



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2025 – 06:21 pm GMT

PDB ID : 8RCT
EMDB ID : EMD-19059
Title : Escherichia coli paused disome complex (Rotated disome interface class 2)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-12-07
Resolution : 5.32 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:

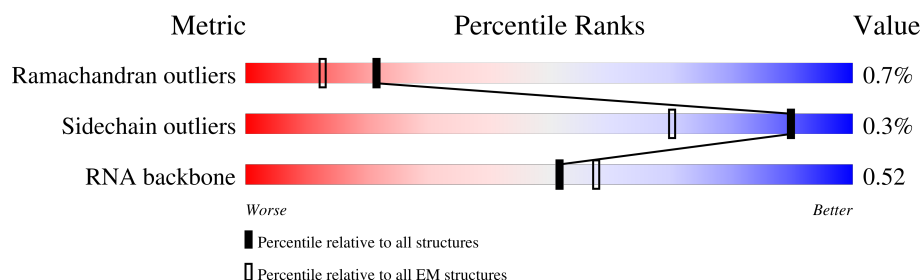
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
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 5.32 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.





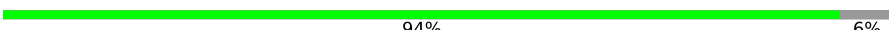







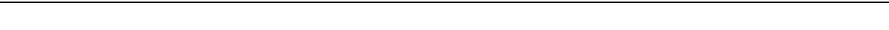

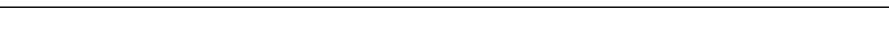
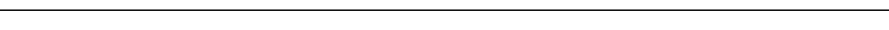
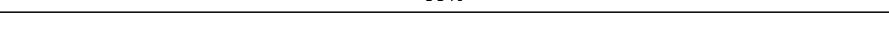
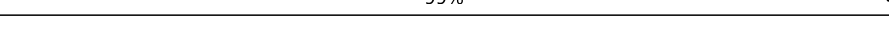
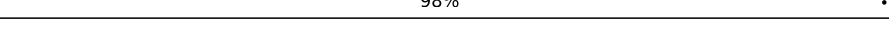
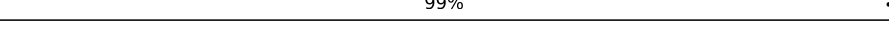
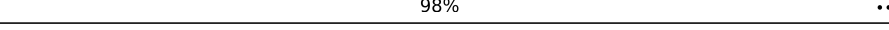
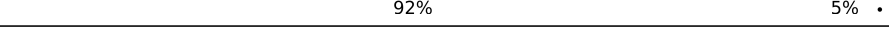


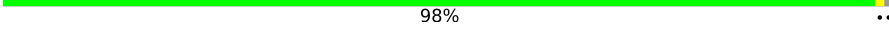
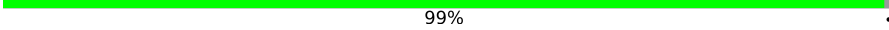
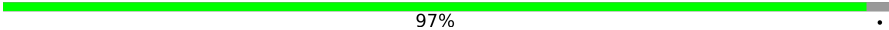
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	94% ..
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%

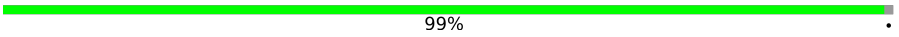
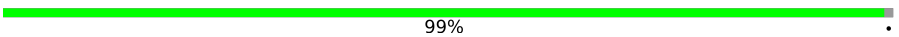
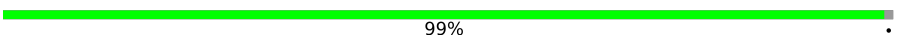
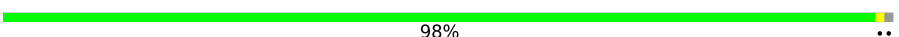
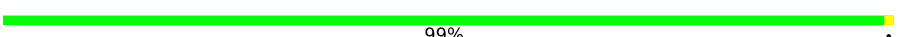
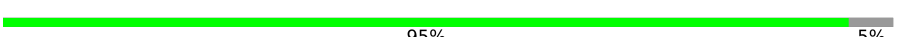




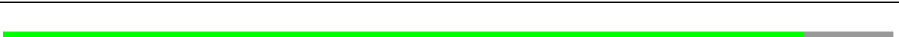


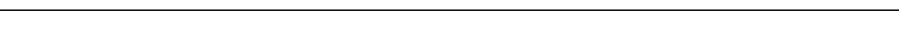
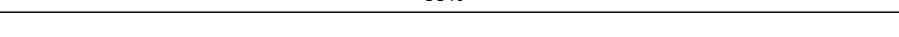
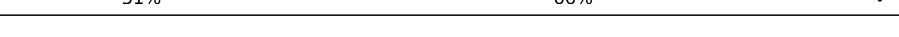



