



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 02:10 AM UTC

PDB ID : 6QDW / pdb_00006qdw
EMDB ID : EMD-4531
Title : Cryo-EM structure of the 50S ribosomal subunit at 2.83 Angstroms with modeled GBC SecM peptide
Authors : Schulte, L.; Reitz, J.; Hodirnau, V.V.; Kudlinzki, D.; Mao, J.; Glaubitz, C.; Frangakis, A.; Schwalbe, H.
Deposited on : 2019-01-03
Resolution : 2.83 Å (reported)
Based on initial model : 3JBU

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
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

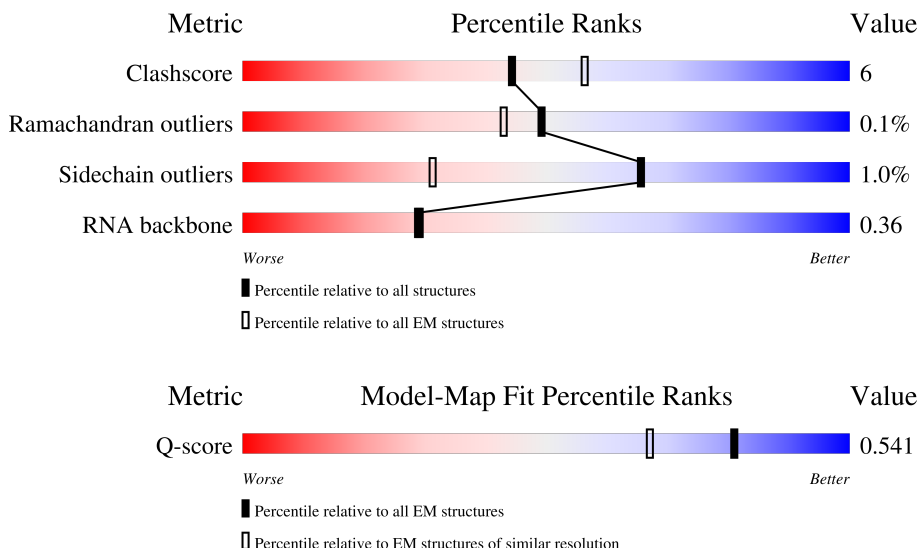
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.83 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.



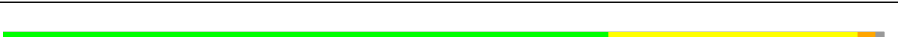
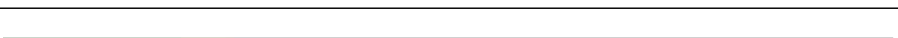
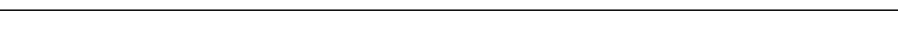
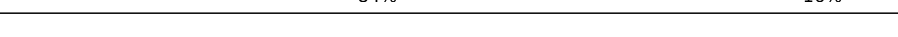
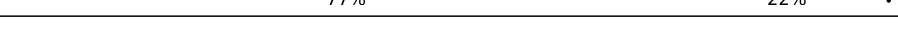
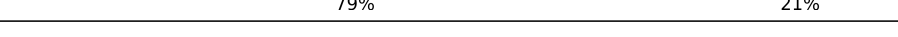
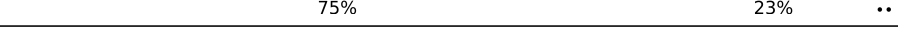
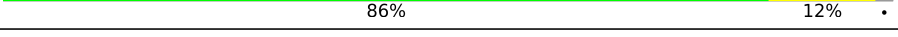
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11847 (2.33 - 3.33)

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	0	78	
2	1	63	
3	2	59	

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Mol	Chain	Length	Quality of chain
4	3	57	
5	4	55	
6	6	46	
7	7	65	
8	8	38	
9	a	120	
10	b	2906	
11	c	273	
12	d	209	
13	e	201	
14	f	179	
15	g	177	
16	h	149	
17	j	142	
18	k	123	
19	l	144	
20	m	136	
21	n	127	
22	o	117	
23	p	115	
24	q	118	
25	r	103	
26	s	110	
27	t	100	
28	u	104	

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Mol	Chain	Length	Quality of chain
29	v	75	 32% 53% 15%
30	w	94	 86% 14%
31	y	85	 68% 18% 13%
32	z	61	 25% 15% 57%

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 90690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 2 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 3 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

- Molecule 4 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 5 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	4	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 6 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 7 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 8 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 9 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	a	118	Total	C	N	O	P	0	0
			2528	1126	464	821	117		

- Molecule 10 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	b	2888	Total	C	N	O	P	0	0
			62008	27660	11413	20047	2888		

- Molecule 11 is a protein called 50S ribosomal protein L2.

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

- Molecule 12 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	d	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 13 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	e	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 14 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 15 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	g	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 16 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	h	39	Total	C	N	O	S	0	0
			287	184	51	51	1		

- Molecule 17 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	k	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	l	143	Total	C	N	O	S	0	0
			1042	648	206	186	2		

- Molecule 20 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	m	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	n	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	o	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 23 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	p	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 24 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	q	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 25 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	r	99	Total	C	N	O	S	0	0
			791	500	149	140	2		

- Molecule 26 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	s	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 27 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	t	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	u	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 29 is a RNA chain called glycine-tRNA glyT.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	v	75	Total	C	N	O	P	0	0
			1583	707	270	531	75		

- Molecule 30 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	w	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 31 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	y	74	Total	C	N	O	S	0	0
			559	348	112	98	1		

- Molecule 32 is a protein called Gamma-crystallin B.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	z	26	Total	C	N	O	S	26	0
			412	266	74	70	2		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	-32	MET	-	initiating methionine	UNP P02526
z	-31	GLY	-	expression tag	UNP P02526
z	-30	HIS	-	expression tag	UNP P02526
z	-29	HIS	-	expression tag	UNP P02526
z	-28	HIS	-	expression tag	UNP P02526
z	-27	HIS	-	expression tag	UNP P02526
z	-26	HIS	-	expression tag	UNP P02526
z	-25	HIS	-	expression tag	UNP P02526
z	-24	HIS	-	expression tag	UNP P02526
z	-23	HIS	-	expression tag	UNP P02526
z	-22	HIS	-	expression tag	UNP P02526
z	-21	HIS	-	expression tag	UNP P02526

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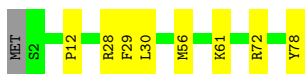
Chain	Residue	Modelled	Actual	Comment	Reference
z	13	PHE	ASN	conflict	UNP P02526
z	15	THR	ILE	conflict	UNP P02526
z	16	PRO	ARG	conflict	UNP P02526
z	18	TRP	-	expression tag	UNP P02526
z	19	ILE	-	expression tag	UNP P02526
z	20	SER	-	expression tag	UNP P02526
z	21	GLN	-	expression tag	UNP P02526
z	22	ALA	-	expression tag	UNP P02526
z	23	GLN	-	expression tag	UNP P02526
z	24	GLY	-	expression tag	UNP P02526
z	25	ILE	-	expression tag	UNP P02526
z	26	ARG	-	expression tag	UNP P02526
z	27	ALA	-	expression tag	UNP P02526
z	28	GLY	-	expression tag	UNP P02526

3 Residue-property plots [i](#)

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

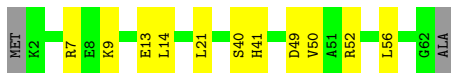
- Molecule 1: 50S ribosomal protein L28

Chain 0:  88% 10% .



- Molecule 2: 50S ribosomal protein L29

Chain 1:  79% 17% .



- Molecule 3: 50S ribosomal protein L30

Chain 2:  85% 12% .



- Molecule 4: 50S ribosomal protein L32

Chain 3:  75% 21% .



- Molecule 5: 50S ribosomal protein L33

Chain 4:  73% 15% 9% .



- Molecule 6: 50S ribosomal protein L34

Chain 6:  80% 20%



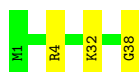
- Molecule 7: 50S ribosomal protein L35

Chain 7:  82% 15% ..



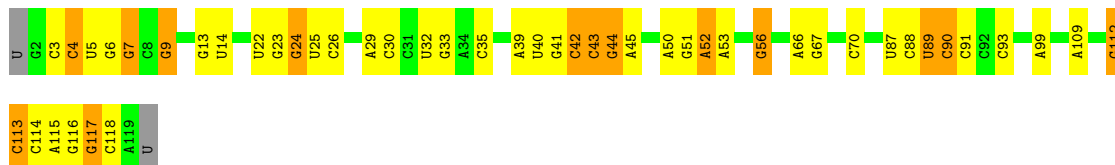
- Molecule 8: 50S ribosomal protein L36

Chain 8:  92% 8%



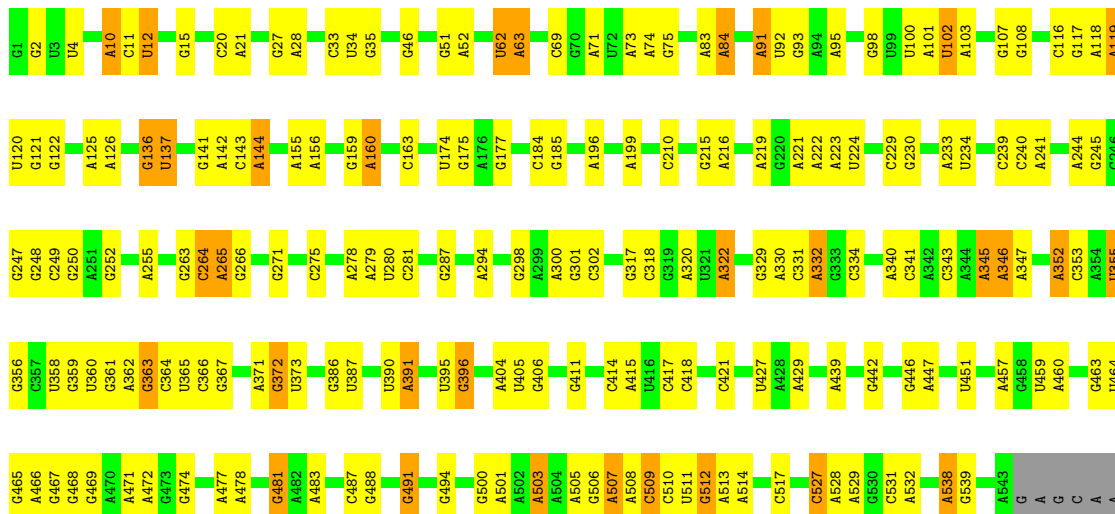
- Molecule 9: 5S rRNA

Chain a:  58% 28% 12% .

