



Full wwPDB EM Validation Report ⓘ

Feb 19, 2025 – 12:25 pm GMT

PDB ID : 8P8B
EMDB ID : EMD-17134
Title : Mycoplasma pneumoniae large ribosomal subunit in chloramphenicol-treated cells
Authors : Schacherl, M.; Xue, L.; Spahn, C.M.T.; Mahamid, J.
Deposited on : 2023-05-31
Resolution : 2.90 Å (reported)
Based on initial models : 7OOC, 7OOD

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
buster-report : 1.1.7 (2018)
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

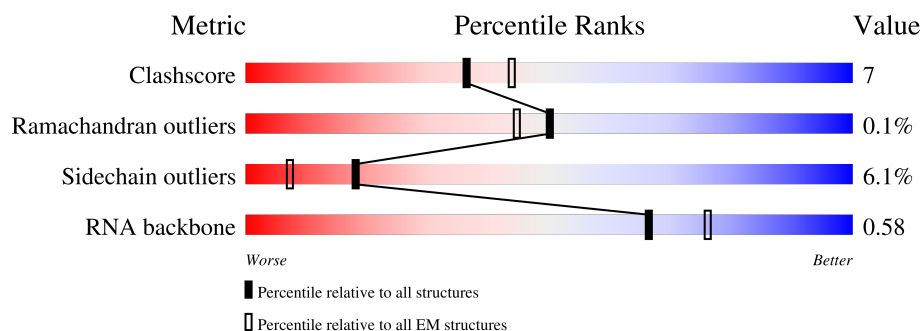
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)
Clashscore	210492	15764
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	0	48	75% 25%
2	1	59	81% 17% .
3	2	37	89% 11%
4	3	2907	69% 27% .
5	4	108	63% 31% 6%
6	5	1520	98% ..
7	6	76	97% .

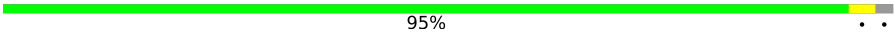


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Mol	Chain	Length	Quality of chain
8	7	75	
9	8	76	
10	X	444	
11	Y	9	
12	Z	36	
13	a	287	
14	b	287	
15	c	212	
16	d	180	
17	e	184	
18	f	149	
19	g	161	
20	h	137	
21	i	146	
22	j	122	
23	k	151	
24	l	139	
25	m	124	
26	n	116	
27	o	119	
28	p	127	
29	q	100	
30	r	159	
31	s	237	
32	t	111	

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Mol	Chain	Length	Quality of chain
33	u	104	
34	v	65	
35	w	111	
36	x	97	
37	y	57	
38	z	53	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 97182 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 L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	48	Total	C	N	O	S	0	0
			392	242	85	63	2		

- Molecule 2 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	59	Total	C	N	O	S	0	0
			477	300	99	77	1		

- Molecule 3 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	37	Total	C	N	O	S	0	0
			304	189	65	46	4		

- Molecule 4 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	2893	Total	C	N	O	P	0	0
			61995	27704	11293	20105	2893		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	108	Total	C	N	O	P	0	0
			2305	1030	415	752	108		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	32	Total	C	N	O	P	0	0
			683	307	124	220	32		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	1003	A	G	conflict	GB 26117688

- Molecule 7 is a RNA chain called tRNA-Ala (E-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	2	Total	C	N	O	P	0	0
			42	19	8	13	2		

- Molecule 8 is a RNA chain called tRNA-Asp (P-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	75	Total	C	N	O	P	0	0
			1599	712	279	533	75		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
7	17	G	-	insertion	GB 26117688
7	55	C	U	conflict	GB 26117688

- Molecule 9 is a RNA chain called tRNA-Lys (A-site).

Mol	Chain	Residues	Atoms					AltConf	Trace
9	8	76	Total	C	N	O	P	0	0
			1615	722	284	533	76		

- Molecule 10 is a protein called Trigger factor.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	30	Total	C	N	O	S	0	0
			242	155	43	43	1		

- Molecule 11 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	9	Total	C	N	O	P	0	0
			195	87	38	61	9		

- Molecule 12 is a protein called nascent peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	Z	36	Total	C	N	O	0	0
			187	112	37	38		

- Molecule 13 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	a	285	Total	C	N	O	S	0	0
			2225	1385	437	397	6		

- Molecule 14 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	b	231	Total	C	N	O	S	0	0
			1778	1129	320	322	7		

- Molecule 15 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	c	211	Total	C	N	O	S	0	0
			1654	1053	299	299	3		

- Molecule 16 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	d	179	Total	C	N	O	S	0	0
			1416	910	251	251	4		

- Molecule 17 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	e	176	Total	C	N	O	0	0
			1396	899	247	250		

- Molecule 18 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	f	149	Total	C	N	O	S	0	0
			1210	780	212	215	3		

- Molecule 19 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	g	125	Total	C	N	O	S	0	0
			951	606	165	177	3		

- Molecule 20 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	h	128	Total	C	N	O	S	0	0
			959	616	160	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	i	144	Total	C	N	O	S	0	0
			1164	737	213	209	5		

- Molecule 22 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	j	122	Total	C	N	O	S	0	0
			944	595	178	167	4		

- Molecule 23 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	k	150	Total	C	N	O	S	0	0
			1170	741	228	200	1		

- Molecule 24 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	l	136	Total	C	N	O	S	0	0
			1079	694	196	182	7		

- Molecule 25 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	m	119	Total	C	N	O	S	0	0
			958	609	175	171	3		

- Molecule 26 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	n	116	Total	C	N	O	S	0	0
			918	573	181	162	2		

- Molecule 27 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	o	118	Total	C	N	O	S	0	0
			966	609	186	170	1		

- Molecule 28 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	p	118	Total	C	N	O	S	0	0
			981	624	194	161	2		

- Molecule 29 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	q	99	Total	C	N	O	S	0	0
			811	525	148	134	4		

- Molecule 30 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	r	142	Total	C	N	O	S	0	0
			1091	677	212	195	7		

- Molecule 31 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	s	95	Total	C	N	O	S	0	0
			740	486	125	128	1		

- Molecule 32 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	t	111	Total	C	N	O	S	0	0
			871	550	166	152	3		

- Molecule 33 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	u	88	Total	C	N	O	S	0	0
			670	416	132	121	1		

- Molecule 34 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	v	64	Total	C	N	O	S	0	0
			520	320	109	90	1		

- Molecule 35 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	w	110	Total	C	N	O	S	0	0
			906	576	168	162			

- Molecule 36 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	x	46	Total	C	N	O	S	0	0
			366	235	59	68	4		

- Molecule 37 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	y	56	Total	C	N	O	S	0	0
			452	274	98	75	5		

- Molecule 38 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	z	50	Total	C	N	O	S	0	0
			408	255	81	68	4		

- Molecule 39 is ZINC ION (three-letter code: ZN) (formula: Zn).

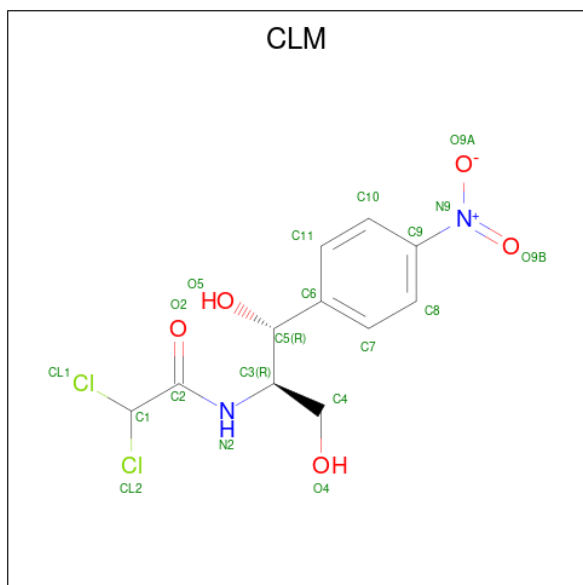
Mol	Chain	Residues	Atoms		AltConf
39	2	1	Total	Zn	0
			1	1	
39	x	1	Total	Zn	0
			1	1	
39	y	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
39	z	1	Total	Zn	0
			1	1	

- Molecule 40 is CHLORAMPHENICOL (three-letter code: CLM) (formula: $C_{11}H_{12}Cl_2N_2O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
40	3	1	Total	C	Cl	N	O	0
			20	11	2	2	5	

- Molecule 41 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
41	3	1	Total	K	0
			1	1	

- Molecule 42 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

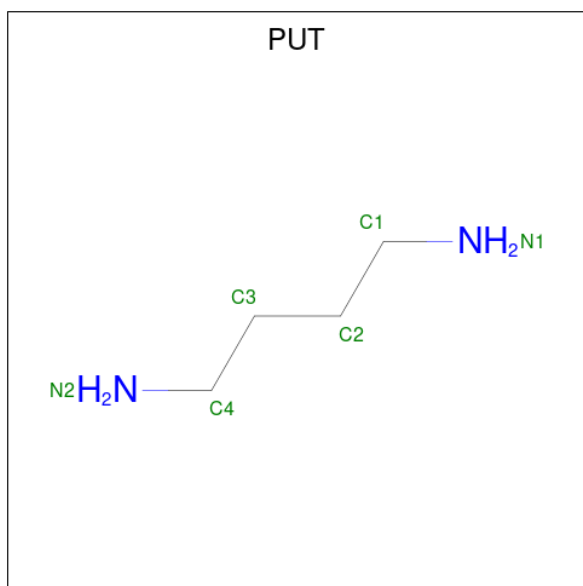
Mol	Chain	Residues	Atoms		AltConf
42	3	219	Total	Mg	0
			219	219	
42	4	1	Total	Mg	0
			1	1	
42	6	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
42	7	1	Total	Mg	0
			1	1	
42	8	2	Total	Mg	0
			2	2	
42	b	2	Total	Mg	0
			2	2	
42	i	1	Total	Mg	0
			1	1	
42	y	2	Total	Mg	0
			2	2	

- Molecule 43 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



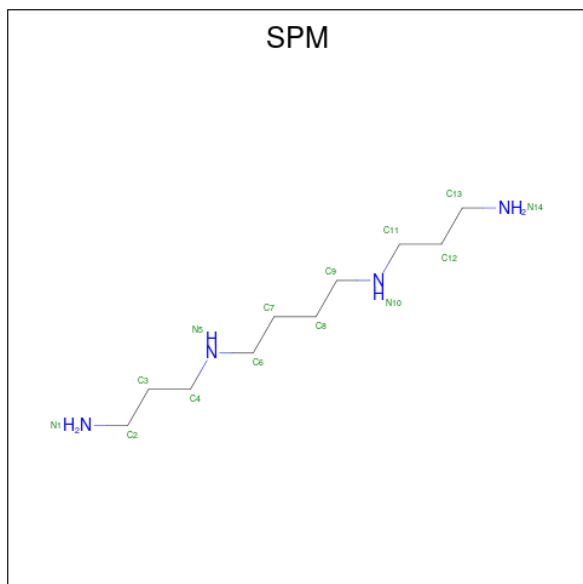
Mol	Chain	Residues	Atoms			AltConf
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	
43	3	1	Total	C	N	0
			6	4	2	

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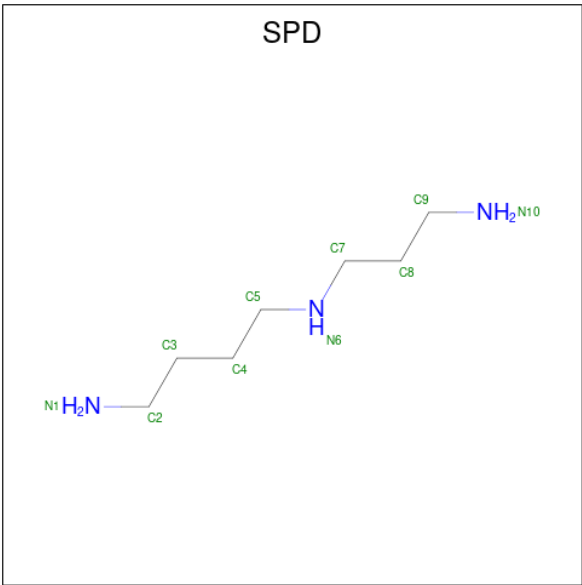
Mol	Chain	Residues	Atoms			AltConf
43	3	1	Total	C	N	0
			6	4	2	

- Molecule 44 is SPERMINE (three-letter code: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
44	3	1	Total	C	N	0
			14	10	4	
44	3	1	Total	C	N	0
			14	10	4	
44	3	1	Total	C	N	0
			14	10	4	
44	b	1	Total	C	N	0
			14	10	4	

- Molecule 45 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



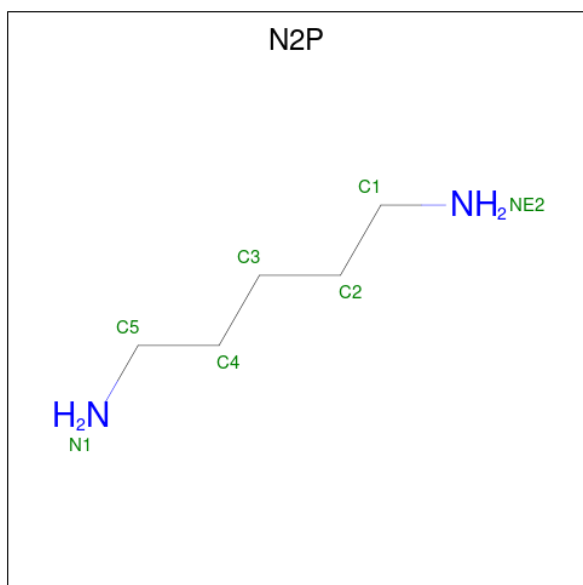
Mol	Chain	Residues	Atoms			AltConf
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	

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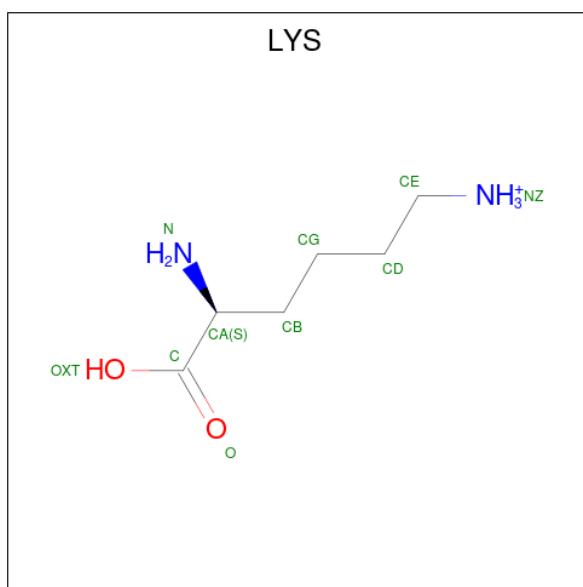
Mol	Chain	Residues	Atoms			AltConf
45	3	1	Total	C	N	0
			10	7	3	
45	3	1	Total	C	N	0
			10	7	3	

- Molecule 46 is PENTANE-1,5-DIAMINE (three-letter code: N2P) (formula: $C_5H_{14}N_2$).



