



wwPDB EM Validation Summary Report ⓘ

Jun 27, 2026 – 02:50 PM EDT

PDB ID : 9P9K / pdb_00009p9k
EMDB ID : EMD-71414
Title : In situ human 60S ribosome with EIF6
Authors : Wei, Z.; Yong, X.
Deposited on : 2025-06-24
Resolution : 2.96 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

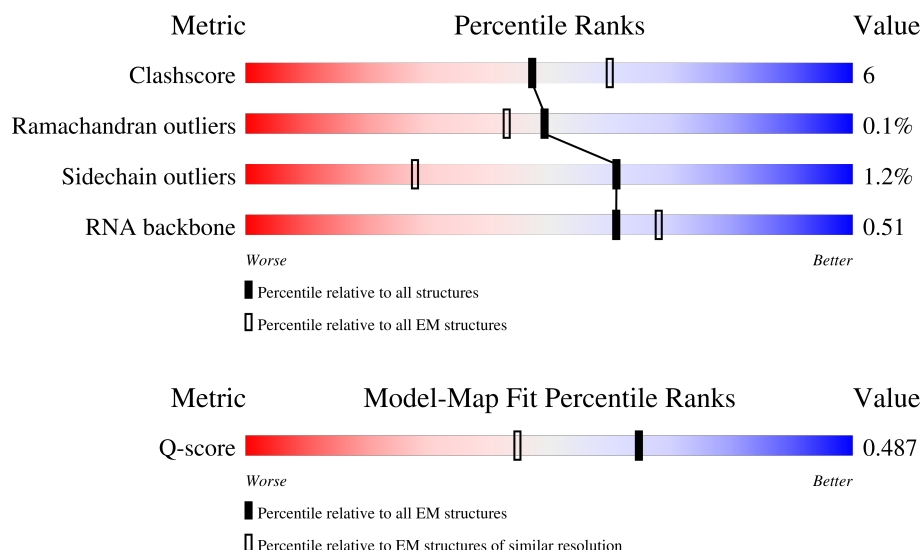
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.96 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.



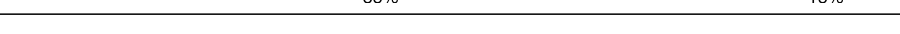
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13155 (2.46 - 3.46)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L5	3675	
2	L7	120	
3	L8	156	

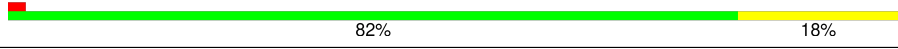
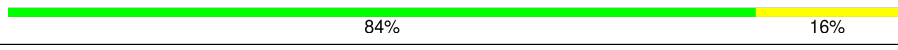
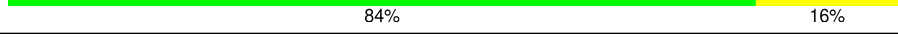
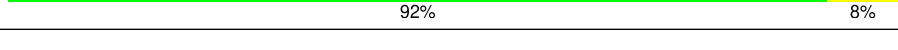
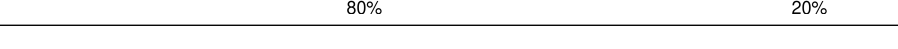
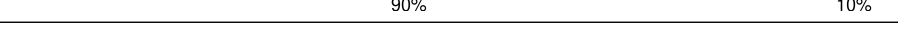
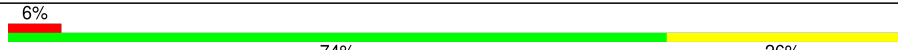
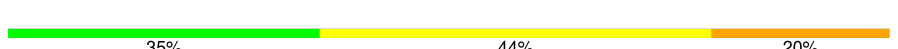
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Mol	Chain	Length	Quality of chain
4	LA	248	 81%19%
5	LB	402	 78%22%
6	LC	368	 88%12%
7	LD	293	 86%14%
8	LE	250	 82%14%
9	LF	225	 88%12%
10	LG	241	 90%10%
11	LH	190	 85%15%
12	LI	213	 83%17%
13	LJ	176	 87%10%
14	LL	210	 88%12%
15	LM	139	 82%18%
16	LN	203	 88%12%
17	LO	201	 82%18%
18	LP	153	 85%15%
19	LQ	187	 87%13%
20	LR	187	 71%11%19%
21	LS	175	 89%11%
22	LT	159	 84%16%
23	LU	101	 83%17%
24	LV	131	 86%14%
25	LX	120	 84%16%
26	LY	134	 85%15%
27	LZ	135	 82%18%
28	La	147	 91%9%

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Mol	Chain	Length	Quality of chain
29	Lb	121	
30	Lc	98	
31	Ld	107	
32	Le	128	
33	Lf	109	
34	Lg	114	
35	Lh	122	
36	Li	102	
37	Lj	86	
38	Lk	69	
39	Ll	50	
40	Lm	52	
41	Lo	105	
42	Lp	91	
43	Lr	125	
44	CA	356	
45	P	225	

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 141030 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	L5	3655	Total	C	N	O	P	1	0
			78444	34968	14346	25475	3655		

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 3 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L8	156	Total	C	N	O	P	0	0
			3315	1481	585	1094	155		

- Molecule 4 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	LA	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 5 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	LB	402	Total	C	N	O	S	0	0
			3238	2060	608	556	14		

- Molecule 6 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	LC	368	Total	C	N	O	S	0	0
			2927	1840	583	489	15		

- Molecule 7 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	LD	293	Total	C	N	O	S	0	0
			2382	1507	434	427	14		

- Molecule 8 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	240	Total	C	N	O	S	0	0
			1935	1242	368	321	4		

- Molecule 9 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	LF	225	Total	C	N	O	S	0	0
			1870	1202	358	301	9		

- Molecule 10 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	LG	241	Total	C	N	O	S	0	0
			1927	1228	371	324	4		

- Molecule 11 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	LH	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 12 is a protein called Ribosomal protein uL16-like.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	213	Total	C	N	O	S	0	0
			1711	1082	329	285	15		

- Molecule 13 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	170	Total	C	N	O	S	0	0
			1362	861	254	241	6		

- Molecule 14 is a protein called Large ribosomal subunit protein eL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 15 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LM	139	Total	C	N	O	S	0	0
			1138	730	218	183	7		

- Molecule 16 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LN	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 17 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LO	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 18 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LP	153	Total	C	N	O	S	0	0
			1242	776	241	216	9		

- Molecule 19 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LQ	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 20 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LR	152	Total	C	N	O	S	0	0
			1273	793	275	196	9		

- Molecule 21 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	175	Total	C	N	O	S	0	0
			1453	925	283	235	10		

- Molecule 22 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	159	Total	C	N	O	S	0	0
			1298	823	252	217	6		

- Molecule 23 is a protein called Heparin-binding protein HBp15.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LU	101	Total	C	N	O	S	0	0
			825	529	144	150	2		

- Molecule 24 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LV	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 25 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LX	120	Total	C	N	O	S	0	0
			985	630	185	169	1		

- Molecule 26 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LY	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 27 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LZ	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 28 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	La	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 29 is a protein called Large ribosomal subunit protein eL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lb	109	Total	C	N	O	S	0	0
			876	546	189	137	4		

- Molecule 30 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lc	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 31 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ld	107	Total	C	N	O	S	0	0
			888	560	171	155	2		

- Molecule 32 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 33 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Lf	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 34 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lg	114	Total	C	N	O	S	0	0
			906	566	187	147	6		

- Molecule 35 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lh	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 36 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Li	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 37 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lj	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 38 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Lk	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 39 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Ll	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 40 is a protein called Large ribosomal subunit protein eL40.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lm	52	Total	C	N	O	S	0	0
			429	266	90	67	6		

- Molecule 41 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lo	105	Total	C	N	O	S	0	0
			862	542	175	139	6		

- Molecule 42 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lp	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 43 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lr	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 44 is a protein called Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	CA	354	Total	C	N	O	S	4	0
			2764	1744	475	528	17		

- Molecule 45 is a protein called Eukaryotic translation initiation factor 6.

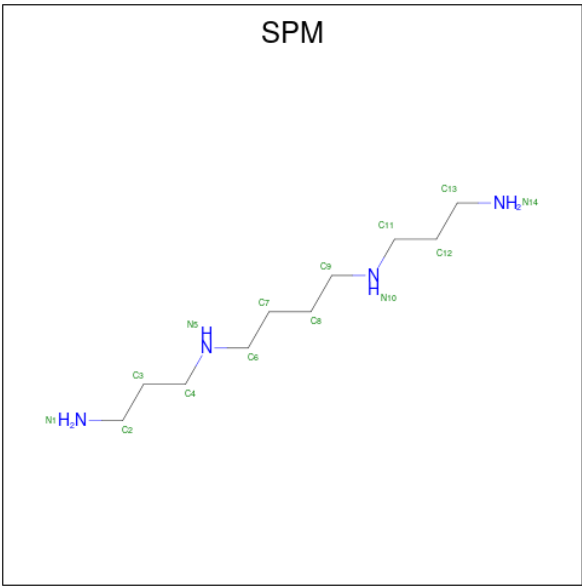
Mol	Chain	Residues	Atoms					AltConf	Trace
45	P	225	Total	C	N	O	S	0	0
			1712	1065	295	340	12		

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
46	L5	178	Total	Mg	0
			178	178	
46	L7	3	Total	Mg	0
			3	3	
46	L8	5	Total	Mg	0
			5	5	
46	LA	1	Total	Mg	0
			1	1	
46	LI	1	Total	Mg	0
			1	1	
46	LP	1	Total	Mg	0
			1	1	
46	LV	1	Total	Mg	0
			1	1	
46	Le	1	Total	Mg	0
			1	1	

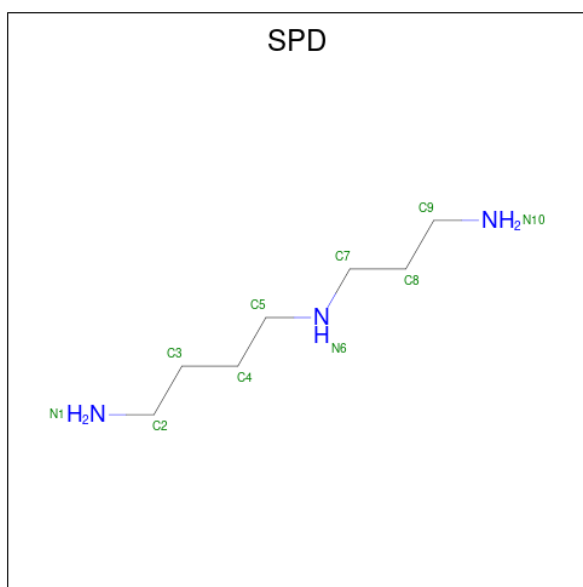
- Molecule 47 is SPERMINE (CCD ID: SPM) (formula: C₁₀H₂₆N₄) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
47	L5	1	Total	C	N	0
			14	10	4	
47	L5	1	Total	C	N	0
			14	10	4	
47	L5	1	Total	C	N	0
			14	10	4	
47	L5	1	Total	C	N	0
			14	10	4	
47	L5	1	Total	C	N	0
			14	10	4	
47	L5	1	Total	C	N	0
			14	10	4	

- Molecule 48 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
48	L5	1	Total	C	N	0
			10	7	3	
48	L5	1	Total	C	N	0
			10	7	3	
48	L5	1	Total	C	N	0
			10	7	3	
48	L5	1	Total	C	N	0
			10	7	3	
48	L5	1	Total	C	N	0
			10	7	3	
48	L5	1	Total	C	N	0
			10	7	3	
48	L5	1	Total	C	N	0
			10	7	3	
48	LN	1	Total	C	N	0
			10	7	3	

- Molecule 49 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
49	Lg	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
49	Lj	1	Total 1	Zn 1	0
49	Lm	1	Total 1	Zn 1	0
49	Lo	1	Total 1	Zn 1	0
49	Lp	1	Total 1	Zn 1	0

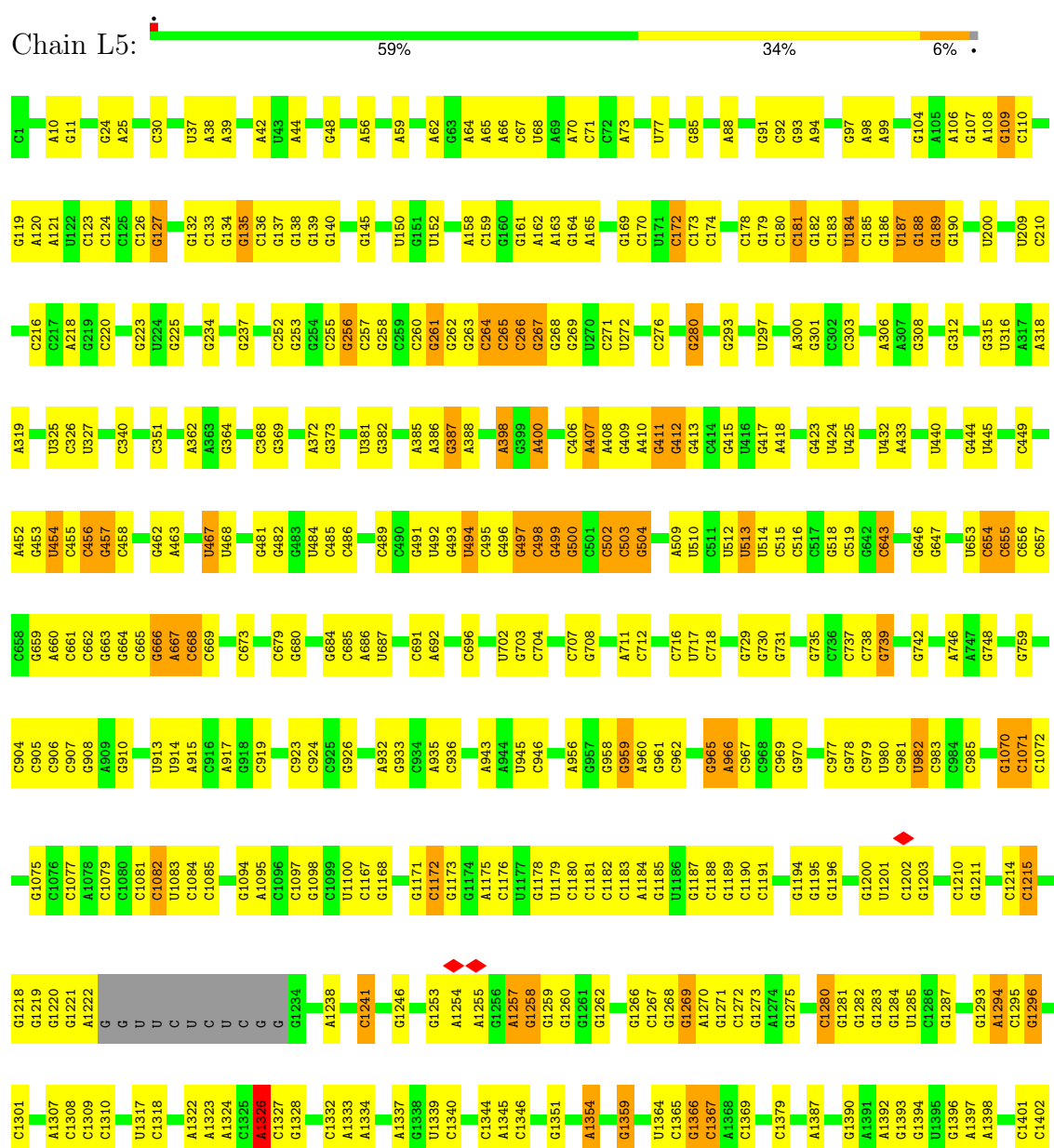
- Molecule 50 is water.