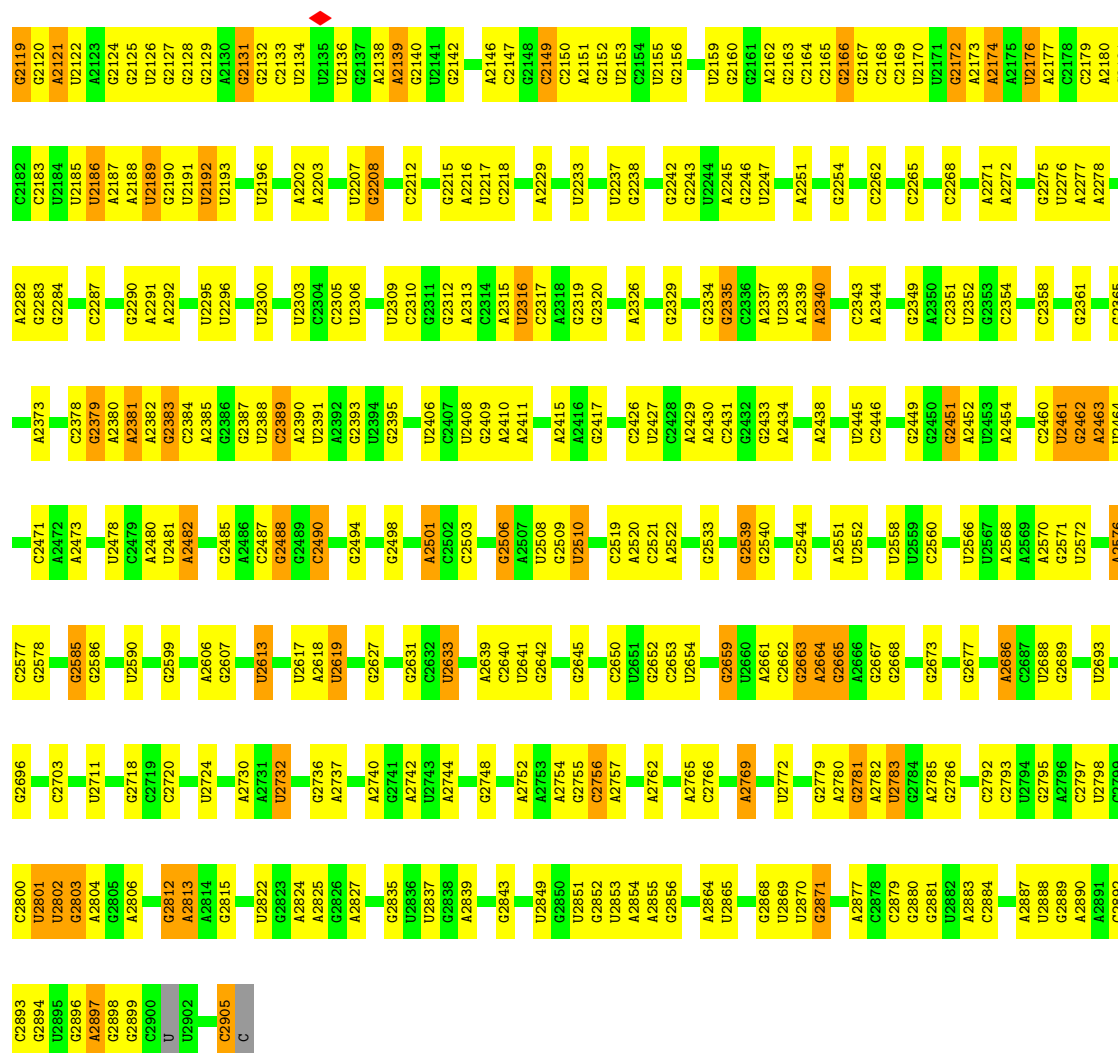


- Molecule 10: 23S rRNA

Chain b:  61% 32% 6% .

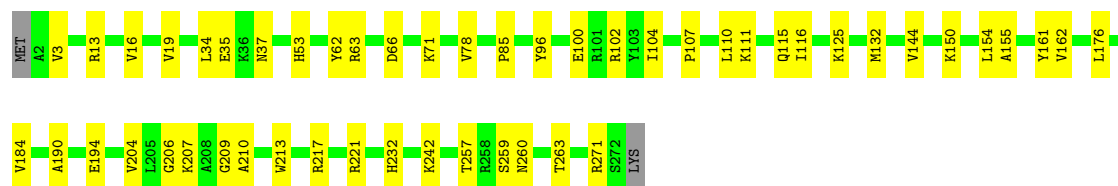


C2027	G1910	U1784	G1568	U1561	U1469	G1366	G1250	U1132	U1063	A986	G877	G759	U648	U
A2034	G1911	A1785	G1669	U1565	U1470	G1367	U1251	G1133	G1064	C989	C878	A763	G649	C
A2035	C1912	A1786	A1670	U1566	A1471	A1368	G1252	U1134	G1065	A899	A879	A764	U	
G2036	G1913	A1787	A1671	C1566	A1472	A1369	A1255	A1135	C1066	A880	A880	G653	G553	
A2037	G1914	A1788	C1672	U1567	G1473	G1370	U1256	A1136	U1067	G881	G881	G765	A558	
U2038	U1915	A1789	G1676	U1568	G1474	A1380	U1257	A1137	U1068	G882	G882	A766	U655	
G2039	A1916	C1792	C1677	G1570	U1477	U1380	G1258	G1138	A1069	G883	G883	C767	C559	
C2040	C1917	A1793	A1680	U1571	U1478	U1381	A1267	U1143	A1071	G884	G884	A657	A565	
U2043	U1921	G1794	A1680	A1574	G1480	G1382	U1268	A1144	A1072	U886	U886	G778	U568	
G2044	A1922	U1799	G1697	U1580	G1484	A1385	G1273	G1165	C1074	A888	A888	A783	U569	
C2047	U1800	G1801	G1705	U1583	U1488	C1388	A1274	G1170	G1075	U889	U889	A785	U570	
A1931	C1802	A1803	C1706	G1584	U1488	C1388	A1275	A1171	G1076	C890	C890	G786	U571	
G2051	A1803	A1803	A1707	C1584	U1488	C1388	A1276	C1172	C1077	G787	G787	A670	G572	
G2052	G1933	A1810	C1708	U1585	C1495	A1394	A1276	A1172	C1078	G893	G893	G671	U575	
G2053	G1934	A1810	G1709	U1586	A1496	A1395	A1278	G1173	A1079	A894	A894	A672	A576	
C2054	U1935	G1813	G1717	C1587	A1497	U1397	G1281	C1174	U1080	C895	C895	C673	U577	
A2055				U1588	A1498	U1398	G1281	U1176	A1081	U896	U896	C674	A578	
A2056	A1940	C1818	G1720	U1591	U1499	U1402	A1286	A1177	U1083	A898	A898	G686	G579	
C2059	A1941	G1819	G1721	A1592	C1500	U1411	A1286	G1179	U1084	C899	C899	G687	G580	
G2060	U1942	U1820	U1722	A1593	A1506	G1412	G1290	G1187	A1086	A795	A795	G688	U582	
A2064	U1943	G1830	G1723	U1594	A1507	U1413	C1291	G1188	A1087	A902	A902	C689	C583	
G2065	U1944	A1831	A1724	A1595	A1507	U1413	C1291	G1188	A1088	G909	G909	A695	A584	
A2066	U1944	A1831	G1725	U1596	A1507	U1413	C1291	G1188	A1088	U809	U809	A695	A584	
C2067	U1944	A1831	G1725	U1596	A1507	U1413	C1291	G1188	A1088	A912	A912	C700	G587	
G2071	U1967	C1835	C1732	U1597	A1510	U1417	G1301	U1190	A1090	A912	A912	A712	G587	
U2072	U1967	C1835	C1732	U1597	A1510	U1417	G1301	U1190	A1090	A912	A912	A712	G587	
G2073	U1967	C1835	C1732	U1597	A1510	U1417	G1301	U1190	A1090	A912	A912	A712	G587	
A2081	U1974	A1856	G1740	A1605	A1530	G1428	G1313	A1206	A1097	U933	U933	A715	U608	
G2084	U1975	G1859	A1741	C1609	G1532	A1429	C1317	A1207	A1098	U933	U933	A715	U608	
U2097	G1976	G1859	C1750	A1611	C1533	C1430	C1321	U1208	A1100	A943	A943	A719	A615	
G2097	G1977	G1864	A1751	A1612	A1534	G1431	G1322	C1209	G1101	G944	G944	A720	A616	
C2100	U1978	G1865	G1752	U1601	C1535	G1432	A1324	G1212	U1103	A947	A947	A723	A617	
A2101	G1979	G1869	G1755	A1620	C1538	G1434	U1328	G1214	A1105	C948	C948	A724	A623	
U2102	A1984	C1870	A1756	A1621	G1539	A1435	U1329	U1226	U1107	A949	A949	C725	G624	
U2103	U1986	G1871	A1757	G1633	U1541	A1436	A1330	U1226	U1107	C950	C950	A725	G624	
G2104	U1986	G1871	G1758	A1636	G1542	A1441	U1331	G1229	G1108	G954	G954	A729	A629	
A2105	U1986	G1871	G1758	A1636	G1542	A1441	U1331	G1229	G1108	G954	G954	A729	A629	
G2106	U1986	G1871	G1758	A1636	G1542	A1441	U1331	G1229	G1108	G954	G954	A729	A629	
C2107	U1997	A	A1759	A1636	C1543	U1442	C1332	G1234	C	U960	U960	G730	G630	
C2108	U1997	A	U1760	A1636	C1543	U1442	C1332	G1234	C	U960	U960	G730	G630	
U2109	C1998	G1877	G1765	G1647	G1545	U1444	G1334	G1238	G1114	C963	C963	A732	G631	
G2111	U1999	C1878	C1766	U1649	C1549	U1445	G1336	A1239	U1115	G964	G964	A732	G631	
A2112	C2000	G1886	U1771	U1650	C1552	G1452	U1342	G1240	G1116	U965	U965	G735	C636	
U2113	C2001	U1886	A1775	A1652	C1553	C1453	U1342	G1240	G1116	U965	U965	G735	C636	
G2114	A2009	U1888	G1778	A1654	A1554	U1455	U1346	U1242	C1119	A974	A974	A736	G638	
U2115	G2014	G1892	G1781	C1660	U1556	G1457	C1353	C1245	G1120	G976	G976	G740	A639	
G2116	U2115	U1886	U1781	C1660	U1557	G1457	U1354	A1246	U1121	G976	G976	A749	U641	
U2117	G2116	U1886	U1781	C1660	U1557	G1457	U1354	A1246	U1121	G976	G976	A749	U641	
A2118	A2023	C1899	U1782	C1558	C1558	U1462	A1355	G1247	G1127	G980	G980	G750	U644	
	A2024		U1783	C1560	C1560	C1463	A1361	A1249	A1128	U1060	U1060	A754	A645	



