



Full wwPDB EM Validation Report ⓘ

Mar 6, 2025 – 03:05 pm GMT

PDB ID : 8RCL
EMDB ID : EMD-19054
Title : Escherichia coli paused disome complex (Non-rotated disome interface class 1)
Authors : Fluegel, T.; Schacherl, M.
Deposited on : 2023-12-06
Resolution : 3.49 Å(reported)
Based on initial model : 7N1P

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

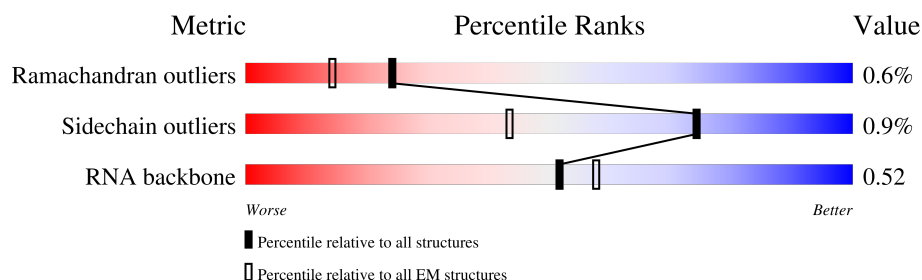
EMDB validation analysis : **FAILED**
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.49 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.



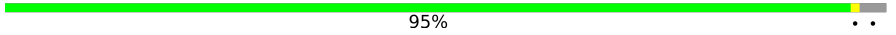
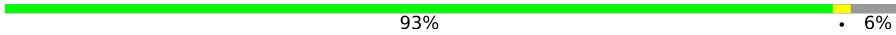


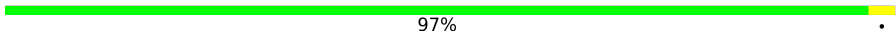
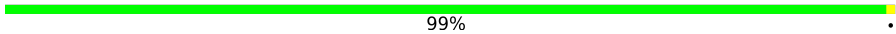
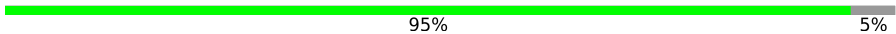
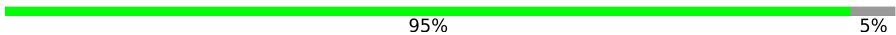






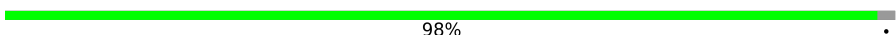
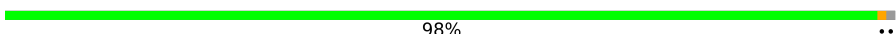
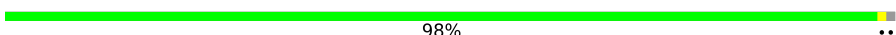



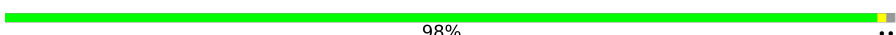
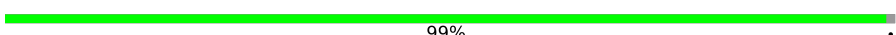
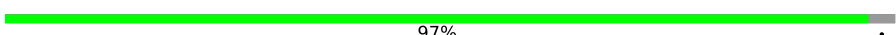
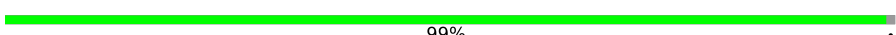
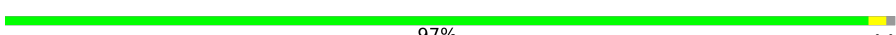
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	
2	32	59	
3	4	70	
4	62	65	
5	71	2904	
5	72	2904	
6	82	120	
7	A1	1542	
7	A2	1542	

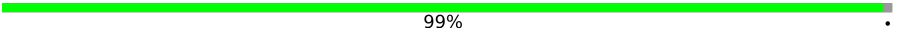
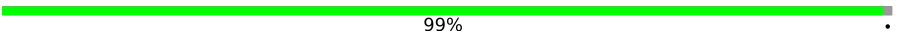
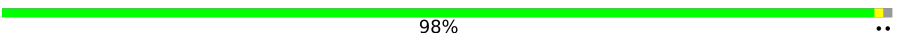
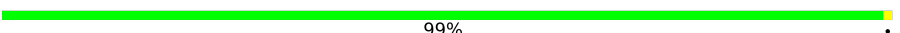
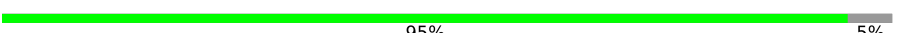

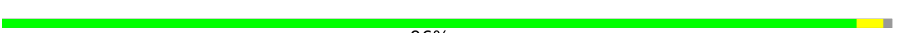













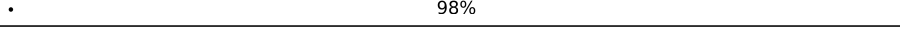

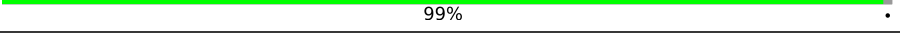
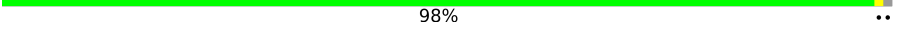
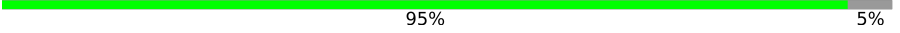
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Mol	Chain	Length	Quality of chain
8	B	241	 95% . .
8	B2	241	 93% . 6%
9	C1	233	 90% . 9%
9	C2	233	 91% 9%
10	D1	206	 97% .
10	D2	206	 99% .
11	E1	167	 95% 5%
11	E2	167	 95% 5%
12	F1	135	 79% 21%
12	F2	135	 77% . 21%
13	G1	179	 87% 13%
13	G2	179	 82% . 14%
14	H1	130	 99% .
14	H2	130	 99% .
15	I1	130	 98% .
15	I2	130	 98% ..
16	J1	103	 98% ..
16	J2	103	 91% 6% .
17	K1	129	 87% . 11%
17	K2	129	 90% . 9%
18	L1	124	 98% ..
18	L2	124	 99% .
19	M1	118	 97% .
19	M2	118	 99% .
20	N1	101	 97% ..

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Mol	Chain	Length	Quality of chain
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	 96% ..
24	R2	75	 93% 5% .
25	S1	92	 89% . 10%
25	S2	92	 90% 10%
26	T1	87	 92% 7% .
27	U1	71	 96% ..
27	U2	71	 96% ..
28	V2	64	 31% 67% .
29	W	76	 59% 32% 9%
30	W1	76	 29% 17% . 53%
31	X2	77	 58% 35% 6%
32	Y1	76	 38% 8% . 53%
33	Y2	76	 64% 32% .
34	Z1	557	 98% .
35	a2	234	 57% 43%
36	b2	273	 99% .
37	e2	179	 98% ..
38	g2	55	 95% 5%
39	h2	136	 100%

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Mol	Chain	Length	Quality of chain
40	i2	149	<div><div></div><div>97%</div><div></div></div>
41	l2	46	<div><div></div><div>98%</div><div></div></div>
42	o2	144	<div><div></div><div>35%</div><div>65%</div></div>
43	p	10	<div><div></div><div>70%</div><div>20%</div><div>10%</div></div>
44	r2	117	<div><div></div><div>99%</div><div></div></div>
45	z2	85	<div><div></div><div>89%</div><div>11%</div></div>

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 188653 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 bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

- 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	30	Total	C	N	O	P	0	0
			644	288	119	207	30		
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
			584	363	122	98	1		

- Molecule 28 is a RNA chain called messenger RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V2	64	Total	C	N	O	P	0	0
			1382	619	267	432	64		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
31	X2	77	Total	C	N	O	P	S	0	0
			1654	740	297	538	77	2		

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

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

- Molecule 33 is a RNA chain called tRNA-Ala (A-site).

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Y2	76	Total	C	N	O	P		0	0
			1628	726	293	533	76			

- Molecule 34 is a protein called 30S ribosomal protein S1.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a2	134	Total	C	N	O	S	0	0
			1026	645	186	193	2		

- Molecule 36 is a protein called 50S ribosomal protein L2.

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

- Molecule 37 is a protein called 50S ribosomal protein L5.

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

- Molecule 38 is a protein called Large ribosomal subunit protein bL33.

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

- Molecule 39 is a protein called 50S ribosomal protein L16.

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

- Molecule 40 is a protein called 50S ribosomal protein L9.

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

- Molecule 41 is a protein called 50S ribosomal protein L34.

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

- Molecule 42 is a protein called 50S ribosomal protein L15.

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

- Molecule 43 is a protein called Nascent chain.

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

- Molecule 44 is a protein called 50S ribosomal protein L18.

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

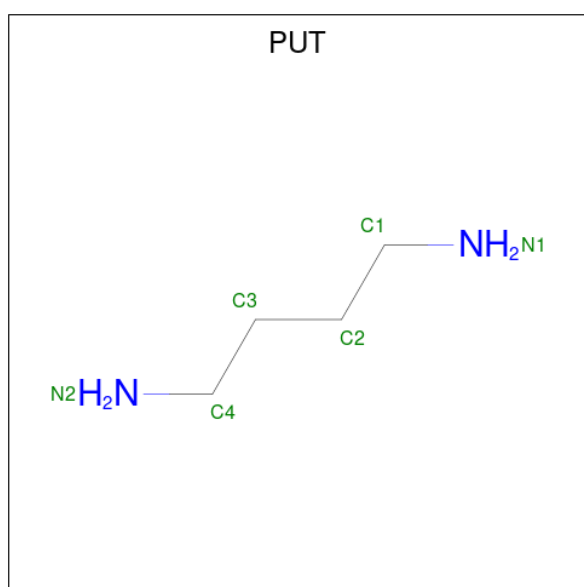
- Molecule 45 is a protein called 50S ribosomal protein L27.

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

- Molecule 46 is ZINC ION (three-letter code: ZN) (formula: Zn).

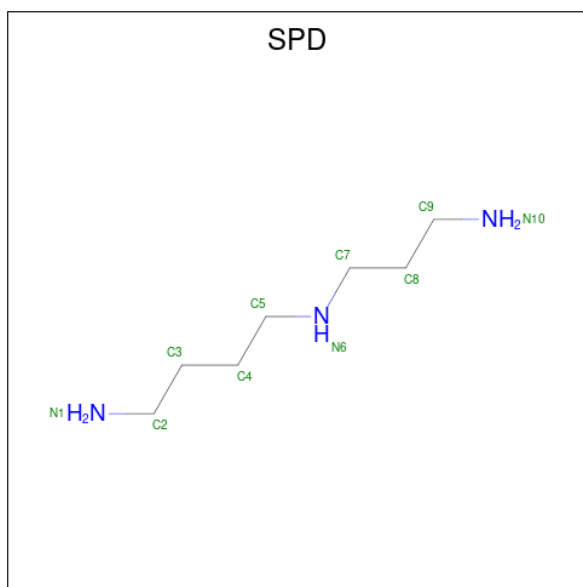
Mol	Chain	Residues	Atoms		AltConf
46	4	1	Total	Zn	0
			1	1	
46	B	1	Total	Zn	0
			1	1	

- Molecule 47 is 1,4-DIAMINOBTUTANE (three-letter code: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
47	72	1	Total	C	N	0
			6	4	2	
47	72	1	Total	C	N	0
			6	4	2	

- Molecule 48 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



Mol	Chain	Residues	Atoms			AltConf
48	72	1	Total	C	N	0
			10	7	3	

- Molecule 49 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

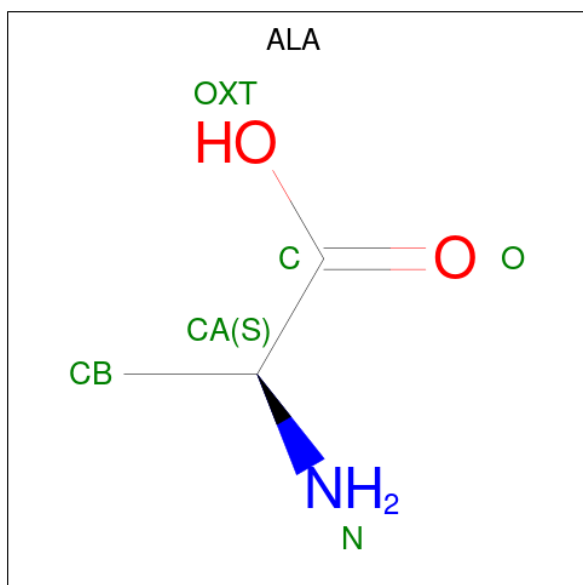
Mol	Chain	Residues	Atoms		AltConf
49	72	189	Total	Mg	0
			189	189	
49	82	1	Total	Mg	0
			1	1	
49	A1	59	Total	Mg	0
			59	59	
49	A2	42	Total	Mg	0
			42	42	
49	V2	1	Total	Mg	0
			1	1	
49	W	1	Total	Mg	0
			1	1	
49	Y2	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
49	b2	1	Total	Mg	0
			1	1	
49	o2	1	Total	Mg	0
			1	1	

- Molecule 50 is ALANINE (three-letter code: ALA) (formula: $C_3H_7NO_2$).



Mol	Chain	Residues	Atoms				AltConf
50	Y2	1	Total	C	N	O	0
			5	3	1	1	

3 Residue-property plots [i](#)

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

- Molecule 1: 50S ribosomal protein L28

Chain 12:  96% ..




- Molecule 2: 50S ribosomal protein L30

Chain 32:  95% ..



- Molecule 3: Large ribosomal subunit protein bL31

Chain 4:  83% 13% .



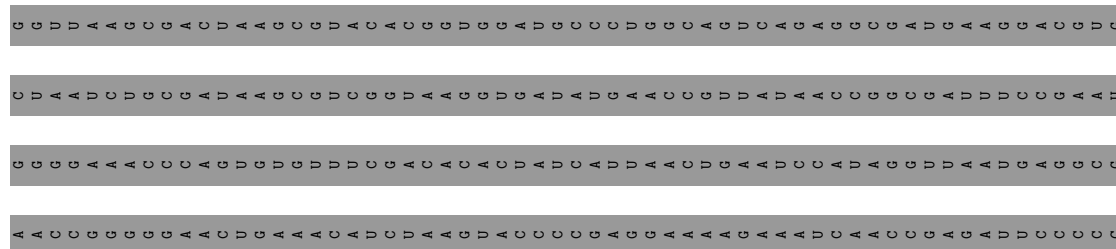
- Molecule 4: 50S ribosomal protein L35

Chain 62:  98% .

