



Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 10:57 AM JST

PDB ID : 8I9R
EMDB ID : EMD-35281
Title : Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit
- State 5S RNP
Authors : Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2023-02-07
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**
Mogul : 1.8.5 (274361), 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) : 2.39

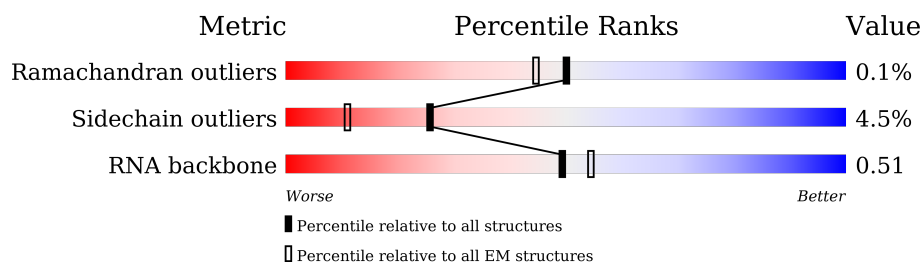
1 Overall quality at a glance

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.




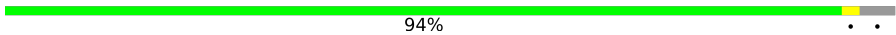
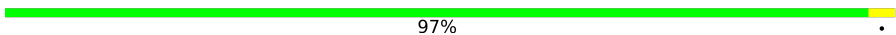








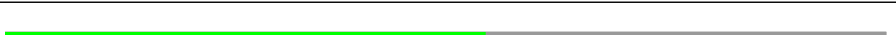

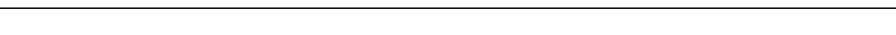
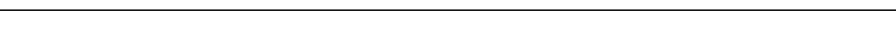
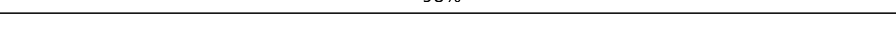

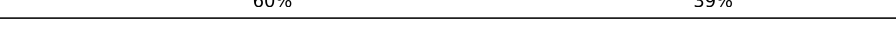
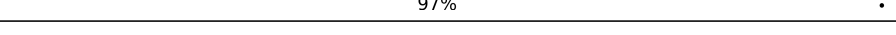

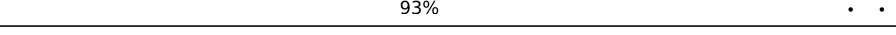
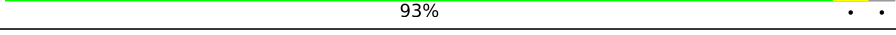
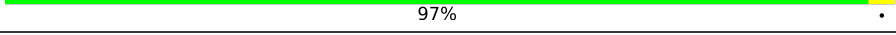
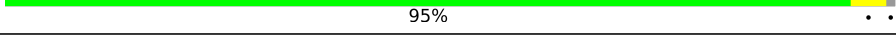

Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	C1	3341	
2	C2	256	
3	CA	316	
4	CB	391	
5	CC	801	
6	CE	598	
7	CH	661	
8	CI	414	
9	CJ	679	














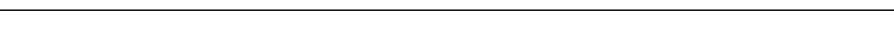
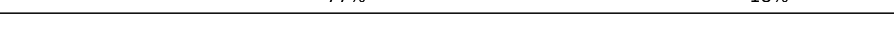
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Mol	Chain	Length	Quality of chain
10	CM	249	
10	LF	249	
11	CN	246	
12	CQ	225	
13	CR	237	
14	CU	451	
15	Ch	354	
16	LB	392	
17	LC	365	
18	LE	200	
19	LG	262	
20	LL	213	
21	LM	142	
22	LN	203	
23	LO	204	
24	LP	187	
25	LQ	213	
26	LS	174	
27	LT	160	
28	LV	139	
29	LY	138	
30	Le	131	
31	Lf	109	
32	Lh	935	
33	Li	110	

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Mol	Chain	Length	Quality of chain
34	Lj	95	 77% 22%
35	Cc	282	 80% 16%
36	Cd	436	 76% 20%
37	Ce	336	 56% 42%
38	Cf	570	 25% 74%
39	Cy	350	 70% 30%
40	Cg	478	 46% 51%
41	CP	751	 43% 57%
42	CG	184	 96%
43	Lq	217	 94% 5%
44	Cx	202	 50% 50%
45	LJ	173	 98%
46	LD	304	 90% 10%
47	C4	119	 77% 18%
48	CX	203	 31% 69%

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 117417 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 RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	2048	Total	C	N	O	P	0	0
			43814	19561	7931	14274	2048		

- Molecule 2 is a RNA chain called RNA (256-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	228	Total	C	N	O	P	0	0
			4846	2162	864	1592	228		

- Molecule 3 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CA	260	Total	C	N	O	S	0	0
			2144	1371	393	373	7		

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CB	260	Total	C	N	O	S	0	0
			2063	1322	367	371	3		

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CC	272	Total	C	N	O	S	0	0
			2258	1438	379	434	7		

- Molecule 6 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CE	463	Total	C	N	O	S	0	0
			3673	2352	643	667	11		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

- Molecule 7 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CH	108	Total	C	N	O	S	0	0
			891	561	146	183	1		

- Molecule 8 is a protein called Putative RNA-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CI	146	Total	C	N	O	S	0	0
			1196	763	224	204	5		

- Molecule 9 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CJ	380	Total	C	N	O	S	0	0
			3109	2003	547	549	10		

- Molecule 10 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CM	187	Total	C	N	O	S	0	0
			1525	987	278	257	3		
10	LF	240	Total	C	N	O	S	0	0
			1967	1264	368	332	3		

- Molecule 11 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CN	246	Total	C	N	O	S	0	0
			1856	1158	322	369	7		

- Molecule 12 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	CQ	112	Total	C	N	O	S	0	0
			960	607	195	148	10		

- Molecule 13 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 14 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	CU	121	Total	C	N	O	S	0	0
			969	604	179	183	3		

- Molecule 15 is a protein called Ribosomal RNA-processing protein 15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ch	71	Total	C	N	O	S	0	0
			562	350	109	102	1		

- Molecule 16 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LB	341	Total	C	N	O	S	0	0
			2708	1721	493	482	12		

- Molecule 17 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LC	362	Total	C	N	O	S	0	0
			2752	1738	526	479	9		

- Molecule 18 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LE	170	Total	C	N	O	S	0	0
			1338	861	241	233	3		

- Molecule 19 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LG	183	Total	C	N	O	S	0	0
			1470	951	263	252	4		

- Molecule 20 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LL	117	Total	C	N	O	S	0	0
			964	608	206	148	2		

- Molecule 21 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LM	137	Total	C	N	O	S	0	0
			1101	699	211	190	1		

- Molecule 22 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LN	183	Total	C	N	O	S	0	0
			1563	974	332	253	4		

- Molecule 23 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LO	204	Total	C	N	O	S	0	0
			1618	1039	306	267	6		

- Molecule 24 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LP	154	Total	C	N	O	S	0	0
			1212	758	233	218	3		

- Molecule 25 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LQ	129	Total	C	N	O	S	0	0
			1021	646	200	173	2		

- Molecule 26 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LS	174	Total	C	N	O	S	0	0
			1433	922	267	239	5		

- Molecule 27 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LT	126	Total	C	N	O	S	0	0
			1014	643	196	173	2		

- Molecule 28 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LV	135	Total	C	N	O	S	0	0
			995	633	185	170	7		

- Molecule 29 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LY	134	Total	C	N	O	S	0	0
			1065	664	215	184	2		

- Molecule 30 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Le	131	Total	C	N	O	S	0	0
			1055	663	213	172	7		

- Molecule 31 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 32 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Lh	121	Total	C	N	O	0	0
			995	633	196	166		

- Molecule 33 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Li	88	Total	C	N	O	S	0	0
			731	449	162	119	1		

- Molecule 34 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lj	74	Total	C	N	O	S	0	0
			595	365	132	93	5		

- Molecule 35 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Cc	236	Total	C	N	O	S	0	0
			1898	1208	337	343	10		

- Molecule 36 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Cd	347	Total	C	N	O	S	0	0
			2800	1764	538	494	4		

- Molecule 37 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Ce	194	Total	C	N	O	S	0	0
			1609	1020	304	276	9		

- Molecule 38 is a protein called 60S ribosome biogenesis protein Rrp14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Cf	147	Total	C	N	O	S	0	0
			1225	755	245	224	1		

- Molecule 39 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Cy	244	Total	C	N	O		0	0
			1210	722	244	244			

- Molecule 40 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Cg	233	Total	C	N	O	S	0	0
			1850	1168	348	324	10		

- Molecule 41 is a protein called RNA methyltransferase nop2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	CP	324	Total	C	N	O		0	0
			1596	948	324	324			

- Molecule 42 is a protein called 60S ribosome subunit biogenesis protein NIP7.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	CG	177	Total	C	N	O	0	0
			873	519	177	177		

- Molecule 43 is a protein called Ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	Lq	207	Total	C	N	O	0	0
			1021	607	207	207		

- Molecule 44 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	Cx	102	Total	C	N	O	0	0
			565	340	114	111		

- Molecule 45 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
45	LJ	169	Total	C	N	O	0	0
			831	492	169	170		

- Molecule 46 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
46	LD	273	Total	C	N	O	0	0
			1346	801	273	272		

- Molecule 47 is a RNA chain called RNA (119-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
47	C4	119	Total	C	N	O	P	0	0
			2536	1131	453	833	119		

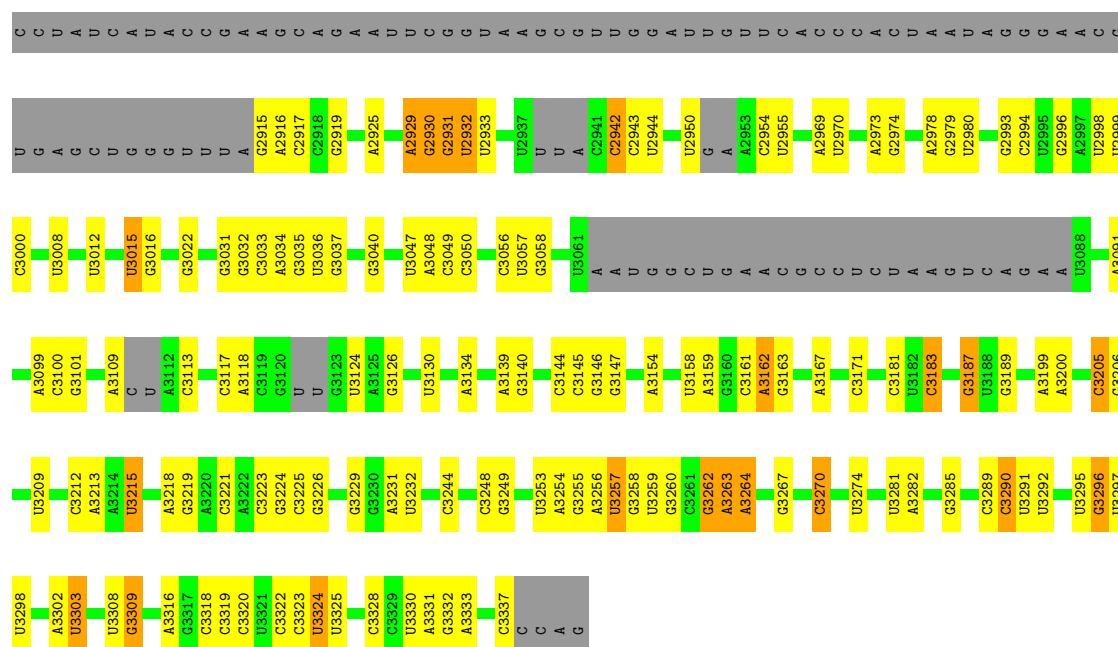
- Molecule 48 is a protein called 60S ribosomal subunit-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
48	CX	63	Total	C	N	O	0	0
			375	233	68	74		

- Molecule 49 is ZINC ION (three-letter code: ZN) (formula: Zn).