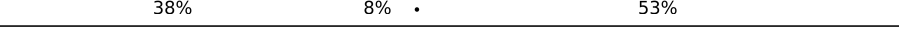
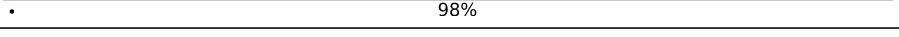
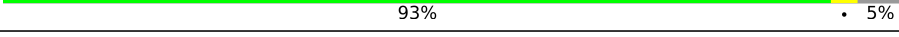
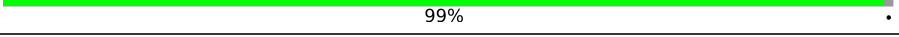
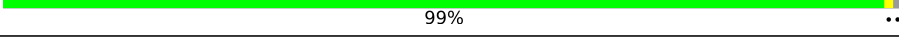
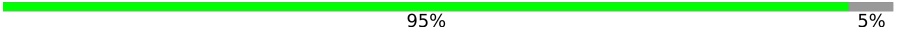
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Mol	Chain	Length	Quality of chain
7	A2	1542	
8	B	241	
8	B2	241	
9	C1	233	
9	C2	233	
10	D1	206	
10	D2	206	
11	E1	167	
11	E2	167	
12	F1	135	
12	F2	135	
13	G1	179	
13	G2	179	
14	H1	130	
14	H2	130	
15	I1	130	
15	I2	130	
16	J1	103	
16	J2	103	
17	K1	129	
17	K2	129	
18	L1	124	
18	L2	124	
19	M1	118	
19	M2	118	


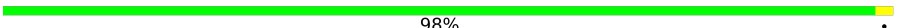

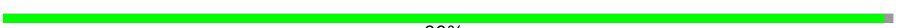
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Mol	Chain	Length	Quality of chain
20	N1	101	 99% .
20	N2	101	 99% .
21	O1	89	 99% .
21	O2	89	 98% ..
22	P1	82	 99% .
23	Q1	84	 95% 5%
23	Q2	84	 94% . 5%
24	R1	75	 97% ..
24	R2	75	 95% . .
25	S1	92	 90% 10%
25	S2	92	 90% 10%
26	T1	87	 94% 5% .
27	U1	71	 97% ..
27	U2	71	 99% .
28	V2	59	 31% 66% .
29	W	76	 54% 37% 9%
30	W1	76	 26% 20% . 53%
31	Y	76	 67% 30% .
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	 95% 5% •
40	l2	46	 98% •
41	o2	144	 35% 65%
42	p	10	 60% 40%
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 187381 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	36	Total	C	N	O	P	S	0	0
			781	352	143	248	36	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		

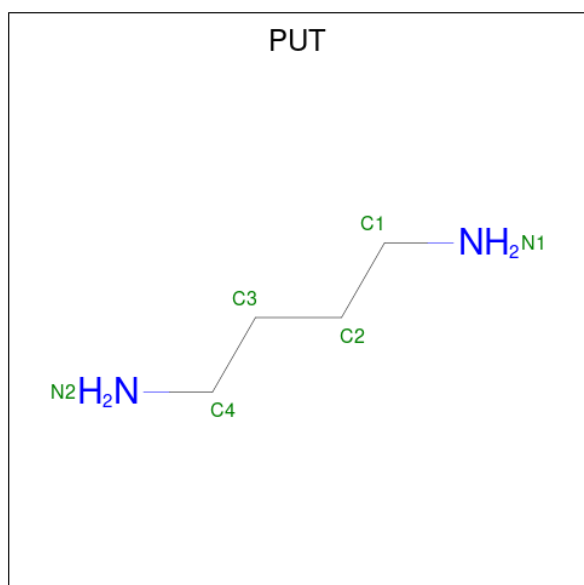
- Molecule 44 is a protein called 50S ribosomal protein L27.

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).

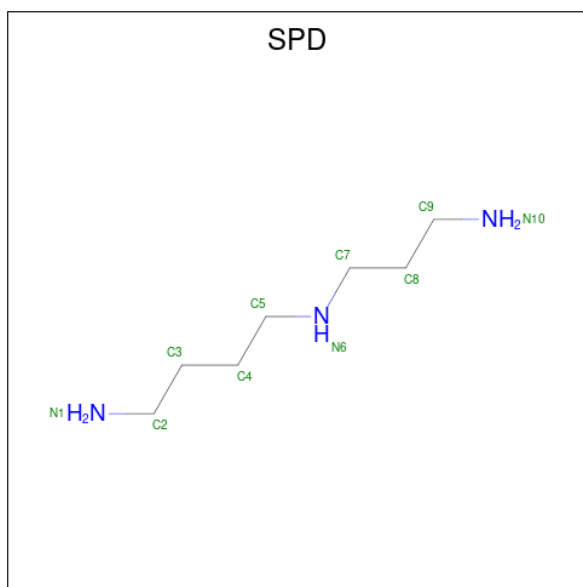
Mol	Chain	Residues	Atoms		AltConf
45	4	1	Total	Zn	0
			1	1	
45	B	1	Total	Zn	0
			1	1	

- 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	163	Total	Mg	0
			163	163	
48	A1	60	Total	Mg	0
			60	60	
48	A2	42	Total	Mg	0
			42	42	
48	Y	2	Total	Mg	0
			2	2	
48	h2	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% ..



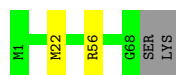
- Molecule 2: 50S ribosomal protein L30

Chain 32:  97% ..



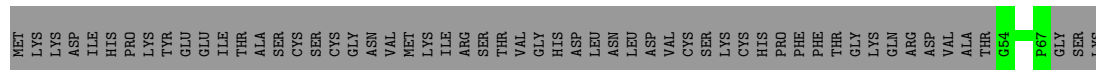
- Molecule 3: Large ribosomal subunit protein bL31A

Chain 4:  94% ..