- Molecule 11: 50S ribosomal protein L2

Chain c: 81% 18%



- Molecule 12: 50S ribosomal protein L3

Chain d: 89% 11%



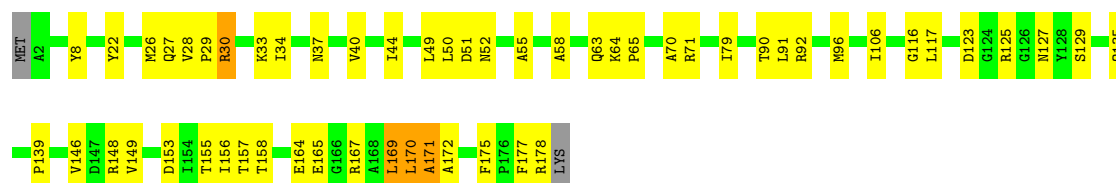
- Molecule 13: 50S ribosomal protein L4

Chain e:  88% 11% .



- Molecule 14: 50S ribosomal protein L5

Chain f:  68% 28% ..



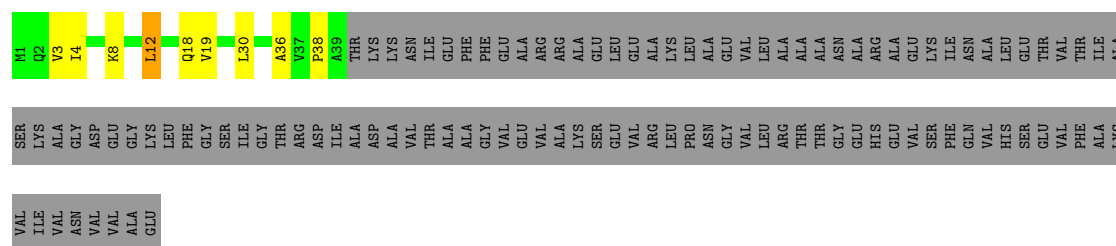
- Molecule 15: 50S ribosomal protein L6

Chain g:  84% 15% ..



- Molecule 16: 50S ribosomal protein L9

Chain h:  20% 5% 74%



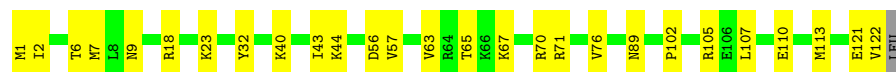
- Molecule 17: 50S ribosomal protein L13

Chain j:  84% 16%

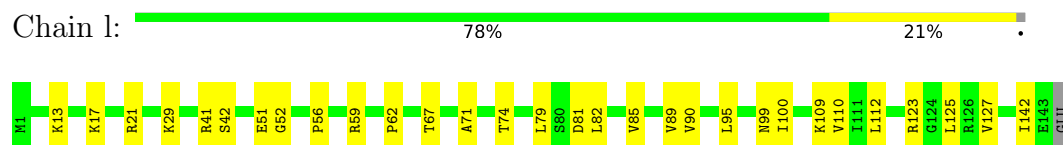


- Molecule 18: 50S ribosomal protein L14

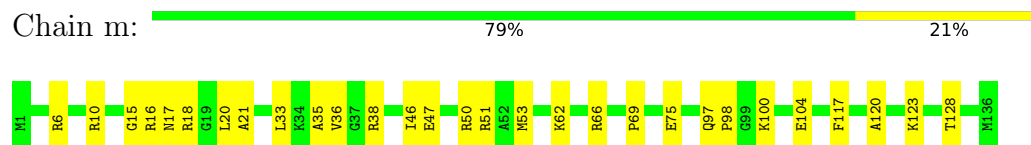
Chain k:  77% 22%



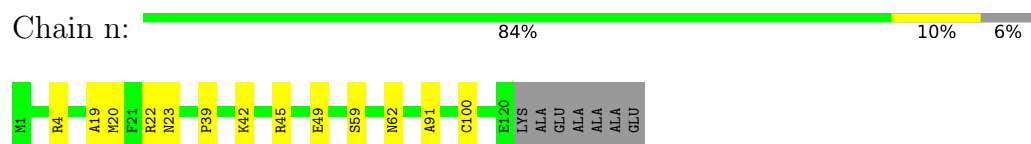
- Molecule 19: 50S ribosomal protein L15



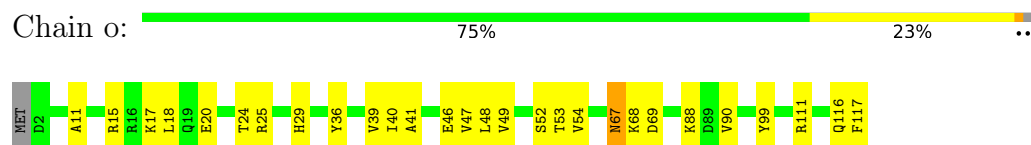
- Molecule 20: 50S ribosomal protein L16



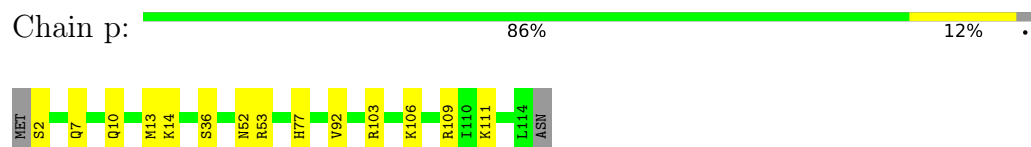
- Molecule 21: 50S ribosomal protein L17



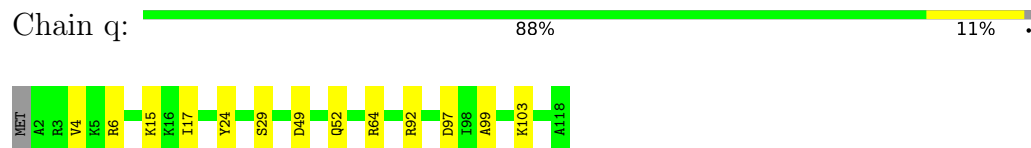
- Molecule 22: 50S ribosomal protein L18



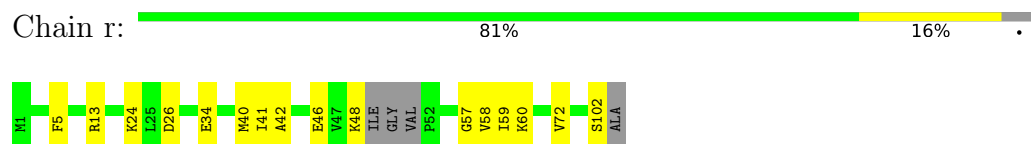
- Molecule 23: 50S ribosomal protein L19



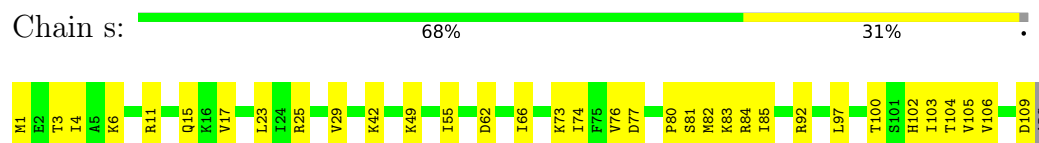
- Molecule 24: 50S ribosomal protein L20



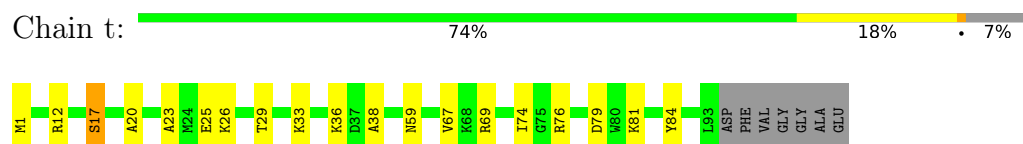
- Molecule 25: 50S ribosomal protein L21



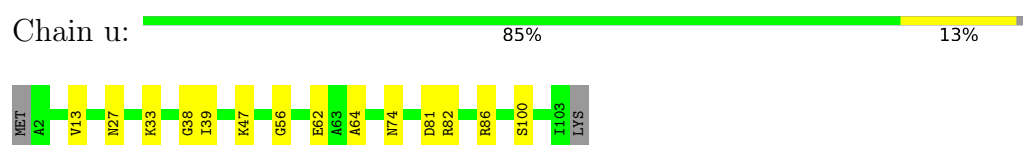
- Molecule 26: 50S ribosomal protein L22



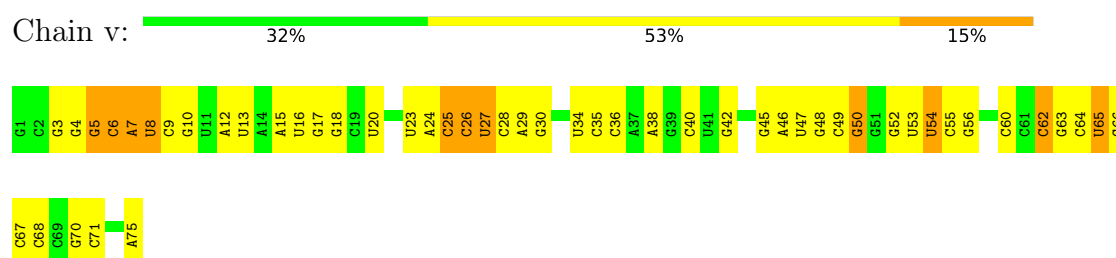
- Molecule 27: 50S ribosomal protein L23