Mol	Chain	Residues	Atoms		AltConf
50	P	1	Total 1	O 1	0

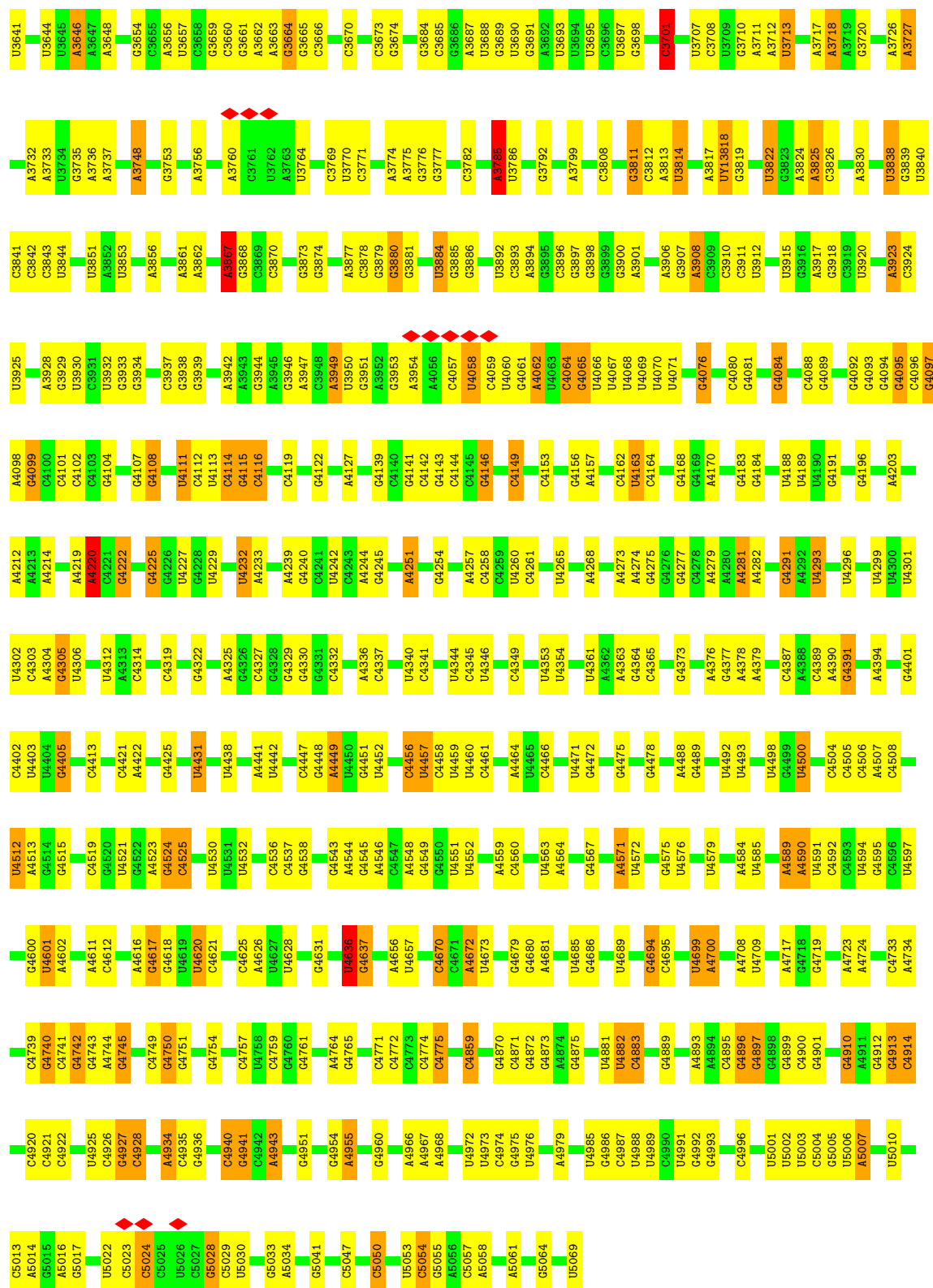
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

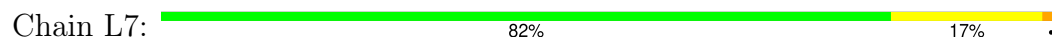
• Molecule 1: 28S rRNA



G2877	C2770	C2684	G2581	C2489	G2397	G2303	G2203	G1935	U1834	G1734	A1642	U1514	G1403
C2892	G2773	U2687	A2582	U2490	U2398	C2271	G2024	C1936	G1835	U1735	C1645	A1515	G1404
G2896	A2783	G2688	C2583	C2491	G2399	G2275	A2026	A1942	A1837	G1739	C1646	G1516	C1406
C2899	A2787	G2694	A2587	U2494	A2401	A2276	A2029	A1943	G1842	A1742	U1647	C1407	G1408
U2900	U2788	A2695	C2588	U2495	A2404	A2279	A2030	G1948	G1846	A1743	G1654	A1523	C1409
G2901	A2789	A2696	C2589	C2496	G2407	U2281	A2033	G1951	C1847	U1744	C1661	A1524	U1410
G2902	U2790	A2697	A2590	C2497	U2408	G2280	G2045	G1961	C1848	G1750	C1662	C1412	C1411
G2903	C2702	C2498	C2591	C2499	U2409	G2284	G2046	A1962	G1855	A1751	C1663	C1413	C1414
U2904	G2706	G2502	G2602	G2502	C2410	C2289	G2047	G1972	C1856	G1752	A1669	C1415	C1416
C2905	U2707	C2607	C2503	G2503	A2411	C2295	U2048	G1973	C1857	U1754	C1676	G1417	G1418
G2906	C2804	U2708	G2605	G2504	A2412	C2298	G2049	U1974	A1858	C1755	U1677	G1545	A1420
G2907	A2806	G2709	G2610	C2505	U2413	C2299	G2052	U1975	C1859	U1756	C1678	C1546	A1425
U2908	A2807	C2710	A2611	G2506	G2414	U2298	G2055	G1976	U1860	U1757	C1679	A1547	G1431
G2909	G2808	G2711	G2612	A2507	U2415	G2299	G2056	U1977	U1861	G1758	G1680	G1548	G1432
G2910	G2811	G2714	C2613	A2507	U2416	A2300	G2057	C1977	U1862	C1759	U1683		C1437
C3584	G2812	G2715	G2618	A2513	A2417	C2301	A2057	A1978	U1866	G1760	C1684		U1438
G3585	A2813	U2718	U2626	G2516	C2422	C2302	A2069	A1979	A1867	C1761	G1685		C1439
C3588	C2814	G2719	C2627	A2517	U2425	C2303	G2076	U1980	A1868	C1762	U1695		C1442
G3591	G2720	G2721	U2630	G2518	A2438	G2306	C2083	G1981	C1869	C1763	U1696		A1443
C3592	G2722	G2723	U2631	C2520	G2439	A2313	C2084	U1982	A1871	A1765	C1697		G1444
C3593	A2725	G2724	U2632	A2537	U2440	G2318	G2092	U1983	C1870	C1766	U1699		U1445
C3594	C2825	U2725	U2633	U2538	G2450	G2319	A2083	U1984	C1871	G1768	C1700		C1446
U3595	U2826	G2726	C2634	G2539	G2451	G2321	G2094	U1985	C1872	A1770	C1701		C1447
C3596	G2827	U2727	U2635	C2540	A2453	C2324	A2095	U1986	C1873	C1702	C1703		C1461
G3597	U2828	U2730	U2636	G2541	G2454	C2325	G2096	U1987	C1874	C1704	G1705		C1468
C3598	U2829	C2731	U2637	A2543	C2458	C2326	G2097	U1988	C1875	C1705	A1706		C1480
A3599	A2832	G2739	U2638	G2544	G2461	G2328	A2098	U1989	C1876	C1706	C		C1481
G3600	C2835	A2742	U2639	U2545	C2462	U2329	G2099	U1990	C1877	C1707	C		G1482
A3604	A2836	G2743	C2641	G2546	G2463	U2330	C2101	C1993	U1878	C1708	A1706		C1483
C3605	C2837	A2744	C2642	G2547	C2464	A2332	G2102	C1994	C1879	C1709	C		U1494
U3607	G2838	U2745	C2643	G2548	C2465	C2333	G2103	G1995	A1896	A1786	C		G1496
C3609	U2839	A2746	U2644	U2549	U2466	C2334	G2104	C1996	A1897	A1787	G		G1497
A3610	A2844	C2749	U2645	U2554	U2467	C2335	A2105	U1997	C1898	A1788	A		C1498
G3611	G2845	G2750	G2646	G2555	C2468	C2336	G2106	A1998	C1899	C1789	C		A1500
U3616	C2846	G2751	U2647	G2556	C2469	A2347	G2107	U1999	G1910	U1792	C		C1502
G3619	G2847	A2755	C2648	G2557	G2470	G2346	C2110	G2000	C1911	A1802	C		A1503
A3624	C2848	G2756	G2649	G2558	G2471	A2349	G2111	G2001	G1912	G1803	C		G1504
G3625	G2855	A2757	U2650	G2559	G2472	U2350	G2112	A2002	A1917	A1804	C		C1509
C3626	C2861	G2758	C2651	G2560	C2473	C2351	C2249	G2003	U1918	G1716	C		U1511
A3630	G2862	G2759	C2652	A2565	G2474	A2360	G2250	U2004	G1919	C1717	C		
U3633	A2863	G2760	C2653	G2566	G2475	G2361	G2251	G2007	C1920	G1805	C		
C3635	C2864	U2761	G2654	G2567	C2476	U2362	G2252	U2008	C1921	G1806	C		
A3636	U2865	G2762	C2655	G2568	G2477	A2363	G2253	A2009	G1922	A1719	C		
C3637	G2866	C2763	U2656	G2569	C2478	G2364	C2254	A2010	G1923	C1720	C		
U3638	C2867	A2764	G2657	U2570	C2479	G2365	C2255	C2011	G1924	G1810	C		
G3639	A2871	U2765	C2658	G2571	A2484	A2382	G2256	A2012	G1925	G1818	C		
U3640		U2766	U2659	A2573	U2485	C2383	G2261	A2017	G1926	G1819	C		
		U2767	G2660	G2574	U2486	G2384	G2262	C2018	C1931	C1820	C		
		U2768	G2661	G2575	G2487	A2395	G2263	C2019	A1932	G1821	C		
		U2769	C2662	G2576	C2488	A2396	U2267	C2020	A1934	G1822	C		
								G2021		G1824	C		
								C2022					

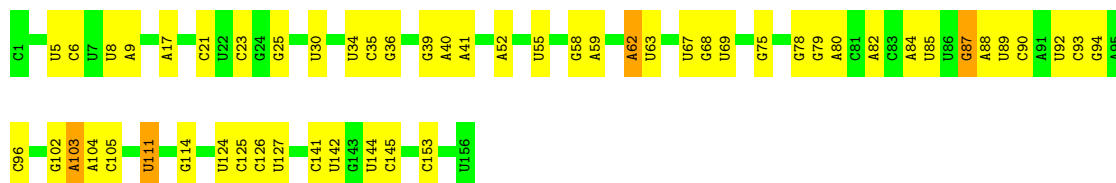


• Molecule 2: 5S rRNA

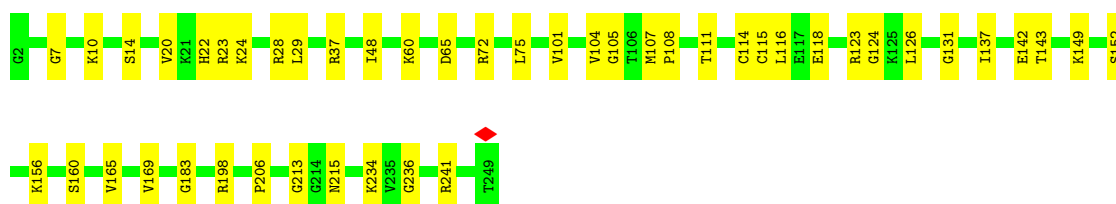
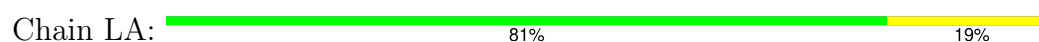




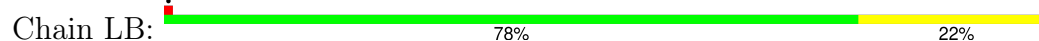
- Molecule 3: 5.8S rRNA



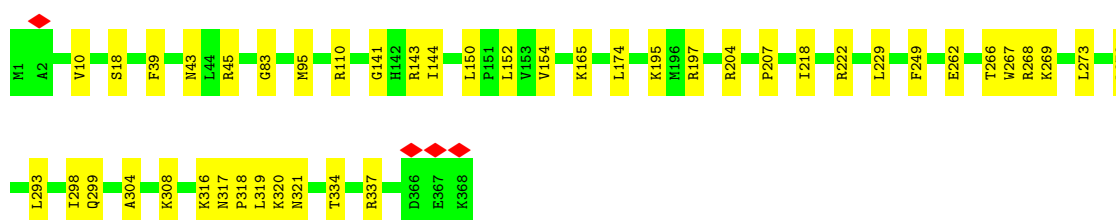
- Molecule 4: 60S ribosomal protein L8



- Molecule 5: Large ribosomal subunit protein uL3

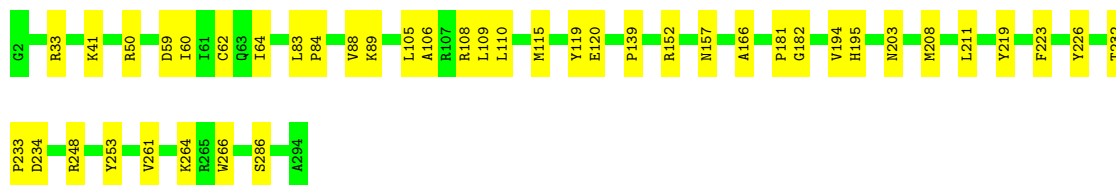


- Molecule 6: 60S ribosomal protein L4



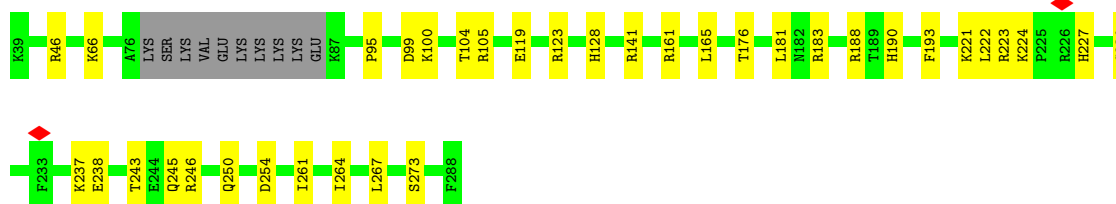
- Molecule 7: Large ribosomal subunit protein uL18

Chain LD:  86% 14%



- Molecule 8: Large ribosomal subunit protein eL6

Chain LE:  82% 14%



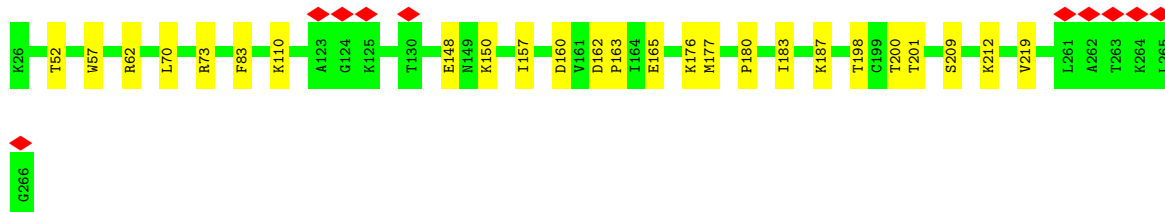
- Molecule 9: 60S ribosomal protein L7

Chain LF:  88% 12%



- Molecule 10: 60S ribosomal protein L7a

Chain LG:  90% 10%



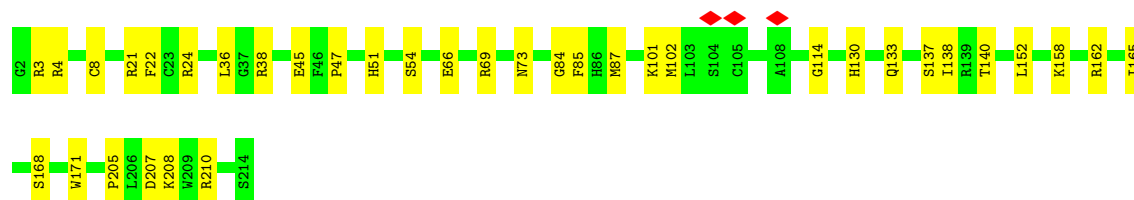
- Molecule 11: 60S ribosomal protein L9

Chain LH:  85% 15%



- Molecule 12: Ribosomal protein uL16-like

Chain LI:  83% 17%



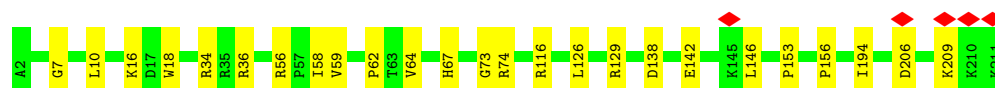
- Molecule 13: 60S ribosomal protein L11

Chain LJ: 87% 10%



- Molecule 14: Large ribosomal subunit protein eL13

Chain LL: 88% 12%



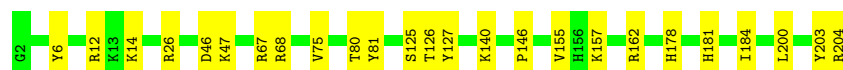
- Molecule 15: 60S ribosomal protein L14

Chain LM: 82% 18%



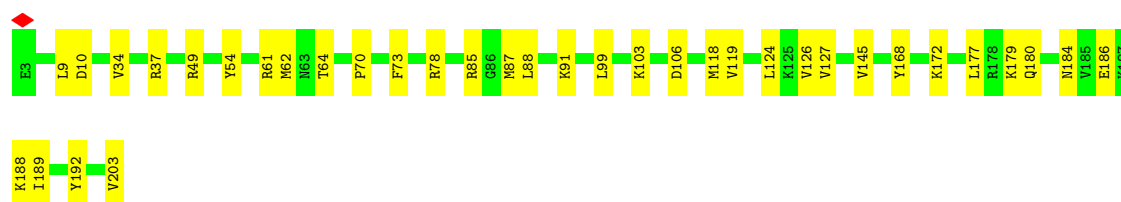
- Molecule 16: 60S ribosomal protein L15

Chain LN: 88% 12%



- Molecule 17: 60S ribosomal protein L13a

Chain LO: 82% 18%

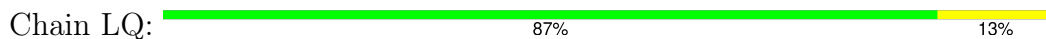


- Molecule 18: 60S ribosomal protein L17

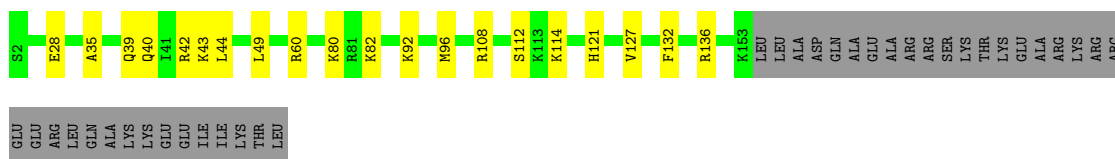
Chain LP: 85% 15%



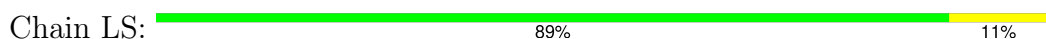
- Molecule 19: 60S ribosomal protein L18



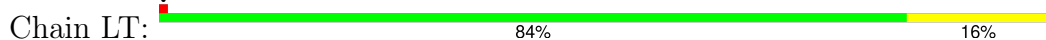
- Molecule 20: 60S ribosomal protein L19



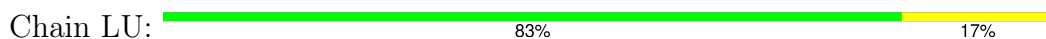
- Molecule 21: 60S ribosomal protein L18a



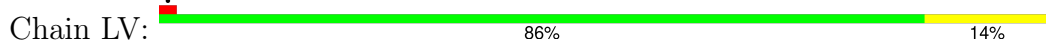
- Molecule 22: 60S ribosomal protein L21



- Molecule 23: Heparin-binding protein HBp15



- Molecule 24: 60S ribosomal protein L23



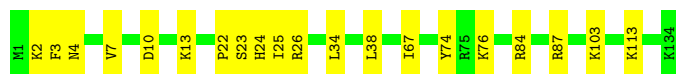
- Molecule 25: 60S ribosomal protein L23a