Mol	Chain	Residues	Atoms			AltConf
46	3	1	Total	C	N	0
			7	5	2	
46	3	1	Total	C	N	0
			7	5	2	
46	3	1	Total	C	N	0
			7	5	2	

- Molecule 47 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
47	8	1	9	6	2	1	0

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 L34

Chain 0: 




- Molecule 2: 50S ribosomal protein L35

Chain 1: 



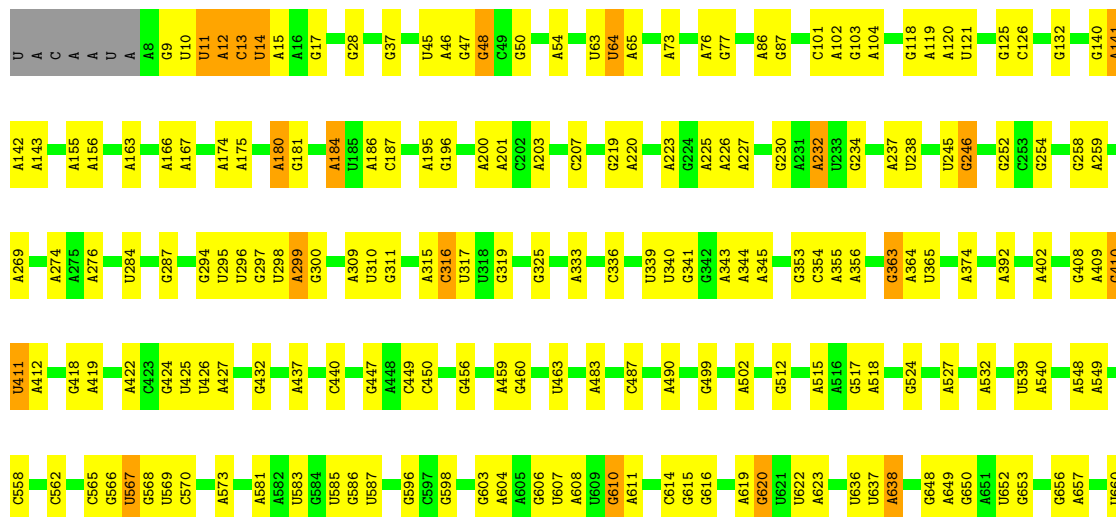
- Molecule 3: 50S ribosomal protein L36

Chain 2: 

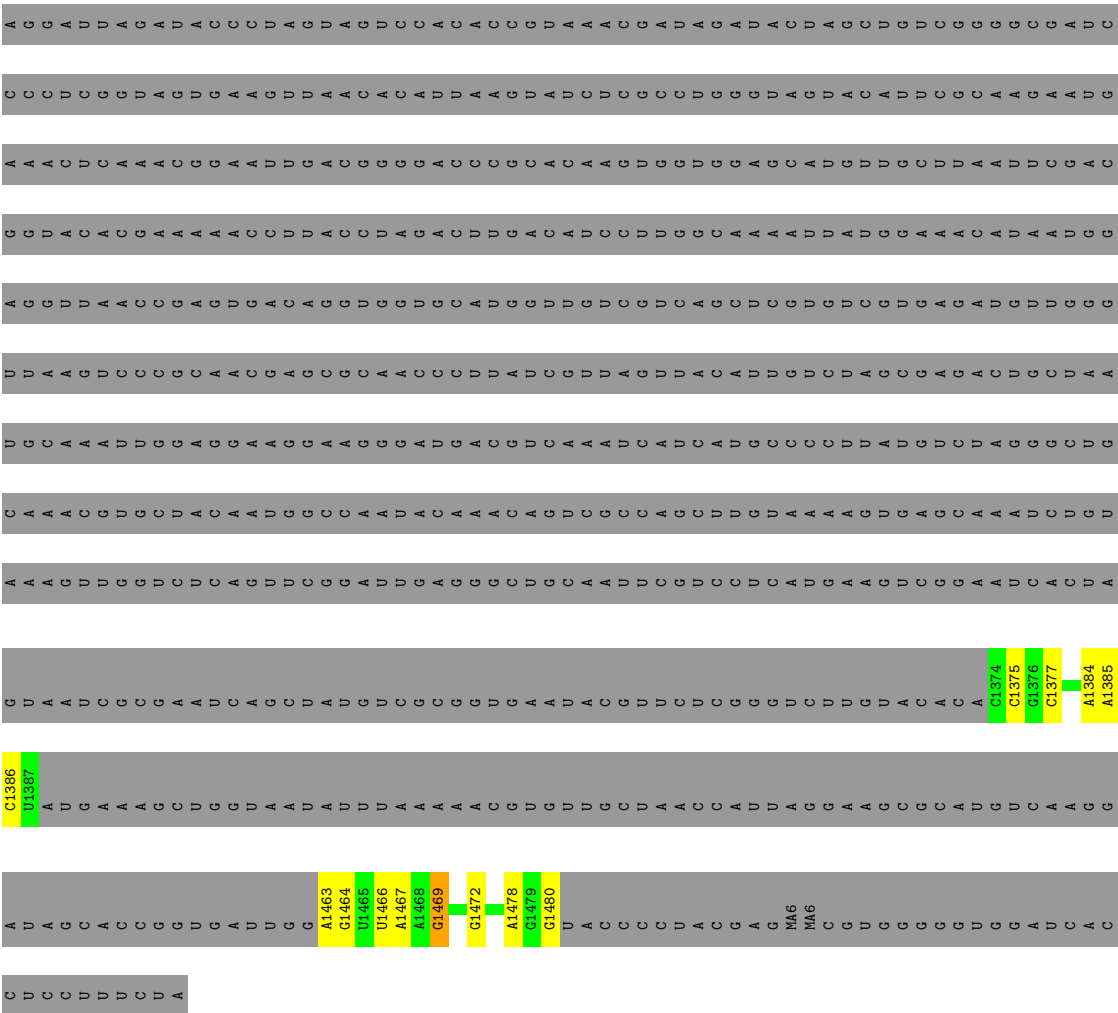


- Molecule 4: 23S ribosomal RNA

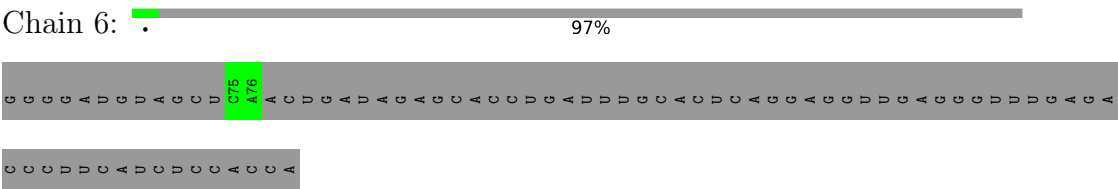
Chain 3: 



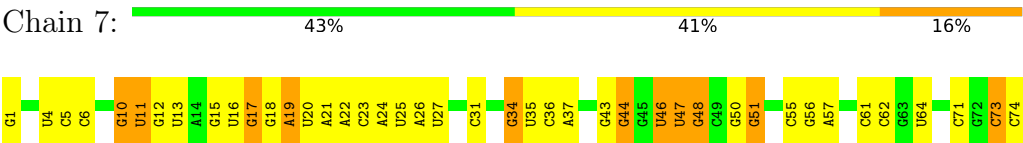
A2344	U2227	G2122	C2024	U1823	G1665	A1545	A1335	U1219	C1111	A1008	C901	A789
G2353	U2228	A2123	C2025	U1823	G1665	U1546	G1338	U1234	A1112	A1009	U902	A663
A2354	A2233	A2124	G2026	G1833	G1668	G1550	U1339	U1235	U1113	G1010	A903	G792
C2355	G2246	U2137	G2027	A1836	U1673	G1557	U1340	G1236	G1114	A1016	U905	G665
U2358	G2247	U2138	G2028	C1837	U1673	U1557	U1341	U1236	U1116	A1019	G906	A667
G2359	G2247	U2138	U2029	C1837	U1673	U1557	C1342	G1239	U1117	A1019	U909	A668
A2366	G2254	C2139	A2030	A1854	A1680	U1564	U1343	U1240	U1118	C1023	G910	A669
G2366	A2255	G2140	C2031	A1855	C1681	G1565	U1344	U1241	A1119	A1026	G910	G810
C2372	A2255	A2145	G2032	A1855	C1682	U1566	G1352	G1242	A1120	A1026	G910	G811
G2372	G2259	A2146	G2033	G1866	A1688	U1567	G1352	U1242	A1121	A1026	U916	G672
G2373	G2259	G2147	G2033	G1866	A1688	C1568	U1341	U1242	A1122	A1026	G916	A673
C2376	C2266	G2151	A2038	G1869	U1691	A1569	G1356	U1246	G1122	A1032	G917	A817
A2377	C2271	G2151	G2039	U1871	A1692	A1570	U1369	A1250	A1123	A1032	G918	A818
A2382	U2274	C2152	A2040	U1871	A1693	U1571	U1369	A1250	G1124	A1036	C924	A881
G2383	A2274	U2153	C2041	A1878	A1694	U1572	U1369	A1251	U1125	A1036	C924	U820
A2386	A2275	A2154	A2042	A1878	G1695	G1573	C1378	G1253	G1126	G1039	U926	A823
U2387	A2276	G2155	A2042	A1878	G1695	G1574	C1379	G1253	G1128	A1045	A927	A824
C2388	A2276	G2156	G2050	C1886	C1696	U1575	C1379	A1256	U1129	A1045	G928	U825
G2386	A2281	U2160	C2057	U1889	C1697	G1576	U1381	G1257	U1130	A1045	G929	G691
C2388	G2287	G2161	G2062	U1890	A1698	U1576	U1381	G1257	A1131	U1049	C930	G827
G2391	U2291	G2164	G2063	G1906	G1708	G1580	U1385	G1266	G1132	U1049	G931	A828
C2393	A2295	A2165	G2063	G1909	U1727	U1581	U1386	A1267	A1133	A1055	U932	A829
G2397	A2296	U2171	A2069	G1913	U1727	G1582	A1387	U1268	G1134	A1055	A933	A830
C2403	G2298	U2175	G2070	G1914	U1727	G1583	U1388	C1269	C1135	U1068	C934	U831
G2404	U2299	C2071	C2071	G1915	U1764	U1584	G1388	U1270	U1136	G1059	U935	C832
A2410	A2300	U2180	C2072	A1920	U1769	U1589	U1391	A1271	C1137	G1060	G936	A705
C2411	C2305	A2181	G2072	A1920	A1770	A1585	U1391	A1271	A1138	A1061	U944	G840
U2414	U2308	C2187	G2076	G1936	C1771	A1603	G1405	G1286	A1162	A1080	U952	A728
G2418	A2309	A2078	A2077	G1937	U1770	A1509	A1406	A1292	U1165	A1081	G953	G853
A2419	C2310	G2193	G2079	U1938	A1780	C1611	U1407	G1296	G1166	A1082	A947	A854
A2420	G2311	U2194	C2080	G1913	U1780	U1612	A1513	G1296	A1083	A1083	U957	C733
C2420	U2081	U2195	U2081	G1914	U1786	U1612	U1514	G1301	G1084	C1084	U963	U862
U2421	G2312	G2196	U2082	A1944	U1786	A1613	A1413	G1301	U1167	U963	U963	U749
G2422	U2313	U2197	U2083	A1944	C1789	G1616	C1414	G1302	A1168	G1091	A964	U869
U2422	G2316	G2198	A2084	U1962	U1790	U1617	A1415	U1303	C1170	A1092	U968	A870
C2430	U2316	C2199	A2084	U1962	A1791	U1618	A1415	U1304	U1176	U1093	U968	C752
U2431	A2319	U2200	U2098	U1974	C1797	U1619	A1420	G1305	A1177	G1094	A969	C755
A2432	U2320	G2201	U2099	U1974	A1798	A1620	A1420	G1306	U1095	U1095	U970	A756
C2433	U2320	U2202	G2100	A1977	A1798	U1620	A1423	G1307	A1178	U1096	A881	A757
A2434	U2327	U2203	G2106	U1978	U1798	U1623	U1424	G1307	A1178	G1097	C882	C882
G2435	C2204	C2204	G2106	U1978	U1801	U1624	U1424	G1313	C1188	G1098	A981	A881
A2436	U2205	U2205	U2110	U1988	C1802	G1530	C1432	G1321	A1204	C1099	A983	A881
G2437	G2329	A2206	U2111	U1998	U1803	A1641	C1432	A1321	A1204	U1100	U989	C755
A2438	A2207	U2207	A2112	U2000	A1804	G1642	U1433	A1322	U1101	U1100	A985	A756
U2438	G2333	G2211	U2113	U2000	C1807	A1643	A1434	C1325	A1208	A1102	U994	C881
A2443	U2334	U2212	U2114	G2004	C1807	A1644	A1435	A1325	U1209	A1102	U994	A893
C2443	A2336	U2212	C2114	A2010	C1808	C1645	C1436	A1328	U1209	G1103	U994	G894
U2449	U2337	U2219	A2115	G2011	A1809	U1650	A1437	A1328	A1210	A1104	G997	A893
U2456	U2342	A2220	U2116	A2201	A1810	G1651	U1438	U1329	U1212	A1105	C998	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897
	A2342	U2221	U2118	G2011	A2201	C1651	U1438	U1330	C1212	G1107	U999	A897