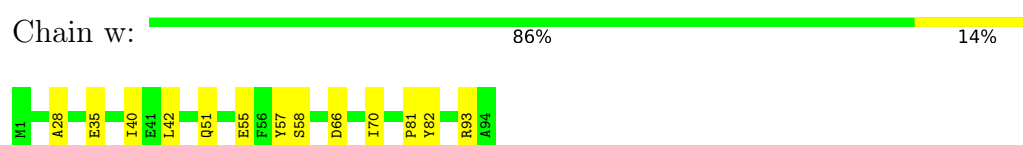
- Molecule 28: 50S ribosomal protein L24



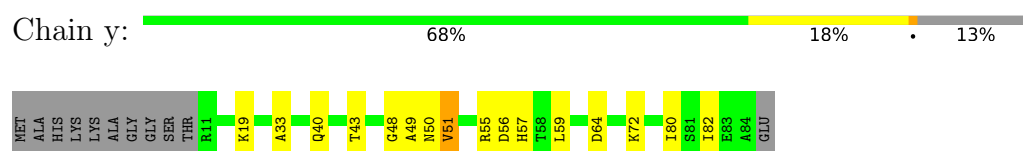
- Molecule 29: glycine-tRNA glyT



- Molecule 30: 50S ribosomal protein L25

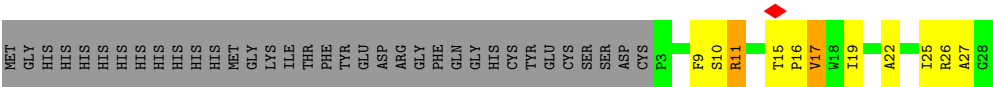


- Molecule 31: 50S ribosomal protein L27



- Molecule 32: Gamma-crystallin B





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196254	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.66	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	0.257	Depositor
Minimum map value	-0.121	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.002	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	0	0.60	0/635	0.62	0/848
2	1	0.45	0/496	0.56	0/660
3	2	0.56	0/443	0.73	1/593 (0.2%)
4	3	0.67	0/440	0.62	0/588
5	4	0.42	0/416	0.65	1/554 (0.2%)
6	6	0.73	0/380	0.60	0/498
7	7	0.65	0/513	0.60	0/676
8	8	0.66	0/303	0.71	0/397
9	a	0.50	0/2824	0.53	0/4402
10	b	0.67	0/69444	0.53	6/108322 (0.0%)
11	c	0.63	0/2121	0.62	0/2852
12	d	0.63	0/1586	0.65	0/2134
13	e	0.58	0/1571	0.66	0/2113
14	f	0.38	0/1434	0.72	0/1926
15	g	0.41	0/1343	0.64	1/1816 (0.1%)
16	h	0.40	0/290	0.74	0/392
17	j	0.59	0/1152	0.55	0/1551
18	k	0.58	0/947	0.62	0/1268
19	l	0.60	0/1051	0.66	2/1400 (0.1%)
20	m	0.59	0/1093	0.58	0/1460
21	n	0.65	0/973	0.69	0/1301
22	o	0.42	0/902	0.69	0/1209
23	p	0.54	0/920	0.55	0/1231
24	q	0.70	0/960	0.61	0/1278
25	r	0.57	0/803	0.59	0/1070
26	s	0.61	0/852	0.57	0/1142
27	t	0.50	0/744	0.62	2/994 (0.2%)
28	u	0.45	0/787	0.75	0/1051
29	v	0.33	0/1764	0.56	0/2744
30	w	0.47	0/766	0.59	0/1025
31	y	0.63	0/566	0.70	0/750
32	z	0.22	0/426	0.52	0/578
All	All	0.64	0/98945	0.56	13/148823 (0.0%)

There are no bond length outliers.

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	4	5	ILE	N-CA-C	-7.47	105.08	112.17
15	g	77	ILE	N-CA-C	-7.09	105.62	112.29
10	b	1301	G	C2'-C3'-O3'	6.89	124.03	113.70
3	2	44	ILE	N-CA-C	-6.51	106.45	112.96
27	t	17	SER	CA-C-N	6.42	133.80	121.54

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	0	625	0	652	5	0
2	1	495	0	526	7	0
3	2	439	0	482	3	0
4	3	434	0	445	10	0
5	4	409	0	440	6	0
6	6	377	0	418	9	0
7	7	504	0	572	10	0
8	8	302	0	341	3	0
9	a	2528	0	1283	49	0
10	b	62008	0	31189	464	0
11	c	2082	0	2154	34	0
12	d	1565	0	1616	16	0
13	e	1552	0	1619	22	0
14	f	1410	0	1444	69	0
15	g	1323	0	1371	15	0
16	h	287	0	307	6	0
17	j	1129	0	1162	16	0
18	k	938	0	1012	15	0
19	l	1042	0	1121	21	0
20	m	1074	0	1157	20	0
21	n	960	0	1000	10	0
22	o	892	0	923	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	p	908	0	956	11	0
24	q	947	0	1019	10	0
25	r	791	0	811	12	0
26	s	845	0	909	24	0
27	t	738	0	807	12	0
28	u	779	0	831	9	0
29	v	1583	0	807	35	0
30	w	753	0	780	9	0
31	y	559	0	575	13	0
32	z	412	0	398	12	0
All	All	90690	0	59127	854	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 854 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)
10:b:511:U:C3'	10:b:512:G:H5'	1.67	1.22
13:e:137:LYS:O	13:e:138:LEU:CG	1.90	1.19
29:v:53:U:H2'	29:v:54:U:H5'	1.25	1.15
13:e:137:LYS:O	13:e:138:LEU:HG	0.97	1.14
10:b:511:U:O3'	10:b:512:G:H5'	1.49	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	1	59/63 (94%)	53 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	2	55/59 (93%)	51 (93%)	4 (7%)	0	100	100
4	3	53/57 (93%)	51 (96%)	2 (4%)	0	100	100
5	4	48/55 (87%)	47 (98%)	1 (2%)	0	100	100
6	6	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
7	7	62/65 (95%)	56 (90%)	6 (10%)	0	100	100
8	8	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
11	c	269/273 (98%)	257 (96%)	12 (4%)	0	100	100
12	d	207/209 (99%)	190 (92%)	17 (8%)	0	100	100
13	e	199/201 (99%)	186 (94%)	12 (6%)	1 (0%)	24	43
14	f	175/179 (98%)	154 (88%)	20 (11%)	1 (1%)	21	39
15	g	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	21	39
16	h	37/149 (25%)	33 (89%)	4 (11%)	0	100	100
17	j	140/142 (99%)	133 (95%)	7 (5%)	0	100	100
18	k	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
19	l	141/144 (98%)	129 (92%)	12 (8%)	0	100	100
20	m	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	n	118/127 (93%)	105 (89%)	13 (11%)	0	100	100
22	o	114/117 (97%)	104 (91%)	10 (9%)	0	100	100
23	p	111/115 (96%)	106 (96%)	5 (4%)	0	100	100
24	q	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
25	r	95/103 (92%)	85 (90%)	10 (10%)	0	100	100
26	s	107/110 (97%)	103 (96%)	4 (4%)	0	100	100
27	t	91/100 (91%)	84 (92%)	7 (8%)	0	100	100
28	u	100/104 (96%)	80 (80%)	20 (20%)	0	100	100
30	w	92/94 (98%)	89 (97%)	2 (2%)	1 (1%)	11	23
31	y	72/85 (85%)	67 (93%)	5 (7%)	0	100	100
32	z	48/61 (79%)	38 (79%)	10 (21%)	0	100	100
All	All	3091/3328 (93%)	2867 (93%)	220 (7%)	4 (0%)	49	69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
13	e	138	LEU

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Mol	Chain	Res	Type
14	f	171	ALA
30	w	66	ASP
15	g	46	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	67/68 (98%)	66 (98%)	1 (2%)	57	77
2	1	54/55 (98%)	54 (100%)	0	100	100
3	2	47/49 (96%)	46 (98%)	1 (2%)	47	70
4	3	46/48 (96%)	46 (100%)	0	100	100
5	4	45/49 (92%)	44 (98%)	1 (2%)	45	69
6	6	38/38 (100%)	38 (100%)	0	100	100
7	7	51/52 (98%)	49 (96%)	2 (4%)	28	53
8	8	34/34 (100%)	34 (100%)	0	100	100
11	c	216/218 (99%)	215 (100%)	1 (0%)	81	90
12	d	164/164 (100%)	162 (99%)	2 (1%)	63	80
13	e	165/165 (100%)	163 (99%)	2 (1%)	63	80
14	f	148/150 (99%)	144 (97%)	4 (3%)	39	63
15	g	137/138 (99%)	136 (99%)	1 (1%)	76	88
16	h	30/114 (26%)	29 (97%)	1 (3%)	33	58
17	j	116/116 (100%)	116 (100%)	0	100	100
18	k	103/104 (99%)	103 (100%)	0	100	100
19	l	102/103 (99%)	102 (100%)	0	100	100
20	m	109/109 (100%)	108 (99%)	1 (1%)	70	84
21	n	100/103 (97%)	100 (100%)	0	100	100
22	o	86/87 (99%)	85 (99%)	1 (1%)	63	80
23	p	98/100 (98%)	97 (99%)	1 (1%)	68	83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	q	89/90 (99%)	89 (100%)	0	100	100
25	r	82/84 (98%)	81 (99%)	1 (1%)	63	80
26	s	92/93 (99%)	91 (99%)	1 (1%)	65	81
27	t	80/84 (95%)	79 (99%)	1 (1%)	61	79
28	u	83/85 (98%)	83 (100%)	0	100	100
30	w	78/78 (100%)	78 (100%)	0	100	100
31	y	55/63 (87%)	54 (98%)	1 (2%)	51	74
32	z	44/53 (83%)	38 (86%)	6 (14%)	3	7
All	All	2559/2694 (95%)	2530 (99%)	29 (1%)	65	81

5 of 29 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	g	43	VAL
32	z	25[A]	ILE
22	o	67	ASN
32	z	11[B]	ARG
20	m	75	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
22	o	98	GLN
26	s	7	HIS
23	p	56	HIS
24	q	71	GLN
26	s	40	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	2882/2906 (99%)	767 (26%)	0
29	v	74/75 (98%)	37 (50%)	0
9	a	116/120 (96%)	33 (28%)	0
All	All	3072/3101 (99%)	837 (27%)	0

5 of 837 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	a	4	C
9	a	5	U
9	a	7	G
9	a	9	G
9	a	13	G

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
10	b	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	b	511:U	O3'	512:G	P	2.42
1	b	512:G	O3'	513:A	P	2.26

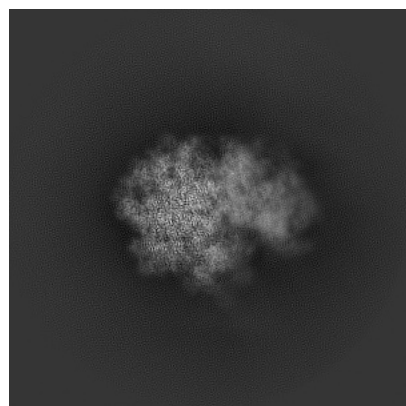
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4531. These allow visual inspection of the internal detail of the map and identification of artifacts.