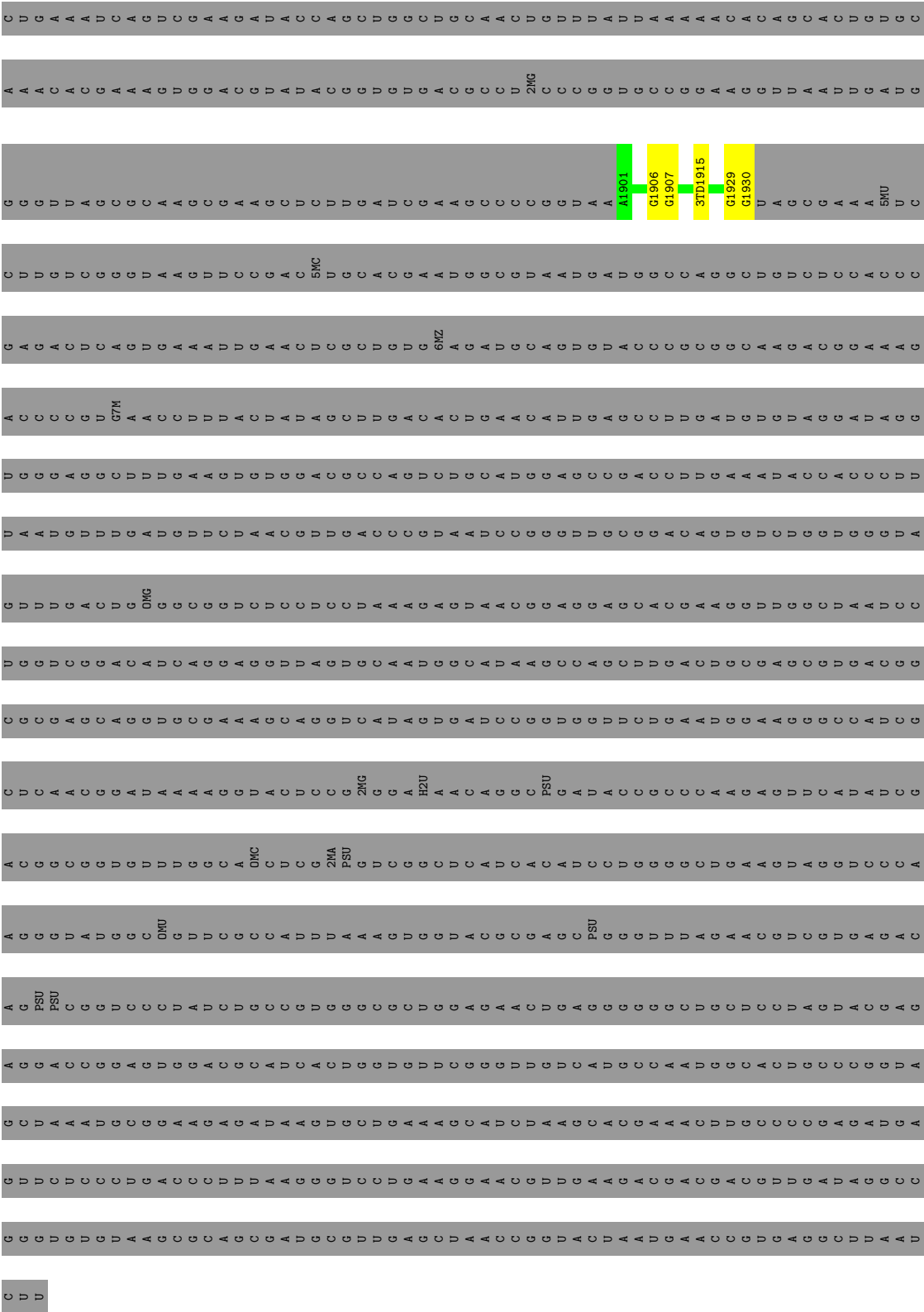


- Molecule 5: 23S ribosomal RNA

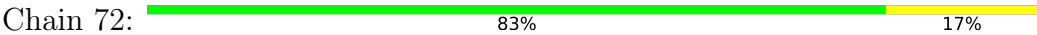
Chain 71:  99%








● Molecule 5: 23S ribosomal RNA



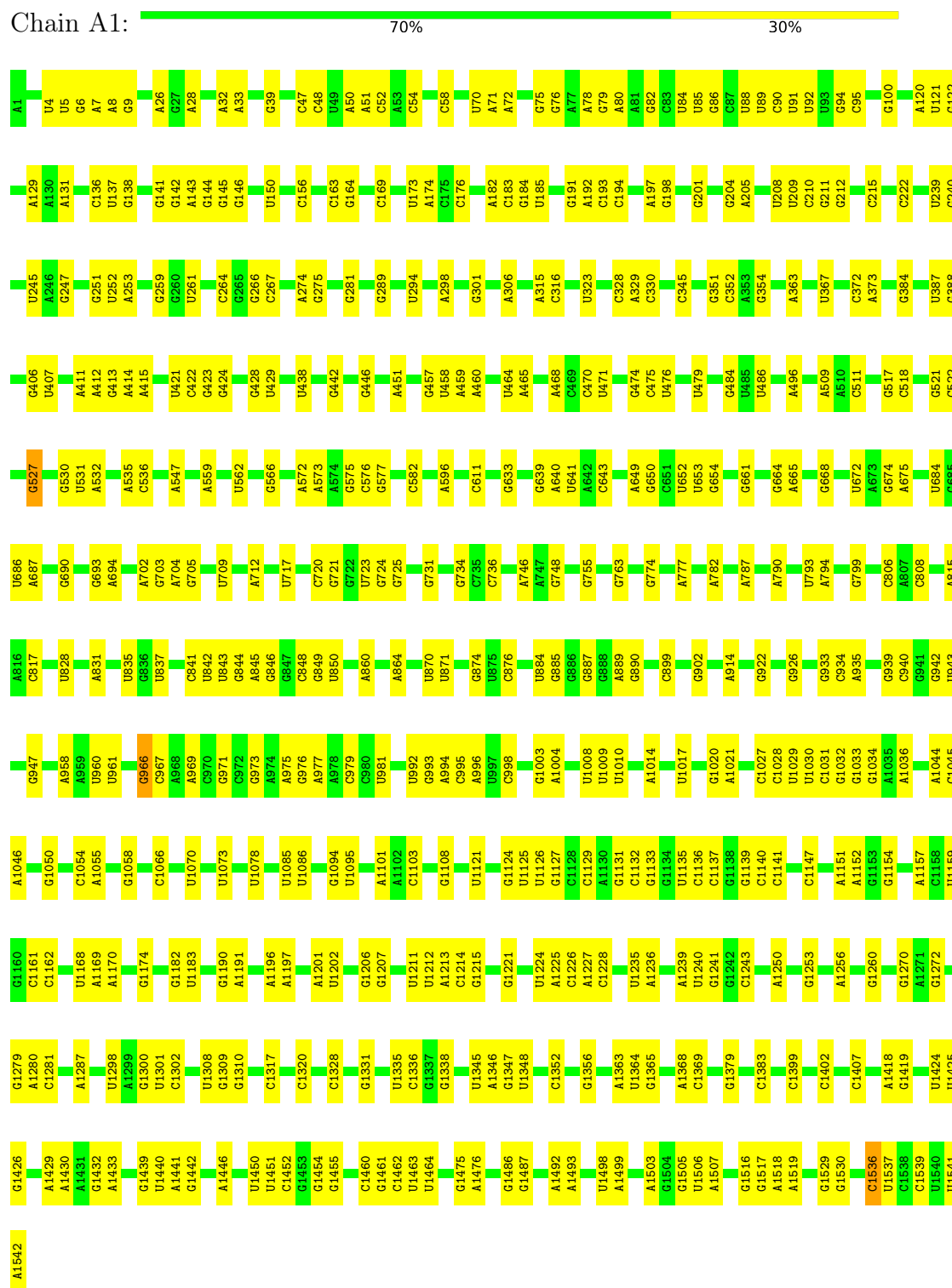
G1	A222	G512	G785	G974	C1172	C1417	U1647	G1929	G2100	A2211	U2402	G2549	A2765
A10	G248	A513	A789	A983	U1173	G1418	U1648	G1930	A2101	A2225	C2403	U2552	A2778
G15	G252	C527	G805	C995	A1175	A1420	U1649	A1937	C2104	G2238	A2406	G2553	U2779
U34	C275	A532	C812	C996	U1176	C1428	G1674	U1938	U2109	G2239	G2410	U2554	U2798
G43	U276	A547	A819	U999	G1177	A1434	C1675	U1940	G2110	G2239	U2423	U2555	A2799
A44	G277	G548	U827	C1005	U1178	A1452	G1715	U1955	G2111	G2239	G2424	A2566	A2800
G45	A278	G549	U827	C1005	U1180	A1453	C1727	U1956	G2112	G2239	A2425	G2567	U2818
G46	A279	A563	G830	U1012	G1211	C1461	U1728	C1961	U2113	G2251	G2429	U2571	U2819
G85	G283	A573	A845	U1013	G1212	C1475	C1730	C1962	G2114	A2268	A2430	U2572	A2820
A71	U284	A574	U847	A1021	G1235	U1476	G1731	U1963	G2115	A2278	U2441	U2580	A2821
A74	G285	A575	U847	A1021	G1236	U1482	G1738	C1965	G2116	A2279	G2445	G2581	U2832
G75	U286	A578	G858	G1026	A1247	G1488	C1764	C1967	G2117	G2283	A2448	G2582	A2835
A101	A311	A603	G859	G1033	G1248	C1489	A1773	A1970	A2126	A2287	U2449	G2583	U2861
U102	A345	A613	G869	A1046	G1250	A1490	A1782	U1971	U2130	U2305	A2457	U2585	G2867
A103	A352	A614	A878	G1047	A1253	G1491	A1783	U1972	U2131	G2308	U2464	U2586	A2873
G110	C353	U615	G883	G1055	G1256	G1492	A1784	G1975	U2132	A2309	G2477	A2602	A2879
A118	G359	A637	U884	U1060	A1262	A1503	A1785	U1982	U2133	G2310	A2478	G2603	C2880
A119	U360	C645	U885	A1070	G1266	U1497	A1786	U1991	G2140	U2312	C2475	U2604	A2883
U120	A361	U646	U886	A1070	G1271	A1508	A1786	U1992	G2141	U2319	A2476	U2605	U2884
A125	G362	G647	U887	U1081	U1272	A1509	A1786	U1993	G2142	U2320	U2477	G2606	U2885
G134	U395	A654	C888	U1082	G1271	A1508	A1786	U1994	U2143	U2321	A2478	U2607	A2886
U135	G396	A655	U895	A1085	U1273	A1509	A1786	U1995	U2144	U2322	A2479	U2608	U2891
U139	A401	U656	A896	A1086	G1300	A1515	A1786	U2022	A2154	G2325	U2491	U2609	U2904
G141	C401	C717	C897	A1087	A1301	G1524	A1786	C2023	A2158	A2333	G2494	U2613	
A142	A404	G726	C902	A1088	U1313	A1532	A1786	A2030	C2161	A2336	C2498	A2614	
U158	U405	G729	G907	A1089	U1321	U1539	A1786	G2032	G2162	G2345	A2502	U2615	
G159	A412	G730	A910	A1090	U1329	A1566	A1786	A2033	A2163	C2347	A2503	U2616	
C163	C455	A730	A917	G1112	C1345	A1569	A1786	C2043	C2165	C2380	U2504	U2617	
U174	C456	U746	A918	U1130	U1352	U1578	A1786	C2055	U2166	C2381	U2505	U2618	
G177	A457	U747	U919	G1131	A1365	A1579	A1786	G2056	U2167	G2382	C2507	U2619	
G178	A470	G748	U931	U1132	A1366	A1580	A1786	A2059	A2170	U2372	U2514	U2732	
G179	G473	A749	U932	A1133	G1368	G1581	A1786	C2061	A2171	G2375	A2518	A2733	
A181	A481	A750	U941	A1134	U1379	C1582	A1786	A2062	U2172	G2379	G2529	U2743	
A196	G491	A764	C946	G1135	U1380	U1584	A1786	G2069	C2179	G2383	G2535	G2744	
A199	A504	G775	U955	A1142	A1383	A1608	A1786	C2072	U2182	U2384	G2536	A2748	
G215	G506	G776	C961	G1149	A1395	A1609	A1786	C2073	A2183	C2385	U2537	G2751	
A216	A782	A783	C962	C1161	U1396	A1610	A1786	G2093	A2198	G2391	A2547	U2756	
A221	G784	A783	G962	A1169	G1416	A1618	A1786	U2098	G2204		U2548	A2757	

● Molecule 6: 5S ribosomal RNA

Chain 82:  78% 21%

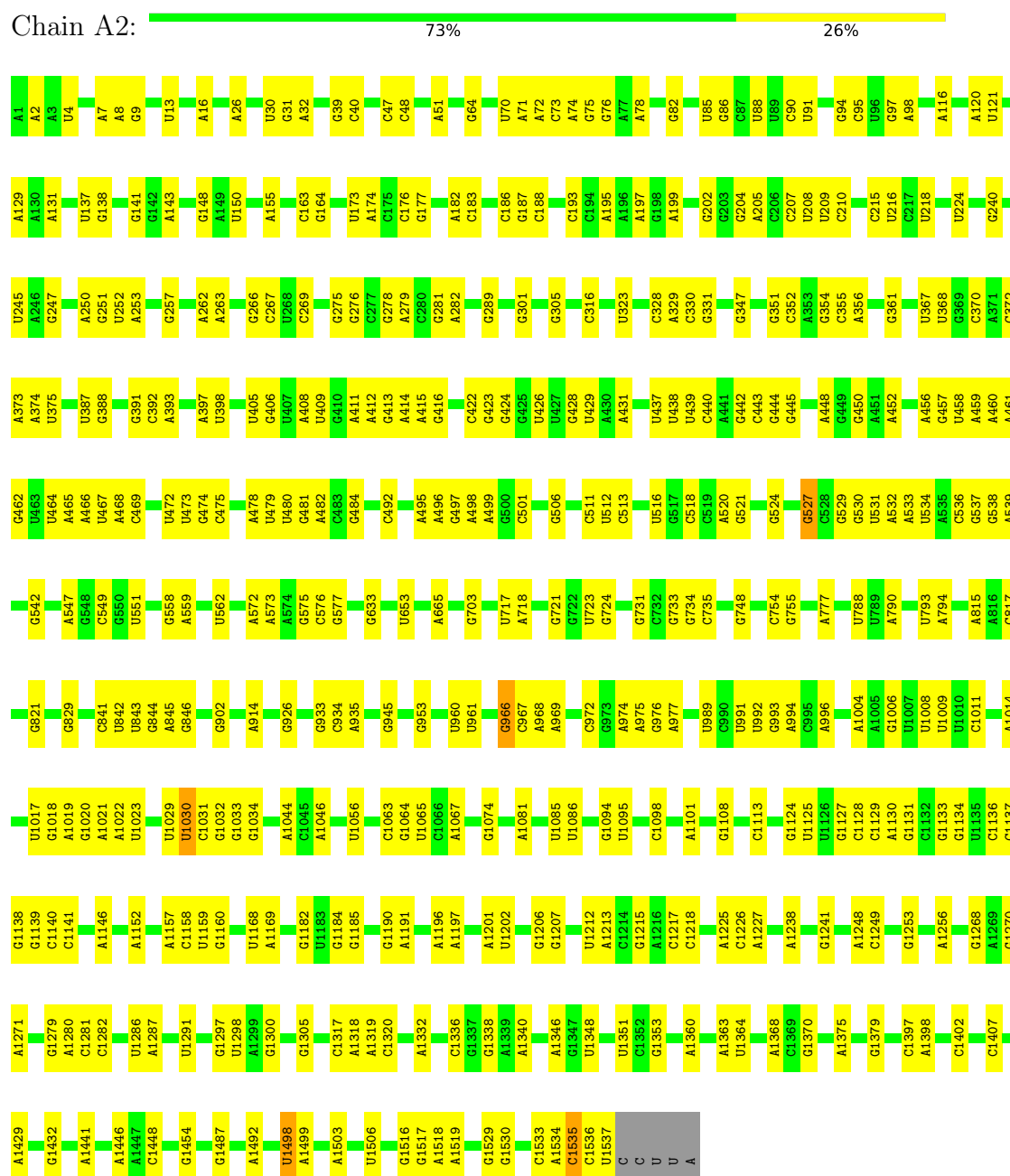


• Molecule 7: 16S ribosomal RNA



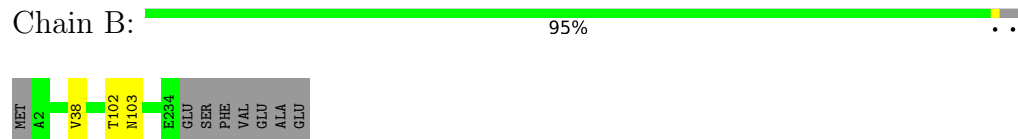
• Molecule 7: 16S ribosomal RNA

Chain A2:



- Molecule 8: Small ribosomal subunit protein uS2

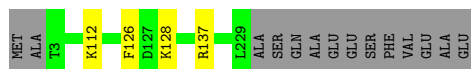
Chain B:



- Molecule 8: Small ribosomal subunit protein uS2

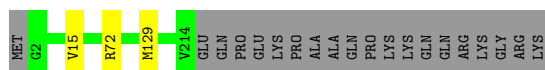
Chain B2:





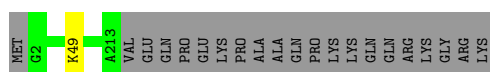
- Molecule 9: Small ribosomal subunit protein uS3

Chain C1: 90% 9%



- Molecule 9: Small ribosomal subunit protein uS3

Chain C2: 91% 9%



- Molecule 10: Small ribosomal subunit protein uS4

Chain D1: 97%



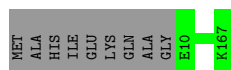
- Molecule 10: Small ribosomal subunit protein uS4

Chain D2: 99%



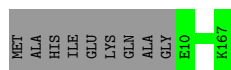
- Molecule 11: Small ribosomal subunit protein uS5

Chain E1: 95% 5%



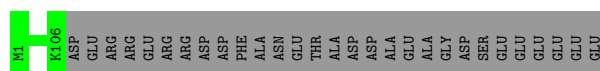
- Molecule 11: Small ribosomal subunit protein uS5

Chain E2: 95% 5%



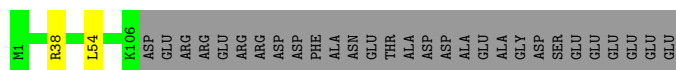
- Molecule 12: 30S ribosomal protein S6

Chain F1: 79% 21%



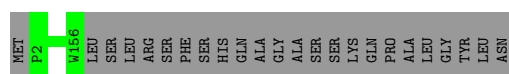
- Molecule 12: 30S ribosomal protein S6

Chain F2: 77% 21%



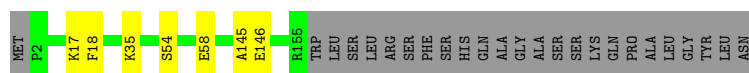
- Molecule 13: 30S ribosomal protein S7

Chain G1: 87% 13%



- Molecule 13: 30S ribosomal protein S7

Chain G2: 82% 14%



- Molecule 14: Small ribosomal subunit protein uS8

Chain H1: 99%



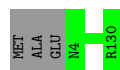
- Molecule 14: Small ribosomal subunit protein uS8

Chain H2: 99%



- Molecule 15: Small ribosomal subunit protein uS9

Chain I1: 98%



- Molecule 15: Small ribosomal subunit protein uS9

Chain I2: 98%



- Molecule 16: 30S ribosomal protein S10

Chain J1: 98% ..



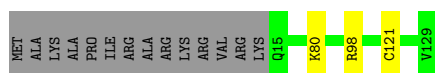
- Molecule 16: 30S ribosomal protein S10

Chain J2: 91% 6% .



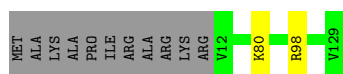
- Molecule 17: Small ribosomal subunit protein uS11

Chain K1: 87% . 11%



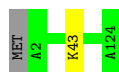
- Molecule 17: Small ribosomal subunit protein uS11

Chain K2: 90% . 9%



- Molecule 18: Small ribosomal subunit protein uS12

Chain L1: 98% ..



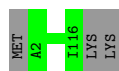
- Molecule 18: Small ribosomal subunit protein uS12

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: 97% ..



- 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% ..



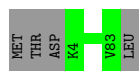
- Molecule 22: 30S ribosomal protein S16

Chain P1: 99% .



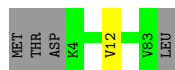
- Molecule 23: Small ribosomal subunit protein uS17

Chain Q1: 95% 5%



- Molecule 23: Small ribosomal subunit protein uS17

Chain Q2: 94% • 5%



- Molecule 24: Small ribosomal subunit protein bS18

Chain R1: 96% • •



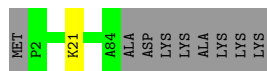
- Molecule 24: Small ribosomal subunit protein bS18

Chain R2: 93% • 5% •



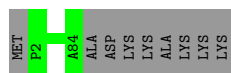
- Molecule 25: Small ribosomal subunit protein uS19

Chain S1: 89% • 10%



- Molecule 25: Small ribosomal subunit protein uS19

Chain S2: 90% 10%



- Molecule 26: Small ribosomal subunit protein bS20

Chain T1: 92% 7% •



- Molecule 27: 30S ribosomal protein S21

Chain U1: 96% • •



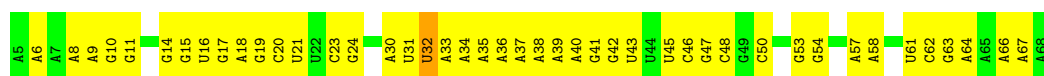
- Molecule 27: 30S ribosomal protein S21

Chain U2: 96%



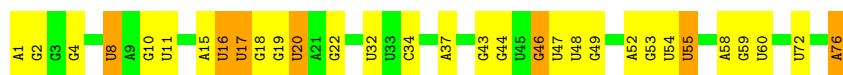
- Molecule 28: messenger RNA

Chain V2: 31% 67%



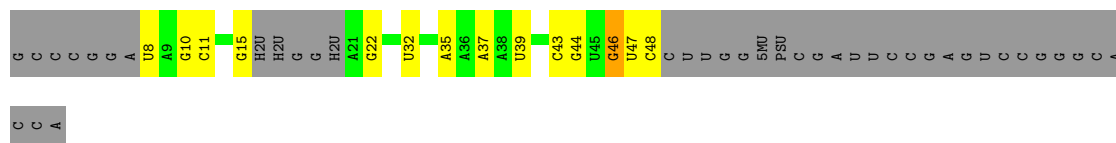
- Molecule 29: tRNA-Trp (P-site)

Chain W: 59% 32% 9%



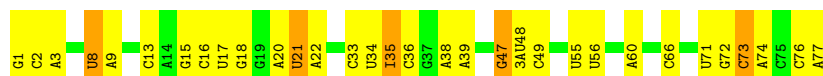
- Molecule 30: tRNA-Phe (P-site)

Chain W1: 29% 17% 53%



- Molecule 31: tRNA-Arg (E-site)

Chain X2: 58% 35% 6%

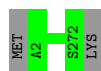


- Molecule 32: tRNA-Val (A-site)

Chain Y1: 38% 8% 53%



- Molecule 33: tRNA-Ala (A-site)



- Molecule 37: 50S ribosomal protein L5



- Molecule 38: Large ribosomal subunit protein bL33



- Molecule 39: 50S ribosomal protein L16



There are no outlier residues recorded for this chain.

