



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 06:56 PM EDT

PDB ID : 9PJ8 / pdb_00009pj8
EMDB ID : EMD-71683
Title : C. acnes 70S ribosome bound to Sarecycline
Authors : Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on : 2025-07-12
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

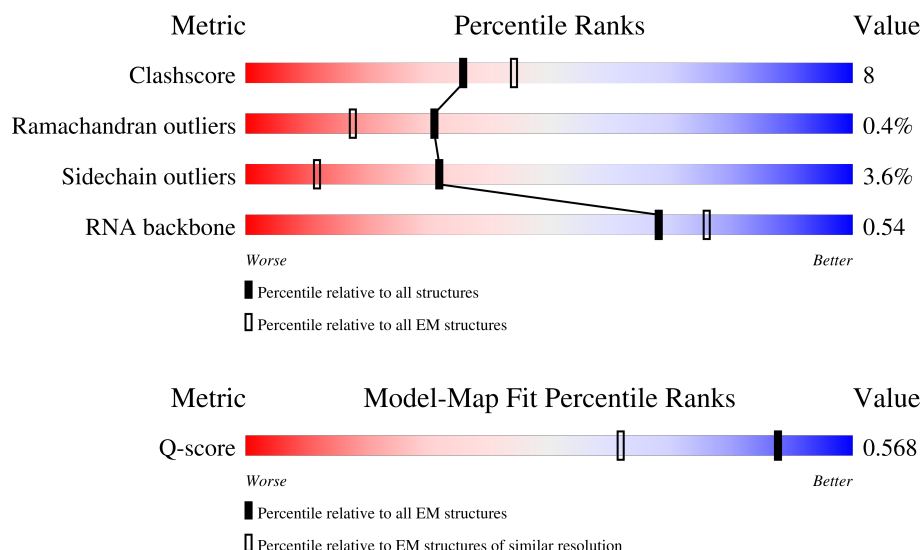
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.50 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.



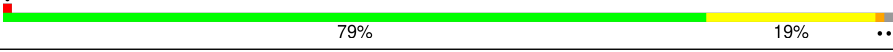
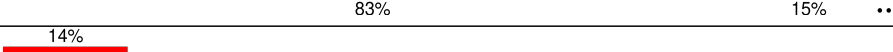
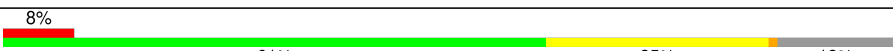
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 (2.00 - 3.00)

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	56	
2	1	44	
3	2	68	

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Mol	Chain	Length	Quality of chain
4	3	37	
5	4	69	
6	A	1537	
7	B	283	
8	C	77	
9	D	201	
10	E	215	
11	F	96	
12	G	269	
13	H	135	
14	I	156	
15	J	173	
16	K	135	
17	L	123	
18	M	103	
19	N	123	
20	O	87	
21	P	147	
22	Q	90	
23	R	79	
24	S	61	
25	T	88	
26	U	93	
27	V	24	
28	X	33	

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Mol	Chain	Length	Quality of chain
29	Y	22	
30	a	3086	
31	b	120	
32	c	278	
33	d	223	
34	e	301	
35	f	210	
36	g	180	
37	i	147	
38	j	122	
39	k	146	
40	l	139	
41	m	187	
42	n	127	
43	o	117	
44	p	123	
45	q	102	
46	r	153	
47	s	102	
48	t	122	
49	u	205	
50	v	89	
51	w	61	
52	x	77	
53	y	60	

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Mol	Chain	Length	Quality of chain
54	z	63	78% 21%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 144415 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 L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	50	Total	C	N	O	S	0	0
			423	253	91	73	6		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			362	213	91	56	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	67	Total	C	N	O	S	0	0
			513	315	110	87	1		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	37	Total	C	N	O	S	0	0
			302	184	66	47	5		

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	66	Total	C	N	O	S	0	0
			512	313	97	97	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1505	Total	C	N	O	P	0	0
			32340	14408	5893	10534	1505		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	233	Total	C	N	O	S	0	0
			1836	1163	326	338	9		

- Molecule 8 is a RNA chain called initiator tRNA Met (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	76	Total	C	N	O	P S	0	0
			1625	725	294	529	76 1		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	200	Total	C	N	O	S	0	0
			1632	1021	313	297	1		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	179	Total	C	N	O	S	0	0
			1309	816	244	245	4		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	96	Total	C	N	O	S	0	0
			785	496	134	149	6		

- Molecule 12 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	206	Total	C	N	O	S	0	0
			1613	1010	305	294	4		

- Molecule 13 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	134	Total	C	N	O	S	0	0
			1021	642	182	194	3		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	155	Total	C	N	O	S	0	0
			1225	764	235	220	6		