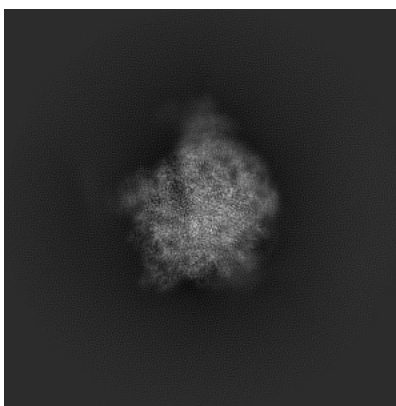
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

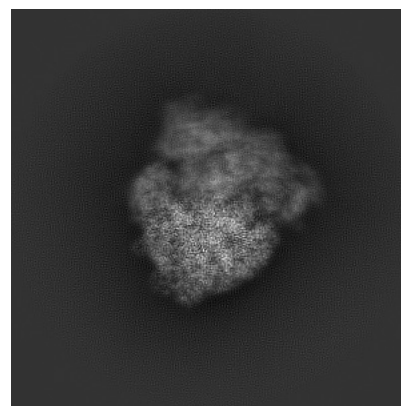
6.1.1 Primary map



X

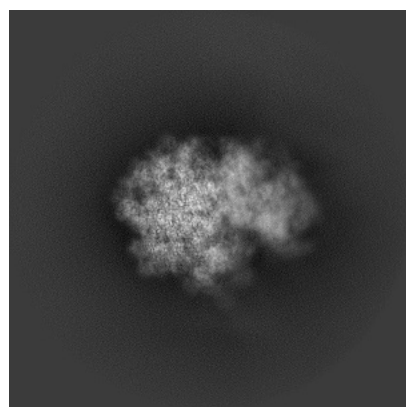


Y

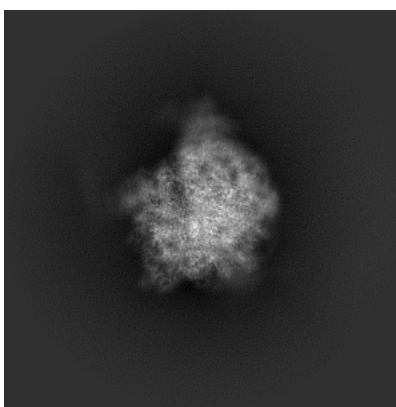


Z

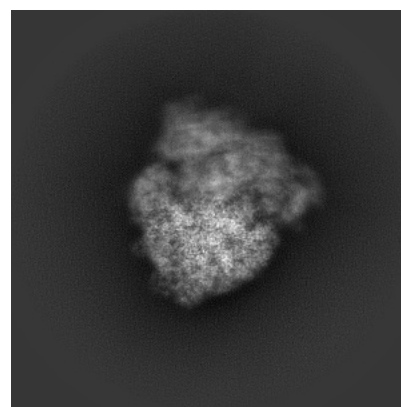
6.1.2 Raw map



X



Y

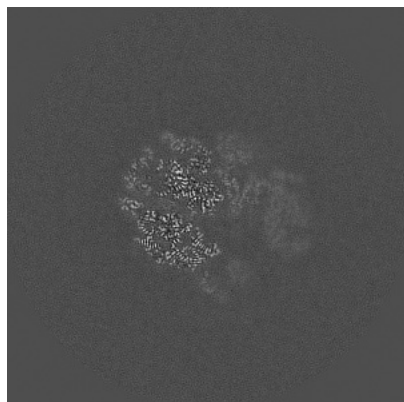


Z

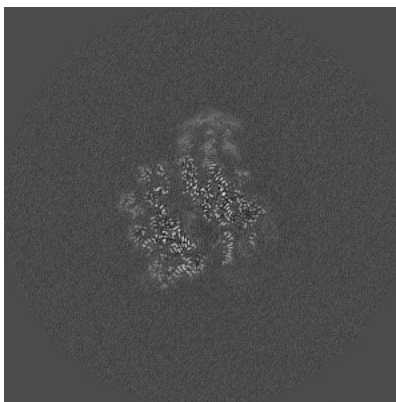
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

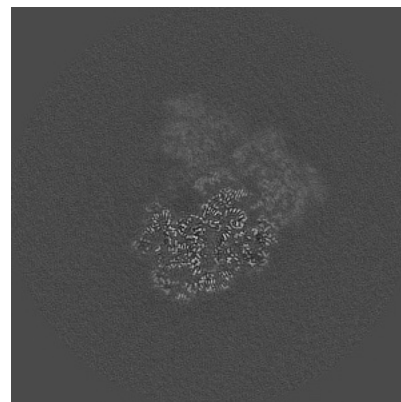
6.2.1 Primary map



X Index: 240

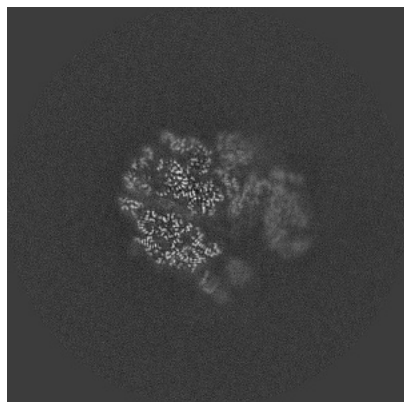


Y Index: 240

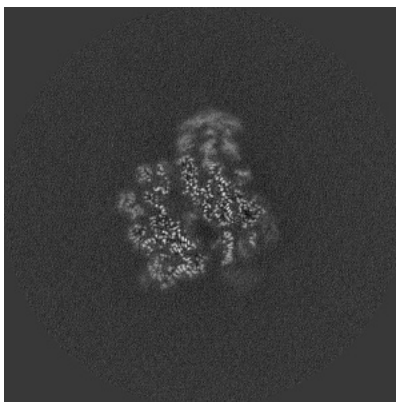


Z Index: 240

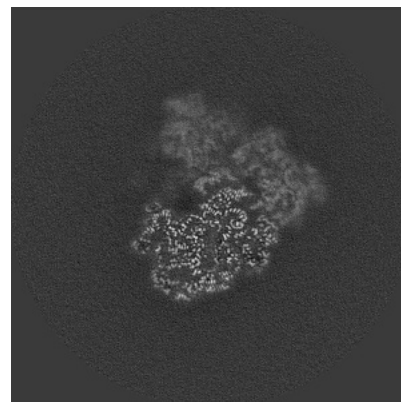
6.2.2 Raw map



X Index: 240



Y Index: 240

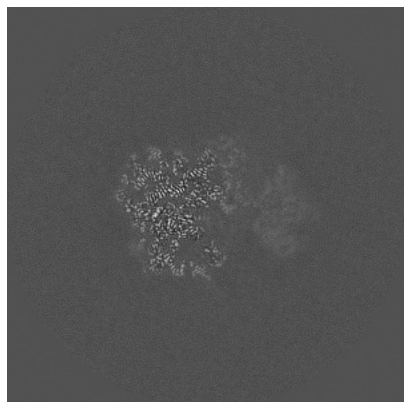


Z Index: 240

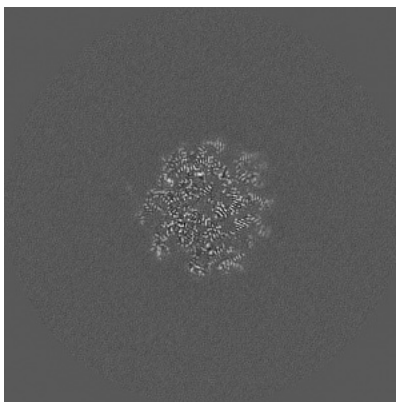
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

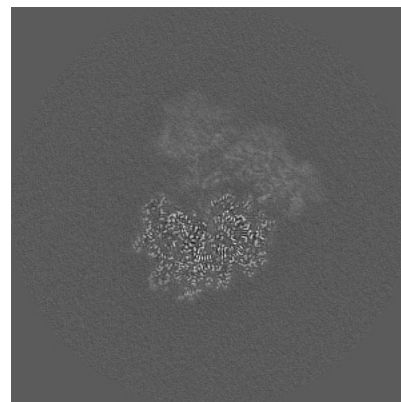
6.3.1 Primary map



X Index: 229

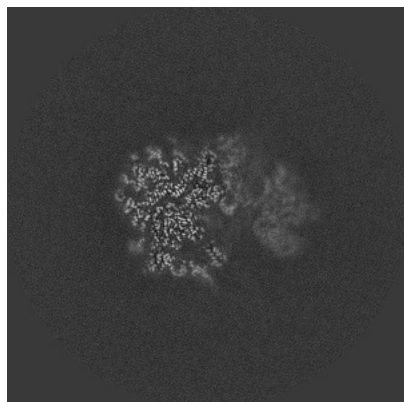


Y Index: 207

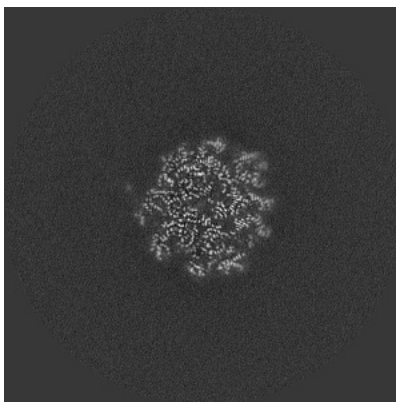


Z Index: 231

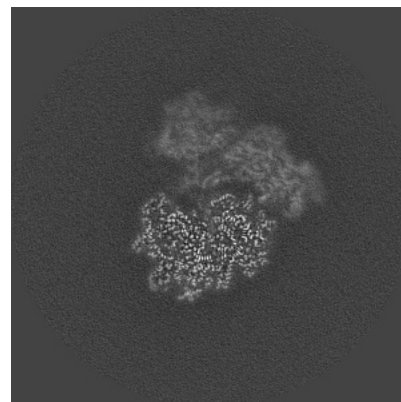
6.3.2 Raw map



X Index: 230



Y Index: 207

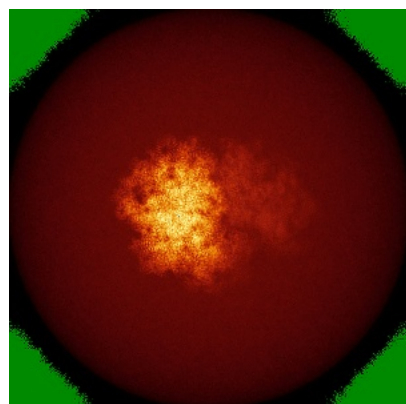


Z Index: 231

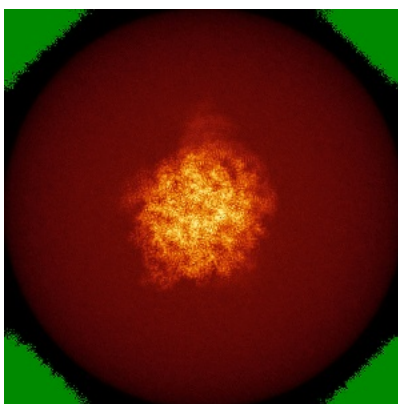
The images above show the largest variance slices of the map in three orthogonal directions.

