



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 06:31 pm GMT

PDB ID : 8RCS
EMDB ID : EMD-19058
Title : Escherichia coli paused disome complex (Rotated disome interface class 1)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-12-07
Resolution : 4.46 Å(reported)
Based on initial model : 7N1P

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

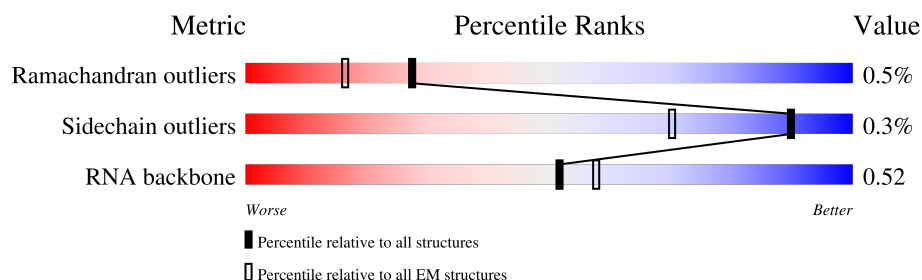
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.46 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.




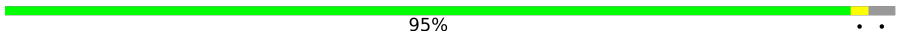



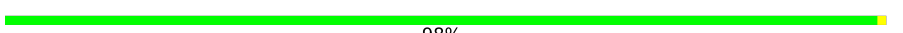
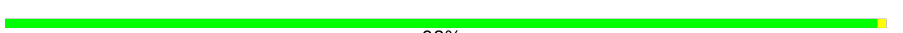








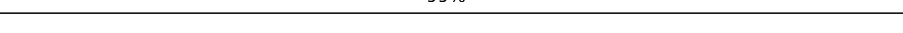
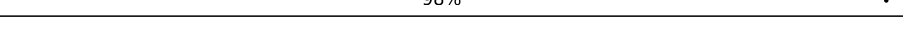
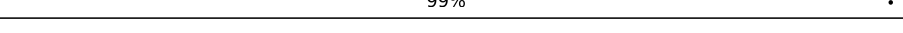
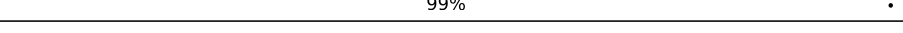



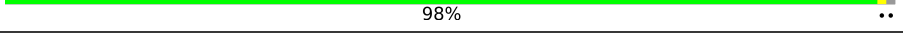
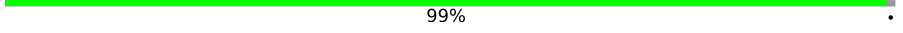
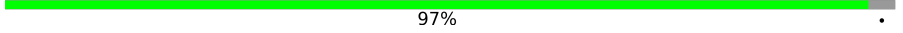
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	12	78	96% ..
2	32	59	97% ..
3	4	70	91% 6% .
3	41	70	20% 80%
4	62	65	98% .
5	71	2904	99%
5	72	2904	83% 17%
6	82	120	80% 19% .
7	A1	1542	70% 30%

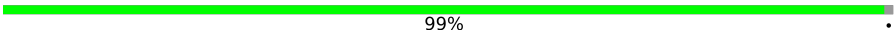
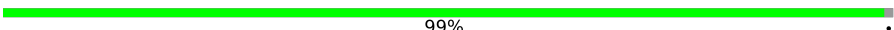
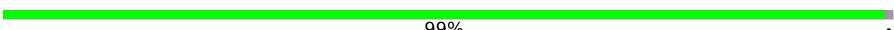
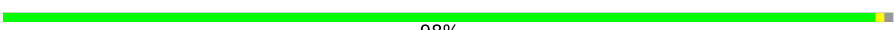
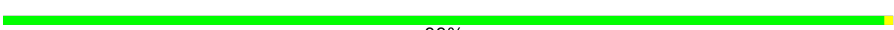





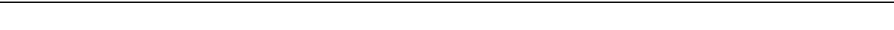

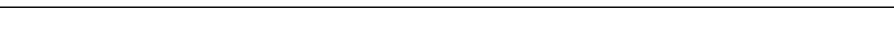
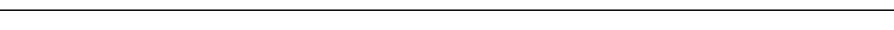
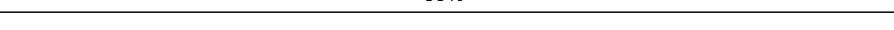





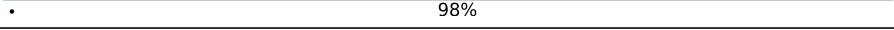
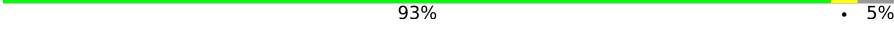
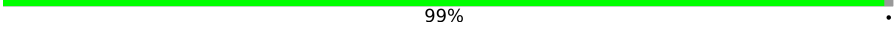
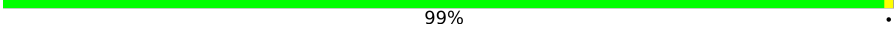
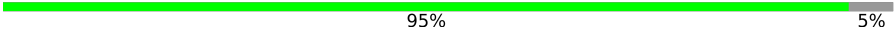
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Mol	Chain	Length	Quality of chain
7	A2	1542	 73%26%
8	B	241	 95%
8	B2	241	 94%6%
9	C1	233	 90%9%
9	C2	233	 91%9%
10	D1	206	 98%
10	D2	206	 98%
11	E1	167	 95%5%
11	E2	167	 95%5%
12	F1	135	 79%21%
12	F2	135	 78%21%
13	G1	179	 87%13%
13	G2	179	 81%5%14%
14	H1	130	 99%
14	H2	130	 99%
15	I1	130	 98%
15	I2	130	 99%
16	J1	103	 99%
16	J2	103	 92%5%
17	K1	129	 88%11%
17	K2	129	 90%9%
18	L1	124	 98%
18	L2	124	 99%
19	M1	118	 97%
19	M2	118	 99%

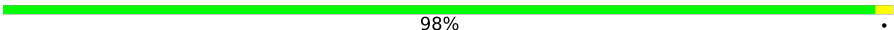

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Mol	Chain	Length	Quality of chain
20	N1	101	 99% .
20	N2	101	 99% .
21	O1	89	 99% .
21	O2	89	 98% ..
22	P1	82	 99% .
23	Q1	84	 95% 5%
23	Q2	84	 94% . 5%
24	R1	75	 97% ..
24	R2	75	 96% . .
25	S1	92	 90% 10%
25	S2	92	 90% 10%
26	T1	87	 94% 5% .
27	U1	71	 97% ..
27	U2	71	 99% .
28	V2	59	 31% 66% .
29	W	76	 54% 37% 9%
30	W1	76	 26% 16% . 57%
31	Y	76	 68% 29% .
32	Y1	76	 38% 8% . 53%
33	Z1	557	 . 98%
34	a2	234	 93% . 5%
35	b2	273	 99% .
36	e2	179	 99% ..
37	g2	55	 95% 5%
38	h2	136	 100%

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Mol	Chain	Length	Quality of chain
39	i2	149	 98% .
40	l2	46	 98% .
41	o2	144	 35% 65%
42	p	10	 70% 30%
43	r2	117	 99% .
44	z2	85	 89% 11%

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 187319 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	12	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	32	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	68	Total	C	N	O	S	0	0
			533	330	101	96	6		
3	41	14	Total	C	N	O		0	0
			118	74	26	18			

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	62	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	71	19	Total	C	N	O	P	0	0
			406	182	73	132	19		
5	72	2904	Total	C	N	O	P	0	0
			62355	27824	11468	20159	2904		