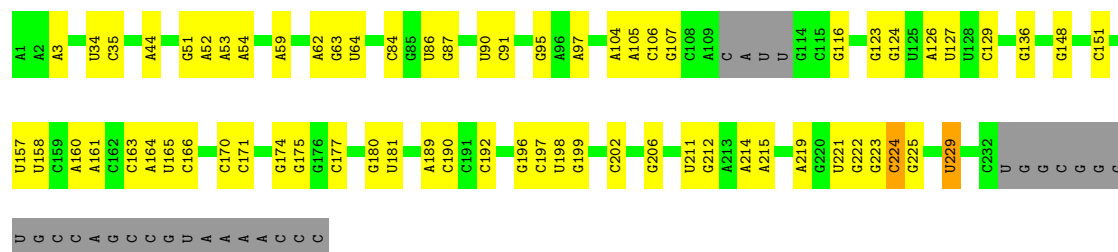
Mol	Chain	Residues	Atoms		AltConf
49	C1	1	Total 1	Zn 1	0
49	Lj	1	Total 1	Zn 1	0
49	Ce	1	Total 1	Zn 1	0





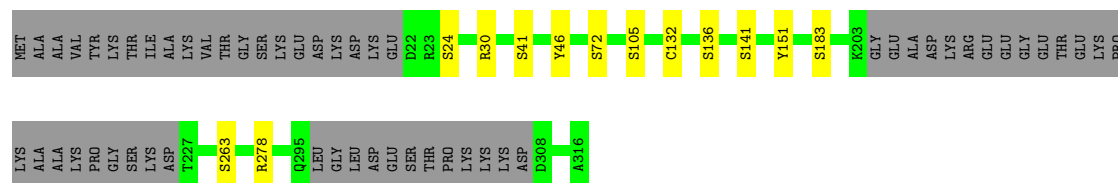
• Molecule 2: RNA (256-MER)

Chain C2: 63% 25% 11%



• Molecule 3: Brix domain-containing protein

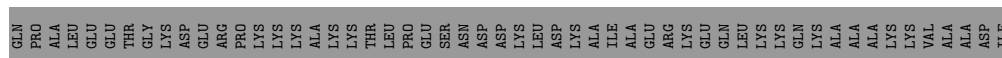
Chain CA: 78% 18%



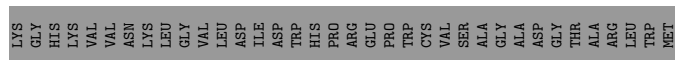
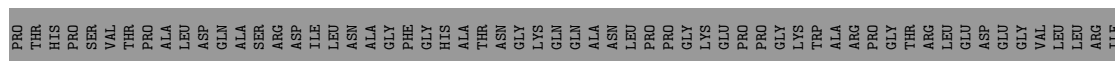
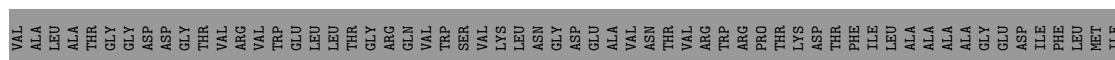
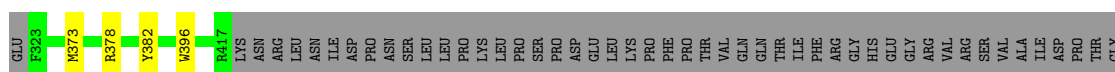
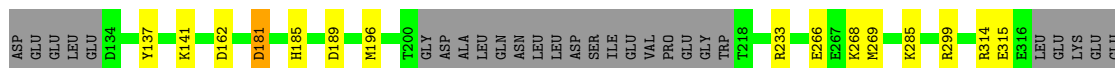
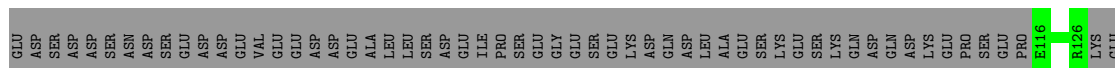
• Molecule 4: Ribosome biogenesis protein C8F11.04

Chain CB: 62% 5% 34%

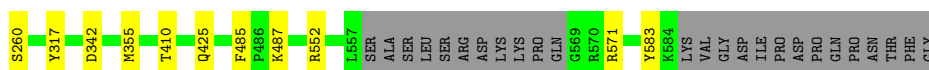
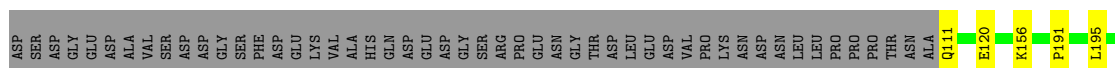
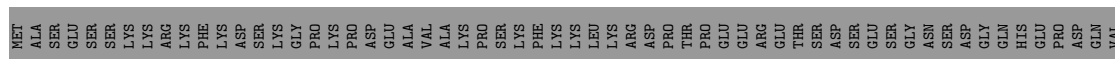




Chain CC:  32% . 66%

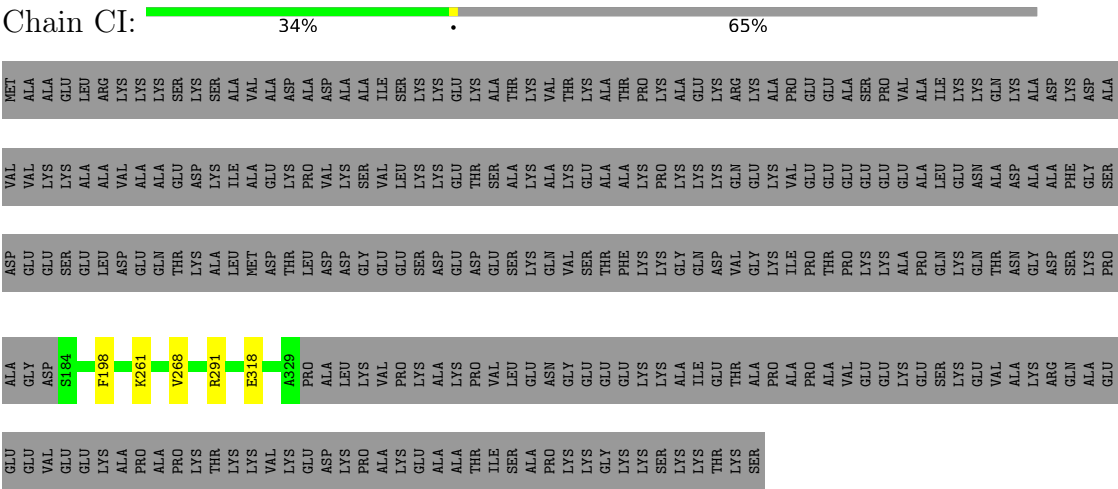


Chain CE: 75% . 23%

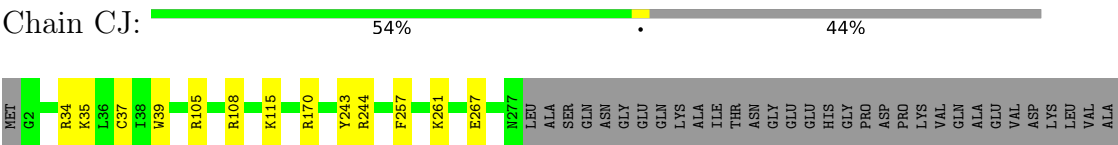


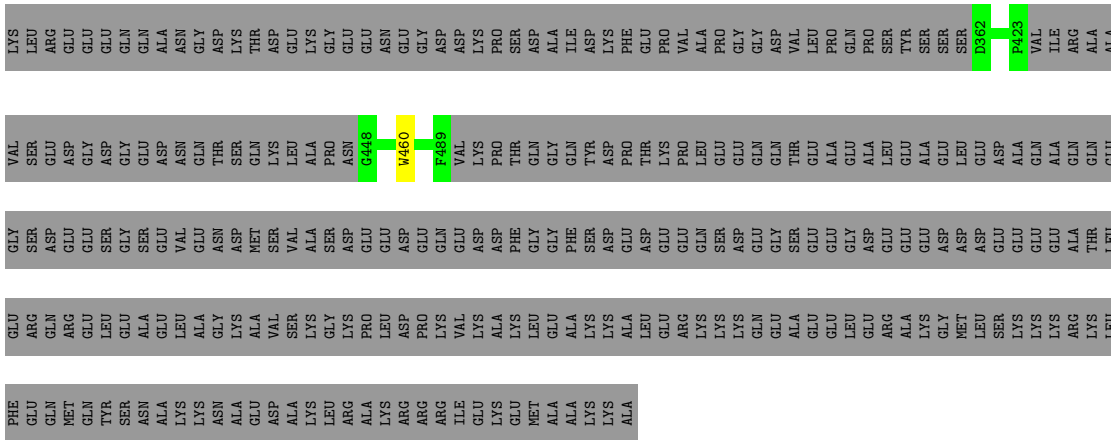


● Molecule 8: Putative RNA-binding protein

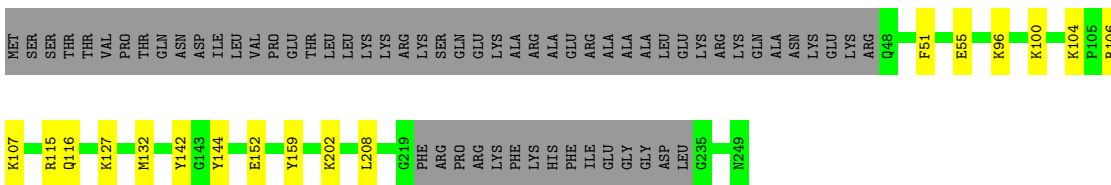


● Molecule 9: Pescadillo homolog





- Molecule 10: 60S ribosomal protein l7-like protein



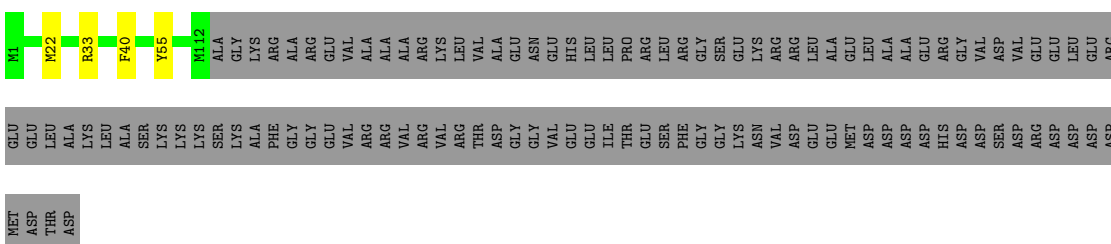
- Molecule 10: 60S ribosomal protein l7-like protein

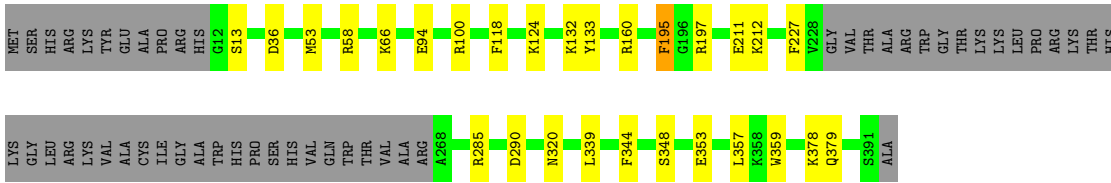


- Molecule 11: Eukaryotic translation initiation factor 6



- Molecule 12: Ribosome biogenesis protein RLP24

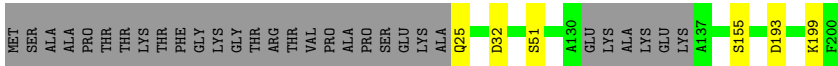
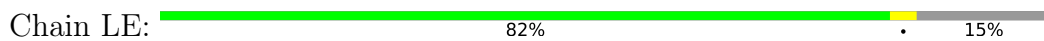