Chain LX:  84% 16%



- Molecule 26: 60S ribosomal protein L26

Chain LY:  85% 15%



- Molecule 27: 60S ribosomal protein L27

Chain LZ:  82% 18%



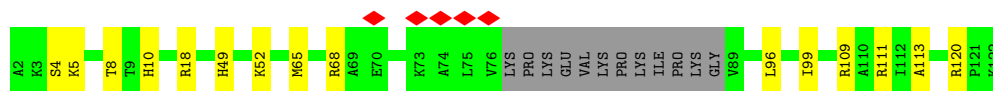
- Molecule 28: 60S ribosomal protein L27a

Chain La:  91% 9%



- Molecule 29: Large ribosomal subunit protein eL29

Chain Lb:  78% 12% 10%



- Molecule 30: 60S ribosomal protein L30

Chain Lc:  87% 13%



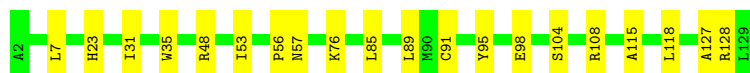
- Molecule 31: 60S ribosomal protein L31

Chain Ld:  82% 18%



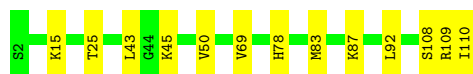
- Molecule 32: 60S ribosomal protein L32

Chain Le:  84% 16%



- Molecule 33: 60S ribosomal protein L35a

Chain Lf:  88% 12%



- Molecule 34: 60S ribosomal protein L34

Chain Lg:  89% 11%



- Molecule 35: 60S ribosomal protein L35

Chain Lh:  84% 16%



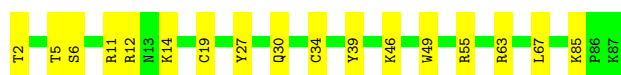
- Molecule 36: 60S ribosomal protein L36

Chain Li:  92% 8%



- Molecule 37: 60S ribosomal protein L37

Chain Lj:  80% 20%



- Molecule 38: 60S ribosomal protein L38

Chain Lk:  90% 10%



- Molecule 39: 60S ribosomal protein L39

Chain Ll:  78% 22%



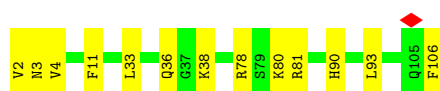
- Molecule 40: Large ribosomal subunit protein eL40

Chain Lm:  88% 12%



- Molecule 41: 60S ribosomal protein L36a

Chain Lo:  88% 12%



- Molecule 42: 60S ribosomal protein L37a

Chain Lp:  90% 10%



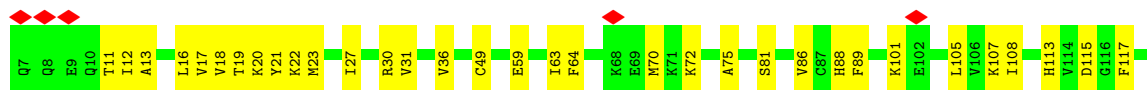
- Molecule 43: 60S ribosomal protein L28

Chain Lr:  90% 10%



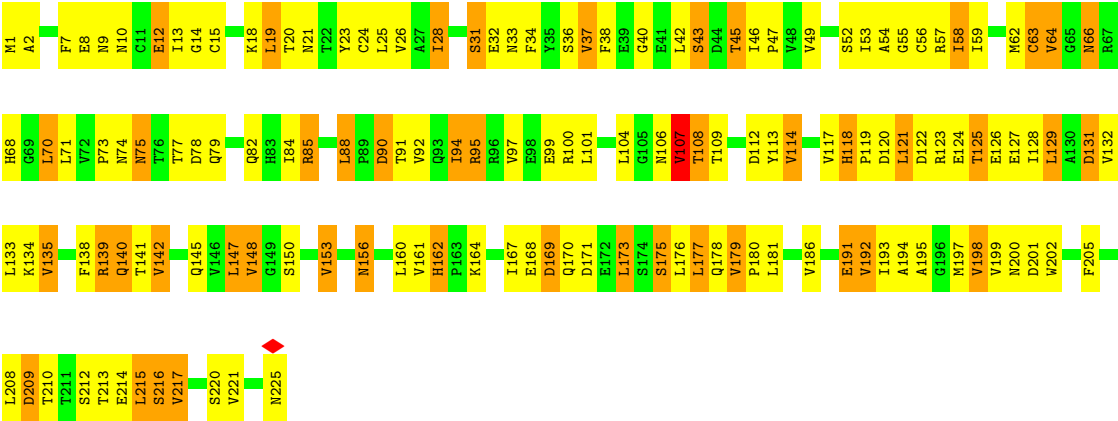
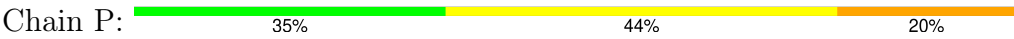
- Molecule 44: Proliferation-associated protein 2G4

Chain CA:  6% 74% 26%





• Molecule 45: Eukaryotic translation initiation factor 6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	132487	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.419	Depositor
Minimum map value	-0.145	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.0354	Depositor
Map size (Å)	546.816, 546.816, 546.816	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.068, 1.068, 1.068	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SPM, 1MA, SPD, UR3, PSU, ZN, OMC, MG, OMU, A2M, UY1, 5MC, OMG, 6MZ

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	L5	0.32	0/85098	0.31	0/132762
2	L7	0.30	0/2861	0.27	0/4459
3	L8	0.32	0/3631	0.29	0/5657
4	LA	0.32	0/1936	0.44	0/2596
5	LB	0.29	0/3306	0.38	0/4424
6	LC	0.30	0/2981	0.41	0/4002
7	LD	0.25	0/2428	0.34	0/3252
8	LE	0.24	0/1973	0.42	0/2645
9	LF	0.29	0/1905	0.30	0/2539
10	LG	0.25	0/1960	0.38	0/2637
11	LH	0.26	0/1537	0.35	0/2066
12	LI	0.25	0/1751	0.33	0/2340
13	LJ	0.20	0/1385	0.34	0/1852
14	LL	0.27	0/1732	0.33	0/2315
15	LM	0.28	0/1161	0.36	0/1554
16	LN	0.31	0/1746	0.35	0/2338
17	LO	0.30	0/1682	0.37	0/2250
18	LP	0.30	0/1268	0.40	0/1701
19	LQ	0.31	0/1537	0.37	0/2052
20	LR	0.26	0/1289	0.31	0/1705
21	LS	0.30	0/1493	0.35	0/2003
22	LT	0.27	0/1326	0.32	0/1770
23	LU	0.22	0/839	0.46	0/1126
24	LV	0.26	0/993	0.38	0/1332
25	LX	0.25	0/1002	0.31	0/1345
26	LY	0.28	0/1132	0.37	0/1504
27	LZ	0.25	0/1130	0.35	0/1507
28	La	0.29	0/1191	0.32	0/1591
29	Lb	0.23	0/889	0.38	0/1175
30	Lc	0.26	0/774	0.35	0/1038
31	Ld	0.27	0/903	0.35	0/1216
32	Le	0.30	0/1071	0.33	0/1429

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Lf	0.31	0/895	0.38	0/1198
34	Lg	0.27	0/916	0.33	0/1220
35	Lh	0.25	0/1023	0.31	0/1351
36	Li	0.23	0/843	0.31	0/1115
37	Lj	0.31	0/720	0.41	0/952
38	Lk	0.21	0/575	0.32	0/761
39	Ll	0.28	0/454	0.31	0/599
40	Lm	0.25	0/435	0.39	1/575 (0.2%)
41	Lo	0.27	0/876	0.35	0/1156
42	Lp	0.27	0/718	0.33	0/953
43	Lr	0.28	0/1017	0.35	0/1364
44	CA	0.18	0/2810	0.40	0/3780
45	P	0.57	0/1736	1.36	10/2362 (0.4%)
All	All	0.31	0/148928	0.36	11/219568 (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
5	LB	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	P	85	ARG	CB-CG-CD	-6.21	97.03	111.30
45	P	90	ASP	CA-CB-CG	6.18	118.78	112.60
45	P	47	PRO	CB-CA-C	-6.17	103.17	111.12
45	P	209	ASP	CB-CA-C	-5.78	101.71	111.02
45	P	107	VAL	N-CA-C	-5.40	107.86	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	LB	174	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	L5	78444	0	39717	757	0
2	L7	2561	0	1295	10	0
3	L8	3315	0	1685	31	0
4	LA	1898	0	1993	35	0
5	LB	3238	0	3376	69	0
6	LC	2927	0	3104	34	0
7	LD	2382	0	2410	28	0
8	LE	1935	0	2096	29	0
9	LF	1870	0	1996	18	0
10	LG	1927	0	2074	18	0
11	LH	1518	0	1601	19	0
12	LI	1711	0	1749	25	0
13	LJ	1362	0	1399	11	0
14	LL	1701	0	1818	20	0
15	LM	1138	0	1204	20	0
16	LN	1701	0	1749	24	0
17	LO	1650	0	1794	27	0
18	LP	1242	0	1269	18	0
19	LQ	1513	0	1628	18	0
20	LR	1273	0	1407	16	0
21	LS	1453	0	1490	12	0
22	LT	1298	0	1366	21	0
23	LU	825	0	850	11	0
24	LV	979	0	1037	23	0
25	LX	985	0	1066	49	0
26	LY	1115	0	1205	14	0
27	LZ	1107	0	1182	16	0
28	La	1162	0	1213	10	0
29	Lb	876	0	948	13	0
30	Lc	764	0	804	7	0
31	Ld	888	0	930	12	0
32	Le	1053	0	1147	14	0
33	Lf	876	0	912	8	0
34	Lg	906	0	998	12	0
35	Lh	1015	0	1148	19	0
36	Li	832	0	917	7	0
37	Lj	705	0	737	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	Lk	569	0	637	5	0
39	Ll	444	0	483	11	0
40	Lm	429	0	465	4	0
41	Lo	862	0	929	8	0
42	Lp	708	0	756	7	0
43	Lr	1002	0	1068	10	0
44	CA	2764	0	2778	113	0
45	P	1712	0	1688	108	0
46	L5	178	0	0	0	0
46	L7	3	0	0	0	0
46	L8	5	0	0	0	0
46	LA	1	0	0	0	0
46	LI	1	0	0	0	0
46	LP	1	0	0	0	0
46	LV	1	0	0	0	0
46	Le	1	0	0	0	0
47	L5	98	0	182	4	0
48	L5	90	0	171	5	0
48	LN	10	0	19	0	0
49	Lg	1	0	0	0	0
49	Lj	1	0	0	0	0
49	Lm	1	0	0	0	0
49	Lo	1	0	0	0	0
49	Lp	1	0	0	0	0
50	P	1	0	0	0	0
All	All	141030	0	102490	1418	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 6.

The worst 5 of 1418 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)
24:LV:131:ARG:NH2	45:P:195:ALA:HB1	1.41	1.33
5:LB:70:LYS:NZ	45:P:55:GLY:HA2	1.63	1.13
1:L5:2709:C:O2'	44:CA:263:ARG:CD	1.96	1.12
5:LB:70:LYS:HZ1	45:P:55:GLY:HA2	1.13	1.06
25:LX:156:ILE:HG12	44:CA:290:ARG:HB3	1.33	1.05

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	
4	LA	246/248 (99%)	229 (93%)	17 (7%)	0	100	100
5	LB	400/402 (100%)	385 (96%)	15 (4%)	0	100	100
6	LC	366/368 (100%)	353 (96%)	13 (4%)	0	100	100
7	LD	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
8	LE	236/250 (94%)	226 (96%)	10 (4%)	0	100	100
9	LF	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
10	LG	239/241 (99%)	226 (95%)	13 (5%)	0	100	100
11	LH	188/190 (99%)	183 (97%)	5 (3%)	0	100	100
12	LI	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
13	LJ	168/176 (96%)	162 (96%)	6 (4%)	0	100	100
14	LL	208/210 (99%)	201 (97%)	7 (3%)	0	100	100
15	LM	137/139 (99%)	130 (95%)	7 (5%)	0	100	100
16	LN	201/203 (99%)	198 (98%)	3 (2%)	0	100	100
17	LO	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
18	LP	151/153 (99%)	145 (96%)	6 (4%)	0	100	100
19	LQ	185/187 (99%)	182 (98%)	3 (2%)	0	100	100
20	LR	150/187 (80%)	146 (97%)	4 (3%)	0	100	100
21	LS	173/175 (99%)	165 (95%)	8 (5%)	0	100	100
22	LT	157/159 (99%)	154 (98%)	3 (2%)	0	100	100
23	LU	99/101 (98%)	93 (94%)	6 (6%)	0	100	100
24	LV	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
25	LX	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
26	LY	132/134 (98%)	128 (97%)	4 (3%)	0	100	100
27	LZ	133/135 (98%)	126 (95%)	7 (5%)	0	100	100
28	La	145/147 (99%)	140 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	Lb	105/121 (87%)	100 (95%)	5 (5%)	0	100	100
30	Lc	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
31	Ld	105/107 (98%)	102 (97%)	3 (3%)	0	100	100
32	Le	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
33	Lf	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
34	Lg	112/114 (98%)	110 (98%)	2 (2%)	0	100	100
35	Lh	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
36	Li	100/102 (98%)	99 (99%)	1 (1%)	0	100	100
37	Lj	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
38	Lk	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
39	Ll	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
40	Lm	50/52 (96%)	50 (100%)	0	0	100	100
41	Lo	103/105 (98%)	98 (95%)	5 (5%)	0	100	100
42	Lp	89/91 (98%)	86 (97%)	3 (3%)	0	100	100
43	Lr	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
44	CA	350/356 (98%)	334 (95%)	16 (5%)	0	100	100
45	P	223/225 (99%)	173 (78%)	44 (20%)	6 (3%)	4	11
All	All	6893/7048 (98%)	6621 (96%)	266 (4%)	6 (0%)	49	72

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
45	P	201	ASP
45	P	139	ARG
45	P	40	GLY
45	P	32	GLU
45	P	192	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	LA	190/190 (100%)	190 (100%)	0	100	100
5	LB	348/348 (100%)	348 (100%)	0	100	100
6	LC	306/306 (100%)	306 (100%)	0	100	100
7	LD	246/247 (100%)	246 (100%)	0	100	100
8	LE	212/222 (96%)	212 (100%)	0	100	100
9	LF	194/194 (100%)	194 (100%)	0	100	100
10	LG	203/205 (99%)	203 (100%)	0	100	100
11	LH	169/169 (100%)	169 (100%)	0	100	100
12	LI	180/180 (100%)	180 (100%)	0	100	100
13	LJ	143/148 (97%)	143 (100%)	0	100	100
14	LL	176/176 (100%)	176 (100%)	0	100	100
15	LM	118/118 (100%)	118 (100%)	0	100	100
16	LN	171/171 (100%)	171 (100%)	0	100	100
17	LO	173/173 (100%)	173 (100%)	0	100	100
18	LP	134/134 (100%)	134 (100%)	0	100	100
19	LQ	164/164 (100%)	164 (100%)	0	100	100
20	LR	136/166 (82%)	136 (100%)	0	100	100
21	LS	156/156 (100%)	156 (100%)	0	100	100
22	LT	139/139 (100%)	139 (100%)	0	100	100
23	LU	91/91 (100%)	91 (100%)	0	100	100
24	LV	101/101 (100%)	101 (100%)	0	100	100
25	LX	108/108 (100%)	108 (100%)	0	100	100
26	LY	124/124 (100%)	124 (100%)	0	100	100
27	LZ	117/117 (100%)	117 (100%)	0	100	100
28	La	120/120 (100%)	120 (100%)	0	100	100
29	Lb	88/101 (87%)	88 (100%)	0	100	100
30	Lc	83/83 (100%)	83 (100%)	0	100	100
31	Ld	98/98 (100%)	98 (100%)	0	100	100
32	Le	114/114 (100%)	114 (100%)	0	100	100
33	Lf	88/88 (100%)	88 (100%)	0	100	100
34	Lg	98/98 (100%)	98 (100%)	0	100	100
35	Lh	109/109 (100%)	109 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
36	Li	86/86 (100%)	86 (100%)	0	100	100
37	Lj	73/73 (100%)	73 (100%)	0	100	100
38	Lk	64/64 (100%)	64 (100%)	0	100	100
39	Ll	47/47 (100%)	47 (100%)	0	100	100
40	Lm	48/48 (100%)	48 (100%)	0	100	100
41	Lo	93/93 (100%)	93 (100%)	0	100	100
42	Lp	74/74 (100%)	74 (100%)	0	100	100
43	Lr	109/109 (100%)	109 (100%)	0	100	100
44	CA	303/305 (99%)	303 (100%)	0	100	100
45	P	195/195 (100%)	122 (63%)	73 (37%)	0	0
All	All	5989/6052 (99%)	5916 (99%)	73 (1%)	61	79

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
45	P	177	LEU
45	P	220	SER
45	P	186	VAL
45	P	209	ASP
45	P	90	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
19	LQ	21	GLN
28	La	34	ASN
20	LR	134	ASN
24	LV	77	HIS
28	La	120	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L5	3643/3675 (99%)	714 (19%)	16 (0%)
2	L7	119/120 (99%)	11 (9%)	0
3	L8	155/156 (99%)	22 (14%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	3917/3951 (99%)	747 (19%)	16 (0%)

5 of 747 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L5	25	A
1	L5	30	C
1	L5	39	A
1	L5	42	A
1	L5	48	G

5 of 16 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L5	4699	U
1	L5	4600	G
1	L5	2416	G
1	L5	3673	C
1	L5	1977	C