- Molecule 6 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	82	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 7 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A1	1542	Total	C	N	O	P	0	0
			33092	14767	6064	10719	1542		
7	A2	1537	Total	C	N	O	P	0	0
			32990	14721	6049	10683	1537		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	233	Total	C	N	O	S	0	0
			1815	1145	325	337	8		
8	B2	227	Total	C	N	O	S	0	0
			1776	1123	318	327	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C1	213	Total	C	N	O	S	0	0
			1665	1054	312	295	4		
9	C2	212	Total	C	N	O	S	0	0
			1658	1049	311	294	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D1	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		
10	D2	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E1	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		
11	E2	158	Total	C	N	O	S	0	0
			1166	725	220	215	6		

- Molecule 12 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	F1	106	Total	C	N	O	S	0	0
			862	545	156	154	7		
12	F2	106	Total	C	N	O	S	0	0
			862	545	156	154	7		

- Molecule 13 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	G1	155	Total	C	N	O	S	0	0
			1228	767	237	220	4		
13	G2	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	H1	129	Total	C	N	O	S	0	0
			979	616	173	184	6		
14	H2	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	I1	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		
15	I2	129	Total	C	N	O	S	0	0
			1036	642	208	183	3		

- Molecule 16 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J1	102	Total	C	N	O	S	0	0
			817	509	157	150	1		
16	J2	100	Total	C	N	O	S	0	0
			803	502	154	146	1		

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K1	115	Total	C	N	O	S	0	0
			857	528	168	158	3		
17	K2	118	Total	C	N	O	S	0	0
			884	545	175	161	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L1	123	Total	C	N	O	S	0	0
			955	590	196	165	4		
18	L2	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M1	115	Total	C	N	O	S	0	0
			891	552	179	157	3		
19	M2	117	Total	C	N	O	S	0	0
			910	564	183	160	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N1	100	Total	C	N	O	S	0	0
			805	499	164	139	3		
20	N2	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 21 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O1	88	Total	C	N	O	S	0	0
			714	439	144	130	1		
21	O2	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 22 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P1	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q1	80	Total	C	N	O	S	0	0
			648	411	121	113	3		
23	Q2	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R1	74	Total	C	N	O	S	0	0
			624	395	122	105	2		
24	R2	74	Total	C	N	O	S	0	0
			626	395	123	107	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S1	83	Total	C	N	O	S	0	0
			663	424	126	111	2		
25	S2	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T1	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 27 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U1	70	Total	C	N	O	S	0	0
			590	366	125	98	1		
27	U2	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	59	Total	C	N	O	P	0	0
			1272	569	242	402	59		

- Molecule 29 is a RNA chain called tRNA-Trp (P/E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
29	W	76	Total	C	N	O	P	S	0	0
			1630	730	286	536	76	2		

- Molecule 30 is a RNA chain called tRNA-Phe (P/E-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
30	W1	33	Total	C	N	O	P	S	0	0
			718	324	133	226	33	2		

- Molecule 31 is a RNA chain called tRNA-Ala (A/P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
31	Y	76	Total	C	N	O	P		0	0
			1628	726	293	533	76			

- Molecule 32 is a RNA chain called tRNA-Val (A/P-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
32	Y1	36	Total	C	N	O	P		0	0
			778	348	142	252	36			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y1	34	CM0	U	variant	GB 1847302804

- Molecule 33 is a protein called 30S ribosomal protein S1.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	Z1	9	Total	C	N	O	0	0
			75	49	10	16		

- Molecule 34 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	a2	223	Total	C	N	O	S		0	0
			1661	1039	302	314	6			

- Molecule 35 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b2	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 36 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	e2	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 37 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	g2	52	Total	C	N	O	0	0
			427	275	78	74		

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h2	136	Total	C	N	O	S	1	0
			1085	692	209	178	6		

- Molecule 39 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i2	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 40 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 41 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o2	51	Total	C	N	O	S	0	0
			377	231	83	62	1		

- Molecule 42 is a protein called Nascent chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	p	10	Total	C	N	O	0	0
			76	47	18	11		

- Molecule 43 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	r2	116	Total	C	N	O	0	0
			891	552	178	161		

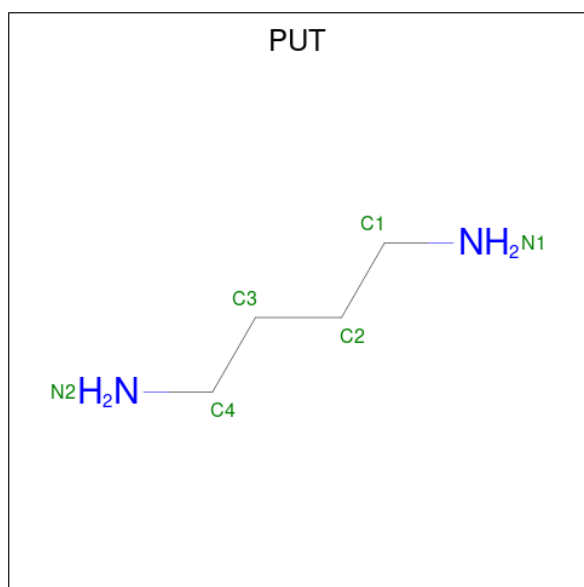
- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	z2	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

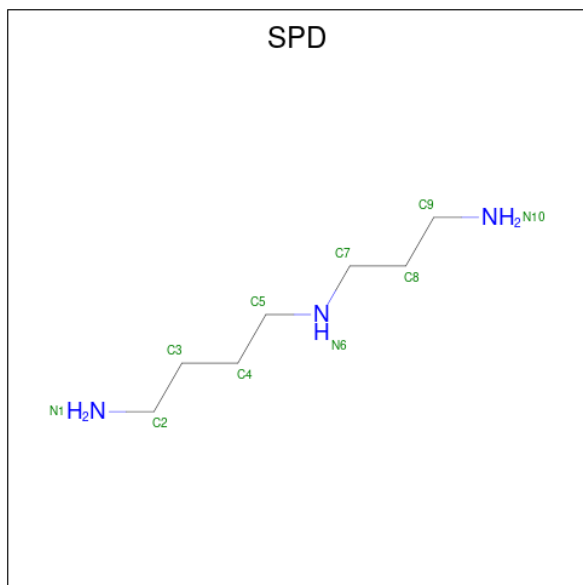
Mol	Chain	Residues	Atoms		AltConf
45	4	1	Total	Zn	0
			1	1	
45	B	1	Total	Zn	0
			1	1	

- Molecule 46 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
46	72	1	Total	C	N	0
			6	4	2	
46	72	1	Total	C	N	0
			6	4	2	

- Molecule 47 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
47	72	1	Total	C	N	0
			10	7	3	

- Molecule 48 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	72	165	Total	Mg	0
			165	165	
48	A1	60	Total	Mg	0
			60	60	
48	A2	41	Total	Mg	0
			41	41	
48	N2	1	Total	Mg	0
			1	1	
48	Y	1	Total	Mg	0
			1	1	
48	o2	1	Total	Mg	0
			1	1	

3 Residue-property plots

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

- Molecule 1: 50S ribosomal protein L28

Chain 12:  96% ..




- Molecule 2: 50S ribosomal protein L30

Chain 32:  97% ..



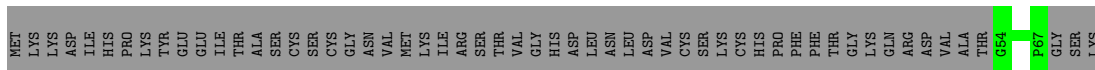
- Molecule 3: Large ribosomal subunit protein bL31A

Chain 4:  91% 6% .



- Molecule 3: Large ribosomal subunit protein bL31A

Chain 41:  20% 80%



- Molecule 4: 50S ribosomal protein L35

Chain 62:  98% .



