



wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 12:21 PM JST

PDB ID : 7F5S / pdb_00007f5s
EMDB ID : EMD-31465
Title : human delta-METTL18 60S ribosome
Authors : Takahashi, M.; Kashiwagi, K.; Ito, T.
Deposited on : 2021-06-22
Resolution : 2.72 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.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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) : 2.49

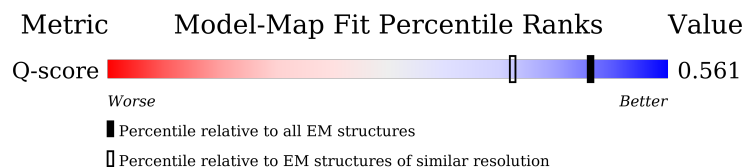
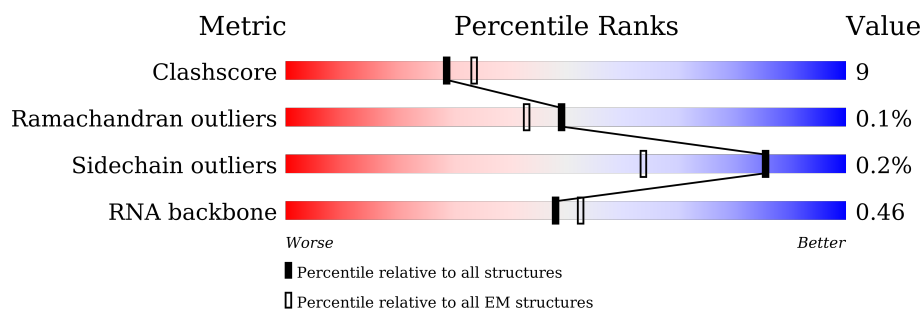
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

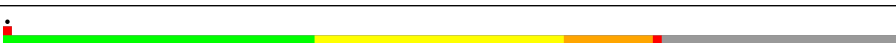
The reported resolution of this entry is 2.72 Å.

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.



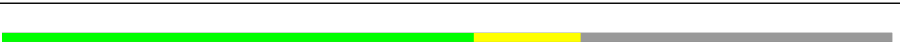
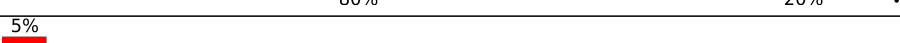
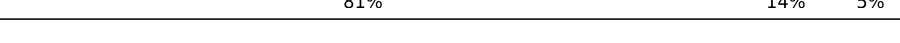
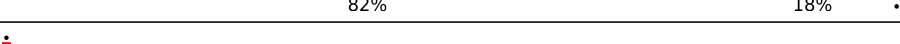
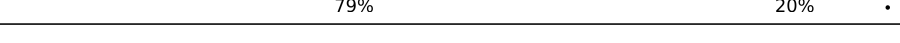
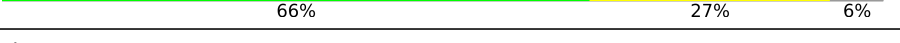
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10355 (2.22 - 3.22)

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	LA	257	
2	LB	403	
3	L5	5070	

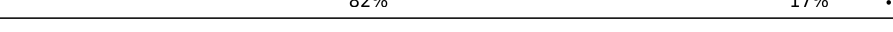
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Mol	Chain	Length	Quality of chain
4	L7	120	
5	L8	156	
6	LC	427	
7	LD	297	
8	LE	288	
9	LF	248	
10	LG	266	
11	LH	192	
12	LI	214	
13	LJ	178	
14	LL	211	
15	LM	215	
16	LN	204	
17	LO	203	
18	LP	184	
19	LQ	188	
20	LR	196	
21	LS	176	
22	LT	160	
23	LU	128	
24	LV	140	
25	LW	157	
26	LX	156	
27	LY	145	
28	LZ	136	

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Mol	Chain	Length	Quality of chain
29	La	148	 79%20%
30	Lb	159	 51%17%32%
31	Lc	115	 70%16%15%
32	Ld	125	 63%22%14%
33	Le	135	 70%25%5%
34	Lf	110	 80%16%...
35	Lg	117	 82%15%.
36	Lh	123	 80%20%.
37	Li	105	 84%13%.
38	Lj	97	 74%12%11%
39	Lk	70	 71%27%.
40	Ll	51	 73%25%.
41	Lm	128	 35%5%59%
42	Ln	25	 88%8%.
43	Lo	106	 72%25%.
44	Lp	92	 82%17%.
45	Lr	137	 72%19%9%

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 138619 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 60S ribosomal protein L8.

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

- Molecule 2 is a protein called 60S ribosomal protein L3.

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

- Molecule 3 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	L5	3715	Total	C	N	O	P	0	0
			79671	35522	14563	25871	3715		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L5	3818	UY1	U	conflict	GB NR_003287

- Molecule 4 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L7	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 5 is a RNA chain called 5.8S rRNA.

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

- 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
			2928	1841	583	489	15		

- Molecule 7 is a protein called 60S ribosomal protein L5.

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 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	LE	223	Total	C	N	O	S	0	0
			1791	1153	338	296	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	240	Total	C	N	O	S	0	0
			1922	1226	370	322	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 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LI	204	Total	C	N	O	S	0	0
			1656	1052	319	272	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LJ	175	Total	C	N	O	S	0	0
			1401	882	261	252	6		

- Molecule 14 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LL	208	Total	C	N	O	S	0	0
			1682	1052	348	278	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	200	Total	C	N	O	S	0	0
			1641	1058	320	258	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	187	Total	C	N	O	S	0	0
			1566	971	336	250	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 60S ribosomal protein L22.

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 L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LW	76	Total	C	N	O	S	0	0
			639	403	128	105	3		

- Molecule 26 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LX	119	Total	C	N	O	S	0	0
			976	624	183	168	1		

- Molecule 27 is a protein called 60S ribosomal protein L26.

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

- Molecule 28 is a protein called 60S ribosomal protein L27.

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

- Molecule 29 is a protein called 60S ribosomal protein L27a.

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

- Molecule 30 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lb	108	Total	C	N	O	S	0	0
			877	546	191	136	4		

- Molecule 31 is a protein called 60S ribosomal protein L30.

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

- Molecule 32 is a protein called 60S ribosomal protein L31.

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

- Molecule 33 is a protein called 60S ribosomal protein L32.

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

- Molecule 34 is a protein called 60S ribosomal protein L35a.

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

- Molecule 35 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Lg	113	Total	C	N	O	S	0	0
			897	560	185	146	6		

- Molecule 36 is a protein called 60S ribosomal protein L35.

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

- Molecule 37 is a protein called 60S ribosomal protein L36.

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

- Molecule 38 is a protein called 60S ribosomal protein L37.

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

- Molecule 39 is a protein called 60S ribosomal protein L38.

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

- Molecule 40 is a protein called 60S ribosomal protein L39.

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

- Molecule 41 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Lm	52	Total	C	N	O	S	0	0
			430	267	90	67	6		

- Molecule 42 is a protein called 60S ribosomal protein L41.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Ln	24	Total	C	N	O	S	0	0
			230	139	62	26	3		

- Molecule 43 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Lo	103	Total	C	N	O	S	0	0
			842	528	172	136	6		

- Molecule 44 is a protein called 60S ribosomal protein L37a.

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

- Molecule 45 is a protein called 60S ribosomal protein L28.

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

- Molecule 46 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
46	LA	1	Total	Mg	0
			1	1	
46	L5	260	Total	Mg	0
			260	260	
46	L7	3	Total	Mg	0
			3	3	
46	L8	5	Total	Mg	0
			5	5	
46	LI	2	Total	Mg	0
			2	2	
46	LN	1	Total	Mg	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
46	LP	1	Total 1	Mg 1	0
46	LR	1	Total 1	Mg 1	0
46	LS	1	Total 1	Mg 1	0
46	LV	1	Total 1	Mg 1	0
46	Le	1	Total 1	Mg 1	0
46	Lf	1	Total 1	Mg 1	0
46	Lg	1	Total 1	Mg 1	0

- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 48 is water.

Mol	Chain	Residues	Atoms		AltConf
48	L5	11	Total 11	O 11	0
48	LH	1	Total 1	O 1	0
48	La	2	Total 2	O 2	0
48	Lb	1	Total 1	O 1	0
48	Le	1	Total 1	O 1	0

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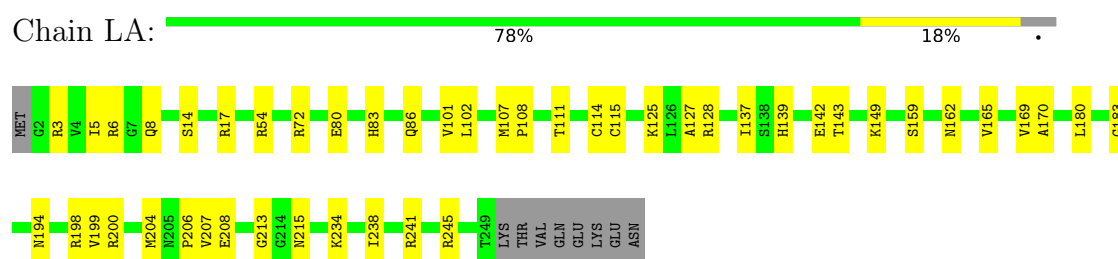
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Mol	Chain	Residues	Atoms		AltConf
48	Lf	1	Total	O	0
			1	1	
48	Lm	1	Total	O	0
			1	1	

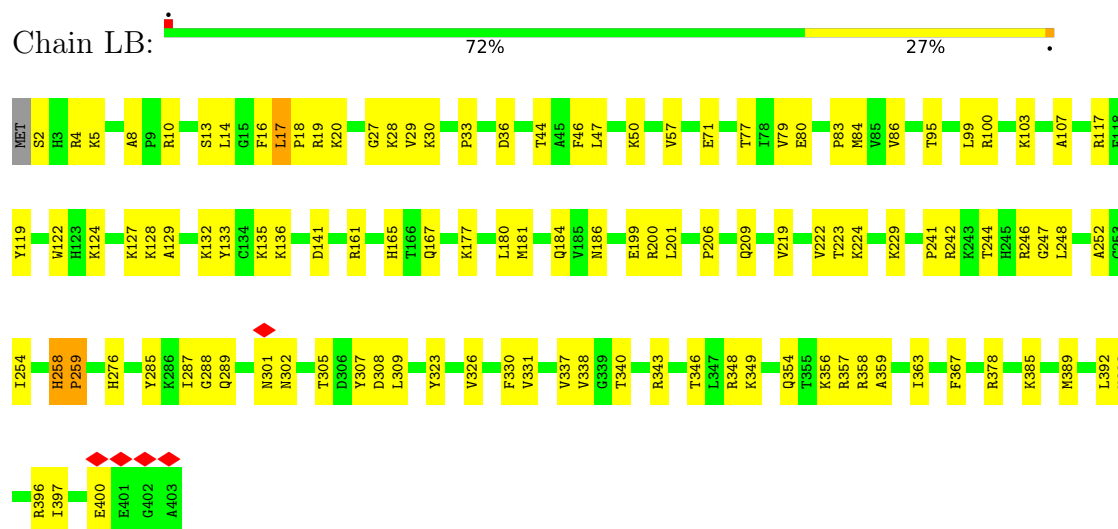
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

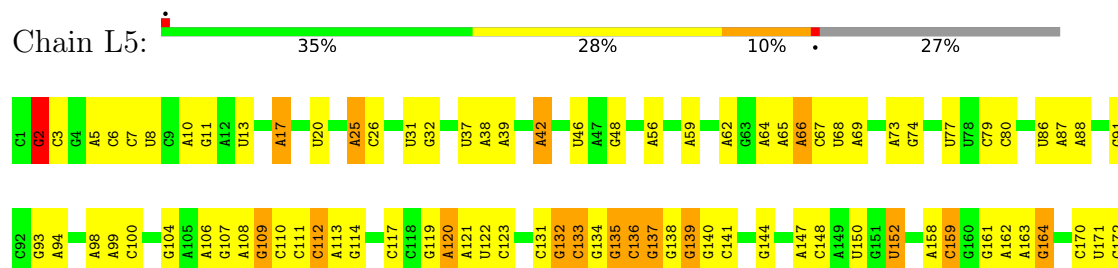
• Molecule 1: 60S ribosomal protein L8



• Molecule 2: 60S ribosomal protein L3



• Molecule 3: 28S rRNA



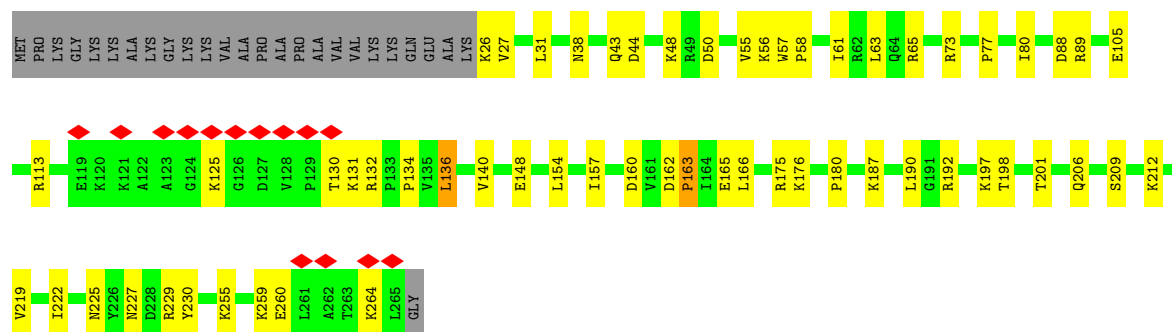
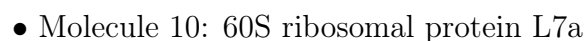
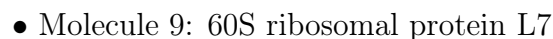