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

114 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	L5	4296	1	18,21,22	1.06	1 (5%)	21,30,33	1.93	4 (19%)
1	A2M	L5	1524	1	22,25,26	1.32	2 (9%)	30,36,39	1.51	6 (20%)
1	OMU	L5	4227	1	19,22,23	3.26	7 (36%)	25,31,34	1.91	4 (16%)
1	PSU	L5	1792	1	18,21,22	1.03	1 (5%)	21,30,33	1.92	4 (19%)
1	OMG	L5	3792	1	23,26,27	0.57	0	32,38,41	0.54	0
1	OMG	L5	4392	1	23,26,27	0.61	0	32,38,41	0.50	0
1	A2M	L5	2401	1	22,25,26	1.23	1 (4%)	30,36,39	1.61	5 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	L5	3825	1	22,25,26	1.17	2 (9%)	30,36,39	1.55	7 (23%)
1	OMG	L5	3744	1	23,26,27	0.57	0	32,38,41	0.51	0
1	PSU	L5	3853	46,1	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
1	PSU	L5	5001	1	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
1	UR3	L5	4530	1	19,22,23	2.66	6 (31%)	26,32,35	1.59	3 (11%)
1	PSU	L5	5010	1	18,21,22	1.08	1 (5%)	21,30,33	1.93	4 (19%)
1	PSU	L5	4312	1	18,21,22	1.07	1 (5%)	21,30,33	1.91	4 (19%)
1	PSU	L5	4673	46,1	18,21,22	1.07	2 (11%)	21,30,33	1.90	4 (19%)
3	OMG	L8	75	3	23,26,27	0.55	0	32,38,41	0.54	0
1	PSU	L5	1860	1	18,21,22	1.07	1 (5%)	21,30,33	1.94	4 (19%)
1	PSU	L5	1536	1	18,21,22	1.05	1 (5%)	21,30,33	1.89	4 (19%)
1	PSU	L5	2839	1	18,21,22	1.02	1 (5%)	21,30,33	1.93	4 (19%)
1	PSU	L5	4576	1	18,21,22	1.06	2 (11%)	21,30,33	1.86	4 (19%)
1	OMC	L5	2861	1	19,22,23	0.63	0	25,31,34	0.82	1 (4%)
1	PSU	L5	4442	1	18,21,22	1.09	2 (11%)	21,30,33	2.04	6 (28%)
1	OMG	L5	4637	1	23,26,27	0.59	0	32,38,41	0.50	0
1	PSU	L5	4579	1	18,21,22	1.08	1 (5%)	21,30,33	1.95	4 (19%)
1	PSU	L5	3844	1	18,21,22	1.11	1 (5%)	21,30,33	1.91	4 (19%)
1	OMG	L5	4228	1	23,26,27	0.58	0	32,38,41	0.67	0
1	PSU	L5	1683	1	18,21,22	1.09	2 (11%)	21,30,33	2.06	5 (23%)
1	PSU	L5	3695	1	18,21,22	1.07	2 (11%)	21,30,33	1.95	4 (19%)
1	OMC	L5	3808	46,1	19,22,23	0.69	0	25,31,34	0.85	1 (4%)
1	OMC	L5	3701	1	19,22,23	0.72	1 (5%)	25,31,34	1.82	4 (16%)
1	PSU	L5	4353	1	18,21,22	1.09	2 (11%)	21,30,33	1.99	6 (28%)
1	OMG	L5	2876	1	23,26,27	0.58	0	32,38,41	0.52	0
1	OMG	L5	4623	1	23,26,27	0.60	0	32,38,41	0.62	0
1	A2M	L5	3718	1	22,25,26	1.16	1 (4%)	30,36,39	1.52	6 (20%)
1	OMU	L5	4498	1	19,22,23	3.23	7 (36%)	25,31,34	1.90	5 (20%)
1	PSU	L5	4521	46,1	18,21,22	1.09	2 (11%)	21,30,33	2.02	6 (28%)
1	1MA	L5	1322	46,1	21,25,26	0.65	0	30,37,40	0.80	2 (6%)
1	PSU	L5	3639	1	18,21,22	1.10	2 (11%)	21,30,33	1.97	5 (23%)
1	A2M	L5	400	1	22,25,26	1.28	3 (13%)	30,36,39	1.57	9 (30%)
1	OMC	L5	3887	1	19,22,23	0.65	0	25,31,34	0.67	0
1	OMC	L5	3841	1	19,22,23	0.67	0	25,31,34	0.73	0
1	5MC	L5	4447	1	19,22,23	0.93	1 (5%)	26,32,35	0.67	0
1	PSU	L5	1862	1	18,21,22	1.05	1 (5%)	21,30,33	2.00	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMG	L5	4494	1	23,26,27	0.59	0	32,38,41	0.49	0
1	OMC	L5	2422	46,1	19,22,23	0.65	0	25,31,34	0.74	1 (4%)
1	PSU	L5	1582	1	18,21,22	1.08	1 (5%)	21,30,33	1.90	4 (19%)
1	OMC	L5	2365	46,1	19,22,23	0.63	0	25,31,34	0.59	0
1	PSU	L5	4293	1	18,21,22	1.08	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	L5	3920	46,1	18,21,22	1.07	1 (5%)	21,30,33	1.97	4 (19%)
1	PSU	L5	4628	1	18,21,22	1.01	1 (5%)	21,30,33	1.86	4 (19%)
1	PSU	L5	3884	1	18,21,22	1.09	2 (11%)	21,30,33	1.97	4 (19%)
1	OMG	L5	2424	1	23,26,27	0.60	0	32,38,41	0.43	0
1	PSU	L5	4403	1	18,21,22	1.07	2 (11%)	21,30,33	2.06	6 (28%)
1	OMU	L5	3925	1	19,22,23	3.22	7 (36%)	25,31,34	1.95	5 (20%)
1	OMC	L5	3869	1	19,22,23	0.64	0	25,31,34	0.79	0
1	A2M	L5	4571	1	22,25,26	1.24	2 (9%)	30,36,39	1.58	9 (30%)
1	A2M	L5	4590	1	22,25,26	1.19	1 (4%)	30,36,39	1.51	5 (16%)
1	A2M	L5	4523	46,1	22,25,26	1.22	3 (13%)	30,36,39	1.53	6 (20%)
1	PSU	L5	4500	1	18,21,22	1.13	2 (11%)	21,30,33	2.06	5 (23%)
1	OMC	L5	4536	1	19,22,23	0.67	0	25,31,34	0.75	0
1	PSU	L5	1744	46,1	18,21,22	1.09	1 (5%)	21,30,33	1.96	4 (19%)
1	PSU	L5	4431	1	18,21,22	1.06	1 (5%)	21,30,33	1.88	4 (19%)
1	OMU	L5	4306	1	19,22,23	3.21	7 (36%)	25,31,34	1.91	4 (16%)
1	OMU	L5	2837	1	19,22,23	3.25	7 (36%)	25,31,34	1.86	4 (16%)
1	OMG	L5	3627	1	23,26,27	0.57	0	32,38,41	0.58	0
1	A2M	L5	2815	1	22,25,26	1.21	2 (9%)	30,36,39	1.51	7 (23%)
1	UY1	L5	3818	1	19,22,23	4.79	9 (47%)	21,31,34	2.04	5 (23%)
3	PSU	L8	69	3	18,21,22	1.06	2 (11%)	21,30,33	1.96	5 (23%)
1	PSU	L5	4972	1	18,21,22	1.04	1 (5%)	21,30,33	1.95	4 (19%)
1	PSU	L5	4457	1	18,21,22	1.05	2 (11%)	21,30,33	1.99	5 (23%)
1	OMG	L5	1625	1	23,26,27	0.58	0	32,38,41	0.50	0
1	OMC	L5	1340	1	19,22,23	0.69	0	25,31,34	0.80	0
1	PSU	L5	4552	1	18,21,22	1.10	2 (11%)	21,30,33	2.03	4 (19%)
1	PSU	L5	4493	1	18,21,22	1.05	1 (5%)	21,30,33	1.85	4 (19%)
1	OMC	L5	2351	46,1	19,22,23	0.71	1 (5%)	25,31,34	1.10	2 (8%)
1	A2M	L5	3867	1	22,25,26	1.28	2 (9%)	30,36,39	1.48	6 (20%)
1	PSU	L5	2632	1	18,21,22	1.06	1 (5%)	21,30,33	1.92	4 (19%)
1	OMG	L5	4618	1	23,26,27	0.59	0	32,38,41	0.53	0
1	A2M	L5	1326	1	22,25,26	1.24	2 (9%)	30,36,39	1.44	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	L5	2363	46,1	22,25,26	1.22	2 (9%)	30,36,39	1.55	9 (30%)
1	A2M	L5	3785	46,1	22,25,26	1.17	2 (9%)	30,36,39	1.59	10 (33%)
1	PSU	L5	3851	1	18,21,22	1.08	1 (5%)	21,30,33	1.94	4 (19%)
1	PSU	L5	3637	1	18,21,22	1.09	1 (5%)	21,30,33	1.97	3 (14%)
1	PSU	L5	4636	1	18,21,22	1.13	2 (11%)	21,30,33	2.08	6 (28%)
1	OMG	L5	4499	1	23,26,27	0.53	0	32,38,41	0.48	0
1	PSU	L5	1781	1	18,21,22	1.07	1 (5%)	21,30,33	1.79	4 (19%)
1	OMC	L5	2824	1	19,22,23	0.64	0	25,31,34	0.65	0
1	PSU	L5	1782	1	18,21,22	1.05	1 (5%)	21,30,33	1.86	4 (19%)
1	PSU	L5	4973	1	18,21,22	1.03	1 (5%)	21,30,33	1.92	4 (19%)
3	PSU	L8	55	3	18,21,22	1.08	1 (5%)	21,30,33	1.88	4 (19%)
1	PSU	L5	4361	1	18,21,22	1.06	2 (11%)	21,30,33	1.88	4 (19%)
1	PSU	L5	4689	1	18,21,22	1.11	2 (11%)	21,30,33	2.07	4 (19%)
1	OMG	L5	3899	1	23,26,27	0.65	0	32,38,41	0.53	0
1	6MZ	L5	4220	1	22,25,26	3.96	11 (50%)	29,36,39	2.49	11 (37%)
1	PSU	L5	4471	1	18,21,22	1.06	1 (5%)	21,30,33	1.90	4 (19%)
1	PSU	L5	3822	1	18,21,22	1.08	1 (5%)	21,30,33	1.99	6 (28%)
1	OMG	L5	2364	46,1	23,26,27	0.60	0	32,38,41	0.44	0
1	OMG	L5	4370	1	23,26,27	0.57	0	32,38,41	0.53	0
1	OMC	L5	4456	1	19,22,23	0.71	1 (5%)	25,31,34	0.79	0
1	OMG	L5	1316	1	23,26,27	0.65	0	32,38,41	0.56	0
1	OMG	L5	4196	1	23,26,27	0.55	0	32,38,41	0.46	0
1	A2M	L5	398	1	22,25,26	1.17	1 (4%)	30,36,39	1.62	7 (23%)
1	OMC	L5	2804	1	19,22,23	0.66	0	25,31,34	0.91	1 (4%)
1	A2M	L5	1871	46,1	22,25,26	1.30	3 (13%)	30,36,39	1.63	7 (23%)
1	OMU	L5	4620	1	19,22,23	3.16	7 (36%)	25,31,34	1.71	4 (16%)
1	A2M	L5	1534	46,1	22,25,26	1.26	3 (13%)	30,36,39	1.46	7 (23%)
1	PSU	L5	4532	1	18,21,22	1.09	1 (5%)	21,30,33	1.86	4 (19%)
1	PSU	L5	4299	1	18,21,22	1.01	1 (5%)	21,30,33	1.90	4 (19%)
1	A2M	L5	2787	1	22,25,26	1.16	1 (4%)	30,36,39	1.49	7 (23%)
1	A2M	L5	3830	1	22,25,26	1.19	1 (4%)	30,36,39	1.57	6 (20%)
1	OMG	L5	1522	1	23,26,27	0.60	0	32,38,41	0.69	1 (3%)
1	PSU	L5	1677	1	18,21,22	1.06	3 (16%)	21,30,33	1.95	5 (23%)
1	A2M	L5	1323	1	22,25,26	1.23	2 (9%)	30,36,39	1.58	7 (23%)
1	5MC	L5	3782	46,1	19,22,23	0.72	0	26,32,35	0.81	1 (3%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	4296	1	-	2/7/25/26	0/2/2/2
1	A2M	L5	1524	1	-	3/9/27/28	0/3/3/3
1	OMU	L5	4227	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	1792	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3792	1	-	2/9/27/28	0/3/3/3
1	OMG	L5	4392	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	2401	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	3825	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	3744	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	3853	46,1	-	0/7/25/26	0/2/2/2
1	PSU	L5	5001	1	-	0/7/25/26	0/2/2/2
1	UR3	L5	4530	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	5010	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4312	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4673	46,1	-	0/7/25/26	0/2/2/2
3	OMG	L8	75	3	-	1/9/27/28	0/3/3/3
1	PSU	L5	1860	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	1536	1	-	2/7/25/26	0/2/2/2
1	PSU	L5	2839	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4576	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2861	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4442	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4637	1	-	3/9/27/28	0/3/3/3
1	PSU	L5	4579	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3844	1	-	1/7/25/26	0/2/2/2
1	OMG	L5	4228	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1683	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3695	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	3808	46,1	-	0/9/27/28	0/2/2/2
1	OMC	L5	3701	1	-	5/9/27/28	0/2/2/2
1	PSU	L5	4353	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2876	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	4623	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	3718	1	-	0/9/27/28	0/3/3/3
1	OMU	L5	4498	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4521	46,1	-	0/7/25/26	0/2/2/2
1	1MA	L5	1322	46,1	-	2/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PSU	L5	3639	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	400	1	-	1/9/27/28	0/3/3/3
1	OMC	L5	3887	1	-	1/9/27/28	0/2/2/2
1	OMC	L5	3841	1	-	0/9/27/28	0/2/2/2
1	5MC	L5	4447	1	-	4/7/25/26	0/2/2/2
1	PSU	L5	1862	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	4494	1	-	1/9/27/28	0/3/3/3
1	OMC	L5	2422	46,1	-	2/9/27/28	0/2/2/2
1	PSU	L5	1582	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2365	46,1	-	0/9/27/28	0/2/2/2
1	PSU	L5	4293	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3920	46,1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4628	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	3884	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2424	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4403	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	3925	1	-	0/9/27/28	0/2/2/2
1	OMC	L5	3869	1	-	1/9/27/28	0/2/2/2
1	A2M	L5	4571	1	-	0/9/27/28	0/3/3/3
1	A2M	L5	4590	1	-	3/9/27/28	0/3/3/3
1	A2M	L5	4523	46,1	-	0/9/27/28	0/3/3/3
1	PSU	L5	4500	1	-	3/7/25/26	0/2/2/2
1	OMC	L5	4536	1	-	0/9/27/28	0/2/2/2
1	PSU	L5	1744	46,1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4431	1	-	0/7/25/26	0/2/2/2
1	OMU	L5	4306	1	-	0/9/27/28	0/2/2/2
1	OMU	L5	2837	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	3627	1	-	1/9/27/28	0/3/3/3
1	A2M	L5	2815	1	-	2/9/27/28	0/3/3/3
1	UY1	L5	3818	1	-	2/9/27/28	0/2/2/2
3	PSU	L8	69	3	-	0/7/25/26	0/2/2/2
1	PSU	L5	4972	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4457	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	1625	1	-	2/9/27/28	0/3/3/3
1	OMC	L5	1340	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	4552	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4493	1	-	0/7/25/26	0/2/2/2
1	OMC	L5	2351	46,1	-	3/9/27/28	0/2/2/2
1	A2M	L5	3867	1	-	2/9/27/28	0/3/3/3
1	PSU	L5	2632	1	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	L5	4618	1	-	2/9/27/28	0/3/3/3
1	A2M	L5	1326	1	-	3/9/27/28	0/3/3/3
1	A2M	L5	2363	46,1	-	0/9/27/28	0/3/3/3
1	A2M	L5	3785	46,1	-	2/9/27/28	0/3/3/3
1	PSU	L5	3851	1	-	1/7/25/26	0/2/2/2
1	PSU	L5	3637	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4636	1	-	1/7/25/26	0/2/2/2
1	OMG	L5	4499	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1781	1	-	1/7/25/26	0/2/2/2
1	OMC	L5	2824	1	-	1/9/27/28	0/2/2/2
1	PSU	L5	1782	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4973	1	-	0/7/25/26	0/2/2/2
3	PSU	L8	55	3	-	0/7/25/26	0/2/2/2
1	PSU	L5	4361	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4689	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	3899	1	-	2/9/27/28	0/3/3/3
1	6MZ	L5	4220	1	-	2/9/27/28	0/3/3/3
1	PSU	L5	4471	1	-	1/7/25/26	0/2/2/2
1	PSU	L5	3822	1	-	0/7/25/26	0/2/2/2
1	OMG	L5	2364	46,1	-	2/9/27/28	0/3/3/3
1	OMG	L5	4370	1	-	0/9/27/28	0/3/3/3
1	OMC	L5	4456	1	-	0/9/27/28	0/2/2/2
1	OMG	L5	1316	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	4196	1	-	1/9/27/28	0/3/3/3
1	A2M	L5	398	1	-	1/9/27/28	0/3/3/3
1	OMC	L5	2804	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	1871	46,1	-	0/9/27/28	0/3/3/3
1	OMU	L5	4620	1	-	0/9/27/28	0/2/2/2
1	A2M	L5	1534	46,1	-	1/9/27/28	0/3/3/3
1	PSU	L5	4532	1	-	0/7/25/26	0/2/2/2
1	PSU	L5	4299	1	-	0/7/25/26	0/2/2/2
1	A2M	L5	2787	1	-	5/9/27/28	0/3/3/3
1	A2M	L5	3830	1	-	0/9/27/28	0/3/3/3
1	OMG	L5	1522	1	-	0/9/27/28	0/3/3/3
1	PSU	L5	1677	1	-	2/7/25/26	0/2/2/2
1	A2M	L5	1323	1	-	2/9/27/28	0/3/3/3
1	5MC	L5	3782	46,1	-	0/7/25/26	0/2/2/2

The worst 5 of 177 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L5	3818	UY1	C6-C5	12.48	1.49	1.35
1	L5	4220	6MZ	C6-N6	12.04	1.48	1.34
1	L5	3818	UY1	C2-N1	11.46	1.51	1.36
1	L5	4220	6MZ	C3'-C2'	-8.41	1.30	1.53
1	L5	4227	OMU	C2-N1	8.03	1.51	1.38

The worst 5 of 406 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L5	3925	OMU	C4-N3-C2	-6.15	118.98	126.61
1	L5	4227	OMU	C4-N3-C2	-6.02	119.13	126.61
1	L5	4498	OMU	C4-N3-C2	-5.91	119.28	126.61
1	L5	4306	OMU	C4-N3-C2	-5.81	119.40	126.61
1	L5	4220	6MZ	N1-C2-N3	-5.81	119.79	128.58

There are no chirality outliers.