- Molecule 5: 23S ribosomal RNA

Chain 71:  99%



G	A	A	A	A	U	C	A	A	G	A	G	C	U	G	A	G	G	C	G	U	G	A	C	G	A	G	A	C	A	C	U	A	C	G	U	G	G	C	U	U	G	A	A	C	A	A	U	G	C	C	U	G
C	U	U	C	C	A	G	G	A	A	A	A	G	C	C	U	U	C	U	A	A	A	G	C	A	A	G	U	A	A	C	A	A	U	C	A	A	A	C	C	C	A	A	A	C	C	6M2	G	G				
U	G	U	U	C	A	C	G	G	U	A	A	G	A	A	A	A	C	C	A	A	A	G	A	A	C	C	U	U	G	A	A	C	A	A	U	C	G	G	U	U	A	A	G	G	C	A	A	A	U			
G	G	U	G	C	C	G	U	A	A	C	U	U	C	C	G	A	G	A	A	G	A	G	A	C	C	G	U	G	A	A	U	A	G	G	U	A	A	C	C	A	C	C	U	A	G	A	A	G				
C	U	G	A	A	A	U	C	A	A	G	U	C	G	A	A	A	U	A	C	C	A	G	C	C	G	U	G	C	C	A	A	C	A	C	A	U	A	A	A	C	U	U	A	A	C	U	G	C				
A	A	A	C	A	A	C	G	A	A	A	G	U	G	G	A	A	U	A	C	A	G	G	U	G	C	C	U	A	A	C	C	2M3	C	C	C	G	U	U	G	U	G	C	C	G	A	A	A	U	G			
G	G	U	U	U	A	G	C	G	G	A	A	G	C	C	G	A	A	U	C	U	U	C	A	U	C	C	G	A	A	C	C	C	C	C	C	G	U	A	A	A	A	A	A	A	A	A	U	G				
C	U	C	C	A	A	5M1	U	C	C	U	U	A	G	U	C	C	G	G	A	A	A	G	U	U	C	G	A	A	C	C	U	U	A	U	G	A	A	A	A	A	A	A	A	A	A	A	A	U	G			
C	G	A	A	5M1	U	C	C	U	U	A	G	U	C	C	G	G	A	A	A	A	A	U	A	A	C	C	U	U	A	A	C	C	6M2	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	G			
A	C	G	G	A	A	A	A	G	A	C	C	C	G	U	A	A	A	C	C	U	U	A	A	C	C	U	U	A	A	C	C	2M3	H2U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U			
A	G	G	A	A	A	G	U	G	A	A	G	A	U	U	A	U	U	G	A	A	A	U	A	A	C	C	U	U	A	A	U	U	C	C	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U			
C	C	A	C	C	C	U	U	A	A	C	U	U	G	A	U	U	C	U	A	A	A	C	C	U	U	A	A	C	C	U	U	A	A	6M2	A	A	A	A	A	A	A	A	A	A	A	A	A	A	G			
A	C	G	G	A	A	A	A	G	A	C	C	C	G	U	A	A	A	C	C	U	U	A	A	C	C	U	U	A	A	C	C	U	U	C	C	A	A	A	A	A	A	A	A	A	A	A	A	A	U			
A	G	G	A	A	U	A	A	G	A	A	G	C	C	U	U	A	U	U	G	A	A	A	C	C	U	U	A	A	C	C	U	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U			
C	C	A	C	C	C	U	U	A	A	C	U	U	G	A	U	U	C	U	A	A	A	A	C	C	U	U	A	A	C	C	U	U	G	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U			
G	G	U	G	G	A	G	U	U	U	U	A	U	A	U	A	U	U	C	U	C	U	C	A	A	A	A	A	A	A	A	G	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U			
G	C	U	A	A	5M1	U	C	C	U	U	A	G	U	C	C	G	G	A	A	A	A	G	U	U	C	G	A	A	C	C	U	U	A	U	G	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U		
C	G	U	G	A	A	5M1	U	C	C	U	U	A	G	U	C	C	G	G	A	A	A	A	G	U	U	C	G	A	A	C	C	6M2	H2U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U		
U	C	A	U	A	U	C	G	A	A	C	C	G	G	U	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	DMC	2M4	PSU	G	U	U	C	C	G	G	C	C	C	C	C	C	U				
A	G	U	C	C	C	A	A	G	G	A	U	U	C	C	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	DMU	G	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	U	
C	G	U	G	A	A	PSU	PSU	C	G	U	U	C	C	C	U	U	A	A	U	C	A	A	U	C	A	A	U	C	C	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U			
A	G	U	A	C	G	A	A	G	G	A	C	C	G	G	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	U			
G	C	C	G	G	U	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	A	C			
C	G	A	G	A	U	G	U	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	C	U			

- Molecule 5: 23S ribosomal RNA

G2403	G2403	A2211	G2103	G1929	U1647	A1419	U1173	A983	A799	A222	G1
	G2406	A2225	G2104	G1930	U1648	A1420	U1174	A513	A799	A222	G1
	G2410	G2238	G2110	A1937	U1649	G1421	A1175	C995	G805	G248	A10
	G2423	G2239	G2112	A1938	G1674	C1428	U1176	A996	C812	G252	G15
	U2425	U2243	U2113	U1939	C1675	A1434	G1177	U999	A819	C276	U34
A2566	G2424	A2117	U1985	G1715	G1452	A1453	U1180	C1005	A547	U276	G43
G2567	G2425	G2251	U1986	C1727	U1729	G1461	C1211	C1012	U827	G277	G44
U2571	G2430	A2268	A1960	G1728	U1730	A1453	G1212	C1013	G830	A278	A44
A2572	G2439	U2431	C1961	U1732	G1731	C1461	G1235	A1020	A845	A279	G45
C2573	U2431	A2278	C1962	U1733	G1731	G1475	G1236	A1021	U847	G283	G46
U2580	U2441	G2279	U1963	G1734	G1731	U1476	G1247	G1026	U847	G285	G55
G2581	U2441	G2279	U1964	G1735	G1734	G1476	A1247	G1026	A575	U286	A71
G2582	G2445	C2283	U2130	C1965	G1738	G1482	G1248	G1026	G858	A311	A74
U2586	A2448	A2287	U2131	C1967	C1764	C1488	U1249	U1033	C859	A311	A74
A2602	U2449	U2305	U2132	A1970	A1773	C1489	G1250	A1046	C869	A330	A75
G2603	U2305	U2305	G2133	U1971	U1773	A1490	A1253	G1047	A603	A330	A75
U2604	U2457	G2308	A2137	G1976	U1782	G1492	G1256	G1055	A613	A345	A101
U2605	G2464	C2310	G2141	G1976	A1784	C1493	G1262	G1060	A614	A352	A103
G2608	C2475	A2311	G2141	U1982	A1786	A1494	A1262	U1060	U615	A352	A103
U2609	A2476	U2312	C2146	U1982	A1786	A1494	A1262	U1060	A637	C353	G110
U2613	U2477	G2319	U2151	U1991	A1791	U1497	G1266	A1070	U887	A359	A118
A2614	A2478	U2320	G2152	G1992	G1799	A1503	G1271	U1081	C889	U360	A119
U2615	U2482	U2321	C2153	U1993	C1800	A1508	A1272	U1082	C890	G361	U120
G2629	G2484	A2322	C2161	C1997	A1801	A1509	U1273	U1083	A896	A362	A125
G2630	G2325	G2325	G2161	U2022	G1807	A1515	G1300	A1085	C898	G386	G134
G2663	A2491	A2333	C2164	C2023	A1808	A1515	A1301	A1086	A999	U395	U135
G2689	G2494	A2336	C2165	A2030	C1816	G1524	U1313	G1087	U866	G396	G135
U2690	C2498	G2345	U2166	G2032	G1835	A1532	A1321	A1089	C717	A401	U139
G2714	G2502	U2346	A2169	A2033	G1835	A1532	A1321	A1090	G726	A404	G141
A2726	U2504	C2347	A2170	C2043	A1847	U1539	U1329	U1097	A910	U405	A142
G2732	G2505	C2350	C2171	G2056	A1848	A1566	G1345	G1112	G729	A412	U158
A2733	U2506	G2361	G2175	A2059	C1870	A1569	U1352	A917	A730	A412	G159
C2507	C2507	G2372	A2176	A2060	A1872	U1578	A1365	A918	G745	C455	C163
U2514	U2514	U2372	C2177	A2062	G1873	A1579	G1368	U931	U747	A457	U174
A2518	A2518	G2375	U2182	A2062	A1901	A1580	G1388	U932	G748	A470	G177
G2529	G2529	G2379	G2190	A2062	A1901	C1582	U1379	U932	A749	A470	G178
G2535	G2535	G2383	U2195	C2072	A1913	A1583	G1380	A941	A764	G473	G181
U2537	U2537</										