- 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%





- Molecule 5: 23S ribosomal RNA

A2547	A2548	A2549	G2391	A2198	U2099	A1927	U1647	U1173	A893	A789	A222	G1
G2549	G2550	G2551	U2402	G2204	G2100	A1928	U1648	U1174	C995	G805	G248	A10
			C2403	A2211	G2102	G1930	G1674	G1177	A996	C527	G252	G15
U2552	U2553	U2554	A2406	A2225	C2104	A1937	C1675	G1178	U999	A532	C275	U34
G2555	G2556	G2557	G2410	G2238	G2110	U1939	G1715	G1179	C1005	A547	U276	G43
U2558	U2559	U2560	G2411	G2239	U2111	U1940	C1727	A1452	U012	U827	G277	G43
G2566	G2567	G2568	C2423	A2243	U2113	C1941	G1728	G1211	U012	G549	A278	A44
A2566	A2567	A2568	U2423	U2243	U2117	U1955	U1729	G1212	C1013	G830	A279	G45
G2567	G2568	G2569	A2425	G2251	A2117	U1956	C1730	C1461	A1020	A845	G283	G46
U2571	U2572	U2573	G2429	A2268	U2118	U1960	G1731	U1475	A1021	U846	U284	G55
A2572	A2573	A2574	A2430	A2269	C1961	U1963	G1738	A1453	G1026	A574	G285	A71
G2573	G2574	G2575	U2431	U2278	G2121	U1964	C1764	G1482	U1033	G578	A311	A74
U2580	U2581	U2582	U2441	G2279	A2126	C1965	A1773	C1488	U1033	G858	A311	G75
G2582	G2583	G2584	G2445	C2283	U2130	U1966	U1778	C1489	A1046	G859	A330	A101
U2586	U2587	U2588	A2448	A2287	U2131	C1967	U1782	A1490	G1047	A603	A330	U102
A2586	A2587	A2588	U2449	U2305	G2132	U1970	A1783	G1492	G1055	A613	A345	A103
A2602	A2603	A2604	U2467	U2306	A2133	U1971	A1784	C1493		A614	A352	G110
G2603	G2604	G2605	U2468	G2308	A2134	G1972	A1785	A1494	U1060	U615	C353	
U2604	U2605	U2606	G2464	A2309	U2137	G1975	A1791	U1497	A1070	A637		A118
G2608	G2609	G2610	C2475	G2310	G2141	U1982	G1799	A1503	U1081	C888	G359	A119
U2609	U2610	U2611	U2476	U2312	C2146	U1983	C1800	U1272	U1082	C899	U360	U120
U2613	U2614	U2615	U2477			U1991	A1801	U1273	U1083	G647	A362	A125
A2614	A2615	A2616	A2478	G2319	U2151	U1992	G1807	G1300	U1084	A654	G386	
U2615	U2616	U2617	U2483	U2320	G2152	U1993	A1808	A1301	A1085	A655	G134	U135
U2629	U2630	U2631	G2483	U2321	C2153	C1997	A1809	U1313	G1087	U686	U395	
G2630	G2631	G2632	G2484	A2322	C2161			U1314	A1088	A901	G396	U139
U2633	U2634	U2635	U2491	G2325	U2167	U2022	C1816	A1321	A1089	C902	A401	C140
G2663	G2664	G2665	G2494	A2333	C2164	C2023	G1835	U1329	A1090	G726	A404	G141
U2689	U2690	U2691	G2498	A2336	U2166	A2030	A1847	U1330	U1097	G729	U405	A142
G2714	G2715	G2716	C2498	G2345	G2168	G2032	A1848	C1345	G1112	A730	A412	U158
A2726	A2727	A2728	G2502	A2346	A2169	A2033	C1870	U1352	A917	A910	G455	G159
U2732	U2733	U2734	A2503	C2347	A2170	G2033	A1871	G1131	U1130	G745	C456	C163
G2732	G2733	G2734	U2504	U2172	C2043	C2043	U1872	A1365	U1132	U747	U457	U174
A2732	A2733	A2734	G2505	C2350	U2173	C2055	G1873	A1579	A1133	U931	G748	
U2733	U2734	U27										