● Molecule 7: tRNA-Ala (E-site)



● Molecule 8: tRNA-Asp (P-site)



● Molecule 9: tRNA-Lys (A-site)



- Molecule 15: 50S ribosomal protein L4

- Molecule 16: 50S ribosomal protein L5

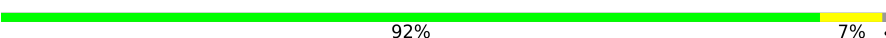
- Molecule 17: 50S ribosomal protein L6

- Molecule 18: 50S ribosomal protein L9

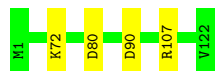
- Molecule 19: 50S ribosomal protein L10

- Molecule 20: 50S ribosomal protein L11

• Molecule 21: 50S ribosomal protein L13

Chain i:  92% 7%

• Molecule 22: 50S ribosomal protein L14

Chain j:  97%


• Molecule 23: 50S ribosomal protein L15

Chain k:  93% 7%

• Molecule 24: 50S ribosomal protein L16

Chain l:  94%

• Molecule 25: 50S ribosomal protein L17

Chain m:  90% 6%

• Molecule 26: 50S ribosomal protein L18

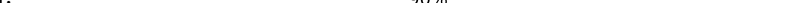
Chain n:  93% 7%

• Molecule 27: 50S ribosomal protein L19

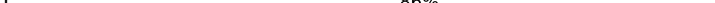
Chain o:  95%

• Molecule 28: 50S ribosomal protein L20

M1	K7	R54	S76	K113	K118	ALA	ALA	LYS	PRO	ALA	ALA	LEU	GLY	ASN
----	----	-----	-----	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain q:  90% 9%

Category	Protein Count
M1	1
V5	1
S9	1
K10	1
K44	1
S75	1
H78	1
T90	1
K91	1
L92	1
H99	1
ASP	1

- Chain r:  86% • 11%

M1		S37	N38	T39	Q78	L107	K141	A142	VAL	THR	SER	SER	VAL	VAL	LYS	ALA	PRO	SER	SER	LYS	THR	GLN	GLY	GLY	VAL	GLN	LYS
----	--	-----	-----	-----	-----	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

- Chain s: 37% . 60%

[illegible]

- Chain t:  93% 7%

Category	Value
M1	10
M28	10
E37	10
N40	10
K47	10
Q84	10
P95	10
N98	10
L111	11

- Chain u: 83% • 15%

MET	ASN	ASN	LYS	TYR	PHE	LEU	THR	LYS	ILE	ASP	LEU	GLN	PHE	PHE	ALA	S17	M44	S96	A104
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

- Chain v:  95%



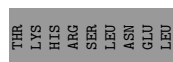
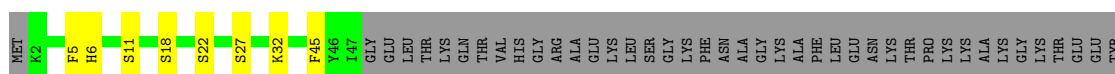
- Molecule 35: 50S ribosomal protein L29

Chain w: 92% 7% .



- Molecule 36: 50S ribosomal protein L31

Chain x: 39% 8% 53%



- Molecule 37: 50S ribosomal protein L32

Chain y: 86% 12% .



- Molecule 38: 50S ribosomal protein L33 1

Chain z: 87% 8% 6%



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	30774	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF estimation and 3D CTF correction are done in Warp	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	137	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3250	Depositor
Magnification	64000	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: 5MC, 1MG, CLM, PUT, B8T, ZN, MG, K, 2MA, SPD, SPM, N2P, OMG

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	0	0.23	0/395	0.56	0/518
2	1	0.24	0/484	0.52	0/637
3	2	0.23	0/306	0.52	0/401
4	3	0.19	0/69363	0.71	8/108161 (0.0%)
5	4	0.17	0/2578	0.72	0/4016
6	5	0.17	0/715	0.71	0/1107
7	6	0.13	0/46	0.62	0/69
8	7	0.30	1/1785 (0.1%)	0.84	2/2779 (0.1%)
9	8	0.53	6/1804 (0.3%)	0.80	0/2807
10	X	0.29	0/245	0.79	1/325 (0.3%)
11	Y	0.28	0/218	0.79	0/338
12	Z	0.75	0/26	1.33	0/33
13	a	0.37	2/2267 (0.1%)	0.60	3/3044 (0.1%)
14	b	0.29	0/1812	0.55	1/2436 (0.0%)
15	c	0.30	0/1681	0.54	1/2257 (0.0%)
16	d	0.32	0/1437	0.66	0/1931
17	e	0.49	2/1420 (0.1%)	0.94	5/1912 (0.3%)
18	f	0.40	1/1233 (0.1%)	0.62	0/1653
19	g	0.32	0/960	0.60	0/1284
20	h	0.78	4/968 (0.4%)	1.19	7/1298 (0.5%)
21	i	0.25	0/1186	0.50	0/1592
22	j	0.27	0/953	0.61	1/1275 (0.1%)
23	k	0.29	0/1187	0.60	0/1581
24	l	0.29	0/1104	0.56	0/1481
25	m	0.29	0/973	0.52	1/1309 (0.1%)
26	n	0.28	0/927	0.58	0/1239
27	o	0.31	0/976	0.59	0/1296
28	p	0.26	0/996	0.54	0/1325
29	q	0.29	0/828	0.55	0/1111
30	r	0.26	0/1100	0.50	0/1471
31	s	0.27	0/752	0.58	0/1015
32	t	0.57	1/878 (0.1%)	0.96	4/1165 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	u	0.25	0/678	0.52	0/902
34	v	0.23	0/526	0.56	0/703
35	w	0.26	0/916	0.56	0/1222
36	x	0.26	0/375	0.46	0/502
37	y	0.28	0/457	0.63	0/601
38	z	0.23	0/412	0.54	0/547
All	All	0.25	17/104967 (0.0%)	0.70	34/157343 (0.0%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	h	52	PRO	CG-CD	-15.31	1.00	1.50
32	t	95	PRO	CG-CD	-13.85	1.04	1.50
17	e	30	PRO	CB-CG	-11.82	0.90	1.50
9	8	76	A	N9-C4	10.38	1.44	1.37
20	h	52	PRO	N-CD	10.15	1.62	1.47
20	h	71	PRO	CG-CD	-9.22	1.20	1.50
18	f	104	LYS	CE-NZ	-8.84	1.26	1.49
9	8	76	A	C6-N6	8.12	1.40	1.33
13	a	151	GLU	CD-OE2	-7.98	1.16	1.25
9	8	76	A	C5-C4	7.71	1.44	1.38
8	7	1	G	OP3-P	-7.58	1.52	1.61
20	h	52	PRO	CB-CG	-7.12	1.14	1.50
9	8	76	A	N3-C4	7.12	1.39	1.34
13	a	151	GLU	CG-CD	-6.78	1.41	1.51
17	e	30	PRO	N-CA	6.69	1.58	1.47
9	8	76	A	N9-C8	6.13	1.42	1.37
9	8	76	A	N1-C2	5.08	1.39	1.34