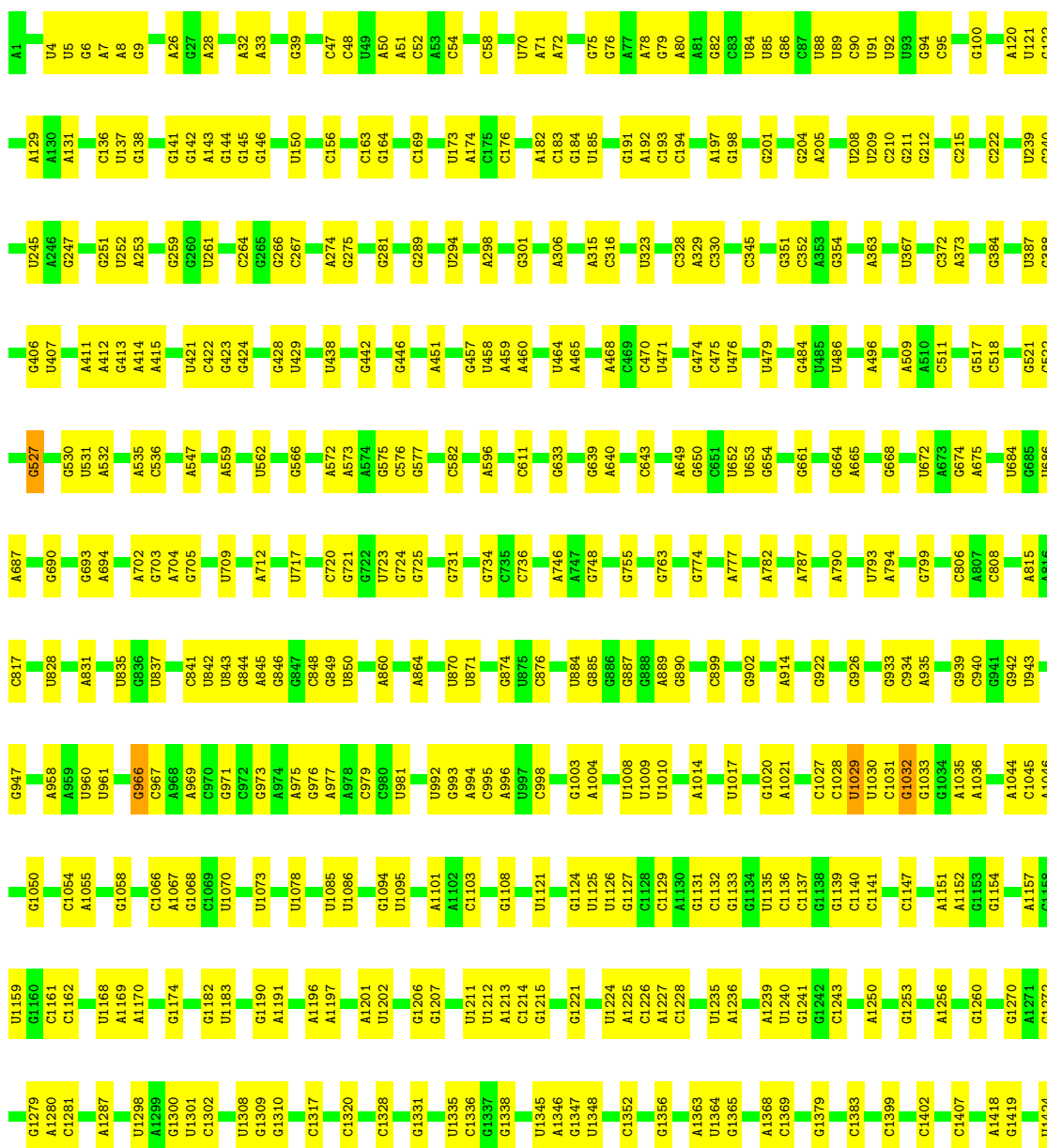
• Molecule 6: 5S ribosomal RNA

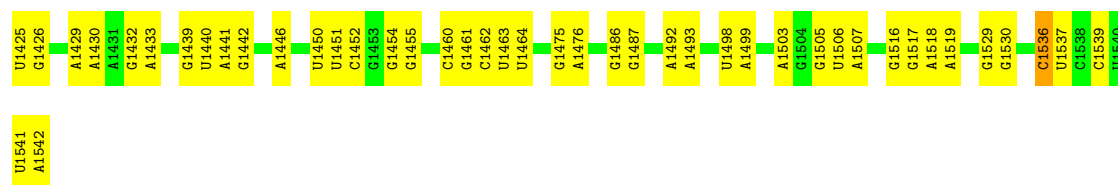
Chain 82: 80% 19%



• Molecule 7: 16S ribosomal RNA

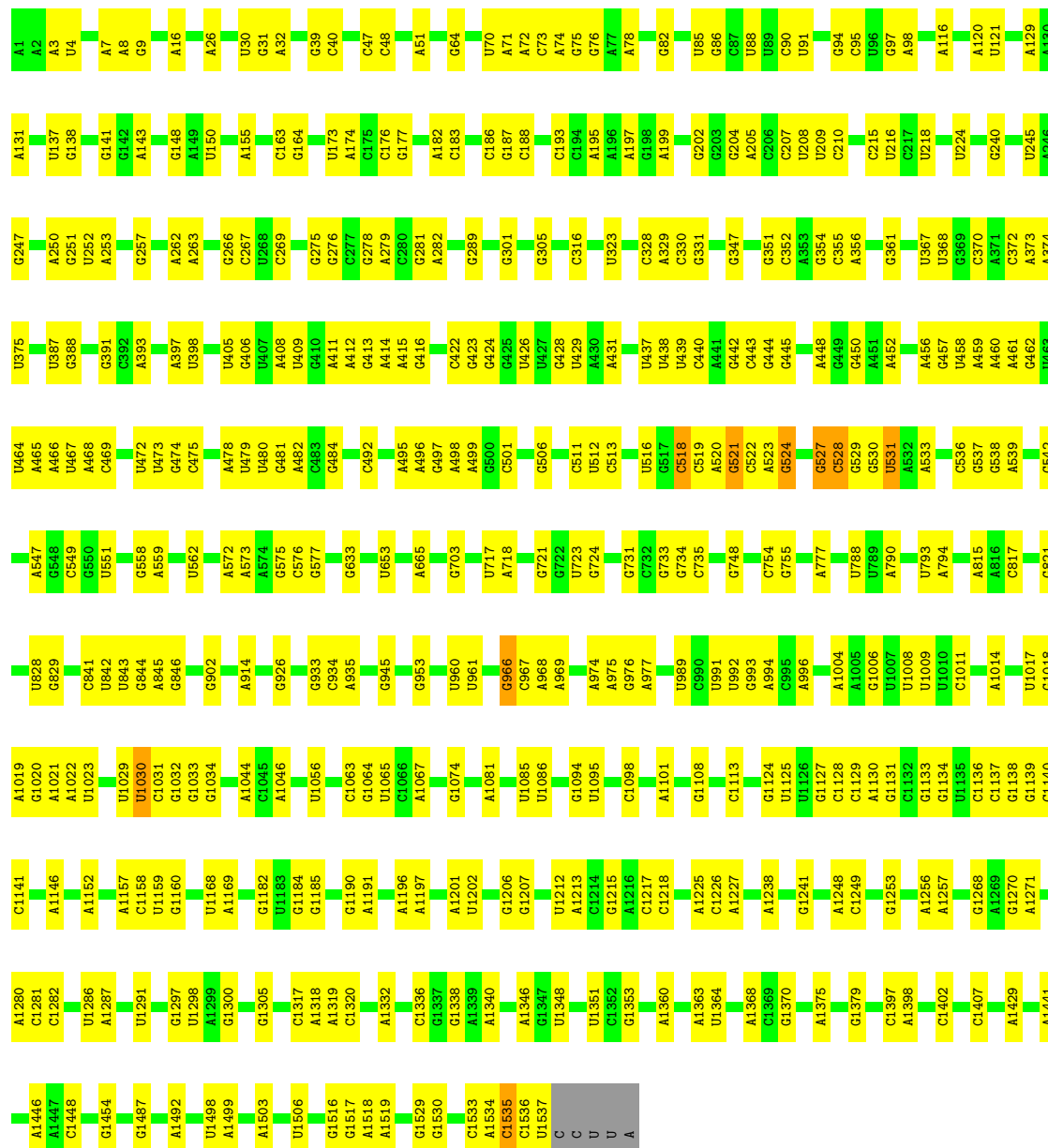
Chain A1: 70% 30%





• Molecule 7: 16S ribosomal RNA

Chain A2: 73% 26%



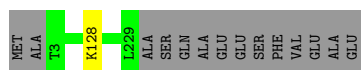
• Molecule 8: Small ribosomal subunit protein uS2

Chain B: 95%



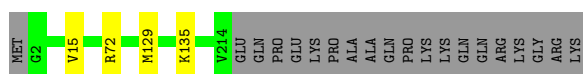
- Molecule 8: Small ribosomal subunit protein uS2

Chain B2: 94% 6%



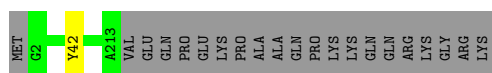
- Molecule 9: Small ribosomal subunit protein uS3

Chain C1: 90% 9%



- Molecule 9: Small ribosomal subunit protein uS3

Chain C2: 91% 9%



- Molecule 10: Small ribosomal subunit protein uS4

Chain D1: 98%



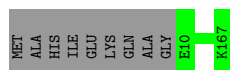
- Molecule 10: Small ribosomal subunit protein uS4

Chain D2: 98%



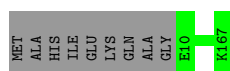
- Molecule 11: Small ribosomal subunit protein uS5

Chain E1: 95% 5%



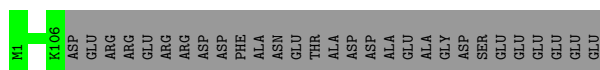
- Molecule 11: Small ribosomal subunit protein uS5

Chain E2: 95% 5%



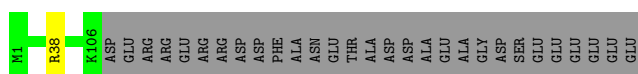
- Molecule 12: 30S ribosomal protein S6

Chain F1: 79% 21%



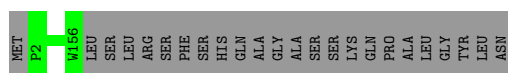
- Molecule 12: 30S ribosomal protein S6

Chain F2: 78% 21%



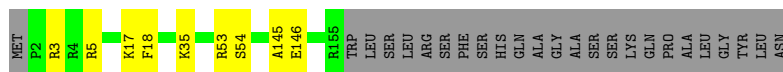
- Molecule 13: 30S ribosomal protein S7

Chain G1: 87% 13%



- Molecule 13: 30S ribosomal protein S7

Chain G2: 81% 5% 14%



- Molecule 14: Small ribosomal subunit protein uS8

Chain H1: 99% .



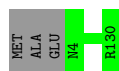
- Molecule 14: Small ribosomal subunit protein uS8

Chain H2: 99% .



- Molecule 15: Small ribosomal subunit protein uS9

Chain I1: 98% .



- Molecule 15: Small ribosomal subunit protein uS9

Chain I2: 99% .



- Molecule 16: 30S ribosomal protein S10

Chain J1: 99% .



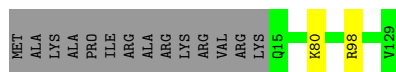
- Molecule 16: 30S ribosomal protein S10

Chain J2: 92% 5% .



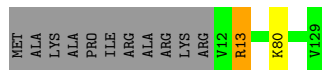
- Molecule 17: Small ribosomal subunit protein uS11

Chain K1: 88% 11% .