G2397	G2297	C	G	U2097	G2007	C1936	G1855	G1761	C1892	G1502	U1410	A1326
U2298	U2298	C	G	G2098	U2008	C1937	G1856	C1762	U1693	A1503	C1411	C1327
G2299	G2299	C	G	G2099	A2009	A1941	C1857	G1763	C1894	G1504	C1414	G1328
A2401	A2300	U	C	A2100	A2010	A1942	C1858	G1764	U1695	C1415	G1416	C1332
G2402	G2301	C	G	G2101	A1943	A1943	C1859	A1766	G1697	A1333	C1417	A1334
G2406	G2302	C	G	G2102	A2012	A1944	U1860	A1767	C1698	U1339	G1418	U1339
G2407	C2303	U	C	G2103	A2013	U1947	U1861	G1768	A1699	C1340	A1420	C1340
C2411	G2306	C	G	G2104	C2014	G1948	U1862	G1769	G1700	U1511	G1419	U1341
A2412	A2105	C	G	G2105	U2015	G1949	U1863	U1770	U1701	G1512	A1426	A1342
G2414	G2106	C	G	G2106	C2016	U1950	U1867	U1771	C1702	U1513	G1426	A1342
U2415	A2313	C	G	G2107	A2017	G1951	U1866	C1772	G1703	U1514	G1426	A1342
G2416	G2316	C	G	G2108	C2018	G1951	A1867	C1773	C1704	A1515	G1431	A1345
A2417	G2317	C	G	G2109	U2019	U1959	A1868	U1774	G1705	G1516	C1431	C1346
G2421	G2318	A	G	G2110	G2021	A1960	G1869	A1775	A1706	G1517	A1433	G1347
C2422	G2321	C	G	G2111	C2022	G1961	C1870	U1776	G1707	A1518	G1434	U1348
A2423	G2322	C	G	G	C2023	A1962	A1871	C1778	G1708	G1522	G1435	G1349
G2424	G2323	C	G	G	C2024	C1963	G1872	U1779	C1709	A1523	C1436	C1350
U2426	A2332	C	G	G	A2025	G1966	A1873	U1780	A	G1524	C1437	G1351
G2434	G2333	C	G	G	A2026	A1967	A1874	U1781	C	A1534	U1440	A1354
G2435	C2334	C	G	G	G2029	G1968	C1875	U1782	C	C1535	C1441	G1355
U2436	G2335	C	G	G	A2030	G1969	U1876	C1783	C	U1536	C1442	U1356
G2437	C2336	U	C	G	G	A1970	G1877	U1787	G1718	A1537	A1443	G1357
U2438	C2337	C	G	G	A2033	C1971	C1881	A1788	A1719	C1538	U1444	G1358
U2439	C2338	C	G	G	G2034	G1972	U1882	U1789	C1720	A1539	U1445	G1359
U2440	G2345	C	G	G	G	G1973	G1883	A1793	C1721	G1539	C1446	G1360
G2441	A2346	C	G	G	G	U1974	U1889	U1802	C1722	A1547	C1447	U1364
U2442	G2347	C	G	G	G	G1975	G1890	G1803	U1725	G1548	C1448	C1365
U2443	A2347	C	G	G	G	G1976	A1891	A1804	U1726	G1552	C1449	G1366
U2444	G2348	C	G	G	G	C1977	A1892	A1805	U1727	A1553	C1450	C1367
U2445	A2349	C	G	G	G	G1978	C1893	A1807	U1728	A1554	G1451	G1370
U2446	U2350	C	G	G	G	U1980	G1894	U1807	U1729	A1558	C1456	G1376
G2447	C2351	C	G	G	G	G1981	G1895	G1810	U1730	G1559	C1457	G1377
U2448	U2352	C	G	G	G	G1982	A1896	G1811	G1733	A1564	C1458	A1387
G2449	G2353	C	G	G	G	A1983	A1897	U1815	G1734	A1565	C1460	U1388
U2450	A2453	C	G	G	G	A1984	C1898	U1816	U1735	C1566	C1461	U1389
G2451	G2360	C	G	G	G	G1985	G1899	G1817	G1739	U1567	C1462	A1392
U2452	U2362	C	G	G	G	U1986	G1909	G1818	C1740	C1568	C1464	G1393
G2453	A2363	C	G	G	G	C1987	C1910	G1819	G1741	G1574	G1475	G1394
U2454	G2364	C	G	G	G	G1988	G1911	G1820	A1742	U1577	C1476	A1397
G2455	C2365	C	G	G	G	G1989	C1912	G1821	U1743	U1578	C1479	A1398
U2456	A2368	C	G	G	G	A1990	A1917	G1822	G1745	C1674	C1480	G1399
G2457	G2369	C	G	G	G	A1991	U1918	U1833	A1749	U1582	C1481	G1400
U2458	U2372	C	G	G	G	G1992	U1919	G1834	G1750	G1586	C1482	C1401
G2459	C2373	C	G	G	G	U1993	C1920	G1835	U1753	G1587	C1483	C1402
U2460	G2376	C	G	G	G	C1994	G1921	G1836	G1754	C1588	G1490	G1403
G2461	C2377	C	G	G	G	G1995	G1922	U1837	U1755	U1589	C1404	C1405
U2462	U2378	C	G	G	G	U1996	G1923	G1842	U1756	C1589	G1406	G1406
G2463	G2379	C	G	G	G	U1997	G1924	A1843	U1757	C1590	C1407	G1407
U2464	C2380	C	G	G	G	A1998	G1925	U1844	G1758	U1591	G1408	G1408
G2465	G2381	C	G	G	G	U1999	G1926	U1845	G1759	U1596	A1500	C1409
U2466	A2382	C	G	G	G	G2000	C1931	G1846	G1760		C1501	
G2467	G2383	C	G	G	G	G2001	A1832	U1847				
U2468	C2384	C	G	G	G	G2002	G1933	C1847				
G2469	G2385	C	G	G	G	G2003	A1934	C1848				
U2470	U2386	C	G	G	G	U2004	C1935					
G2471	G2387	C	G	G	G	G2005						
U2472	A2388	C	G	G	G	U2006						
G2473	G2389	C	G	G	G							
U2474	A2390	C	G	G	G							
G2475	G2391	C	G	G	G							
U2476	C2392	C	G	G	G							
G2477	G2393	C	G	G	G							
U2478	A2394	C	G	G	G							
G2479	G2395	C	G	G	G							
U2480	U2396	C	G	G	G							
G2481	G2397	C	G	G	G							
U2482	A2398	C	G	G	G							
G2483	G2399	C	G	G	G							
A2484	U2400	C	G	G	G							

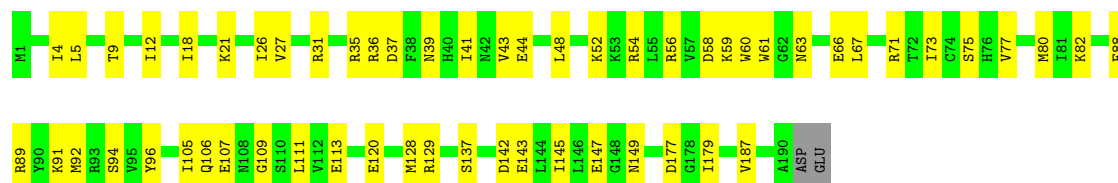




Chain LE:



Chain LH: 69% 30%





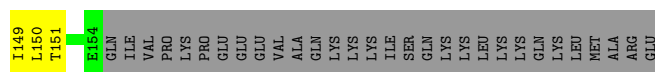
- Molecule 17: 60S ribosomal protein L13a

Chain LO: 76% 22%



- Molecule 18: 60S ribosomal protein L17

Chain LP: 63% 20% 17%



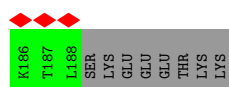
- Molecule 19: 60S ribosomal protein L18

Chain LQ: 80% 20%



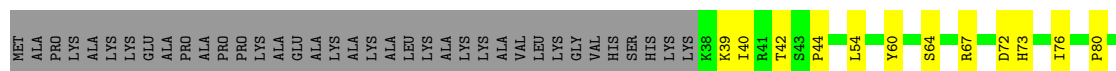
- Molecule 20: 60S ribosomal protein L19

Chain LR: 5% 81% 14% 5%



- Molecule 21: 60S ribosomal protein L18a

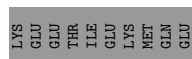
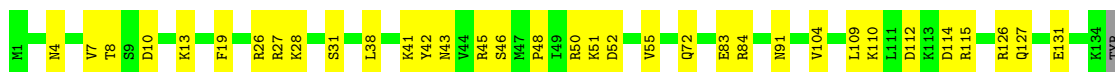
Chain LS: 82% 18%





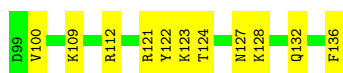
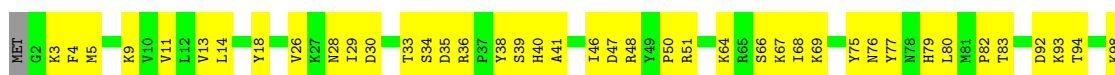
- Molecule 27: 60S ribosomal protein L26

Chain LY: 69% 23% 8%



- Molecule 28: 60S ribosomal protein L27

Chain LZ: 61% 38% .



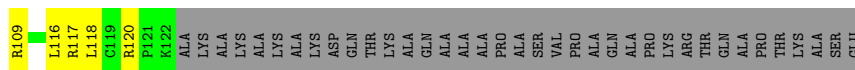
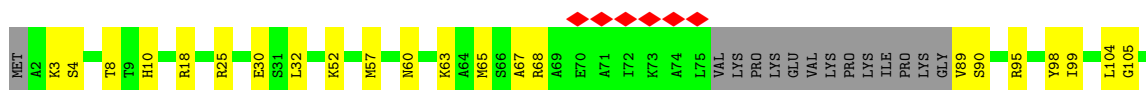
- Molecule 29: 60S ribosomal protein L27a

Chain La: 79% 20% .



- Molecule 30: 60S ribosomal protein L29

Chain Lb: 51% 17% 32%



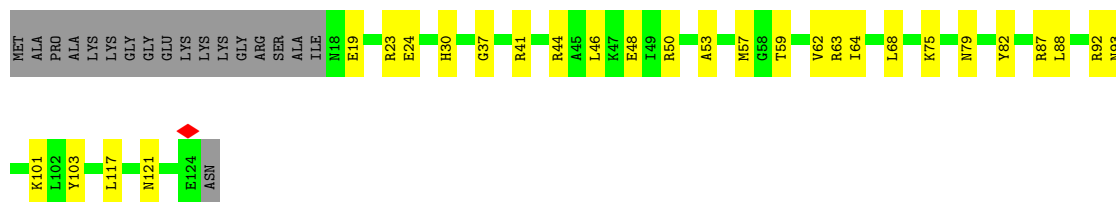
- Molecule 31: 60S ribosomal protein L30

Chain Lc: 70% 16% 15%



- Molecule 32: 60S ribosomal protein L31

Chain Ld: 



- Molecule 33: 60S ribosomal protein L32

Chain Le: 



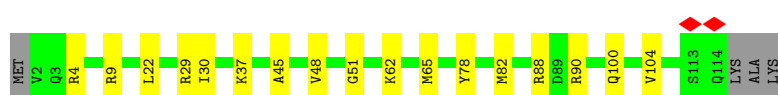
- Molecule 34: 60S ribosomal protein L35a

Chain Lf: 



- Molecule 35: 60S ribosomal protein L34

Chain Lg: 



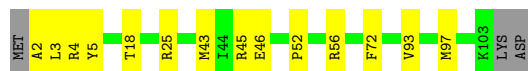
- Molecule 36: 60S ribosomal protein L35

Chain Lh: 



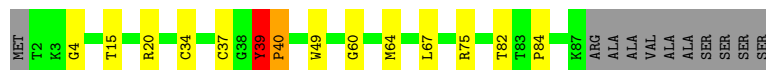
- Molecule 37: 60S ribosomal protein L36

Chain Li: 



- Molecule 38: 60S ribosomal protein L37

Chain Lj:  74% 12% .. 11%



- Molecule 39: 60S ribosomal protein L38

Chain Lk:  71% 27% .