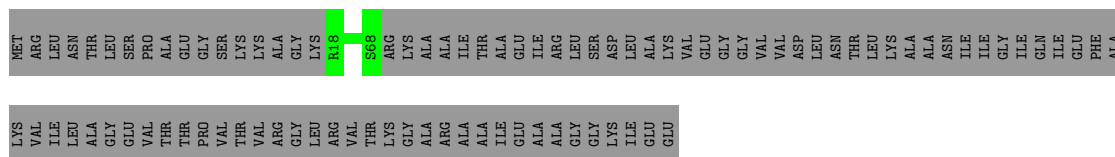
- Molecule 40: 50S ribosomal protein L9



- Molecule 41: 50S ribosomal protein L34



- Molecule 42: 50S ribosomal protein L15



- Molecule 43: Nascent chain

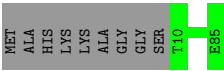
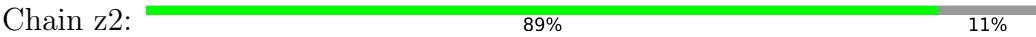




- Molecule 44: 50S ribosomal protein L18



- Molecule 45: 50S ribosomal protein L27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39441	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: RSP, PUT, 2MG, 3TD, PSU, 5MU, 4OC, 7MG, MG, MA6, ZN, G7M, SPD, CM0, OMG, 1MG, 6MZ, 2MA, 4SU, 3AU, OMC, UR3, MIA, OMU, 5MC, H2U

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	0.24	0/635	0.60	0/848
2	32	0.23	0/453	0.52	0/605
3	4	0.63	0/539	0.63	0/721
4	62	0.24	0/513	0.56	0/676
5	71	0.18	0/696	0.70	0/1081
5	72	0.20	1/69306 (0.0%)	0.70	20/108116 (0.0%)
6	82	0.22	1/2872 (0.0%)	0.75	2/4478 (0.0%)
7	A1	0.25	0/36794	0.77	1/57392 (0.0%)
7	A2	0.25	0/36681	0.75	7/57217 (0.0%)
8	B	0.24	0/1846	0.52	0/2488
8	B2	0.25	0/1807	0.49	0/2435
9	C1	0.25	0/1692	0.54	0/2280
9	C2	0.26	0/1685	0.56	0/2270
10	D1	0.25	0/1665	0.54	0/2227
10	D2	0.25	0/1665	0.55	0/2227
11	E1	0.27	0/1179	0.52	0/1584
11	E2	0.27	0/1179	0.53	0/1584
12	F1	0.24	0/881	0.51	0/1189
12	F2	0.25	0/881	0.50	0/1189
13	G1	0.25	0/1246	0.53	0/1672
13	G2	0.25	0/1230	0.56	0/1649
14	H1	0.26	0/989	0.54	0/1326
14	H2	0.26	0/989	0.54	0/1326
15	I1	0.25	0/1034	0.58	0/1375
15	I2	0.26	0/1048	0.58	0/1394
16	J1	0.28	0/827	0.59	0/1117
16	J2	0.26	0/813	0.63	0/1100
17	K1	0.25	0/873	0.55	0/1180
17	K2	0.26	0/900	0.56	0/1215
18	L1	0.27	0/969	0.61	0/1300
18	L2	0.27	0/969	0.61	0/1300

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	M1	0.24	0/900	0.57	0/1204
19	M2	0.24	0/919	0.58	0/1226
20	N1	0.26	0/817	0.57	0/1088
20	N2	0.25	0/817	0.59	0/1088
21	O1	0.24	0/722	0.57	0/964
21	O2	0.24	0/722	0.59	0/964
22	P1	0.26	0/659	0.60	0/884
23	Q1	0.27	0/657	0.58	0/881
23	Q2	0.25	0/657	0.56	0/881
24	R1	0.25	0/635	0.57	0/849
24	R2	0.25	0/637	0.59	0/851
25	S1	0.25	0/680	0.51	0/915
25	S2	0.26	0/680	0.53	0/915
26	T1	0.25	0/676	0.52	0/895
27	U1	0.26	0/598	0.62	0/792
27	U2	0.25	0/592	0.58	0/785
28	V2	0.31	0/1552	0.88	3/2419 (0.1%)
29	W	0.41	1/1604 (0.1%)	0.81	1/2496 (0.0%)
30	W1	0.18	0/747	0.73	0/1161
31	X2	0.49	3/1628 (0.2%)	0.81	1/2526 (0.0%)
32	Y1	0.20	0/786	0.75	0/1216
33	Y2	0.38	1/1725 (0.1%)	0.82	2/2687 (0.1%)
34	Z1	0.27	0/76	0.34	0/101
35	a2	0.24	0/1033	0.47	0/1387
36	b2	0.26	0/2121	0.59	0/2852
37	e2	0.25	0/1444	0.52	0/1937
38	g2	0.25	0/434	0.51	0/576
39	h2	0.25	0/1104	0.57	0/1474
40	i2	0.25	0/1122	0.51	0/1515
41	l2	0.24	0/380	0.63	0/498
42	o2	0.27	0/383	0.69	0/501
43	p	0.58	0/77	0.86	0/104
44	r2	0.25	0/901	0.60	0/1209
45	z2	0.26	0/589	0.55	0/779
All	All	0.25	7/203930 (0.0%)	0.70	37/307181 (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
3	4	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	D1	0	2
10	D2	0	1
15	I2	0	1
16	J2	0	2
17	K1	0	1
17	K2	0	1
21	O2	0	1
22	P1	0	1
43	p	0	1
All	All	0	13

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	1	A	OP3-P	-10.60	1.48	1.61
5	72	1	G	OP3-P	-10.59	1.48	1.61
31	X2	1	G	OP3-P	-10.57	1.48	1.61
33	Y2	1	G	OP3-P	-10.57	1.48	1.61
31	X2	35	I	C5-C6	7.33	1.54	1.39
31	X2	35	I	N3-C4	7.04	1.50	1.35
6	82	120	U	C1'-N1	5.91	1.57	1.48

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2584	U	P-O3'-C3'	-13.29	103.75	119.70
5	72	2585	U	P-O3'-C3'	-12.31	104.93	119.70
5	72	1939	5MU	P-O3'-C3'	-11.85	105.48	119.70
5	72	747	5MU	P-O3'-C3'	-11.14	106.33	119.70
5	72	749	A	P-O3'-C3'	-10.63	106.94	119.70
33	Y2	52	G	P-O3'-C3'	-9.84	107.89	119.70
5	72	748	G	P-O3'-C3'	-9.64	108.13	119.70
33	Y2	74	C	P-O3'-C3'	-9.24	108.61	119.70
5	72	2585	U	C3'-C2'-C1'	-8.26	94.89	101.50
5	72	2583	G	P-O3'-C3'	-6.59	111.79	119.70
28	V2	32	U	N1-C2-O2	6.29	127.20	122.80
7	A2	1030	U	C2-N1-C1'	6.27	125.22	117.70
5	72	1937	A	P-O3'-C3'	-6.18	112.28	119.70
5	72	1313	U	N1-C2-O2	6.07	127.05	122.80
28	V2	32	U	C2-N1-C1'	6.07	124.98	117.70
5	72	1313	U	C2-N1-C1'	5.99	124.89	117.70
5	72	1211	C	OP2-P-O3'	5.88	118.14	105.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	V2	32	U	N3-C2-O2	-5.83	118.12	122.20
7	A1	1536	C	OP2-P-O3'	5.76	117.88	105.20
6	82	3	C	OP1-P-O3'	5.75	117.86	105.20
29	W	76	A	OP1-P-OP2	-5.74	110.99	119.60
5	72	1020	A	P-O3'-C3'	5.62	126.44	119.70
7	A2	1030	U	N3-C2-O2	-5.60	118.28	122.20
6	82	3	C	P-O3'-C3'	5.53	126.33	119.70
5	72	1313	U	N3-C2-O2	-5.51	118.34	122.20
7	A2	1030	U	N1-C2-O2	5.49	126.64	122.80
5	72	1675	C	N1-C2-O2	5.36	122.12	118.90
5	72	1675	C	C2-N1-C1'	5.33	124.67	118.80
5	72	1130	U	P-O3'-C3'	5.32	126.08	119.70
5	72	1020	A	OP2-P-O3'	5.30	116.87	105.20
7	A2	1535	C	P-O3'-C3'	5.29	126.05	119.70
5	72	2585	U	C2'-C3'-O3'	-5.15	98.16	109.50
5	72	1938	A	C3'-C2'-C1'	-5.12	97.40	101.50
31	X2	73	C	N1-C2-O2	5.12	121.97	118.90
7	A2	754	C	C2-N1-C1'	5.10	124.41	118.80
7	A2	392	C	N1-C2-O2	5.01	121.91	118.90
7	A2	1030	U	C5-C6-N1	5.00	125.20	122.70

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	56	ARG	Sidechain
3	4	59	ARG	Sidechain
10	D1	104	ARG	Sidechain
10	D1	15	GLU	Peptide
10	D2	104	ARG	Sidechain
15	I2	113	ARG	Sidechain
16	J2	37	ARG	Sidechain
16	J2	48	ARG	Sidechain
17	K1	98	ARG	Sidechain
17	K2	98	ARG	Sidechain
21	O2	84	ARG	Sidechain
22	P1	51	ARG	Sidechain
43	p	35	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	12	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
2	32	56/59 (95%)	52 (93%)	3 (5%)	1 (2%)	7	35
3	4	65/70 (93%)	54 (83%)	10 (15%)	1 (2%)	8	39
4	62	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
8	B	231/241 (96%)	193 (84%)	35 (15%)	3 (1%)	10	41
8	B2	225/241 (93%)	189 (84%)	36 (16%)	0	100	100
9	C1	211/233 (91%)	186 (88%)	23 (11%)	2 (1%)	14	49
9	C2	210/233 (90%)	184 (88%)	26 (12%)	0	100	100
10	D1	203/206 (98%)	181 (89%)	21 (10%)	1 (0%)	25	59
10	D2	203/206 (98%)	199 (98%)	4 (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%)	79 (76%)	23 (22%)	2 (2%)	6	34
13	G1	153/179 (86%)	151 (99%)	2 (1%)	0	100	100
13	G2	152/179 (85%)	122 (80%)	24 (16%)	6 (4%)	2	21
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
16	J1	100/103 (97%)	92 (92%)	8 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	J2	98/103 (95%)	86 (88%)	8 (8%)	4 (4%)	2	20
17	K1	113/129 (88%)	97 (86%)	15 (13%)	1 (1%)	14	49
17	K2	116/129 (90%)	100 (86%)	15 (13%)	1 (1%)	14	49
18	L1	121/124 (98%)	114 (94%)	6 (5%)	1 (1%)	16	51
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%)	85 (87%)	13 (13%)	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%)	74 (92%)	6 (8%)	0	100	100
23	Q1	78/84 (93%)	77 (99%)	1 (1%)	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	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%)	80 (99%)	1 (1%)	0	100	100
26	T1	84/87 (97%)	79 (94%)	3 (4%)	2 (2%)	5	30
27	U1	68/71 (96%)	57 (84%)	11 (16%)	0	100	100
27	U2	68/71 (96%)	59 (87%)	7 (10%)	2 (3%)	3	27
34	Z1	7/557 (1%)	7 (100%)	0	0	100	100
35	a2	130/234 (56%)	123 (95%)	7 (5%)	0	100	100
36	b2	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
37	e2	176/179 (98%)	172 (98%)	4 (2%)	0	100	100
38	g2	50/55 (91%)	50 (100%)	0	0	100	100
39	h2	135/136 (99%)	135 (100%)	0	0	100	100
40	i2	147/149 (99%)	116 (79%)	29 (20%)	2 (1%)	9	40
41	l2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
42	o2	49/144 (34%)	45 (92%)	4 (8%)	0	100	100
43	p	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	r2	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
45	z2	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
All	All	6102/7240 (84%)	5611 (92%)	457 (8%)	34 (1%)	24	56

All (34) 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
23	Q2	12	VAL
10	D1	175	ALA
12	F2	38	ARG
13	G2	17	LYS
13	G2	145	ALA
16	J2	89	ARG
16	J2	94	ALA
40	i2	89	LYS
43	p	30	ALA
8	B	102	THR
8	B	103	ASN
17	K1	80	LYS
17	K2	80	LYS
18	L1	43	LYS
24	R1	21	ILE
26	T1	55	GLN
2	32	33	HIS
9	C1	129	MET
3	4	55	GLY
12	F2	54	LEU
16	J2	88	MET
40	i2	86	ASP
16	J2	79	PRO
8	B	38	VAL
26	T1	56	PRO
27	U2	6	VAL
43	p	31	VAL
27	U2	11	PRO
24	R2	69	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	12	67/68 (98%)	65 (97%)	2 (3%)	36	63
2	32	48/49 (98%)	47 (98%)	1 (2%)	48	71
3	4	60/62 (97%)	54 (90%)	6 (10%)	6	26
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%)	185 (98%)	4 (2%)	48	71
9	C1	173/190 (91%)	172 (99%)	1 (1%)	84	91
9	C2	172/190 (90%)	171 (99%)	1 (1%)	84	91
10	D1	172/173 (99%)	169 (98%)	3 (2%)	56	75
10	D2	172/173 (99%)	171 (99%)	1 (1%)	84	91
11	E1	120/126 (95%)	120 (100%)	0	100	100
11	E2	120/126 (95%)	120 (100%)	0	100	100
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%)	126 (99%)	1 (1%)	79	88
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%)	105 (99%)	1 (1%)	75	86
16	J1	89/90 (99%)	88 (99%)	1 (1%)	70	83
16	J2	88/90 (98%)	88 (100%)	0	100	100
17	K1	88/99 (89%)	87 (99%)	1 (1%)	70	83
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	81 (98%)	2 (2%)	44	68
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%)	63 (98%)	1 (2%)	58	76
24	R2	64/65 (98%)	61 (95%)	3 (5%)	22	51
25	S1	72/79 (91%)	71 (99%)	1 (1%)	62	79
25	S2	72/79 (91%)	72 (100%)	0	100	100
26	T1	65/66 (98%)	61 (94%)	4 (6%)	15	42
27	U1	60/61 (98%)	58 (97%)	2 (3%)	33	61
27	U2	59/61 (97%)	59 (100%)	0	100	100
34	Z1	8/461 (2%)	8 (100%)	0	100	100
35	a2	110/181 (61%)	109 (99%)	1 (1%)	75	86
36	b2	216/218 (99%)	216 (100%)	0	100	100
37	e2	149/150 (99%)	147 (99%)	2 (1%)	65	81
38	g2	47/49 (96%)	47 (100%)	0	100	100
39	h2	110/109 (101%)	110 (100%)	0	100	100
40	i2	114/114 (100%)	111 (97%)	3 (3%)	41	66
41	l2	38/38 (100%)	37 (97%)	1 (3%)	41	66
42	o2	35/103 (34%)	35 (100%)	0	100	100
43	p	5/5 (100%)	4 (80%)	1 (20%)	1	6
44	r2	86/87 (99%)	86 (100%)	0	100	100
45	z2	58/63 (92%)	58 (100%)	0	100	100
All	All	5107/5932 (86%)	5063 (99%)	44 (1%)	74	86

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	12	72	ARG
1	12	77	LYS
2	32	36	GLU
3	4	1	MET
3	4	6	HIS
3	4	9	TYR
3	4	31	ASP
3	4	33	ASN
3	4	40	CYS
8	B2	112	LYS
8	B2	126	PHE
8	B2	128	LYS
8	B2	137	ARG
9	C1	72	ARG
9	C2	49	LYS
10	D1	20	PHE
10	D1	26	ARG
10	D1	58	LYS
10	D2	44	ARG
13	G2	58	GLU
15	I2	113	ARG
16	J1	102	LEU
17	K1	121	CYS
20	N1	13	ARG
20	N1	53	ARG
24	R1	8	ARG
24	R2	7	ARG
24	R2	10	PHE
24	R2	16	GLU
25	S1	21	LYS
26	T1	49	LYS
26	T1	53	GLU
26	T1	71	LYS
26	T1	85	LYS
27	U1	38	TYR
27	U1	66	ARG
35	a2	30	LEU
37	e2	3	LYS
37	e2	178	ARG
40	i2	25	TYR
40	i2	51	ARG
40	i2	114	GLU
41	l2	3	ARG

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Mol	Chain	Res	Type
43	p	35	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
3	4	6	HIS
3	4	33	ASN
3	4	41	HIS
3	4	61	ASN
8	B	94	HIS
8	B	203	ASN
8	B2	89	GLN
8	B2	177	ASN
9	C2	190	HIS
10	D1	59	GLN
10	D2	85	ASN
16	J2	35	GLN
18	L2	29	GLN
45	z2	50	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	V2	63/64 (98%)	42 (66%)	8 (12%)
29	W	74/76 (97%)	26 (35%)	4 (5%)
30	W1	33/76 (43%)	8 (24%)	2 (6%)
31	X2	73/77 (94%)	26 (35%)	5 (6%)
32	Y1	32/76 (42%)	4 (12%)	2 (6%)
33	Y2	75/76 (98%)	23 (30%)	2 (2%)
5	71	28/2904 (0%)	4 (14%)	0
5	72	2899/2904 (99%)	460 (15%)	33 (1%)
6	82	119/120 (99%)	21 (17%)	4 (3%)
7	A1	1538/1542 (99%)	449 (29%)	36 (2%)
7	A2	1533/1542 (99%)	397 (25%)	33 (2%)
All	All	6467/9457 (68%)	1460 (22%)	129 (1%)

All (1460) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	71	1906	G

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Mol	Chain	Res	Type
5	71	1907	G
5	71	1929	G
5	71	1930	G
5	72	10	A
5	72	15	G
5	72	34	U
5	72	44	A
5	72	46	G
5	72	55	G
5	72	71	A
5	72	74	A
5	72	75	G
5	72	101	A
5	72	102	U
5	72	103	A
5	72	110	G
5	72	118	A
5	72	119	A
5	72	120	U
5	72	125	A
5	72	135	U
5	72	139	U
5	72	141	G
5	72	142	A
5	72	159	G
5	72	163	C
5	72	174	U
5	72	177	G
5	72	178	G
5	72	181	A
5	72	196	A
5	72	199	A
5	72	215	G
5	72	216	A
5	72	221	A
5	72	222	A
5	72	248	G
5	72	252	G
5	72	275	C
5	72	277	G
5	72	278	A
5	72	279	A

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Mol	Chain	Res	Type
5	72	283	G
5	72	284	U
5	72	285	G
5	72	286	U
5	72	311	A
5	72	330	A
5	72	345	A
5	72	353	C
5	72	359	G
5	72	361	G
5	72	362	A
5	72	386	G
5	72	395	U
5	72	396	G
5	72	401	A
5	72	405	U
5	72	412	A
5	72	455	C
5	72	456	C
5	72	457	A
5	72	470	A
5	72	473	G
5	72	481	G
5	72	491	G
5	72	505	A
5	72	506	G
5	72	509	C
5	72	513	A
5	72	527	C
5	72	532	A
5	72	547	A
5	72	549	G
5	72	563	A
5	72	573	U
5	72	575	A
5	72	578	G
5	72	603	A
5	72	613	A
5	72	614	A
5	72	615	U
5	72	637	A
5	72	645	C

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Mol	Chain	Res	Type
5	72	646	U
5	72	647	G
5	72	654	A
5	72	655	A
5	72	686	U
5	72	717	C
5	72	726	G
5	72	729	G
5	72	730	A
5	72	747	5MU
5	72	748	G
5	72	749	A
5	72	750	A
5	72	764	A
5	72	765	C
5	72	775	G
5	72	776	G
5	72	782	A
5	72	784	G
5	72	785	G
5	72	789	A
5	72	805	G
5	72	812	C
5	72	819	A
5	72	827	U
5	72	830	G
5	72	845	A
5	72	846	U
5	72	847	U
5	72	858	G
5	72	859	G
5	72	869	G
5	72	878	A
5	72	883	G
5	72	885	C
5	72	887	U
5	72	888	C
5	72	891	G
5	72	895	U
5	72	896	A
5	72	897	C
5	72	902	C

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Mol	Chain	Res	Type
5	72	907	G
5	72	910	A
5	72	917	A
5	72	919	U
5	72	931	U
5	72	932	U
5	72	941	A
5	72	946	C
5	72	961	C
5	72	962	G
5	72	974	G
5	72	983	A
5	72	995	C
5	72	996	A
5	72	999	U
5	72	1005	C
5	72	1012	U
5	72	1013	C
5	72	1021	A
5	72	1026	G
5	72	1033	U
5	72	1046	A
5	72	1047	G
5	72	1055	G
5	72	1060	U
5	72	1070	A
5	72	1081	U
5	72	1083	U
5	72	1084	A
5	72	1085	A
5	72	1087	G
5	72	1088	A
5	72	1090	A
5	72	1097	U
5	72	1112	G
5	72	1130	U
5	72	1131	G
5	72	1132	U
5	72	1133	A
5	72	1134	A
5	72	1135	C
5	72	1136	G

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Mol	Chain	Res	Type
5	72	1142	A
5	72	1149	G
5	72	1161	C
5	72	1169	A
5	72	1172	C
5	72	1173	U
5	72	1174	U
5	72	1176	U
5	72	1178	C
5	72	1179	G
5	72	1180	U
5	72	1212	G
5	72	1235	G
5	72	1236	G
5	72	1247	A
5	72	1249	U
5	72	1250	G
5	72	1253	A
5	72	1256	G
5	72	1262	A
5	72	1271	G
5	72	1272	A
5	72	1273	U
5	72	1300	G
5	72	1301	A
5	72	1321	A
5	72	1329	U
5	72	1345	C
5	72	1352	U
5	72	1365	A
5	72	1368	G
5	72	1379	U
5	72	1380	G
5	72	1383	A
5	72	1395	A
5	72	1396	U
5	72	1416	G
5	72	1417	C
5	72	1419	A
5	72	1420	A
5	72	1428	C
5	72	1434	A

