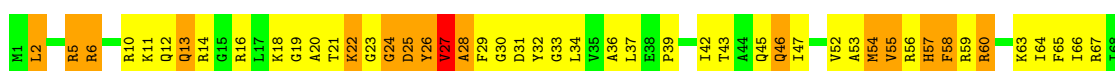
• Molecule 11: 50S ribosomal protein L14

Chain P:



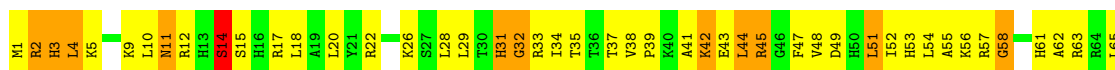
• Molecule 12: 50S ribosomal protein L15

Chain Q:



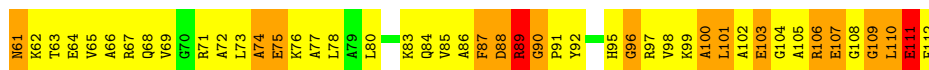
• Molecule 13: 50S ribosomal protein L16

Chain R:



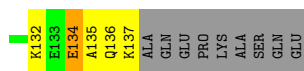
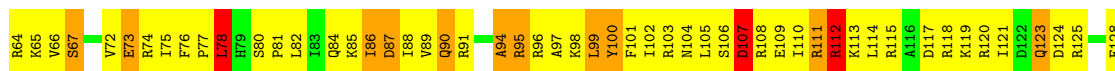
• Molecule 14: 50S ribosomal protein L17

Chain S:



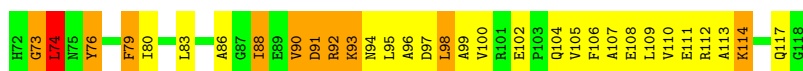
• Molecule 15: 50S ribosomal protein L18

Chain T:



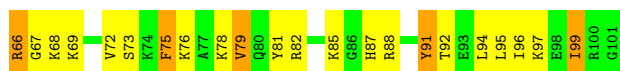
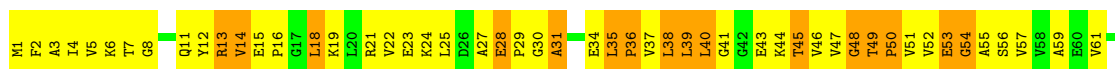
• Molecule 16: 50S ribosomal protein L19

Chain U:



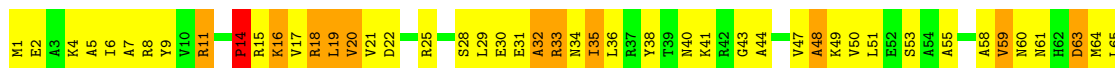
• Molecule 17: 50S ribosomal protein L20

Chain V:



• Molecule 18: 50S ribosomal protein L21

Chain W:





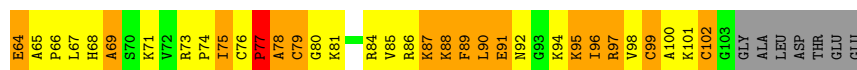
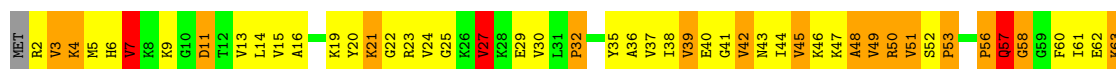
• Molecule 19: 50S ribosomal protein L22

Chain X:



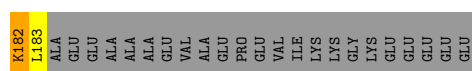
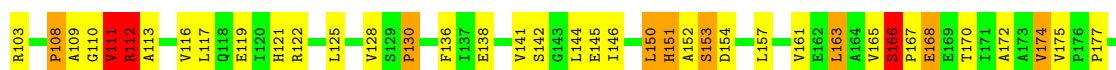
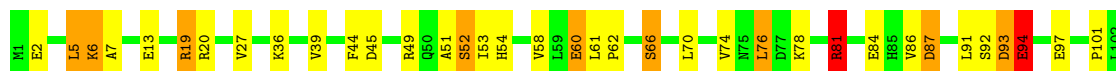
• Molecule 20: 50S ribosomal protein L23

Chain Y:



• Molecule 21: 50S ribosomal protein L24

Chain Z:



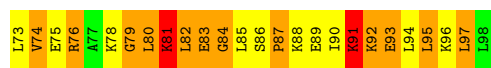
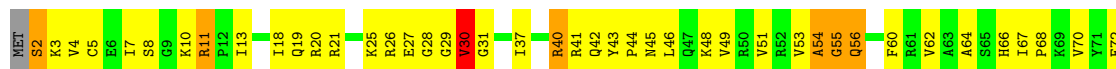
• Molecule 22: 50S ribosomal protein L25