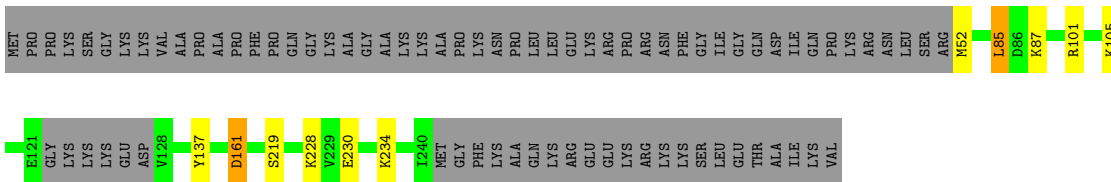
- Molecule 17: 60S ribosomal protein L4-like protein



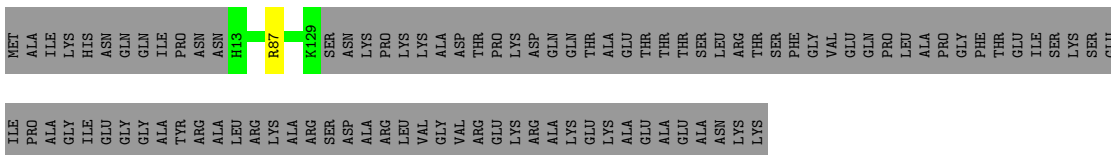
- Molecule 18: 60S ribosomal protein L6



- Molecule 19: 60S ribosomal protein L8



- Molecule 20: 60S ribosomal protein L13

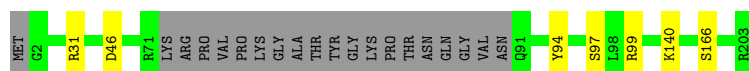


- Molecule 21: 60S ribosomal protein L14-like protein



- Molecule 22: Ribosomal protein L15





- Molecule 23: 60S ribosomal protein L16-like protein

Chain LO: 98%



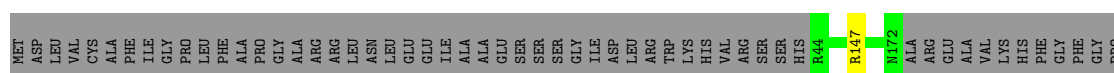
- Molecule 24: 60S ribosomal protein l17-like protein

Chain LP: 81% 18%



- Molecule 25: Ribosomal protein L18-like protein

Chain LQ: 60% 39%



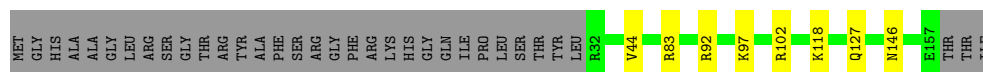
- Molecule 26: 60S ribosomal protein L20

Chain LS: 97%



- Molecule 27: 60S ribosomal protein l21-like protein

Chain LT: 74% 5% 21%



- Molecule 28: 60S ribosomal protein l23-like protein

Chain LV: 93%



- Molecule 29: 60S ribosomal protein L26-like protein

Sequence logo for the 13th position. The y-axis represents information content in bits, ranging from 0 to 1.5. The x-axis shows the amino acid sequence: M1, S8, K63, K68, Y73, K76, K134, LYS, THR, ALA, ALA. The bar for K134 is the tallest, reaching approximately 1.4 bits. The bars for LYS, THR, ALA, and ALA are very short, near 0.1 bits.

- Chain Le: 97%

```

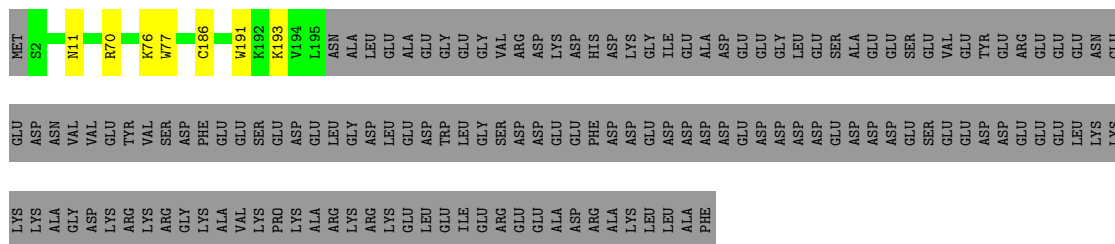
graph LR
    M1[M1] --- K5_K6[K5  
K6]
    K5_K6 --- R20[R20]
    R20 --- K124[K124]
    K124 --- V131[V131]

```

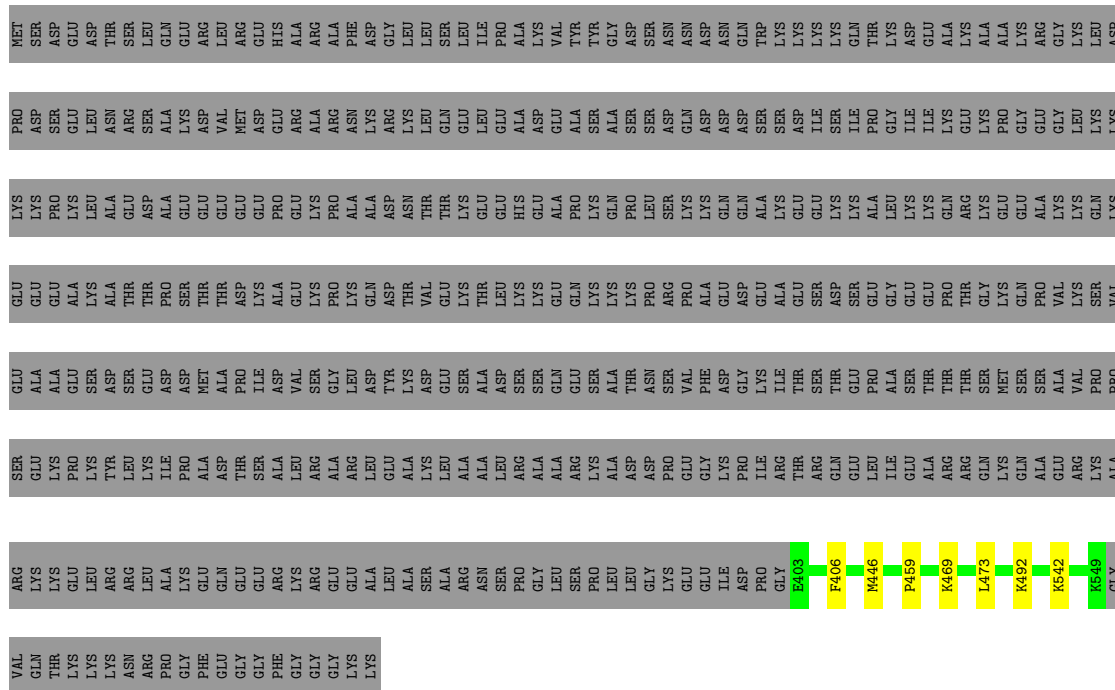
- Chain Lf: 95% ..

- Chain Lh:  13% 87%

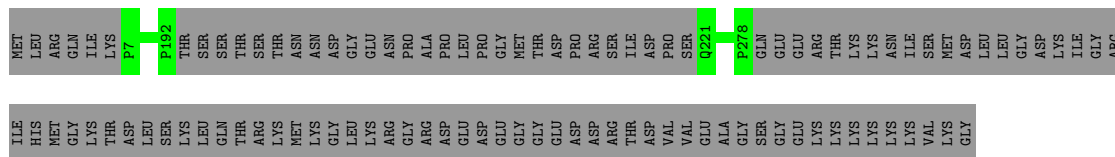
[illegible]



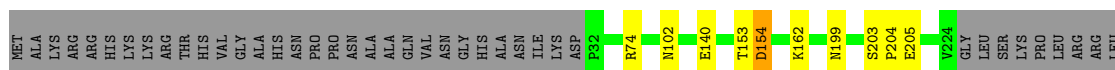
- Molecule 38: 60S ribosome biogenesis protein Rrp14