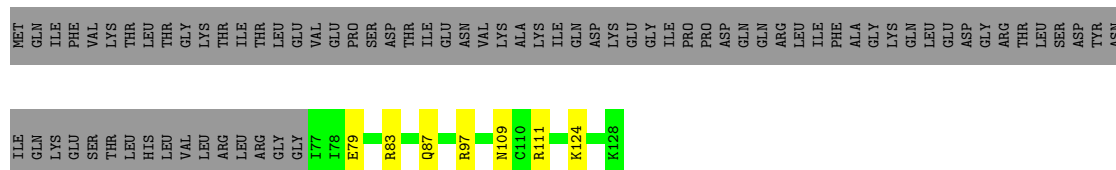
- Molecule 40: 60S ribosomal protein L39

Chain Ll:  73% 25% .



- Molecule 41: Ubiquitin-60S ribosomal protein L40

Chain Lm:  35% 5% 59%



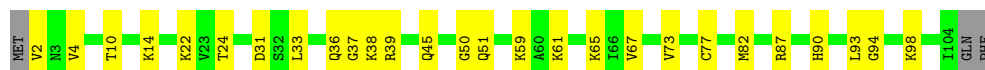
- Molecule 42: 60S ribosomal protein L41

Chain Ln:  88% 8% .



- Molecule 43: 60S ribosomal protein L36a

Chain Lo:  72% 25% .

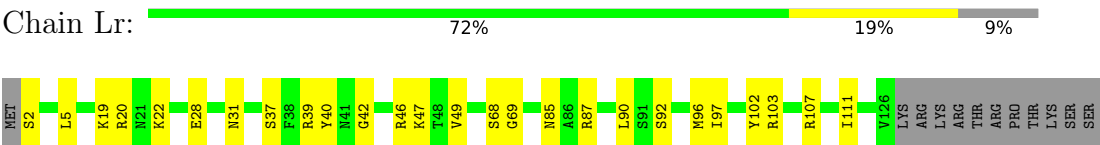


- Molecule 44: 60S ribosomal protein L37a

Chain Lp:  82% 17% .



● Molecule 45: 60S ribosomal protein L28



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	118470	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TECNAI ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	32.789	Depositor
Minimum map value	-7.797	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.5	Depositor
Map size (Å)	485.0, 485.0, 485.0	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: JMH, ZN, MLZ, OMG, UY1, A2M, 2MG, MG, PSU, 5MU, 5MC, 6MZ, OMU, B8T, UR3, OMC, 1MA

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	LA	0.50	0/1936	0.53	0/2596
2	LB	0.51	0/3306	0.61	7/4424 (0.2%)
3	L5	0.48	1/85750 (0.0%)	0.42	82/133763 (0.1%)
4	L7	0.48	0/2858	0.30	0/4455
5	L8	0.49	0/3679	0.33	0/5732
6	LC	0.48	0/2971	0.52	0/3988
7	LD	0.41	0/2428	0.49	0/3252
8	LE	0.40	0/1825	0.67	3/2448 (0.1%)
9	LF	0.49	0/1905	0.51	0/2539
10	LG	0.45	0/1955	0.61	2/2632 (0.1%)
11	LH	0.42	0/1537	0.50	0/2066
12	LI	0.48	0/1694	0.54	0/2261
13	LJ	0.38	0/1424	0.59	2/1904 (0.1%)
14	LL	0.44	0/1713	0.52	0/2293
15	LM	0.43	0/1161	0.48	0/1554
16	LN	0.53	0/1746	0.55	0/2338
17	LO	0.48	0/1673	0.47	0/2238
18	LP	0.49	0/1268	0.49	0/1701
19	LQ	0.50	0/1537	0.53	1/2052 (0.0%)
20	LR	0.40	0/1582	0.48	1/2091 (0.0%)
21	LS	0.48	0/1493	0.45	0/2003
22	LT	0.45	0/1326	0.47	0/1770
23	LU	0.35	0/839	0.57	1/1126 (0.1%)
24	LV	0.49	0/993	0.56	0/1332
25	LW	0.37	0/652	0.47	0/866
26	LX	0.40	0/993	0.41	0/1334
27	LY	0.46	0/1132	0.50	0/1504
28	LZ	0.40	0/1130	0.45	0/1507
29	La	0.51	0/1191	0.49	0/1591
30	Lb	0.35	0/890	0.50	0/1175
31	Lc	0.41	0/774	0.46	0/1038

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ld	0.45	0/903	0.46	0/1216
33	Le	0.50	0/1071	0.50	0/1429
34	Lf	0.52	0/895	0.71	3/1198 (0.3%)
35	Lg	0.56	0/907	0.71	1/1209 (0.1%)
36	Lh	0.40	0/1023	0.43	0/1351
37	Li	0.35	0/843	0.45	0/1115
38	Lj	0.54	0/720	0.69	2/952 (0.2%)
39	Lk	0.35	0/575	0.41	0/761
40	Ll	0.47	0/454	0.51	0/599
41	Lm	0.42	0/425	0.53	0/561
42	Ln	0.35	0/231	0.53	0/294
43	Lo	0.44	0/855	0.50	0/1128
44	Lp	0.46	0/718	0.47	0/953
45	Lr	0.47	0/1017	0.49	0/1364
All	All	0.48	1/145998 (0.0%)	0.45	105/215703 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	1326	A2M	O3'-P	6.47	1.62	1.56

The worst 5 of 105 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	3921	U	C1'-C2'-O2'	-15.04	85.84	108.40
8	LE	101	ASN	N-CA-C	-15.02	95.60	112.72
34	Lf	104	MET	N-CA-C	13.28	129.70	113.23
3	L5	1783	C	C1'-C2'-O2'	-12.53	89.61	108.40
3	L5	3731	C	C1'-C2'-O2'	-12.24	90.04	108.40

There are no chirality outliers.

There are no planarity outliers.

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	LA	1898	0	1993	42	0
2	LB	3238	0	3376	87	0
3	L5	79671	0	40317	1311	0
4	L7	2558	0	1296	17	0
5	L8	3315	0	1685	60	0
6	LC	2928	0	3105	64	0
7	LD	2382	0	2410	50	0
8	LE	1791	0	1947	46	0
9	LF	1870	0	1996	48	0
10	LG	1922	0	2071	44	0
11	LH	1518	0	1601	43	0
12	LI	1656	0	1706	36	0
13	LJ	1401	0	1428	45	0
14	LL	1682	0	1792	40	0
15	LM	1138	0	1204	20	0
16	LN	1701	0	1749	41	0
17	LO	1641	0	1788	36	0
18	LP	1242	0	1269	23	0
19	LQ	1513	0	1628	28	0
20	LR	1566	0	1729	22	0
21	LS	1453	0	1490	22	0
22	LT	1298	0	1366	30	0
23	LU	825	0	850	34	0
24	LV	979	0	1039	28	0
25	LW	639	0	663	9	0
26	LX	976	0	1053	22	0
27	LY	1115	0	1205	24	0
28	LZ	1107	0	1182	40	0
29	La	1162	0	1213	25	0
30	Lb	877	0	957	32	0
31	Lc	764	0	804	12	0
32	Ld	888	0	930	19	0
33	Le	1053	0	1147	29	0
34	Lf	876	0	912	15	0
35	Lg	897	0	985	14	0
36	Lh	1015	0	1148	23	0
37	Li	832	0	917	13	0
38	Lj	705	0	737	12	0
39	Lk	569	0	637	16	0
40	Ll	444	0	483	14	0
41	Lm	430	0	465	7	0
42	Ln	230	0	276	1	0
43	Lo	842	0	912	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	Lp	708	0	756	13	0
45	Lr	1002	0	1068	21	0
46	L5	260	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	2	0	0	0	0
46	LN	1	0	0	0	0
46	LP	1	0	0	0	0
46	LR	1	0	0	0	0
46	LS	1	0	0	0	0
46	LV	1	0	0	0	0
46	Le	1	0	0	0	0
46	Lf	1	0	0	0	0
46	Lg	1	0	0	0	0
47	Lg	1	0	0	0	0
47	Lj	1	0	0	0	0
47	Lm	1	0	0	0	0
47	Lo	1	0	0	0	0
47	Lp	1	0	0	0	0
48	L5	11	0	0	0	0
48	LH	1	0	0	0	0
48	La	2	0	0	0	0
48	Lb	1	0	0	0	0
48	Le	1	0	0	0	0
48	Lf	1	0	0	0	0
48	Lm	1	0	0	0	0
All	All	138619	0	99285	2197	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 9.

The worst 5 of 2197 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)
3:L5:4576:PSU:H6	3:L5:4576:PSU:H5"	1.13	1.10
30:Lb:89:VAL:HG12	30:Lb:90:SER:N	1.64	1.09
30:Lb:89:VAL:CG1	30:Lb:90:SER:H	1.66	1.09
30:Lb:89:VAL:HG12	30:Lb:90:SER:H	0.84	1.00
3:L5:4576:PSU:H5"	3:L5:4576:PSU:C6	1.98	0.98

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	LA	246/257 (96%)	220 (89%)	26 (11%)	0	100	100
2	LB	400/403 (99%)	375 (94%)	25 (6%)	0	100	100
6	LC	365/427 (86%)	336 (92%)	28 (8%)	1 (0%)	36	59
7	LD	291/297 (98%)	276 (95%)	15 (5%)	0	100	100
8	LE	217/288 (75%)	197 (91%)	19 (9%)	1 (0%)	24	46
9	LF	223/248 (90%)	211 (95%)	12 (5%)	0	100	100
10	LG	238/266 (90%)	220 (92%)	17 (7%)	1 (0%)	30	52
11	LH	188/192 (98%)	175 (93%)	13 (7%)	0	100	100
12	LI	200/214 (94%)	187 (94%)	13 (6%)	0	100	100
13	LJ	173/178 (97%)	161 (93%)	12 (7%)	0	100	100
14	LL	206/211 (98%)	188 (91%)	18 (9%)	0	100	100
15	LM	137/215 (64%)	131 (96%)	6 (4%)	0	100	100
16	LN	201/204 (98%)	188 (94%)	11 (6%)	2 (1%)	12	30
17	LO	198/203 (98%)	193 (98%)	5 (2%)	0	100	100
18	LP	151/184 (82%)	142 (94%)	9 (6%)	0	100	100
19	LQ	185/188 (98%)	178 (96%)	7 (4%)	0	100	100
20	LR	185/196 (94%)	181 (98%)	4 (2%)	0	100	100
21	LS	173/176 (98%)	162 (94%)	11 (6%)	0	100	100
22	LT	157/160 (98%)	148 (94%)	9 (6%)	0	100	100
23	LU	99/128 (77%)	84 (85%)	15 (15%)	0	100	100
24	LV	129/140 (92%)	122 (95%)	7 (5%)	0	100	100
25	LW	74/157 (47%)	67 (90%)	7 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	LX	117/156 (75%)	116 (99%)	1 (1%)	0	100	100
27	LY	132/145 (91%)	124 (94%)	8 (6%)	0	100	100
28	LZ	133/136 (98%)	123 (92%)	10 (8%)	0	100	100
29	La	145/148 (98%)	137 (94%)	8 (6%)	0	100	100
30	Lb	104/159 (65%)	97 (93%)	7 (7%)	0	100	100
31	Lc	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
32	Ld	105/125 (84%)	95 (90%)	10 (10%)	0	100	100
33	Le	126/135 (93%)	119 (94%)	7 (6%)	0	100	100
34	Lf	107/110 (97%)	101 (94%)	5 (5%)	1 (1%)	14	33
35	Lg	111/117 (95%)	111 (100%)	0	0	100	100
36	Lh	120/123 (98%)	117 (98%)	3 (2%)	0	100	100
37	Li	100/105 (95%)	94 (94%)	6 (6%)	0	100	100
38	Lj	84/97 (87%)	78 (93%)	4 (5%)	2 (2%)	4	11
39	Lk	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
40	Ll	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
41	Lm	49/128 (38%)	47 (96%)	2 (4%)	0	100	100
42	Ln	22/25 (88%)	21 (96%)	1 (4%)	0	100	100
43	Lo	101/106 (95%)	97 (96%)	4 (4%)	0	100	100
44	Lp	89/92 (97%)	85 (96%)	4 (4%)	0	100	100
45	Lr	123/137 (90%)	112 (91%)	11 (9%)	0	100	100
All	All	6415/7212 (89%)	6018 (94%)	389 (6%)	8 (0%)	49	72