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

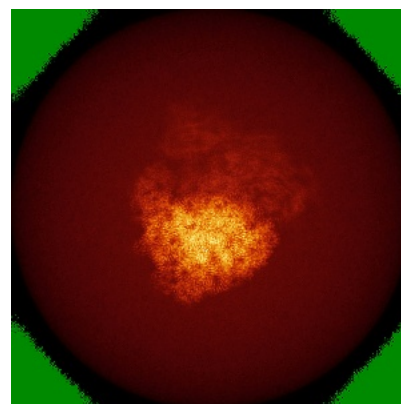
6.4.1 Primary map



X

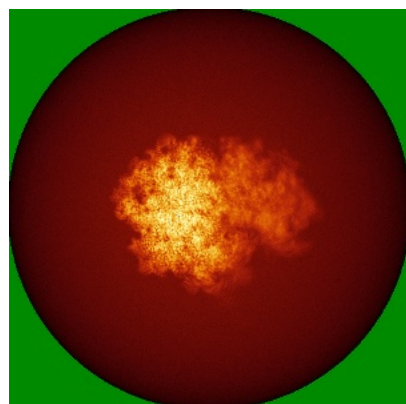


Y

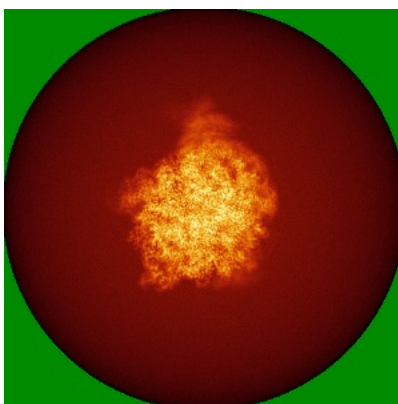


Z

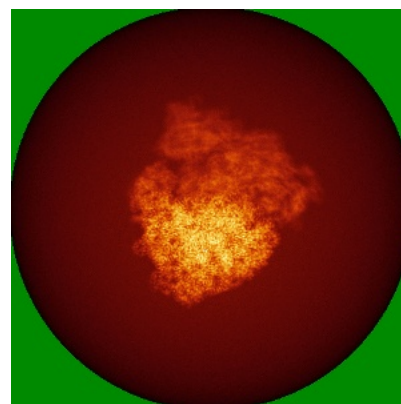
6.4.2 Raw map



X



Y

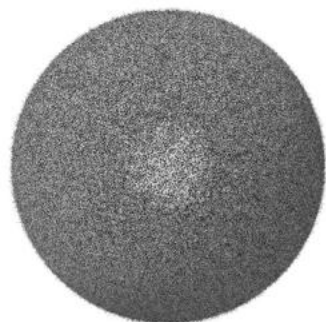


Z

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](#)

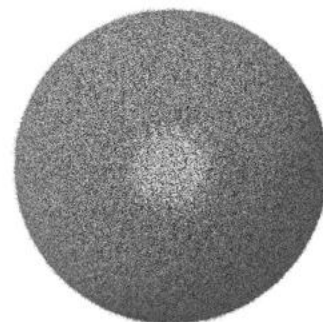
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.002. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

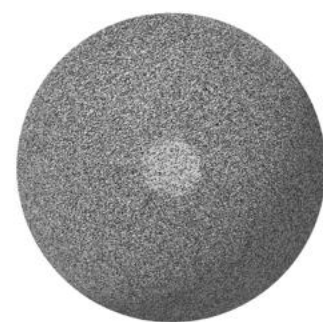
6.5.2 Raw map



X



Y



Z

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.

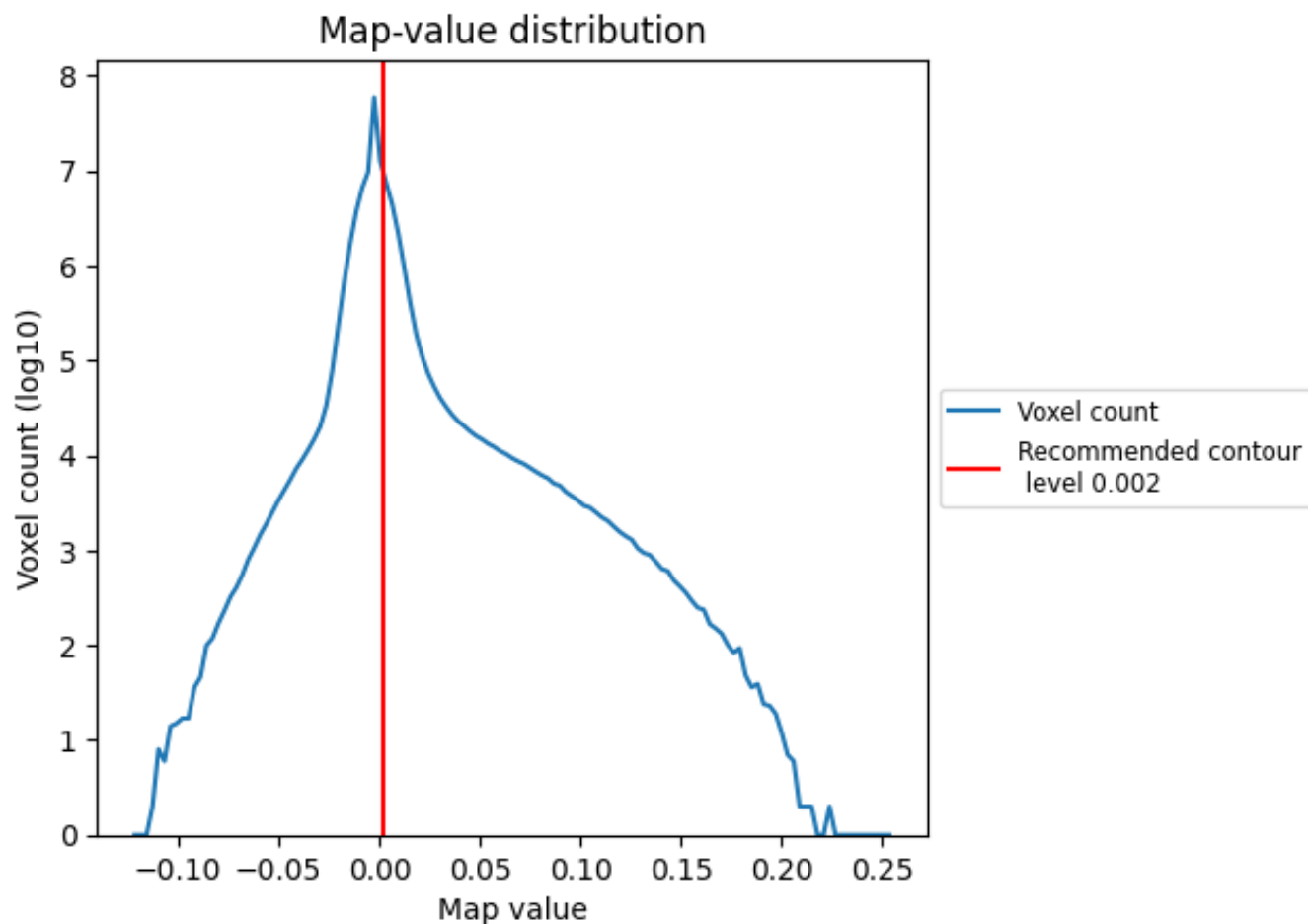
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