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	h	52	PRO	N-CD-CG	-20.95	71.77	103.20
32	t	95	PRO	N-CD-CG	-19.84	73.44	103.20
17	e	30	PRO	N-CD-CG	-19.64	73.73	103.20
17	e	30	PRO	CB-CG-CD	18.83	179.95	106.50
17	e	30	PRO	CA-CB-CG	-16.62	72.43	104.00
20	h	52	PRO	CB-CG-CD	16.08	169.21	106.50
32	t	95	PRO	CA-CB-CG	-15.20	75.13	104.00
20	h	71	PRO	N-CD-CG	-13.67	82.69	103.20
20	h	52	PRO	CA-CB-CG	-13.67	78.02	104.00
20	h	71	PRO	CA-N-CD	-10.78	96.41	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	h	71	PRO	CA-CB-CG	-9.63	85.71	104.00
20	h	52	PRO	CA-N-CD	-9.45	98.27	111.50
10	X	38	MET	CA-CB-CG	8.06	127.00	113.30
8	7	73	C	P-O3'-C3'	-7.63	110.54	119.70
4	3	1486	U	C2-N1-C1'	7.15	126.28	117.70
32	t	95	PRO	N-CA-CB	-7.01	94.89	103.30
4	3	1486	U	N1-C2-O2	6.71	127.50	122.80
17	e	30	PRO	CA-N-CD	-6.67	102.16	111.50
4	3	1486	U	N3-C2-O2	-6.19	117.87	122.20
13	a	128	ILE	CG1-CB-CG2	-6.00	98.20	111.40
4	3	1341	U	C2-N1-C1'	5.80	124.66	117.70
13	a	151	GLU	CG-CD-OE2	-5.68	106.94	118.30
32	t	95	PRO	CA-N-CD	-5.66	103.58	111.50
15	c	193	LEU	CA-CB-CG	5.62	128.23	115.30
4	3	1303	U	C2-N1-C1'	5.60	124.42	117.70
17	e	92	LEU	CA-CB-CG	5.53	128.01	115.30
13	a	151	GLU	CG-CD-OE1	5.50	129.29	118.30
14	b	45	ASP	CB-CG-OD1	5.41	123.16	118.30
22	j	90	ASP	CB-CG-OD1	5.33	123.09	118.30
4	3	1303	U	N3-C2-O2	-5.31	118.48	122.20
4	3	1303	U	N1-C2-O2	5.22	126.46	122.80
25	m	79	MET	CA-CB-CG	5.12	122.00	113.30
8	7	31	C	N1-C2-O2	5.09	121.95	118.90
4	3	2187	C	N1-C2-O2	5.01	121.91	118.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	392	0	442	8	0
2	1	477	0	530	7	0
3	2	304	0	348	3	0
4	3	61995	0	31115	341	0
5	4	2305	0	1164	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	5	683	0	339	4	0
7	6	42	0	23	0	0
8	7	1599	0	805	24	0
9	8	1615	0	816	19	0
10	X	242	0	263	9	0
11	Y	195	0	99	1	0
12	Z	187	0	68	5	0
13	a	2225	0	2301	0	0
14	b	1778	0	1821	0	0
15	c	1654	0	1744	0	0
16	d	1416	0	1500	0	0
17	e	1396	0	1481	0	0
18	f	1210	0	1259	0	0
19	g	951	0	1001	0	0
20	h	959	0	1039	0	0
21	i	1164	0	1192	0	0
22	j	944	0	1019	0	0
23	k	1170	0	1274	0	0
24	l	1079	0	1134	0	0
25	m	958	0	1011	0	0
26	n	918	0	979	0	0
27	o	966	0	1042	0	0
28	p	981	0	1062	0	0
29	q	811	0	858	0	0
30	r	1091	0	1178	0	0
31	s	740	0	819	0	0
32	t	871	0	972	0	0
33	u	670	0	704	0	0
34	v	520	0	565	0	0
35	w	906	0	981	0	0
36	x	366	0	356	0	0
37	y	452	0	471	0	0
38	z	408	0	436	0	0
39	2	1	0	0	0	0
39	x	1	0	0	0	0
39	y	1	0	0	0	0
39	z	1	0	0	0	0
40	3	20	0	11	4	0
41	3	1	0	0	0	0
42	3	219	0	0	0	0
42	4	1	0	0	0	0
42	6	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	7	1	0	0	0	0
42	8	2	0	0	0	0
42	b	2	0	0	0	0
42	i	1	0	0	0	0
42	y	2	0	0	0	0
43	3	42	0	84	1	0
44	3	42	0	78	7	0
44	b	14	0	26	0	0
45	3	160	0	304	3	0
46	3	21	0	42	0	0
47	8	9	0	12	0	0
All	All	97182	0	64768	416	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (416) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:50:G:H1	9:8:64:U:H3	1.21	0.88
4:3:2736:U:HO2'	4:3:2737:G:H8	1.24	0.85
10:X:29:LYS:HE3	10:X:30:GLN:HG2	1.60	0.82
3:2:4:ARG:NH2	4:3:2485:U:O2	2.12	0.82
10:X:38:MET:SD	10:X:57:LEU:HD22	2.20	0.81
4:3:2312:G:H22	4:3:2320:U:H3	1.28	0.80
8:7:34:G:H1	11:Y:42:U:H3	1.29	0.79
4:3:47:G:H5''	4:3:48:G:H5'	1.64	0.79
8:7:10:G:H1	8:7:25:U:H3	1.31	0.79
4:3:1344:U:O2'	10:X:44:ARG:NH2	2.15	0.78
4:3:2066:A:H2'	4:3:2511:2MA:HM23	1.72	0.71
8:7:48:G:H1	8:7:64:U:H3	1.37	0.71
1:0:9:LYS:NZ	4:3:1338:G:OP2	2.24	0.70
4:3:2799:U:OP1	4:3:2896:G:N1	2.21	0.70
4:3:1446:G:O2'	4:3:1613:A:N6	2.26	0.68
4:3:619:A:H62	4:3:1281:A:H2	1.40	0.68
5:4:83:U:H5'	5:4:84:C:H5'	1.77	0.67
4:3:656:G:H4'	4:3:657:A:H5'	1.76	0.67
1:0:24:THR:HG23	1:0:27:GLY:H	1.60	0.66
4:3:2465:U:H3	4:3:2502:G:H1	1.44	0.65
10:X:38:MET:SD	10:X:38:MET:O	2.54	0.65
4:3:1096:U:H1'	4:3:1105:A:H1'	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:925:C:H4'	4:3:926:U:O4'	1.97	0.64
4:3:2589:G:N2	4:3:2589:G:OP2	2.29	0.64
4:3:1619:A:H2'	4:3:1620:A:C8	2.33	0.64
4:3:2805:A:H4'	4:3:2807:G:H5''	1.80	0.64
4:3:881:A:H1'	4:3:882:C:H5''	1.80	0.64
4:3:1518:C:N4	4:3:2220:A:OP1	2.31	0.63
5:4:84:C:HO2'	5:4:85:A:H8	1.44	0.63
4:3:2823:A:O2'	4:3:2825:A:N7	2.30	0.63
8:7:19:A:H61	8:7:55:C:H42	1.46	0.63
4:3:2481:U:OP1	4:3:2483:C:N4	2.31	0.63
4:3:499:G:N2	4:3:502:A:OP2	2.29	0.62
4:3:487:C:N4	4:3:490:A:OP2	2.27	0.62
4:3:2308:U:H2'	4:3:2309:A:H8	1.64	0.62
4:3:1557:G:O6	4:3:1571:G:O2'	2.18	0.61
4:3:1786:U:OP2	4:3:1791:A:N6	2.25	0.61
4:3:2667:G:N2	4:3:2670:A:OP2	2.30	0.61
4:3:341:G:N1	4:3:344:A:OP2	2.32	0.60
4:3:1095:U:H1'	4:3:1096:U:H3'	1.83	0.60
4:3:2490:A:O2'	9:8:63:C:O2'	2.19	0.59
4:3:13:C:H3'	4:3:14:U:H5'	1.84	0.59
4:3:1137:C:H2'	4:3:1138:A:H8	1.66	0.59
4:3:196:G:OP2	4:3:196:G:N2	2.34	0.59
4:3:2098:U:H3'	4:3:2099:U:H5''	1.84	0.59
4:3:1129:U:N3	4:3:1132:C:OP2	2.25	0.59
40:3:3001:CLM:CL2	12:Z:33:LYS:HG2	2.39	0.58
4:3:1092:A:N6	4:3:1122:G:OP1	2.36	0.58
8:7:27:U:H3	8:7:43:G:H1	1.49	0.58
10:X:53:ALA:HB3	10:X:54:LYS:HE2	1.83	0.58
10:X:44:ARG:HH11	10:X:47:LYS:HE3	1.68	0.58
4:3:1906:G:H21	4:3:1909:C:H41	1.50	0.57
4:3:195:A:H3'	4:3:196:G:H21	1.69	0.57
4:3:1391:U:O2'	4:3:1816:A:N3	2.34	0.57
4:3:166:A:C6	4:3:167:A:C5	2.93	0.57
4:3:1833:G:O2'	4:3:1978:U:OP2	2.23	0.57
4:3:1055:A:N1	4:3:1176:U:O2'	2.35	0.56
4:3:2266:C:O2'	4:3:2435:C:OP2	2.23	0.56
4:3:879:U:O4	4:3:968:U:O2'	2.23	0.56
4:3:720:A:OP1	4:3:721:G:N2	2.39	0.56
8:7:36:C:H2'	8:7:37:A:C8	2.39	0.56
4:3:933:A:O2'	9:8:56:C:N3	2.39	0.56
8:7:50:G:H1	8:7:62:C:H42	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:512:G:N1	4:3:515:A:OP2	2.35	0.56
4:3:733:C:O2'	4:3:769:A:N6	2.39	0.56
4:3:1103:G:N2	4:3:1130:A:O2'	2.38	0.56
4:3:343:A:N3	4:3:363:G:O2'	2.38	0.55
4:3:585:U:H2'	4:3:586:G:H8	1.71	0.55
4:3:2383:G:N2	4:3:2386:A:OP2	2.35	0.55
4:3:1386:G:O2'	4:3:1401:A:N6	2.39	0.55
4:3:9:G:H2'	4:3:10:U:C6	2.42	0.55
4:3:1111:C:H2'	4:3:1112:A:O4'	2.05	0.55
8:7:36:C:H2'	8:7:37:A:H8	1.71	0.55
4:3:1125:U:H2'	4:3:1126:G:C8	2.42	0.55
1:0:1:MET:HE3	4:3:788:G:H5'	1.87	0.55
4:3:2299:U:H2'	4:3:2300:A:C8	2.42	0.55
4:3:196:G:O2'	4:3:712:A:N1	2.40	0.54
4:3:933:A:H3'	4:3:934:C:O4'	2.08	0.54
4:3:2296:A:H1'	45:3:3248:SPD:H91	1.87	0.54
4:3:1569:A:H2'	4:3:1570:A:C2	2.42	0.54
4:3:2513:G:C4	12:Z:33:LYS:HD2	2.43	0.54
4:3:1076:U:H3	4:3:1149:G:H1	1.55	0.54
2:1:15:LYS:HD3	4:3:664:G:H5''	1.89	0.54
4:3:410:G:H4'	4:3:411:U:O5'	2.07	0.54
4:3:901:C:H4'	4:3:902:U:C5'	2.38	0.54
4:3:1292:A:H61	4:3:2024:C:H42	1.55	0.54
5:4:2:U:O2	5:4:107:G:N2	2.41	0.54
9:8:29:U:H3	9:8:41:A:H61	1.54	0.54
4:3:1106:G:N2	4:3:1124:G:O2'	2.41	0.53
4:3:2122:G:O2'	4:3:2175:U:O2	2.25	0.53
4:3:2516:G:HO2'	4:3:2562:U:HO2'	1.56	0.53
4:3:201:A:N6	4:3:2438:A:O2'	2.41	0.53
4:3:619:A:N1	4:3:844:G:O2'	2.34	0.53
4:3:897:A:N3	5:4:77:G:O2'	2.42	0.53
4:3:2797:C:O2	4:3:2895:A:O2'	2.23	0.53
4:3:2820:G:N3	4:3:2887:A:O2'	2.41	0.53
4:3:2854:A:N7	4:3:2872:A:O2'	2.35	0.53
4:3:549:A:N3	4:3:614:C:O2'	2.41	0.53
9:8:27:A:H61	9:8:43:U:H3	1.57	0.53
4:3:2137:A:O2'	4:3:2165:A:N6	2.42	0.53
4:3:2630:U:O2'	4:3:2829:G:N7	2.40	0.53
4:3:427:A:H1'	4:3:447:G:O4'	2.09	0.53
4:3:892:G:H2'	4:3:893:A:C8	2.43	0.53
4:3:184:A:O2'	4:3:186:A:N7	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:620:G:H5'	44:3:3227:SPM:H61	1.91	0.52
4:3:2477:A:H2'	4:3:2478:G:O4'	2.09	0.52
4:3:87:G:O2'	4:3:104:A:N1	2.39	0.52
4:3:1588:A:H2'	4:3:1589:A:C8	2.45	0.52
4:3:2081:U:HO2'	4:3:2605:G:HO2'	1.58	0.52
4:3:2004:G:OP2	45:3:3250:SPD:H41	2.10	0.52
9:8:40:C:H2'	9:8:41:A:C8	2.45	0.52
9:8:28:A:H2'	9:8:29:U:C6	2.44	0.51
4:3:2813:A:H2'	4:3:2814:A:C8	2.45	0.51
2:1:5:SER:HA	2:1:8:LYS:HE2	1.91	0.51
4:3:316:C:H2'	4:3:392:A:H61	1.75	0.51
4:3:917:G:H2'	4:3:918:G:C8	2.45	0.51
4:3:2151:G:H1'	4:3:2154:A:H61	1.76	0.51
4:3:788:G:H2'	4:3:789:A:H8	1.75	0.51
4:3:86:A:N6	4:3:101:C:O4'	2.44	0.51
4:3:620:G:H5'	44:3:3227:SPM:H82	1.92	0.51
4:3:118:G:OP2	4:3:120:A:O2'	2.27	0.51
4:3:2308:U:H2'	4:3:2309:A:C8	2.45	0.51
4:3:180:A:H5'	4:3:181:G:C8	2.46	0.50
4:3:823:A:OP1	4:3:826:C:N4	2.39	0.50
4:3:196:G:O6	4:3:207:C:O2'	2.23	0.50
4:3:853:G:N1	4:3:1219:U:OP2	2.38	0.50
4:3:1566:A:H2'	4:3:1567:U:O4'	2.12	0.50
4:3:2299:U:OP1	4:3:2388:C:O2'	2.29	0.50
4:3:408:G:OP2	4:3:459:A:N6	2.45	0.50
4:3:1023:C:O2'	4:3:1036:A:N3	2.42	0.50
4:3:1091:G:H4'	4:3:1121:A:H8	1.76	0.50
4:3:1617:U:H5''	4:3:1619:A:C4	2.47	0.50
4:3:622:U:H2'	4:3:623:A:C8	2.47	0.50
4:3:1583:G:O2'	4:3:1584:U:OP1	2.25	0.50
4:3:1343:C:O2'	4:3:1420:A:N3	2.36	0.50
4:3:1166:G:N2	4:3:1167:U:O4	2.38	0.50
4:3:1445:U:H2'	4:3:1446:G:O4'	2.11	0.50
4:3:1920:A:C8	6:5:1469:G:H4'	2.46	0.49
4:3:2299:U:H2'	4:3:2300:A:H8	1.77	0.49
4:3:1132:C:H3'	4:3:1133:A:H8	1.77	0.49
4:3:1270:C:H2'	4:3:1271:A:H8	1.76	0.49
4:3:615:G:H2'	4:3:616:G:H8	1.77	0.49
4:3:1485:A:H4'	4:3:1486:U:C4	2.47	0.49
4:3:140:G:N2	4:3:143:A:OP2	2.28	0.49
4:3:917:G:H2'	4:3:918:G:H8	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:8:5:C:H2'	9:8:6:U:H6	1.78	0.49
4:3:666:G:N2	4:3:669:A:OP2	2.33	0.49
4:3:1104:A:H5''	4:3:1105:A:C5	2.47	0.49
4:3:2797:C:H5'	4:3:2798:A:O5'	2.13	0.49
4:3:1568:C:H3'	4:3:1569:A:C8	2.48	0.48
4:3:1618:U:H4'	4:3:1619:A:OP2	2.12	0.48
4:3:246:G:O2'	4:3:258:G:O6	2.29	0.48
5:4:11:A:H2'	5:4:12:U:H5''	1.95	0.48
4:3:518:A:O2'	4:3:532:A:N1	2.44	0.48
4:3:638:A:H62	4:3:660:U:H3	1.60	0.48
4:3:728:A:O2'	4:3:1381:A:N3	2.40	0.48
8:7:10:G:O2'	8:7:11:U:OP1	2.25	0.48
10:X:40:ILE:HD11	10:X:48:VAL:HG13	1.94	0.48
4:3:700:U:H2'	4:3:701:A:H8	1.79	0.48
5:4:2:U:H2'	5:4:3:U:C6	2.49	0.48
4:3:892:G:H2'	4:3:893:A:H8	1.79	0.48
4:3:1117:U:H2'	4:3:1118:U:O4'	2.14	0.48
4:3:1696:C:O2'	4:3:2695:U:OP1	2.31	0.48
4:3:50:G:H22	4:3:180:A:H5''	1.79	0.48
4:3:916:U:H3	4:3:935:U:H3	1.61	0.48
4:3:12:A:H2'	4:3:13:C:O4'	2.13	0.48
4:3:2847:C:H2'	4:3:2848:A:H8	1.79	0.48
2:1:19:ILE:HD12	2:1:47:VAL:HG21	1.95	0.47
4:3:615:G:H2'	4:3:616:G:C8	2.49	0.47
4:3:2180:U:H4'	4:3:2181:A:OP2	2.13	0.47
40:3:3001:CLM:CL1	12:Z:35:ALA:HB2	2.50	0.47
4:3:619:A:OP1	44:3:3227:SPM:N14	2.47	0.47
4:3:652:U:H2'	4:3:653:G:C8	2.49	0.47
4:3:1544:G:H2'	4:3:1545:A:H8	1.79	0.47
4:3:1665:G:N1	4:3:1668:G:OP2	2.37	0.47
4:3:2254:G:H2'	4:3:2255:A:H8	1.80	0.47
4:3:818:A:H2'	4:3:819:U:H4'	1.97	0.47
4:3:703:A:H2'	4:3:705:A:H62	1.79	0.47
8:7:50:G:H2'	8:7:51:G:C8	2.49	0.47
1:0:1:MET:CE	4:3:788:G:H5'	2.44	0.47
4:3:1306:G:H2'	4:3:1307:G:H8	1.80	0.47
4:3:652:U:H2'	4:3:653:G:H8	1.80	0.47
4:3:1392:G:N2	4:3:1395:A:OP2	2.42	0.47
4:3:2376:C:H2'	4:3:2377:A:H8	1.79	0.47
4:3:2548:G:O2'	4:3:2748:A:N3	2.44	0.47
4:3:355:A:O2'	4:3:374:A:N3	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1103:G:O2'	4:3:1104:A:H5'	2.15	0.47
4:3:2160:U:H2'	4:3:2161:G:H8	1.80	0.47
4:3:1045:A:N3	4:3:1188:C:O2'	2.45	0.47
4:3:1093:U:H3	4:3:1115:G:H1	1.62	0.47
4:3:1137:C:H2'	4:3:1138:A:C8	2.48	0.47
4:3:2254:G:H2'	4:3:2255:A:C8	2.50	0.47
4:3:2653:G:OP2	4:3:2653:G:N2	2.29	0.47
9:8:28:A:H2'	9:8:29:U:H6	1.79	0.47
4:3:1296:G:O2'	4:3:2019:G:O6	2.27	0.47
4:3:1000:U:O2'	4:3:2281:A:N3	2.34	0.46
4:3:1124:G:N2	4:3:1125:U:O4	2.48	0.46
4:3:1436:C:H2'	4:3:1437:A:C8	2.50	0.46
4:3:933:A:H2'	4:3:933:A:N3	2.29	0.46
4:3:2838:G:H2'	4:3:2883:A:H61	1.79	0.46
9:8:37:A:H3'	9:8:38:A:H8	1.79	0.46
2:1:42:ARG:NH1	4:3:2358:U:OP2	2.48	0.46
4:3:1121:A:H5''	4:3:1122:G:H5'	1.96	0.46
4:3:755:C:H2'	4:3:756:A:H8	1.79	0.46
4:3:1437:A:H2'	4:3:1438:G:C8	2.51	0.46
6:5:1463:A:H2'	6:5:1464:G:C8	2.51	0.46
4:3:1091:G:H4'	4:3:1121:A:C8	2.50	0.46
4:3:1583:G:H2'	4:3:1584:U:C6	2.51	0.46
4:3:2540:G:N2	4:3:2671:G:O2'	2.48	0.46
1:0:48:ARG:HH12	4:3:1339:U:H2'	1.81	0.46
4:3:230:G:O2'	4:3:232:A:N6	2.48	0.46
4:3:1465:U:HO2'	4:3:1542:G:HO2'	1.60	0.46
4:3:2118:U:OP2	4:3:2152:C:N4	2.49	0.46
9:8:18:G:N2	9:8:58:A:OP2	2.45	0.46
10:X:44:ARG:NH1	10:X:47:LYS:HE3	2.31	0.46
4:3:1440:U:H2'	4:3:1441:A:C8	2.51	0.46
44:3:3249:SPM:H62	44:3:3249:SPM:H92	1.78	0.46
8:7:35:U:H2'	8:7:36:C:C6	2.50	0.46
4:3:604:A:O2'	4:3:606:G:OP2	2.28	0.46
4:3:1797:C:H2'	4:3:1798:A:C8	2.51	0.46
4:3:2863:G:OP2	4:3:2863:G:H8	1.99	0.46
4:3:1436:C:H2'	4:3:1437:A:H8	1.80	0.45
4:3:1529:U:H2'	4:3:1530:G:H8	1.81	0.45
4:3:356:A:H5'	4:3:374:A:H1'	1.98	0.45
4:3:569:U:H2'	4:3:570:C:C6	2.50	0.45
1:0:6:GLN:O	4:3:721:G:H8	1.99	0.45
4:3:606:G:N2	4:3:2038:A:OP1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:756:A:H2'	4:3:757:A:C8	2.51	0.45
4:3:901:C:H4'	4:3:902:U:O5'	2.17	0.45
4:3:916:U:H2'	4:3:917:G:C8	2.52	0.45
4:3:963:U:H2'	4:3:964:A:H8	1.81	0.45
4:3:1437:A:H2'	4:3:1438:G:H8	1.82	0.45
4:3:2372:C:H2'	4:3:2373:G:O4'	2.16	0.45
44:3:3227:SPM:H121	44:3:3227:SPM:H92	1.76	0.45
9:8:41:A:H2'	9:8:42:U:O4'	2.16	0.45
4:3:894:G:N3	4:3:2276:A:H2'	2.31	0.45
5:4:40:U:HO2'	5:4:41:C:H6	1.60	0.45
6:5:1384:A:H2'	6:5:1385:A:C8	2.51	0.45
9:8:74:C:OP1	9:8:75:C:H5'	2.17	0.45
4:3:340:U:H2'	4:3:341:G:O4'	2.17	0.45
4:3:668:A:H2'	4:3:669:A:C8	2.52	0.45
4:3:2813:A:H61	4:3:2894:G:H2'	1.81	0.45
4:3:299:A:H2'	4:3:300:G:C8	2.51	0.45
4:3:411:U:H2'	4:3:412:A:H8	1.82	0.45
4:3:1135:C:H2'	4:3:1136:U:O4'	2.17	0.45
5:4:3:U:O2'	5:4:24:A:N1	2.47	0.45
4:3:1974:U:OP1	43:3:3231:PUT:N1	2.49	0.45
4:3:1575:C:H2'	4:3:1576:G:O4'	2.17	0.45
9:8:70:U:H2'	9:8:71:G:C8	2.51	0.45
4:3:166:A:N6	4:3:167:A:C6	2.85	0.44
4:3:680:A:H2'	4:3:682:A:N7	2.32	0.44
4:3:1092:A:H2'	4:3:1093:U:C6	2.52	0.44
5:4:104:C:H2'	5:4:105:A:C8	2.52	0.44
4:3:1102:A:N3	4:3:1102:A:H2'	2.31	0.44
4:3:1598:U:H2'	4:3:1599:C:C6	2.52	0.44
4:3:2110:U:H3	4:3:2194:G:H1	1.65	0.44
4:3:1099:C:H3'	4:3:1100:U:H6	1.83	0.44
4:3:1128:G:H2'	4:3:1129:U:C6	2.53	0.44
4:3:2853:U:O2'	4:3:2870:U:O2	2.31	0.44
4:3:2863:G:H2'	4:3:2864:A:C8	2.53	0.44
8:7:46:U:O2'	8:7:47:U:OP1	2.24	0.44
3:2:9:PRO:HD3	3:2:16:ILE:HD11	2.00	0.44
4:3:2299:U:O2'	4:3:2382:A:N3	2.48	0.44
4:3:2802:C:N4	4:3:2803:G:H21	2.15	0.44
4:3:524:G:N2	4:3:527:A:OP2	2.34	0.44
4:3:603:G:H2'	4:3:2037:A:N7	2.32	0.44
44:3:3241:SPM:H121	44:3:3241:SPM:H92	1.77	0.44
5:4:82:U:H2'	5:4:83:U:H4'	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:223:A:N3	4:3:238:U:O2'	2.39	0.44
4:3:1801:U:H2'	4:3:1802:C:C6	2.53	0.44
10:X:40:ILE:HD12	10:X:40:ILE:H	1.83	0.44
4:3:15:A:O2'	4:3:17:G:N7	2.48	0.43
4:3:174:A:H2'	4:3:175:A:H8	1.83	0.43
4:3:333:A:N3	4:3:353:G:O2'	2.45	0.43
4:3:1691:U:H2'	4:3:1692:A:C8	2.53	0.43
4:3:2811:G:H2'	4:3:2812:U:C6	2.53	0.43
4:3:299:A:H2'	4:3:300:G:H8	1.84	0.43
4:3:340:U:H1'	4:3:1241:U:H5	1.82	0.43
4:3:2155:G:H2'	4:3:2156:G:H8	1.81	0.43
4:3:2459:A:C2	40:3:3001:CLM:H8	2.53	0.43
4:3:2896:G:H3'	4:3:2897:G:H5'	2.00	0.43
1:0:44:VAL:O	1:0:47:GLU:HG3	2.18	0.43
4:3:756:A:H2'	4:3:757:A:H8	1.83	0.43
4:3:1414:C:H2'	4:3:1415:A:C8	2.52	0.43
4:3:1529:U:H2'	4:3:1530:G:C8	2.53	0.43
8:7:61:C:H2'	8:7:62:C:H6	1.83	0.43
4:3:610:G:H5''	4:3:2510:G:C2	2.53	0.43
4:3:1415:A:H5'	4:3:1495:A:H1'	2.00	0.43
4:3:1521:A:N3	4:3:1611:C:O2'	2.40	0.43
4:3:2565:G:H2'	4:3:2566:C:C6	2.53	0.43
1:0:32:LYS:O	1:0:36:LYS:HG3	2.19	0.43
4:3:1623:U:H2'	4:3:1624:A:C8	2.53	0.43
4:3:339:U:H2'	4:3:340:U:C6	2.53	0.43
4:3:610:G:H2'	4:3:611:A:C8	2.54	0.43
4:3:2146:A:H2'	4:3:2147:G:H8	1.83	0.43
4:3:1306:G:H2'	4:3:1307:G:C8	2.54	0.43
4:3:2031:C:OP1	45:3:3237:SPD:H81	2.18	0.43
4:3:2081:U:H2'	4:3:2082:U:C6	2.53	0.43
4:3:2813:A:H2'	4:3:2814:A:H8	1.84	0.43
4:3:1495:A:H2'	4:3:1496:A:C8	2.54	0.43
8:7:23:C:H2'	8:7:24:A:C8	2.54	0.43
4:3:848:U:H2'	4:3:849:C:C6	2.53	0.43
4:3:1585:A:N3	4:3:1585:A:H2'	2.34	0.43
4:3:1619:A:H8	4:3:1619:A:H5''	1.82	0.43
4:3:1915:C:O2'	8:7:12:G:H5''	2.19	0.43
4:3:2032:G:H2'	4:3:2033:G:C8	2.54	0.43
4:3:2798:A:O3'	4:3:2896:G:N2	2.52	0.43
9:8:63:C:H6	9:8:63:C:H5''	1.84	0.43
4:3:354:C:HO2'	4:3:356:A:H8	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1414:C:H2'	4:3:1415:A:H8	1.84	0.42
8:7:26:A:H61	8:7:44:G:H1	1.67	0.42
3:2:1:MET:CE	4:3:2750:A:H5''	2.49	0.42
4:3:1697:C:HO2'	4:3:1698:A:H8	1.66	0.42
4:3:1815:U:O2'	4:3:1816:A:O4'	2.37	0.42
4:3:2336:A:H2'	4:3:2337:U:C6	2.54	0.42
4:3:2358:U:H2'	4:3:2359:G:O4'	2.18	0.42
4:3:2655:U:H2'	4:3:2656:G:H8	1.84	0.42
4:3:831:U:H2'	4:3:832:C:C6	2.53	0.42
4:3:1836:A:H3'	4:3:1837:C:H6	1.84	0.42
4:3:2537:G:H5''	4:3:2538:A:H5''	2.01	0.42
4:3:2764:U:H1'	4:3:2765:A:H5''	2.01	0.42
4:3:63:U:O2'	4:3:64:U:O2	2.37	0.42
4:3:1101:U:H2'	4:3:1103:G:N7	2.34	0.42
4:3:1798:A:H8	4:3:1798:A:P	2.43	0.42
4:3:2271:C:H4'	4:3:2337:U:H4'	2.00	0.42
4:3:54:A:OP2	4:3:118:G:N1	2.43	0.42
4:3:1120:A:H2'	4:3:1121:A:N9	2.34	0.42
4:3:1321:C:H2'	4:3:1322:A:O4'	2.19	0.42
4:3:1385:U:H2'	4:3:1386:G:O4'	2.19	0.42
6:5:1385:A:H2'	6:5:1386:C:C6	2.55	0.42
8:7:61:C:H2'	8:7:62:C:C6	2.54	0.42
4:3:899:A:H2'	4:3:900:G:C8	2.54	0.42
4:3:2438:A:H2'	4:3:2438:A:N3	2.33	0.42
4:3:2638:G:H2'	4:3:2639:G:H8	1.85	0.42
9:8:48:C:OP2	9:8:48:C:H6	2.02	0.42
4:3:558:C:H1'	4:3:587:U:H1'	2.01	0.42
4:3:1536:C:H2'	4:3:1537:A:C8	2.54	0.42
4:3:1572:U:H2'	4:3:1573:A:H8	1.85	0.42
4:3:1809:A:H2'	4:3:1810:A:C8	2.55	0.42
4:3:2334:U:H3	4:3:2397:G:H1	1.67	0.42
40:3:3001:CLM:CL1	12:Z:35:ALA:CB	3.04	0.42
4:3:141:A:H2	4:3:1437:A:H1'	1.83	0.42
4:3:449:C:H2'	4:3:450:C:C6	2.55	0.42
4:3:1673:U:O2'	4:3:2707:A:H4'	2.20	0.42
4:3:1691:U:H2'	4:3:1692:A:H8	1.85	0.42
4:3:2070:C:H1'	12:Z:36:ASP:HA	2.02	0.42
4:3:776:U:H2'	4:3:777:C:H6	1.85	0.42
4:3:1460:G:H2'	4:3:1461:A:C8	2.55	0.42
4:3:1871:U:OP1	4:3:2418:G:O2'	2.33	0.42
4:3:2204:C:H2'	4:3:2205:U:C6	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:606:G:N1	4:3:2038:A:OP1	2.53	0.42
4:3:1114:C:H3'	4:3:1115:G:H8	1.84	0.42
4:3:1239:G:O2'	4:3:1267:A:N1	2.37	0.42
4:3:622:U:H2'	4:3:623:A:H8	1.81	0.41
4:3:1444:C:N4	4:3:1616:G:O6	2.53	0.41
4:3:125:G:OP1	4:3:1404:C:O2'	2.28	0.41
4:3:155:A:H2'	4:3:156:A:H8	1.84	0.41
4:3:2376:C:H2'	4:3:2377:A:C8	2.55	0.41
4:3:2420:A:H2'	4:3:2421:U:O4'	2.20	0.41
2:1:10:ARG:NH1	4:3:254:G:OP2	2.46	0.41
4:3:259:A:O2'	4:3:422:A:OP1	2.36	0.41
4:3:274:A:OP2	4:3:294:G:N1	2.53	0.41
4:3:1313:G:N2	4:3:1356:G:H5''	2.35	0.41
4:3:1464:G:H1	4:3:1590:U:H3	1.67	0.41
4:3:166:A:C6	4:3:167:A:C6	3.09	0.41
4:3:749:U:H1'	4:3:752:C:H5	1.85	0.41
4:3:890:U:H2'	4:3:891:G:C8	2.55	0.41
4:3:2403:C:H2'	4:3:2404:G:C8	2.55	0.41
5:4:65:G:H2'	5:4:66:A:H8	1.86	0.41
4:3:155:A:H2'	4:3:156:A:C8	2.55	0.41
8:7:10:G:HO2'	8:7:11:U:P	2.43	0.41
9:8:5:C:H2'	9:8:6:U:C6	2.55	0.41
4:3:10:U:H2'	4:3:11:U:H4'	2.02	0.41
4:3:1697:C:O2'	4:3:2694:A:H4'	2.21	0.41
4:3:1803:U:H2'	4:3:1804:A:C8	2.55	0.41
4:3:2071:C:H2'	4:3:2072:C:C6	2.55	0.41
4:3:2638:G:H2'	4:3:2639:G:C8	2.56	0.41
4:3:2803:G:O2'	4:3:2804:C:O5'	2.35	0.41
2:1:28:HIS:HE1	4:3:2430:C:C5	2.39	0.41
4:3:1208:A:H2'	4:3:1209:U:H4'	2.01	0.41
4:3:2025:C:H2'	4:3:2026:A:H8	1.86	0.41
4:3:45:U:H2'	4:3:46:A:O4'	2.21	0.41
4:3:893:A:H61	4:3:957:G:H1	1.69	0.41
4:3:1334:U:H2'	4:3:1335:A:H8	1.86	0.41
4:3:1485:A:H4'	4:3:1486:U:C5	2.56	0.41
4:3:1564:U:H2'	4:3:1565:G:C8	2.56	0.41
4:3:1619:A:H2'	4:3:1620:A:H8	1.81	0.41
4:3:2335:A:H2'	4:3:2336:A:C8	2.56	0.41
4:3:2713:A:O2'	4:3:2856:G:OP1	2.33	0.41
4:3:2736:U:O2'	4:3:2737:G:H8	1.94	0.41
5:4:81:U:H2'	5:4:82:U:O4'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:7:18:G:O2'	8:7:56:G:N2	2.32	0.41
4:3:227:A:O2'	4:3:456:G:N3	2.45	0.41
4:3:869:U:H2'	4:3:870:A:H8	1.86	0.41
4:3:909:U:H2'	4:3:910:G:C8	2.56	0.41
2:1:51:ASP:O	2:1:55:ILE:HG12	2.21	0.40
4:3:984:C:H2'	4:3:985:A:H8	1.85	0.40
4:3:1162:A:N3	44:3:3249:SPM:H21	2.36	0.40
4:3:1583:G:HO2'	4:3:1584:U:P	2.43	0.40
4:3:2010:A:H2'	4:3:2011:G:O4'	2.21	0.40
8:7:17:G:H4'	8:7:18:G:H5''	2.03	0.40
4:3:567:U:H4'	4:3:568:G:C8	2.56	0.40
4:3:2078:A:H2'	4:3:2079:G:C8	2.56	0.40
8:7:5:C:H2'	8:7:6:C:H6	1.86	0.40
9:8:71:G:H2'	9:8:72:C:C6	2.57	0.40
4:3:881:A:H2	4:3:968:U:H3	1.63	0.40
8:7:10:G:H2'	8:7:11:U:C6	2.56	0.40
4:3:1543:U:H2'	4:3:1544:G:C8	2.57	0.40
4:3:1889:U:H2'	4:3:1890:U:C6	2.57	0.40
4:3:2145:A:H2'	4:3:2146:A:H8	1.85	0.40
4:3:2200:U:H2'	4:3:2201:G:H5'	2.04	0.40
8:7:74:C:H5''	8:7:75:A:OP2	2.21	0.40
4:3:670:G:H2'	4:3:671:C:C6	2.56	0.40
4:3:1433:U:H2'	4:3:1434:U:C6	2.57	0.40
8:7:5:C:H2'	8:7:6:C:C6	2.56	0.40
9:8:30:G:H3'	9:8:31:A:H8	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	0	46/48 (96%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	1	57/59 (97%)	57 (100%)	0	0	100	100
3	2	35/37 (95%)	35 (100%)	0	0	100	100
10	X	28/444 (6%)	24 (86%)	4 (14%)	0	100	100
12	Z	3/36 (8%)	3 (100%)	0	0	100	100
13	a	283/287 (99%)	268 (95%)	14 (5%)	1 (0%)	30	60
14	b	229/287 (80%)	221 (96%)	8 (4%)	0	100	100
15	c	209/212 (99%)	198 (95%)	11 (5%)	0	100	100
16	d	177/180 (98%)	169 (96%)	8 (4%)	0	100	100
17	e	174/184 (95%)	161 (92%)	13 (8%)	0	100	100
18	f	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	9	31
19	g	123/161 (76%)	116 (94%)	7 (6%)	0	100	100
20	h	126/137 (92%)	121 (96%)	5 (4%)	0	100	100
21	i	142/146 (97%)	134 (94%)	8 (6%)	0	100	100
22	j	120/122 (98%)	115 (96%)	5 (4%)	0	100	100
23	k	148/151 (98%)	139 (94%)	9 (6%)	0	100	100
24	l	134/139 (96%)	132 (98%)	2 (2%)	0	100	100
25	m	117/124 (94%)	112 (96%)	5 (4%)	0	100	100
26	n	114/116 (98%)	109 (96%)	5 (4%)	0	100	100
27	o	116/119 (98%)	107 (92%)	9 (8%)	0	100	100
28	p	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
29	q	97/100 (97%)	93 (96%)	4 (4%)	0	100	100
30	r	140/159 (88%)	136 (97%)	4 (3%)	0	100	100
31	s	93/237 (39%)	89 (96%)	4 (4%)	0	100	100
32	t	109/111 (98%)	102 (94%)	7 (6%)	0	100	100
33	u	86/104 (83%)	82 (95%)	4 (5%)	0	100	100
34	v	62/65 (95%)	62 (100%)	0	0	100	100
35	w	108/111 (97%)	102 (94%)	6 (6%)	0	100	100
36	x	44/97 (45%)	35 (80%)	8 (18%)	1 (2%)	5	20
37	y	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
38	z	48/53 (91%)	47 (98%)	1 (2%)	0	100	100
All	All	3485/4359 (80%)	3310 (95%)	171 (5%)	4 (0%)	50	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	a	128	ILE
18	f	12	LEU
18	f	74	GLN
36	x	18	SER