Chain 0:



• Molecule 23: 50S ribosomal protein L27

Chain 1:



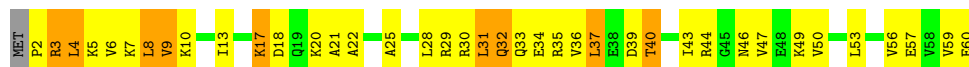
• Molecule 24: 50S ribosomal protein L28

Chain 2:



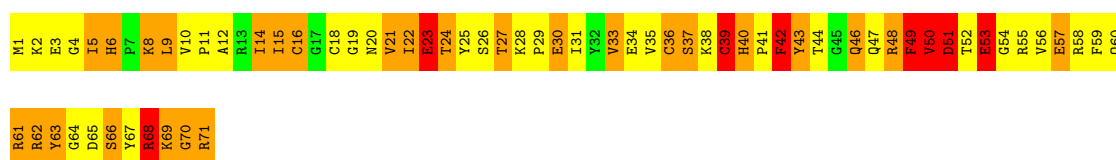
- Molecule 25: 50S ribosomal protein L29

Chain 3:



- Molecule 26: 50S ribosomal protein L30

Chain 4:



- Molecule 27: 50S ribosomal protein L32

Chain 5:



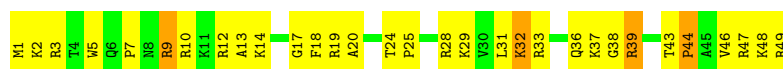
- Molecule 28: 50S ribosomal protein L33

Chain 6:



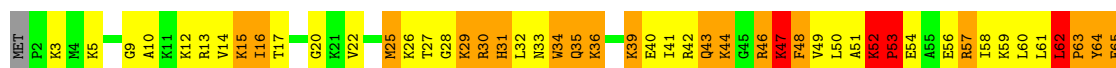
- Molecule 29: 50S ribosomal protein L34

Chain 7:



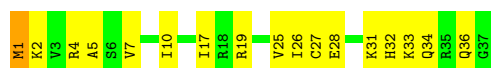
- Molecule 30: 50S ribosomal protein L35

Chain 8:



- Molecule 31: 50S ribosomal protein L36

Chain 9:



- Molecule 32: tRNA acceptor end mimic

Chain a: 

C74
C75
A76

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	209.21Å 448.45Å 619.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	189.60 – 3.14	Depositor
% Data completeness (in resolution range)	99.6 (189.60-3.14)	Depositor
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.230 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	92242	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.39	0/69521	0.88	70/108529 (0.1%)
2	B	0.32	0/2878	0.84	0/4490
3	D	0.60	2/2165 (0.1%)	0.90	4/2919 (0.1%)
4	E	0.52	0/1601	0.91	2/2160 (0.1%)
5	F	0.50	0/1620	0.76	0/2194
6	G	0.40	0/1499	0.66	0/2016
7	H	0.45	0/1332	0.85	3/1802 (0.2%)
8	I	0.28	0/1151	0.56	0/1558
9	N	0.46	0/1131	0.78	1/1525 (0.1%)
10	O	0.54	0/943	0.71	0/1269
11	P	0.50	0/1162	0.95	3/1544 (0.2%)
12	Q	0.54	0/1143	0.91	3/1527 (0.2%)
13	R	0.45	0/982	0.80	1/1312 (0.1%)
14	S	0.46	0/892	0.82	1/1187 (0.1%)
15	T	0.47	0/1155	0.73	2/1542 (0.1%)
16	U	0.48	0/982	0.78	0/1306
17	V	0.47	0/790	0.82	0/1057
18	W	0.45	0/911	0.75	0/1220
19	X	0.56	0/739	0.77	0/993
20	Y	0.52	0/798	0.80	0/1064
21	Z	0.27	0/1493	0.52	0/2026
22	0	0.30	0/657	0.54	0/874
23	1	0.49	0/770	0.85	1/1022 (0.1%)
24	2	0.51	0/583	0.83	1/771 (0.1%)
25	3	0.47	0/474	0.72	0/635
26	4	0.38	0/594	0.78	1/795 (0.1%)
27	5	0.51	0/473	0.74	0/639
28	6	0.42	0/431	0.76	0/575
29	7	0.56	0/438	0.76	0/575
30	8	0.62	0/525	0.93	1/691 (0.1%)
31	9	0.35	0/310	0.59	0/407
32	a	0.79	0/40	1.81	1/60 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.41	2/100183 (0.0%)	0.86	95/150284 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	236	GLY	C-N	8.57	1.53	1.34
3	D	241	PRO	N-CD	5.19	1.55	1.47