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Mol	Chain	Res	Type
5	72	1452	G
5	72	1453	A
5	72	1461	C
5	72	1476	U
5	72	1482	G
5	72	1488	C
5	72	1490	A
5	72	1491	G
5	72	1493	C
5	72	1494	A
5	72	1497	U
5	72	1503	A
5	72	1508	A
5	72	1509	A
5	72	1515	A
5	72	1524	G
5	72	1532	A
5	72	1539	U
5	72	1566	A
5	72	1569	A
5	72	1578	U
5	72	1581	G
5	72	1583	A
5	72	1584	U
5	72	1608	A
5	72	1610	A
5	72	1619	G
5	72	1647	U
5	72	1648	U
5	72	1649	G
5	72	1674	G
5	72	1715	G
5	72	1727	C
5	72	1729	U
5	72	1730	C
5	72	1731	G
5	72	1738	G
5	72	1764	C
5	72	1773	A
5	72	1782	U
5	72	1784	A
5	72	1786	A

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Mol	Chain	Res	Type
5	72	1791	A
5	72	1799	G
5	72	1800	C
5	72	1801	A
5	72	1807	G
5	72	1808	A
5	72	1816	C
5	72	1848	A
5	72	1870	C
5	72	1872	A
5	72	1873	G
5	72	1901	A
5	72	1906	G
5	72	1907	G
5	72	1913	A
5	72	1920	C
5	72	1929	G
5	72	1930	G
5	72	1937	A
5	72	1939	5MU
5	72	1940	U
5	72	1955	U
5	72	1956	U
5	72	1960	A
5	72	1963	U
5	72	1964	G
5	72	1966	A
5	72	1967	C
5	72	1970	A
5	72	1971	U
5	72	1972	G
5	72	1975	G
5	72	1982	U
5	72	1991	U
5	72	1993	U
5	72	1997	C
5	72	2022	U
5	72	2023	C
5	72	2032	G
5	72	2033	A
5	72	2043	C
5	72	2055	C

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Mol	Chain	Res	Type
5	72	2056	G
5	72	2059	A
5	72	2060	A
5	72	2061	G
5	72	2062	A
5	72	2069	G7M
5	72	2072	C
5	72	2093	G
5	72	2098	U
5	72	2100	G
5	72	2101	A
5	72	2104	C
5	72	2109	U
5	72	2110	G
5	72	2111	U
5	72	2112	G
5	72	2113	U
5	72	2114	A
5	72	2115	G
5	72	2116	G
5	72	2117	A
5	72	2118	U
5	72	2119	A
5	72	2120	G
5	72	2126	A
5	72	2130	U
5	72	2131	U
5	72	2132	U
5	72	2133	G
5	72	2134	A
5	72	2139	U
5	72	2140	G
5	72	2141	G
5	72	2145	C
5	72	2146	C
5	72	2149	U
5	72	2154	A
5	72	2158	A
5	72	2161	C
5	72	2162	G
5	72	2164	C
5	72	2165	C

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Mol	Chain	Res	Type
5	72	2166	U
5	72	2167	U
5	72	2170	A
5	72	2171	A
5	72	2172	U
5	72	2173	A
5	72	2179	C
5	72	2182	U
5	72	2183	A
5	72	2198	A
5	72	2204	G
5	72	2211	A
5	72	2225	A
5	72	2238	G
5	72	2239	G
5	72	2243	U
5	72	2251	OMG
5	72	2268	A
5	72	2278	A
5	72	2279	G
5	72	2283	C
5	72	2287	A
5	72	2305	U
5	72	2308	G
5	72	2309	A
5	72	2311	A
5	72	2312	U
5	72	2319	G
5	72	2321	U
5	72	2322	A
5	72	2325	G
5	72	2333	A
5	72	2336	A
5	72	2345	G
5	72	2347	C
5	72	2350	C
5	72	2361	G
5	72	2372	U
5	72	2375	G
5	72	2379	G
5	72	2383	G
5	72	2385	C

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Mol	Chain	Res	Type
5	72	2391	G
5	72	2402	U
5	72	2403	C
5	72	2406	A
5	72	2410	G
5	72	2423	U
5	72	2425	A
5	72	2429	G
5	72	2430	A
5	72	2431	U
5	72	2441	U
5	72	2448	A
5	72	2457	PSU
5	72	2464	G
5	72	2475	C
5	72	2476	A
5	72	2478	A
5	72	2482	A
5	72	2484	G
5	72	2491	U
5	72	2494	G
5	72	2498	OMC
5	72	2502	G
5	72	2504	PSU
5	72	2505	G
5	72	2507	C
5	72	2514	U
5	72	2518	A
5	72	2529	G
5	72	2535	G
5	72	2537	U
5	72	2547	A
5	72	2549	G
5	72	2554	U
5	72	2556	C
5	72	2566	A
5	72	2567	G
5	72	2571	U
5	72	2572	A
5	72	2573	C
5	72	2581	G
5	72	2582	G

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Mol	Chain	Res	Type
5	72	2585	U
5	72	2586	U
5	72	2602	A
5	72	2608	G
5	72	2609	U
5	72	2613	U
5	72	2614	A
5	72	2615	U
5	72	2629	U
5	72	2630	G
5	72	2663	G
5	72	2689	U
5	72	2690	U
5	72	2714	G
5	72	2726	A
5	72	2732	G
5	72	2733	A
5	72	2743	U
5	72	2744	G
5	72	2748	A
5	72	2751	G
5	72	2757	A
5	72	2765	A
5	72	2778	A
5	72	2779	U
5	72	2798	U
5	72	2800	A
5	72	2818	U
5	72	2820	A
5	72	2821	A
5	72	2832	U
5	72	2835	A
5	72	2861	U
5	72	2867	G
5	72	2873	A
5	72	2879	A
5	72	2880	C
5	72	2883	A
5	72	2884	U
5	72	2885	G
5	72	2886	A
5	72	2891	U

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Mol	Chain	Res	Type
5	72	2904	U
6	82	4	C
6	82	9	G
6	82	13	G
6	82	33	G
6	82	34	A
6	82	35	C
6	82	37	C
6	82	40	U
6	82	41	G
6	82	45	A
6	82	48	U
6	82	50	A
6	82	51	G
6	82	66	A
6	82	67	G
6	82	87	U
6	82	89	U
6	82	90	C
6	82	91	C
6	82	99	A
6	82	109	A
7	A1	4	U
7	A1	5	U
7	A1	6	G
7	A1	7	A
7	A1	8	A
7	A1	9	G
7	A1	26	A
7	A1	28	A
7	A1	32	A
7	A1	33	A
7	A1	39	G
7	A1	47	C
7	A1	48	C
7	A1	50	A
7	A1	51	A
7	A1	52	C
7	A1	54	C
7	A1	58	C
7	A1	70	U
7	A1	71	A

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Mol	Chain	Res	Type
7	A1	72	A
7	A1	75	G
7	A1	76	G
7	A1	78	A
7	A1	79	G
7	A1	80	A
7	A1	82	G
7	A1	84	U
7	A1	85	U
7	A1	86	G
7	A1	88	U
7	A1	89	U
7	A1	90	C
7	A1	91	U
7	A1	92	U
7	A1	94	G
7	A1	95	C
7	A1	100	G
7	A1	120	A
7	A1	121	U
7	A1	122	G
7	A1	129	A
7	A1	131	A
7	A1	136	C
7	A1	137	U
7	A1	138	G
7	A1	141	G
7	A1	142	G
7	A1	143	A
7	A1	144	G
7	A1	145	G
7	A1	146	G
7	A1	150	U
7	A1	156	C
7	A1	163	C
7	A1	164	G
7	A1	169	C
7	A1	173	U
7	A1	174	A
7	A1	176	C
7	A1	182	A
7	A1	183	C

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Mol	Chain	Res	Type
7	A1	184	G
7	A1	185	U
7	A1	191	G
7	A1	192	A
7	A1	193	C
7	A1	194	C
7	A1	197	A
7	A1	198	G
7	A1	201	G
7	A1	204	G
7	A1	205	A
7	A1	208	U
7	A1	209	U
7	A1	210	C
7	A1	211	G
7	A1	212	G
7	A1	215	C
7	A1	222	C
7	A1	239	U
7	A1	240	G
7	A1	245	U
7	A1	247	G
7	A1	251	G
7	A1	252	U
7	A1	253	A
7	A1	259	G
7	A1	261	U
7	A1	264	C
7	A1	266	G
7	A1	267	C
7	A1	275	G
7	A1	281	G
7	A1	289	G
7	A1	294	U
7	A1	298	A
7	A1	301	G
7	A1	306	A
7	A1	315	A
7	A1	316	C
7	A1	323	U
7	A1	328	C
7	A1	329	A

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Mol	Chain	Res	Type
7	A1	330	C
7	A1	345	C
7	A1	351	G
7	A1	352	C
7	A1	354	G
7	A1	363	A
7	A1	367	U
7	A1	372	C
7	A1	373	A
7	A1	384	G
7	A1	387	U
7	A1	388	G
7	A1	406	G
7	A1	407	U
7	A1	411	A
7	A1	412	A
7	A1	413	G
7	A1	414	A
7	A1	415	A
7	A1	421	U
7	A1	422	C
7	A1	423	G
7	A1	424	G
7	A1	428	G
7	A1	429	U
7	A1	438	U
7	A1	442	G
7	A1	446	G
7	A1	451	A
7	A1	457	G
7	A1	458	U
7	A1	459	A
7	A1	460	A
7	A1	464	U
7	A1	465	A
7	A1	468	A
7	A1	470	C
7	A1	471	U
7	A1	474	G
7	A1	475	C
7	A1	476	U
7	A1	479	U

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Mol	Chain	Res	Type
7	A1	484	G
7	A1	486	U
7	A1	496	A
7	A1	509	A
7	A1	511	C
7	A1	517	G
7	A1	518	C
7	A1	521	G
7	A1	522	C
7	A1	527	G7M
7	A1	530	G
7	A1	531	U
7	A1	532	A
7	A1	536	C
7	A1	547	A
7	A1	559	A
7	A1	562	U
7	A1	566	G
7	A1	572	A
7	A1	573	A
7	A1	575	G
7	A1	576	C
7	A1	577	G
7	A1	582	C
7	A1	596	A
7	A1	611	C
7	A1	633	G
7	A1	639	G
7	A1	640	A
7	A1	641	U
7	A1	643	C
7	A1	649	A
7	A1	650	G
7	A1	652	U
7	A1	653	U
7	A1	654	G
7	A1	661	G
7	A1	664	G
7	A1	665	A
7	A1	668	G
7	A1	672	U
7	A1	674	G

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Mol	Chain	Res	Type
7	A1	675	A
7	A1	684	U
7	A1	686	U
7	A1	687	A
7	A1	690	G
7	A1	693	G
7	A1	694	A
7	A1	702	A
7	A1	703	G
7	A1	704	A
7	A1	705	G
7	A1	709	U
7	A1	712	A
7	A1	717	U
7	A1	720	C
7	A1	721	G
7	A1	723	U
7	A1	724	G
7	A1	725	G
7	A1	731	G
7	A1	734	G
7	A1	736	C
7	A1	746	A
7	A1	748	G
7	A1	755	G
7	A1	763	G
7	A1	774	G
7	A1	777	A
7	A1	782	A
7	A1	787	A
7	A1	790	A
7	A1	793	U
7	A1	794	A
7	A1	799	G
7	A1	806	C
7	A1	808	C
7	A1	815	A
7	A1	817	C
7	A1	828	U
7	A1	831	A
7	A1	835	U
7	A1	837	U

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Mol	Chain	Res	Type
7	A1	841	C
7	A1	842	U
7	A1	843	U
7	A1	844	G
7	A1	845	A
7	A1	846	G
7	A1	848	C
7	A1	849	G
7	A1	850	U
7	A1	860	A
7	A1	864	A
7	A1	870	U
7	A1	871	U
7	A1	874	G
7	A1	876	C
7	A1	884	U
7	A1	885	G
7	A1	887	G
7	A1	889	A
7	A1	890	G
7	A1	899	C
7	A1	902	G
7	A1	914	A
7	A1	922	G
7	A1	926	G
7	A1	933	G
7	A1	934	C
7	A1	935	A
7	A1	939	G
7	A1	940	C
7	A1	942	G
7	A1	943	U
7	A1	947	G
7	A1	958	A
7	A1	960	U
7	A1	961	U
7	A1	966	2MG
7	A1	969	A
7	A1	971	G
7	A1	973	G
7	A1	975	A
7	A1	976	G

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Mol	Chain	Res	Type
7	A1	977	A
7	A1	979	C
7	A1	981	U
7	A1	992	U
7	A1	993	G
7	A1	994	A
7	A1	995	C
7	A1	996	A
7	A1	998	C
7	A1	1003	G
7	A1	1004	A
7	A1	1008	U
7	A1	1009	U
7	A1	1010	U
7	A1	1014	A
7	A1	1017	U
7	A1	1020	G
7	A1	1021	A
7	A1	1027	C
7	A1	1028	C
7	A1	1029	U
7	A1	1030	U
7	A1	1031	C
7	A1	1032	G
7	A1	1033	G
7	A1	1034	G
7	A1	1036	A
7	A1	1044	A
7	A1	1045	C
7	A1	1046	A
7	A1	1050	G
7	A1	1054	C
7	A1	1055	A
7	A1	1058	G
7	A1	1066	C
7	A1	1070	U
7	A1	1073	U
7	A1	1078	U
7	A1	1085	U
7	A1	1086	U
7	A1	1094	G
7	A1	1095	U

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Mol	Chain	Res	Type
7	A1	1101	A
7	A1	1103	C
7	A1	1108	G
7	A1	1121	U
7	A1	1124	G
7	A1	1125	U
7	A1	1126	U
7	A1	1127	G
7	A1	1129	C
7	A1	1131	G
7	A1	1132	C
7	A1	1133	G
7	A1	1135	U
7	A1	1136	C
7	A1	1137	C
7	A1	1139	G
7	A1	1140	C
7	A1	1141	C
7	A1	1147	C
7	A1	1151	A
7	A1	1152	A
7	A1	1154	G
7	A1	1157	A
7	A1	1159	U
7	A1	1161	C
7	A1	1162	C
7	A1	1168	U
7	A1	1169	A
7	A1	1170	A
7	A1	1174	G
7	A1	1182	G
7	A1	1183	U
7	A1	1191	A
7	A1	1196	A
7	A1	1197	A
7	A1	1201	A
7	A1	1202	U
7	A1	1206	G
7	A1	1211	U
7	A1	1212	U
7	A1	1213	A
7	A1	1214	C

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Mol	Chain	Res	Type
7	A1	1215	G
7	A1	1221	G
7	A1	1224	U
7	A1	1225	A
7	A1	1226	C
7	A1	1227	A
7	A1	1228	C
7	A1	1235	U
7	A1	1236	A
7	A1	1239	A
7	A1	1240	U
7	A1	1241	G
7	A1	1243	C
7	A1	1250	A
7	A1	1253	G
7	A1	1256	A
7	A1	1260	G
7	A1	1270	G
7	A1	1272	G
7	A1	1279	G
7	A1	1280	A
7	A1	1281	C
7	A1	1287	A
7	A1	1298	U
7	A1	1300	G
7	A1	1301	U
7	A1	1302	C
7	A1	1308	U
7	A1	1309	G
7	A1	1310	G
7	A1	1317	C
7	A1	1320	C
7	A1	1328	C
7	A1	1331	G
7	A1	1335	U
7	A1	1336	C
7	A1	1338	G
7	A1	1345	U
7	A1	1346	A
7	A1	1347	G
7	A1	1348	U
7	A1	1352	C

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Mol	Chain	Res	Type
7	A1	1356	G
7	A1	1363	A
7	A1	1364	U
7	A1	1365	G
7	A1	1368	A
7	A1	1369	C
7	A1	1379	G
7	A1	1383	C
7	A1	1399	C
7	A1	1418	A
7	A1	1419	G
7	A1	1424	U
7	A1	1425	U
7	A1	1426	G
7	A1	1429	A
7	A1	1430	A
7	A1	1432	G
7	A1	1433	A
7	A1	1439	G
7	A1	1440	U
7	A1	1441	A
7	A1	1442	G
7	A1	1446	A
7	A1	1450	U
7	A1	1451	U
7	A1	1452	C
7	A1	1454	G
7	A1	1455	G
7	A1	1460	C
7	A1	1461	G
7	A1	1462	C
7	A1	1464	U
7	A1	1475	G
7	A1	1476	A
7	A1	1486	G
7	A1	1487	G
7	A1	1492	A
7	A1	1493	A
7	A1	1499	A
7	A1	1503	A
7	A1	1505	G
7	A1	1506	U

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Mol	Chain	Res	Type
7	A1	1507	A
7	A1	1517	G
7	A1	1529	G
7	A1	1530	G
7	A1	1536	C
7	A1	1537	U
7	A1	1539	C
7	A1	1541	U
7	A1	1542	A
7	A2	2	A
7	A2	4	U
7	A2	7	A
7	A2	8	A
7	A2	9	G
7	A2	16	A
7	A2	26	A
7	A2	30	U
7	A2	31	G
7	A2	32	A
7	A2	39	G
7	A2	40	C
7	A2	47	C
7	A2	48	C
7	A2	51	A
7	A2	64	G
7	A2	70	U
7	A2	71	A
7	A2	72	A
7	A2	73	C
7	A2	74	A
7	A2	75	G
7	A2	76	G
7	A2	78	A
7	A2	82	G
7	A2	85	U
7	A2	86	G
7	A2	88	U
7	A2	90	C
7	A2	91	U
7	A2	94	G
7	A2	95	C
7	A2	97	G

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Mol	Chain	Res	Type
7	A2	98	A
7	A2	116	A
7	A2	120	A
7	A2	121	U
7	A2	129	A
7	A2	131	A
7	A2	137	U
7	A2	138	G
7	A2	141	G
7	A2	143	A
7	A2	148	G
7	A2	150	U
7	A2	155	A
7	A2	163	C
7	A2	164	G
7	A2	173	U
7	A2	174	A
7	A2	176	C
7	A2	177	G
7	A2	182	A
7	A2	183	C
7	A2	186	C
7	A2	187	G
7	A2	188	C
7	A2	193	C
7	A2	195	A
7	A2	197	A
7	A2	199	A
7	A2	202	G
7	A2	204	G
7	A2	205	A
7	A2	207	C
7	A2	208	U
7	A2	209	U
7	A2	210	C
7	A2	215	C
7	A2	216	U
7	A2	218	U
7	A2	224	U
7	A2	240	G
7	A2	245	U
7	A2	247	G

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Mol	Chain	Res	Type
7	A2	250	A
7	A2	251	G
7	A2	252	U
7	A2	253	A
7	A2	257	G
7	A2	262	A
7	A2	263	A
7	A2	266	G
7	A2	267	C
7	A2	269	C
7	A2	275	G
7	A2	276	G
7	A2	278	G
7	A2	279	A
7	A2	281	G
7	A2	282	A
7	A2	289	G
7	A2	301	G
7	A2	305	G
7	A2	316	C
7	A2	323	U
7	A2	328	C
7	A2	329	A
7	A2	330	C
7	A2	331	G
7	A2	347	G
7	A2	351	G
7	A2	352	C
7	A2	354	G
7	A2	355	C
7	A2	356	A
7	A2	361	G
7	A2	367	U
7	A2	368	U
7	A2	370	C
7	A2	372	C
7	A2	373	A
7	A2	374	A
7	A2	375	U
7	A2	387	U
7	A2	388	G
7	A2	391	G

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Mol	Chain	Res	Type
7	A2	393	A
7	A2	397	A
7	A2	398	U
7	A2	405	U
7	A2	406	G
7	A2	408	A
7	A2	409	U
7	A2	411	A
7	A2	412	A
7	A2	413	G
7	A2	414	A
7	A2	415	A
7	A2	416	G
7	A2	422	C
7	A2	423	G
7	A2	424	G
7	A2	426	U
7	A2	428	G
7	A2	429	U
7	A2	431	A
7	A2	437	U
7	A2	439	U
7	A2	440	C
7	A2	442	G
7	A2	443	C
7	A2	444	G
7	A2	445	G
7	A2	448	A
7	A2	450	G
7	A2	452	A
7	A2	456	A
7	A2	457	G
7	A2	458	U
7	A2	459	A
7	A2	460	A
7	A2	461	A
7	A2	462	G
7	A2	464	U
7	A2	465	A
7	A2	466	A
7	A2	467	U
7	A2	468	A