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	LC	222	ARG
8	LE	100	LYS
16	LN	124	ASP
34	Lf	107	PRO
38	Lj	39	TYR

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	LA	190/199 (96%)	190 (100%)	0	100	100
2	LB	348/349 (100%)	348 (100%)	0	100	100
6	LC	305/347 (88%)	305 (100%)	0	100	100
7	LD	246/250 (98%)	246 (100%)	0	100	100
8	LE	197/252 (78%)	195 (99%)	2 (1%)	68	85
9	LF	194/215 (90%)	194 (100%)	0	100	100
10	LG	203/223 (91%)	201 (99%)	2 (1%)	68	85
11	LH	169/171 (99%)	169 (100%)	0	100	100
12	LI	174/181 (96%)	173 (99%)	1 (1%)	78	90
13	LJ	147/149 (99%)	145 (99%)	2 (1%)	59	80
14	LL	174/177 (98%)	174 (100%)	0	100	100
15	LM	118/161 (73%)	118 (100%)	0	100	100
16	LN	171/172 (99%)	171 (100%)	0	100	100
17	LO	172/174 (99%)	172 (100%)	0	100	100
18	LP	134/163 (82%)	134 (100%)	0	100	100
19	LQ	164/165 (99%)	164 (100%)	0	100	100
20	LR	166/175 (95%)	166 (100%)	0	100	100
21	LS	156/157 (99%)	156 (100%)	0	100	100
22	LT	139/140 (99%)	139 (100%)	0	100	100
23	LU	91/115 (79%)	90 (99%)	1 (1%)	65	84
24	LV	101/107 (94%)	101 (100%)	0	100	100
25	LW	67/126 (53%)	67 (100%)	0	100	100
26	LX	107/133 (80%)	107 (100%)	0	100	100
27	LY	124/135 (92%)	124 (100%)	0	100	100
28	LZ	117/118 (99%)	117 (100%)	0	100	100
29	La	120/121 (99%)	120 (100%)	0	100	100
30	Lb	89/126 (71%)	89 (100%)	0	100	100
31	Lc	83/97 (86%)	83 (100%)	0	100	100
32	Ld	98/110 (89%)	98 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	Le	114/121 (94%)	114 (100%)	0	100	100
34	Lf	88/89 (99%)	87 (99%)	1 (1%)	65	84
35	Lg	97/100 (97%)	96 (99%)	1 (1%)	68	85
36	Lh	109/110 (99%)	109 (100%)	0	100	100
37	Li	86/89 (97%)	86 (100%)	0	100	100
38	Lj	73/80 (91%)	73 (100%)	0	100	100
39	Lk	64/65 (98%)	64 (100%)	0	100	100
40	Ll	47/48 (98%)	47 (100%)	0	100	100
41	Lm	47/115 (41%)	46 (98%)	1 (2%)	47	73
42	Ln	23/24 (96%)	23 (100%)	0	100	100
43	Lo	91/94 (97%)	91 (100%)	0	100	100
44	Lp	74/75 (99%)	74 (100%)	0	100	100
45	Lr	109/121 (90%)	109 (100%)	0	100	100
All	All	5586/6139 (91%)	5575 (100%)	11 (0%)	85	95

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	LU	111	GLU
34	Lf	107	PRO
41	Lm	79	GLU
35	Lg	48	VAL
12	LI	203	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
17	LO	50	ASN
23	LU	50	ASN
34	Lf	56	ASN
17	LO	72	HIS
20	LR	141	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	L5	3698/5070 (72%)	895 (24%)	39 (1%)
4	L7	119/120 (99%)	13 (10%)	0
5	L8	155/156 (99%)	30 (19%)	1 (0%)
All	All	3972/5346 (74%)	938 (23%)	40 (1%)

5 of 938 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	L5	2	G
3	L5	13	U
3	L5	17	A
3	L5	25	A
3	L5	39	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	L5	4354	U
3	L5	4699	U
3	L5	4378	A
3	L5	4576	PSU
3	L5	4913	G

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

143 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	$\# Z > 2$
3	A2M	L5	4523	46,3	22,25,26	1.45	5 (22%)	31,36,39	2.13	8 (25%)
3	A2M	L5	1326	3	22,25,26	1.45	5 (22%)	31,36,39	2.01	8 (25%)
3	PSU	L5	4450	46,3	18,21,22	1.47	3 (16%)	22,30,33	2.01	4 (18%)
3	UR3	L5	4530	3	19,22,23	0.91	1 (5%)	26,32,35	1.41	1 (3%)
3	OMG	L5	3944	3	23,26,27	1.35	4 (17%)	33,38,41	1.92	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMU	L5	3925	3	19,22,23	1.93	5 (26%)	26,31,34	2.37	9 (34%)
3	A2M	L5	4571	3	22,25,26	1.48	5 (22%)	31,36,39	2.05	9 (29%)
3	PSU	L5	4579	3	18,21,22	1.96	6 (33%)	22,30,33	2.43	5 (22%)
3	PSU	L5	1782	3	18,21,22	1.92	6 (33%)	22,30,33	2.44	7 (31%)
3	OMC	L5	3887	3	19,22,23	0.88	2 (10%)	26,31,34	0.88	0
3	PSU	L5	4521	46,3	18,21,22	1.54	5 (27%)	22,30,33	2.02	4 (18%)
3	PSU	L5	4420	3	18,21,22	1.45	3 (16%)	22,30,33	2.25	4 (18%)
3	OMG	L5	4196	46,3	23,26,27	1.29	4 (17%)	33,38,41	1.94	6 (18%)
3	OMC	L5	2824	3	19,22,23	0.87	0	26,31,34	0.92	1 (3%)
3	PSU	L5	3637	3	18,21,22	2.21	7 (38%)	22,30,33	2.45	7 (31%)
3	2MG	L5	4872	3	23,26,27	1.36	4 (17%)	32,38,41	2.27	8 (25%)
3	PSU	L5	1677	3	18,21,22	2.02	6 (33%)	22,30,33	2.32	7 (31%)
3	A2M	L5	2787	46,3	22,25,26	1.43	5 (22%)	31,36,39	2.06	9 (29%)
3	OMG	L5	4187	3	23,26,27	1.59	5 (21%)	33,38,41	2.50	13 (39%)
3	PSU	L5	4353	3	18,21,22	1.97	5 (27%)	22,30,33	2.21	6 (27%)
3	PSU	L5	1683	3	18,21,22	1.58	3 (16%)	22,30,33	2.01	4 (18%)
3	A2M	L5	3723	3	22,25,26	1.40	5 (22%)	31,36,39	2.14	10 (32%)
3	OMG	L5	4370	3	23,26,27	1.27	4 (17%)	33,38,41	1.94	7 (21%)
3	PSU	L5	4576	3	18,21,22	1.98	4 (22%)	22,30,33	2.45	9 (40%)
3	OMC	L5	2351	46,3	19,22,23	1.05	2 (10%)	26,31,34	1.22	3 (11%)
3	OMG	L5	373	3	23,26,27	1.30	4 (17%)	33,38,41	2.01	8 (24%)
3	B8T	L5	4483	3	19,22,23	1.05	2 (10%)	26,31,34	0.86	0
3	OMG	L5	4623	3	23,26,27	1.29	4 (17%)	33,38,41	2.00	7 (21%)
3	PSU	L5	2632	3	18,21,22	1.79	5 (27%)	22,30,33	2.24	5 (22%)
3	PSU	L5	4493	46,3	18,21,22	1.91	4 (22%)	22,30,33	2.20	5 (22%)
3	PSU	L5	4689	3	18,21,22	2.15	5 (27%)	22,30,33	2.44	8 (36%)
3	PSU	L5	4293	3	18,21,22	1.57	4 (22%)	22,30,33	1.88	3 (13%)
3	PSU	L5	4673	3	18,21,22	2.00	6 (33%)	22,30,33	2.46	7 (31%)
3	PSU	L5	1860	3	18,21,22	1.88	6 (33%)	22,30,33	2.26	5 (22%)
3	PSU	L5	1536	3	18,21,22	2.14	5 (27%)	22,30,33	2.48	6 (27%)
3	UR3	L5	4597	3	19,22,23	0.91	1 (5%)	26,32,35	1.32	2 (7%)
3	OMG	L5	2424	3	23,26,27	1.30	4 (17%)	33,38,41	1.84	6 (18%)
3	PSU	L5	3734	3	18,21,22	1.43	4 (22%)	22,30,33	2.05	4 (18%)
3	A2M	L5	398	3	22,25,26	1.43	4 (18%)	31,36,39	2.09	7 (22%)
3	OMC	L5	1340	3	19,22,23	0.94	2 (10%)	26,31,34	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMG	L5	2773	3	23,26,27	1.23	4 (17%)	33,38,41	1.92	6 (18%)
3	2MG	L5	1517	3	23,26,27	1.30	4 (17%)	32,38,41	2.32	9 (28%)
3	PSU	L5	4531	3	18,21,22	1.43	2 (11%)	22,30,33	1.95	4 (18%)
3	OMC	L5	2861	3	19,22,23	0.88	2 (10%)	26,31,34	0.85	1 (3%)
3	UY1	L5	3818	46,3	19,22,23	2.56	9 (47%)	22,31,34	1.90	4 (18%)
3	PSU	L5	2843	3	18,21,22	2.01	6 (33%)	22,30,33	2.19	5 (22%)
3	OMU	L5	2837	3	19,22,23	1.68	4 (21%)	26,31,34	2.23	8 (30%)
3	PSU	L5	4471	3	18,21,22	1.99	5 (27%)	22,30,33	2.19	6 (27%)
3	A2M	L5	400	3	22,25,26	1.54	4 (18%)	31,36,39	2.10	10 (32%)
3	PSU	L5	4431	3	18,21,22	1.95	5 (27%)	22,30,33	2.29	6 (27%)
3	OMU	L5	2415	3	19,22,23	1.51	4 (21%)	26,31,34	2.09	7 (26%)
6	MLZ	LC	333	6	8,9,10	0.89	0	4,9,11	0.72	0
3	PSU	L5	4532	3	18,21,22	1.93	4 (22%)	22,30,33	2.23	9 (40%)
3	PSU	L5	3730	3	18,21,22	1.66	4 (22%)	22,30,33	2.17	5 (22%)
3	A2M	L5	1524	3	22,25,26	1.44	5 (22%)	31,36,39	2.13	11 (35%)
3	OMG	L5	4228	3	23,26,27	1.25	4 (17%)	33,38,41	1.92	6 (18%)
3	OMG	L5	2876	3	23,26,27	1.30	3 (13%)	33,38,41	2.11	8 (24%)
3	OMG	L5	3899	3	23,26,27	1.30	4 (17%)	33,38,41	1.91	7 (21%)
3	OMG	L5	4637	3	23,26,27	1.32	4 (17%)	33,38,41	1.94	7 (21%)
3	A2M	L5	3785	3	22,25,26	1.40	5 (22%)	31,36,39	2.39	11 (35%)
3	PSU	L5	4299	3	18,21,22	2.08	7 (38%)	22,30,33	2.24	9 (40%)
3	PSU	L5	4423	3	18,21,22	1.73	4 (22%)	22,30,33	2.04	4 (18%)
3	A2M	L5	3718	3	22,25,26	1.47	5 (22%)	31,36,39	1.93	6 (19%)
3	5MC	L5	4335	3	18,22,23	1.02	2 (11%)	26,32,35	1.23	2 (7%)
3	A2M	L5	1534	46,3	22,25,26	1.46	5 (22%)	31,36,39	2.11	10 (32%)
3	OMG	L5	4618	3	23,26,27	1.27	4 (17%)	33,38,41	1.98	7 (21%)
3	A2M	L5	1323	3	22,25,26	1.48	5 (22%)	31,36,39	2.06	8 (25%)
3	A2M	L5	2401	3	22,25,26	1.43	5 (22%)	31,36,39	2.10	10 (32%)
3	PSU	L5	1582	3	18,21,22	1.49	4 (22%)	22,30,33	1.89	3 (13%)
3	OMC	L5	3841	3	19,22,23	0.94	2 (10%)	26,31,34	0.75	0
3	PSU	L5	3920	46,3	18,21,22	2.20	6 (33%)	22,30,33	2.26	7 (31%)
3	5MC	L5	4447	46,3	18,22,23	1.06	2 (11%)	26,32,35	1.38	3 (11%)
3	PSU	L5	3822	3	18,21,22	1.49	5 (27%)	22,30,33	1.93	3 (13%)
3	PSU	L5	3764	3	18,21,22	1.41	4 (22%)	22,30,33	1.88	4 (18%)
3	5MC	L5	3782	46,3	18,22,23	0.99	2 (11%)	26,32,35	1.17	3 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	A2M	L5	3830	3	22,25,26	1.44	4 (18%)	31,36,39	2.07	10 (32%)
3	PSU	L5	4500	3	18,21,22	1.49	5 (27%)	22,30,33	2.07	4 (18%)
3	PSU	L5	3695	3	18,21,22	1.87	5 (27%)	22,30,33	2.38	5 (22%)
3	PSU	L5	3715	3	18,21,22	1.42	4 (22%)	22,30,33	1.97	5 (22%)
3	OMG	L5	4392	3	23,26,27	1.31	4 (17%)	33,38,41	1.97	8 (24%)
3	PSU	L5	4457	3	18,21,22	1.55	4 (22%)	22,30,33	2.06	6 (27%)
41	MLZ	Lm	98	41	8,9,10	0.82	0	4,9,11	0.68	0
3	2MG	L5	729	46,3	23,26,27	1.34	3 (13%)	32,38,41	2.20	7 (21%)
3	UR3	L5	1866	3	19,22,23	0.95	2 (10%)	26,32,35	1.37	2 (7%)
3	2MG	L5	978	3	23,26,27	1.32	4 (17%)	32,38,41	2.20	8 (25%)
3	OMG	L5	3627	3	23,26,27	1.33	4 (17%)	33,38,41	2.08	7 (21%)
3	PSU	L5	4312	3	18,21,22	1.91	5 (27%)	22,30,33	2.42	5 (22%)
3	PSU	L5	4442	3	18,21,22	1.52	5 (27%)	22,30,33	2.05	5 (22%)
3	PSU	L5	4361	3	18,21,22	1.98	5 (27%)	22,30,33	2.24	5 (22%)
3	PSU	L5	3639	3	18,21,22	1.55	4 (22%)	22,30,33	1.98	4 (18%)
3	A2M	L5	2815	3	22,25,26	1.53	4 (18%)	31,36,39	2.27	11 (35%)
3	JMH	L5	1456	3	18,22,23	1.24	2 (11%)	21,32,35	0.84	0
3	A2M	L5	3825	3	22,25,26	1.44	5 (22%)	31,36,39	2.13	9 (29%)
3	PSU	L5	3762	3	18,21,22	1.39	2 (11%)	22,30,33	1.89	3 (13%)
3	PSU	L5	4628	3	18,21,22	1.49	3 (16%)	22,30,33	1.96	3 (13%)
5	OMU	L8	14	5,3	19,22,23	1.39	4 (21%)	26,31,34	1.85	5 (19%)
3	1MA	L5	1322	46,3	21,25,26	1.40	4 (19%)	31,37,40	1.72	5 (16%)
3	A2M	L5	4590	3	22,25,26	1.46	3 (13%)	31,36,39	2.10	8 (25%)
3	PSU	L5	4636	3	18,21,22	1.48	3 (16%)	22,30,33	2.05	5 (22%)
3	PSU	L5	3758	3	18,21,22	1.39	3 (16%)	22,30,33	2.03	6 (27%)
3	PSU	L5	4403	3	18,21,22	2.12	7 (38%)	22,30,33	2.77	7 (31%)
3	PSU	L5	1744	46,3	18,21,22	1.79	5 (27%)	22,30,33	2.22	7 (31%)
3	B8T	L5	4671	3	19,22,23	1.04	2 (10%)	26,31,34	0.95	1 (3%)
3	OMG	L5	2050	3	23,26,27	1.32	4 (17%)	33,38,41	1.91	7 (21%)
3	A2M	L5	2363	46,3	22,25,26	1.45	4 (18%)	31,36,39	2.05	8 (25%)
3	PSU	L5	2839	3	18,21,22	1.83	5 (27%)	22,30,33	2.20	5 (22%)
3	6MZ	L5	4220	3	22,25,26	1.35	4 (18%)	30,36,39	2.30	9 (30%)
3	OMC	L5	2804	3	19,22,23	0.93	2 (10%)	26,31,34	0.89	1 (3%)
3	OMC	L5	2422	46,3	19,22,23	0.90	2 (10%)	26,31,34	0.90	0
3	1MA	L5	4415	3	21,25,26	1.39	4 (19%)	31,37,40	1.62	4 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	OMC	L5	3808	3	19,22,23	0.93	2 (10%)	26,31,34	0.87	1 (3%)
3	OMG	L5	3744	3	23,26,27	1.34	4 (17%)	33,38,41	1.96	8 (24%)
3	5MU	L5	4083	3	19,22,23	1.40	3 (15%)	28,32,35	2.21	6 (21%)
3	PSU	L5	1781	3	18,21,22	1.88	5 (27%)	22,30,33	2.26	5 (22%)
3	OMC	L5	3909	3	19,22,23	0.92	2 (10%)	26,31,34	0.98	2 (7%)
3	A2M	L5	3867	3	22,25,26	1.46	5 (22%)	31,36,39	2.08	9 (29%)
3	OMC	L5	3869	3	19,22,23	0.91	2 (10%)	26,31,34	0.78	0
3	PSU	L5	1779	3	18,21,22	1.73	4 (22%)	22,30,33	2.20	5 (22%)
3	PSU	L5	4552	3	18,21,22	1.98	5 (27%)	22,30,33	2.17	5 (22%)
3	A2M	L5	1871	46,3	22,25,26	1.45	4 (18%)	31,36,39	2.16	9 (29%)
3	OMG	L5	1625	3	23,26,27	1.28	3 (13%)	33,38,41	1.98	6 (18%)
3	PSU	L5	3770	3	18,21,22	1.41	3 (16%)	22,30,33	1.97	4 (18%)
3	PSU	L5	1792	3	18,21,22	1.97	4 (22%)	22,30,33	2.27	5 (22%)
3	OMG	L5	4494	3	23,26,27	1.59	6 (26%)	33,38,41	2.10	9 (27%)
3	OMG	L5	1522	3	23,26,27	1.30	4 (17%)	33,38,41	2.00	8 (24%)
3	PSU	L5	1862	3	18,21,22	2.08	6 (33%)	22,30,33	2.43	7 (31%)
3	OMG	L5	3792	3	23,26,27	1.28	4 (17%)	33,38,41	1.92	6 (18%)
3	OMC	L5	3701	46,3	19,22,23	0.87	1 (5%)	26,31,34	0.78	0
3	OMU	L5	4227	3	19,22,23	1.40	4 (21%)	26,31,34	1.87	5 (19%)
3	OMC	L5	4456	3	19,22,23	1.20	2 (10%)	26,31,34	1.16	3 (11%)
3	OMG	L5	4499	3	23,26,27	1.31	3 (13%)	33,38,41	2.00	7 (21%)
3	OMG	L5	1316	3	23,26,27	1.35	5 (21%)	33,38,41	2.01	7 (21%)
3	OMU	L5	4498	46,3	19,22,23	1.37	4 (21%)	26,31,34	1.79	6 (23%)
3	OMG	L5	4870	3	23,26,27	1.27	4 (17%)	33,38,41	1.90	6 (18%)
3	OMG	L5	1883	3	23,26,27	1.32	4 (17%)	33,38,41	2.00	6 (18%)
3	OMC	L5	4536	3	19,22,23	0.94	2 (10%)	26,31,34	0.84	0
3	OMC	L5	2365	46,3	19,22,23	0.91	2 (10%)	26,31,34	0.81	0
3	PSU	L5	3768	3	18,21,22	1.44	3 (16%)	22,30,33	2.03	4 (18%)
3	OMU	L5	4620	3	19,22,23	1.40	4 (21%)	26,31,34	1.86	5 (19%)
3	OMU	L5	4306	3	19,22,23	1.37	4 (21%)	26,31,34	1.73	4 (15%)
3	PSU	L5	2508	3	18,21,22	1.49	4 (22%)	22,30,33	1.94	4 (18%)
3	PSU	L5	4296	3	18,21,22	1.83	4 (22%)	22,30,33	2.28	6 (27%)
3	OMG	L5	2364	3	23,26,27	1.30	4 (17%)	33,38,41	1.94	6 (18%)