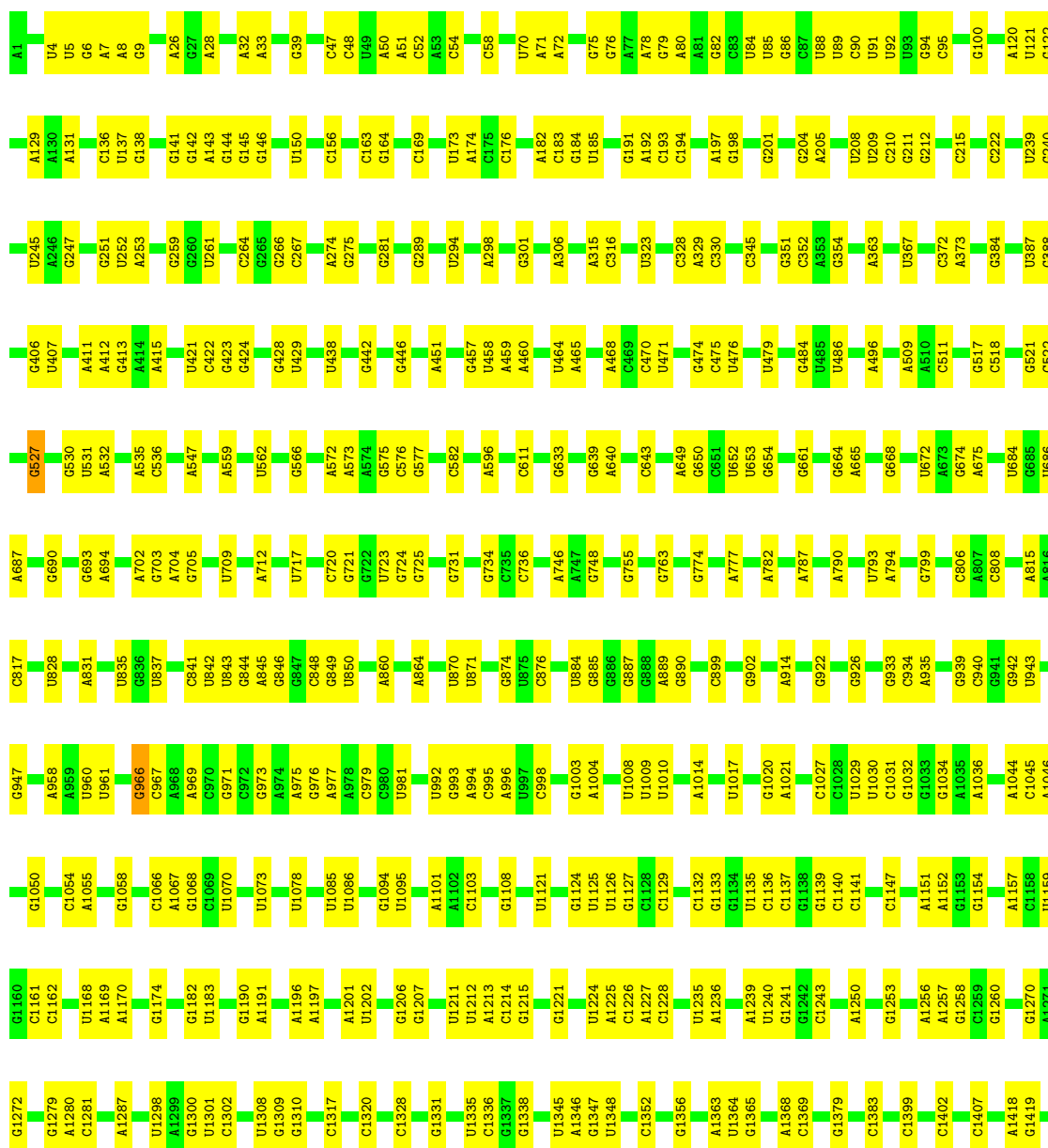
• Molecule 6: 5S ribosomal RNA

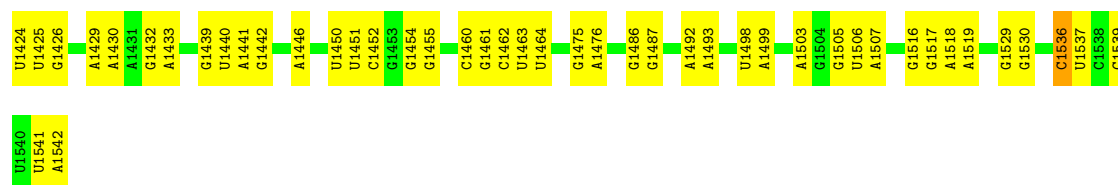
Chain 82: 80% 19%



• Molecule 7: 16S ribosomal RNA

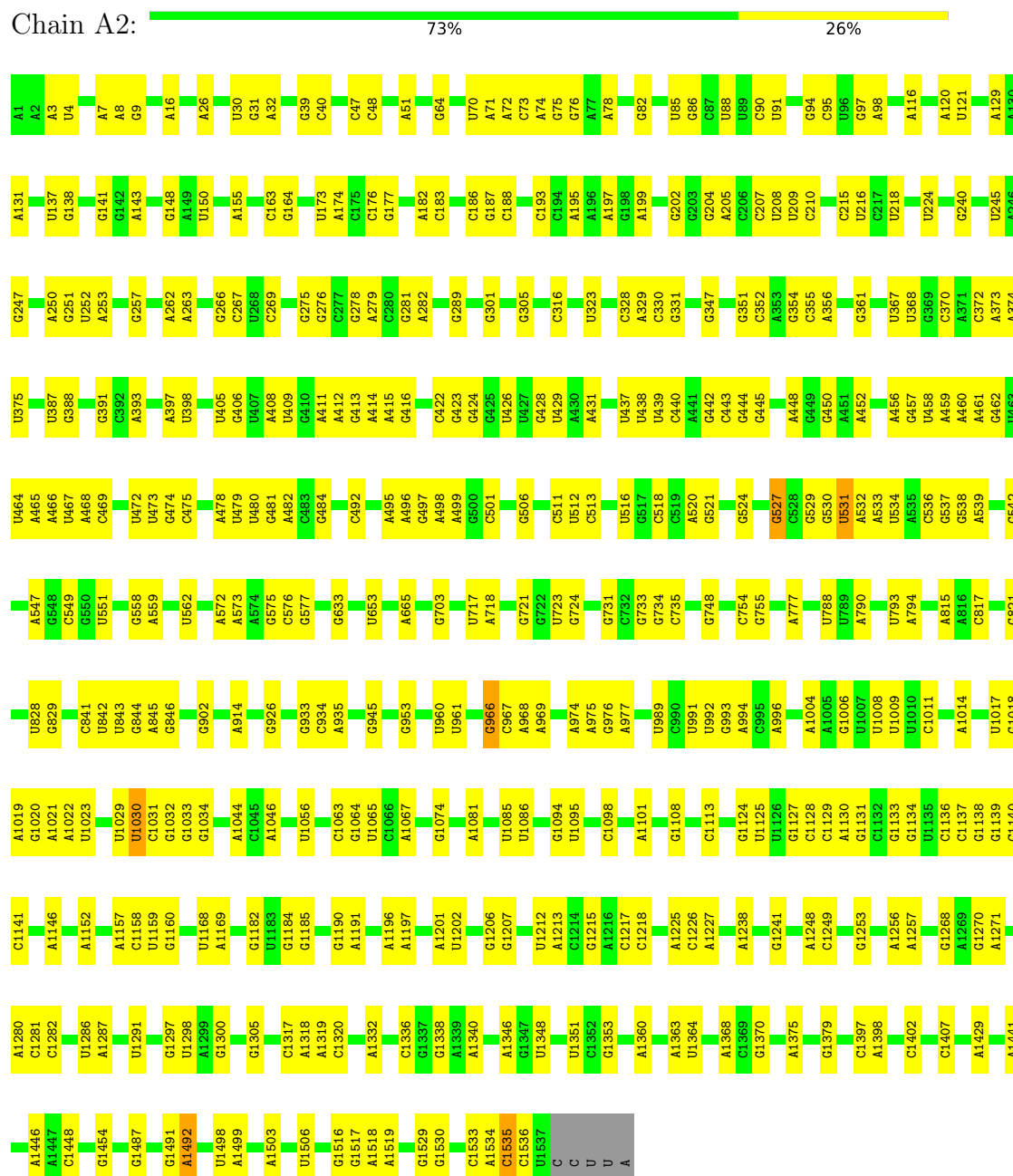
Chain A1: 70% 30%





• Molecule 7: 16S ribosomal RNA

Chain A2:



• Molecule 8: Small ribosomal subunit protein uS2

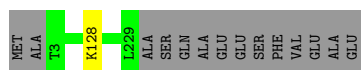
Chain B:

95%



- Molecule 8: Small ribosomal subunit protein uS2

Chain B2: 94% 6%



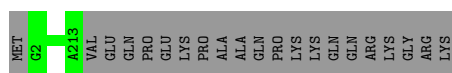
- Molecule 9: Small ribosomal subunit protein uS3

Chain C1: 88% 9%



- Molecule 9: Small ribosomal subunit protein uS3

Chain C2: 91% 9%



- Molecule 10: Small ribosomal subunit protein uS4

Chain D1: 98%



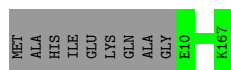
- Molecule 10: Small ribosomal subunit protein uS4

Chain D2: 98%



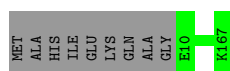
- Molecule 11: Small ribosomal subunit protein uS5

Chain E1: 95% 5%



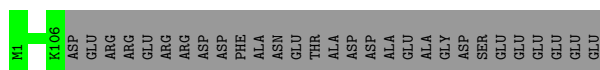
- Molecule 11: Small ribosomal subunit protein uS5

Chain E2: 95% 5%



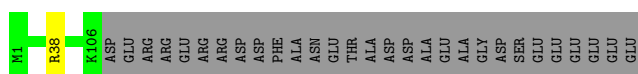
- Molecule 12: 30S ribosomal protein S6

Chain F1: 79% 21%



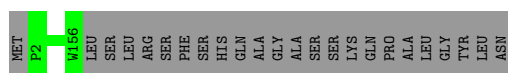
- Molecule 12: 30S ribosomal protein S6

Chain F2: 78% 21%



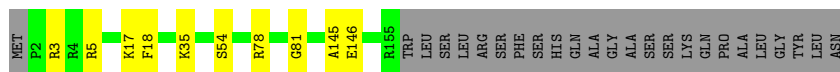
- Molecule 13: 30S ribosomal protein S7

Chain G1: 87% 13%



- Molecule 13: 30S ribosomal protein S7

Chain G2: 80% 6% 14%



- Molecule 14: Small ribosomal subunit protein uS8

Chain H1: 99%



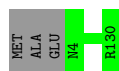
- Molecule 14: Small ribosomal subunit protein uS8

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: 98% ..



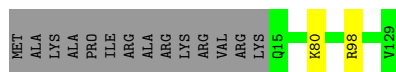
- Molecule 16: 30S ribosomal protein S10

Chain J2: 92% 5% .



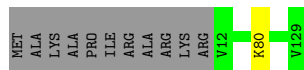
- Molecule 17: Small ribosomal subunit protein uS11

Chain K1: 88% . 11%



- Molecule 17: Small ribosomal subunit protein uS11

Chain K2: 91% . 9%



- Molecule 18: Small ribosomal subunit protein uS12

Chain L1: 98% ..



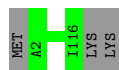
- Molecule 18: Small ribosomal subunit protein uS12

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%



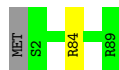
- Molecule 21: 30S ribosomal protein S15

Chain O1:  99%



- Molecule 21: 30S ribosomal protein S15

Chain O2:  98%



- Molecule 22: 30S ribosomal protein S16

Chain P1:  99%

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:  95% 5% •



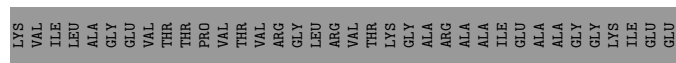
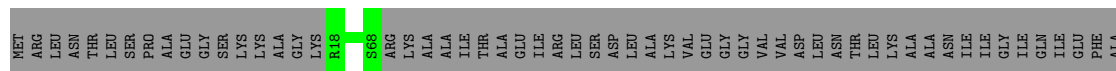
- Molecule 40: 50S ribosomal protein L34

Chain l2:  98% •



- Molecule 41: 50S ribosomal protein L15

Chain o2:  35% 65%



- Molecule 42: Nascent chain

Chain p:  60% 40%





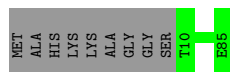
- Molecule 43: 50S ribosomal protein L18

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	6999	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, OMG, 6MZ, UR3, 3TD, MA6, MG, H2U, 4OC, PSU, OMC, 5MU, G7M, CM0, MIA, 2MG, 5MC, OMU, 7MG, 1MG, PUT, 4SU, SPD, 2MA