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	0	41/41 (100%)	39 (95%)	2 (5%)	21	53
2	1	51/51 (100%)	49 (96%)	2 (4%)	27	62
3	2	35/35 (100%)	35 (100%)	0	100	100
10	X	27/406 (7%)	22 (82%)	5 (18%)	1	4
12	Z	2/2 (100%)	2 (100%)	0	100	100
13	a	241/243 (99%)	232 (96%)	9 (4%)	29	64
14	b	188/233 (81%)	180 (96%)	8 (4%)	25	57
15	c	183/184 (100%)	170 (93%)	13 (7%)	12	36
16	d	153/154 (99%)	143 (94%)	10 (6%)	14	40
17	e	153/159 (96%)	147 (96%)	6 (4%)	27	62
18	f	134/134 (100%)	129 (96%)	5 (4%)	29	64
19	g	100/129 (78%)	90 (90%)	10 (10%)	6	20
20	h	102/110 (93%)	97 (95%)	5 (5%)	21	53
21	i	126/128 (98%)	116 (92%)	10 (8%)	10	30
22	j	103/103 (100%)	100 (97%)	3 (3%)	37	72
23	k	125/126 (99%)	115 (92%)	10 (8%)	10	30
24	l	113/115 (98%)	108 (96%)	5 (4%)	24	57
25	m	105/109 (96%)	99 (94%)	6 (6%)	17	47
26	n	99/99 (100%)	91 (92%)	8 (8%)	9	29
27	o	104/105 (99%)	99 (95%)	5 (5%)	21	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	p	104/108 (96%)	100 (96%)	4 (4%)	28	63
29	q	90/91 (99%)	81 (90%)	9 (10%)	6	20
30	r	118/132 (89%)	113 (96%)	5 (4%)	25	59
31	s	84/208 (40%)	76 (90%)	8 (10%)	7	22
32	t	96/96 (100%)	89 (93%)	7 (7%)	11	34
33	u	70/85 (82%)	68 (97%)	2 (3%)	37	72
34	v	59/60 (98%)	57 (97%)	2 (3%)	32	67
35	w	97/98 (99%)	89 (92%)	8 (8%)	9	29
36	x	44/86 (51%)	37 (84%)	7 (16%)	2	6
37	y	48/49 (98%)	41 (85%)	7 (15%)	2	8
38	z	47/50 (94%)	43 (92%)	4 (8%)	8	27
All	All	3042/3729 (82%)	2857 (94%)	185 (6%)	18	43