The worst 5 of 95 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	21	VAL	C-N-CD	-10.09	98.41	120.60
1	A	2506	U	N3-C2-O2	-9.83	115.32	122.20
1	A	2506	U	N1-C2-O2	8.71	128.90	122.80
12	Q	81	VAL	CB-CA-C	-8.63	94.99	111.40
1	A	2614	A	C6-N1-C2	-8.11	113.73	118.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	62071	0	31288	983	0
2	B	2573	0	1306	62	0
3	D	2115	0	2195	319	0
4	E	1568	0	1634	270	0
5	F	1585	0	1632	181	0
6	G	1474	0	1535	206	0
7	H	1307	0	1382	225	0
8	I	1136	0	1223	42	0
9	N	1104	0	1180	191	0
10	O	933	0	996	122	0
11	P	1145	0	1228	250	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	Q	1122	0	1179	159	0
13	R	968	0	1033	113	0
14	S	882	0	943	165	0
15	T	1141	0	1202	150	0
16	U	964	0	1022	131	0
17	V	779	0	852	129	0
18	W	900	0	964	99	0
19	X	725	0	778	69	0
20	Y	785	0	878	163	0
21	Z	1461	0	1493	46	0
22	0	648	0	672	20	0
23	1	763	0	848	146	0
24	2	581	0	629	81	0
25	3	469	0	518	41	0
26	4	581	0	574	132	0
27	5	459	0	480	77	0
28	6	424	0	450	92	0
29	7	430	0	480	43	0
30	8	517	0	582	106	0
31	9	307	0	338	18	0
32	a	74	0	51	0	0
33	0	1	0	0	0	0
33	5	1	0	0	0	0
33	A	240	0	0	0	0
33	B	2	0	0	0	0
33	D	1	0	0	0	0
33	E	2	0	0	0	0
33	F	1	0	0	0	0
33	P	1	0	0	0	0
33	R	2	0	0	0	0
All	All	92242	0	61565	4341	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 28.

The worst 5 of 4341 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
7:H:127:GLU:CG	7:H:128:PRO:HD3	1.35	1.53
23:1:81:LYS:NZ	23:1:81:LYS:HA	1.43	1.34
23:1:81:LYS:HE2	23:1:81:LYS:N	1.50	1.26
12:Q:59:ARG:O	12:Q:60:ARG:HD2	1.38	1.22
7:H:127:GLU:HG2	7:H:128:PRO:CD	1.69	1.20

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 X-ray entries followed by that with respect to entries of similar resolution.

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	
3	D	270/276 (98%)	203 (75%)	48 (18%)	19 (7%)	2	14
4	E	203/206 (98%)	120 (59%)	41 (20%)	42 (21%)	0	0
5	F	200/210 (95%)	144 (72%)	36 (18%)	20 (10%)	1	6
6	G	179/182 (98%)	119 (66%)	39 (22%)	21 (12%)	1	4
7	H	168/180 (93%)	94 (56%)	36 (21%)	38 (23%)	0	0
8	I	144/148 (97%)	102 (71%)	27 (19%)	15 (10%)	1	6
9	N	136/140 (97%)	84 (62%)	30 (22%)	22 (16%)	0	1
10	O	120/122 (98%)	90 (75%)	21 (18%)	9 (8%)	2	12
11	P	148/150 (99%)	97 (66%)	19 (13%)	32 (22%)	0	0
12	Q	139/141 (99%)	95 (68%)	30 (22%)	14 (10%)	1	6
13	R	116/118 (98%)	83 (72%)	19 (16%)	14 (12%)	1	4
14	S	109/112 (97%)	62 (57%)	28 (26%)	19 (17%)	0	0
15	T	135/146 (92%)	83 (62%)	32 (24%)	20 (15%)	0	2
16	U	115/118 (98%)	87 (76%)	19 (16%)	9 (8%)	1	11
17	V	99/101 (98%)	73 (74%)	16 (16%)	10 (10%)	1	6
18	W	111/113 (98%)	75 (68%)	22 (20%)	14 (13%)	0	3
19	X	90/96 (94%)	77 (86%)	8 (9%)	5 (6%)	3	22
20	Y	100/110 (91%)	58 (58%)	16 (16%)	26 (26%)	0	0
21	Z	181/206 (88%)	126 (70%)	35 (19%)	20 (11%)	1	5
22	0	80/85 (94%)	71 (89%)	7 (9%)	2 (2%)	9	47
23	1	95/98 (97%)	64 (67%)	20 (21%)	11 (12%)	1	4
24	2	67/72 (93%)	46 (69%)	12 (18%)	9 (13%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	3	57/60 (95%)	45 (79%)	9 (16%)	3 (5%)	3	24
26	4	69/71 (97%)	23 (33%)	20 (29%)	26 (38%)	0	0
27	5	57/60 (95%)	33 (58%)	9 (16%)	15 (26%)	0	0
28	6	47/54 (87%)	15 (32%)	18 (38%)	14 (30%)	0	0
29	7	47/49 (96%)	37 (79%)	7 (15%)	3 (6%)	2	17
30	8	62/65 (95%)	36 (58%)	15 (24%)	11 (18%)	0	0
31	9	35/37 (95%)	31 (89%)	4 (11%)	0	100	100
All	All	3379/3526 (96%)	2273 (67%)	643 (19%)	463 (14%)	0	2