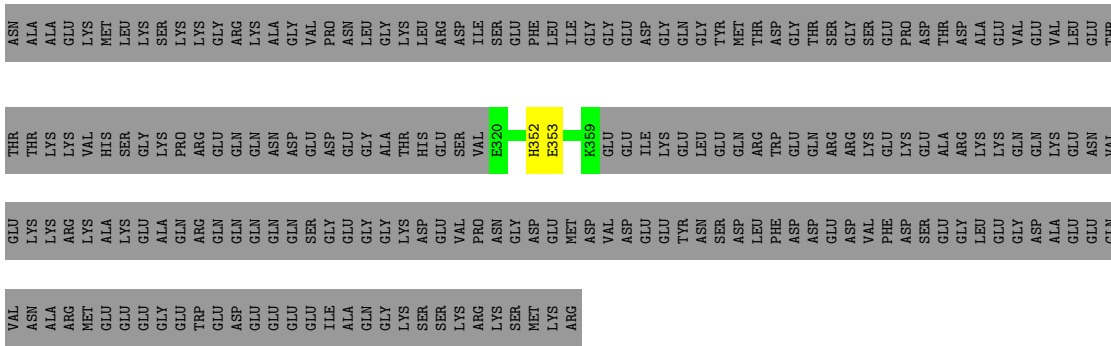


- Molecule 39: Ribosome production factor 2 homolog

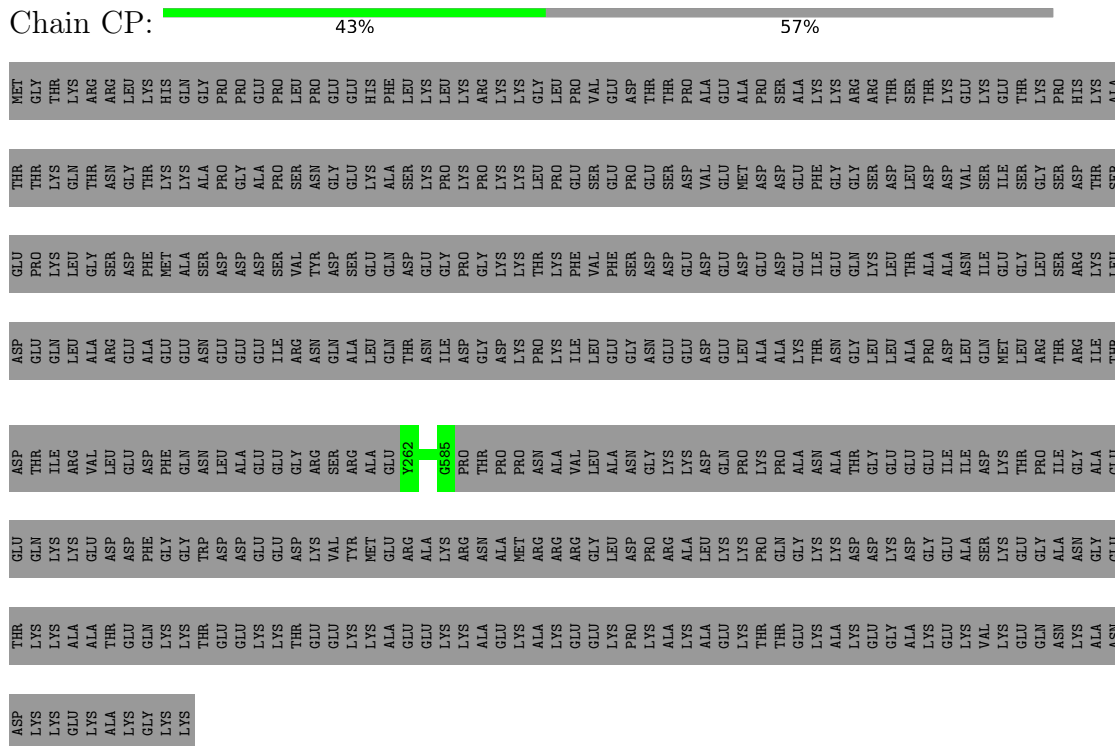


- Molecule 40: Brix domain-containing protein

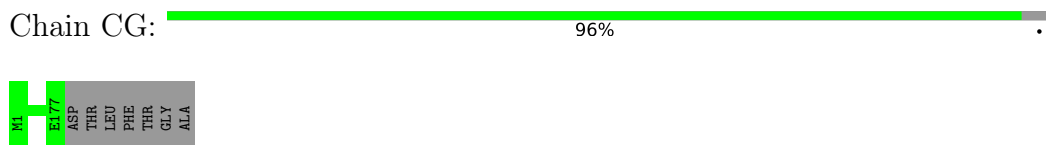




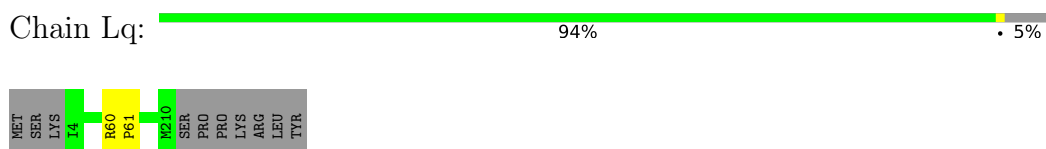
- Molecule 41: RNA methyltransferase nop2-like protein



- Molecule 42: 60S ribosome subunit biogenesis protein NIP7



- Molecule 43: Ribosomal protein



- Molecule 44: Ribosome biogenesis regulatory protein

ALA	LYS	GLU	ALA	MET	ARG	PRO	GLU	GLY	THR	SER	VAL	GLN	ASP	LYS	ARG	GLY	PRO	LYS	GLU	THR	LYS	ILE	GLU	ASN	ARG	LEU	MET	GLN	LYS	GLN	ASN	GLN	ARG	ILE	ALA	ALA	R123	R137	TRP	GLY	TYR	LYS	GLY	ALA	ASN	LYS	ARG	GLY	GIU	THR	ASP	PRO	ILE	ILE	GLU	VAL	SER
MET	SER	THR	ASP	THR	SER	LYS	PRO	ALA	ARG	L11	P97	GLN	PRO	LYS	PRO	GLU	THR	LYS	TRP	GLN	ALA	ALA	PHE	ALA	ARG	ASN	ARG	GLY	ILE	LYS	PRO	PHO	LYS	THR	ARG	R123	R137	TRP	GLY	TYR	LYS	GLY	ALA	ASN	LYS	ARG	GLY	GIU	THR	ASP	PRO	ILE	ILE	GLU	VAL	SER	

- Chain LJ: 98%

MET
SER
SER
GLU
K5
R173

- Chain LD: 

MET	ALA	PHE	HIS	K5	D116	LYS	THR	PHE	THR	GLY	VAL	GLU	GLU	PRO	ASN	G127	R287	LYS	ALA	ARG	VAL	GLU	ALA	ALA	LYS	ILE	LYS	GLN	LEU	LEU	ALA	GLU	GLN	ASP	GLU
-----	-----	-----	-----	----	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain C4: 77% 18% .

A1	G7	A8	C9	G15	A22	C26	G29	C42	U54	A55	A64	G65	G66	A75	G76	G82	G83	G84	U85	C96	U89	C92	G93	A94	C95	C99	G100	A101	G111	H119
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- Chain CX:  31% 69%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41599	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	C1	0.55	1/48945 (0.0%)	1.02	181/76270 (0.2%)
2	C2	0.57	0/5415	0.96	11/8436 (0.1%)
3	CA	0.34	0/2190	0.68	0/2940
4	CB	0.34	0/2109	0.65	2/2866 (0.1%)
5	CC	0.33	0/2325	0.67	4/3164 (0.1%)
6	CE	0.35	0/3743	0.61	1/5045 (0.0%)
7	CH	0.31	0/909	0.68	0/1229
8	CI	0.34	0/1225	0.64	0/1645
9	CJ	0.28	0/3189	0.58	2/4309 (0.0%)
10	CM	0.31	0/1555	0.65	1/2091 (0.0%)
10	LF	0.37	0/2004	0.60	1/2686 (0.0%)
11	CN	0.30	0/1881	0.66	1/2560 (0.0%)
12	CQ	0.34	0/981	0.70	0/1301
13	CR	0.33	0/1369	0.62	0/1828
14	CU	0.28	0/980	0.64	1/1314 (0.1%)
15	Ch	0.26	0/563	0.68	1/746 (0.1%)
16	LB	0.35	0/2760	0.72	5/3701 (0.1%)
17	LC	0.36	0/2809	0.58	0/3787
18	LE	0.34	0/1363	0.57	0/1833
19	LG	0.36	0/1492	0.59	1/2003 (0.0%)
20	LL	0.36	0/983	0.66	0/1318
21	LM	0.34	0/1120	0.64	1/1507 (0.1%)
22	LN	0.37	0/1595	0.63	1/2132 (0.0%)
23	LO	0.36	0/1652	0.64	1/2215 (0.0%)
24	LP	0.29	0/1231	0.56	0/1658
25	LQ	0.35	0/1033	0.61	0/1391
26	LS	0.35	0/1468	0.63	0/1975
27	LT	0.31	0/1033	0.62	0/1389
28	LV	0.32	0/1013	0.66	2/1361 (0.1%)
29	LY	0.34	0/1079	0.59	0/1443
30	Le	0.34	0/1073	0.57	0/1431
31	Lf	0.38	0/883	0.62	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Lh	0.30	0/1006	0.56	0/1338
33	Li	0.32	0/738	0.63	0/971
34	Lj	0.37	0/606	0.64	0/803
35	Cc	0.33	0/1934	0.58	1/2614 (0.0%)
36	Cd	0.33	0/2857	0.59	0/3843
37	Ce	0.38	0/1638	0.63	1/2196 (0.0%)
38	Cf	0.31	0/1238	0.67	2/1631 (0.1%)
39	Cy	0.24	0/1208	0.43	0/1682
40	Cg	0.51	2/1887 (0.1%)	0.85	4/2544 (0.2%)
41	CP	0.24	0/1595	0.46	0/2217
42	CG	0.26	0/872	0.50	0/1212
43	Lq	0.26	0/1020	0.49	0/1418
44	Cx	0.25	0/567	0.49	0/783
45	LJ	0.24	0/830	0.44	0/1150
46	LD	0.23	0/1344	0.41	0/1868
47	C4	0.30	0/2833	1.08	19/4414 (0.4%)
48	CX	0.58	0/377	0.66	0/518
All	All	0.44	3/124520 (0.0%)	0.84	244/179963 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	CB	0	1
15	Ch	0	1
16	LB	0	1
19	LG	0	1
25	LQ	0	1
40	Cg	0	1
43	Lq	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	Cg	204	PRO	CG-CD	-15.22	1.00	1.50
40	Cg	204	PRO	N-CD	6.92	1.57	1.47
1	C1	3215	U	C1'-N1	6.65	1.58	1.48