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	22	MET
1	0	28	ARG
2	1	1	MET
2	1	28	HIS
10	X	29	LYS
10	X	40	ILE
10	X	44	ARG
10	X	45	LYS
10	X	56	TYR
13	a	9	ARG
13	a	16	HIS
13	a	21	ASP
13	a	37	LEU
13	a	70	ASP
13	a	107	SER
13	a	140	PHE
13	a	227	THR
13	a	262	HIS
14	b	39	VAL
14	b	42	GLU
14	b	58	GLU
14	b	74	ASN

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Mol	Chain	Res	Type
14	b	100	ASN
14	b	158	ARG
14	b	186	GLU
14	b	231	GLU
15	c	10	ASP
15	c	19	LYS
15	c	36	ASP
15	c	75	ARG
15	c	151	LYS
15	c	153	LEU
15	c	162	ASN
15	c	166	THR
15	c	169	GLU
15	c	173	SER
15	c	176	LYS
15	c	179	GLN
15	c	180	VAL
16	d	15	GLU
16	d	26	MET
16	d	31	LEU
16	d	88	LYS
16	d	95	ARG
16	d	114	PHE
16	d	125	ARG
16	d	128	TYR
16	d	133	LYS
16	d	179	LYS
17	e	41	ASN
17	e	48	LEU
17	e	84	GLN
17	e	108	LEU
17	e	109	GLN
17	e	135	THR
18	f	8	ASP
18	f	23	ASP
18	f	84	HIS
18	f	104	LYS
18	f	106	MET
19	g	10	GLN
19	g	24	PHE
19	g	25	VAL
19	g	32	MET

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Mol	Chain	Res	Type
19	g	42	LYS
19	g	55	LYS
19	g	64	LYS
19	g	67	LYS
19	g	108	PHE
19	g	125	LYS
20	h	46	LYS
20	h	50	MET
20	h	58	TYR
20	h	123	MET
20	h	131	MET
21	i	6	MET
21	i	7	LEU
21	i	62	SER
21	i	63	ASP
21	i	80	HIS
21	i	87	ILE
21	i	89	LYS
21	i	95	MET
21	i	132	LYS
21	i	146	SER
22	j	72	LYS
22	j	80	ASP
22	j	107	ARG
23	k	8	SER
23	k	11	LYS
23	k	36	GLN
23	k	75	GLN
23	k	76	GLU
23	k	108	SER
23	k	113	LYS
23	k	120	LEU
23	k	137	LYS
23	k	147	LYS
24	l	6	ARG
24	l	60	LYS
24	l	63	LYS
24	l	73	SER
24	l	83	MET
25	m	10	THR
25	m	71	ASN
25	m	84	SER

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Mol	Chain	Res	Type
25	m	85	LYS
25	m	97	TYR
25	m	107	ARG
26	n	1	MET
26	n	12	HIS
26	n	20	ARG
26	n	36	LEU
26	n	61	LYS
26	n	64	ASN
26	n	66	ASN
26	n	89	VAL
27	o	24	GLU
27	o	38	LYS
27	o	87	SER
27	o	98	ARG
27	o	116	GLU
28	p	7	LYS
28	p	54	ARG
28	p	76	SER
28	p	113	LYS
29	q	1	MET
29	q	5	VAL
29	q	9	SER
29	q	10	LYS
29	q	44	LYS
29	q	75	SER
29	q	78	HIS
29	q	90	THR
29	q	92	LEU
30	r	37	SER
30	r	39	THR
30	r	78	GLN
30	r	107	LEU
30	r	141	LYS
31	s	12	LEU
31	s	18	PHE
31	s	24	THR
31	s	34	LYS
31	s	47	VAL
31	s	51	LYS
31	s	64	THR
31	s	84	THR

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Mol	Chain	Res	Type
32	t	1	MET
32	t	28	MET
32	t	37	GLU
32	t	40	ASN
32	t	47	LYS
32	t	84	GLN
32	t	98	ASN
33	u	44	MET
33	u	96	SER
34	v	26	ARG
34	v	49	LEU
35	w	38	LEU
35	w	48	ARG
35	w	55	LEU
35	w	68	GLU
35	w	72	TYR
35	w	76	THR
35	w	101	SER
35	w	107	ASP
36	x	5	PHE
36	x	6	HIS
36	x	11	SER
36	x	22	SER
36	x	27	SER
36	x	32	LYS
36	x	45	PHE
37	y	6	ARG
37	y	10	LYS
37	y	18	SER
37	y	35	LYS
37	y	43	CYS
37	y	47	MET
37	y	52	ARG
38	z	5	ARG
38	z	6	SER
38	z	12	ASN
38	z	18	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
14	b	66	GLN

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Mol	Chain	Res	Type
14	b	135	HIS
14	b	148	GLN
14	b	157	GLN
14	b	188	ASN
18	f	96	GLN
21	i	80	HIS
23	k	134	GLN
26	n	64	ASN
28	p	8	GLN
28	p	71	GLN
28	p	106	ASN
33	u	100	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
11	Y	8/9 (88%)	4 (50%)	1 (12%)
4	3	2891/2907 (99%)	503 (17%)	12 (0%)
5	4	107/108 (99%)	29 (27%)	0
6	5	29/1520 (1%)	6 (20%)	0
7	6	1/76 (1%)	0	0
8	7	74/75 (98%)	20 (27%)	2 (2%)
9	8	75/76 (98%)	23 (30%)	0
All	All	3185/4771 (66%)	585 (18%)	15 (0%)

All (585) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	3	11	U
4	3	12	A
4	3	13	C
4	3	14	U
4	3	28	G
4	3	37	G
4	3	48	G
4	3	64	U
4	3	65	A
4	3	73	A
4	3	76	A
4	3	77	G
4	3	102	A

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Mol	Chain	Res	Type
4	3	103	G
4	3	119	A
4	3	121	U
4	3	126	C
4	3	132	G
4	3	141	A
4	3	142	A
4	3	163	A
4	3	180	A
4	3	184	A
4	3	187	C
4	3	200	A
4	3	203	A
4	3	219	G
4	3	220	A
4	3	225	A
4	3	226	A
4	3	232	A
4	3	234	G
4	3	237	A
4	3	245	U
4	3	246	G
4	3	252	G
4	3	269	A
4	3	276	A
4	3	284	U
4	3	287	G
4	3	295	U
4	3	296	U
4	3	297	G
4	3	298	U
4	3	299	A
4	3	309	A
4	3	310	U
4	3	311	G
4	3	315	A
4	3	316	C
4	3	317	U
4	3	319	G
4	3	325	G
4	3	336	C
4	3	345	A