- Molecule 15 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	134	Total	C	N	O	S	0	0
			1012	629	204	177	2		

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			858	532	168	154	4		

- Molecule 17 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	122	Total	C	N	O	S	0	0
			948	587	195	164	2		

- Molecule 18 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	98	Total	C	N	O	S	0	0
			786	496	146	141	3		

- Molecule 19 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	122	Total	C	N	O	S	0	0
			976	598	205	173			

- Molecule 20 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	87	Total	C	N	O	S	0	0
			708	440	140	125	3		

- Molecule 21 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	128	Total	C	N	O	S	0	0
			994	621	185	187	1		

- Molecule 22 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	90	Total	C	N	O	S	0	0
			728	446	142	134	6		

- Molecule 23 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	67	Total	C	N	O		0	0
			527	334	103	90			

- Molecule 24 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	60	Total	C	N	O	S	0	0
			474	298	98	73	5		

- Molecule 25 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	87	Total	C	N	O		0	0
			673	408	144	121			

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	84	Total	C	N	O	S	0	0
			658	416	126	113	3		

- Molecule 27 is a protein called 50S ribosomal protein bL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	23	Total	C	N	O		0	0
			183	106	50	27			

- Molecule 28 is a protein called AURKAIP1/COX24 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	32	Total	C	N	O	S	0	0
			277	170	71	35	1		

- Molecule 29 is a RNA chain called mRNA 32MF.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	10	Total	C	N	O	P	0	0
			211	95	35	71	10		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2903	Total	C	N	O	P	1	0
			62432	27805	11391	20332	2904		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	63	A	G	conflict	GB CP012350
a	524	C	G	conflict	GB CP012350
a	1038	PSU	G	conflict	GB CP012350

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	120	Total	C	N	O	P	0	0
			2567	1145	466	836	120		

- Molecule 32 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	274	Total	C	N	O	S	0	0
			2091	1289	425	372	5		

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	214	Total	C	N	O	S	0	0
			1586	984	304	291	7		

- Molecule 34 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	210	Total	C	N	O	S	0	0
			1577	979	301	295	2		

- Molecule 35 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	f	184	Total	C	N	O	S	0	0
			1468	924	269	266	9		

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	177	Total	C	N	O	S	0	0
			1376	867	250	258	1		

- Molecule 37 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	146	Total	C	N	O	S	0	0
			1139	718	213	205	3		

- Molecule 38 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	122	Total	C	N	O	S	0	0
			946	596	177	169	4		

- Molecule 39 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	144	Total	C	N	O	S	0	0
			1072	675	196	199	2		

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	136	Total	C	N	O	S	0	0
			1082	685	210	181	6		

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	120	Total	C	N	O	S	0	0
			936	583	188	163	2		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
m	124	ALA	THR	conflict	UNP A0A8B2VJI7
m	185	PRO	SER	conflict	UNP A0A8B2VJI7

- Molecule 42 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	126	Total	C	N	O	S	0	0
			952	583	190	176	3		

- Molecule 43 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	114	Total	C	N	O	S	0	0
			896	559	174	162	1		

- Molecule 44 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	119	Total	C	N	O	S	0	0
			958	589	196	171	2		

- Molecule 45 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	102	Total	C	N	O	S	0	0
			778	487	140	150	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
q	52	ALA	VAL	conflict	UNP Q6A9I3

- Molecule 46 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	132	Total	C	N	O	S	0	0
			1017	624	204	182	7		

- Molecule 47 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	95	Total	C	N	O	S	0	0
			751	474	138	138	1		

- Molecule 48 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	107	Total	C	N	O	S	0	0
			833	516	163	153	1		

- Molecule 49 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	179	Total	C	N	O	S	0	0
			1376	865	240	268	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
50	v	78	Total	C	N	O	0	0
			591	355	127	109		

- Molecule 51 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	60	Total	C	N	O	S	0	0
			474	290	102	77	5		

- Molecule 52 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	x	69	Total	C	N	O	0	0
			564	348	108	108		

- Molecule 53 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	58	Total	C	N	O	S	0	0
			467	290	91	83	3		

- Molecule 54 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	62	Total	C	N	O	S	0	0
			477	287	102	83	5		