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Mol	Chain	Res	Type
7	A2	469	C
7	A2	472	U
7	A2	473	U
7	A2	474	G
7	A2	475	C
7	A2	478	A
7	A2	479	U
7	A2	480	U
7	A2	481	G
7	A2	482	A
7	A2	484	G
7	A2	492	C
7	A2	495	A
7	A2	496	A
7	A2	497	G
7	A2	498	A
7	A2	499	A
7	A2	501	C
7	A2	506	G
7	A2	511	C
7	A2	512	U
7	A2	513	C
7	A2	516	U
7	A2	518	C
7	A2	520	A
7	A2	521	G
7	A2	524	G
7	A2	527	G7M
7	A2	529	G
7	A2	530	G
7	A2	531	U
7	A2	532	A
7	A2	533	A
7	A2	534	U
7	A2	536	C
7	A2	538	G
7	A2	539	A
7	A2	542	G
7	A2	547	A
7	A2	549	C
7	A2	551	U
7	A2	558	G

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Mol	Chain	Res	Type
7	A2	559	A
7	A2	562	U
7	A2	572	A
7	A2	573	A
7	A2	575	G
7	A2	576	C
7	A2	577	G
7	A2	633	G
7	A2	653	U
7	A2	665	A
7	A2	703	G
7	A2	718	A
7	A2	721	G
7	A2	723	U
7	A2	724	G
7	A2	731	G
7	A2	733	G
7	A2	734	G
7	A2	735	C
7	A2	748	G
7	A2	755	G
7	A2	777	A
7	A2	788	U
7	A2	790	A
7	A2	793	U
7	A2	794	A
7	A2	815	A
7	A2	817	C
7	A2	821	G
7	A2	829	G
7	A2	841	C
7	A2	842	U
7	A2	843	U
7	A2	844	G
7	A2	845	A
7	A2	846	G
7	A2	902	G
7	A2	914	A
7	A2	926	G
7	A2	933	G
7	A2	934	C
7	A2	935	A

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Mol	Chain	Res	Type
7	A2	945	G
7	A2	953	G
7	A2	960	U
7	A2	961	U
7	A2	966	2MG
7	A2	968	A
7	A2	969	A
7	A2	972	C
7	A2	974	A
7	A2	975	A
7	A2	976	G
7	A2	977	A
7	A2	989	U
7	A2	991	U
7	A2	992	U
7	A2	993	G
7	A2	994	A
7	A2	996	A
7	A2	1004	A
7	A2	1006	G
7	A2	1008	U
7	A2	1009	U
7	A2	1011	C
7	A2	1014	A
7	A2	1017	U
7	A2	1018	G
7	A2	1019	A
7	A2	1020	G
7	A2	1021	A
7	A2	1022	A
7	A2	1023	U
7	A2	1029	U
7	A2	1030	U
7	A2	1031	C
7	A2	1032	G
7	A2	1033	G
7	A2	1034	G
7	A2	1044	A
7	A2	1046	A
7	A2	1056	U
7	A2	1063	C
7	A2	1064	G

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Mol	Chain	Res	Type
7	A2	1065	U
7	A2	1067	A
7	A2	1074	G
7	A2	1081	A
7	A2	1085	U
7	A2	1086	U
7	A2	1094	G
7	A2	1095	U
7	A2	1098	C
7	A2	1101	A
7	A2	1108	G
7	A2	1113	C
7	A2	1124	G
7	A2	1125	U
7	A2	1127	G
7	A2	1128	C
7	A2	1129	C
7	A2	1130	A
7	A2	1131	G
7	A2	1133	G
7	A2	1134	G
7	A2	1136	C
7	A2	1137	C
7	A2	1138	G
7	A2	1139	G
7	A2	1140	C
7	A2	1141	C
7	A2	1146	A
7	A2	1152	A
7	A2	1157	A
7	A2	1158	C
7	A2	1159	U
7	A2	1160	G
7	A2	1168	U
7	A2	1169	A
7	A2	1182	G
7	A2	1184	G
7	A2	1185	G
7	A2	1191	A
7	A2	1196	A
7	A2	1197	A
7	A2	1201	A

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Mol	Chain	Res	Type
7	A2	1202	U
7	A2	1206	G
7	A2	1212	U
7	A2	1213	A
7	A2	1215	G
7	A2	1217	C
7	A2	1218	C
7	A2	1225	A
7	A2	1226	C
7	A2	1227	A
7	A2	1238	A
7	A2	1241	G
7	A2	1248	A
7	A2	1249	C
7	A2	1253	G
7	A2	1256	A
7	A2	1268	G
7	A2	1270	G
7	A2	1271	A
7	A2	1279	G
7	A2	1280	A
7	A2	1281	C
7	A2	1282	C
7	A2	1286	U
7	A2	1287	A
7	A2	1291	U
7	A2	1297	G
7	A2	1298	U
7	A2	1300	G
7	A2	1305	G
7	A2	1317	C
7	A2	1318	A
7	A2	1320	C
7	A2	1332	A
7	A2	1336	C
7	A2	1338	G
7	A2	1340	A
7	A2	1346	A
7	A2	1348	U
7	A2	1351	U
7	A2	1353	G
7	A2	1360	A

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Mol	Chain	Res	Type
7	A2	1363	A
7	A2	1364	U
7	A2	1368	A
7	A2	1370	G
7	A2	1375	A
7	A2	1379	G
7	A2	1397	C
7	A2	1398	A
7	A2	1429	A
7	A2	1432	G
7	A2	1441	A
7	A2	1446	A
7	A2	1448	C
7	A2	1454	G
7	A2	1487	G
7	A2	1492	A
7	A2	1498	UR3
7	A2	1499	A
7	A2	1503	A
7	A2	1506	U
7	A2	1517	G
7	A2	1529	G
7	A2	1530	G
7	A2	1533	C
7	A2	1534	A
7	A2	1535	C
7	A2	1536	C
7	A2	1537	U
28	V2	6	A
28	V2	8	A
28	V2	9	A
28	V2	10	G
28	V2	11	G
28	V2	14	G
28	V2	15	G
28	V2	16	U
28	V2	17	G
28	V2	18	A
28	V2	19	G
28	V2	20	C
28	V2	21	U
28	V2	23	C

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Mol	Chain	Res	Type
28	V2	24	G
28	V2	30	A
28	V2	32	U
28	V2	33	A
28	V2	34	A
28	V2	35	A
28	V2	37	A
28	V2	38	A
28	V2	39	A
28	V2	40	A
28	V2	41	G
28	V2	42	G
28	V2	43	U
28	V2	45	U
28	V2	46	C
28	V2	47	G
28	V2	48	C
28	V2	50	C
28	V2	53	G
28	V2	54	G
28	V2	57	A
28	V2	58	A
28	V2	61	U
28	V2	62	C
28	V2	63	G
28	V2	64	A
28	V2	66	A
28	V2	67	A
29	W	2	G
29	W	4	G
29	W	8	4SU
29	W	11	U
29	W	15	A
29	W	16	H2U
29	W	17	H2U
29	W	18	G
29	W	19	G
29	W	20	H2U
29	W	22	G
29	W	34	C
29	W	44	G
29	W	46	G7M

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Mol	Chain	Res	Type
29	W	47	U
29	W	48	U
29	W	49	G
29	W	52	A
29	W	53	G
29	W	54	5MU
29	W	55	PSU
29	W	58	A
29	W	59	G
29	W	60	U
29	W	72	U
29	W	76	A
30	W1	11	C
30	W1	15	G
30	W1	22	G
30	W1	35	A
30	W1	44	G
30	W1	46	G7M
30	W1	47	U
30	W1	48	C
31	X2	2	C
31	X2	3	A
31	X2	8	4SU
31	X2	9	A
31	X2	13	C
31	X2	15	G
31	X2	16	C
31	X2	18	G
31	X2	20	A
31	X2	21	H2U
31	X2	22	A
31	X2	34	U
31	X2	35	I
31	X2	36	C
31	X2	39	A
31	X2	47	G7M
31	X2	49	C
31	X2	55	5MU
31	X2	60	A
31	X2	66	C
31	X2	71	U
31	X2	72	G

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Mol	Chain	Res	Type
31	X2	73	C
31	X2	74	A
31	X2	76	C
31	X2	77	A
32	Y1	10	G
32	Y1	11	C
32	Y1	46	7MG
32	Y1	48	C
33	Y2	15	G
33	Y2	16	C
33	Y2	17	H2U
33	Y2	18	G
33	Y2	19	G
33	Y2	20	G
33	Y2	21	A
33	Y2	22	G
33	Y2	34	G
33	Y2	36	C
33	Y2	39	G
33	Y2	45	G
33	Y2	46	G7M
33	Y2	48	C
33	Y2	49	A
33	Y2	54	5MU
33	Y2	56	C
33	Y2	64	C
33	Y2	72	C
33	Y2	73	A
33	Y2	74	C
33	Y2	75	C
33	Y2	76	A

All (129) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	72	43	G
5	72	134	G
5	72	158	U
5	72	277	G
5	72	285	G
5	72	352	A
5	72	404	A

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Mol	Chain	Res	Type
5	72	504	A
5	72	512	G
5	72	613	A
5	72	747	5MU
5	72	748	G
5	72	749	A
5	72	784	G
5	72	827	U
5	72	1020	A
5	72	1046	A
5	72	1130	U
5	72	1211	C
5	72	1266	G
5	72	1416	G
5	72	1475	G
5	72	1490	A
5	72	1580	A
5	72	1847	A
5	72	1940	U
5	72	2061	G
5	72	2118	U
5	72	2172	U
5	72	2430	A
5	72	2581	G
5	72	2585	U
5	72	2756	U
6	82	3	C
6	82	15	A
6	82	39	A
6	82	88	C
7	A1	5	U
7	A1	7	A
7	A1	51	A
7	A1	70	U
7	A1	129	A
7	A1	173	U
7	A1	197	A
7	A1	209	U
7	A1	251	G
7	A1	274	A
7	A1	372	C
7	A1	412	A

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Mol	Chain	Res	Type
7	A1	421	U
7	A1	428	G
7	A1	438	U
7	A1	535	A
7	A1	559	A
7	A1	575	G
7	A1	653	U
7	A1	686	U
7	A1	870	U
7	A1	884	U
7	A1	992	U
7	A1	993	G
7	A1	1054	C
7	A1	1085	U
7	A1	1182	G
7	A1	1190	G
7	A1	1201	A
7	A1	1302	C
7	A1	1335	U
7	A1	1432	G
7	A1	1440	U
7	A1	1452	C
7	A1	1463	U
7	A1	1536	C
7	A2	7	A
7	A2	13	U
7	A2	30	U
7	A2	70	U
7	A2	183	C
7	A2	208	U
7	A2	209	U
7	A2	251	G
7	A2	367	U
7	A2	411	A
7	A2	428	G
7	A2	438	U
7	A2	532	A
7	A2	537	G
7	A2	717	U
7	A2	845	A
7	A2	992	U
7	A2	993	G

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Mol	Chain	Res	Type
7	A2	1085	U
7	A2	1101	A
7	A2	1129	C
7	A2	1136	C
7	A2	1140	C
7	A2	1168	U
7	A2	1190	G
7	A2	1201	A
7	A2	1256	A
7	A2	1281	C
7	A2	1297	G
7	A2	1319	A
7	A2	1533	C
7	A2	1534	A
7	A2	1535	C
28	V2	8	A
28	V2	23	C
28	V2	31	U
28	V2	36	A
28	V2	37	A
28	V2	39	A
28	V2	46	C
28	V2	53	G
29	W	10	G
29	W	18	G
29	W	19	G
29	W	43	G
30	W1	10	G
30	W1	43	C
31	X2	15	G
31	X2	22	A
31	X2	47	G7M
31	X2	49	C
31	X2	73	C
32	Y1	10	G
32	Y1	47	U
33	Y2	17	H2U
33	Y2	63	G

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

73 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
7	2MG	A1	1207	7	18,26,27	2.84	7 (38%)	16,38,41	1.34	3 (18%)
7	5MC	A1	967	7	18,22,23	4.03	7 (38%)	26,32,35	1.01	2 (7%)
31	H2U	X2	17	31	18,21,22	3.09	5 (27%)	21,30,33	1.95	5 (23%)
5	OMU	72	2552	5	19,22,23	3.22	8 (42%)	26,31,34	1.68	5 (19%)
30	4SU	W1	8	30	18,21,22	3.80	7 (38%)	26,30,33	2.21	4 (15%)
7	2MG	A1	1516	7	18,26,27	2.84	7 (38%)	16,38,41	1.36	3 (18%)
5	5MU	72	747	5	19,22,23	0.34	0	28,32,35	0.58	0
7	MA6	A2	1518	7	18,26,27	1.07	2 (11%)	19,38,41	3.41	3 (15%)
5	2MG	72	1835	5	18,26,27	2.80	7 (38%)	16,38,41	1.41	4 (25%)
32	CM0	Y1	34	32	23,26,27	3.73	6 (26%)	27,37,40	1.52	2 (7%)
5	6MZ	72	2030	5	18,25,26	2.07	3 (16%)	16,36,39	2.31	3 (18%)
31	G7M	X2	47	31	20,26,27	2.81	7 (35%)	17,39,42	1.21	1 (5%)
31	5MU	X2	55	31	19,22,23	0.25	0	28,32,35	0.18	0
5	G7M	72	2069	5	20,26,27	2.77	7 (35%)	17,39,42	1.04	1 (5%)
5	PSU	72	746	5	18,21,22	0.99	2 (11%)	22,30,33	0.95	1 (4%)
33	5MU	Y2	54	33	19,22,23	0.24	0	28,32,35	0.24	0
5	PSU	72	2605	5	18,21,22	4.64	8 (44%)	22,30,33	1.85	5 (22%)
29	PSU	W	32	29	18,21,22	4.63	8 (44%)	22,30,33	1.88	5 (22%)
7	2MG	A2	1516	7	18,26,27	2.81	7 (38%)	16,38,41	1.36	3 (18%)
5	H2U	72	2449	49,5	18,21,22	3.04	5 (27%)	21,30,33	2.03	5 (23%)
5	3TD	71	1915	5	19,22,23	4.09	7 (36%)	21,32,35	1.70	2 (9%)
7	4OC	A1	1402	7	20,23,24	3.22	8 (40%)	26,32,35	0.93	1 (3%)
7	UR3	A2	1498	7	19,22,23	2.73	8 (42%)	26,32,35	1.29	2 (7%)
5	2MG	72	2445	5	18,26,27	2.82	7 (38%)	16,38,41	1.41	4 (25%)
31	3AU	X2	48	31	24,28,29	2.84	7 (29%)	33,40,43	1.29	3 (9%)
31	H2U	X2	21	31	18,21,22	3.07	5 (27%)	21,30,33	2.04	5 (23%)
30	PSU	W1	32	30	18,21,22	4.65	8 (44%)	22,30,33	1.82	5 (22%)
29	G7M	W	46	29	20,26,27	2.79	7 (35%)	17,39,42	1.12	1 (5%)
5	OMC	72	2498	49,5	19,22,23	3.29	8 (42%)	26,31,34	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	1MG	72	745	5	18,26,27	2.75	6 (33%)	19,39,42	1.43	3 (15%)
29	5MU	W	54	29	19,22,23	0.25	0	28,32,35	0.39	0
5	6MZ	72	1618	5	18,25,26	2.03	2 (11%)	16,36,39	2.20	4 (25%)
7	2MG	A2	1207	7	18,26,27	2.86	7 (38%)	16,38,41	1.37	3 (18%)
7	UR3	A1	1498	7	19,22,23	2.75	8 (42%)	26,32,35	1.29	3 (11%)
5	2MA	72	2503	5	19,25,26	3.58	6 (31%)	21,37,40	3.66	4 (19%)
31	4SU	X2	8	31	18,21,22	3.79	7 (38%)	26,30,33	2.27	4 (15%)
31	PSU	X2	56	31	18,21,22	0.87	1 (5%)	22,30,33	0.49	0
33	H2U	Y2	17	33	18,21,22	3.07	5 (27%)	21,30,33	2.01	5 (23%)
33	PSU	Y2	55	33	18,21,22	0.88	1 (5%)	22,30,33	0.64	0
5	OMG	72	2251	29,5	18,26,27	2.82	7 (38%)	19,38,41	1.55	4 (21%)
29	H2U	W	16	29	18,21,22	3.05	5 (27%)	21,30,33	1.98	5 (23%)
5	PSU	72	2504	49,5	18,21,22	4.67	8 (44%)	22,30,33	1.92	5 (22%)
30	MIA	W1	37	30	24,31,32	2.34	3 (12%)	26,44,47	2.67	7 (26%)
5	PSU	72	2604	5	18,21,22	4.64	8 (44%)	22,30,33	1.83	5 (22%)
30	PSU	W1	39	30	18,21,22	4.64	8 (44%)	22,30,33	1.84	5 (22%)
31	RSP	X2	33	31	17,21,22	4.13	7 (41%)	22,30,33	0.78	0
29	4SU	W	8	29	18,21,22	3.77	7 (38%)	26,30,33	2.26	5 (19%)
7	G7M	A1	527	7	20,26,27	2.79	8 (40%)	17,39,42	1.04	1 (5%)
29	MIA	W	37	29	24,31,32	2.32	3 (12%)	26,44,47	2.53	7 (26%)
7	5MC	A1	1407	7	18,22,23	4.03	7 (38%)	26,32,35	0.99	2 (7%)
7	5MC	A2	1407	7	18,22,23	4.00	7 (38%)	26,32,35	0.97	2 (7%)
32	6MZ	Y1	37	32	18,25,26	2.06	3 (16%)	16,36,39	2.35	4 (25%)
29	H2U	W	17	29	18,21,22	3.08	5 (27%)	21,30,33	2.01	5 (23%)
33	G7M	Y2	46	33	20,26,27	2.81	8 (40%)	17,39,42	1.09	1 (5%)
5	PSU	72	955	5	18,21,22	4.67	8 (44%)	22,30,33	1.87	5 (22%)
29	PSU	W	55	29	18,21,22	0.85	1 (5%)	22,30,33	0.79	1 (4%)
7	MA6	A1	1518	7	18,26,27	1.06	2 (11%)	19,38,41	3.38	3 (15%)
31	2MA	X2	38	31	19,25,26	3.64	6 (31%)	21,37,40	3.60	3 (14%)
29	H2U	W	20	29	18,21,22	3.04	5 (27%)	21,30,33	2.02	5 (23%)
5	3TD	72	1915	5	19,22,23	4.03	7 (36%)	21,32,35	1.78	3 (14%)
7	4OC	A2	1402	7	20,23,24	3.24	8 (40%)	26,32,35	0.90	1 (3%)
7	2MG	A1	966	7	18,26,27	2.85	7 (38%)	16,38,41	1.41	3 (18%)
7	G7M	A2	527	7	20,26,27	2.77	7 (35%)	17,39,42	1.02	1 (5%)
7	2MG	A2	966	7	18,26,27	2.85	7 (38%)	16,38,41	1.35	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	5MU	72	1939	5	19,22,23	0.74	0	28,32,35	1.27	2 (7%)
5	PSU	72	2580	5	18,21,22	4.65	8 (44%)	22,30,33	1.85	6 (27%)
30	G7M	W1	46	30	20,26,27	2.81	7 (35%)	17,39,42	1.12	1 (5%)
7	MA6	A1	1519	7	18,26,27	1.08	2 (11%)	19,38,41	3.47	3 (15%)
5	5MC	72	1962	5	18,22,23	4.01	7 (38%)	26,32,35	1.06	2 (7%)
7	5MC	A2	967	7	18,22,23	4.01	7 (38%)	26,32,35	1.00	2 (7%)
32	7MG	Y1	46	32	22,26,27	3.89	10 (45%)	29,39,42	2.07	9 (31%)
7	MA6	A2	1519	7	18,26,27	1.08	2 (11%)	19,38,41	3.42	3 (15%)
5	PSU	72	2457	5	18,21,22	4.65	8 (44%)	22,30,33	1.88	5 (22%)