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Mol	Chain	Res	Type
4	3	363	G
4	3	364	A
4	3	365	U
4	3	402	A
4	3	409	A
4	3	410	G
4	3	411	U
4	3	418	G
4	3	419	A
4	3	424	G
4	3	425	U
4	3	426	U
4	3	432	G
4	3	437	A
4	3	440	C
4	3	460	G
4	3	463	U
4	3	483	A
4	3	517	G
4	3	539	U
4	3	540	A
4	3	548	A
4	3	562	C
4	3	565	C
4	3	566	G
4	3	567	U
4	3	573	A
4	3	581	A
4	3	583	U
4	3	596	G
4	3	598	G
4	3	607	U
4	3	608	A
4	3	610	G
4	3	620	G
4	3	636	U
4	3	637	U
4	3	638	A
4	3	648	G
4	3	649	A
4	3	650	G
4	3	663	A

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Mol	Chain	Res	Type
4	3	670	G
4	3	673	A
4	3	681	A
4	3	682	A
4	3	689	U
4	3	691	G
4	3	705	A
4	3	712	A
4	3	716	G
4	3	721	G
4	3	722	C
4	3	765	A
4	3	775	C
4	3	782	U
4	3	792	G
4	3	797	U
4	3	800	C
4	3	810	G
4	3	811	G
4	3	817	A
4	3	819	U
4	3	820	U
4	3	824	A
4	3	828	A
4	3	829	A
4	3	840	G
4	3	846	U
4	3	847	C
4	3	854	A
4	3	862	U
4	3	881	A
4	3	882	C
4	3	883	A
4	3	901	C
4	3	902	U
4	3	904	C
4	3	906	G
4	3	918	G
4	3	924	C
4	3	926	U
4	3	927	A
4	3	928	G

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Mol	Chain	Res	Type
4	3	930	C
4	3	932	U
4	3	934	C
4	3	935	U
4	3	936	G
4	3	944	U
4	3	947	A
4	3	949	C
4	3	951	C
4	3	952	U
4	3	953	G
4	3	970	U
4	3	981	A
4	3	982	G
4	3	994	U
4	3	997	G
4	3	998	C
4	3	1008	A
4	3	1010	G
4	3	1016	A
4	3	1019	A
4	3	1026	A
4	3	1032	A
4	3	1039	G
4	3	1045	A
4	3	1049	U
4	3	1058	U
4	3	1060	G
4	3	1061	A
4	3	1068	U
4	3	1074	A
4	3	1080	A
4	3	1082	A
4	3	1084	C
4	3	1096	U
4	3	1097	G
4	3	1098	G
4	3	1099	C
4	3	1102	A
4	3	1104	A
4	3	1105	A
4	3	1106	G

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Mol	Chain	Res	Type
4	3	1107	C
4	3	1110	C
4	3	1111	C
4	3	1113	U
4	3	1114	C
4	3	1115	G
4	3	1120	A
4	3	1122	G
4	3	1123	A
4	3	1125	U
4	3	1130	A
4	3	1132	C
4	3	1138	A
4	3	1145	G
4	3	1146	A
4	3	1147	G
4	3	1165	U
4	3	1167	U
4	3	1168	A
4	3	1170	C
4	3	1176	U
4	3	1177	A
4	3	1178	A
4	3	1204	A
4	3	1208	A
4	3	1209	U
4	3	1210	A
4	3	1212	C
4	3	1215	G
4	3	1234	U
4	3	1235	U
4	3	1236	G
4	3	1242	G
4	3	1246	U
4	3	1250	A
4	3	1251	G
4	3	1253	G
4	3	1256	A
4	3	1257	G
4	3	1266	G
4	3	1268	U
4	3	1280	G

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Mol	Chain	Res	Type
4	3	1281	A
4	3	1283	A
4	3	1285	U
4	3	1286	G
4	3	1292	A
4	3	1301	G
4	3	1304	U
4	3	1313	G
4	3	1325	C
4	3	1328	A
4	3	1329	U
4	3	1330	U
4	3	1369	U
4	3	1378	C
4	3	1380	U
4	3	1388	G
4	3	1393	A
4	3	1406	A
4	3	1407	U
4	3	1412	A
4	3	1423	A
4	3	1424	U
4	3	1431	A
4	3	1444	C
4	3	1445	U
4	3	1446	G
4	3	1448	U
4	3	1456	C
4	3	1463	G
4	3	1467	U
4	3	1480	A
4	3	1481	U
4	3	1483	G
4	3	1486	U
4	3	1487	U
4	3	1502	A
4	3	1504	G
4	3	1508	G
4	3	1510	A
4	3	1513	A
4	3	1514	U
4	3	1515	A

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Mol	Chain	Res	Type
4	3	1519	A
4	3	1522	U
4	3	1534	A
4	3	1535	A
4	3	1541	A
4	3	1546	U
4	3	1550	G
4	3	1569	A
4	3	1570	A
4	3	1571	G
4	3	1580	G
4	3	1582	G
4	3	1584	U
4	3	1585	A
4	3	1588	A
4	3	1589	A
4	3	1603	A
4	3	1612	U
4	3	1617	U
4	3	1618	U
4	3	1619	A
4	3	1641	A
4	3	1642	G
4	3	1643	A
4	3	1644	A
4	3	1645	C
4	3	1650	A
4	3	1651	C
4	3	1661	A
4	3	1668	G
4	3	1680	A
4	3	1681	G
4	3	1682	C
4	3	1688	A
4	3	1694	A
4	3	1708	G
4	3	1727	U
4	3	1737	G
4	3	1748	U
4	3	1749	A
4	3	1764	U
4	3	1769	A

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Mol	Chain	Res	Type
4	3	1770	A
4	3	1771	C
4	3	1780	A
4	3	1789	C
4	3	1791	A
4	3	1807	C
4	3	1808	C
4	3	1809	A
4	3	1816	A
4	3	1823	U
4	3	1836	A
4	3	1854	A
4	3	1855	A
4	3	1866	G
4	3	1869	G
4	3	1878	A
4	3	1886	C
4	3	1910	G
4	3	1913	G
4	3	1920	A
4	3	1936	G
4	3	1937	G
4	3	1938	U
4	3	1943	A
4	3	1944	A
4	3	1962	U
4	3	1974	U
4	3	1977	A
4	3	1978	U
4	3	1979	G
4	3	1998	U
4	3	1999	G
4	3	2000	U
4	3	2004	G
4	3	2028	G
4	3	2030	A
4	3	2038	A
4	3	2040	A
4	3	2041	C
4	3	2042	A
4	3	2050	G
4	3	2057	C

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Mol	Chain	Res	Type
4	3	2062	C
4	3	2063	G
4	3	2067	A
4	3	2068	G
4	3	2069	A
4	3	2076	G
4	3	2084	A
4	3	2099	U
4	3	2100	G
4	3	2106	G
4	3	2110	U
4	3	2111	U
4	3	2112	A
4	3	2114	C
4	3	2115	A
4	3	2117	G
4	3	2123	A
4	3	2124	A
4	3	2125	U
4	3	2139	C
4	3	2140	G
4	3	2153	U
4	3	2154	A
4	3	2164	G
4	3	2166	U
4	3	2171	A
4	3	2180	U
4	3	2181	A
4	3	2193	U
4	3	2195	U
4	3	2196	G
4	3	2197	U
4	3	2198	G
4	3	2199	C
4	3	2200	U
4	3	2201	G
4	3	2202	U
4	3	2207	A
4	3	2211	G
4	3	2212	U
4	3	2219	U
4	3	2220	A

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Mol	Chain	Res	Type
4	3	2221	U
4	3	2227	U
4	3	2228	U
4	3	2233	A
4	3	2246	G
4	3	2247	G
4	3	2259	OMG
4	3	2274	A
4	3	2276	A
4	3	2287	G
4	3	2291	U
4	3	2295	A
4	3	2298	G
4	3	2305	C
4	3	2311	G
4	3	2313	U
4	3	2316	G
4	3	2319	A
4	3	2327	U
4	3	2329	G
4	3	2333	G
4	3	2335	A
4	3	2336	A
4	3	2342	U
4	3	2343	A
4	3	2344	A
4	3	2353	G
4	3	2355	C
4	3	2358	U
4	3	2366	A
4	3	2391	G
4	3	2393	C
4	3	2397	G
4	3	2410	C
4	3	2411	C
4	3	2414	U
4	3	2422	G
4	3	2431	U
4	3	2433	A
4	3	2437	G
4	3	2438	A
4	3	2443	A

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Mol	Chain	Res	Type
4	3	2449	U
4	3	2456	A
4	3	2477	A
4	3	2481	U
4	3	2482	U
4	3	2483	C
4	3	2484	A
4	3	2486	A
4	3	2488	C
4	3	2499	U
4	3	2510	G
4	3	2512	U
4	3	2513	G
4	3	2521	A
4	3	2526	A
4	3	2537	G
4	3	2543	G
4	3	2574	A
4	3	2575	G
4	3	2580	A
4	3	2585	A
4	3	2593	U
4	3	2594	C
4	3	2605	G
4	3	2610	A
4	3	2617	U
4	3	2618	C
4	3	2621	U
4	3	2623	U
4	3	2637	A
4	3	2638	G
4	3	2654	U
4	3	2668	A
4	3	2669	G
4	3	2697	C
4	3	2698	U
4	3	2722	G
4	3	2734	C
4	3	2737	G
4	3	2741	A
4	3	2752	G
4	3	2756	A

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Mol	Chain	Res	Type
4	3	2760	C
4	3	2764	U
4	3	2765	A
4	3	2773	A
4	3	2786	A
4	3	2798	A
4	3	2799	U
4	3	2804	C
4	3	2806	A
4	3	2807	G
4	3	2808	A
4	3	2810	A
4	3	2813	A
4	3	2822	C
4	3	2824	A
4	3	2829	G
4	3	2839	A
4	3	2853	U
4	3	2862	U
4	3	2863	G
4	3	2871	G
4	3	2876	G
4	3	2884	C
4	3	2887	A
4	3	2888	U
4	3	2895	A
4	3	2896	G
4	3	2899	C
5	4	9	C
5	4	10	C
5	4	11	A
5	4	13	G
5	4	14	U
5	4	22	G
5	4	23	A
5	4	28	C
5	4	33	U
5	4	35	C
5	4	39	U
5	4	41	C
5	4	48	A
5	4	49	G

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Mol	Chain	Res	Type
5	4	54	U
5	4	56	A
5	4	60	C
5	4	64	G
5	4	65	G
5	4	80	G
5	4	82	U
5	4	83	U
5	4	84	C
5	4	85	A
5	4	88	G
5	4	89	A
5	4	99	A
5	4	106	A
5	4	108	C
6	5	1466	U
6	5	1467	A
6	5	1469	G
6	5	1472	G
6	5	1478	A
6	5	1480	G
8	7	4	U
8	7	11	U
8	7	13	U
8	7	15	G
8	7	16	U
8	7	17	G
8	7	19	A
8	7	20	U
8	7	21	A
8	7	22	A
8	7	34	G
8	7	44	G
8	7	46	U
8	7	47	U
8	7	48	G
8	7	51	G
8	7	57	A
8	7	71	C
8	7	73	C
8	7	75	A
9	8	3	A

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Mol	Chain	Res	Type
9	8	9	A
9	8	10	G
9	8	15	G
9	8	16	U
9	8	17	U
9	8	18	G
9	8	19	G
9	8	20	U
9	8	21	A
9	8	30	G
9	8	31	A
9	8	41	A
9	8	46	G
9	8	47	U
9	8	48	C
9	8	58	A
9	8	60	C
9	8	71	G
9	8	73	A
9	8	74	C
9	8	75	C
9	8	76	A
11	Y	40	G
11	Y	42	U
11	Y	43	A
11	Y	46	G

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	3	315	A
4	3	410	G
4	3	881	A
4	3	901	C
4	3	1124	G
4	3	1209	U
4	3	1352	G
4	3	1583	G
4	3	1618	U
4	3	2180	U
4	3	2410	C
4	3	2764	U

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Mol	Chain	Res	Type
8	7	10	G
8	7	46	U
11	Y	42	U

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

5 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$
4	2MA	3	2511	42,4	17,25,26	2.62	5 (29%)	17,37,40	1.35	3 (17%)
4	OMG	3	2259	42,8,4	18,26,27	2.83	7 (38%)	19,38,41	1.57	4 (21%)
6	B8T	5	1377	6	19,22,23	3.28	8 (42%)	26,31,34	0.84	1 (3%)
4	1MG	3	783	4	18,26,27	2.73	6 (33%)	19,39,42	1.50	3 (15%)
6	5MC	5	1375	6	18,22,23	4.07	7 (38%)	26,32,35	1.04	2 (7%)

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
4	2MA	3	2511	42,4	-	2/3/25/26	0/3/3/3
4	OMG	3	2259	42,8,4	-	3/5/27/28	0/3/3/3
6	B8T	5	1377	6	-	2/7/27/28	0/2/2/2
4	1MG	3	783	4	-	0/3/25/26	0/3/3/3
6	5MC	5	1375	6	-	0/7/25/26	0/2/2/2