- Molecule 17: Small ribosomal subunit protein uS11

Chain K2: 90% 9% ..



- Molecule 18: Small ribosomal subunit protein uS12

Chain L1: 98% ..



- Molecule 18: Small ribosomal subunit protein uS12

Chain L2: 99% .



- Molecule 19: Small ribosomal subunit protein uS13

Chain M1:  97%



- Molecule 19: Small ribosomal subunit protein uS13

Chain M2:  99%



- Molecule 20: Small ribosomal subunit protein uS14

Chain N1:  99%



- Molecule 20: Small ribosomal subunit protein uS14

Chain N2:  99%



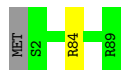
- Molecule 21: 30S ribosomal protein S15

Chain O1:  99%



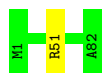
- Molecule 21: 30S ribosomal protein S15

Chain O2:  98%



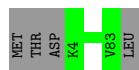
- Molecule 22: 30S ribosomal protein S16

Chain P1:  99%



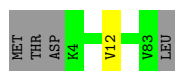
- Molecule 23: Small ribosomal subunit protein uS17

Chain Q1: 95% 5%



- Molecule 23: Small ribosomal subunit protein uS17

Chain Q2: 94% 5%



- Molecule 24: Small ribosomal subunit protein bS18

Chain R1: 97% ..



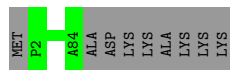
- Molecule 24: Small ribosomal subunit protein bS18

Chain R2: 96% ..



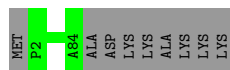
- Molecule 25: Small ribosomal subunit protein uS19

Chain S1: 90% 10%



- Molecule 25: Small ribosomal subunit protein uS19

Chain S2: 90% 10%



- Molecule 26: Small ribosomal subunit protein bS20

Chain T1: 94% 5%

Chain e2:  99% ..



- Molecule 37: 50S ribosomal protein L33

Chain g2:  95% 5%



- Molecule 38: 50S ribosomal protein L16

Chain h2:  100%

There are no outlier residues recorded for this chain.

- Molecule 39: 50S ribosomal protein L9

Chain i2:  98% .



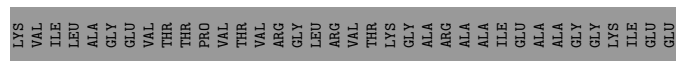
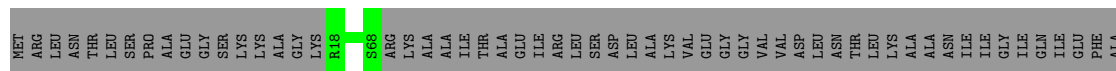
- Molecule 40: 50S ribosomal protein L34

Chain l2:  98% .



- Molecule 41: 50S ribosomal protein L15

Chain o2:  35% 65%



- Molecule 42: Nascent chain

Chain p:  70% 30%





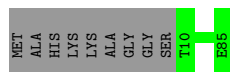
- Molecule 43: 50S ribosomal protein L18

Chain r2:  99% .