5 of 80 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L8	75	OMG	C1'-C2'-O2'-CM2
1	L5	400	A2M	C1'-C2'-O2'-CM'
1	L5	1326	A2M	O4'-C4'-C5'-O5'
1	L5	1340	OMC	C1'-C2'-O2'-CM2
1	L5	1625	OMG	O4'-C4'-C5'-O5'

There are no ring outliers.

37 monomers are involved in 47 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	3825	A2M	1	0
3	L8	75	OMG	2	0
1	L5	4637	OMG	1	0
1	L5	1683	PSU	1	0
1	L5	3701	OMC	1	0
1	L5	3718	A2M	3	0
1	L5	400	A2M	1	0
1	L5	3841	OMC	1	0
1	L5	2422	OMC	1	0
1	L5	4293	PSU	1	0
1	L5	3884	PSU	1	0
1	L5	4571	A2M	1	0
1	L5	4536	OMC	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	L5	4431	PSU	1	0
1	L5	3818	UY1	1	0
1	L5	4457	PSU	1	0
1	L5	1625	OMG	1	0
1	L5	1340	OMC	2	0
1	L5	2351	OMC	2	0
1	L5	3867	A2M	4	0
1	L5	2632	PSU	1	0
1	L5	4618	OMG	1	0
1	L5	1326	A2M	2	0
1	L5	2363	A2M	1	0
1	L5	3785	A2M	1	0
1	L5	4636	PSU	1	0
1	L5	2824	OMC	1	0
1	L5	4220	6MZ	1	0
1	L5	3822	PSU	1	0
1	L5	4456	OMC	1	0
1	L5	4196	OMG	1	0
1	L5	398	A2M	1	0
1	L5	2804	OMC	1	0
1	L5	1871	A2M	1	0
1	L5	4620	OMU	2	0
1	L5	1534	A2M	1	0
1	L5	1677	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 213 ligands modelled in this entry, 196 are monoatomic - leaving 17 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
47	SPM	L5	5292	-	13,13,13	0.37	0	12,12,12	0.97	0
48	SPD	LN	301	-	9,9,9	0.34	0	8,8,8	0.85	0
48	SPD	L5	5291	-	9,9,9	0.33	0	8,8,8	0.81	0
48	SPD	L5	5283	-	9,9,9	0.33	0	8,8,8	0.82	0
47	SPM	L5	5267	-	13,13,13	0.36	0	12,12,12	1.12	0
48	SPD	L5	5286	-	9,9,9	0.32	0	8,8,8	0.82	0
47	SPM	L5	5259	-	13,13,13	0.36	0	12,12,12	0.98	0
47	SPM	L5	5264	-	13,13,13	0.36	0	12,12,12	0.97	0
47	SPM	L5	5293	-	13,13,13	0.36	0	12,12,12	0.89	0
48	SPD	L5	5285	-	9,9,9	0.32	0	8,8,8	0.90	0
48	SPD	L5	5288	-	9,9,9	0.31	0	8,8,8	0.87	0
48	SPD	L5	5290	-	9,9,9	0.31	0	8,8,8	0.81	0
48	SPD	L5	5261	-	9,9,9	0.31	0	8,8,8	0.97	0
48	SPD	L5	5287	-	9,9,9	0.31	0	8,8,8	0.89	0
47	SPM	L5	5289	-	13,13,13	0.38	0	12,12,12	1.01	0
47	SPM	L5	5263	-	13,13,13	0.36	0	12,12,12	0.92	0
48	SPD	L5	5284	-	9,9,9	0.31	0	8,8,8	0.81	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
47	SPM	L5	5292	-	-	4/11/11/11	-
48	SPD	LN	301	-	-	1/7/7/7	-
48	SPD	L5	5291	-	-	3/7/7/7	-
48	SPD	L5	5283	-	-	2/7/7/7	-
47	SPM	L5	5267	-	-	4/11/11/11	-
48	SPD	L5	5286	-	-	0/7/7/7	-
47	SPM	L5	5259	-	-	3/11/11/11	-
47	SPM	L5	5264	-	-	3/11/11/11	-
47	SPM	L5	5293	-	-	4/11/11/11	-
48	SPD	L5	5285	-	-	5/7/7/7	-
48	SPD	L5	5288	-	-	1/7/7/7	-
48	SPD	L5	5290	-	-	2/7/7/7	-
48	SPD	L5	5261	-	-	0/7/7/7	-
48	SPD	L5	5287	-	-	3/7/7/7	-
47	SPM	L5	5289	-	-	5/11/11/11	-
47	SPM	L5	5263	-	-	7/11/11/11	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	SPD	L5	5284	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

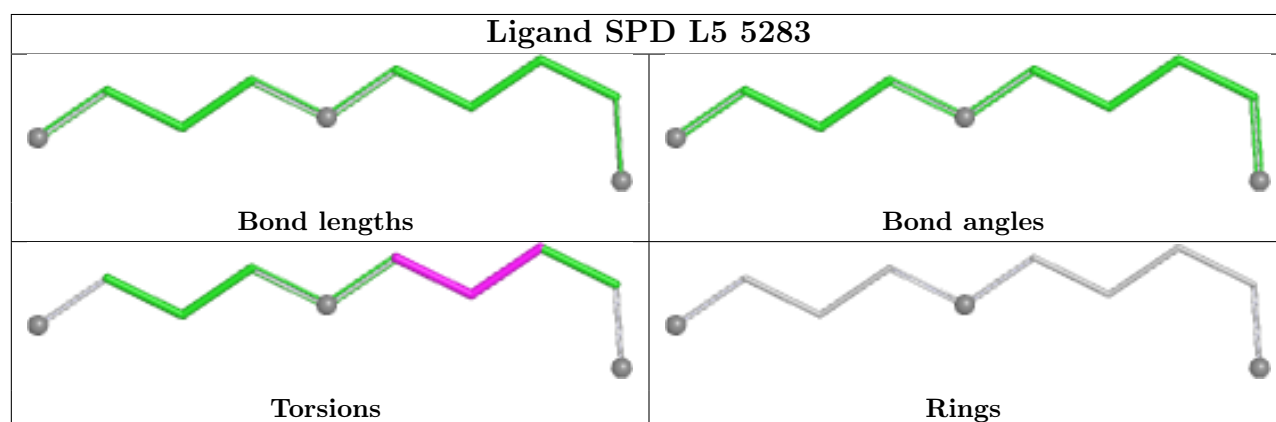
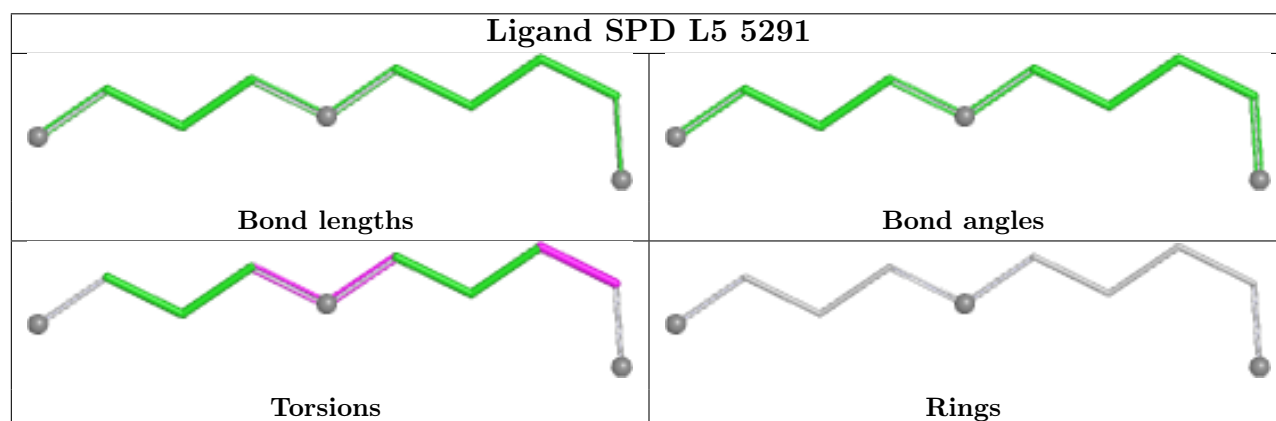
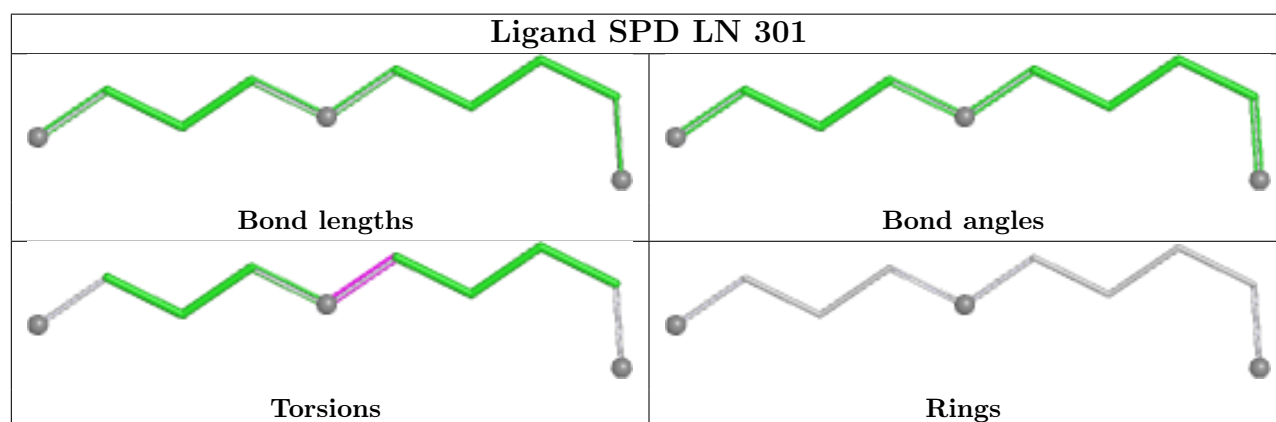
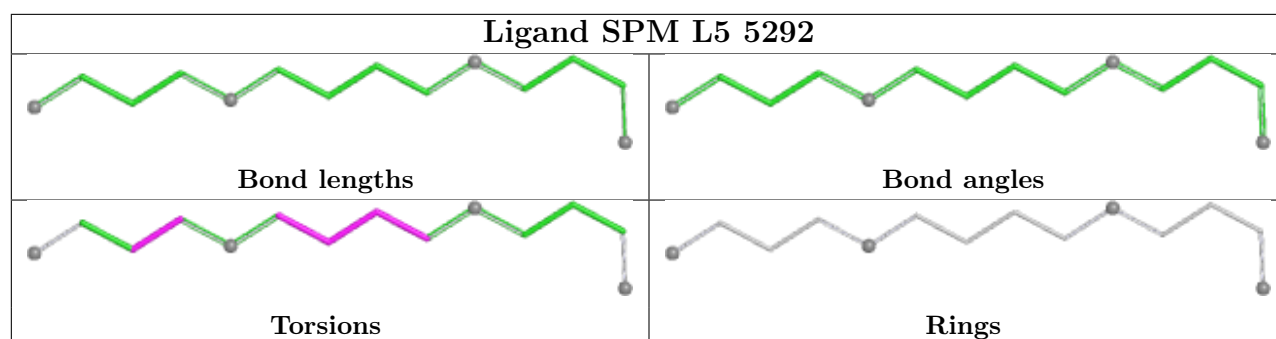
Mol	Chain	Res	Type	Atoms
48	L5	5285	SPD	N6-C7-C8-C9
47	L5	5292	SPM	C7-C8-C9-N10
48	L5	5285	SPD	C3-C4-C5-N6
48	L5	5287	SPD	C3-C4-C5-N6
47	L5	5264	SPM	C2-C3-C4-N5

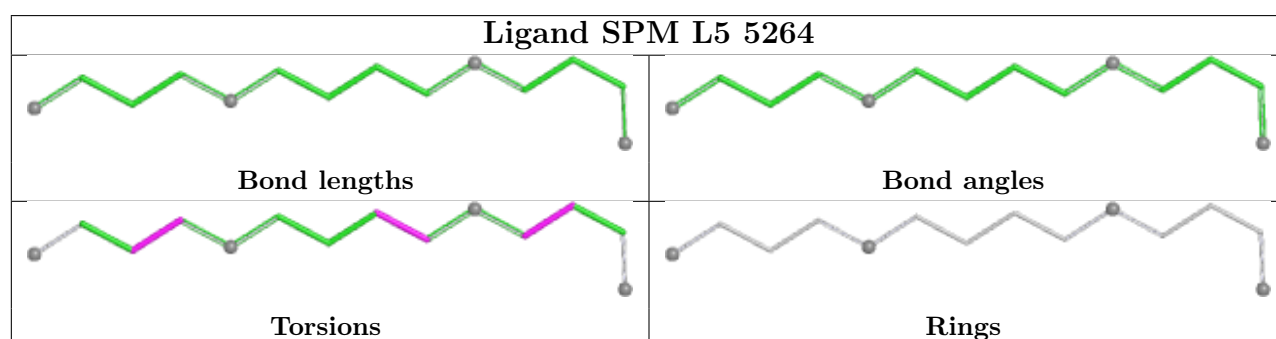
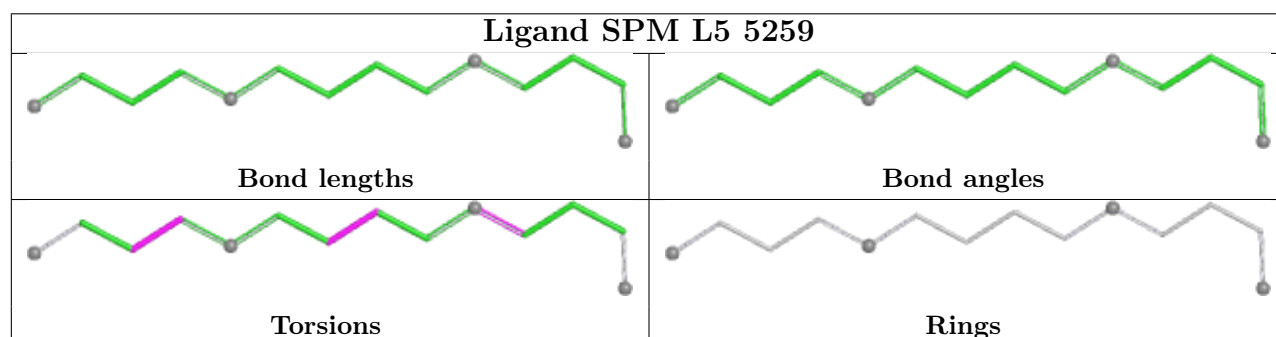
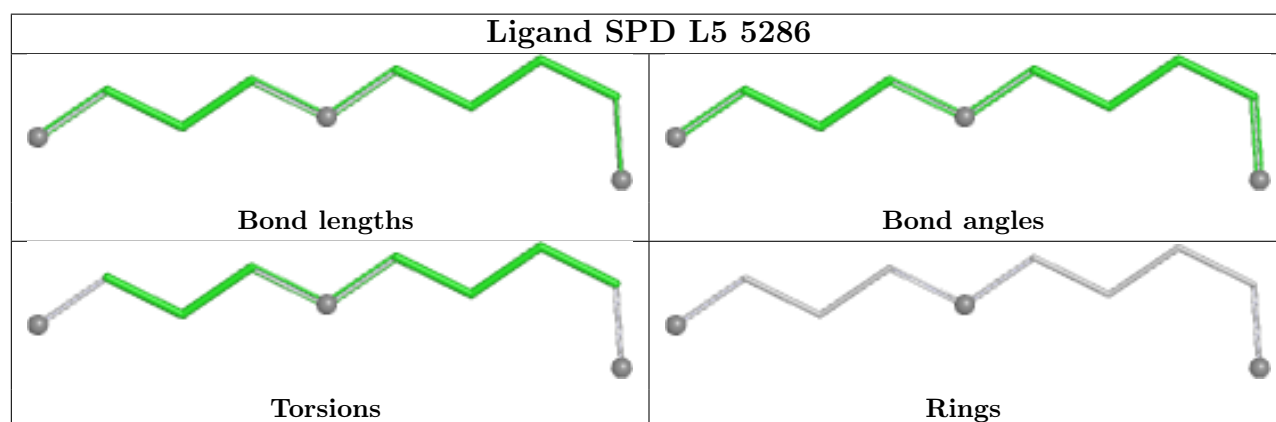
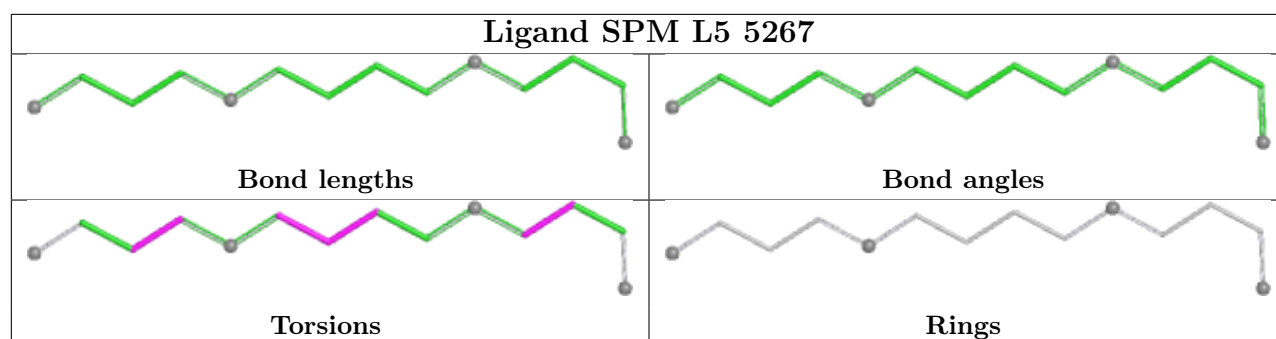
There are no ring outliers.