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	0.53	0/605
3	4	0.25	0/543	0.60	1/726 (0.1%)
3	41	0.25	0/120	0.59	0/158
4	62	0.24	0/513	0.55	0/676
5	71	0.15	0/429	0.69	0/664
5	72	0.18	1/69306 (0.0%)	0.70	15/108116 (0.0%)
6	82	0.18	0/2872	0.74	2/4478 (0.0%)
7	A1	0.22	0/36794	0.76	1/57392 (0.0%)
7	A2	0.22	0/36681	0.75	9/57217 (0.0%)
8	B	0.24	0/1846	0.53	0/2488
8	B2	0.25	0/1807	0.50	0/2435
9	C1	0.25	0/1692	0.56	0/2280
9	C2	0.27	0/1685	0.59	0/2270
10	D1	0.26	0/1665	0.54	0/2227
10	D2	0.24	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	0.26	0/881	0.50	0/1189
13	G1	0.24	0/1246	0.53	0/1672
13	G2	0.25	0/1230	0.56	0/1649
14	H1	0.25	0/989	0.53	0/1326
14	H2	0.25	0/989	0.52	0/1326
15	I1	0.25	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.26	0/827	0.63	0/1117
16	J2	0.25	0/813	0.63	0/1100
17	K1	0.26	0/873	0.55	0/1180
17	K2	0.26	0/900	0.56	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	0.24	0/900	0.57	0/1204
19	M2	0.24	0/919	0.58	0/1226
20	N1	0.25	0/817	0.59	0/1088
20	N2	0.25	0/817	0.58	0/1088
21	O1	0.23	0/722	0.55	0/964
21	O2	0.24	0/722	0.57	0/964
22	P1	0.25	0/659	0.61	0/884
23	Q1	0.27	0/657	0.58	0/881
23	Q2	0.25	0/657	0.56	0/881
24	R1	0.24	0/635	0.57	0/849
24	R2	0.24	0/637	0.61	0/851
25	S1	0.25	0/680	0.52	0/915
25	S2	0.25	0/680	0.53	0/915
26	T1	0.25	0/676	0.54	0/895
27	U1	0.25	0/598	0.61	0/792
27	U2	0.24	0/598	0.58	0/792
28	V2	0.31	0/1427	0.91	5/2224 (0.2%)
29	W	0.39	1/1604 (0.1%)	1.29	5/2496 (0.2%)
30	W1	0.27	0/747	0.88	0/1161
31	Y	0.34	1/1725 (0.1%)	0.78	0/2687
32	Y1	0.20	0/786	0.79	0/1216
33	Z1	0.26	0/76	0.34	0/101
34	a2	0.25	0/1676	0.49	0/2259
35	b2	0.25	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	0.24	0/1104	0.57	0/1474
39	i2	0.31	0/1122	0.57	0/1515
40	l2	0.24	0/380	0.62	0/498
41	o2	0.26	0/383	0.67	0/501
42	p	0.59	0/77	0.66	0/104
43	r2	0.25	0/901	0.58	0/1209
44	z2	0.26	0/589	0.54	0/779
All	All	0.22	3/202683 (0.0%)	0.70	38/305085 (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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Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	1
10	D1	0	1
10	D2	0	1
13	G2	0	3
16	J1	0	1
16	J2	0	2
17	K1	0	1
21	O2	0	1
22	P1	0	1
34	a2	0	1
39	i2	0	3
42	p	0	1
All	All	0	18

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	1	G	OP3-P	-10.61	1.48	1.61
5	72	1	G	OP3-P	-10.59	1.48	1.61
29	W	1	A	OP3-P	-10.57	1.48	1.61

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	43	G	O5'-P-OP2	-28.04	77.05	110.70
29	W	43	G	OP1-P-OP2	-27.57	78.24	119.60
29	W	43	G	O5'-P-OP1	15.99	129.89	110.70
29	W	42	G	OP1-P-O3'	-14.69	72.88	105.20
29	W	42	G	OP2-P-O3'	14.47	137.04	105.20

There are no chirality outliers.

5 of 18 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	12	74	ARG	Sidechain
3	4	56	ARG	Sidechain
10	D1	104	ARG	Sidechain
10	D2	104	ARG	Sidechain
13	G2	3	ARG	Sidechain

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	33
3	4	66/70 (94%)	57 (86%)	9 (14%)	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	35
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100	100
9	C1	211/233 (91%)	178 (84%)	26 (12%)	7 (3%)	3	20
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%)	121 (80%)	24 (16%)	7 (5%)	2	16
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%)	116 (91%)	11 (9%)	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	21
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	14	51
17	K2	116/129 (90%)	101 (87%)	14 (12%)	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%)	84 (86%)	14 (14%)	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	41
24	R1	72/75 (96%)	65 (90%)	6 (8%)	1 (1%)	9	39
24	R2	72/75 (96%)	53 (74%)	17 (24%)	2 (3%)	4	24
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	26
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	27
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%)	115 (78%)	26 (18%)	6 (4%)	2	17
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%)	5 (62%)	2 (25%)	1 (12%)	0	4
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%)	5700 (92%)	461 (7%)	45 (1%)	21	56

5 of 45 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C1	15	VAL
13	G2	18	PHE
13	G2	35	LYS
13	G2	54	SER
13	G2	146	GLU

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%)	60 (100%)	0	100	100
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%)	172 (99%)	1 (1%)	84	88
9	C2	172/190 (90%)	172 (100%)	0	100	100
10	D1	172/173 (99%)	170 (99%)	2 (1%)	67	79
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%)	91 (100%)	0	100	100
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	60
41	o2	35/103 (34%)	35 (100%)	0	100	100
42	p	5/5 (100%)	3 (60%)	2 (40%)	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%)	5169 (100%)	15 (0%)	90	92