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Cg	204	PRO	N-CD-CG	-16.54	78.39	103.20
1	C1	1050	C	N3-C2-O2	-12.57	113.10	121.90
1	C1	1050	C	N1-C2-O2	10.13	124.98	118.90
37	Ce	186	CYS	C-N-CA	10.04	146.80	121.70
1	C1	625	C	C6-N1-C2	-10.02	116.29	120.30
40	Cg	204	PRO	CA-N-CD	-10.00	97.49	111.50
40	Cg	204	PRO	CA-CB-CG	-9.85	85.28	104.00
1	C1	739	C	N3-C2-O2	-9.20	115.46	121.90
1	C1	2931	G	P-O3'-C3'	-8.85	109.09	119.70
1	C1	2324	C	C2-N1-C1'	8.80	128.48	118.80
1	C1	398	G	O4'-C1'-N9	8.70	115.16	108.20
1	C1	2932	U	P-O3'-C3'	-8.62	109.35	119.70
1	C1	625	C	N3-C2-O2	-8.57	115.90	121.90
5	CC	181	ASP	CB-CG-OD1	8.35	125.82	118.30
1	C1	2723	C	N3-C2-O2	-8.27	116.11	121.90
1	C1	2680	U	N3-C2-O2	-8.22	116.45	122.20
1	C1	3290	C	N3-C2-O2	-8.16	116.19	121.90
1	C1	3320	C	N3-C2-O2	-8.14	116.20	121.90
1	C1	1050	C	C6-N1-C2	-8.06	117.08	120.30
1	C1	2943	C	N3-C2-O2	-8.00	116.30	121.90
22	LN	46	ASP	CB-CG-OD1	7.92	125.43	118.30
1	C1	3253	U	N1-C2-O2	7.75	128.23	122.80
5	CC	189	ASP	CB-CG-OD1	7.72	125.25	118.30
1	C1	3319	C	N1-C2-O2	7.71	123.53	118.90
2	C2	171	C	N3-C2-O2	-7.69	116.52	121.90
1	C1	1841	U	N3-C2-O2	-7.64	116.85	122.20
1	C1	2558	C	C2-N1-C1'	7.63	127.20	118.80
1	C1	3267	G	N1-C6-O6	-7.56	115.37	119.90
2	C2	170	C	N1-C2-O2	7.51	123.41	118.90
1	C1	2406	C	C2-N1-C1'	7.49	127.04	118.80
47	C4	95	C	N3-C2-O2	-7.47	116.67	121.90
1	C1	36	C	N1-C2-O2	7.42	123.35	118.90
1	C1	2417	U	C2-N1-C1'	7.29	126.45	117.70
47	C4	89	U	C2-N1-C1'	7.29	126.44	117.70
1	C1	1051	C	N3-C2-O2	-7.28	116.80	121.90
1	C1	2324	C	N1-C2-O2	7.26	123.26	118.90
47	C4	42	C	N1-C2-O2	7.25	123.25	118.90
1	C1	2680	U	N1-C2-O2	7.25	127.88	122.80
16	LB	36	ASP	CB-CG-OD1	7.21	124.79	118.30
1	C1	590	C	C6-N1-C2	-7.18	117.43	120.30
1	C1	3267	G	C5-C6-O6	7.10	132.86	128.60
1	C1	3253	U	C2-N1-C1'	7.09	126.21	117.70
1	C1	3264	A	O5'-P-OP1	-7.06	99.34	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1137	C	C2-N1-C1'	6.81	126.29	118.80
1	C1	2930	G	P-O3'-C3'	-6.79	111.55	119.70
1	C1	2915	G	C4-N9-C1'	6.76	135.29	126.50
1	C1	263	C	N1-C2-O2	6.74	122.94	118.90
1	C1	2431	G	N3-C4-N9	-6.64	122.02	126.00
14	CU	253	LEU	CA-CB-CG	6.58	130.43	115.30
1	C1	3253	U	N3-C2-O2	-6.52	117.63	122.20
47	C4	95	C	N1-C2-O2	6.51	122.81	118.90
1	C1	3187	G	N1-C6-O6	-6.48	116.01	119.90
1	C1	473	C	C2-N1-C1'	6.45	125.90	118.80
1	C1	2324	C	C6-N1-C1'	-6.45	113.06	120.80
1	C1	887	G	P-O3'-C3'	6.44	127.43	119.70
16	LB	357	LEU	CA-CB-CG	6.39	130.00	115.30
1	C1	550	C	C2-N1-C1'	6.36	125.80	118.80
1	C1	2417	U	N3-C2-O2	-6.36	117.75	122.20
1	C1	2929	A	P-O3'-C3'	6.34	127.31	119.70
1	C1	3187	G	C5-C6-O6	6.33	132.40	128.60
1	C1	2328	C	C5-C6-N1	6.32	124.16	121.00
1	C1	590	C	N1-C2-O2	6.30	122.68	118.90
1	C1	3158	U	C2-N1-C1'	6.29	125.25	117.70
28	LV	73	LYS	CA-CB-CG	6.29	127.23	113.40
47	C4	82	G	C4-N9-C1'	6.29	134.67	126.50
1	C1	78	U	N3-C2-O2	-6.28	117.81	122.20
1	C1	3290	C	N1-C2-O2	6.28	122.67	118.90
1	C1	3257	U	P-O3'-C3'	6.24	127.18	119.70
1	C1	2998	U	N1-C2-O2	6.23	127.16	122.80
47	C4	89	U	N1-C2-O2	6.23	127.16	122.80
1	C1	102	C	N1-C2-O2	6.22	122.63	118.90
1	C1	2417	U	N1-C2-O2	6.21	127.15	122.80
23	LO	53	LEU	CA-CB-CG	6.20	129.56	115.30
47	C4	15	C	N3-C2-O2	-6.20	117.56	121.90
1	C1	3320	C	N1-C2-N3	6.19	123.53	119.20
1	C1	3015	U	N3-C2-O2	-6.19	117.87	122.20
47	C4	99	C	C2-N1-C1'	6.19	125.61	118.80
1	C1	263	C	C2-N1-C1'	6.17	125.59	118.80
1	C1	2998	U	C2-N1-C1'	6.16	125.10	117.70
1	C1	940	C	N3-C2-O2	-6.13	117.61	121.90
1	C1	590	C	N3-C2-O2	-6.12	117.61	121.90
1	C1	463	C	C2-N1-C1'	6.12	125.53	118.80
2	C2	64	U	N3-C2-O2	-6.12	117.92	122.20
1	C1	374	U	C2-N1-C1'	6.10	125.02	117.70
1	C1	433	U	C2-N1-C1'	6.09	125.01	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1072	G	N1-C2-N2	-6.08	110.72	116.20
1	C1	3205	C	N1-C2-O2	6.05	122.53	118.90
1	C1	3320	C	C6-N1-C2	-6.01	117.90	120.30
1	C1	3270	C	N1-C2-O2	6.01	122.50	118.90
1	C1	1092	C	C2-N1-C1'	6.00	125.39	118.80
21	LM	104	LEU	CA-CB-CG	5.97	129.02	115.30
1	C1	2681	U	N1-C2-O2	5.96	126.97	122.80
1	C1	1841	U	O4'-C1'-N1	5.96	112.97	108.20
1	C1	2915	G	N3-C4-C5	-5.95	125.62	128.60
6	CE	342	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C1	940	C	C6-N1-C2	-5.92	117.93	120.30
47	C4	26	C	N1-C2-O2	5.90	122.44	118.90
40	Cg	203	SER	C-N-CD	5.87	140.73	128.40
1	C1	150	G	P-O3'-C3'	5.87	126.74	119.70
1	C1	2915	G	N3-C4-N9	5.86	129.52	126.00
38	Cf	459	PRO	CA-N-CD	-5.86	103.30	111.50
16	LB	212	LYS	CA-CB-CG	5.86	126.28	113.40
1	C1	2681	U	C2-N1-C1'	5.85	124.72	117.70
1	C1	1841	U	N1-C2-O2	5.85	126.89	122.80
1	C1	1051	C	C6-N1-C2	-5.83	117.97	120.30
1	C1	167	C	C2-N1-C1'	5.83	125.21	118.80
1	C1	3309	G	N3-C4-C5	-5.82	125.69	128.60
1	C1	243	G	C4-N9-C1'	5.81	134.05	126.50
1	C1	2406	C	N1-C2-O2	5.81	122.38	118.90
1	C1	2942	C	N3-C2-O2	-5.81	117.84	121.90
1	C1	639	G	N1-C6-O6	-5.80	116.42	119.90
1	C1	1071	G	N1-C2-N2	-5.79	110.99	116.20
28	LV	111	MET	CA-CB-CG	5.78	123.13	113.30
1	C1	3183	C	C5-C4-N4	5.78	124.25	120.20
1	C1	2667	C	C2-N1-C1'	5.77	125.15	118.80
1	C1	2752	G	C5-C6-O6	5.76	132.06	128.60
1	C1	437	C	C2-N1-C1'	5.75	125.12	118.80
1	C1	3225	C	C2-N1-C1'	5.75	125.12	118.80
47	C4	42	C	C2-N1-C1'	5.75	125.12	118.80
47	C4	42	C	N3-C2-O2	-5.72	117.89	121.90
1	C1	3309	G	C4-N9-C1'	5.72	133.94	126.50
1	C1	3324	U	C2-N1-C1'	5.71	124.56	117.70
1	C1	2942	C	N1-C2-O2	5.71	122.33	118.90
1	C1	72	C	C2-N3-C4	-5.71	117.05	119.90
1	C1	101	G	C4-N9-C1'	5.69	133.90	126.50
1	C1	2356	G	N1-C2-N2	-5.69	111.08	116.20
1	C1	3319	C	N3-C2-O2	-5.68	117.92	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2583	C	C2-N1-C1'	5.68	125.05	118.80
1	C1	2998	U	N3-C2-O2	-5.66	118.24	122.20
1	C1	2915	G	C8-N9-C1'	-5.66	119.64	127.00
15	Ch	282	LEU	CA-CB-CG	5.65	128.30	115.30
5	CC	314	ARG	CA-CB-CG	5.65	125.83	113.40
1	C1	939	C	N1-C2-O2	5.64	122.28	118.90
1	C1	739	C	C6-N1-C2	-5.64	118.04	120.30
1	C1	2431	G	C4-N9-C1'	-5.63	119.17	126.50
38	Cf	459	PRO	N-CD-CG	-5.62	94.76	103.20
1	C1	2731	C	C2-N1-C1'	5.62	124.99	118.80
1	C1	625	C	N1-C2-N3	5.62	123.13	119.20
1	C1	3183	C	N3-C4-N4	-5.59	114.08	118.00
1	C1	102	C	N3-C2-O2	-5.59	117.99	121.90
1	C1	2999	U	N1-C2-O2	5.58	126.70	122.80
1	C1	1071	G	N3-C2-N2	5.57	123.80	119.90
47	C4	82	G	C8-N9-C1'	-5.57	119.76	127.00
1	C1	2731	C	N1-C2-O2	5.57	122.24	118.90
1	C1	101	G	C8-N9-C1'	-5.57	119.76	127.00
47	C4	42	C	C6-N1-C2	-5.56	118.08	120.30
1	C1	625	C	N3-C4-C5	-5.55	119.68	121.90
47	C4	15	C	N1-C2-O2	5.55	122.23	118.90
1	C1	133	G	N3-C4-C5	-5.55	125.83	128.60
1	C1	3320	C	C5-C4-N4	5.54	124.08	120.20
1	C1	2999	U	N3-C2-O2	-5.54	118.33	122.20
1	C1	36	C	N3-C2-O2	-5.53	118.03	121.90
1	C1	162	U	N3-C2-O2	-5.52	118.33	122.20
2	C2	202	C	C5-C6-N1	5.52	123.76	121.00
1	C1	243	G	N3-C4-C5	-5.52	125.84	128.60
1	C1	896	A	P-O3'-C3'	5.51	126.31	119.70
1	C1	2431	G	C8-N9-C1'	5.50	134.15	127.00
1	C1	2722	C	N1-C2-O2	5.50	122.20	118.90
1	C1	592	G	O4'-C1'-N9	5.49	112.59	108.20
35	Cc	251	ASP	CB-CG-OD1	5.49	123.24	118.30
4	CB	141	GLU	CA-CB-CG	5.48	125.46	113.40
1	C1	2406	C	C5-C6-N1	5.47	123.74	121.00
16	LB	53	MET	CA-CB-CG	5.47	122.60	113.30
1	C1	963	C	C2-N1-C1'	5.46	124.81	118.80
1	C1	2406	C	C6-N1-C2	-5.45	118.12	120.30
2	C2	224	C	C2-N1-C1'	5.44	124.78	118.80
1	C1	3289	C	N1-C2-O2	5.44	122.16	118.90
1	C1	2408	U	C2-N1-C1'	5.43	124.22	117.70
2	C2	170	C	C2-N1-C1'	5.43	124.77	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	CJ	261	LYS	CA-CB-CG	5.40	125.28	113.40
2	C2	64	U	N1-C2-O2	5.40	126.58	122.80
1	C1	2680	U	C2-N1-C1'	5.39	124.17	117.70
16	LB	195	PHE	CB-CG-CD1	5.39	124.57	120.80
1	C1	1198	C	N1-C2-O2	5.38	122.13	118.90
2	C2	229	U	N1-C2-O2	5.38	126.57	122.80
1	C1	3296	G	N1-C2-N2	-5.37	111.36	116.20
1	C1	113	C	C2-N1-C1'	5.37	124.70	118.80
1	C1	2558	C	C6-N1-C1'	-5.36	114.37	120.80
1	C1	1072	G	N3-C2-N2	5.34	123.64	119.90
1	C1	639	G	C5-C6-O6	5.34	131.81	128.60
1	C1	2451	C	N1-C2-O2	5.34	122.11	118.90
1	C1	722	C	C2-N1-C1'	5.33	124.66	118.80
1	C1	3158	U	N3-C2-O2	-5.30	118.49	122.20
1	C1	738	C	N1-C2-O2	5.29	122.08	118.90
1	C1	3162	A	P-O3'-C3'	5.29	126.05	119.70
47	C4	82	G	P-O3'-C3'	5.28	126.04	119.70
1	C1	3320	C	C6-N1-C1'	5.28	127.14	120.80
1	C1	3296	G	P-O3'-C3'	5.26	126.02	119.70
1	C1	2681	U	N3-C2-O2	-5.26	118.52	122.20
47	C4	83	G	N3-C4-N9	5.26	129.16	126.00
1	C1	2440	C	N1-C2-O2	5.26	122.06	118.90
1	C1	738	C	N3-C2-O2	-5.26	118.22	121.90
47	C4	85	U	N3-C2-O2	-5.25	118.53	122.20
1	C1	249	C	N3-C2-O2	-5.24	118.23	121.90
1	C1	3309	G	C2-N3-C4	5.24	114.52	111.90
1	C1	1051	C	N1-C2-O2	5.23	122.04	118.90
1	C1	2458	U	N3-C2-O2	-5.22	118.54	122.20
1	C1	3319	C	C2-N1-C1'	5.22	124.54	118.80
1	C1	3324	U	N1-C2-O2	5.22	126.45	122.80
4	CB	251	GLU	CA-CB-CG	5.22	124.88	113.40
1	C1	3309	G	N3-C4-N9	5.21	129.13	126.00
1	C1	1092	C	C5-C6-N1	5.21	123.60	121.00
1	C1	263	C	N3-C2-O2	-5.20	118.26	121.90
10	LF	13	LEU	CA-CB-CG	5.20	127.25	115.30
1	C1	3262	G	O4'-C1'-N9	5.19	112.36	108.20
1	C1	590	C	C5-C6-N1	5.19	123.59	121.00
1	C1	724	C	N1-C2-O2	5.19	122.01	118.90
1	C1	2723	C	C6-N1-C2	-5.19	118.22	120.30
11	CN	224	LEU	CB-CG-CD1	-5.19	102.18	111.00
1	C1	3325	U	C2-N1-C1'	5.18	123.92	117.70
1	C1	34	A	O4'-C1'-N9	5.18	112.34	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	3303	U	N3-C2-O2	-5.18	118.58	122.20
47	C4	89	U	C6-N1-C1'	-5.18	113.95	121.20
1	C1	2355	G	N3-C4-N9	5.17	129.10	126.00
1	C1	953	U	C2-N1-C1'	5.17	123.90	117.70
1	C1	75	G	N3-C4-N9	5.16	129.09	126.00
1	C1	2943	C	N1-C2-O2	5.16	122.00	118.90
1	C1	3289	C	N3-C2-O2	-5.15	118.29	121.90
1	C1	2752	G	N1-C6-O6	-5.14	116.81	119.90
9	CJ	35	LYS	CA-CB-CG	5.14	124.71	113.40
10	CM	208	LEU	C-N-CA	5.12	134.50	121.70
1	C1	2558	C	C5-C6-N1	5.12	123.56	121.00
1	C1	1090	C	C2-N1-C1'	5.11	124.42	118.80
1	C1	101	G	O4'-C1'-N9	5.11	112.29	108.20
1	C1	3263	A	P-O3'-C3'	-5.10	113.58	119.70
1	C1	2354	C	N1-C2-O2	5.10	121.96	118.90
1	C1	133	G	C4-N9-C1'	5.09	133.12	126.50
1	C1	2731	C	C6-N1-C2	-5.08	118.27	120.30
1	C1	1137	C	C6-N1-C2	-5.08	118.27	120.30
19	LG	85	LEU	CA-CB-CG	5.07	126.97	115.30
2	C2	171	C	C6-N1-C2	-5.07	118.27	120.30
1	C1	2583	C	N1-C2-O2	5.06	121.94	118.90
1	C1	463	C	C6-N1-C2	-5.06	118.28	120.30
2	C2	177	C	C2-N1-C1'	5.04	124.34	118.80
1	C1	2558	C	N1-C2-O2	5.04	121.92	118.90
2	C2	170	C	N3-C2-O2	-5.04	118.38	121.90
1	C1	239	C	C2-N1-C1'	5.03	124.33	118.80
1	C1	892	C	N1-C2-O2	5.02	121.91	118.90
1	C1	2980	U	N1-C2-O2	5.02	126.32	122.80
1	C1	3270	C	N3-C2-O2	-5.02	118.38	121.90
1	C1	1074	C	C6-N1-C2	-5.01	118.30	120.30
1	C1	2406	C	C6-N1-C1'	-5.01	114.79	120.80
47	C4	42	C	C5-C6-N1	5.00	123.50	121.00
5	CC	196	MET	CA-CB-CG	5.00	121.80	113.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	CB	42	ARG	Peptide
40	Cg	154	ASP	Peptide
15	Ch	282	LEU	Peptide
16	LB	58	ARG	Sidechain