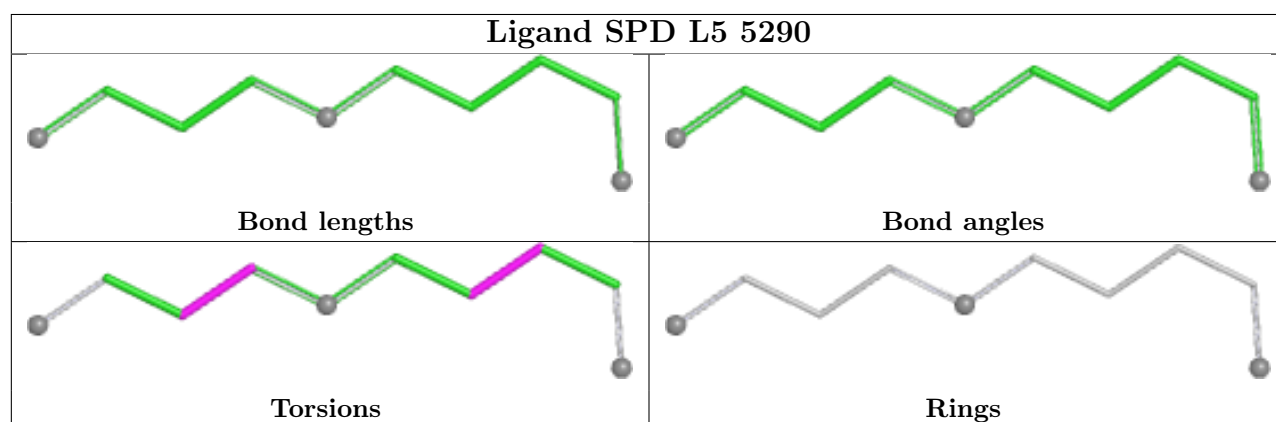
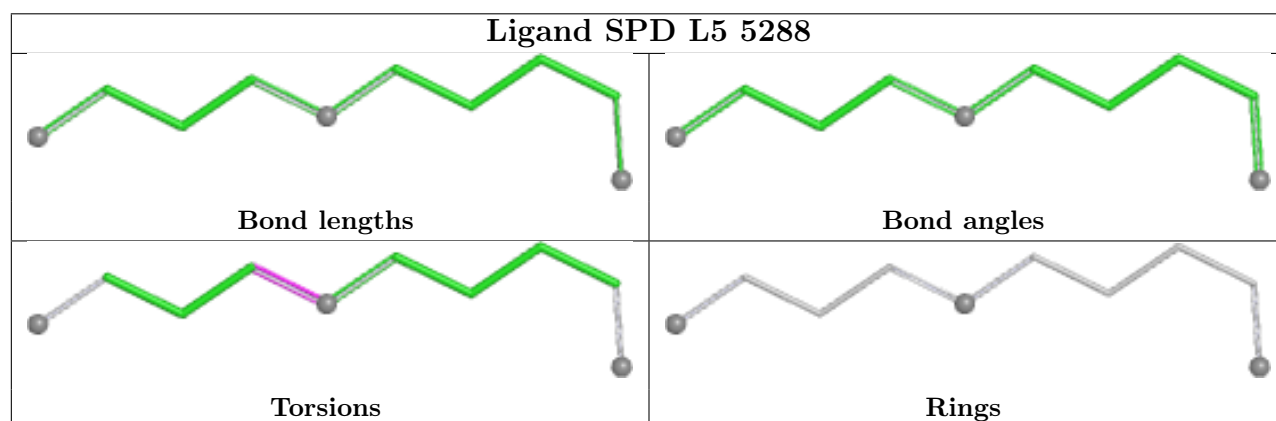
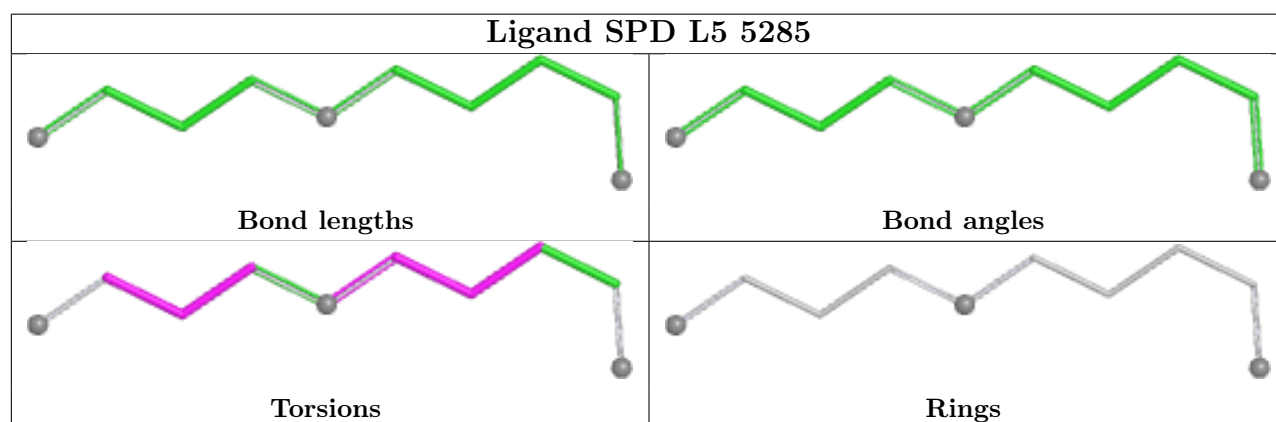
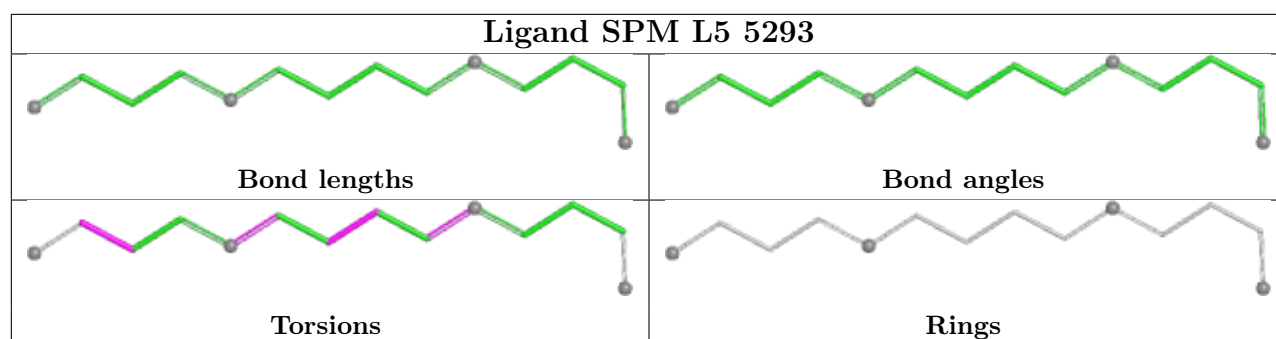
8 monomers are involved in 9 short contacts:

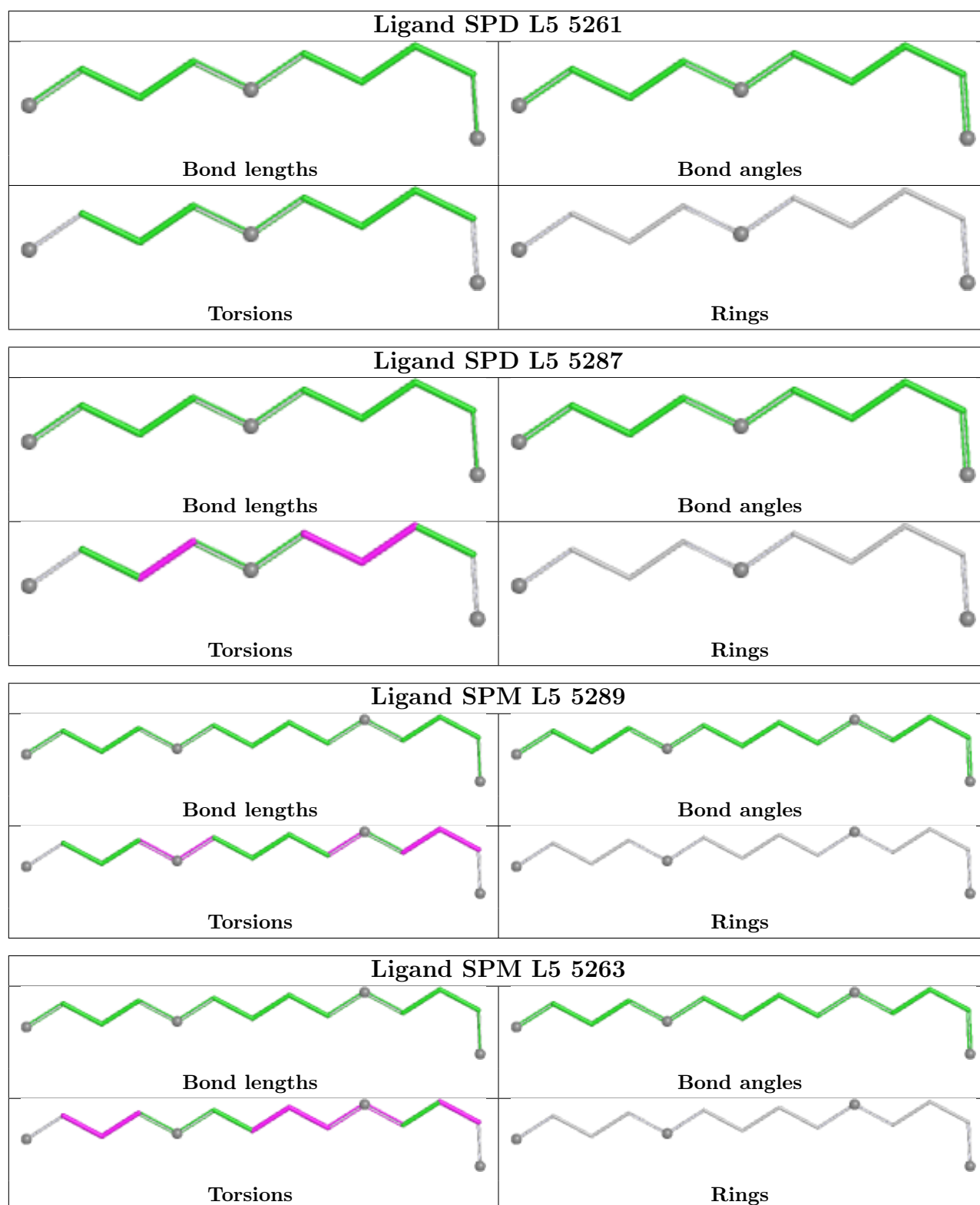
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	L5	5292	SPM	1	0
48	L5	5291	SPD	1	0
48	L5	5286	SPD	1	0
47	L5	5264	SPM	2	0
47	L5	5293	SPM	1	0
48	L5	5290	SPD	1	0
48	L5	5261	SPD	1	0
48	L5	5284	SPD	1	0

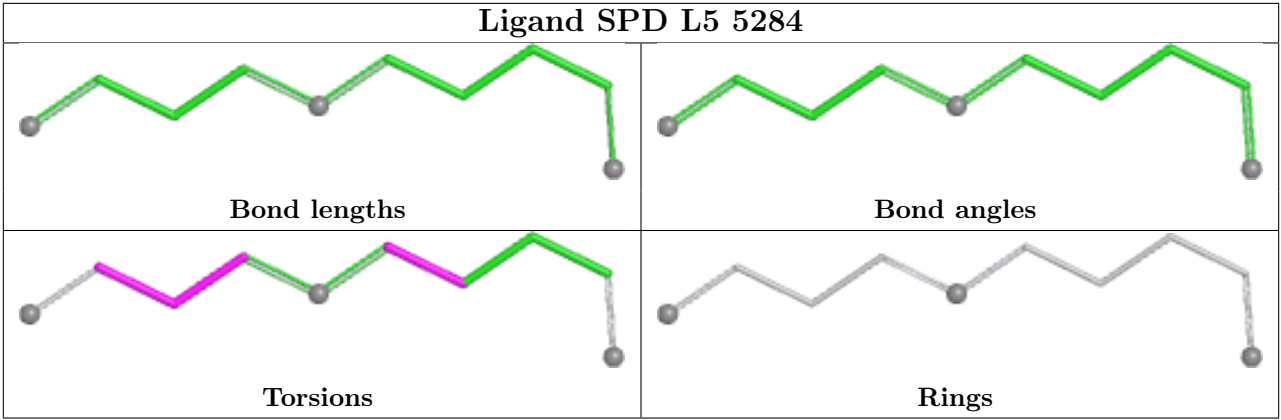
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	L5	8

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L5	2910:G	O3'	3584:C	P	21.32
1	L5	760:G	O3'	903:C	P	16.88
1	L5	519:C	O3'	642:G	P	15.66
1	L5	4776:G	O3'	4858:C	P	15.18
1	L5	2112:G	O3'	2249:C	P	14.87

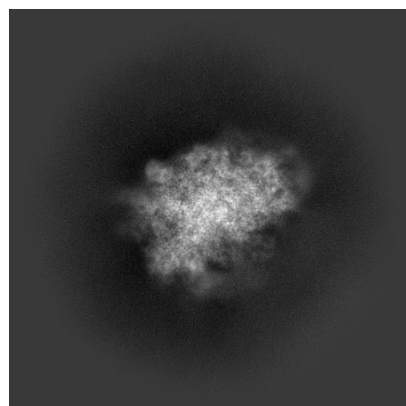
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71414. These allow visual inspection of the internal detail of the map and identification of artifacts.

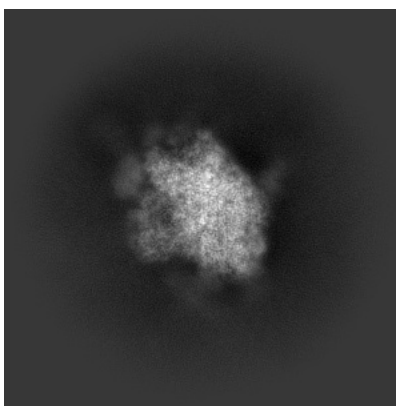
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

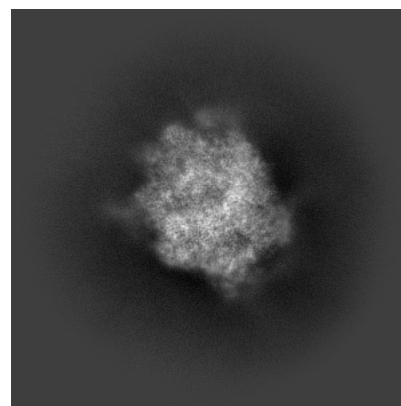
6.1.1 Primary map



X

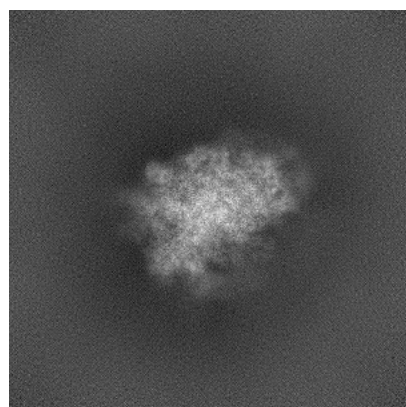


Y

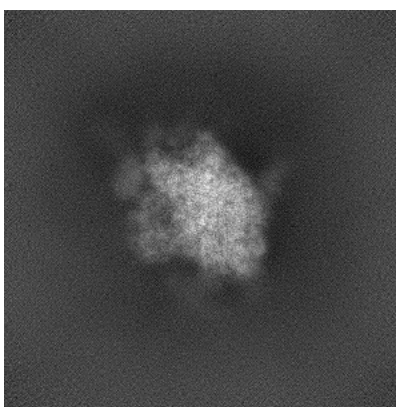


Z

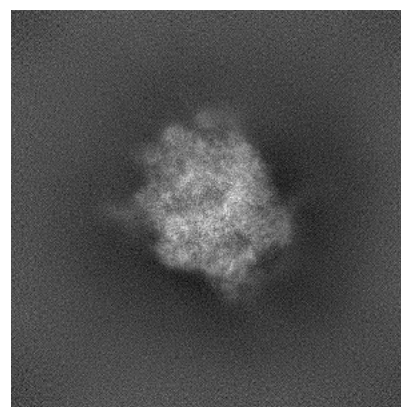
6.1.2 Raw map



X



Y

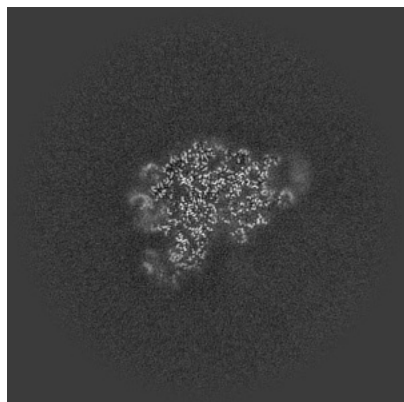


Z

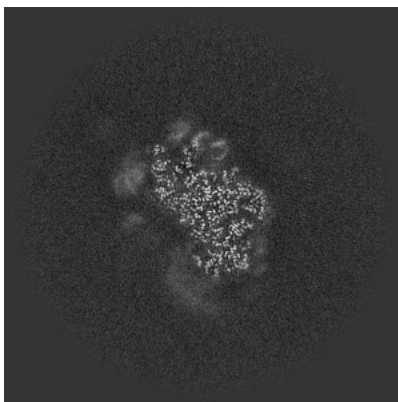
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