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	R2	7	ARG
42	p	34	ARG
26	T1	49	LYS
42	p	35	TRP
36	e2	3	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
15	I2	75	GLN
17	K2	119	ASN
18	L2	29	GLN
12	F2	46	GLN
13	G2	148	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	58/59 (98%)	40 (68%)	9 (15%)
29	W	74/76 (97%)	28 (37%)	3 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	W1	34/76 (44%)	10 (29%)	2 (5%)
31	Y	75/76 (98%)	21 (28%)	2 (2%)
32	Y1	32/76 (42%)	5 (15%)	2 (6%)
5	71	17/2904 (0%)	1 (5%)	0
5	72	2899/2904 (99%)	460 (15%)	38 (1%)
6	82	119/120 (99%)	21 (17%)	3 (2%)
7	A1	1538/1542 (99%)	447 (29%)	36 (2%)
7	A2	1533/1542 (99%)	393 (25%)	30 (1%)
All	All	6379/9375 (68%)	1426 (22%)	125 (1%)

5 of 1426 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 125 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A1	575	G
28	V2	35	A
7	A1	1335	U
28	V2	31	U
29	W	48	U

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	PSU	72	2504	5	18,21,22	4.69	8 (44%)	22,30,33	1.83	5 (22%)
7	UR3	A2	1498	7	19,22,23	2.79	8 (42%)	26,32,35	1.32	3 (11%)
7	5MC	A2	1407	7	18,22,23	4.04	7 (38%)	26,32,35	0.97	2 (7%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.69	5 (19%)
29	H2U	W	16	29	18,21,22	3.04	5 (27%)	21,30,33	1.99	5 (23%)
31	H2U	Y	17	31	18,21,22	3.08	5 (27%)	21,30,33	2.02	5 (23%)
7	4OC	A1	1402	7	20,23,24	3.25	8 (40%)	26,32,35	0.89	1 (3%)
30	G7M	W1	46	30	20,26,27	2.82	7 (35%)	17,39,42	1.13	1 (5%)
29	MIA	W	37	29	24,31,32	2.32	3 (12%)	26,44,47	3.04	8 (30%)
30	MIA	W1	37	30	24,31,32	2.36	3 (12%)	26,44,47	2.76	7 (26%)
7	5MC	A1	967	7	18,22,23	4.06	7 (38%)	26,32,35	1.02	2 (7%)
5	5MC	72	1962	5	18,22,23	4.03	7 (38%)	26,32,35	1.07	2 (7%)
29	5MU	W	54	29	19,22,23	4.09	14 (73%)	28,32,35	4.01	13 (46%)
32	CM0	Y1	34	32	23,26,27	3.71	6 (26%)	27,37,40	1.58	3 (11%)
7	MA6	A2	1519	7	18,26,27	1.06	2 (11%)	19,38,41	3.35	3 (15%)
30	PSU	W1	32	30	18,21,22	4.65	8 (44%)	22,30,33	1.83	5 (22%)
5	H2U	72	2449	5,48	18,21,22	3.06	5 (27%)	21,30,33	2.04	5 (23%)
5	3TD	71	1915	5	19,22,23	4.08	7 (36%)	21,32,35	1.69	2 (9%)
5	5MU	72	747	5	19,22,23	0.27	0	28,32,35	0.52	0
5	PSU	72	746	5	18,21,22	0.89	1 (5%)	22,30,33	0.61	0
7	4OC	A2	1402	7	20,23,24	3.26	8 (40%)	26,32,35	0.90	1 (3%)
7	5MC	A2	967	7	18,22,23	4.03	7 (38%)	26,32,35	0.99	2 (7%)
7	G7M	A2	527	7	20,26,27	2.79	8 (40%)	17,39,42	1.01	1 (5%)
7	G7M	A1	527	7	20,26,27	2.79	8 (40%)	17,39,42	1.02	1 (5%)
7	2MG	A2	966	7	18,26,27	2.85	7 (38%)	16,38,41	1.34	3 (18%)
32	7MG	Y1	46	32	22,26,27	3.90	10 (45%)	29,39,42	2.04	9 (31%)
31	G7M	Y	46	31	20,26,27	2.82	8 (40%)	17,39,42	1.08	1 (5%)
5	PSU	72	955	5	18,21,22	4.67	8 (44%)	22,30,33	1.86	5 (22%)
5	2MA	72	2503	5,48	19,25,26	3.63	6 (31%)	21,37,40	3.73	3 (14%)
29	PSU	W	32	29	18,21,22	4.67	8 (44%)	22,30,33	1.91	5 (22%)
29	4SU	W	8	29	18,21,22	3.81	7 (38%)	26,30,33	2.26	4 (15%)
29	G7M	W	46	29	20,26,27	2.81	8 (40%)	17,39,42	1.11	1 (5%)
5	PSU	72	2604	5	18,21,22	4.66	8 (44%)	22,30,33	1.86	5 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	2MG	A2	1207	7	18,26,27	2.86	7 (38%)	16,38,41	1.36	3 (18%)
31	5MU	Y	54	31	19,22,23	4.14	14 (73%)	28,32,35	4.14	12 (42%)
32	6MZ	Y1	37	32	18,25,26	2.06	3 (16%)	16,36,39	2.45	4 (25%)
7	5MC	A1	1407	7	18,22,23	4.06	7 (38%)	26,32,35	0.96	2 (7%)
7	UR3	A1	1498	7	19,22,23	2.78	8 (42%)	26,32,35	1.28	2 (7%)
5	2MG	72	1835	5	18,26,27	2.85	6 (33%)	16,38,41	1.43	4 (25%)
7	MA6	A2	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.34	3 (15%)
5	PSU	72	2605	5	18,21,22	4.66	8 (44%)	22,30,33	1.81	5 (22%)
7	2MG	A2	1516	7	18,26,27	2.84	7 (38%)	16,38,41	1.34	3 (18%)
30	PSU	W1	39	30	18,21,22	4.68	8 (44%)	22,30,33	1.82	5 (22%)
5	OMC	72	2498	5,48	19,22,23	3.30	8 (42%)	26,31,34	0.77	0
5	PSU	72	2580	5	18,21,22	4.66	8 (44%)	22,30,33	1.84	6 (27%)
5	6MZ	72	1618	5	18,25,26	2.03	3 (16%)	16,36,39	2.24	4 (25%)
29	PSU	W	55	29	18,21,22	0.87	1 (5%)	22,30,33	0.58	0
5	3TD	72	1915	5	19,22,23	0.82	1 (5%)	21,32,35	0.66	0
5	2MG	72	2445	5	18,26,27	2.85	7 (38%)	16,38,41	1.39	3 (18%)
7	MA6	A1	1519	7	18,26,27	1.06	2 (11%)	19,38,41	3.41	3 (15%)
5	5MU	72	1939	5	19,22,23	4.14	15 (78%)	28,32,35	4.12	12 (42%)
5	OMG	72	2251	5,31	18,26,27	2.85	7 (38%)	19,38,41	1.53	4 (21%)
5	6MZ	72	2030	5	18,25,26	2.06	4 (22%)	16,36,39	2.33	3 (18%)
5	1MG	72	745	5	18,26,27	2.75	6 (33%)	19,39,42	1.43	3 (15%)
29	H2U	W	20	29	18,21,22	3.07	5 (27%)	21,30,33	2.02	5 (23%)
7	2MG	A1	1516	7	18,26,27	2.88	7 (38%)	16,38,41	1.35	3 (18%)
30	4SU	W1	8	30	18,21,22	3.81	7 (38%)	26,30,33	2.24	4 (15%)
7	2MG	A1	1207	7	18,26,27	2.86	6 (33%)	16,38,41	1.34	3 (18%)
31	PSU	Y	55	31	18,21,22	0.87	1 (5%)	22,30,33	0.58	0
5	PSU	72	2457	5	18,21,22	4.67	8 (44%)	22,30,33	1.87	5 (22%)
7	2MG	A1	966	7	18,26,27	2.85	6 (33%)	16,38,41	1.40	4 (25%)
7	MA6	A1	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.37	3 (15%)
29	H2U	W	17	29	18,21,22	3.06	5 (27%)	21,30,33	2.02	5 (23%)
5	G7M	72	2069	5	20,26,27	2.80	8 (40%)	17,39,42	1.04	1 (5%)