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
7	2MG	A1	1207	7	-	0/5/27/28	0/3/3/3
7	5MC	A1	967	7	-	0/7/25/26	0/2/2/2
31	H2U	X2	17	31	-	6/7/38/39	0/2/2/2
5	OMU	72	2552	5	-	0/9/27/28	0/2/2/2
30	4SU	W1	8	30	-	2/7/25/26	0/2/2/2
7	2MG	A1	1516	7	-	0/5/27/28	0/3/3/3
5	5MU	72	747	5	-	0/7/25/26	0/2/2/2
7	MA6	A2	1518	7	-	0/7/29/30	0/3/3/3
5	2MG	72	1835	5	-	0/5/27/28	0/3/3/3
32	CM0	Y1	34	32	-	2/12/30/31	0/2/2/2
5	6MZ	72	2030	5	-	3/5/27/28	0/3/3/3
31	G7M	X2	47	31	-	3/3/25/26	0/3/3/3
31	5MU	X2	55	31	-	2/7/25/26	0/2/2/2
5	G7M	72	2069	5	-	2/3/25/26	0/3/3/3
5	PSU	72	746	5	-	1/7/25/26	0/2/2/2
33	5MU	Y2	54	33	-	2/7/25/26	0/2/2/2
5	PSU	72	2605	5	-	0/7/25/26	0/2/2/2
29	PSU	W	32	29	-	0/7/25/26	0/2/2/2
7	2MG	A2	1516	7	-	0/5/27/28	0/3/3/3
5	H2U	72	2449	49,5	-	1/7/38/39	0/2/2/2
5	3TD	71	1915	5	-	1/7/25/26	0/2/2/2
7	4OC	A1	1402	7	-	2/9/29/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	UR3	A2	1498	7	-	2/7/25/26	0/2/2/2
5	2MG	72	2445	5	-	0/5/27/28	0/3/3/3
31	3AU	X2	48	31	-	6/16/34/35	0/2/2/2
31	H2U	X2	21	31	-	3/7/38/39	0/2/2/2
30	PSU	W1	32	30	-	0/7/25/26	0/2/2/2
29	G7M	W	46	29	-	3/3/25/26	0/3/3/3
5	OMC	72	2498	49,5	-	2/9/27/28	0/2/2/2
5	1MG	72	745	5	-	0/3/25/26	0/3/3/3
29	5MU	W	54	29	-	3/7/25/26	0/2/2/2
5	6MZ	72	1618	5	-	4/5/27/28	0/3/3/3
7	2MG	A2	1207	7	-	0/5/27/28	0/3/3/3
7	UR3	A1	1498	7	-	2/7/25/26	0/2/2/2
5	2MA	72	2503	5	-	0/3/25/26	0/3/3/3
31	4SU	X2	8	31	-	2/7/25/26	0/2/2/2
31	PSU	X2	56	31	-	2/7/25/26	0/2/2/2
33	H2U	Y2	17	33	-	7/7/38/39	0/2/2/2
33	PSU	Y2	55	33	-	0/7/25/26	0/2/2/2
5	OMG	72	2251	29,5	-	3/5/27/28	0/3/3/3
29	H2U	W	16	29	-	1/7/38/39	0/2/2/2
5	PSU	72	2504	49,5	-	1/7/25/26	0/2/2/2
30	MIA	W1	37	30	-	6/11/33/34	0/3/3/3
5	PSU	72	2604	5	-	0/7/25/26	0/2/2/2
30	PSU	W1	39	30	-	0/7/25/26	0/2/2/2
31	RSP	X2	33	31	-	1/7/25/26	0/2/2/2
29	4SU	W	8	29	-	2/7/25/26	0/2/2/2
7	G7M	A1	527	7	-	1/3/25/26	0/3/3/3
29	MIA	W	37	29	-	1/11/33/34	0/3/3/3
7	5MC	A1	1407	7	-	0/7/25/26	0/2/2/2
7	5MC	A2	1407	7	-	0/7/25/26	0/2/2/2
32	6MZ	Y1	37	32	-	2/5/27/28	0/3/3/3
29	H2U	W	17	29	-	1/7/38/39	0/2/2/2
33	G7M	Y2	46	33	-	2/3/25/26	0/3/3/3
5	PSU	72	955	5	-	0/7/25/26	0/2/2/2
29	PSU	W	55	29	-	3/7/25/26	0/2/2/2
7	MA6	A1	1518	7	-	3/7/29/30	0/3/3/3
31	2MA	X2	38	31	-	3/3/25/26	0/3/3/3
29	H2U	W	20	29	-	1/7/38/39	0/2/2/2
5	3TD	72	1915	5	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	4OC	A2	1402	7	-	1/9/29/30	0/2/2/2
7	2MG	A1	966	7	-	0/5/27/28	0/3/3/3
7	G7M	A2	527	7	-	3/3/25/26	0/3/3/3
7	2MG	A2	966	7	-	0/5/27/28	0/3/3/3
5	5MU	72	1939	5	-	2/7/25/26	0/2/2/2
5	PSU	72	2580	5	-	0/7/25/26	0/2/2/2
30	G7M	W1	46	30	-	3/3/25/26	0/3/3/3
7	MA6	A1	1519	7	-	6/7/29/30	0/3/3/3
5	5MC	72	1962	5	-	0/7/25/26	0/2/2/2
7	5MC	A2	967	7	-	1/7/25/26	0/2/2/2
32	7MG	Y1	46	32	-	1/7/37/38	0/3/3/3
7	MA6	A2	1519	7	-	2/7/29/30	0/3/3/3
5	PSU	72	2457	5	-	2/7/25/26	0/2/2/2

All (414) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y1	34	CM0	C6-C5	12.87	1.48	1.34
5	71	1915	3TD	C6-C5	12.74	1.50	1.35
5	72	1915	3TD	C6-C5	12.52	1.49	1.35
5	72	2504	PSU	C6-C5	12.20	1.49	1.35
5	72	955	PSU	C6-C5	12.17	1.49	1.35
5	72	2457	PSU	C6-C5	12.13	1.49	1.35
30	W1	32	PSU	C6-C5	12.13	1.49	1.35
30	W1	39	PSU	C6-C5	12.12	1.49	1.35
29	W	32	PSU	C6-C5	12.10	1.49	1.35
5	72	2605	PSU	C6-C5	12.09	1.49	1.35
5	72	2580	PSU	C6-C5	12.06	1.49	1.35
5	72	2604	PSU	C6-C5	12.06	1.49	1.35
31	X2	33	RSP	C2-N3	11.76	1.48	1.36
32	Y1	46	7MG	C8-N9	9.99	1.51	1.46
7	A1	967	5MC	C6-C5	9.98	1.51	1.34
7	A1	1407	5MC	C6-C5	9.89	1.50	1.34
5	72	1962	5MC	C6-C5	9.89	1.50	1.34
7	A2	967	5MC	C6-C5	9.87	1.50	1.34
7	A2	1407	5MC	C6-C5	9.84	1.50	1.34
5	72	2504	PSU	C2-N1	9.63	1.49	1.36
31	X2	17	H2U	C2-N1	9.62	1.49	1.35
5	72	955	PSU	C2-N1	9.58	1.49	1.36
5	72	2580	PSU	C2-N1	9.56	1.49	1.36
30	W1	32	PSU	C2-N1	9.55	1.49	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2604	PSU	C2-N1	9.54	1.49	1.36
30	W1	39	PSU	C2-N1	9.53	1.49	1.36
5	72	2457	PSU	C2-N1	9.53	1.49	1.36
5	72	2605	PSU	C2-N1	9.52	1.49	1.36
29	W	32	PSU	C2-N1	9.49	1.49	1.36
29	W	17	H2U	C2-N1	9.46	1.49	1.35
31	X2	21	H2U	C2-N1	9.44	1.49	1.35
33	Y2	17	H2U	C2-N1	9.42	1.49	1.35
29	W	16	H2U	C2-N1	9.39	1.49	1.35
5	72	2449	H2U	C2-N1	9.36	1.49	1.35
29	W	20	H2U	C2-N1	9.34	1.49	1.35
31	X2	38	2MA	C4-N3	9.29	1.50	1.35
5	72	2503	2MA	C4-N3	9.02	1.49	1.35
30	W1	8	4SU	C4-N3	8.98	1.47	1.37
5	71	1915	3TD	C2-N1	8.86	1.48	1.37
29	W	8	4SU	C4-N3	8.85	1.47	1.37
5	72	1915	3TD	C2-N1	8.85	1.48	1.37
31	X2	8	4SU	C4-N3	8.83	1.47	1.37
5	72	2504	PSU	C2-N3	8.24	1.51	1.37
5	72	955	PSU	C2-N3	8.23	1.51	1.37
30	W1	32	PSU	C2-N3	8.21	1.51	1.37
29	W	32	PSU	C2-N3	8.21	1.51	1.37
5	72	2605	PSU	C2-N3	8.20	1.51	1.37
5	72	2580	PSU	C2-N3	8.19	1.51	1.37
5	72	2604	PSU	C2-N3	8.19	1.51	1.37
5	72	2457	PSU	C2-N3	8.19	1.51	1.37
30	W1	39	PSU	C2-N3	8.14	1.51	1.37
31	X2	48	3AU	C2-N1	8.13	1.50	1.38
31	X2	38	2MA	C2-N3	8.06	1.48	1.34
32	Y1	46	7MG	C5-N7	7.90	1.44	1.35
5	72	2503	2MA	C2-N3	7.86	1.48	1.34
30	W1	37	MIA	C2-S10	7.71	1.82	1.75
29	W	37	MIA	C2-S10	7.69	1.82	1.75
5	72	1962	5MC	C4-N3	7.46	1.46	1.34
7	A2	967	5MC	C4-N3	7.45	1.46	1.34
7	A1	967	5MC	C4-N3	7.44	1.46	1.34
5	72	2030	6MZ	C6-N6	7.42	1.47	1.35
32	Y1	34	CM0	C2-N1	7.39	1.50	1.38
7	A1	1407	5MC	C4-N3	7.35	1.46	1.34
32	Y1	37	6MZ	C6-N6	7.34	1.47	1.35
7	A2	1407	5MC	C4-N3	7.30	1.46	1.34
5	72	1618	6MZ	C6-N6	7.22	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	2251	OMG	C2-N2	7.18	1.51	1.34
7	A2	1402	4OC	C4-N3	7.12	1.45	1.32
7	A1	1498	UR3	C2-N1	7.04	1.48	1.38
5	72	2498	OMC	C2-N3	7.00	1.50	1.36
7	A2	1498	UR3	C2-N1	6.98	1.48	1.38
32	Y1	34	CM0	C2-N3	6.98	1.50	1.38
5	72	2552	OMU	C2-N3	6.97	1.50	1.38
7	A1	1407	5MC	C2-N3	6.96	1.50	1.36
7	A1	1402	4OC	C4-N3	6.95	1.44	1.32
7	A1	967	5MC	C2-N3	6.94	1.50	1.36
7	A2	967	5MC	C2-N3	6.92	1.50	1.36
30	W1	8	4SU	C2-N3	6.91	1.50	1.38
30	W1	37	MIA	C6-N6	6.91	1.47	1.34
5	72	1962	5MC	C2-N3	6.90	1.50	1.36
7	A2	1407	5MC	C2-N3	6.90	1.50	1.36
31	X2	8	4SU	C2-N3	6.86	1.50	1.38
29	W	8	4SU	C2-N3	6.82	1.50	1.38
5	72	745	1MG	C2-N3	6.80	1.47	1.34
29	W	37	MIA	C6-N6	6.80	1.47	1.34
31	X2	33	RSP	C6-C5	6.72	1.50	1.35
31	X2	33	RSP	C4-N4	6.65	1.49	1.33
33	Y2	46	G7M	C2-N2	6.61	1.49	1.34
31	X2	47	G7M	C2-N2	6.59	1.49	1.34
29	W	46	G7M	C2-N2	6.58	1.49	1.34
5	72	2069	G7M	C2-N2	6.58	1.49	1.34
30	W1	46	G7M	C2-N2	6.56	1.49	1.34
7	A2	527	G7M	C2-N2	6.55	1.49	1.34
7	A2	1207	2MG	C2-N2	6.54	1.47	1.33
7	A1	527	G7M	C2-N2	6.53	1.49	1.34
5	72	2552	OMU	C2-N1	6.53	1.48	1.38
29	W	17	H2U	C2-N3	6.52	1.49	1.38
31	X2	17	H2U	C2-N3	6.49	1.49	1.38
33	Y2	17	H2U	C2-N3	6.49	1.49	1.38
7	A1	1516	2MG	C2-N2	6.48	1.47	1.33
31	X2	21	H2U	C2-N3	6.47	1.49	1.38
7	A1	966	2MG	C2-N2	6.47	1.47	1.33
29	W	20	H2U	C2-N3	6.46	1.49	1.38
7	A1	1207	2MG	C2-N2	6.45	1.47	1.33
7	A2	966	2MG	C2-N2	6.45	1.47	1.33
7	A1	1402	4OC	C6-C5	6.43	1.50	1.35
5	72	1835	2MG	C2-N2	6.43	1.47	1.33
29	W	16	H2U	C2-N3	6.42	1.49	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	1516	2MG	C2-N2	6.41	1.47	1.33
5	72	745	1MG	C2-N2	6.41	1.45	1.34
5	72	2449	H2U	C2-N3	6.40	1.49	1.38
31	X2	48	3AU	C2-N3	6.38	1.50	1.38
5	72	2445	2MG	C2-N2	6.38	1.47	1.33
7	A2	1402	4OC	C6-C5	6.36	1.49	1.35
7	A2	1402	4OC	C2-N3	6.33	1.49	1.36
7	A1	1402	4OC	C2-N3	6.21	1.48	1.36
31	X2	38	2MA	C2-N1	6.20	1.45	1.34
5	72	2503	2MA	C2-N1	6.17	1.45	1.34
7	A1	1498	UR3	C6-C5	6.16	1.49	1.35
7	A2	1498	UR3	C6-C5	6.13	1.49	1.35
5	72	2498	OMC	C6-C5	6.11	1.49	1.35
31	X2	8	4SU	C4-S4	-6.07	1.56	1.68
5	72	2503	2MA	C6-N1	6.05	1.44	1.33
31	X2	48	3AU	C6-C5	6.04	1.49	1.35
31	X2	38	2MA	C6-N1	6.03	1.44	1.33
29	W	8	4SU	C4-S4	-5.96	1.57	1.68
30	W1	8	4SU	C4-S4	-5.93	1.57	1.68
32	Y1	46	7MG	C2-N3	5.92	1.47	1.33
31	X2	8	4SU	C2-N1	5.86	1.47	1.38
30	W1	8	4SU	C6-C5	5.84	1.48	1.35
5	72	955	PSU	C6-N1	5.83	1.45	1.36
33	Y2	46	G7M	C2-N3	5.83	1.47	1.33
30	W1	8	4SU	C2-N1	5.83	1.47	1.38
29	W	8	4SU	C6-C5	5.82	1.48	1.35
30	W1	39	PSU	C6-N1	5.82	1.45	1.36
31	X2	8	4SU	C6-C5	5.82	1.48	1.35
30	W1	46	G7M	C2-N3	5.80	1.47	1.33
5	72	2457	PSU	C6-N1	5.80	1.45	1.36
7	A1	527	G7M	C2-N3	5.80	1.47	1.33
5	72	2580	PSU	C6-N1	5.79	1.45	1.36
5	72	2504	PSU	C6-N1	5.79	1.45	1.36
30	W1	32	PSU	C6-N1	5.77	1.45	1.36
5	72	2605	PSU	C6-N1	5.77	1.45	1.36
5	72	2604	PSU	C6-N1	5.76	1.45	1.36
31	X2	47	G7M	C2-N3	5.74	1.47	1.33
7	A2	527	G7M	C2-N3	5.74	1.47	1.33
5	72	2069	G7M	C2-N3	5.74	1.47	1.33
29	W	46	G7M	C2-N3	5.74	1.47	1.33
29	W	32	PSU	C6-N1	5.73	1.45	1.36
29	W	8	4SU	C2-N1	5.72	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y1	46	7MG	C4-N9	5.67	1.44	1.37
7	A1	967	5MC	C4-N4	5.66	1.48	1.34
7	A1	1407	5MC	C4-N4	5.66	1.48	1.34
7	A2	1407	5MC	C4-N4	5.64	1.48	1.34
7	A2	967	5MC	C4-N4	5.63	1.48	1.34
5	72	1962	5MC	C4-N4	5.62	1.48	1.34
7	A1	1407	5MC	C6-N1	5.61	1.47	1.38
32	Y1	46	7MG	C4-N3	5.59	1.47	1.34
5	72	2445	2MG	C4-N3	5.55	1.50	1.37
7	A1	966	2MG	C4-N3	5.54	1.50	1.37
7	A2	1407	5MC	C6-N1	5.53	1.47	1.38
5	71	1915	3TD	C6-N1	5.53	1.45	1.36
7	A1	1516	2MG	C4-N3	5.52	1.50	1.37
5	72	2498	OMC	C4-N3	5.51	1.45	1.34
7	A2	1207	2MG	C4-N3	5.51	1.50	1.37
7	A1	967	5MC	C6-N1	5.49	1.47	1.38
5	72	1915	3TD	C6-N1	5.49	1.45	1.36
5	72	1962	5MC	C6-N1	5.47	1.47	1.38
7	A2	966	2MG	C4-N3	5.47	1.50	1.37
5	72	2552	OMU	C6-C5	5.47	1.47	1.35
5	72	1835	2MG	C4-N3	5.46	1.50	1.37
7	A2	967	5MC	C6-N1	5.44	1.47	1.38
7	A1	1207	2MG	C4-N3	5.42	1.50	1.37
7	A1	1207	2MG	C2-N1	5.42	1.45	1.36
31	X2	33	RSP	C4-N3	5.41	1.45	1.34
7	A1	966	2MG	C2-N1	5.40	1.45	1.36
7	A2	1207	2MG	C2-N1	5.40	1.45	1.36
7	A2	966	2MG	C2-N1	5.39	1.45	1.36
7	A2	1516	2MG	C4-N3	5.38	1.50	1.37
7	A1	1516	2MG	C2-N1	5.38	1.45	1.36
7	A2	1516	2MG	C2-N1	5.36	1.45	1.36
30	W1	46	G7M	C4-N3	5.34	1.50	1.37
31	X2	47	G7M	C4-N3	5.33	1.50	1.37
5	72	2445	2MG	C2-N1	5.29	1.45	1.36
29	W	46	G7M	C4-N3	5.28	1.50	1.37
5	72	1835	2MG	C2-N1	5.24	1.45	1.36
5	72	2498	OMC	C4-N4	5.21	1.46	1.33
33	Y2	46	G7M	C4-N3	5.21	1.50	1.37
5	72	2251	OMG	C2-N3	5.18	1.45	1.33
7	A1	1498	UR3	C2-N3	5.13	1.48	1.39
7	A2	1402	4OC	C4-N4	5.12	1.46	1.35
5	72	2069	G7M	C4-N3	5.11	1.49	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A2	527	G7M	C4-N3	5.11	1.49	1.37
5	72	745	1MG	C4-N3	5.09	1.49	1.37
7	A1	527	G7M	C4-N3	5.09	1.49	1.37
7	A1	1402	4OC	C4-N4	5.09	1.46	1.35
7	A2	1498	UR3	C2-N3	5.03	1.48	1.39
29	W	20	H2U	C4-N3	4.97	1.46	1.37
29	W	17	H2U	C4-N3	4.97	1.46	1.37
31	X2	21	H2U	C4-N3	4.92	1.46	1.37
31	X2	17	H2U	C4-N3	4.92	1.46	1.37
5	72	2449	H2U	C4-N3	4.90	1.45	1.37
33	Y2	17	H2U	C4-N3	4.90	1.45	1.37
29	W	16	H2U	C4-N3	4.86	1.45	1.37
32	Y1	46	7MG	C2-N2	4.74	1.45	1.34
5	72	2552	OMU	C4-N3	4.64	1.46	1.38
7	A2	967	5MC	C2-N1	4.56	1.49	1.40
7	A1	1407	5MC	C2-N1	4.56	1.49	1.40
5	72	1962	5MC	C2-N1	4.55	1.49	1.40
5	72	2251	OMG	C4-N3	4.53	1.48	1.37
32	Y1	34	CM0	C6-N1	4.53	1.45	1.38
7	A1	967	5MC	C2-N1	4.52	1.49	1.40
5	72	2552	OMU	O4-C4	-4.49	1.15	1.24
7	A2	1407	5MC	C2-N1	4.48	1.49	1.40
33	Y2	46	G7M	C6-N1	4.46	1.44	1.37
5	72	2498	OMC	C2-N1	4.45	1.49	1.40
5	72	2504	PSU	C4-N3	4.40	1.47	1.38
5	72	2580	PSU	C4-N3	4.39	1.47	1.38
30	W1	32	PSU	C4-N3	4.38	1.47	1.38
7	A1	527	G7M	C6-N1	4.37	1.44	1.37
5	72	955	PSU	C4-N3	4.35	1.46	1.38
5	72	2605	PSU	C4-N3	4.34	1.46	1.38
5	72	2457	PSU	C4-N3	4.33	1.46	1.38
30	W1	46	G7M	C6-N1	4.33	1.44	1.37
30	W1	39	PSU	C4-N3	4.32	1.46	1.38
29	W	32	PSU	C4-N3	4.32	1.46	1.38
5	72	2069	G7M	C6-N1	4.31	1.44	1.37
29	W	46	G7M	C6-N1	4.30	1.44	1.37
7	A2	527	G7M	C6-N1	4.29	1.44	1.37
31	X2	47	G7M	C6-N1	4.29	1.44	1.37
5	72	2604	PSU	C4-N3	4.28	1.46	1.38
7	A2	1402	4OC	C2-N1	4.26	1.49	1.40
5	71	1915	3TD	C2-N3	4.21	1.47	1.38
7	A1	1402	4OC	C2-N1	4.20	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	1915	3TD	C2-N3	4.18	1.47	1.38
7	A1	966	2MG	C6-N1	4.14	1.44	1.37
5	72	2498	OMC	O2-C2	-4.13	1.16	1.23
7	A2	1516	2MG	C6-N1	4.08	1.44	1.37
7	A2	966	2MG	C6-N1	4.07	1.43	1.37
7	A1	1516	2MG	C6-N1	4.03	1.43	1.37
5	72	2445	2MG	C6-N1	4.03	1.43	1.37
7	A2	1207	2MG	C6-N1	4.01	1.43	1.37
5	72	1835	2MG	C6-N1	3.99	1.43	1.37
7	A1	1402	4OC	C5-C4	3.97	1.49	1.40
7	A1	1207	2MG	C6-N1	3.96	1.43	1.37
7	A2	966	2MG	C5-C6	3.87	1.55	1.47
7	A2	1402	4OC	C5-C4	3.86	1.49	1.40
32	Y1	46	7MG	C2-N1	3.84	1.47	1.37
7	A1	966	2MG	C5-C6	3.81	1.55	1.47
5	72	2445	2MG	C5-C6	3.80	1.55	1.47
5	72	2498	OMC	C6-N1	3.79	1.47	1.38
5	72	1835	2MG	C5-C6	3.79	1.55	1.47
7	A2	1207	2MG	C5-C6	3.78	1.55	1.47
7	A1	1207	2MG	C5-C6	3.78	1.55	1.47
7	A1	1516	2MG	C5-C6	3.76	1.55	1.47
7	A2	1516	2MG	C5-C6	3.75	1.55	1.47
32	Y1	34	CM0	C4-N3	3.71	1.45	1.38
5	72	2552	OMU	C6-N1	3.70	1.46	1.38
5	72	2552	OMU	O2-C2	-3.57	1.16	1.23
31	X2	48	3AU	C4-N3	3.57	1.46	1.40
31	X2	33	RSP	C5-C4	3.56	1.51	1.42
30	W1	46	G7M	C5-C6	3.53	1.54	1.45
32	Y1	46	7MG	C5-C6	3.52	1.52	1.43
31	X2	47	G7M	C5-C6	3.50	1.54	1.45
29	W	8	4SU	C5-C4	3.49	1.47	1.42
30	W1	8	4SU	C6-N1	3.48	1.46	1.38
30	W1	8	4SU	C5-C4	3.48	1.47	1.42
29	W	46	G7M	C5-C6	3.47	1.54	1.45
31	X2	8	4SU	C5-C4	3.47	1.47	1.42
7	A1	527	G7M	C5-C6	3.47	1.54	1.45
33	Y2	46	G7M	C5-C6	3.45	1.54	1.45
32	Y1	46	7MG	C6-N1	3.44	1.45	1.38
33	Y2	55	PSU	C6-C5	3.43	1.39	1.35
31	X2	38	2MA	C6-C5	3.40	1.55	1.43
31	X2	8	4SU	C6-N1	3.38	1.46	1.38
5	72	2069	G7M	C5-C6	3.38	1.54	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	8	4SU	C6-N1	3.38	1.46	1.38
7	A2	527	G7M	C5-C6	3.37	1.54	1.45
31	X2	56	PSU	C6-C5	3.34	1.39	1.35
5	72	2503	2MA	C6-C5	3.33	1.55	1.43
5	72	2251	OMG	C2-N1	3.30	1.45	1.37
7	A1	1402	4OC	C6-N1	3.28	1.45	1.38
31	X2	48	3AU	C6-N1	3.27	1.45	1.38
29	W	55	PSU	C6-C5	3.25	1.39	1.35
5	72	955	PSU	O4-C4	-3.24	1.17	1.23
30	W1	32	PSU	O4-C4	-3.22	1.17	1.23
30	W1	39	PSU	O4-C4	-3.21	1.17	1.23
5	72	2604	PSU	O4-C4	-3.21	1.17	1.23
7	A2	1402	4OC	C6-N1	3.21	1.45	1.38
29	W	32	PSU	O4-C4	-3.18	1.17	1.23
5	72	2605	PSU	O4-C4	-3.18	1.17	1.23
5	72	2457	PSU	O4-C4	-3.17	1.17	1.23
31	X2	33	RSP	C2-S2	-3.17	1.59	1.67
5	72	2580	PSU	O4-C4	-3.15	1.17	1.23
5	72	2504	PSU	O4-C4	-3.13	1.17	1.23
31	X2	33	RSP	C6-N1	3.10	1.45	1.38
33	Y2	46	G7M	C2-N1	3.09	1.45	1.37
5	72	746	PSU	C6-C5	3.06	1.38	1.35
7	A1	1498	UR3	C6-N1	3.03	1.45	1.38
31	X2	48	3AU	C11-C10	3.03	1.59	1.52
5	72	2069	G7M	C2-N1	3.02	1.45	1.37
5	72	2251	OMG	C6-N1	3.02	1.42	1.37
7	A1	527	G7M	C2-N1	3.00	1.45	1.37
7	A2	527	G7M	C2-N1	3.00	1.45	1.37
7	A2	1498	UR3	C6-N1	2.99	1.45	1.38
30	W1	46	G7M	C2-N1	2.97	1.45	1.37
29	W	46	G7M	C2-N1	2.97	1.45	1.37
31	X2	47	G7M	C2-N1	2.95	1.45	1.37
5	72	2251	OMG	C5-C6	2.85	1.53	1.47
5	72	2498	OMC	C5-C4	2.81	1.49	1.42
7	A1	1402	4OC	O2-C2	-2.81	1.18	1.23
5	72	2580	PSU	C1'-C5	2.79	1.56	1.50
5	72	2604	PSU	C1'-C5	2.78	1.56	1.50
5	72	2605	PSU	C1'-C5	2.76	1.56	1.50
30	W1	32	PSU	C1'-C5	2.74	1.56	1.50
5	72	2457	PSU	C1'-C5	2.73	1.56	1.50
7	A2	1402	4OC	O2-C2	-2.72	1.18	1.23
31	X2	48	3AU	C5-C4	2.72	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	72	955	PSU	C1'-C5	2.72	1.56	1.50
7	A1	1519	MA6	C2-N3	2.71	1.36	1.32
5	72	2504	PSU	C1'-C5	2.70	1.56	1.50
30	W1	39	PSU	C1'-C5	2.67	1.56	1.50
5	72	2604	PSU	O2-C2	-2.65	1.17	1.23
5	72	955	PSU	O2-C2	-2.65	1.17	1.23
29	W	32	PSU	C1'-C5	2.64	1.56	1.50
7	A1	1518	MA6	C2-N3	2.63	1.36	1.32
7	A2	1519	MA6	C2-N3	2.61	1.36	1.32
30	W1	39	PSU	O2-C2	-2.61	1.17	1.23
29	W	32	PSU	O2-C2	-2.61	1.17	1.23
5	71	1915	3TD	C1'-C5	2.61	1.56	1.50
32	Y1	34	CM0	O5-C7	-2.60	1.38	1.44
5	72	2580	PSU	O2-C2	-2.60	1.17	1.23
5	72	2457	PSU	O2-C2	-2.59	1.18	1.23
5	72	2605	PSU	O2-C2	-2.59	1.18	1.23
5	72	2504	PSU	O2-C2	-2.58	1.18	1.23
7	A2	1518	MA6	C2-N3	2.57	1.36	1.32
30	W1	32	PSU	O2-C2	-2.57	1.18	1.23
7	A2	966	2MG	C5-C4	-2.56	1.36	1.43
7	A2	1516	2MG	C5-C4	-2.55	1.36	1.43
7	A1	966	2MG	C5-C4	-2.53	1.36	1.43
7	A1	1516	2MG	C5-C4	-2.53	1.36	1.43
29	W	37	MIA	C5-C4	-2.53	1.34	1.40
7	A1	1207	2MG	C5-C4	-2.52	1.36	1.43
5	71	1915	3TD	C4-N3	2.52	1.45	1.40
5	72	1915	3TD	C4-N3	2.50	1.45	1.40
7	A2	1207	2MG	C5-C4	-2.49	1.36	1.43
5	72	1835	2MG	C5-C4	-2.46	1.36	1.43
32	Y1	46	7MG	O6-C6	-2.46	1.18	1.23
5	72	746	PSU	C4-C5	-2.43	1.37	1.44
5	72	2445	2MG	C5-C4	-2.43	1.36	1.43
5	72	1915	3TD	C1'-C5	2.43	1.55	1.50
5	72	745	1MG	C5-C4	-2.42	1.36	1.43
5	72	2251	OMG	C5-C4	-2.41	1.36	1.43
30	W1	37	MIA	C5-C4	-2.40	1.34	1.40
7	A2	1519	MA6	C5-C4	-2.39	1.34	1.40
5	72	745	1MG	C6-N1	2.36	1.43	1.39
7	A2	1407	5MC	O2-C2	-2.35	1.19	1.23
7	A1	1518	MA6	C5-C4	-2.34	1.34	1.40
7	A2	1518	MA6	C5-C4	-2.34	1.34	1.40
5	72	2552	OMU	C5-C4	2.33	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	W	16	H2U	O2-C2	-2.29	1.18	1.23
5	71	1915	3TD	O4-C4	-2.29	1.18	1.23
7	A1	1519	MA6	C5-C4	-2.29	1.34	1.40
5	72	1915	3TD	O4-C4	-2.28	1.18	1.23
31	X2	17	H2U	O2-C2	-2.27	1.18	1.23
7	A2	967	5MC	O2-C2	-2.26	1.19	1.23
7	A1	967	5MC	O2-C2	-2.25	1.19	1.23
5	72	745	1MG	C5-C6	2.25	1.54	1.47
29	W	17	H2U	O2-C2	-2.25	1.18	1.23
32	Y1	37	6MZ	C5-C4	-2.25	1.35	1.40
5	72	2449	H2U	O2-C2	-2.25	1.18	1.23
5	72	1962	5MC	O2-C2	-2.24	1.19	1.23
33	Y2	17	H2U	O2-C2	-2.24	1.19	1.23
29	W	20	H2U	O2-C2	-2.23	1.19	1.23
5	72	2030	6MZ	C5-C4	-2.22	1.35	1.40
7	A1	1498	UR3	C5-C4	2.22	1.49	1.43
30	W1	46	G7M	O6-C6	-2.22	1.18	1.23
7	A1	1407	5MC	O2-C2	-2.21	1.19	1.23
5	72	1618	6MZ	C5-C4	-2.20	1.35	1.40
31	X2	21	H2U	O2-C2	-2.20	1.19	1.23
7	A2	527	G7M	O6-C6	-2.19	1.18	1.23
31	X2	47	G7M	O6-C6	-2.19	1.18	1.23
7	A2	1498	UR3	O4-C4	-2.19	1.18	1.23
7	A2	1498	UR3	C5-C4	2.18	1.49	1.43
31	X2	21	H2U	O4-C4	-2.17	1.18	1.23
7	A2	1498	UR3	O2-C2	-2.16	1.18	1.22
7	A1	527	G7M	O6-C6	-2.16	1.18	1.23
7	A1	1498	UR3	O4-C4	-2.15	1.18	1.23
5	72	2449	H2U	O4-C4	-2.14	1.18	1.23
29	W	46	G7M	O6-C6	-2.13	1.19	1.23
7	A1	1498	UR3	C4-N3	2.13	1.45	1.40
33	Y2	17	H2U	O4-C4	-2.13	1.18	1.23
7	A1	1498	UR3	O2-C2	-2.12	1.18	1.22
5	72	2069	G7M	O6-C6	-2.12	1.19	1.23
29	W	17	H2U	O4-C4	-2.12	1.19	1.23
29	W	20	H2U	O4-C4	-2.12	1.19	1.23
29	W	16	H2U	O4-C4	-2.12	1.19	1.23
31	X2	17	H2U	O4-C4	-2.11	1.19	1.23
7	A2	1498	UR3	C4-N3	2.09	1.45	1.40
33	Y2	46	G7M	O6-C6	-2.09	1.19	1.23
7	A2	1207	2MG	O6-C6	-2.09	1.19	1.23
7	A1	527	G7M	C8-N7	2.08	1.36	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A1	1207	2MG	O6-C6	-2.08	1.19	1.23
32	Y1	37	6MZ	C2-N3	2.07	1.35	1.32
5	72	1835	2MG	O6-C6	-2.07	1.19	1.23
31	X2	38	2MA	C5-N7	-2.07	1.32	1.39
33	Y2	46	G7M	C8-N7	2.06	1.36	1.33
7	A1	1516	2MG	O6-C6	-2.05	1.19	1.23
7	A2	1516	2MG	O6-C6	-2.05	1.19	1.23
5	72	2445	2MG	O6-C6	-2.04	1.19	1.23
7	A2	966	2MG	O6-C6	-2.04	1.19	1.23
7	A1	966	2MG	O6-C6	-2.04	1.19	1.23
5	72	2030	6MZ	C2-N3	2.04	1.35	1.32
5	72	2503	2MA	C5-N7	-2.04	1.32	1.39