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
3	A2M	L5	4523	46,3	-	0/9/27/28	0/3/3/3
3	A2M	L5	1326	3	-	3/9/27/28	0/3/3/3
3	PSU	L5	4450	46,3	-	3/7/25/26	0/2/2/2
3	UR3	L5	4530	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3944	3	-	2/9/27/28	0/3/3/3
3	OMU	L5	3925	3	-	2/9/27/28	0/2/2/2
3	A2M	L5	4571	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4579	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	1782	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	3887	3	-	1/9/27/28	0/2/2/2
3	PSU	L5	4521	46,3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4420	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	4196	46,3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2824	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3637	3	-	3/7/25/26	0/2/2/2
3	2MG	L5	4872	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1677	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2787	46,3	-	3/9/27/28	0/3/3/3
3	OMG	L5	4187	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4353	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1683	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3723	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4370	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4576	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	2351	46,3	-	4/9/27/28	0/2/2/2
3	OMG	L5	373	3	-	1/9/27/28	0/3/3/3
3	B8T	L5	4483	3	-	0/7/27/28	0/2/2/2
3	OMG	L5	4623	3	-	1/9/27/28	0/3/3/3
3	PSU	L5	2632	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4493	46,3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4689	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4293	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4673	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	1860	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	1536	3	-	0/7/25/26	0/2/2/2
3	UR3	L5	4597	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	2424	3	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	3734	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	398	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	1340	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	2773	3	-	0/9/27/28	0/3/3/3
3	2MG	L5	1517	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4531	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	2861	3	-	0/9/27/28	0/2/2/2
3	UY1	L5	3818	46,3	-	4/9/27/28	0/2/2/2
3	PSU	L5	2843	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	2837	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	4471	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	400	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4431	3	-	1/7/25/26	0/2/2/2
3	OMU	L5	2415	3	-	2/9/27/28	0/2/2/2
6	MLZ	LC	333	6	-	2/7/8/10	-
3	PSU	L5	4532	3	-	1/7/25/26	0/2/2/2
3	PSU	L5	3730	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1524	3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4228	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	2876	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	3899	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	4637	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	3785	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4299	3	-	2/7/25/26	0/2/2/2
3	PSU	L5	4423	3	-	2/7/25/26	0/2/2/2
3	A2M	L5	3718	3	-	0/9/27/28	0/3/3/3
3	5MC	L5	4335	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	1534	46,3	-	1/9/27/28	0/3/3/3
3	OMG	L5	4618	3	-	1/9/27/28	0/3/3/3
3	A2M	L5	1323	3	-	3/9/27/28	0/3/3/3
3	A2M	L5	2401	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1582	3	-	1/7/25/26	0/2/2/2
3	OMC	L5	3841	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3920	46,3	-	0/7/25/26	0/2/2/2
3	5MC	L5	4447	46,3	-	4/7/25/26	0/2/2/2
3	PSU	L5	3822	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3764	3	-	3/7/25/26	0/2/2/2
3	5MC	L5	3782	46,3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3830	3	-	1/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PSU	L5	4500	3	-	5/7/25/26	0/2/2/2
3	PSU	L5	3695	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3715	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4392	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	4457	3	-	2/7/25/26	0/2/2/2
41	MLZ	Lm	98	41	-	1/7/8/10	-
3	2MG	L5	729	46,3	-	3/9/27/28	0/3/3/3
3	UR3	L5	1866	3	-	0/7/25/26	0/2/2/2
3	2MG	L5	978	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	3627	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	4312	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4442	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4361	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	3639	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	2815	3	-	2/9/27/28	0/3/3/3
3	JMH	L5	1456	3	-	0/7/25/26	0/2/2/2
3	A2M	L5	3825	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	3762	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4628	3	-	0/7/25/26	0/2/2/2
5	OMU	L8	14	5,3	-	1/9/27/28	0/2/2/2
3	1MA	L5	1322	46,3	-	1/7/25/26	0/3/3/3
3	A2M	L5	4590	3	-	5/9/27/28	0/3/3/3
3	PSU	L5	4636	3	-	4/7/25/26	0/2/2/2
3	PSU	L5	3758	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4403	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1744	46,3	-	0/7/25/26	0/2/2/2
3	B8T	L5	4671	3	-	1/7/27/28	0/2/2/2
3	OMG	L5	2050	3	-	0/9/27/28	0/3/3/3
3	A2M	L5	2363	46,3	-	1/9/27/28	0/3/3/3
3	PSU	L5	2839	3	-	0/7/25/26	0/2/2/2
3	6MZ	L5	4220	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	2804	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2422	46,3	-	1/9/27/28	0/2/2/2
3	1MA	L5	4415	3	-	0/7/25/26	0/3/3/3
3	OMC	L5	3808	3	-	0/9/27/28	0/2/2/2
3	OMG	L5	3744	3	-	0/9/27/28	0/3/3/3
3	5MU	L5	4083	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1781	3	-	0/7/25/26	0/2/2/2
3	OMC	L5	3909	3	-	2/9/27/28	0/2/2/2
3	A2M	L5	3867	3	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OMC	L5	3869	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	1779	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4552	3	-	1/7/25/26	0/2/2/2
3	A2M	L5	1871	46,3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1625	3	-	2/9/27/28	0/3/3/3
3	PSU	L5	3770	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	1792	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	4494	3	-	0/9/27/28	0/3/3/3
3	OMG	L5	1522	3	-	0/9/27/28	0/3/3/3
3	PSU	L5	1862	3	-	0/7/25/26	0/2/2/2
3	OMG	L5	3792	3	-	0/9/27/28	0/3/3/3
3	OMC	L5	3701	46,3	-	4/9/27/28	0/2/2/2
3	OMU	L5	4227	3	-	3/9/27/28	0/2/2/2
3	OMC	L5	4456	3	-	1/9/27/28	0/2/2/2
3	OMG	L5	4499	3	-	2/9/27/28	0/3/3/3
3	OMG	L5	1316	3	-	0/9/27/28	0/3/3/3
3	OMU	L5	4498	46,3	-	0/9/27/28	0/2/2/2
3	OMG	L5	4870	3	-	3/9/27/28	0/3/3/3
3	OMG	L5	1883	3	-	1/9/27/28	0/3/3/3
3	OMC	L5	4536	3	-	0/9/27/28	0/2/2/2
3	OMC	L5	2365	46,3	-	0/9/27/28	0/2/2/2
3	PSU	L5	3768	3	-	0/7/25/26	0/2/2/2
3	OMU	L5	4620	3	-	0/9/27/28	0/2/2/2
3	OMU	L5	4306	3	-	0/9/27/28	0/2/2/2
3	PSU	L5	2508	3	-	0/7/25/26	0/2/2/2
3	PSU	L5	4296	3	-	2/7/25/26	0/2/2/2
3	OMG	L5	2364	3	-	2/9/27/28	0/3/3/3