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	PSU	72	2504	5	-	0/7/25/26	0/2/2/2
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
31	H2U	Y	17	31	-	7/7/38/39	0/2/2/2
7	4OC	A1	1402	7	-	1/9/29/30	0/2/2/2
30	G7M	W1	46	30	-	2/3/25/26	0/3/3/3
29	MIA	W	37	29	-	6/11/33/34	0/3/3/3
30	MIA	W1	37	30	-	4/11/33/34	0/3/3/3
7	5MC	A1	967	7	-	1/7/25/26	0/2/2/2
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2
32	CM0	Y1	34	32	-	4/12/30/31	0/2/2/2
7	MA6	A2	1519	7	-	2/7/29/30	0/3/3/3
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
5	H2U	72	2449	5,48	-	0/7/38/39	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
5	5MU	72	747	5	-	2/7/25/26	0/2/2/2
5	PSU	72	746	5	-	4/7/25/26	0/2/2/2
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
7	G7M	A2	527	7	-	3/3/25/26	0/3/3/3
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
31	G7M	Y	46	31	-	2/3/25/26	0/3/3/3
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
5	2MA	72	2503	5,48	-	0/3/25/26	0/3/3/3
29	PSU	W	32	29	-	5/7/25/26	0/2/2/2
29	4SU	W	8	29	-	0/7/25/26	0/2/2/2
29	G7M	W	46	29	-	1/3/25/26	0/3/3/3
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
31	5MU	Y	54	31	-	0/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MA6	A2	1518	7	-	2/7/29/30	0/3/3/3
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
5	OMC	72	2498	5,48	-	2/9/27/28	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
29	PSU	W	55	29	-	0/7/25/26	0/2/2/2
5	3TD	72	1915	5	-	0/7/25/26	0/2/2/2
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
7	MA6	A1	1519	7	-	3/7/29/30	0/3/3/3
5	5MU	72	1939	5	-	3/7/25/26	0/2/2/2
5	OMG	72	2251	5,31	-	3/5/27/28	0/3/3/3
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
29	H2U	W	20	29	-	3/7/38/39	0/2/2/2
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
31	PSU	Y	55	31	-	0/7/25/26	0/2/2/2
5	PSU	72	2457	5	-	0/7/25/26	0/2/2/2
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
29	H2U	W	17	29	-	2/7/38/39	0/2/2/2
5	G7M	72	2069	5	-	2/3/25/26	0/3/3/3

The worst 5 of 407 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	71	1915	3TD	C6-C5	12.66	1.50	1.35
32	Y1	34	CM0	C6-C5	12.62	1.48	1.34
5	72	2504	PSU	C6-C5	12.23	1.49	1.35
5	72	955	PSU	C6-C5	12.20	1.49	1.35
30	W1	39	PSU	C6-C5	12.20	1.49	1.35

The worst 5 of 232 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2503	2MA	C1'-N9-C4	15.31	153.54	126.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A1	1519	MA6	N1-C6-N6	-12.47	103.93	117.06
7	A1	1518	MA6	N1-C6-N6	-12.27	104.14	117.06
7	A2	1519	MA6	N1-C6-N6	-12.21	104.21	117.06
7	A2	1518	MA6	N1-C6-N6	-12.05	104.38	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	1402	4OC	C1'-C2'-O2'-CM2

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 273 ligands modelled in this entry, 270 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	0.26	0	4,4,4	0.54	0
47	SPD	72	3003	-	9,9,9	0.32	0	8,8,8	0.84	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.