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	2503	2MA	C1'-N9-C4	14.94	152.89	126.64
31	X2	38	2MA	C1'-N9-C4	14.60	152.28	126.64
7	A2	1519	MA6	N1-C6-N6	-12.56	103.84	117.06
7	A1	1519	MA6	N1-C6-N6	-12.55	103.85	117.06
7	A2	1518	MA6	N1-C6-N6	-12.40	104.00	117.06
7	A1	1518	MA6	N1-C6-N6	-12.15	104.26	117.06
30	W1	37	MIA	C11-S10-C2	10.55	110.15	102.27
29	W	37	MIA	C11-S10-C2	8.92	108.93	102.27
29	W	8	4SU	C4-N3-C2	-7.97	119.60	127.34
31	X2	8	4SU	C4-N3-C2	-7.92	119.65	127.34
30	W1	8	4SU	C4-N3-C2	-7.71	119.85	127.34
31	X2	21	H2U	C4-N3-C2	-7.16	119.85	125.79
5	72	2449	H2U	C4-N3-C2	-7.14	119.87	125.79
29	W	20	H2U	C4-N3-C2	-7.02	119.97	125.79
33	Y2	17	H2U	C4-N3-C2	-7.00	119.98	125.79
29	W	17	H2U	C4-N3-C2	-6.89	120.07	125.79
29	W	16	H2U	C4-N3-C2	-6.81	120.15	125.79
31	X2	17	H2U	C4-N3-C2	-6.76	120.18	125.79
7	A1	1519	MA6	C1'-N9-C4	6.09	137.34	126.64
7	A1	1518	MA6	C1'-N9-C4	5.79	136.82	126.64
31	X2	38	2MA	C2-N3-C4	5.69	120.15	115.52
31	X2	8	4SU	C5-C4-N3	5.64	119.92	114.69
7	A2	1519	MA6	N3-C2-N1	-5.62	119.89	128.68
32	Y1	37	6MZ	C1'-N9-C4	-5.61	116.79	126.64
7	A2	1518	MA6	C1'-N9-C4	5.60	136.48	126.64
29	W	8	4SU	C5-C4-N3	5.59	119.87	114.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	72	1618	6MZ	N3-C2-N1	-5.57	119.98	128.68
5	72	2503	2MA	C2-N3-C4	5.53	120.02	115.52
7	A2	1518	MA6	N3-C2-N1	-5.52	120.05	128.68
7	A1	1518	MA6	N3-C2-N1	-5.50	120.09	128.68
32	Y1	37	6MZ	N3-C2-N1	-5.49	120.10	128.68
5	72	1915	3TD	N1-C2-N3	5.47	120.45	116.14
7	A1	1519	MA6	N3-C2-N1	-5.46	120.14	128.68
30	W1	8	4SU	C5-C4-N3	5.45	119.74	114.69
5	72	2030	6MZ	N3-C2-N1	-5.44	120.17	128.68
5	72	2030	6MZ	C1'-N9-C4	-5.44	117.09	126.64
32	Y1	34	CM0	C4-N3-C2	-5.41	120.34	127.35
5	71	1915	3TD	N1-C2-N3	5.30	120.32	116.14
7	A2	1519	MA6	C1'-N9-C4	5.19	135.76	126.64
5	72	2552	OMU	C4-N3-C2	-5.06	119.91	126.58
32	Y1	46	7MG	C5-C6-N1	5.01	119.82	110.99
5	72	955	PSU	C4-N3-C2	-4.74	119.51	126.34
5	72	2504	PSU	C4-N3-C2	-4.71	119.55	126.34
29	W	37	MIA	C1'-N9-C4	-4.71	118.37	126.64
7	A2	1498	UR3	C4-N3-C2	-4.67	120.17	124.56
5	72	2604	PSU	C4-N3-C2	-4.67	119.61	126.34
5	72	2580	PSU	C4-N3-C2	-4.64	119.65	126.34
5	72	2605	PSU	C4-N3-C2	-4.63	119.67	126.34
7	A1	1498	UR3	C4-N3-C2	-4.63	120.21	124.56
5	72	2457	PSU	C4-N3-C2	-4.61	119.69	126.34
30	W1	39	PSU	C4-N3-C2	-4.54	119.80	126.34
29	W	32	PSU	C4-N3-C2	-4.53	119.81	126.34
30	W1	32	PSU	C4-N3-C2	-4.51	119.83	126.34
32	Y1	46	7MG	C2-N3-C4	4.50	120.31	112.30
5	72	2504	PSU	N1-C2-N3	4.34	120.05	115.13
5	72	2030	6MZ	C2-N1-C6	4.27	120.25	116.59
5	72	2457	PSU	N1-C2-N3	4.20	119.89	115.13
5	72	955	PSU	N1-C2-N3	4.19	119.88	115.13
5	72	2605	PSU	N1-C2-N3	4.19	119.88	115.13
32	Y1	46	7MG	C5-C4-N3	-4.17	120.18	128.13
5	72	1915	3TD	C4-N3-C2	-4.16	120.10	124.61
30	W1	39	PSU	N1-C2-N3	4.15	119.83	115.13
29	W	32	PSU	N1-C2-N3	4.14	119.82	115.13
32	Y1	37	6MZ	C2-N1-C6	4.14	120.14	116.59
5	72	2604	PSU	N1-C2-N3	4.11	119.79	115.13
5	72	2580	PSU	N1-C2-N3	4.11	119.78	115.13
30	W1	32	PSU	N1-C2-N3	4.09	119.76	115.13
5	72	745	1MG	C5-C6-N1	4.08	120.03	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	71	1915	3TD	C4-N3-C2	-4.04	120.22	124.61
29	W	8	4SU	N3-C2-N1	3.85	120.00	114.89
5	72	1618	6MZ	C1'-N9-C4	-3.82	119.93	126.64
31	X2	8	4SU	N3-C2-N1	3.82	119.96	114.89
30	W1	8	4SU	N3-C2-N1	3.78	119.90	114.89
5	72	1618	6MZ	C9-N6-C6	-3.77	119.62	122.87
5	72	2552	OMU	N3-C2-N1	3.76	119.89	114.89
31	X2	48	3AU	C4-N3-C2	-3.74	119.94	124.63
29	W	37	MIA	N3-C2-N1	-3.70	120.17	126.98
30	W1	37	MIA	C12-C13-C14	-3.69	119.96	127.14
5	72	1618	6MZ	C2-N1-C6	3.68	119.74	116.59
5	72	2445	2MG	C5-C6-N1	3.61	120.33	113.95
5	72	1835	2MG	C5-C6-N1	3.60	120.31	113.95
32	Y1	34	CM0	N3-C2-N1	3.59	119.65	114.89
30	W1	37	MIA	N3-C2-N1	-3.59	120.38	126.98
7	A1	966	2MG	C5-C6-N1	3.55	120.21	113.95
7	A1	1516	2MG	C5-C6-N1	3.52	120.17	113.95
5	72	2251	OMG	C5-C6-N1	3.50	120.14	113.95
30	W1	8	4SU	C5-C4-S4	-3.50	119.96	124.47
29	W	37	MIA	C12-C13-C14	-3.49	120.34	127.14
7	A2	966	2MG	C5-C6-N1	3.48	120.10	113.95
7	A2	1207	2MG	C5-C6-N1	3.48	120.10	113.95
29	W	8	4SU	C5-C4-S4	-3.47	120.00	124.47
5	72	1962	5MC	C5-C6-N1	-3.47	119.77	123.34
31	X2	8	4SU	C5-C4-S4	-3.45	120.02	124.47
30	W1	37	MIA	C2-N3-C4	3.44	120.07	115.32
7	A1	967	5MC	C5-C6-N1	-3.43	119.81	123.34
7	A2	1516	2MG	C5-C6-N1	3.40	119.95	113.95
5	72	2504	PSU	C6-C5-C4	3.38	120.56	118.20
7	A1	1207	2MG	C5-C6-N1	3.38	119.92	113.95
29	W	32	PSU	C6-C5-C4	3.37	120.55	118.20
5	72	1939	5MU	O3'-C3'-C2'	-3.34	101.02	111.82
31	X2	48	3AU	C5-C4-N3	3.33	119.89	115.50
29	W	37	MIA	C2-N3-C4	3.33	119.91	115.32
5	72	2457	PSU	C6-C5-C4	3.28	120.49	118.20
5	72	2552	OMU	C5-C4-N3	3.27	119.74	114.84
30	W1	39	PSU	C6-C5-C4	3.25	120.47	118.20
32	Y1	46	7MG	C4-C5-N7	3.21	109.99	105.53
5	72	2449	H2U	N3-C2-N1	3.21	120.05	116.65
31	X2	21	H2U	N3-C2-N1	3.19	120.02	116.65
29	W	17	H2U	N3-C2-N1	3.17	120.01	116.65
29	W	20	H2U	N3-C2-N1	3.16	120.00	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A2	967	5MC	C5-C6-N1	-3.15	120.09	123.34
31	X2	17	H2U	N3-C2-N1	3.14	119.97	116.65
33	Y2	17	H2U	N3-C2-N1	3.14	119.97	116.65
30	W1	46	G7M	C2-N1-C6	-3.12	119.35	125.10
31	X2	38	2MA	N3-C2-N1	-3.12	120.03	125.73
5	72	2580	PSU	C6-C5-C4	3.12	120.38	118.20
29	W	46	G7M	C2-N1-C6	-3.11	119.37	125.10
5	72	2503	2MA	N3-C2-N1	-3.07	120.13	125.73
5	72	955	PSU	C6-C5-C4	3.07	120.34	118.20
30	W1	37	MIA	C1'-N9-C4	-3.03	121.31	126.64
31	X2	47	G7M	C2-N1-C6	-3.01	119.56	125.10
5	72	2251	OMG	C2-N1-C6	-3.00	119.56	125.10
30	W1	32	PSU	C6-C5-C4	3.00	120.30	118.20
7	A2	527	G7M	C2-N1-C6	-2.99	119.60	125.10
7	A1	527	G7M	C2-N1-C6	-2.99	119.60	125.10
29	W	16	H2U	C5-C4-N3	2.98	119.99	116.65
29	W	16	H2U	N3-C2-N1	2.98	119.80	116.65
5	72	2504	PSU	C6-N1-C2	-2.97	119.65	122.68
5	72	2604	PSU	C6-C5-C4	2.97	120.27	118.20
32	Y1	46	7MG	C5-C4-N9	2.96	110.19	106.35
5	72	2605	PSU	C6-N1-C2	-2.96	119.66	122.68
5	72	2069	G7M	C2-N1-C6	-2.92	119.72	125.10
33	Y2	46	G7M	C2-N1-C6	-2.91	119.73	125.10
30	W1	32	PSU	C6-N1-C2	-2.91	119.71	122.68
5	72	1939	5MU	O2'-C2'-C1'	-2.90	100.34	110.02
5	72	2552	OMU	O4-C4-C5	-2.89	120.08	125.16
7	A1	1407	5MC	C5-C6-N1	-2.89	120.37	123.34
29	W	32	PSU	C6-N1-C2	-2.89	119.73	122.68
5	72	2449	H2U	C5-C4-N3	2.88	119.89	116.65
32	Y1	46	7MG	C2-N1-C6	-2.88	119.86	125.10
30	W1	39	PSU	C6-N1-C2	-2.87	119.74	122.68
5	72	2251	OMG	C8-N7-C5	2.87	108.46	102.99
29	W	37	MIA	S10-C2-N3	2.86	126.03	116.10
31	X2	21	H2U	C5-C4-N3	2.85	119.85	116.65
5	72	2457	PSU	C6-N1-C2	-2.85	119.77	122.68
32	Y1	46	7MG	O6-C6-C5	-2.85	120.55	127.54
5	72	2605	PSU	C6-C5-C4	2.84	120.18	118.20
29	W	17	H2U	C5-C4-N3	2.82	119.82	116.65
33	Y2	17	H2U	C5-C4-N3	2.80	119.79	116.65
5	72	955	PSU	C6-N1-C2	-2.79	119.83	122.68
29	W	20	H2U	C5-C4-N3	2.79	119.78	116.65
32	Y1	46	7MG	N9-C4-N3	2.78	129.62	125.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	16	H2U	C5-C6-N1	2.77	120.73	111.61
29	W	17	H2U	C5-C6-N1	2.75	120.69	111.61
31	X2	17	H2U	C5-C4-N3	2.73	119.71	116.65
30	W1	37	MIA	S10-C2-N3	2.72	125.54	116.10
31	X2	17	H2U	C5-C6-N1	2.72	120.58	111.61
7	A2	1407	5MC	C5-C6-N1	-2.71	120.55	123.34
5	72	2580	PSU	C6-N1-C2	-2.70	119.92	122.68
5	72	745	1MG	C8-N7-C5	2.70	108.14	102.99
7	A2	966	2MG	C8-N7-C5	2.68	108.10	102.99
5	72	2604	PSU	C6-N1-C2	-2.67	119.96	122.68
7	A1	966	2MG	C8-N7-C5	2.66	108.05	102.99
7	A1	1516	2MG	C8-N7-C5	2.63	108.00	102.99
29	W	20	H2U	C5-C6-N1	2.62	120.26	111.61
33	Y2	17	H2U	C5-C6-N1	2.62	120.24	111.61
7	A1	1207	2MG	C8-N7-C5	2.61	107.97	102.99
7	A2	1516	2MG	C8-N7-C5	2.61	107.97	102.99
5	72	2449	H2U	C5-C6-N1	2.61	120.20	111.61
31	X2	21	H2U	C5-C6-N1	2.58	120.11	111.61
5	72	2445	2MG	C8-N7-C5	2.57	107.89	102.99
7	A2	1207	2MG	C8-N7-C5	2.57	107.89	102.99
5	72	2605	PSU	O2-C2-N1	-2.55	119.98	122.79
7	A1	1402	4OC	C6-C5-C4	2.55	120.08	116.96
5	72	1835	2MG	C8-N7-C5	2.54	107.83	102.99
29	W	32	PSU	O2-C2-N1	-2.54	119.99	122.79
5	72	955	PSU	O2-C2-N1	-2.51	120.03	122.79
5	72	2457	PSU	O2-C2-N1	-2.51	120.03	122.79
5	72	2504	PSU	O2-C2-N1	-2.50	120.03	122.79
29	W	17	H2U	O2-C2-N1	-2.48	120.00	123.11
5	72	745	1MG	O6-C6-C5	-2.45	119.85	124.19
29	W	20	H2U	O2-C2-N1	-2.45	120.03	123.11
32	Y1	46	7MG	N9-C8-N7	2.41	106.83	103.38
5	72	2580	PSU	O2-C2-N1	-2.41	120.14	122.79
33	Y2	17	H2U	O2-C2-N1	-2.41	120.09	123.11
30	W1	39	PSU	O2-C2-N1	-2.40	120.14	122.79
30	W1	32	PSU	O2-C2-N1	-2.39	120.16	122.79
5	72	2604	PSU	O2-C2-N1	-2.39	120.16	122.79
29	W	16	H2U	O2-C2-N1	-2.39	120.11	123.11
29	W	37	MIA	C16-C14-C15	2.37	119.83	114.60
30	W1	37	MIA	C16-C14-C15	2.36	119.83	114.60
29	W	55	PSU	C2'-C3'-C4'	-2.36	98.05	102.64
5	72	1835	2MG	O6-C6-C5	-2.36	119.76	124.37
7	A2	1402	4OC	C6-C5-C4	2.35	119.83	116.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A1	1516	2MG	O6-C6-C5	-2.34	119.80	124.37
5	72	2445	2MG	O6-C6-C5	-2.33	119.81	124.37
5	72	1915	3TD	C6-C5-C4	2.32	119.82	118.22
32	Y1	37	6MZ	C9-N6-C6	-2.32	120.88	122.87
7	A2	1516	2MG	O6-C6-C5	-2.31	119.87	124.37
7	A1	966	2MG	O6-C6-C5	-2.30	119.89	124.37
31	X2	21	H2U	O2-C2-N1	-2.29	120.23	123.11
5	72	2449	H2U	O2-C2-N1	-2.28	120.25	123.11
7	A2	966	2MG	O6-C6-C5	-2.26	119.95	124.37
7	A2	1207	2MG	O6-C6-C5	-2.25	119.98	124.37
7	A1	1207	2MG	O6-C6-C5	-2.23	120.01	124.37
5	72	2503	2MA	CM2-C2-N1	2.23	120.63	117.15
5	72	2251	OMG	O6-C6-C5	-2.23	120.02	124.37
5	72	746	PSU	C5-C6-N1	-2.17	118.85	122.11
7	A1	1407	5MC	CM5-C5-C6	-2.15	119.97	122.85
7	A2	1407	5MC	CM5-C5-C6	-2.13	120.00	122.85
5	72	2580	PSU	O4'-C1'-C2'	2.12	108.14	105.14
5	72	2552	OMU	O2-C2-N1	-2.12	119.97	122.79
7	A1	1498	UR3	C6-N1-C2	-2.12	119.89	121.79
7	A1	967	5MC	CM5-C5-C6	-2.11	120.03	122.85
29	W	8	4SU	O2-C2-N1	-2.09	120.01	122.79
5	72	2445	2MG	CM2-N2-C2	-2.08	119.26	123.86
7	A1	1498	UR3	C1'-N1-C2	2.08	120.50	116.99
5	72	1962	5MC	CM5-C5-C6	-2.08	120.07	122.85
7	A2	1498	UR3	C6-N1-C2	-2.07	119.93	121.79
5	72	1835	2MG	CM2-N2-C2	-2.06	119.31	123.86
31	X2	48	3AU	C6-N1-C2	-2.04	119.96	121.79
7	A2	967	5MC	CM5-C5-C6	-2.02	120.15	122.85
31	X2	17	H2U	O2-C2-N1	-2.01	120.59	123.11