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Mol	Chain	Res	Type	Group
19	LG	161	ASP	Peptide
25	LQ	147	ARG	Sidechain
43	Lq	60	ARG	Peptide

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	
3	CA	254/316 (80%)	236 (93%)	18 (7%)	0	100	100
4	CB	256/391 (66%)	235 (92%)	20 (8%)	1 (0%)	30	63
5	CC	264/801 (33%)	250 (95%)	14 (5%)	0	100	100
6	CE	459/598 (77%)	440 (96%)	19 (4%)	0	100	100
7	CH	106/661 (16%)	101 (95%)	4 (4%)	1 (1%)	14	45
8	CI	144/414 (35%)	133 (92%)	10 (7%)	1 (1%)	19	51
9	CJ	374/679 (55%)	357 (96%)	16 (4%)	1 (0%)	37	68
10	CM	183/249 (74%)	171 (93%)	12 (7%)	0	100	100
10	LF	238/249 (96%)	230 (97%)	7 (3%)	1 (0%)	30	63
11	CN	244/246 (99%)	228 (93%)	16 (7%)	0	100	100
12	CQ	110/225 (49%)	107 (97%)	3 (3%)	0	100	100
13	CR	159/237 (67%)	153 (96%)	6 (4%)	0	100	100
14	CU	119/451 (26%)	113 (95%)	6 (5%)	0	100	100
15	Ch	69/354 (20%)	66 (96%)	3 (4%)	0	100	100
16	LB	337/392 (86%)	319 (95%)	18 (5%)	0	100	100
17	LC	360/365 (99%)	349 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	LE	166/200 (83%)	161 (97%)	5 (3%)	0	100	100
19	LG	179/262 (68%)	174 (97%)	5 (3%)	0	100	100
20	LL	115/213 (54%)	111 (96%)	4 (4%)	0	100	100
21	LM	135/142 (95%)	131 (97%)	4 (3%)	0	100	100
22	LN	179/203 (88%)	175 (98%)	4 (2%)	0	100	100
23	LO	202/204 (99%)	194 (96%)	8 (4%)	0	100	100
24	LP	150/187 (80%)	148 (99%)	2 (1%)	0	100	100
25	LQ	127/213 (60%)	123 (97%)	4 (3%)	0	100	100
26	LS	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
27	LT	124/160 (78%)	115 (93%)	8 (6%)	1 (1%)	16	48
28	LV	133/139 (96%)	127 (96%)	6 (4%)	0	100	100
29	LY	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
30	Le	129/131 (98%)	127 (98%)	2 (2%)	0	100	100
31	Lf	106/109 (97%)	102 (96%)	2 (2%)	2 (2%)	6	27
32	Lh	119/935 (13%)	117 (98%)	2 (2%)	0	100	100
33	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
34	Lj	72/95 (76%)	71 (99%)	1 (1%)	0	100	100
35	Cc	232/282 (82%)	222 (96%)	10 (4%)	0	100	100
36	Cd	343/436 (79%)	321 (94%)	22 (6%)	0	100	100
37	Ce	192/336 (57%)	188 (98%)	4 (2%)	0	100	100
38	Cf	145/570 (25%)	136 (94%)	9 (6%)	0	100	100
39	Cy	240/350 (69%)	238 (99%)	2 (1%)	0	100	100
40	Cg	229/478 (48%)	215 (94%)	12 (5%)	2 (1%)	14	45
41	CP	322/751 (43%)	314 (98%)	8 (2%)	0	100	100
42	CG	175/184 (95%)	171 (98%)	4 (2%)	0	100	100
43	Lq	205/217 (94%)	183 (89%)	21 (10%)	1 (0%)	25	58
44	Cx	98/202 (48%)	98 (100%)	0	0	100	100
45	LJ	167/173 (96%)	167 (100%)	0	0	100	100
46	LD	269/304 (88%)	266 (99%)	3 (1%)	0	100	100
48	CX	59/203 (29%)	56 (95%)	3 (5%)	0	100	100
All	All	8678/14729 (59%)	8315 (96%)	352 (4%)	11 (0%)	50	79

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CB	117	PRO
8	CI	268	VAL
40	Cg	154	ASP
31	Lf	93	ALA
7	CH	403	LEU
10	LF	12	ILE
9	CJ	267	GLU
40	Cg	153	THR
27	LT	44	VAL
31	Lf	92	PRO
43	Lq	61	PRO

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	
3	CA	231/276 (84%)	218 (94%)	13 (6%)	17	46
4	CB	222/329 (68%)	206 (93%)	16 (7%)	12	38
5	CC	252/710 (36%)	236 (94%)	16 (6%)	15	42
6	CE	398/517 (77%)	383 (96%)	15 (4%)	28	59
7	CH	95/575 (16%)	88 (93%)	7 (7%)	11	36
8	CI	121/336 (36%)	117 (97%)	4 (3%)	33	62
9	CJ	332/579 (57%)	321 (97%)	11 (3%)	33	62
10	CM	161/215 (75%)	145 (90%)	16 (10%)	6	24
10	LF	206/215 (96%)	202 (98%)	4 (2%)	52	75
11	CN	206/206 (100%)	199 (97%)	7 (3%)	32	62
12	CQ	100/192 (52%)	96 (96%)	4 (4%)	27	58
13	CR	144/206 (70%)	136 (94%)	8 (6%)	17	46
14	CU	104/376 (28%)	98 (94%)	6 (6%)	17	45
15	Ch	58/291 (20%)	56 (97%)	2 (3%)	32	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	LB	290/331 (88%)	267 (92%)	23 (8%)	10	34
17	LC	283/285 (99%)	274 (97%)	9 (3%)	34	63
18	LE	143/166 (86%)	137 (96%)	6 (4%)	25	56
19	LG	157/222 (71%)	146 (93%)	11 (7%)	12	39
20	LL	99/176 (56%)	98 (99%)	1 (1%)	73	86
21	LM	115/117 (98%)	110 (96%)	5 (4%)	25	55
22	LN	164/180 (91%)	158 (96%)	6 (4%)	29	59
23	LO	163/163 (100%)	160 (98%)	3 (2%)	54	76
24	LP	125/152 (82%)	122 (98%)	3 (2%)	44	70
25	LQ	110/178 (62%)	110 (100%)	0	100	100
26	LS	154/154 (100%)	148 (96%)	6 (4%)	27	58
27	LT	109/135 (81%)	102 (94%)	7 (6%)	14	42
28	LV	99/102 (97%)	95 (96%)	4 (4%)	27	58
29	LY	117/119 (98%)	112 (96%)	5 (4%)	25	55
30	Le	114/114 (100%)	110 (96%)	4 (4%)	31	61
31	Lf	89/90 (99%)	87 (98%)	2 (2%)	47	71
32	Lh	108/781 (14%)	104 (96%)	4 (4%)	29	59
33	Li	75/93 (81%)	69 (92%)	6 (8%)	10	34
34	Lj	61/78 (78%)	60 (98%)	1 (2%)	58	79
35	Cc	204/244 (84%)	194 (95%)	10 (5%)	21	51
36	Cd	295/367 (80%)	279 (95%)	16 (5%)	18	47
37	Ce	173/297 (58%)	167 (96%)	6 (4%)	31	61
38	Cf	127/482 (26%)	121 (95%)	6 (5%)	22	52
40	Cg	210/417 (50%)	202 (96%)	8 (4%)	28	59
44	Cx	14/176 (8%)	14 (100%)	0	100	100
48	CX	22/172 (13%)	21 (96%)	1 (4%)	23	53
All	All	6250/10814 (58%)	5968 (96%)	282 (4%)	26	53

All (282) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CA	24	SER
3	CA	30	ARG

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Mol	Chain	Res	Type
3	CA	41	SER
3	CA	46	TYR
3	CA	72	SER
3	CA	105	SER
3	CA	132	CYS
3	CA	136	SER
3	CA	141	SER
3	CA	151	TYR
3	CA	183	SER
3	CA	263	SER
3	CA	278	ARG
4	CB	22	GLN
4	CB	31	LEU
4	CB	44	ASP
4	CB	48	ASN
4	CB	75	SER
4	CB	87	HIS
4	CB	93	GLU
4	CB	97	VAL
4	CB	98	CYS
4	CB	107	PHE
4	CB	121	ARG
4	CB	173	LYS
4	CB	240	ASN
4	CB	251	GLU
4	CB	264	ARG
4	CB	281	PHE
5	CC	137	TYR
5	CC	141	LYS
5	CC	162	ASP
5	CC	181	ASP
5	CC	185	HIS
5	CC	233	ARG
5	CC	266	GLU
5	CC	268	LYS
5	CC	269	MET
5	CC	285	LYS
5	CC	299	ARG
5	CC	315	GLU
5	CC	373	MET
5	CC	378	ARG
5	CC	382	TYR