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	1375	5MC	C6-C5	9.99	1.51	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	3	2511	2MA	C2-N3	7.81	1.47	1.31
6	5	1375	5MC	C4-N3	7.53	1.46	1.34
6	5	1377	B8T	C4-N3	7.25	1.45	1.32
4	3	2259	OMG	C2-N2	7.16	1.51	1.34
6	5	1375	5MC	C2-N3	7.03	1.50	1.36
4	3	783	1MG	C2-N3	6.87	1.47	1.34
6	5	1377	B8T	C2-N3	6.41	1.49	1.36
4	3	783	1MG	C2-N2	6.38	1.45	1.34
6	5	1377	B8T	C6-C5	6.07	1.49	1.35
6	5	1375	5MC	C4-N4	5.69	1.48	1.34
6	5	1375	5MC	C6-N1	5.59	1.47	1.38
4	3	2259	OMG	C2-N3	5.15	1.45	1.33
4	3	2511	2MA	C4-N3	5.09	1.49	1.37
4	3	783	1MG	C4-N3	5.05	1.49	1.37
6	5	1377	B8T	C4-N4	4.73	1.45	1.35
6	5	1375	5MC	C2-N1	4.66	1.50	1.40
4	3	2259	OMG	C4-N3	4.54	1.48	1.37
6	5	1377	B8T	C2-N1	4.34	1.49	1.40
6	5	1377	B8T	C5-C4	3.90	1.49	1.40
4	3	2259	OMG	C2-N1	3.27	1.45	1.37
4	3	2511	2MA	C6-N1	3.16	1.44	1.38
6	5	1377	B8T	C6-N1	3.14	1.45	1.38
4	3	2259	OMG	C6-N1	3.10	1.42	1.37
4	3	2259	OMG	C5-C6	2.89	1.53	1.47
4	3	2511	2MA	C2-N1	2.76	1.45	1.36
6	5	1377	B8T	O2-C2	-2.62	1.18	1.23
4	3	2259	OMG	C5-C4	-2.48	1.36	1.43
4	3	783	1MG	C5-C4	-2.37	1.37	1.43
4	3	783	1MG	C6-N1	2.33	1.43	1.39
4	3	2511	2MA	C5-C4	-2.28	1.37	1.43
4	3	783	1MG	C5-C6	2.27	1.54	1.47
6	5	1375	5MC	O2-C2	-2.22	1.19	1.23

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	783	1MG	C5-C6-N1	4.12	120.09	113.90
4	3	2259	OMG	C5-C6-N1	3.44	120.03	113.95
4	3	2511	2MA	C5-C6-N1	3.39	119.88	114.02
6	5	1375	5MC	C5-C6-N1	-3.16	120.09	123.34
4	3	2259	OMG	C2-N1-C6	-2.89	119.77	125.10
4	3	2259	OMG	C8-N7-C5	2.84	108.40	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	3	783	1MG	C8-N7-C5	2.73	108.19	102.99
4	3	2511	2MA	C8-N7-C5	2.73	108.19	102.99
6	5	1377	B8T	C6-C5-C4	2.52	120.04	116.96
4	3	783	1MG	O6-C6-C5	-2.32	120.08	124.19
4	3	2511	2MA	CM2-C2-N1	2.23	121.19	116.23
6	5	1375	5MC	CM5-C5-C6	-2.22	119.88	122.85
4	3	2259	OMG	O6-C6-C5	-2.20	120.08	124.37

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	3	2259	OMG	O4'-C4'-C5'-O5'
4	3	2259	OMG	C3'-C4'-C5'-O5'
4	3	2259	OMG	C1'-C2'-O2'-CM2
6	5	1377	B8T	O4'-C4'-C5'-O5'
4	3	2511	2MA	O4'-C4'-C5'-O5'
6	5	1377	B8T	C3'-C4'-C5'-O5'
4	3	2511	2MA	C4'-C5'-O5'-P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	3	2511	2MA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 266 ligands modelled in this entry, 234 are monoatomic - leaving 32 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
45	SPD	3	3239	-	9,9,9	0.32	0	8,8,8	0.88	0
45	SPD	3	3248	-	9,9,9	0.31	0	8,8,8	0.88	0
40	CLM	3	3001	-	19,20,20	0.55	1 (5%)	23,27,27	0.61	0
45	SPD	3	3234	-	9,9,9	0.32	0	8,8,8	0.78	0
46	N2P	3	3244	-	6,6,6	0.25	0	5,5,5	0.63	0
43	PUT	3	3231	-	5,5,5	0.25	0	4,4,4	0.51	0
45	SPD	3	3235	-	9,9,9	0.33	0	8,8,8	0.87	0
43	PUT	3	3223	-	5,5,5	0.23	0	4,4,4	0.56	0
45	SPD	3	3230	-	9,9,9	0.33	0	8,8,8	0.80	0
45	SPD	3	3236	-	9,9,9	0.33	0	8,8,8	0.82	0
45	SPD	3	3229	-	9,9,9	0.32	0	8,8,8	0.87	0
46	N2P	3	3243	-	6,6,6	0.25	0	5,5,5	0.65	0
45	SPD	3	3245	-	9,9,9	0.32	0	8,8,8	0.89	0
44	SPM	3	3249	-	13,13,13	0.35	0	12,12,12	0.87	0
45	SPD	3	3240	-	9,9,9	0.32	0	8,8,8	0.86	0
44	SPM	3	3227	-	13,13,13	0.35	0	12,12,12	0.90	0
45	SPD	3	3238	-	9,9,9	0.32	0	8,8,8	0.85	0
45	SPD	3	3237	-	9,9,9	0.32	0	8,8,8	0.96	0
43	PUT	3	3226	-	5,5,5	0.26	0	4,4,4	0.52	0
45	SPD	3	3232	-	9,9,9	0.35	0	8,8,8	0.75	0
47	LYS	8	103	9	7,8,9	1.79	1 (14%)	3,8,10	0.37	0
45	SPD	3	3246	-	9,9,9	0.33	0	8,8,8	0.82	0
43	PUT	3	3222	-	5,5,5	0.24	0	4,4,4	0.55	0
43	PUT	3	3225	-	5,5,5	0.25	0	4,4,4	0.52	0
45	SPD	3	3228	-	9,9,9	0.32	0	8,8,8	0.87	0
46	N2P	3	3247	-	6,6,6	0.24	0	5,5,5	0.67	0
44	SPM	3	3241	-	13,13,13	0.34	0	12,12,12	0.93	0
45	SPD	3	3233	-	9,9,9	0.32	0	8,8,8	0.89	0
45	SPD	3	3250	-	9,9,9	0.17	0	8,8,8	0.19	0
44	SPM	b	303	-	13,13,13	0.16	0	12,12,12	0.32	0
43	PUT	3	3242	-	5,5,5	0.25	0	4,4,4	0.54	0
43	PUT	3	3224	-	5,5,5	0.25	0	4,4,4	0.54	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
45	SPD	3	3239	-	-	2/7/7/7	-
45	SPD	3	3248	-	-	0/7/7/7	-
40	CLM	3	3001	-	-	2/20/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SPD	3	3234	-	-	1/7/7/7	-
46	N2P	3	3244	-	-	2/4/4/4	-
43	PUT	3	3231	-	-	0/3/3/3	-
45	SPD	3	3235	-	-	0/7/7/7	-
43	PUT	3	3223	-	-	0/3/3/3	-
45	SPD	3	3230	-	-	0/7/7/7	-
45	SPD	3	3236	-	-	0/7/7/7	-
45	SPD	3	3229	-	-	1/7/7/7	-
46	N2P	3	3243	-	-	1/4/4/4	-
45	SPD	3	3245	-	-	0/7/7/7	-
44	SPM	3	3249	-	-	1/11/11/11	-
45	SPD	3	3240	-	-	0/7/7/7	-
44	SPM	3	3227	-	-	4/11/11/11	-
45	SPD	3	3238	-	-	0/7/7/7	-
45	SPD	3	3237	-	-	1/7/7/7	-
43	PUT	3	3226	-	-	0/3/3/3	-
45	SPD	3	3232	-	-	2/7/7/7	-
47	LYS	8	103	9	-	3/6/7/9	-
45	SPD	3	3246	-	-	1/7/7/7	-
43	PUT	3	3222	-	-	0/3/3/3	-
43	PUT	3	3225	-	-	1/3/3/3	-
45	SPD	3	3228	-	-	0/7/7/7	-
46	N2P	3	3247	-	-	1/4/4/4	-
44	SPM	3	3241	-	-	2/11/11/11	-
45	SPD	3	3233	-	-	0/7/7/7	-
45	SPD	3	3250	-	-	0/7/7/7	-
44	SPM	b	303	-	-	2/11/11/11	-
43	PUT	3	3242	-	-	0/3/3/3	-
43	PUT	3	3224	-	-	0/3/3/3	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	8	103	LYS	CB-CA	4.20	1.59	1.53
40	3	3001	CLM	C1-C2	-2.11	1.50	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	8	103	LYS	O-C-CA-CB
47	8	103	LYS	C-CA-CB-CG
46	3	3243	N2P	C2-C3-C4-C5
44	3	3227	SPM	C7-C8-C9-N10
40	3	3001	CLM	C5-C3-N2-C2
45	3	3229	SPD	N6-C7-C8-C9
44	3	3241	SPM	C7-C6-N5-C4
46	3	3247	N2P	C2-C3-C4-C5
46	3	3244	N2P	C2-C3-C4-C5
44	3	3249	SPM	C6-C7-C8-C9
45	3	3234	SPD	C8-C7-N6-C5
44	3	3227	SPM	C7-C6-N5-C4
45	3	3232	SPD	N1-C2-C3-C4
43	3	3225	PUT	C1-C2-C3-C4
45	3	3239	SPD	C8-C7-N6-C5
45	3	3237	SPD	C8-C7-N6-C5
44	3	3227	SPM	N10-C11-C12-C13
44	3	3241	SPM	N10-C11-C12-C13
40	3	3001	CLM	C4-C3-N2-C2
44	b	303	SPM	C3-C4-N5-C6
46	3	3244	N2P	C3-C4-C5-N1
45	3	3239	SPD	C2-C3-C4-C5
44	b	303	SPM	C7-C6-N5-C4
44	3	3227	SPM	C6-C7-C8-C9
47	8	103	LYS	N-CA-CB-CG
45	3	3246	SPD	C3-C4-C5-N6
45	3	3232	SPD	C2-C3-C4-C5

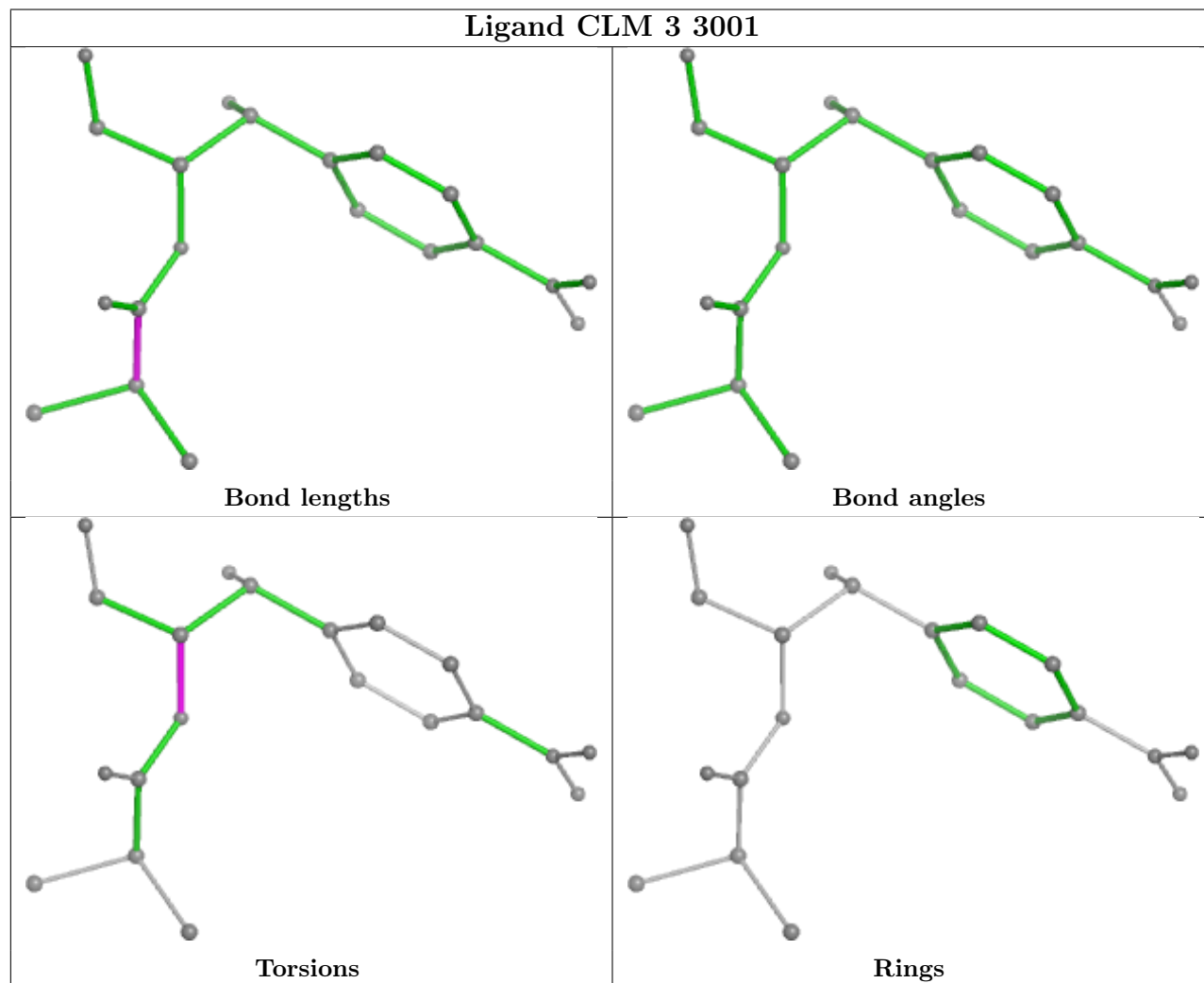
There are no ring outliers.

8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	3	3248	SPD	1	0
40	3	3001	CLM	4	0
43	3	3231	PUT	1	0
44	3	3249	SPM	2	0
44	3	3227	SPM	4	0
45	3	3237	SPD	1	0
44	3	3241	SPM	1	0
45	3	3250	SPD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.