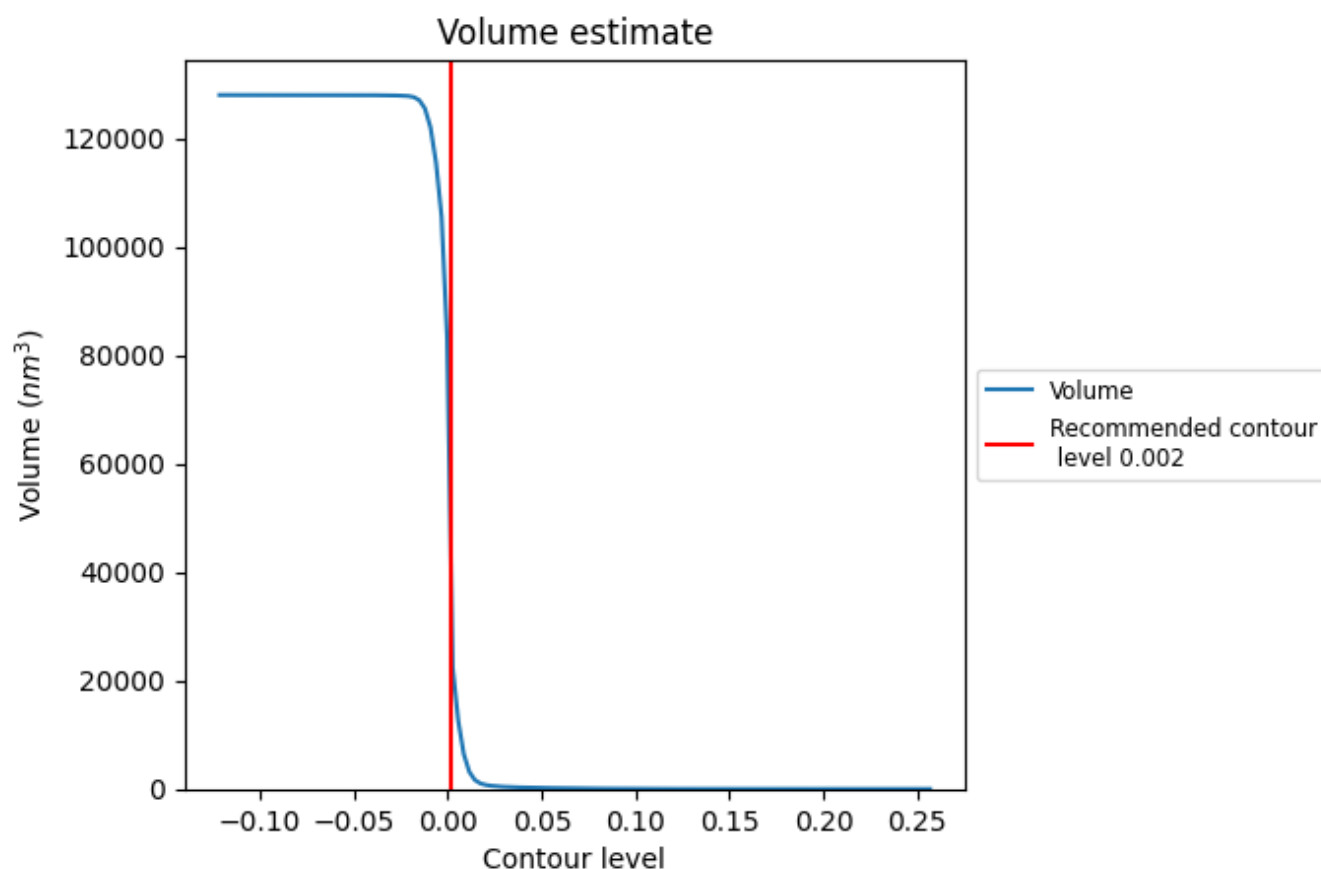
This section contains the results of statistical analysis of the map.

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.

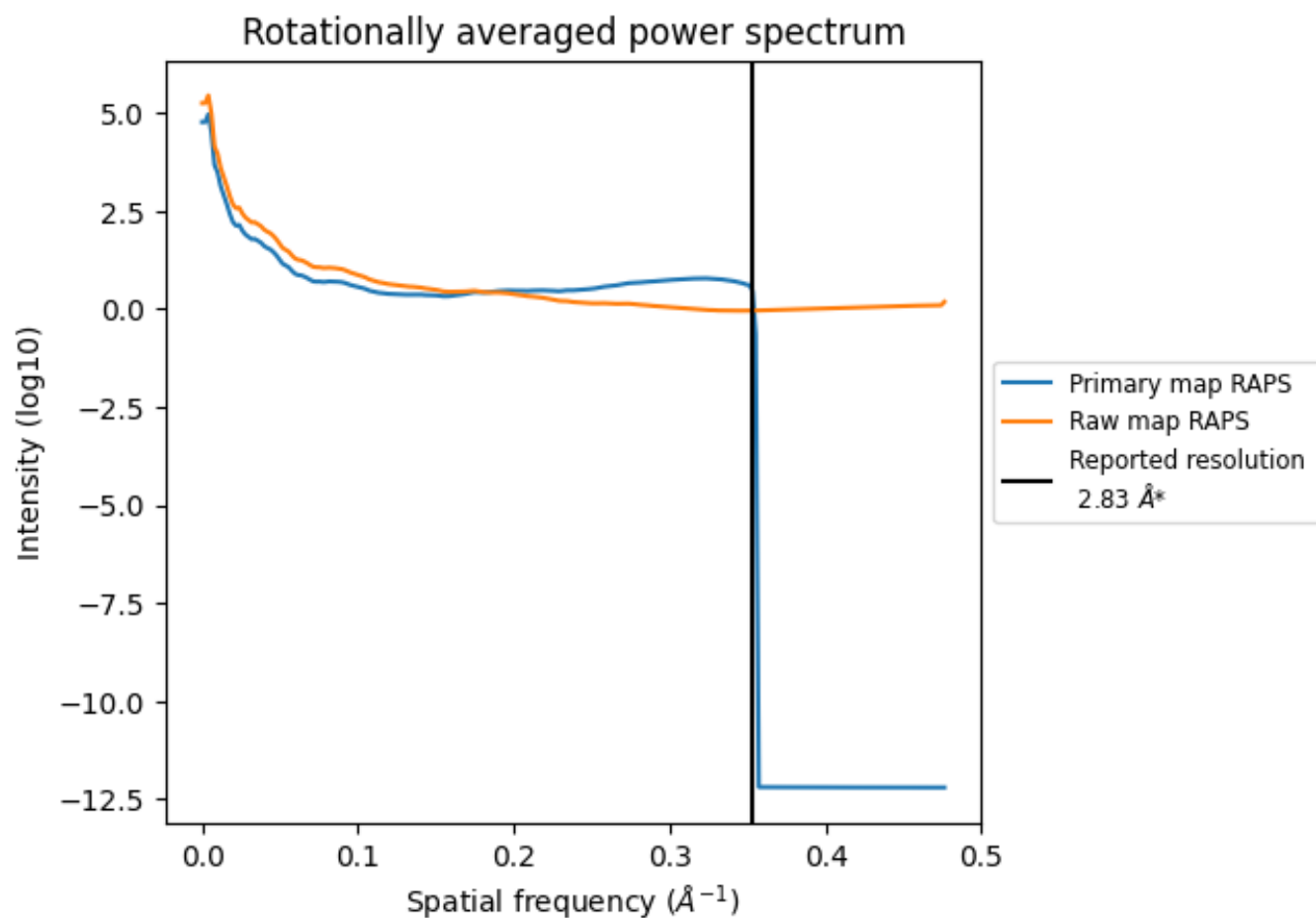
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 35519 nm^3 ; this corresponds to an approximate mass of 32085 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 ⓘ