- Molecule 44: 50S ribosomal protein L27

Chain z2:  89%  11%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	10748	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 ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k 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, SPD, OMU, MA6, CM0, 1MG, 7MG, 2MA, OMC, 4SU, 5MC, H2U, 3TD, 5MU, MIA, OMG, 4OC, UR3, 6MZ, MG, G7M, PUT, PSU, 2MG

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	12	0.25	0/635	0.63	0/848
2	32	0.22	0/453	0.52	0/605
3	4	0.37	0/543	0.65	1/726 (0.1%)
3	41	0.25	0/120	0.60	0/158
4	62	0.24	0/513	0.56	0/676
5	71	0.16	0/429	0.69	0/664
5	72	0.18	1/69306 (0.0%)	0.70	12/108116 (0.0%)
6	82	0.18	0/2872	0.73	2/4478 (0.0%)
7	A1	0.24	0/36794	0.77	7/57392 (0.0%)
7	A2	0.24	0/36681	0.76	16/57217 (0.0%)
8	B	0.24	0/1846	0.53	0/2488
8	B2	0.25	0/1807	0.50	0/2435
9	C1	0.26	0/1692	0.55	0/2280
9	C2	0.29	0/1685	0.61	0/2270
10	D1	0.25	0/1665	0.53	0/2227
10	D2	0.25	0/1665	0.54	0/2227
11	E1	0.26	0/1179	0.52	0/1584
11	E2	0.26	0/1179	0.52	0/1584
12	F1	0.24	0/881	0.51	0/1189
12	F2	0.25	0/881	0.51	0/1189
13	G1	0.24	0/1246	0.53	0/1672
13	G2	0.28	0/1230	0.58	0/1649
14	H1	0.25	0/989	0.53	0/1326
14	H2	0.25	0/989	0.53	0/1326
15	I1	0.25	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.25	0/827	0.61	0/1117
16	J2	0.25	0/813	0.63	0/1100
17	K1	0.26	0/873	0.56	0/1180
17	K2	0.28	0/900	0.57	0/1215
18	L1	0.26	0/969	0.60	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	L2	0.26	0/969	0.61	0/1300
19	M1	0.25	0/900	0.57	0/1204
19	M2	0.24	0/919	0.58	0/1226
20	N1	0.26	0/817	0.60	0/1088
20	N2	0.25	0/817	0.57	0/1088
21	O1	0.23	0/722	0.55	0/964
21	O2	0.23	0/722	0.57	0/964
22	P1	0.25	0/659	0.60	0/884
23	Q1	0.27	0/657	0.58	0/881
23	Q2	0.25	0/657	0.58	0/881
24	R1	0.24	0/635	0.57	0/849
24	R2	0.25	0/637	0.62	0/851
25	S1	0.25	0/680	0.52	0/915
25	S2	0.26	0/680	0.53	0/915
26	T1	0.25	0/676	0.53	0/895
27	U1	0.26	0/598	0.61	0/792
27	U2	0.25	0/598	0.58	0/792
28	V2	0.32	0/1427	0.92	6/2224 (0.3%)
29	W	0.40	1/1604 (0.1%)	1.29	5/2496 (0.2%)
30	W1	0.28	0/677	0.89	0/1052
31	Y	0.35	1/1725 (0.1%)	0.79	2/2687 (0.1%)
32	Y1	0.20	0/786	0.79	0/1216
33	Z1	0.26	0/76	0.35	0/101
34	a2	0.24	0/1676	0.49	0/2259
35	b2	0.26	0/2121	0.59	0/2852
36	e2	0.25	0/1444	0.52	0/1937
37	g2	0.25	0/434	0.51	0/576
38	h2	0.25	0/1104	0.57	0/1474
39	i2	0.26	0/1122	0.55	0/1515
40	l2	0.24	0/380	0.63	0/498
41	o2	0.26	0/383	0.67	0/501
42	p	0.72	0/77	0.64	0/104
43	r2	0.25	0/901	0.59	0/1209
44	z2	0.26	0/589	0.54	0/779
All	All	0.23	3/202613 (0.0%)	0.71	51/304976 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	12	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	1
9	C2	0	1
10	D1	0	2
10	D2	0	1
13	G2	0	3
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
34	a2	0	1
39	i2	0	1
All	All	0	17

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	1	G	OP3-P	-10.65	1.48	1.61
31	Y	1	G	OP3-P	-10.59	1.48	1.61
29	W	1	A	OP3-P	-10.58	1.48	1.61

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	43	G	O5'-P-OP2	-28.03	77.06	110.70
29	W	43	G	OP1-P-OP2	-27.59	78.22	119.60
29	W	43	G	O5'-P-OP1	15.97	129.86	110.70
29	W	42	G	OP1-P-O3'	-14.70	72.86	105.20
29	W	42	G	OP2-P-O3'	14.49	137.08	105.20

There are no chirality outliers.

5 of 17 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	12	74	ARG	Sidechain
3	4	56	ARG	Sidechain
9	C2	42	TYR	Mainchain
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	12	75/78 (96%)	72 (96%)	3 (4%)	0	100	100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	34
3	4	66/70 (94%)	55 (83%)	11 (17%)	0	100	100
3	41	12/70 (17%)	10 (83%)	2 (17%)	0	100	100
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	B	231/241 (96%)	193 (84%)	34 (15%)	4 (2%)	7	36
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100	100
9	C1	211/233 (91%)	185 (88%)	24 (11%)	2 (1%)	14	51
9	C2	210/233 (90%)	185 (88%)	25 (12%)	0	100	100
10	D1	203/206 (98%)	183 (90%)	19 (9%)	1 (0%)	25	64
10	D2	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
11	E1	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
11	E2	156/167 (93%)	152 (97%)	4 (3%)	0	100	100
12	F1	104/135 (77%)	104 (100%)	0	0	100	100
12	F2	104/135 (77%)	80 (77%)	23 (22%)	1 (1%)	13	49
13	G1	153/179 (86%)	151 (99%)	2 (1%)	0	100	100
13	G2	152/179 (85%)	122 (80%)	24 (16%)	6 (4%)	2	19
14	H1	127/130 (98%)	127 (100%)	0	0	100	100
14	H2	127/130 (98%)	127 (100%)	0	0	100	100
15	I1	125/130 (96%)	103 (82%)	22 (18%)	0	100	100
15	I2	127/130 (98%)	117 (92%)	10 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J1	100/103 (97%)	92 (92%)	8 (8%)	0	100	100
16	J2	98/103 (95%)	86 (88%)	9 (9%)	3 (3%)	3	22
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	14	51
17	K2	116/129 (90%)	100 (86%)	15 (13%)	1 (1%)	14	51
18	L1	121/124 (98%)	115 (95%)	5 (4%)	1 (1%)	16	54
18	L2	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
19	M1	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	M2	115/118 (98%)	108 (94%)	7 (6%)	0	100	100
20	N1	98/101 (97%)	86 (88%)	12 (12%)	0	100	100
20	N2	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
21	O1	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
21	O2	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P1	80/82 (98%)	75 (94%)	5 (6%)	0	100	100
23	Q1	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
23	Q2	78/84 (93%)	75 (96%)	2 (3%)	1 (1%)	10	42
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9	40
24	R2	72/75 (96%)	53 (74%)	18 (25%)	1 (1%)	9	40
25	S1	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
25	S2	81/92 (88%)	79 (98%)	2 (2%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	5	28
27	U1	68/71 (96%)	58 (85%)	10 (15%)	0	100	100
27	U2	68/71 (96%)	60 (88%)	8 (12%)	0	100	100
33	Z1	7/557 (1%)	7 (100%)	0	0	100	100
34	a2	221/234 (94%)	201 (91%)	15 (7%)	5 (2%)	5	29
35	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
36	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
37	g2	50/55 (91%)	50 (100%)	0	0	100	100
38	h2	135/136 (99%)	135 (100%)	0	0	100	100
39	i2	147/149 (99%)	120 (82%)	25 (17%)	2 (1%)	9	40
40	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
41	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	p	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
43	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
44	z2	74/85 (87%)	74 (100%)	0	0	100	100
All	All	6206/7310 (85%)	5715 (92%)	458 (7%)	33 (0%)	27	64