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Mol	Chain	Res	Type
5	CC	396	TRP
6	CE	111	GLN
6	CE	120	GLU
6	CE	156	LYS
6	CE	191	PRO
6	CE	195	LEU
6	CE	260	SER
6	CE	317	TYR
6	CE	355	MET
6	CE	410	THR
6	CE	425	GLN
6	CE	485	PHE
6	CE	487	LYS
6	CE	552	ARG
6	CE	571	ARG
6	CE	583	TYR
7	CH	379	ARG
7	CH	392	LYS
7	CH	401	ARG
7	CH	447	TYR
7	CH	459	GLN
7	CH	467	ARG
7	CH	473	PHE
8	CI	198	PHE
8	CI	261	LYS
8	CI	291	ARG
8	CI	318	GLU
9	CJ	34	ARG
9	CJ	37	CYS
9	CJ	39	TRP
9	CJ	105	ARG
9	CJ	108	ARG
9	CJ	115	LYS
9	CJ	170	ARG
9	CJ	243	TYR
9	CJ	244	ARG
9	CJ	257	PHE
9	CJ	460	TRP
10	CM	51	PHE
10	CM	55	GLU
10	CM	96	LYS
10	CM	100	LYS

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Mol	Chain	Res	Type
10	CM	104	LYS
10	CM	106	ARG
10	CM	107	LYS
10	CM	115	ARG
10	CM	116	GLN
10	CM	127	LYS
10	CM	132	MET
10	CM	142	TYR
10	CM	144	TYR
10	CM	152	GLU
10	CM	159	TYR
10	CM	202	LYS
11	CN	4	ARG
11	CN	7	PHE
11	CN	9	ASN
11	CN	50	ARG
11	CN	136	GLU
11	CN	138	PHE
11	CN	209	ASP
12	CQ	22	MET
12	CQ	33	ARG
12	CQ	40	PHE
12	CQ	55	TYR
13	CR	8	ARG
13	CR	22	ARG
13	CR	24	LYS
13	CR	60	LYS
13	CR	70	LYS
13	CR	73	LEU
13	CR	135	GLN
13	CR	230	LYS
14	CU	216	PHE
14	CU	249	GLU
14	CU	255	ARG
14	CU	258	LEU
14	CU	289	LEU
14	CU	310	LYS
15	Ch	273	GLU
15	Ch	292	LYS
16	LB	13	SER
16	LB	66	LYS
16	LB	94	GLU

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Mol	Chain	Res	Type
16	LB	100	ARG
16	LB	118	PHE
16	LB	124	LYS
16	LB	132	LYS
16	LB	133	TYR
16	LB	160	ARG
16	LB	195	PHE
16	LB	197	ARG
16	LB	211	GLU
16	LB	227	PHE
16	LB	285	ARG
16	LB	290	ASP
16	LB	320	ASN
16	LB	339	LEU
16	LB	344	PHE
16	LB	348	SER
16	LB	353	GLU
16	LB	359	TRP
16	LB	378	LYS
16	LB	379	GLN
17	LC	47	LYS
17	LC	56	LYS
17	LC	94	MET
17	LC	121	PHE
17	LC	137	MET
17	LC	199	ARG
17	LC	273	LYS
17	LC	308	ARG
17	LC	323	LYS
18	LE	25	GLN
18	LE	32	ASP
18	LE	51	SER
18	LE	155	SER
18	LE	193	ASP
18	LE	199	LYS
10	LF	23	LYS
10	LF	67	GLU
10	LF	106	ARG
10	LF	131	GLU
19	LG	52	MET
19	LG	85	LEU
19	LG	87	LYS

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Mol	Chain	Res	Type
19	LG	101	ARG
19	LG	105	LYS
19	LG	137	TYR
19	LG	161	ASP
19	LG	219	SER
19	LG	228	LYS
19	LG	230	GLU
19	LG	234	LYS
20	LL	87	ARG
21	LM	12	ARG
21	LM	49	LYS
21	LM	71	LYS
21	LM	102	LYS
21	LM	109	ARG
22	LN	31	ARG
22	LN	94	TYR
22	LN	97	SER
22	LN	99	ARG
22	LN	140	LYS
22	LN	166	SER
23	LO	69	ARG
23	LO	170	TYR
23	LO	173	LYS
24	LP	30	ARG
24	LP	55	LYS
24	LP	141	SER
26	LS	57	GLU
26	LS	79	LEU
26	LS	81	TYR
26	LS	88	HIS
26	LS	90	MET
26	LS	98	SER
27	LT	83	ARG
27	LT	92	ARG
27	LT	97	LYS
27	LT	102	ARG
27	LT	118	LYS
27	LT	127	GLN
27	LT	146	ASN
28	LV	85	LYS
28	LV	90	PHE
28	LV	114	SER

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Mol	Chain	Res	Type
28	LV	122	LYS
29	LY	8	SER
29	LY	63	LYS
29	LY	68	LYS
29	LY	73	TYR
29	LY	76	LYS
30	Le	5	LYS
30	Le	6	LYS
30	Le	20	ARG
30	Le	124	LYS
31	Lf	56	ARG
31	Lf	62	ARG
32	Lh	35	ARG
32	Lh	76	LYS
32	Lh	99	LYS
32	Lh	100	GLU
33	Li	25	LYS
33	Li	36	SER
33	Li	37	ARG
33	Li	68	GLU
33	Li	84	LYS
33	Li	107	ARG
34	Lj	36	SER
35	Cc	16	SER
35	Cc	19	ARG
35	Cc	28	SER
35	Cc	61	CYS
35	Cc	174	ARG
35	Cc	207	ARG
35	Cc	226	SER
35	Cc	228	MET
35	Cc	238	SER
35	Cc	244	ARG
36	Cd	39	LYS
36	Cd	62	GLU
36	Cd	71	LYS
36	Cd	76	ASP
36	Cd	80	ASP
36	Cd	93	LYS
36	Cd	95	ARG
36	Cd	260	GLN
36	Cd	261	GLU

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Mol	Chain	Res	Type
36	Cd	263	GLN
36	Cd	267	SER
36	Cd	296	LYS
36	Cd	327	SER
36	Cd	381	GLU
36	Cd	417	ASP
36	Cd	436	LEU
37	Ce	11	ASN
37	Ce	70	ARG
37	Ce	76	LYS
37	Ce	77	TRP
37	Ce	191	TRP
37	Ce	193	LYS
38	Cf	406	PHE
38	Cf	446	MET
38	Cf	469	LYS
38	Cf	473	LEU
38	Cf	492	LYS
38	Cf	542	LYS
40	Cg	74	ARG
40	Cg	102	ASN
40	Cg	140	GLU
40	Cg	162	LYS
40	Cg	199	ASN
40	Cg	205	GLU
40	Cg	352	HIS
40	Cg	353	GLU
48	CX	69	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
4	CB	240	ASN
5	CC	243	GLN
9	CJ	177	HIS
10	CM	242	ASN
12	CQ	45	ASN
15	Ch	321	GLN
32	Lh	47	ASN
40	Cg	100	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	2026/3341 (60%)	482 (23%)	17 (0%)
2	C2	225/256 (87%)	61 (27%)	1 (0%)
47	C4	118/119 (99%)	23 (19%)	0
All	All	2369/3716 (63%)	566 (23%)	18 (0%)

All (566) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	14	U
1	C1	26	A
1	C1	40	A
1	C1	43	A
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	73	A
1	C1	75	G
1	C1	91	G
1	C1	92	G
1	C1	94	G
1	C1	96	G
1	C1	105	C
1	C1	109	A
1	C1	110	G
1	C1	113	C
1	C1	116	A
1	C1	122	A
1	C1	131	U
1	C1	132	C
1	C1	133	G
1	C1	134	G
1	C1	136	C
1	C1	143	G
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	162	U
1	C1	163	U
1	C1	164	G

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Mol	Chain	Res	Type
1	C1	176	U
1	C1	180	G
1	C1	183	U
1	C1	192	A
1	C1	193	C
1	C1	203	C
1	C1	204	A
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	213	G
1	C1	224	A
1	C1	225	G
1	C1	240	U
1	C1	242	U
1	C1	244	U
1	C1	253	U
1	C1	257	A
1	C1	258	C
1	C1	261	G
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	291	G
1	C1	300	A
1	C1	302	U
1	C1	309	A
1	C1	310	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	329	G
1	C1	331	C
1	C1	343	A
1	C1	368	G
1	C1	376	A
1	C1	377	A
1	C1	390	U
1	C1	391	A
1	C1	393	C
1	C1	394	A

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Mol	Chain	Res	Type
1	C1	395	C
1	C1	412	G
1	C1	413	G
1	C1	416	G
1	C1	421	U
1	C1	432	U
1	C1	434	G
1	C1	446	U
1	C1	448	A
1	C1	450	C
1	C1	457	U
1	C1	459	U
1	C1	460	C
1	C1	467	G
1	C1	474	G
1	C1	485	G
1	C1	493	C
1	C1	500	G
1	C1	504	G
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	520	G
1	C1	526	G
1	C1	535	C
1	C1	536	C
1	C1	543	G
1	C1	544	U
1	C1	545	U
1	C1	546	A
1	C1	547	U
1	C1	548	A
1	C1	549	G
1	C1	558	G
1	C1	569	G
1	C1	582	A
1	C1	587	G
1	C1	590	C
1	C1	592	G
1	C1	593	C
1	C1	596	G

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Mol	Chain	Res	Type
1	C1	598	A
1	C1	624	C
1	C1	625	C
1	C1	629	U
1	C1	633	A
1	C1	634	A
1	C1	636	A
1	C1	647	A
1	C1	664	A
1	C1	668	U
1	C1	678	A
1	C1	708	G
1	C1	718	U
1	C1	719	C
1	C1	723	G
1	C1	730	C
1	C1	731	G
1	C1	744	G
1	C1	746	A
1	C1	748	U
1	C1	751	G
1	C1	755	G
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	766	G
1	C1	787	A
1	C1	798	A
1	C1	887	G
1	C1	888	G
1	C1	896	A
1	C1	897	G
1	C1	905	G
1	C1	906	A
1	C1	907	A
1	C1	918	G
1	C1	924	U
1	C1	925	A
1	C1	932	A
1	C1	934	G
1	C1	937	U

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Mol	Chain	Res	Type
1	C1	940	C
1	C1	943	A
1	C1	944	G
1	C1	954	G
1	C1	957	G
1	C1	958	A
1	C1	960	C
1	C1	975	G
1	C1	976	U
1	C1	978	A
1	C1	1033	U
1	C1	1034	U
1	C1	1036	A
1	C1	1039	A
1	C1	1045	G
1	C1	1046	A
1	C1	1047	A
1	C1	1057	A
1	C1	1063	C
1	C1	1064	U
1	C1	1073	G
1	C1	1075	A
1	C1	1076	U
1	C1	1077	U
1	C1	1078	C
1	C1	1079	G
1	C1	1080	A
1	C1	1084	U
1	C1	1085	A
1	C1	1091	A
1	C1	1092	C
1	C1	1094	A
1	C1	1096	U
1	C1	1097	G
1	C1	1099	G
1	C1	1126	U
1	C1	1132	A
1	C1	1136	A
1	C1	1137	C
1	C1	1141	A
1	C1	1142	C
1	C1	1163	U

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Mol	Chain	Res	Type
1	C1	1164	G
1	C1	1186	A
1	C1	1198	C
1	C1	1271	G
1	C1	1272	U
1	C1	1277	G
1	C1	1278	C
1	C1	1279	C
1	C1	1295	G
1	C1	1298	C
1	C1	1309	C
1	C1	1312	A
1	C1	1313	U
1	C1	1314	A
1	C1	1330	A
1	C1	1331	G
1	C1	1332	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1368	A
1	C1	1369	G
1	C1	1381	A
1	C1	1382	G
1	C1	1384	G
1	C1	1400	A
1	C1	1401	A
1	C1	1416	G
1	C1	1419	C
1	C1	1432	G
1	C1	1443	A
1	C1	1444	A
1	C1	1448	G
1	C1	1841	U
1	C1	1843	A
1	C1	1844	A
1	C1	1845	C
1	C1	1846	A
1	C1	1859	U
1	C1	1861	G
1	C1	1863	A