5 of 463 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	D	26	LYS
3	D	28	GLU
3	D	123	ALA
3	D	231	HIS
4	E	4	ILE

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 X-ray entries followed by that with respect to entries of similar resolution. 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	
3	D	214/218 (98%)	177 (83%)	37 (17%)	3	13
4	E	165/166 (99%)	128 (78%)	37 (22%)	1	6
5	F	161/166 (97%)	140 (87%)	21 (13%)	6	26
6	G	155/156 (99%)	130 (84%)	25 (16%)	3	15
7	H	142/148 (96%)	114 (80%)	28 (20%)	2	9
8	I	122/124 (98%)	100 (82%)	22 (18%)	2	12
9	N	117/119 (98%)	98 (84%)	19 (16%)	3	15
10	O	100/100 (100%)	90 (90%)	10 (10%)	11	41
11	P	116/116 (100%)	89 (77%)	27 (23%)	1	5
12	Q	111/111 (100%)	93 (84%)	18 (16%)	3	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
13	R	101/101 (100%)	84 (83%)	17 (17%)	3	13
14	S	87/88 (99%)	74 (85%)	13 (15%)	4	19
15	T	120/127 (94%)	97 (81%)	23 (19%)	2	10
16	U	93/94 (99%)	80 (86%)	13 (14%)	5	23
17	V	82/82 (100%)	71 (87%)	11 (13%)	6	25
18	W	92/92 (100%)	77 (84%)	15 (16%)	3	15
19	X	74/78 (95%)	63 (85%)	11 (15%)	4	19
20	Y	85/91 (93%)	70 (82%)	15 (18%)	3	12
21	Z	162/179 (90%)	138 (85%)	24 (15%)	4	19
22	0	65/67 (97%)	58 (89%)	7 (11%)	9	37
23	1	82/83 (99%)	67 (82%)	15 (18%)	2	11
24	2	64/67 (96%)	57 (89%)	7 (11%)	9	37
25	3	51/52 (98%)	40 (78%)	11 (22%)	1	7
26	4	63/63 (100%)	44 (70%)	19 (30%)	0	1
27	5	51/52 (98%)	39 (76%)	12 (24%)	1	5
28	6	48/52 (92%)	38 (79%)	10 (21%)	2	8
29	7	42/42 (100%)	39 (93%)	3 (7%)	21	64
30	8	54/55 (98%)	39 (72%)	15 (28%)	0	1
31	9	34/34 (100%)	32 (94%)	2 (6%)	28	72
All	All	2853/2923 (98%)	2366 (83%)	487 (17%)	3	13

5 of 487 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	P	91	PHE
14	S	106	ARG
27	5	25	LEU
12	Q	2	LEU
13	R	44	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
12	Q	123	HIS

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Mol	Chain	Res	Type
15	T	58	ASN
25	3	19	GLN
13	R	3	HIS
16	U	81	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2879/2916 (98%)	618 (21%)	67 (2%)
2	B	119/122 (97%)	24 (20%)	2 (1%)
32	a	1/3 (33%)	0	0
All	All	2999/3041 (98%)	642 (21%)	69 (2%)

5 of 642 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	9	U
1	A	14	A
1	A	15	G
1	A	28	A
1	A	34	C

5 of 69 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1045	A
1	A	1210	A
1	A	2776	A
1	A	1078	U
1	A	1141	U

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

1 non-standard protein/DNA/RNA residue is 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	PPU	a	76	1,32	38,40,41	2.42	8 (21%)	54,57,60	2.62	14 (25%)

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	PPU	a	76	1,32	-	0/26/43/44	0/4/4/4

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	76	PPU	O-C	9.24	1.41	1.23
32	a	76	PPU	C9-N6	-5.44	1.32	1.45
32	a	76	PPU	C-N3'	5.41	1.46	1.34
32	a	76	PPU	C10-N6	-5.14	1.32	1.45
32	a	76	PPU	C4-N9	-3.07	1.33	1.37

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	a	76	PPU	N3-C2-N1	-8.46	121.45	128.89
32	a	76	PPU	C3'-N3'-C	-8.17	110.18	123.19
32	a	76	PPU	C5-C4-N3	-6.41	119.72	125.98
32	a	76	PPU	C2'-C1'-N9	-5.45	98.50	113.35
32	a	76	PPU	C2'-C3'-N3'	5.18	125.11	113.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 251 ligands modelled in this entry, 251 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.

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.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.