The worst 5 of 558 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L5	3818	UY1	C3'-C4'	-5.54	1.38	1.53
3	L5	4403	PSU	C4-N3	-4.67	1.30	1.38
3	L5	3637	PSU	C4-N3	-4.52	1.30	1.38
3	L5	4689	PSU	C2'-C1'	-4.49	1.47	1.53
3	L5	3920	PSU	C4-N3	-4.37	1.30	1.38

The worst 5 of 787 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	4403	PSU	N1-C2-N3	8.22	124.45	115.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L5	1517	2MG	C2-N3-C4	7.48	121.31	112.04
3	L5	3695	PSU	N1-C2-N3	7.43	123.55	115.13
3	L5	1536	PSU	N1-C2-N3	7.29	123.39	115.13
3	L5	1860	PSU	N1-C2-N3	7.17	123.25	115.13

There are no chirality outliers.

5 of 129 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	L5	729	2MG	N1-C2-N2-CM2
3	L5	729	2MG	N3-C2-N2-CM2
3	L5	1860	PSU	C3'-C4'-C5'-O5'
3	L5	2351	OMC	C3'-C4'-C5'-O5'
3	L5	2351	OMC	O4'-C4'-C5'-O5'

There are no ring outliers.

87 monomers are involved in 146 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4523	A2M	1	0
3	L5	1326	A2M	2	0
3	L5	4530	UR3	1	0
3	L5	3944	OMG	4	0
3	L5	3925	OMU	1	0
3	L5	4571	A2M	2	0
3	L5	4579	PSU	3	0
3	L5	1782	PSU	2	0
3	L5	3887	OMC	1	0
3	L5	4420	PSU	1	0
3	L5	4196	OMG	1	0
3	L5	3637	PSU	3	0
3	L5	4872	2MG	6	0
3	L5	1677	PSU	1	0
3	L5	4187	OMG	2	0
3	L5	4353	PSU	2	0
3	L5	1683	PSU	1	0
3	L5	4576	PSU	4	0
3	L5	2351	OMC	3	0
3	L5	2632	PSU	1	0
3	L5	4493	PSU	1	0
3	L5	4689	PSU	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4673	PSU	1	0
3	L5	1860	PSU	3	0
3	L5	4597	UR3	1	0
3	L5	2424	OMG	2	0
3	L5	398	A2M	1	0
3	L5	1340	OMC	1	0
3	L5	1517	2MG	1	0
3	L5	4531	PSU	1	0
3	L5	2843	PSU	1	0
3	L5	2837	OMU	2	0
3	L5	4471	PSU	1	0
3	L5	4431	PSU	1	0
3	L5	2415	OMU	4	0
6	LC	333	MLZ	1	0
3	L5	4532	PSU	2	0
3	L5	3730	PSU	2	0
3	L5	1524	A2M	1	0
3	L5	4228	OMG	2	0
3	L5	4637	OMG	2	0
3	L5	3785	A2M	2	0
3	L5	4299	PSU	6	0
3	L5	3718	A2M	4	0
3	L5	1534	A2M	2	0
3	L5	4618	OMG	1	0
3	L5	3920	PSU	1	0
3	L5	4447	5MC	1	0
3	L5	3822	PSU	1	0
3	L5	3764	PSU	1	0
3	L5	3830	A2M	1	0
3	L5	4500	PSU	2	0
3	L5	3695	PSU	1	0
3	L5	4392	OMG	1	0
3	L5	4457	PSU	2	0
3	L5	729	2MG	1	0
3	L5	1866	UR3	1	0
3	L5	4442	PSU	1	0
3	L5	4361	PSU	1	0
3	L5	2815	A2M	2	0
3	L5	4628	PSU	1	0
5	L8	14	OMU	1	0
3	L5	1322	1MA	1	0
3	L5	4590	A2M	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L5	4636	PSU	1	0
3	L5	1744	PSU	1	0
3	L5	2050	OMG	1	0
3	L5	2363	A2M	1	0
3	L5	4220	6MZ	1	0
3	L5	2422	OMC	1	0
3	L5	1781	PSU	2	0
3	L5	3909	OMC	2	0
3	L5	3867	A2M	3	0
3	L5	1779	PSU	1	0
3	L5	1871	A2M	2	0
3	L5	3770	PSU	2	0
3	L5	1792	PSU	2	0
3	L5	1522	OMG	1	0
3	L5	1862	PSU	1	0
3	L5	4456	OMC	3	0
3	L5	4499	OMG	1	0
3	L5	1883	OMG	3	0
3	L5	4536	OMC	2	0
3	L5	3768	PSU	2	0
3	L5	4620	OMU	2	0
3	L5	4306	OMU	1	0
3	L5	4296	PSU	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 284 ligands modelled in this entry, 284 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

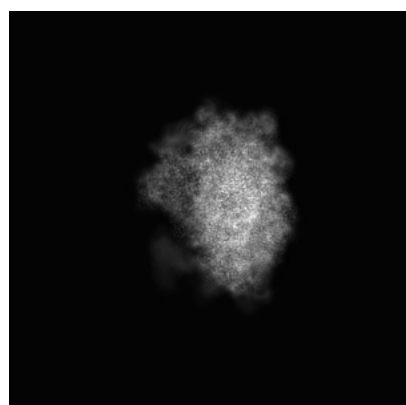
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31465. These allow visual inspection of the internal detail of the map and identification of artifacts.

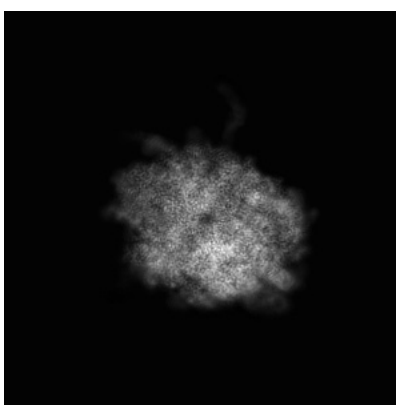
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

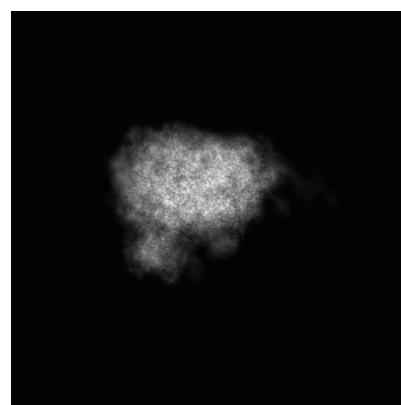
6.1.1 Primary map



X



Y

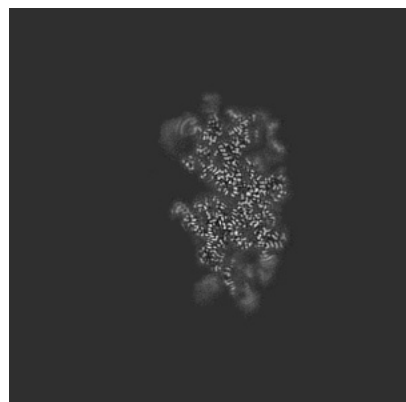


Z

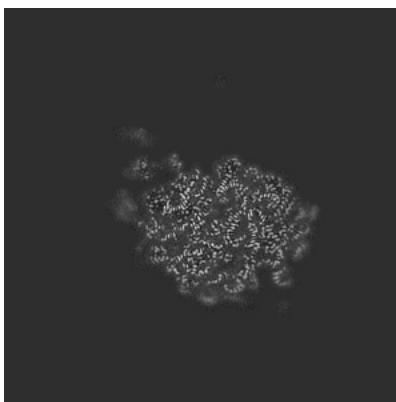
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

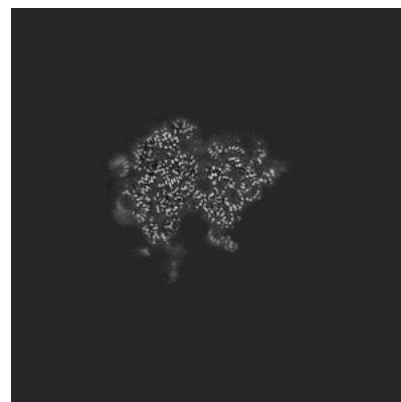
6.2.1 Primary map



X Index: 250



Y Index: 250

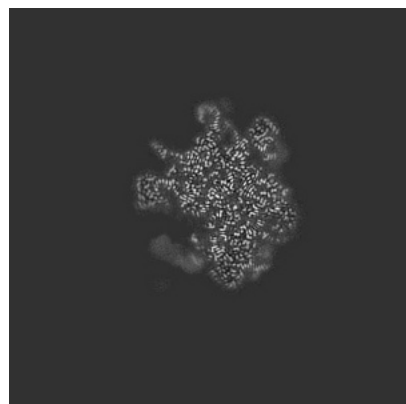


Z Index: 250

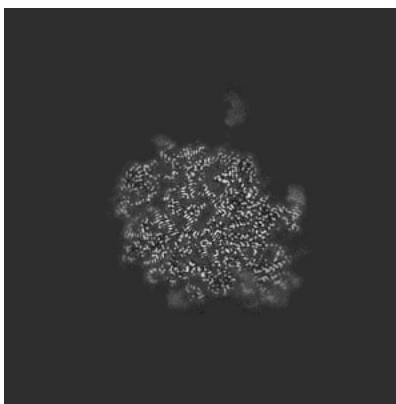
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

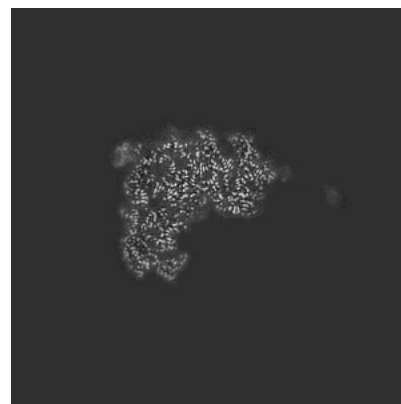
6.3.1 Primary map



X Index: 201



Y Index: 281

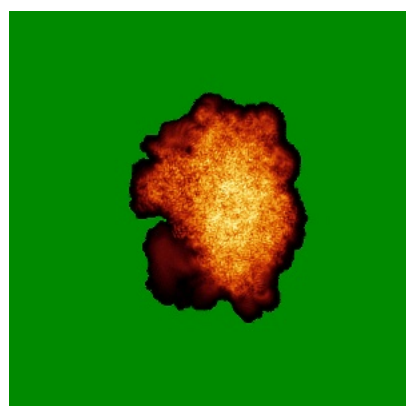


Z Index: 274

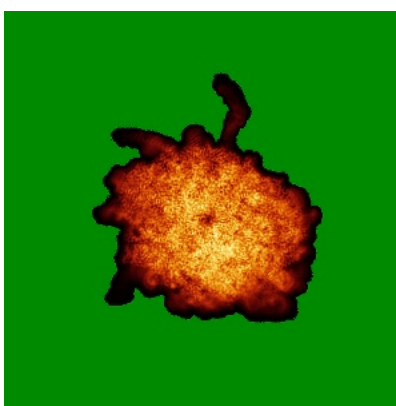
The images above show the largest variance slices of the map in three orthogonal directions.