5 of 33 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
13	G2	18	PHE
13	G2	35	LYS
13	G2	146	GLU
23	Q2	12	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	12	67/68 (98%)	66 (98%)	1 (2%)	60	75
2	32	48/49 (98%)	48 (100%)	0	100	100
3	4	60/62 (97%)	58 (97%)	2 (3%)	33	54
3	41	12/62 (19%)	12 (100%)	0	100	100
4	62	51/52 (98%)	51 (100%)	0	100	100
8	B	192/199 (96%)	192 (100%)	0	100	100
8	B2	189/199 (95%)	188 (100%)	1 (0%)	86	89
9	C1	173/190 (91%)	171 (99%)	2 (1%)	67	79
9	C2	172/190 (90%)	172 (100%)	0	100	100
10	D1	172/173 (99%)	172 (100%)	0	100	100
10	D2	172/173 (99%)	170 (99%)	2 (1%)	67	79
11	E1	120/126 (95%)	120 (100%)	0	100	100
11	E2	120/126 (95%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	F1	92/116 (79%)	92 (100%)	0	100	100
12	F2	92/116 (79%)	92 (100%)	0	100	100
13	G1	128/147 (87%)	128 (100%)	0	100	100
13	G2	127/147 (86%)	127 (100%)	0	100	100
14	H1	104/105 (99%)	104 (100%)	0	100	100
14	H2	104/105 (99%)	104 (100%)	0	100	100
15	I1	105/107 (98%)	105 (100%)	0	100	100
15	I2	106/107 (99%)	106 (100%)	0	100	100
16	J1	89/90 (99%)	89 (100%)	0	100	100
16	J2	88/90 (98%)	88 (100%)	0	100	100
17	K1	88/99 (89%)	88 (100%)	0	100	100
17	K2	91/99 (92%)	90 (99%)	1 (1%)	70	80
18	L1	103/104 (99%)	103 (100%)	0	100	100
18	L2	103/104 (99%)	103 (100%)	0	100	100
19	M1	93/96 (97%)	93 (100%)	0	100	100
19	M2	95/96 (99%)	95 (100%)	0	100	100
20	N1	83/84 (99%)	83 (100%)	0	100	100
20	N2	83/84 (99%)	83 (100%)	0	100	100
21	O1	76/77 (99%)	76 (100%)	0	100	100
21	O2	76/77 (99%)	76 (100%)	0	100	100
22	P1	65/65 (100%)	65 (100%)	0	100	100
23	Q1	74/78 (95%)	74 (100%)	0	100	100
23	Q2	74/78 (95%)	74 (100%)	0	100	100
24	R1	64/65 (98%)	64 (100%)	0	100	100
24	R2	64/65 (98%)	63 (98%)	1 (2%)	58	74
25	S1	72/79 (91%)	72 (100%)	0	100	100
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	63 (97%)	2 (3%)	35	55
27	U1	60/61 (98%)	59 (98%)	1 (2%)	56	72
27	U2	60/61 (98%)	60 (100%)	0	100	100
33	Z1	8/461 (2%)	8 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
34	a2	174/181 (96%)	174 (100%)	0	100	100
35	b2	216/218 (99%)	216 (100%)	0	100	100
36	e2	149/150 (99%)	148 (99%)	1 (1%)	81	87
37	g2	47/49 (96%)	47 (100%)	0	100	100
38	h2	110/109 (101%)	110 (100%)	0	100	100
39	i2	114/114 (100%)	114 (100%)	0	100	100
40	l2	38/38 (100%)	37 (97%)	1 (3%)	41	61
41	o2	35/103 (34%)	35 (100%)	0	100	100
42	p	5/5 (100%)	2 (40%)	3 (60%)	0	0
43	r2	86/87 (99%)	86 (100%)	0	100	100
44	z2	58/63 (92%)	58 (100%)	0	100	100
All	All	5184/5994 (86%)	5166 (100%)	18 (0%)	90	91

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
40	l2	3	ARG
42	p	35	TRP
42	p	34	ARG
17	K2	13	ARG
36	e2	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
18	L2	29	GLN
35	b2	243	HIS
15	I1	75	GLN
15	I2	75	GLN
17	K1	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	58/59 (98%)	39 (67%)	8 (13%)
29	W	74/76 (97%)	28 (37%)	3 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	W1	31/76 (40%)	7 (22%)	2 (6%)
31	Y	75/76 (98%)	19 (25%)	2 (2%)
32	Y1	32/76 (42%)	5 (15%)	2 (6%)
5	71	17/2904 (0%)	1 (5%)	0
5	72	2899/2904 (99%)	458 (15%)	36 (1%)
6	82	119/120 (99%)	21 (17%)	3 (2%)
7	A1	1538/1542 (99%)	445 (28%)	36 (2%)
7	A2	1533/1542 (99%)	392 (25%)	30 (1%)
All	All	6376/9375 (68%)	1415 (22%)	122 (1%)

5 of 1415 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1907	G
5	72	10	A
5	72	15	G
5	72	34	U
5	72	44	A

5 of 122 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A1	686	U
28	V2	39	A
7	A1	1440	U
28	V2	37	A
31	Y	17	H2U