There are no chirality outliers.

All (117) 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	A1	1519	MA6	C5-C6-N6-C10
7	A2	1402	4OC	C1'-C2'-O2'-CM2
5	72	1618	6MZ	N1-C6-N6-C9
5	72	1618	6MZ	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	72	1618	6MZ	C3'-C4'-C5'-O5'
5	72	1939	5MU	C3'-C4'-C5'-O5'
5	72	1939	5MU	O4'-C4'-C5'-O5'
5	72	2030	6MZ	C5-C6-N6-C9
5	72	2030	6MZ	N1-C6-N6-C9
5	72	2251	OMG	O4'-C4'-C5'-O5'
5	72	2251	OMG	C1'-C2'-O2'-CM2
30	W1	37	MIA	O4'-C4'-C5'-O5'
30	W1	37	MIA	C3'-C4'-C5'-O5'
30	W1	37	MIA	N1-C2-S10-C11
30	W1	37	MIA	N3-C2-S10-C11
31	X2	8	4SU	C3'-C4'-C5'-O5'
31	X2	8	4SU	O4'-C4'-C5'-O5'
31	X2	17	H2U	O4'-C1'-N1-C6
31	X2	33	RSP	C4'-C5'-O5'-P
31	X2	47	G7M	O4'-C4'-C5'-O5'
31	X2	47	G7M	C3'-C4'-C5'-O5'
31	X2	48	3AU	C10-C11-C12-N40
31	X2	55	5MU	C3'-C4'-C5'-O5'
32	Y1	34	CM0	O5-C7-C8-O8
32	Y1	37	6MZ	N1-C6-N6-C9
33	Y2	17	H2U	O4'-C4'-C5'-O5'
33	Y2	17	H2U	C3'-C4'-C5'-O5'
33	Y2	17	H2U	O4'-C1'-N1-C6
33	Y2	17	H2U	C2'-C1'-N1-C2
33	Y2	17	H2U	C2'-C1'-N1-C6
32	Y1	34	CM0	O5-C7-C8-O9
31	X2	47	G7M	C4'-C5'-O5'-P
7	A1	1498	UR3	O4'-C4'-C5'-O5'
7	A1	1498	UR3	C3'-C4'-C5'-O5'
7	A1	1519	MA6	O4'-C4'-C5'-O5'
7	A2	1498	UR3	O4'-C4'-C5'-O5'
7	A2	1498	UR3	C3'-C4'-C5'-O5'
7	A2	1519	MA6	O4'-C4'-C5'-O5'
5	72	2251	OMG	C3'-C4'-C5'-O5'
5	72	2498	OMC	C3'-C4'-C5'-O5'
5	72	2498	OMC	O4'-C4'-C5'-O5'
29	W	8	4SU	C3'-C4'-C5'-O5'
29	W	8	4SU	O4'-C4'-C5'-O5'
30	W1	8	4SU	O4'-C4'-C5'-O5'
33	Y2	46	G7M	C3'-C4'-C5'-O5'
30	W1	8	4SU	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
31	X2	48	3AU	O4'-C4'-C5'-O5'
31	X2	55	5MU	O4'-C4'-C5'-O5'
7	A1	1518	MA6	N1-C6-N6-C10
7	A2	1519	MA6	C3'-C4'-C5'-O5'
5	72	1915	3TD	O4'-C4'-C5'-O5'
29	W	54	5MU	C3'-C4'-C5'-O5'
33	Y2	54	5MU	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C4'-C5'-O5'-P
29	W	55	PSU	O4'-C4'-C5'-O5'
31	X2	17	H2U	C3'-C4'-C5'-O5'
31	X2	48	3AU	C3'-C4'-C5'-O5'
7	A1	1519	MA6	C5-C6-N6-C9
31	X2	38	2MA	C4'-C5'-O5'-P
31	X2	17	H2U	C4'-C5'-O5'-P
31	X2	21	H2U	C4'-C5'-O5'-P
29	W	55	PSU	C3'-C4'-C5'-O5'
31	X2	17	H2U	O4'-C4'-C5'-O5'
33	Y2	46	G7M	O4'-C4'-C5'-O5'
33	Y2	54	5MU	O4'-C4'-C5'-O5'
5	72	1618	6MZ	C5-C6-N6-C9
32	Y1	37	6MZ	C5-C6-N6-C9
30	W1	46	G7M	O4'-C4'-C5'-O5'
7	A1	527	G7M	C4'-C5'-O5'-P
29	W	46	G7M	C4'-C5'-O5'-P
30	W1	46	G7M	C4'-C5'-O5'-P
31	X2	48	3AU	C4'-C5'-O5'-P
32	Y1	46	7MG	C4'-C5'-O5'-P
29	W	54	5MU	O4'-C4'-C5'-O5'
7	A2	527	G7M	C3'-C4'-C5'-O5'
30	W1	37	MIA	C5-C6-N6-C12
7	A2	527	G7M	C4'-C5'-O5'-P
33	Y2	17	H2U	C4'-C5'-O5'-P
5	72	2069	G7M	C4'-C5'-O5'-P
29	W	16	H2U	C4'-C5'-O5'-P
29	W	55	PSU	C4'-C5'-O5'-P
29	W	46	G7M	O4'-C4'-C5'-O5'
31	X2	38	2MA	C3'-C4'-C5'-O5'
30	W1	37	MIA	N1-C6-N6-C12
5	72	1915	3TD	C3'-C4'-C5'-O5'
33	Y2	17	H2U	O4'-C1'-N1-C2
29	W	37	MIA	N6-C12-C13-C14
5	72	2069	G7M	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
5	72	746	PSU	O4'-C1'-C5-C4
5	72	2457	PSU	O4'-C1'-C5-C4
5	72	2504	PSU	O4'-C1'-C5-C4
31	X2	56	PSU	O4'-C1'-C5-C4
7	A1	1519	MA6	N1-C6-N6-C10
31	X2	48	3AU	C11-C12-C13-O31
7	A2	527	G7M	O4'-C4'-C5'-O5'
7	A2	967	5MC	O4'-C4'-C5'-O5'
29	W	17	H2U	O4'-C4'-C5'-O5'
30	W1	46	G7M	C3'-C4'-C5'-O5'
31	X2	38	2MA	O4'-C4'-C5'-O5'
31	X2	48	3AU	C11-C12-C13-O30
5	72	2449	H2U	O4'-C1'-N1-C6
5	72	2457	PSU	O4'-C1'-C5-C6
31	X2	21	H2U	O4'-C1'-N1-C6
31	X2	56	PSU	O4'-C1'-C5-C6
29	W	54	5MU	C2'-C1'-N1-C2
31	X2	17	H2U	O4'-C1'-N1-C2
29	W	20	H2U	C4'-C5'-O5'-P
31	X2	17	H2U	C2'-C1'-N1-C2
7	A1	1402	4OC	O4'-C4'-C5'-O5'
5	71	1915	3TD	C3'-C4'-C5'-O5'
5	72	2030	6MZ	O4'-C4'-C5'-O5'
29	W	46	G7M	C3'-C4'-C5'-O5'
31	X2	21	H2U	C2'-C1'-N1-C2

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 302 ligands modelled in this entry, 298 are monoatomic - leaving 4 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	$\# Z > 2$
48	SPD	72	3003	-	9,9,9	0.32	0	8,8,8	0.87	0
47	PUT	72	3002	-	5,5,5	0.24	0	4,4,4	0.56	0
50	ALA	Y2	102	33	3,4,5	0.48	0	2,4,6	2.56	2 (100%)
47	PUT	72	3001	-	5,5,5	0.26	0	4,4,4	0.52	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
48	SPD	72	3003	-	-	0/7/7/7	-
47	PUT	72	3002	-	-	0/3/3/3	-
50	ALA	Y2	102	33	-	0/0/2/4	-
47	PUT	72	3001	-	-	1/3/3/3	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Y2	102	ALA	CB-CA-N	-3.01	100.32	109.85
50	Y2	102	ALA	O-C-CA	-2.02	117.88	124.28

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	72	3001	PUT	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.