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

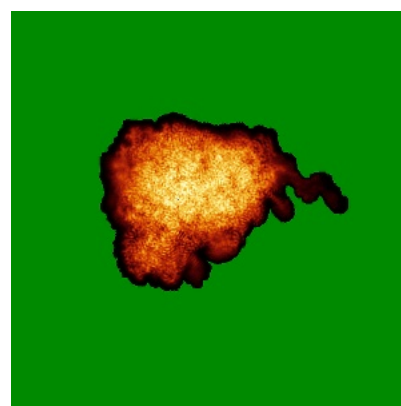
6.4.1 Primary map



X



Y

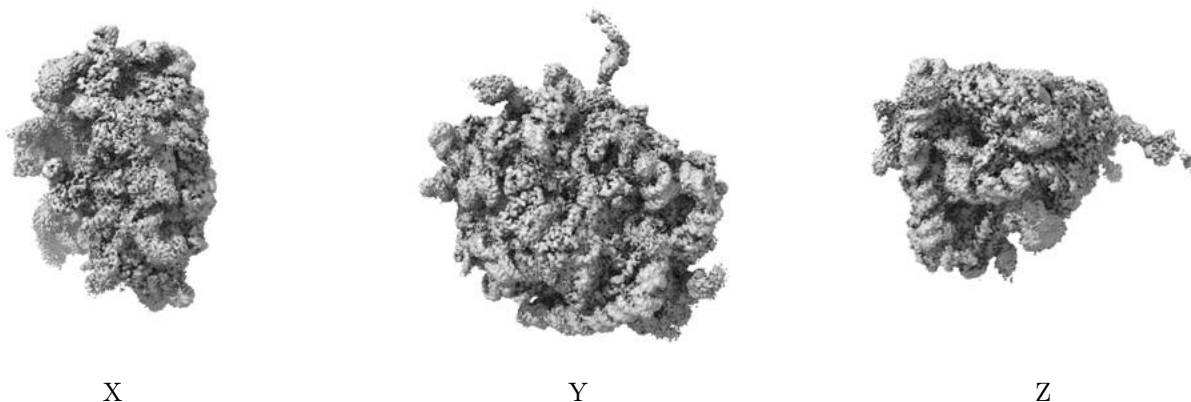


Z

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 2.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

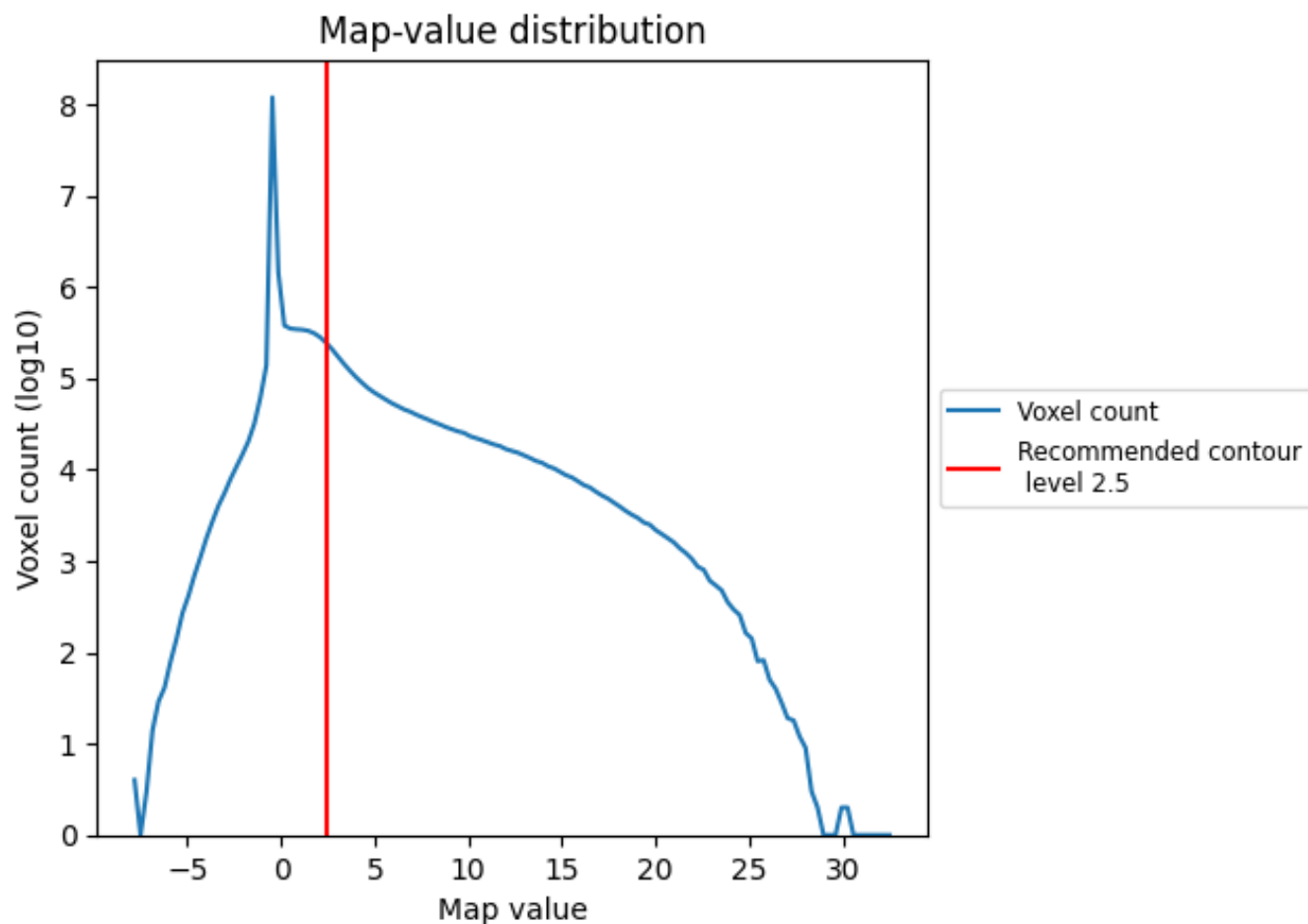
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

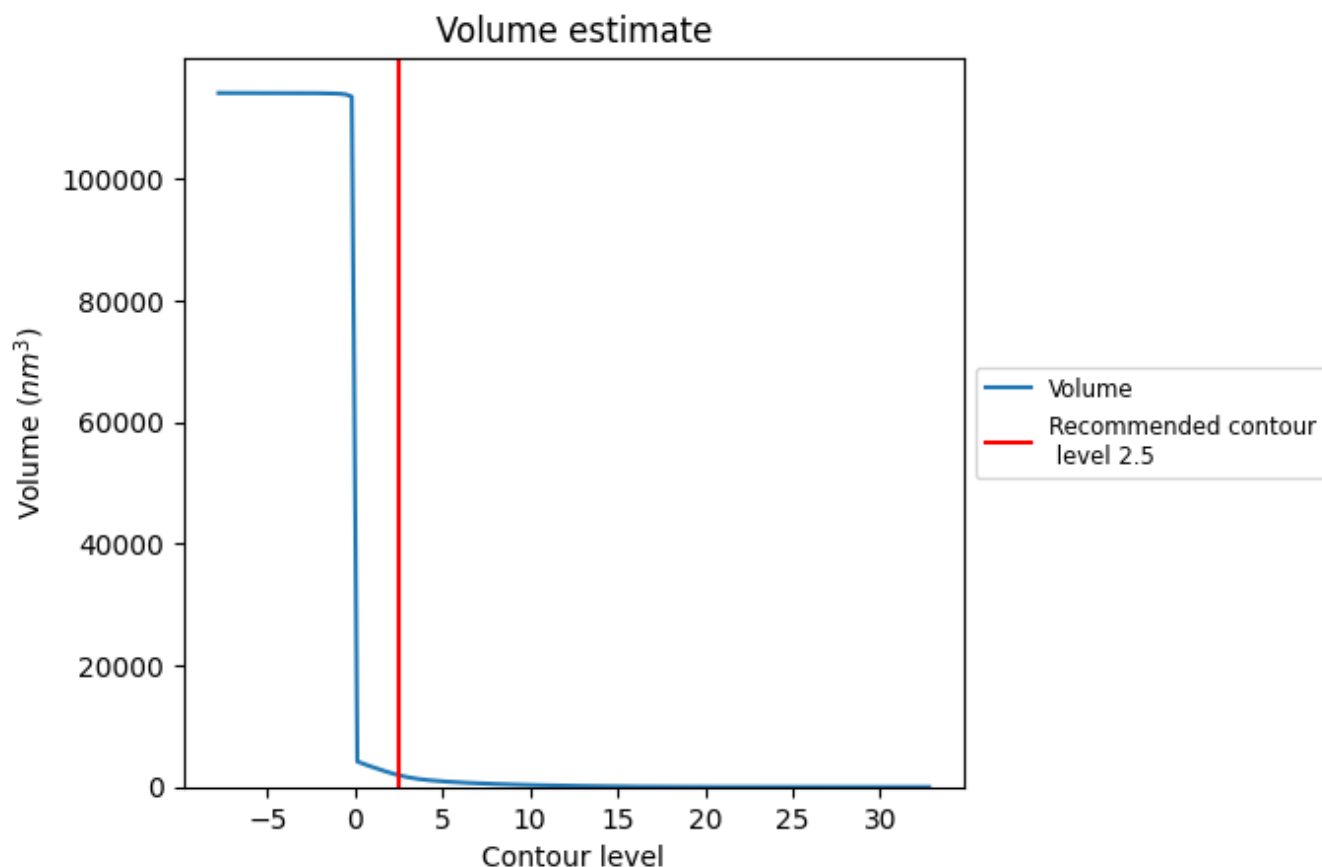
This section contains the results of statistical analysis of the map.

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.

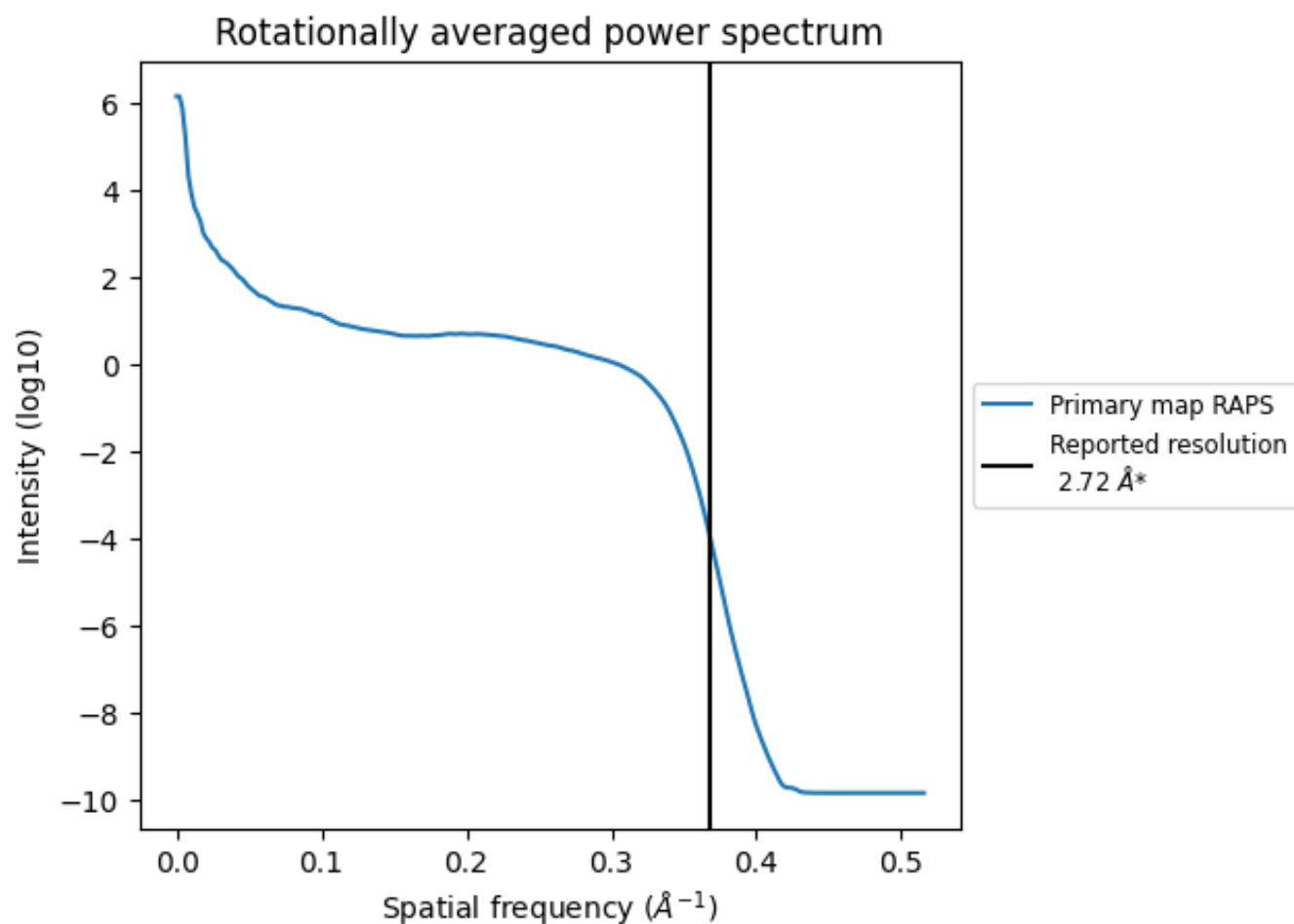
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1927 nm^3 ; this corresponds to an approximate mass of 1741 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.368 Å⁻¹