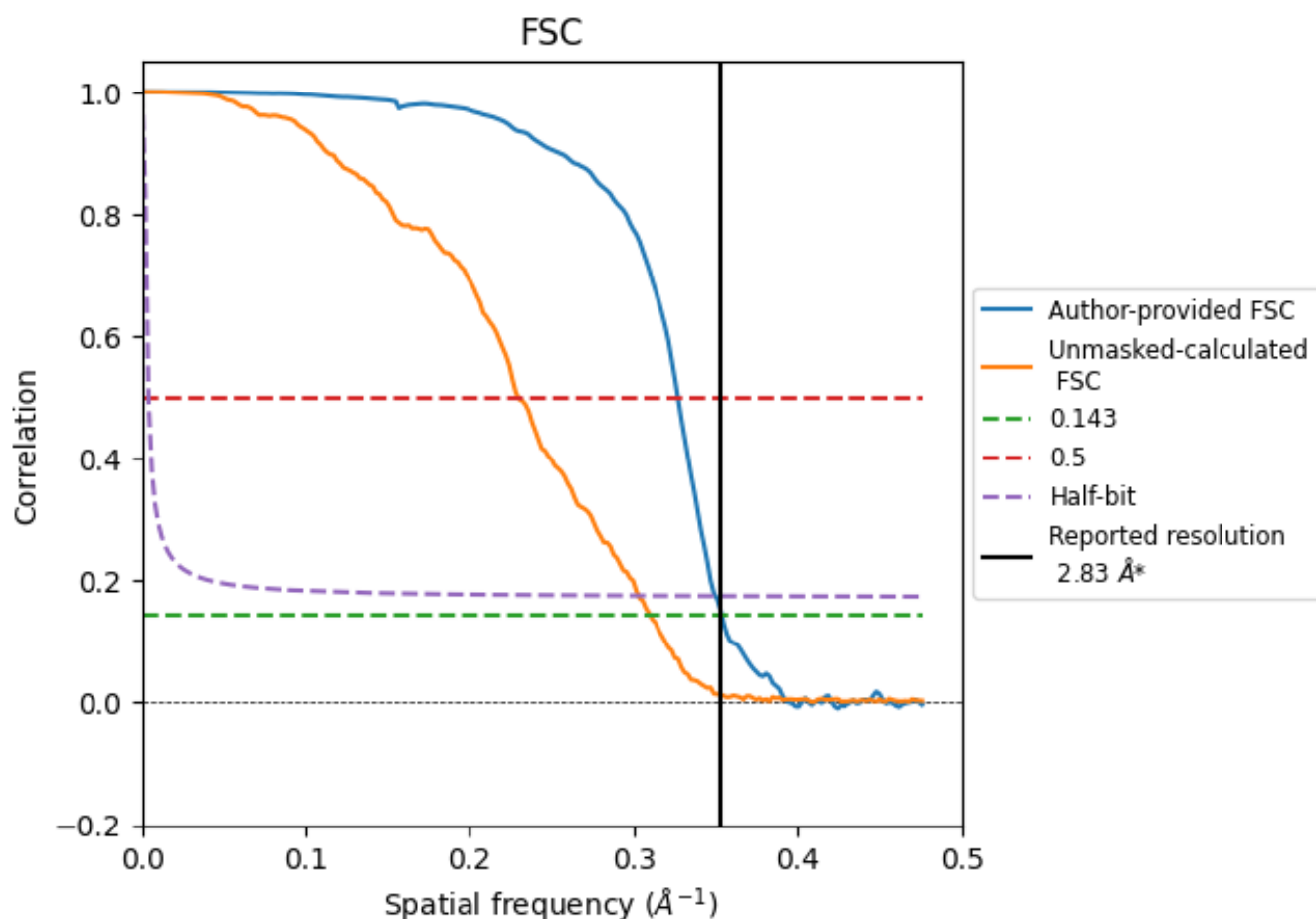


*Reported resolution corresponds to spatial frequency of 0.353 $\text{\AA}^{-1}$

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 0.353 Å⁻¹

8.2 Resolution estimates [i](#)

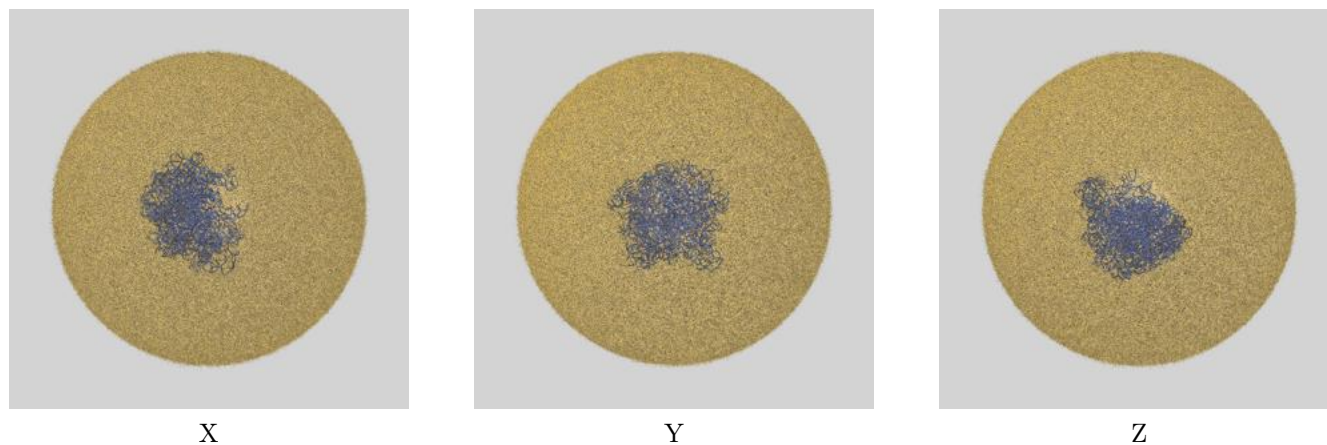
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.83	-	-
Author-provided FSC curve	2.83	3.06	2.86
Unmasked-calculated*	3.22	4.36	3.30

*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 3.22 differs from the reported value 2.83 by more than 10 %

9 Map-model fit [i](#)

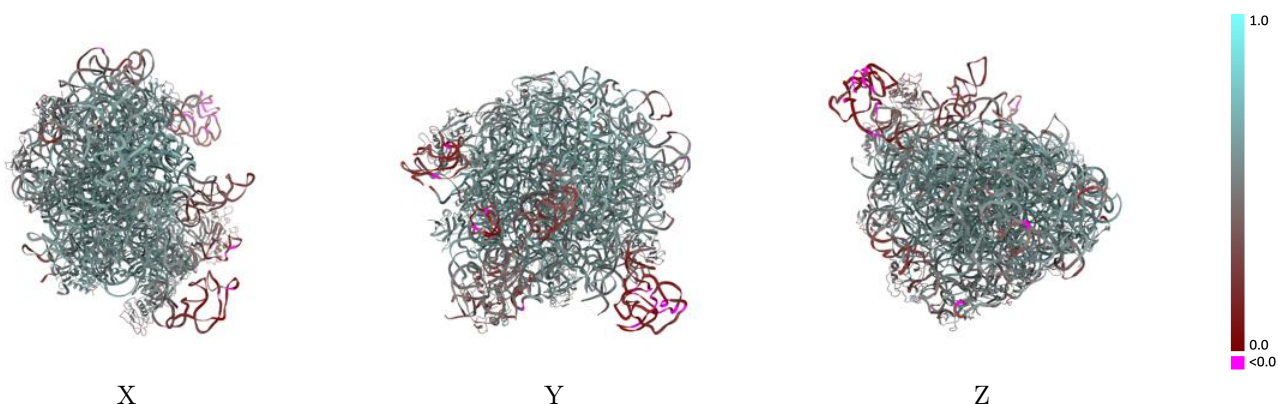
This section contains information regarding the fit between EMDB map EMD-4531 and PDB model 6QDW. Per-residue inclusion information can be found in [section 3](#) on [page 11](#).

9.1 Map-model overlay [i](#)



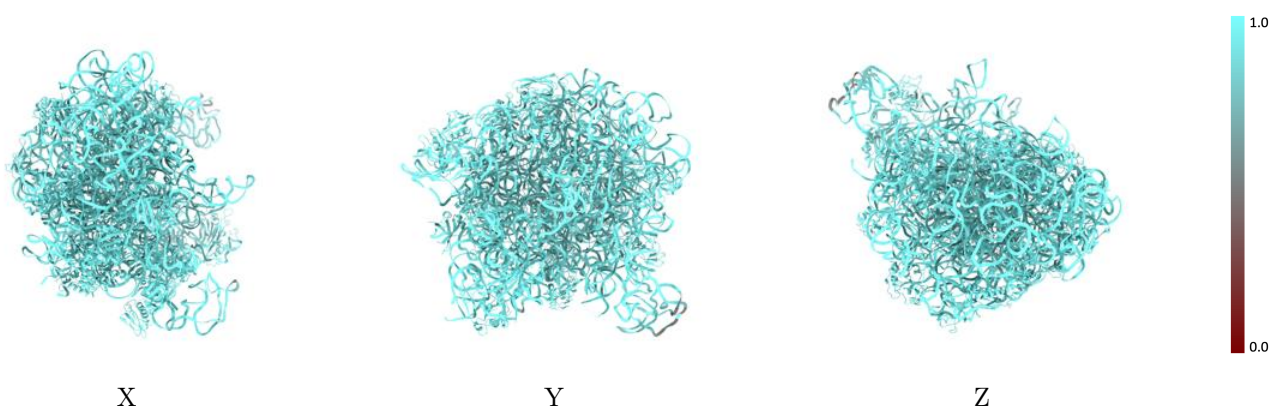
The images above show the 3D surface view of the map at the recommended contour level 0.002 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



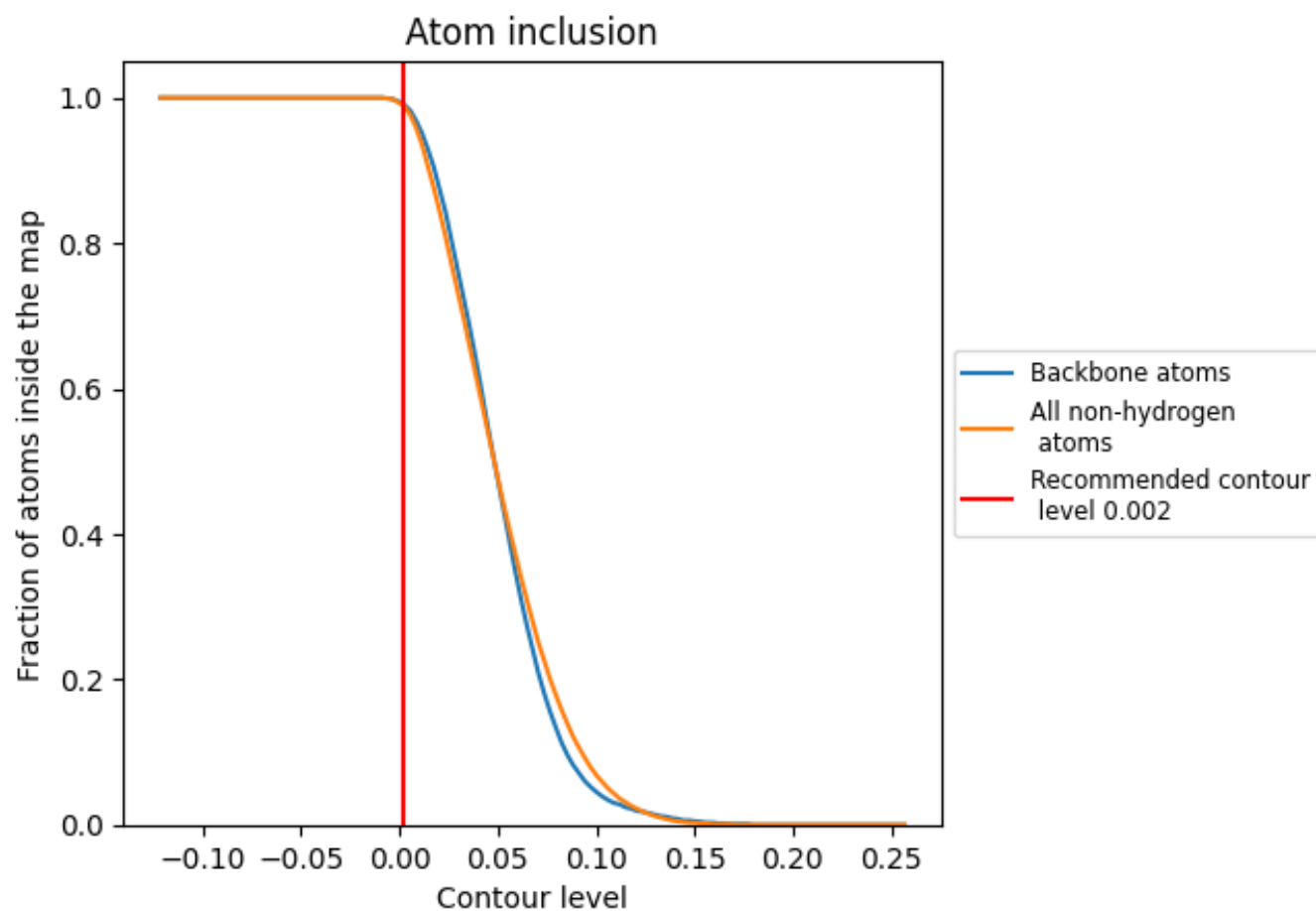
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.002).

9.4 Atom inclusion ⓘ



At the recommended contour level, 99% of all backbone atoms, 99% 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 (0.002) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9890	 0.5410
0	 0.9880	 0.5580
1	 0.9770	 0.4710
2	 0.9980	 0.5990
3	 0.9950	 0.5550
4	 0.9680	 0.5120
6	 0.9920	 0.6080
7	 0.9960	 0.6150
8	 1.0000	 0.5820
a	 0.9930	 0.5000
b	 0.9910	 0.5510
c	 0.9930	 0.5910
d	 0.9890	 0.5650
e	 0.9850	 0.5240
f	 0.9830	 0.3410
g	 0.9870	 0.4600
h	 0.9790	 0.4550
j	 0.9950	 0.5910
k	 0.9920	 0.5730
l	 0.9850	 0.5590
m	 0.9940	 0.5920
n	 0.9940	 0.5660
o	 0.9880	 0.4670
p	 0.9840	 0.5340
q	 0.9970	 0.6130
r	 0.9900	 0.5800
s	 0.9930	 0.5770
t	 0.9890	 0.5100
u	 0.9840	 0.4570
v	 0.9260	 0.2810
w	 0.9930	 0.5560
y	 0.9910	 0.5980
z	 0.8500	 0.2500