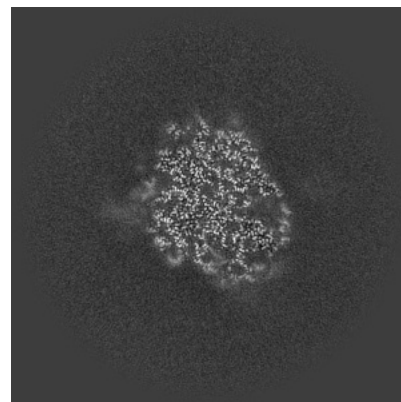
6.2.1 Primary map



X Index: 256

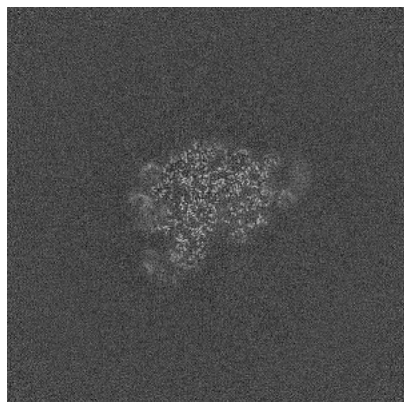


Y Index: 256

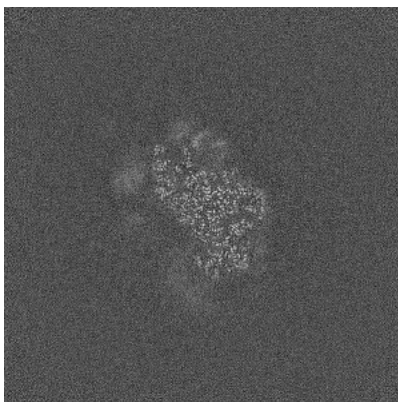


Z Index: 256

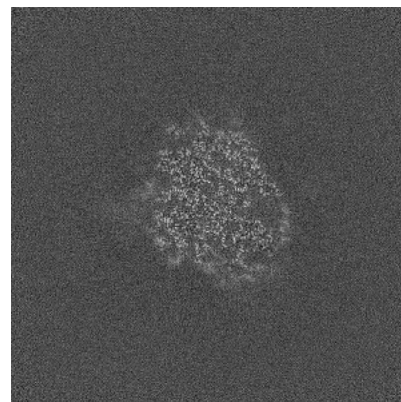
6.2.2 Raw map



X Index: 256



Y Index: 256

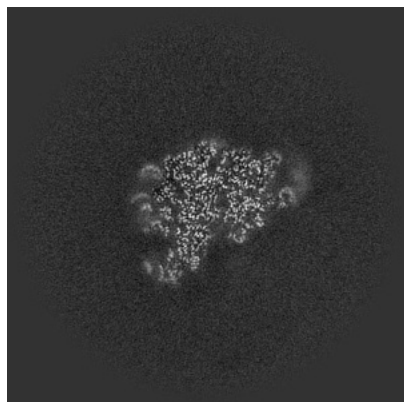


Z Index: 256

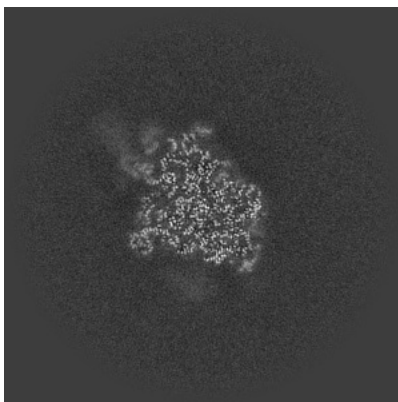
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

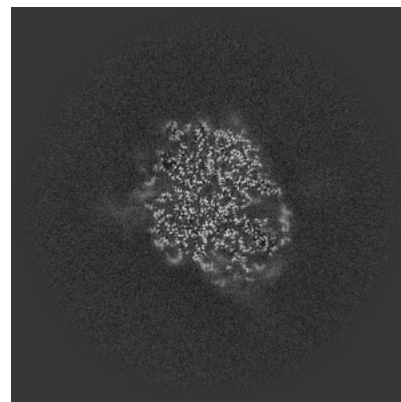
6.3.1 Primary map



X Index: 253

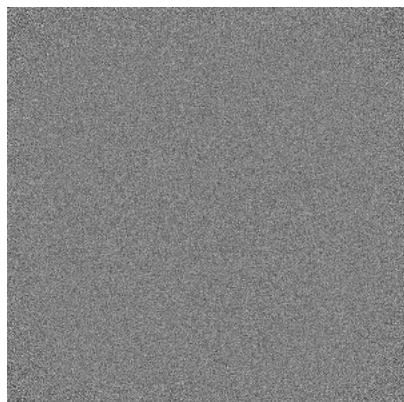


Y Index: 233

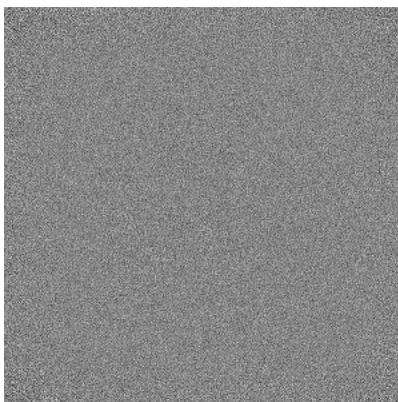


Z Index: 258

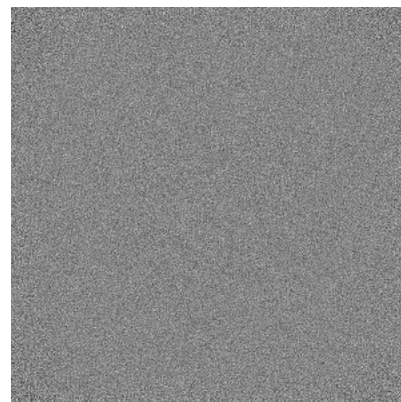
6.3.2 Raw map



X Index: 0



Y Index: 0

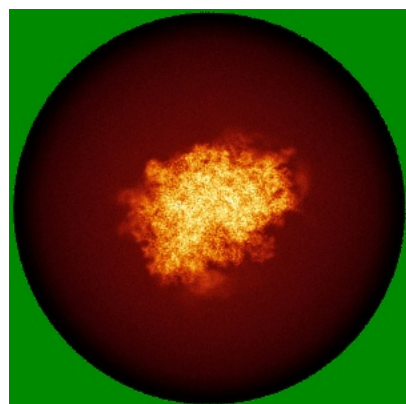


Z Index: 0

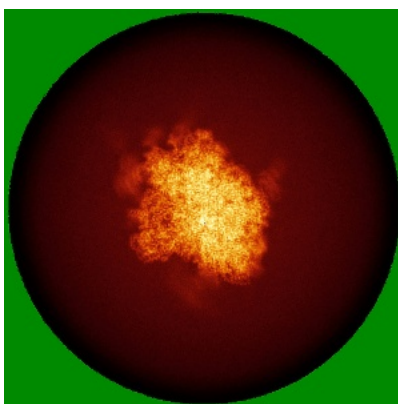
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

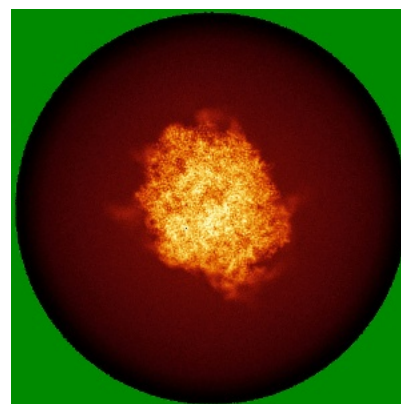
6.4.1 Primary map



X

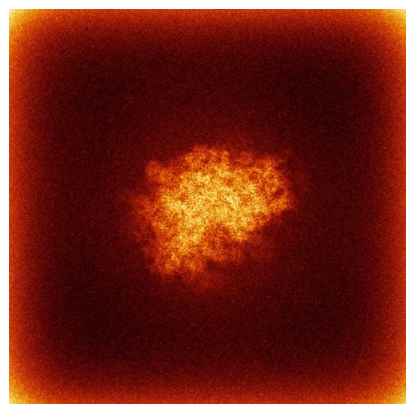


Y

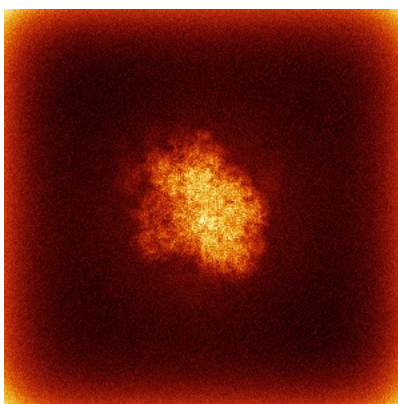


Z

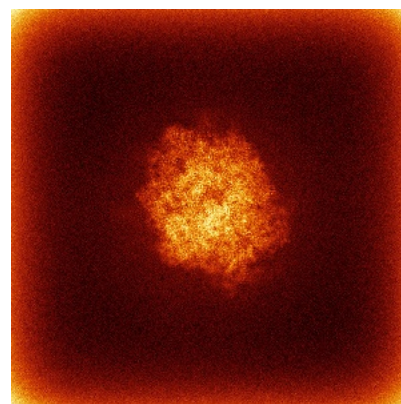
6.4.2 Raw map



X



Y

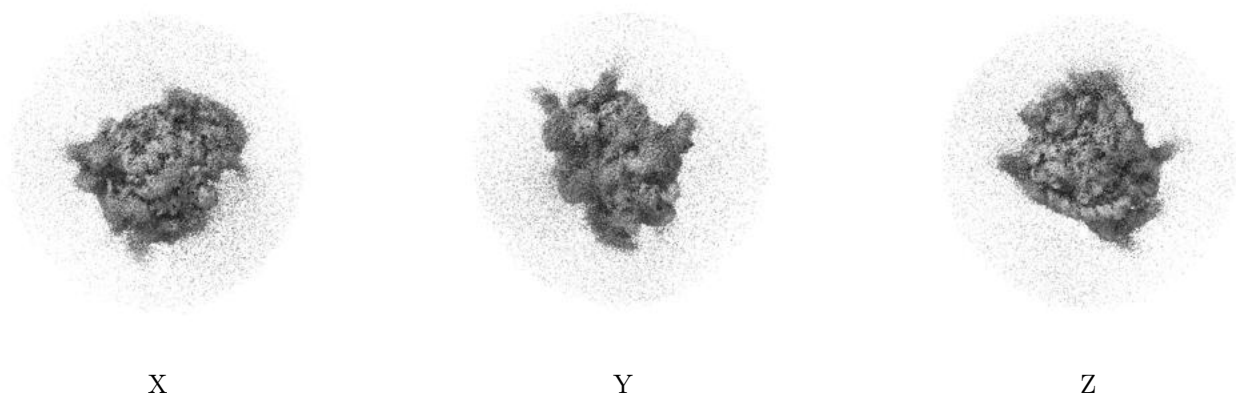


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

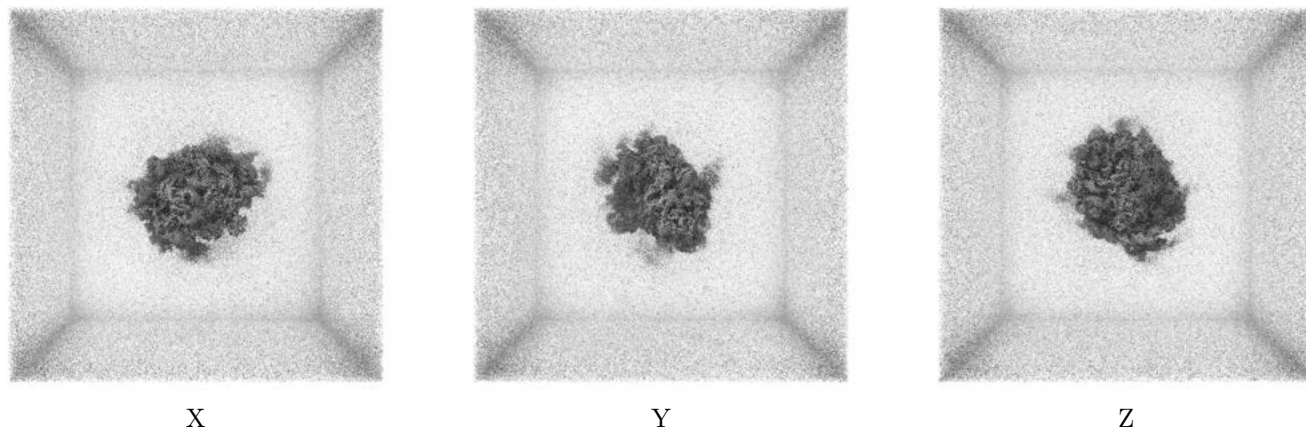
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0354. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

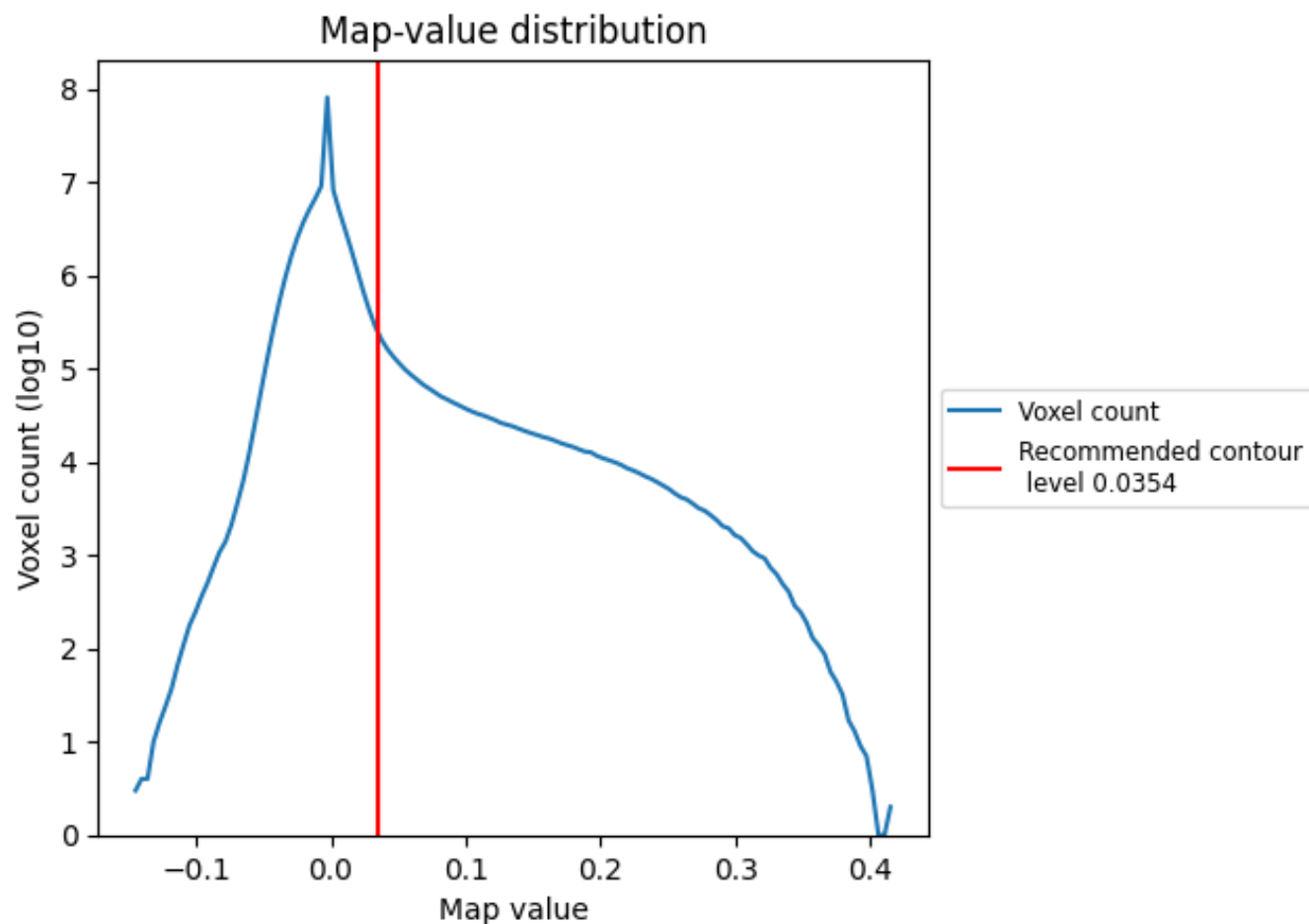
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

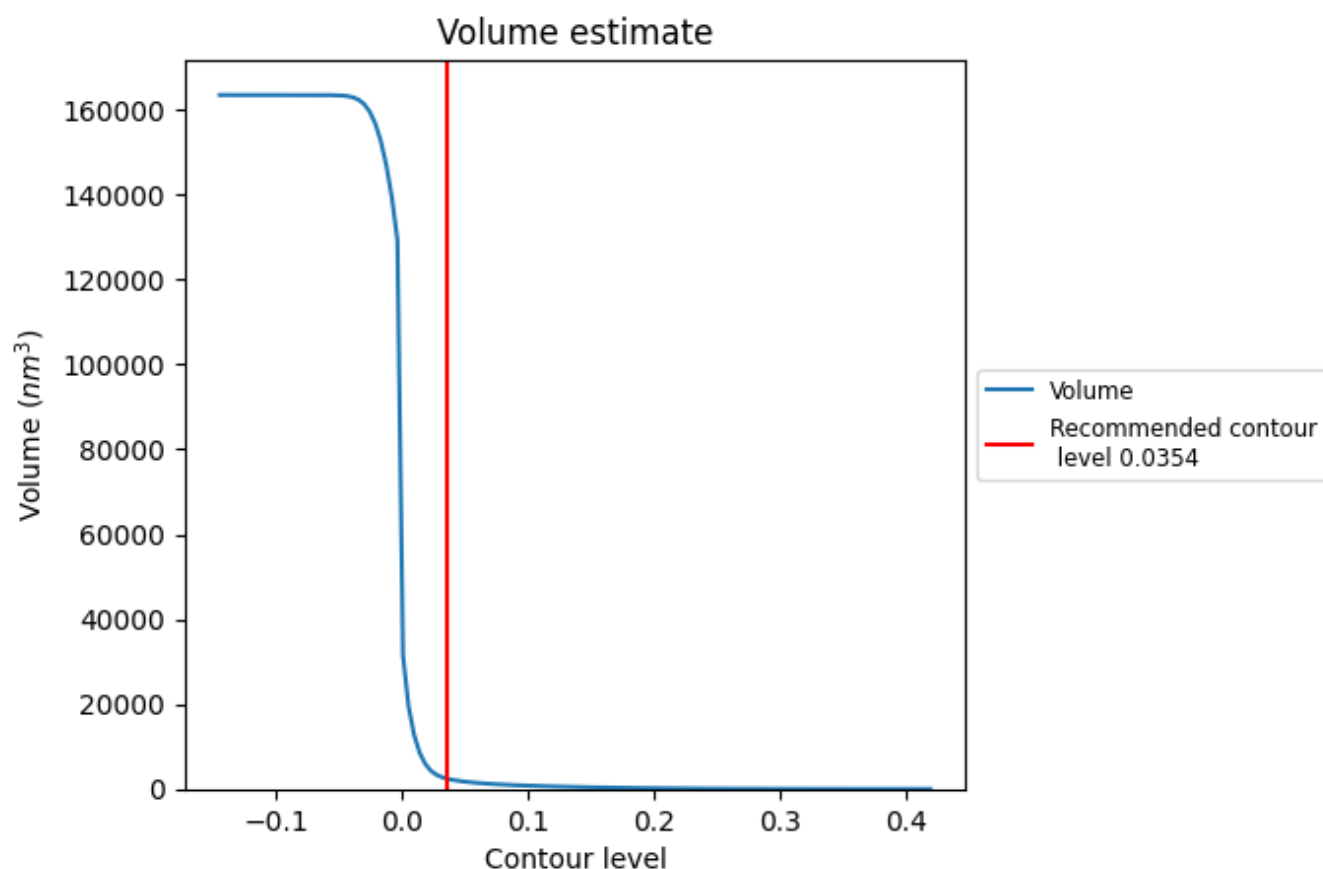
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