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

64 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
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
7	5MC	A1	1407	7	18,22,23	4.04	7 (38%)	26,32,35	0.96	2 (7%)
7	5MC	A2	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.00	2 (7%)
5	OMC	72	2498	48,5	19,22,23	3.29	8 (42%)	26,31,34	0.75	0
5	2MG	72	2445	5	18,26,27	2.85	7 (38%)	16,38,41	1.37	3 (18%)
7	MA6	A2	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.37	3 (15%)
5	6MZ	72	2030	5	18,25,26	2.07	4 (22%)	16,36,39	2.33	3 (18%)
7	2MG	A1	1516	7	18,26,27	2.86	7 (38%)	16,38,41	1.35	3 (18%)
30	PSU	W1	32	30	18,21,22	4.66	8 (44%)	22,30,33	1.83	5 (22%)
7	4OC	A2	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.91	1 (3%)
5	PSU	72	955	5	18,21,22	4.68	8 (44%)	22,30,33	1.87	5 (22%)
7	G7M	A1	527	7	20,26,27	2.80	8 (40%)	17,39,42	1.02	1 (5%)
5	G7M	72	2069	5	20,26,27	2.79	8 (40%)	17,39,42	1.03	1 (5%)
32	7MG	Y1	46	32	22,26,27	3.89	10 (45%)	29,39,42	2.03	9 (31%)
30	MIA	W1	37	30	24,31,32	2.34	3 (12%)	26,44,47	2.74	7 (26%)
30	4SU	W1	8	30	18,21,22	3.80	7 (38%)	26,30,33	2.24	5 (19%)
31	H2U	Y	17	31	18,21,22	3.09	5 (27%)	21,30,33	2.02	5 (23%)
30	G7M	W1	46	30	20,26,27	2.82	7 (35%)	17,39,42	1.13	1 (5%)
7	2MG	A2	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.38	3 (18%)
7	2MG	A2	1516	7	18,26,27	2.85	7 (38%)	16,38,41	1.36	3 (18%)
5	6MZ	72	1618	5	18,25,26	2.04	2 (11%)	16,36,39	2.27	4 (25%)
32	CM0	Y1	34	32	23,26,27	3.74	6 (26%)	27,37,40	1.60	3 (11%)
7	5MC	A2	1407	7	18,22,23	4.04	7 (38%)	26,32,35	0.96	2 (7%)
5	5MU	72	1939	5	19,22,23	4.16	15 (78%)	28,32,35	4.12	12 (42%)
5	3TD	72	1915	5	19,22,23	0.83	1 (5%)	21,32,35	0.70	0
7	MA6	A2	1519	7	18,26,27	1.06	2 (11%)	19,38,41	3.38	3 (15%)
5	PSU	72	2504	48,5	18,21,22	4.69	8 (44%)	22,30,33	1.85	5 (22%)
5	1MG	72	745	5	18,26,27	2.74	6 (33%)	19,39,42	1.45	3 (15%)
7	UR3	A1	1498	7	19,22,23	2.77	8 (42%)	26,32,35	1.28	1 (3%)
29	MIA	W	37	29	24,31,32	2.28	3 (12%)	26,44,47	3.01	8 (30%)
5	2MG	72	1835	5	18,26,27	2.84	7 (38%)	16,38,41	1.45	4 (25%)
7	UR3	A2	1498	7	19,22,23	2.78	8 (42%)	26,32,35	1.33	3 (11%)
31	G7M	Y	46	31	20,26,27	2.82	8 (40%)	17,39,42	1.10	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	G7M	A2	527	7	20,26,27	6.09	12 (60%)	17,39,42	1.54	4 (23%)
7	2MG	A2	966	7	18,26,27	2.84	7 (38%)	16,38,41	1.35	3 (18%)
29	G7M	W	46	29	20,26,27	2.81	7 (35%)	17,39,42	1.11	1 (5%)
5	PSU	72	746	5	18,21,22	0.91	1 (5%)	22,30,33	0.61	0
7	5MC	A1	967	7	18,22,23	4.04	7 (38%)	26,32,35	1.02	2 (7%)
5	PSU	72	2605	5	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
7	2MG	A1	966	7	18,26,27	2.84	7 (38%)	16,38,41	1.41	4 (25%)
7	MA6	A1	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.39	3 (15%)
5	2MA	72	2503	48,5	19,25,26	3.61	6 (31%)	21,37,40	3.69	3 (14%)
29	H2U	W	20	29	18,21,22	3.06	5 (27%)	21,30,33	2.03	5 (23%)
29	PSU	W	55	29	18,21,22	5.78	13 (72%)	22,30,33	2.12	5 (22%)
7	4OC	A1	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.89	1 (3%)
5	OMG	72	2251	5,31	18,26,27	2.84	7 (38%)	19,38,41	1.53	4 (21%)
30	PSU	W1	39	30	18,21,22	4.67	8 (44%)	22,30,33	1.85	5 (22%)
7	MA6	A1	1519	7	18,26,27	1.07	2 (11%)	19,38,41	3.40	3 (15%)
31	5MU	Y	54	31	19,22,23	4.12	14 (73%)	28,32,35	3.97	12 (42%)
31	PSU	Y	55	31	18,21,22	5.79	14 (77%)	22,30,33	1.98	5 (22%)
5	H2U	72	2449	48,5	18,21,22	3.05	5 (27%)	21,30,33	2.05	5 (23%)
29	4SU	W	8	29	18,21,22	3.81	7 (38%)	26,30,33	2.28	4 (15%)
5	5MC	72	1962	5	18,22,23	4.04	7 (38%)	26,32,35	1.05	2 (7%)
5	5MU	72	747	5	19,22,23	0.27	0	28,32,35	0.58	0
5	PSU	72	2604	5	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)
5	PSU	72	2457	5	18,21,22	4.65	8 (44%)	22,30,33	1.89	5 (22%)
29	H2U	W	16	29	18,21,22	3.04	5 (27%)	21,30,33	1.99	5 (23%)
29	PSU	W	32	29	18,21,22	4.66	8 (44%)	22,30,33	1.88	5 (22%)
5	3TD	71	1915	5	19,22,23	4.07	7 (36%)	21,32,35	1.75	3 (14%)
29	5MU	W	54	29	19,22,23	4.11	14 (73%)	28,32,35	3.89	14 (50%)
32	6MZ	Y1	37	32	18,25,26	2.05	4 (22%)	16,36,39	2.44	4 (25%)
7	2MG	A1	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.32	3 (18%)
5	PSU	72	2580	5	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
29	H2U	W	17	29	18,21,22	3.06	5 (27%)	21,30,33	2.02	5 (23%)

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
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
5	OMC	72	2498	48,5	-	2/9/27/28	0/2/2/2
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
7	MA6	A2	1518	7	-	0/7/29/30	0/3/3/3
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3
5	G7M	72	2069	5	-	2/3/25/26	0/3/3/3
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
30	MIA	W1	37	30	-	6/11/33/34	0/3/3/3
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
31	H2U	Y	17	31	-	7/7/38/39	0/2/2/2
30	G7M	W1	46	30	-	2/3/25/26	0/3/3/3
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
32	CM0	Y1	34	32	-	4/12/30/31	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
5	5MU	72	1939	5	-	2/7/25/26	0/2/2/2
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2
7	MA6	A2	1519	7	-	2/7/29/30	0/3/3/3
5	PSU	72	2504	48,5	-	0/7/25/26	0/2/2/2
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
29	MIA	W	37	29	-	6/11/33/34	0/3/3/3
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
31	G7M	Y	46	31	-	2/3/25/26	0/3/3/3
7	G7M	A2	527	7	-	2/3/25/26	0/3/3/3
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
29	G7M	W	46	29	-	1/3/25/26	0/3/3/3
5	PSU	72	746	5	-	4/7/25/26	0/2/2/2
7	5MC	A1	967	7	-	0/7/25/26	0/2/2/2
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	2MG	A1	966	7	-	0/5/27/28	0/3/3/3
7	MA6	A1	1518	7	-	3/7/29/30	0/3/3/3
5	2MA	72	2503	48,5	-	0/3/25/26	0/3/3/3
29	H2U	W	20	29	-	3/7/38/39	0/2/2/2
29	PSU	W	55	29	-	1/7/25/26	0/2/2/2
7	4OC	A1	1402	7	-	1/9/29/30	0/2/2/2
5	OMG	72	2251	5,31	-	3/5/27/28	0/3/3/3
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
7	MA6	A1	1519	7	-	4/7/29/30	0/3/3/3
31	5MU	Y	54	31	-	0/7/25/26	0/2/2/2
31	PSU	Y	55	31	-	2/7/25/26	0/2/2/2
5	H2U	72	2449	48,5	-	0/7/38/39	0/2/2/2
29	4SU	W	8	29	-	0/7/25/26	0/2/2/2
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
5	5MU	72	747	5	-	1/7/25/26	0/2/2/2
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
5	PSU	72	2457	5	-	0/7/25/26	0/2/2/2
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
29	PSU	W	32	29	-	3/7/25/26	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
29	H2U	W	17	29	-	2/7/38/39	0/2/2/2

The worst 5 of 438 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	527	G7M	C2'-C1'	-18.04	1.26	1.53
32	Y1	34	CM0	C6-C5	12.73	1.48	1.34
5	71	1915	3TD	C6-C5	12.65	1.50	1.35
5	72	955	PSU	C6-C5	12.25	1.49	1.35
5	72	2504	PSU	C6-C5	12.20	1.49	1.35

The worst 5 of 247 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2503	2MA	C1'-N9-C4	15.11	153.20	126.64
7	A1	1519	MA6	N1-C6-N6	-12.36	104.05	117.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	1519	MA6	N1-C6-N6	-12.35	104.06	117.06
7	A1	1518	MA6	N1-C6-N6	-12.22	104.19	117.06
7	A2	1518	MA6	N1-C6-N6	-12.12	104.30	117.06

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A1	1402	4OC	C1'-C2'-O2'-CM2
7	A1	1518	MA6	C5-C6-N6-C9
7	A1	1518	MA6	C5-C6-N6-C10
7	A1	1519	MA6	C3'-C4'-C5'-O5'
7	A2	527	G7M	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 274 ligands modelled in this entry, 271 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
46	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.52	0
46	PUT	72	3002	-	5,5,5	0.25	0	4,4,4	0.54	0
47	SPD	72	3003	-	9,9,9	0.33	0	8,8,8	0.88	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PUT	72	3001	-	-	1/3/3/3	-
46	PUT	72	3002	-	-	0/3/3/3	-
47	SPD	72	3003	-	-	0/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	72	3001	PUT	C1-C2-C3-C4

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.