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Mol	Chain	Res	Type
1	C1	1864	C
1	C1	1866	A
1	C1	1868	G
1	C1	1874	A
1	C1	1875	A
1	C1	1883	C
1	C1	2297	G
1	C1	2302	U
1	C1	2309	U
1	C1	2310	A
1	C1	2325	A
1	C1	2326	G
1	C1	2327	C
1	C1	2332	G
1	C1	2334	A
1	C1	2335	A
1	C1	2336	C
1	C1	2337	G
1	C1	2339	G
1	C1	2346	A
1	C1	2347	A
1	C1	2348	A
1	C1	2349	A
1	C1	2350	U
1	C1	2351	C
1	C1	2352	A
1	C1	2353	G
1	C1	2355	G
1	C1	2356	G
1	C1	2358	G
1	C1	2365	G
1	C1	2376	G
1	C1	2388	U
1	C1	2396	U
1	C1	2402	A
1	C1	2407	A
1	C1	2414	G
1	C1	2415	U
1	C1	2421	A
1	C1	2422	U
1	C1	2423	A
1	C1	2424	G

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Mol	Chain	Res	Type
1	C1	2425	G
1	C1	2428	G
1	C1	2429	G
1	C1	2430	A
1	C1	2432	C
1	C1	2433	U
1	C1	2434	U
1	C1	2435	C
1	C1	2436	G
1	C1	2438	C
1	C1	2439	G
1	C1	2443	G
1	C1	2449	U
1	C1	2450	A
1	C1	2452	C
1	C1	2453	A
1	C1	2455	U
1	C1	2456	A
1	C1	2457	C
1	C1	2459	C
1	C1	2465	G
1	C1	2466	U
1	C1	2467	U
1	C1	2484	G
1	C1	2551	A
1	C1	2558	C
1	C1	2560	G
1	C1	2564	G
1	C1	2565	G
1	C1	2570	U
1	C1	2581	G
1	C1	2583	C
1	C1	2584	A
1	C1	2588	C
1	C1	2605	A
1	C1	2608	U
1	C1	2614	A
1	C1	2630	G
1	C1	2632	A
1	C1	2634	A
1	C1	2635	G
1	C1	2645	G

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Mol	Chain	Res	Type
1	C1	2646	U
1	C1	2650	A
1	C1	2655	A
1	C1	2656	G
1	C1	2657	G
1	C1	2662	A
1	C1	2663	A
1	C1	2666	C
1	C1	2670	U
1	C1	2671	U
1	C1	2672	G
1	C1	2673	A
1	C1	2674	U
1	C1	2679	A
1	C1	2688	G
1	C1	2689	OMU
1	C1	2690	G
1	C1	2707	G
1	C1	2712	G
1	C1	2713	C
1	C1	2730	C
1	C1	2735	G
1	C1	2739	U
1	C1	2749	G
1	C1	2759	A
1	C1	2766	A
1	C1	2916	A
1	C1	2917	C
1	C1	2919	G
1	C1	2925	A
1	C1	2929	A
1	C1	2930	G
1	C1	2931	G
1	C1	2932	U
1	C1	2933	U
1	C1	2942	C
1	C1	2944	U
1	C1	2950	U
1	C1	2954	C
1	C1	2955	U
1	C1	2969	A
1	C1	2970	U

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Mol	Chain	Res	Type
1	C1	2973	A
1	C1	2974	G
1	C1	2978	A
1	C1	2979	G
1	C1	2993	G
1	C1	2994	C
1	C1	2996	G
1	C1	3000	C
1	C1	3008	U
1	C1	3012	U
1	C1	3015	U
1	C1	3016	G
1	C1	3022	G
1	C1	3031	G
1	C1	3032	G
1	C1	3033	C
1	C1	3034	A
1	C1	3035	G
1	C1	3036	U
1	C1	3037	G
1	C1	3040	G
1	C1	3047	U
1	C1	3048	A
1	C1	3049	C
1	C1	3050	C
1	C1	3056	C
1	C1	3057	U
1	C1	3058	G
1	C1	3091	A
1	C1	3099	A
1	C1	3100	C
1	C1	3101	G
1	C1	3109	A
1	C1	3113	C
1	C1	3117	C
1	C1	3118	A
1	C1	3124	U
1	C1	3126	G
1	C1	3130	U
1	C1	3134	A
1	C1	3139	A
1	C1	3140	G

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Mol	Chain	Res	Type
1	C1	3144	C
1	C1	3145	C
1	C1	3146	G
1	C1	3147	G
1	C1	3154	A
1	C1	3159	A
1	C1	3161	C
1	C1	3162	A
1	C1	3163	G
1	C1	3167	A
1	C1	3171	C
1	C1	3181	C
1	C1	3183	C
1	C1	3187	G
1	C1	3189	G
1	C1	3199	A
1	C1	3200	A
1	C1	3205	C
1	C1	3206	G
1	C1	3209	U
1	C1	3212	C
1	C1	3213	A
1	C1	3215	U
1	C1	3218	A
1	C1	3219	G
1	C1	3221	C
1	C1	3223	C
1	C1	3224	G
1	C1	3226	G
1	C1	3229	G
1	C1	3231	A
1	C1	3232	U
1	C1	3244	C
1	C1	3248	C
1	C1	3249	G
1	C1	3254	A
1	C1	3256	A
1	C1	3257	U
1	C1	3258	G
1	C1	3259	U
1	C1	3260	G
1	C1	3262	G

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Mol	Chain	Res	Type
1	C1	3263	A
1	C1	3264	A
1	C1	3270	C
1	C1	3274	U
1	C1	3281	U
1	C1	3282	A
1	C1	3285	G
1	C1	3290	C
1	C1	3291	U
1	C1	3292	U
1	C1	3295	U
1	C1	3296	G
1	C1	3297	U
1	C1	3298	U
1	C1	3302	A
1	C1	3303	U
1	C1	3308	U
1	C1	3309	G
1	C1	3316	A
1	C1	3318	C
1	C1	3322	C
1	C1	3323	C
1	C1	3324	U
1	C1	3328	C
1	C1	3330	U
1	C1	3331	A
1	C1	3332	G
1	C1	3333	A
1	C1	3337	C
2	C2	3	A
2	C2	34	U
2	C2	35	C
2	C2	44	A
2	C2	51	G
2	C2	52	A
2	C2	53	A
2	C2	54	A
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	84	C
2	C2	86	U

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Mol	Chain	Res	Type
2	C2	87	G
2	C2	90	U
2	C2	91	C
2	C2	95	G
2	C2	97	A
2	C2	104	A
2	C2	105	A
2	C2	106	C
2	C2	107	G
2	C2	116	G
2	C2	124	G
2	C2	126	A
2	C2	127	U
2	C2	129	C
2	C2	136	G
2	C2	148	G
2	C2	151	C
2	C2	157	U
2	C2	158	U
2	C2	160	A
2	C2	161	A
2	C2	163	C
2	C2	164	A
2	C2	165	U
2	C2	166	C
2	C2	174	G
2	C2	175	G
2	C2	180	G
2	C2	181	U
2	C2	189	A
2	C2	190	C
2	C2	192	C
2	C2	196	G
2	C2	197	C
2	C2	198	U
2	C2	199	G
2	C2	206	G
2	C2	211	U
2	C2	212	G
2	C2	214	A
2	C2	215	A
2	C2	219	A

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Mol	Chain	Res	Type
2	C2	221	U
2	C2	222	G
2	C2	223	G
2	C2	224	C
2	C2	225	G
2	C2	229	U
47	C4	7	G
47	C4	9	C
47	C4	22	A
47	C4	29	G
47	C4	54	U
47	C4	55	A
47	C4	64	A
47	C4	66	G
47	C4	75	A
47	C4	76	G
47	C4	82	G
47	C4	83	G
47	C4	84	G
47	C4	85	U
47	C4	86	C
47	C4	89	U
47	C4	92	C
47	C4	93	G
47	C4	94	A
47	C4	99	C
47	C4	100	G
47	C4	101	A
47	C4	111	G

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	519	A
1	C1	887	G
1	C1	896	A
1	C1	906	A
1	C1	1044	A
1	C1	1046	A
1	C1	2301	C
1	C1	2569	U

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Mol	Chain	Res	Type
1	C1	2929	A
1	C1	2932	U
1	C1	3015	U
1	C1	3162	A
1	C1	3255	G
1	C1	3257	U
1	C1	3296	G
1	C1	3297	U
2	C2	123	G

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

3 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
1	OMU	C1	2682	1	19,22,23	2.97	8 (42%)	26,31,34	1.64	4 (15%)
1	OMU	C1	2687	1	19,22,23	2.96	8 (42%)	26,31,34	1.67	4 (15%)
1	OMU	C1	2689	1	19,22,23	2.98	8 (42%)	26,31,34	1.68	4 (15%)

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
1	OMU	C1	2682	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	2687	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2689	1	-	2/9/27/28	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2682	OMU	C2-N1	7.20	1.50	1.38
1	C1	2689	OMU	C2-N1	7.20	1.50	1.38
1	C1	2687	OMU	C2-N1	7.15	1.49	1.38
1	C1	2689	OMU	C2-N3	6.72	1.49	1.38
1	C1	2682	OMU	C2-N3	6.71	1.49	1.38
1	C1	2687	OMU	C2-N3	6.70	1.49	1.38
1	C1	2682	OMU	C6-C5	5.92	1.48	1.35
1	C1	2689	OMU	C6-C5	5.91	1.48	1.35
1	C1	2687	OMU	C6-C5	5.89	1.48	1.35
1	C1	2689	OMU	C4-N3	3.61	1.45	1.38
1	C1	2687	OMU	C4-N3	3.56	1.44	1.38
1	C1	2682	OMU	C4-N3	3.50	1.44	1.38
1	C1	2687	OMU	O4-C4	-2.58	1.19	1.24
1	C1	2689	OMU	O4-C4	-2.58	1.19	1.24
1	C1	2682	OMU	O2-C2	-2.57	1.18	1.23
1	C1	2682	OMU	O4-C4	-2.57	1.19	1.24
1	C1	2689	OMU	O2-C2	-2.54	1.18	1.23
1	C1	2687	OMU	O2-C2	-2.52	1.18	1.23
1	C1	2687	OMU	C6-N1	2.14	1.43	1.38
1	C1	2682	OMU	C6-N1	2.14	1.43	1.38
1	C1	2687	OMU	C5-C4	2.13	1.48	1.43
1	C1	2689	OMU	C6-N1	2.12	1.43	1.38
1	C1	2689	OMU	C5-C4	2.11	1.48	1.43
1	C1	2682	OMU	C5-C4	2.05	1.48	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2689	OMU	C4-N3-C2	-5.14	119.80	126.58
1	C1	2687	OMU	C4-N3-C2	-5.12	119.83	126.58
1	C1	2682	OMU	C4-N3-C2	-4.98	120.01	126.58
1	C1	2689	OMU	N3-C2-N1	3.71	119.82	114.89
1	C1	2687	OMU	N3-C2-N1	3.67	119.77	114.89
1	C1	2682	OMU	N3-C2-N1	3.59	119.66	114.89
1	C1	2687	OMU	C5-C4-N3	3.29	119.76	114.84
1	C1	2682	OMU	C5-C4-N3	3.28	119.75	114.84
1	C1	2689	OMU	C5-C4-N3	3.27	119.73	114.84
1	C1	2687	OMU	O4-C4-C5	-2.86	120.12	125.16
1	C1	2689	OMU	O4-C4-C5	-2.86	120.13	125.16
1	C1	2682	OMU	O4-C4-C5	-2.86	120.14	125.16

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	2682	OMU	C1'-C2'-O2'-CM2
1	C1	2689	OMU	C3'-C4'-C5'-O5'
1	C1	2689	OMU	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 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.