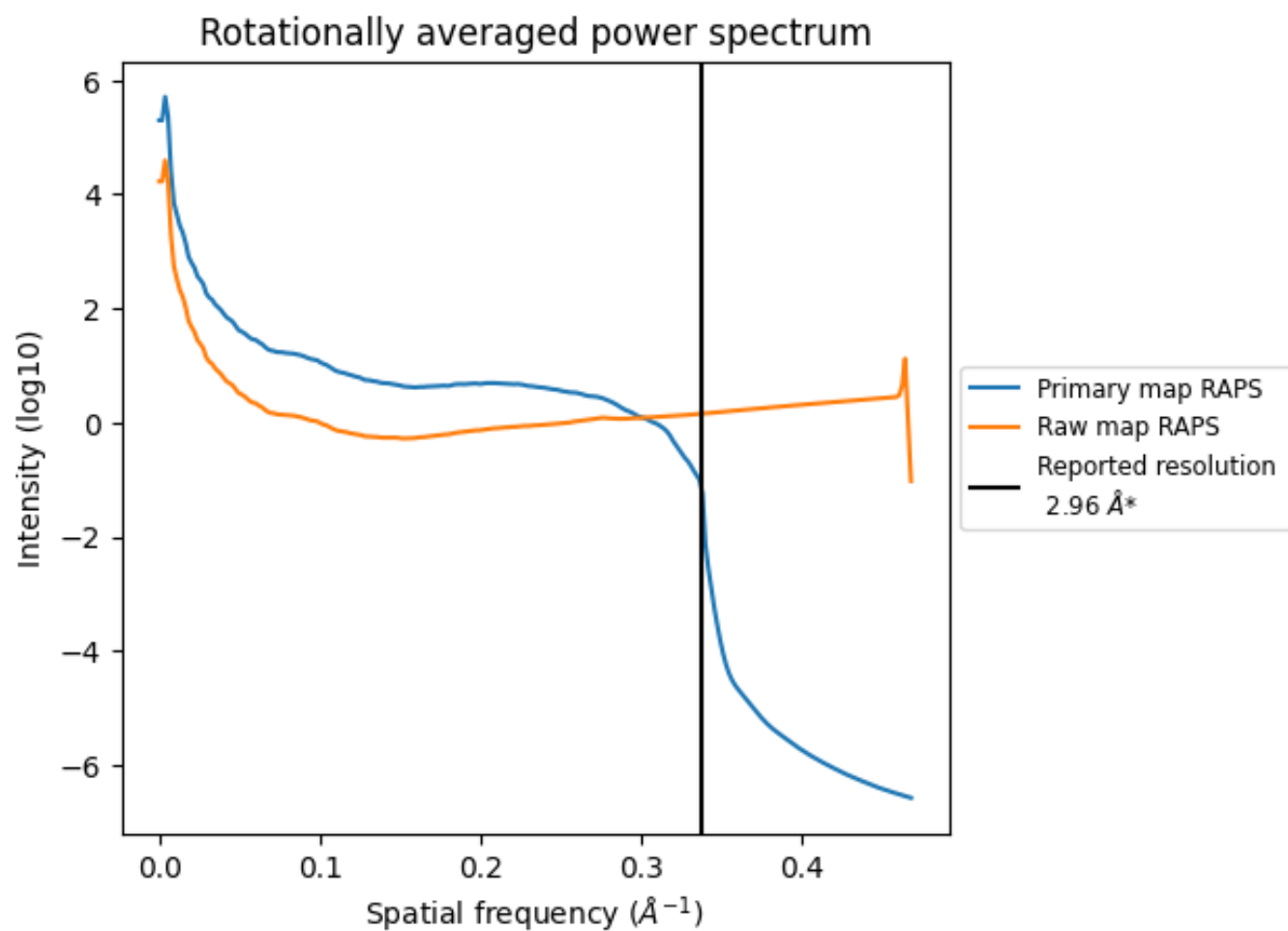
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2437 nm³; this corresponds to an approximate mass of 2202 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

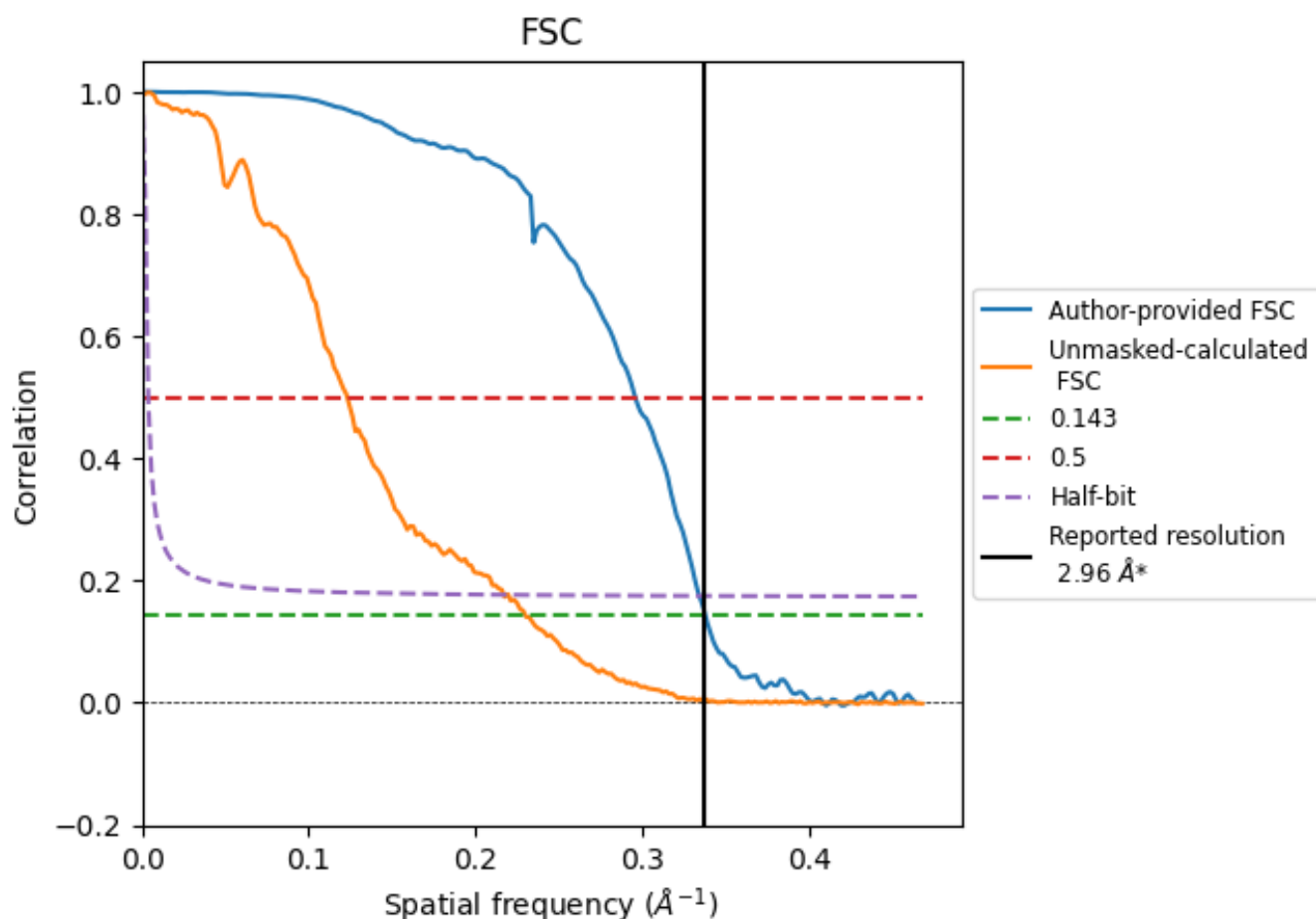


*Reported resolution corresponds to spatial frequency of 0.338 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.338 Å⁻¹

8.2 Resolution estimates [i](#)

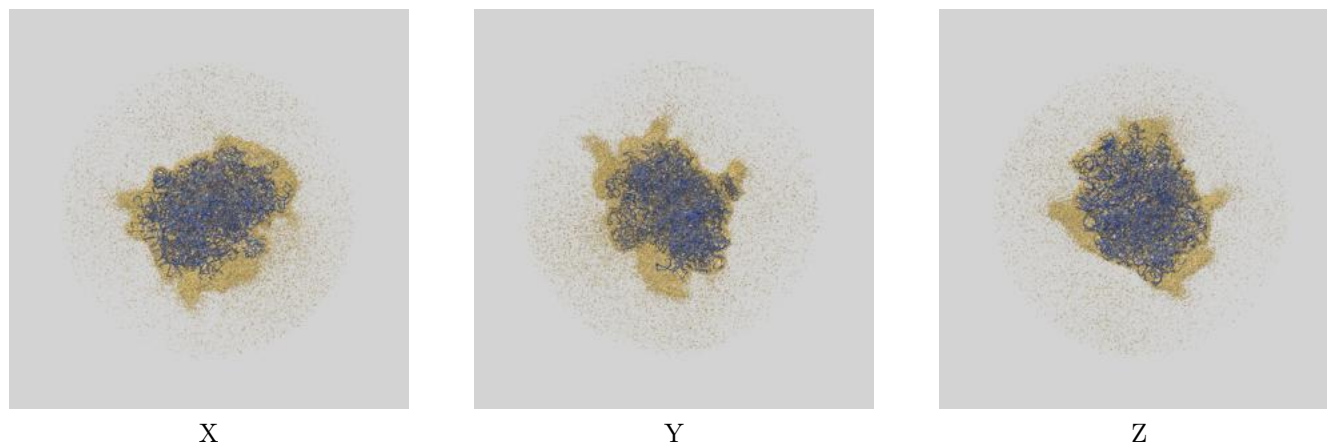
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.96	-	-
Author-provided FSC curve	2.96	3.38	2.99
Unmasked-calculated*	4.35	8.13	4.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.35 differs from the reported value 2.96 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-71414 and PDB model 9P9K. Per-residue inclusion information can be found in [section 3](#) on [page 15](#).

9.1 Map-model overlay [i](#)



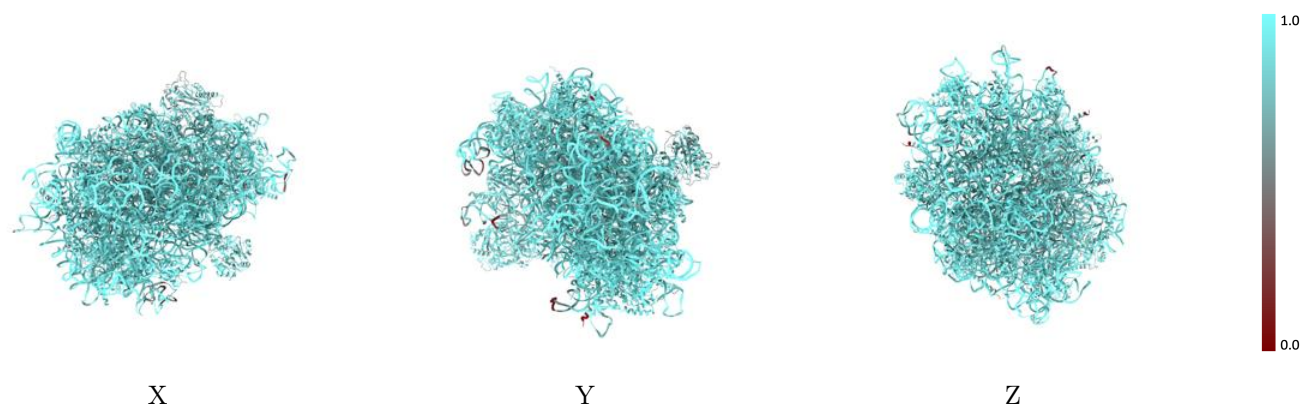
The images above show the 3D surface view of the map at the recommended contour level 0.0354 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



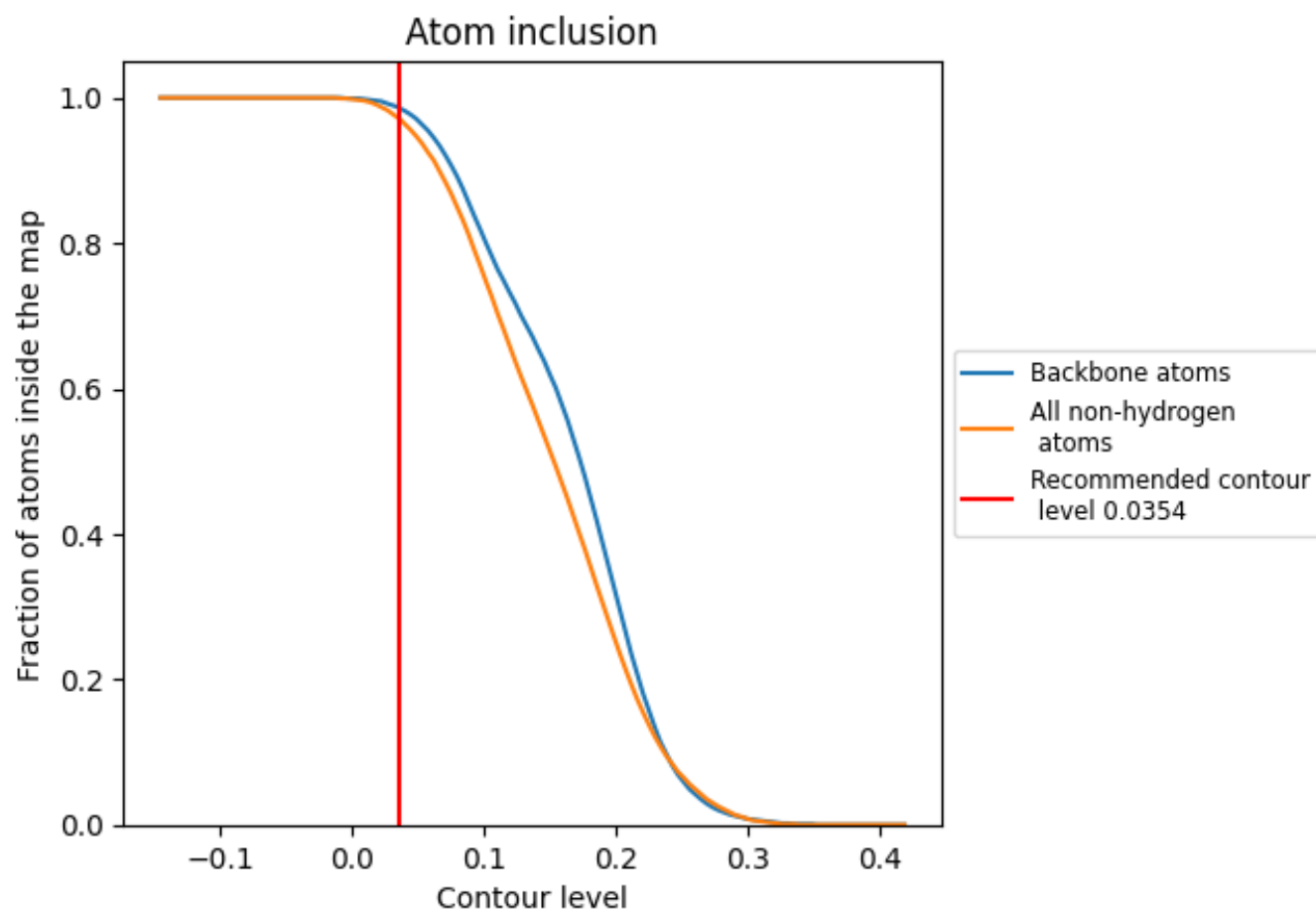
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0354).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 97% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0354) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9720	 0.4870
CA	 0.7660	 0.2560
L5	 0.9840	 0.4770
L7	 1.0000	 0.5260
L8	 0.9920	 0.5100
LA	 0.9860	 0.5510
LB	 0.9630	 0.5330
LC	 0.9670	 0.5350
LD	 0.9650	 0.4800
LE	 0.9480	 0.4670
LF	 0.9780	 0.5350
LG	 0.9290	 0.4690
LH	 0.9720	 0.5180
LI	 0.9510	 0.5140
LJ	 0.9390	 0.4360
LL	 0.9500	 0.5060
LM	 0.9710	 0.5080
LN	 0.9950	 0.5700
LO	 0.9690	 0.5320
LP	 0.9780	 0.5490
LQ	 0.9800	 0.5570
LR	 0.9730	 0.5160
LS	 0.9840	 0.5550
LT	 0.9680	 0.5200
LU	 0.9340	 0.3940
LV	 0.9650	 0.5250
LX	 0.9660	 0.5200
LY	 0.9670	 0.5270
LZ	 0.9790	 0.5080
La	 0.9810	 0.5630
Lb	 0.9220	 0.4640
Lc	 0.9480	 0.4820
Ld	 0.9630	 0.5080
Le	 0.9830	 0.5530
Lf	 0.9870	 0.5570



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Chain	Atom inclusion	Q-score
Lg	 0.9680	 0.5180
Lh	 0.9540	 0.5100
Li	 0.9600	 0.5020
Lj	 0.9870	 0.5570
Lk	 0.9280	 0.4490
Ll	 0.9880	 0.5470
Lm	 0.9540	 0.5260
Lo	 0.9620	 0.5240
Lp	 0.9700	 0.5240
Lr	 0.9750	 0.5450
P	 0.8790	 0.3410