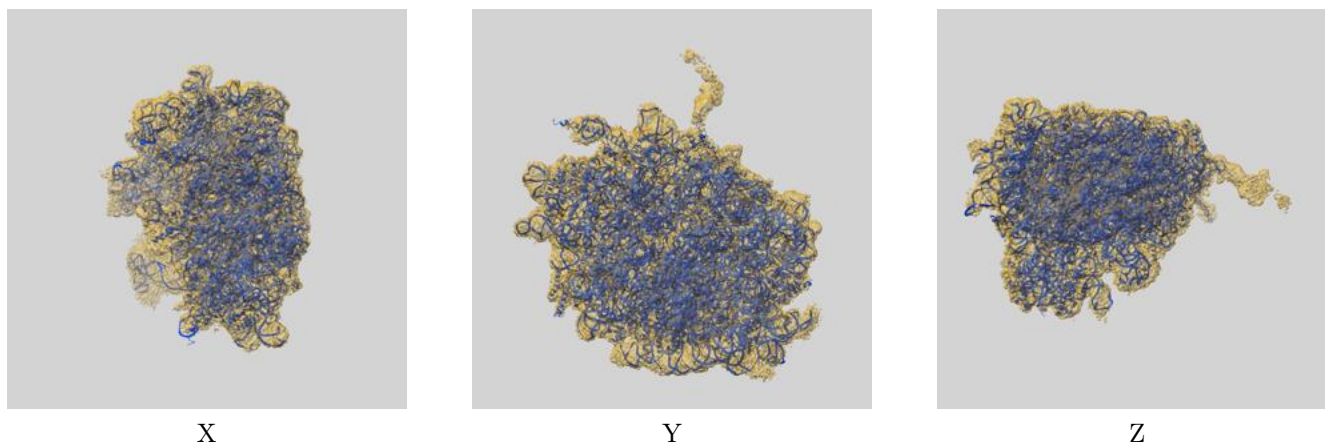
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

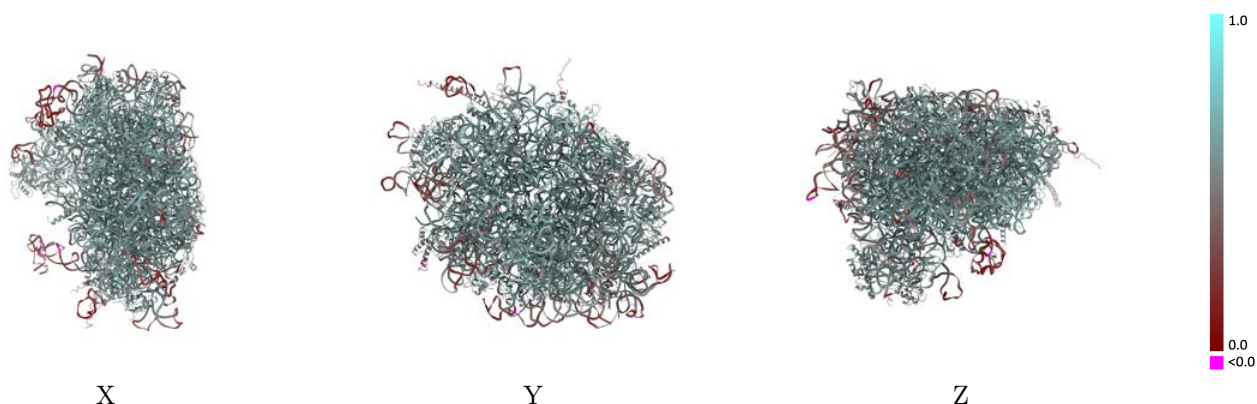
This section contains information regarding the fit between EMDB map EMD-31465 and PDB model 7F5S. Per-residue inclusion information can be found in [section 3](#) on [page 14](#).

9.1 Map-model overlay [i](#)



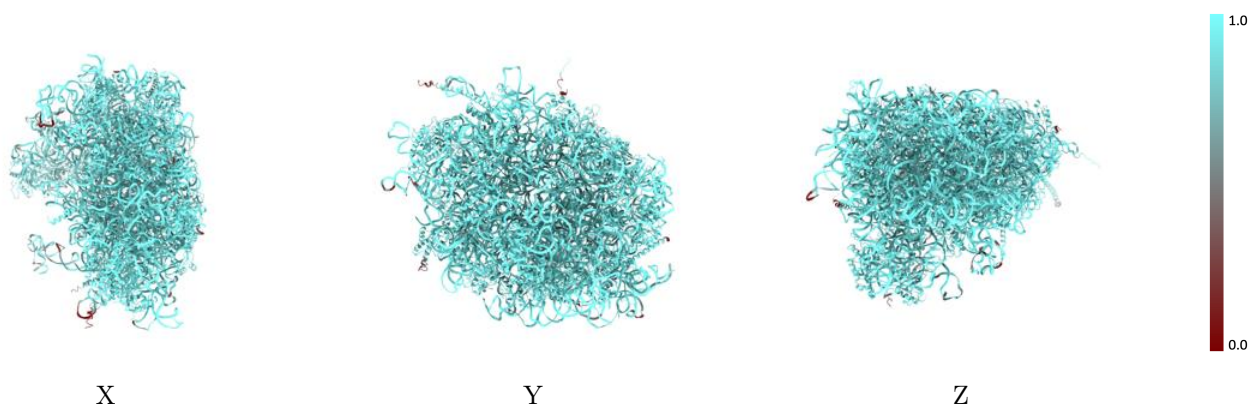
The images above show the 3D surface view of the map at the recommended contour level 2.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



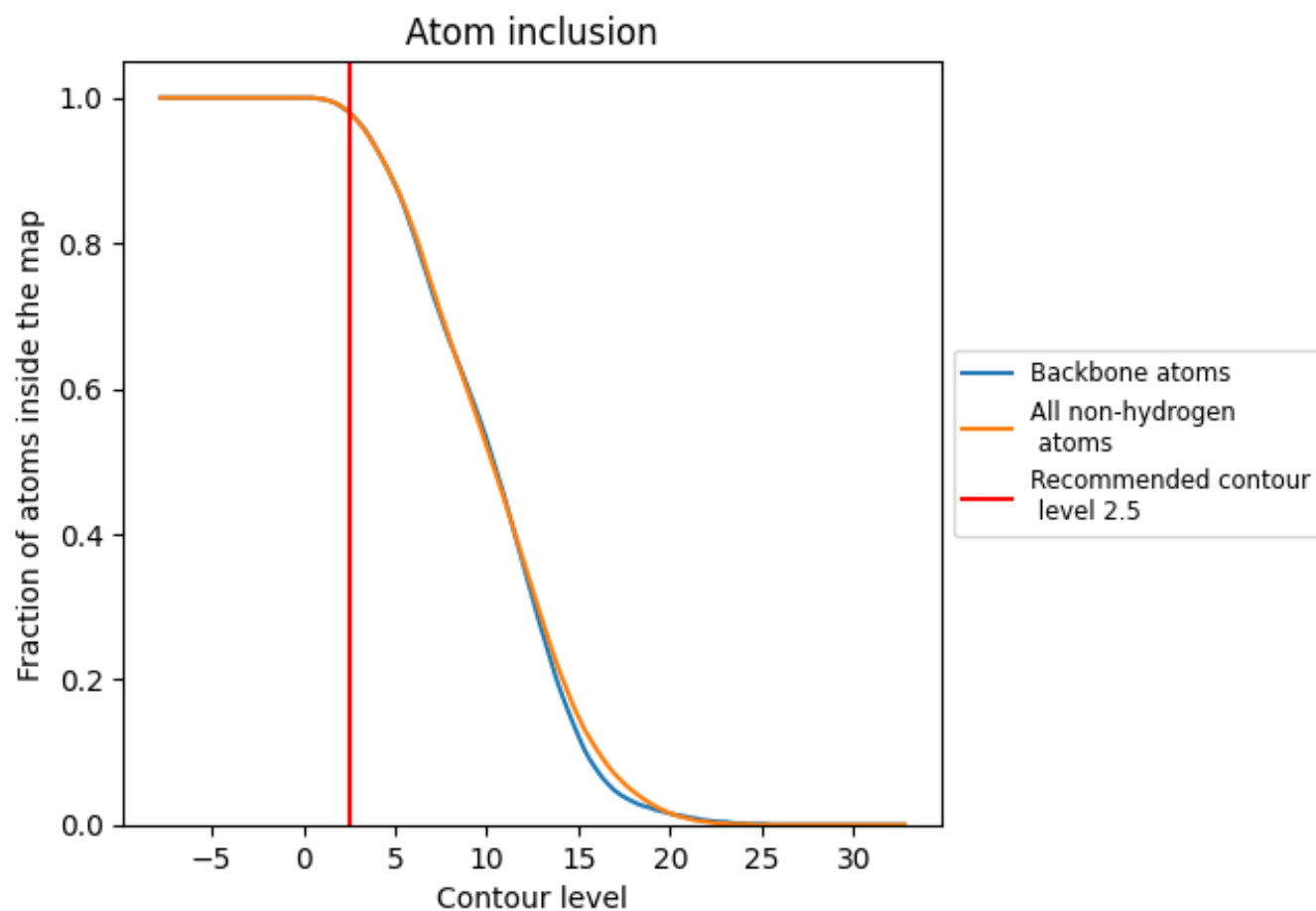
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (2.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9800	 0.5610
L5	 0.9830	 0.5480
L7	 0.9980	 0.5990
L8	 0.9850	 0.5760
LA	 0.9950	 0.6110
LB	 0.9770	 0.5930
LC	 0.9820	 0.5890
LD	 0.9750	 0.5620
LE	 0.9820	 0.5540
LF	 0.9930	 0.5900
LG	 0.9250	 0.5330
LH	 0.9810	 0.5810
LI	 0.9730	 0.5810
LJ	 0.9290	 0.5170
LL	 0.9600	 0.5700
LM	 0.9820	 0.5730
LN	 0.9960	 0.6120
LO	 0.9890	 0.5960
LP	 0.9910	 0.6020
LQ	 0.9940	 0.6100
LR	 0.9170	 0.5480
LS	 0.9940	 0.6060
LT	 0.9770	 0.5750
LU	 0.9530	 0.5120
LV	 0.9840	 0.5950
LW	 0.9120	 0.5180
LX	 0.9830	 0.5790
LY	 0.9830	 0.5820
LZ	 0.9900	 0.5760
La	 0.9940	 0.6120
Lb	 0.9210	 0.5280
Lc	 0.9600	 0.5590
Ld	 0.9720	 0.5850
Le	 0.9950	 0.6040
Lf	 0.9910	 0.6140



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Chain	Atom inclusion	Q-score
Lg	 0.9780	 0.5850
Lh	 0.9770	 0.5750
Li	 0.9800	 0.5670
Lj	 0.9990	 0.6060
Lk	 0.9440	 0.5470
Ll	 0.9910	 0.5840
Lm	 0.9780	 0.5880
Ln	 0.9760	 0.5480
Lo	 0.9820	 0.5850
Lp	 0.9810	 0.5870
Lr	 0.9910	 0.5940