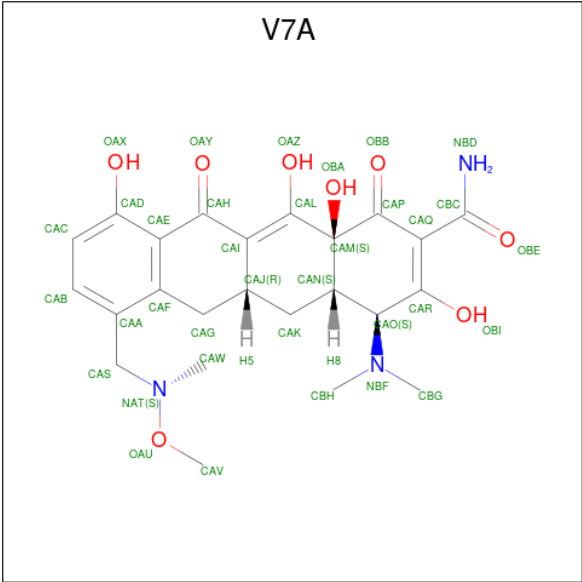
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	0	1	Total	Zn	0
			1	1	
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	
55	S	1	Total	Zn	0
			1	1	
55	w	1	Total	Zn	0
			1	1	
55	z	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	63	Total	Mg	0
			63	63	
56	a	233	Total	Mg	0
			233	233	
56	b	2	Total	Mg	0
			2	2	
56	c	1	Total	Mg	0
			1	1	
56	d	1	Total	Mg	0
			1	1	
56	k	1	Total	Mg	0
			1	1	

- Molecule 57 is Sarecycline (CCD ID: V7A) (formula: C₂₄H₂₉N₃O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	N	O	0
			35	24	3	8	
57	a	1	Total	C	N	O	0
			35	24	3	8	

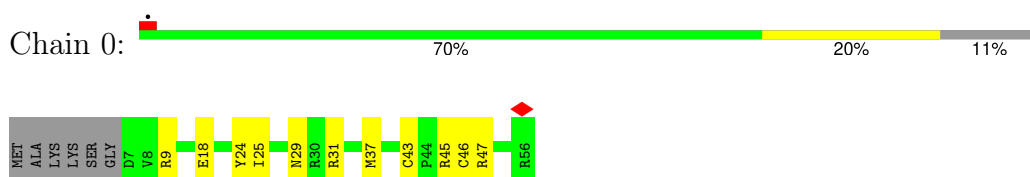
- Molecule 58 is water.

Mol	Chain	Residues	Atoms		AltConf
58	A	11	Total	O	0
			11	11	
58	a	108	Total	O	0
			108	108	
58	b	1	Total	O	0
			1	1	
58	c	1	Total	O	0
			1	1	

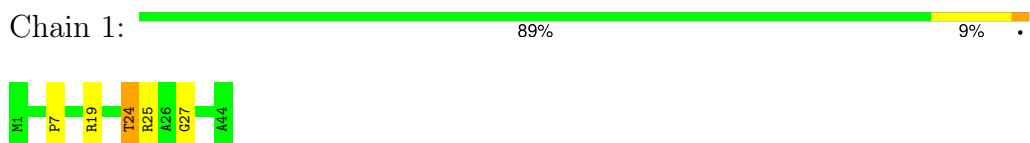
3 Residue-property plots [i](#)

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

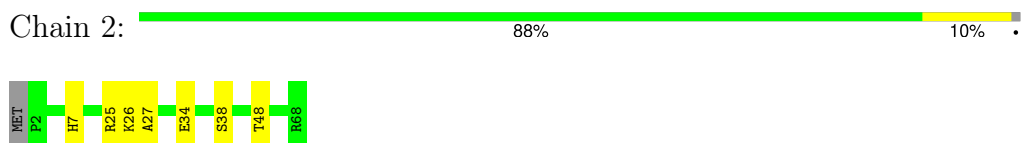
- Molecule 1: 50S ribosomal protein L33



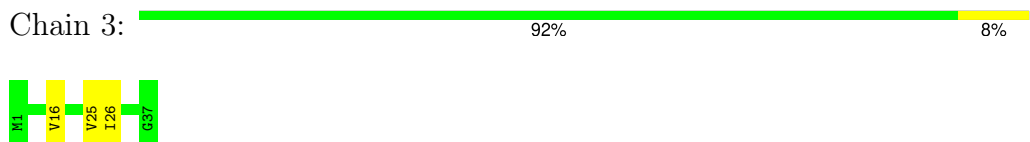
- Molecule 2: 50S ribosomal protein L34



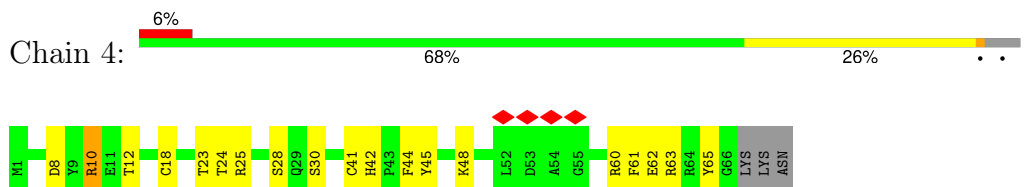
- Molecule 3: Large ribosomal subunit protein bL35



- Molecule 4: 50S ribosomal protein L36



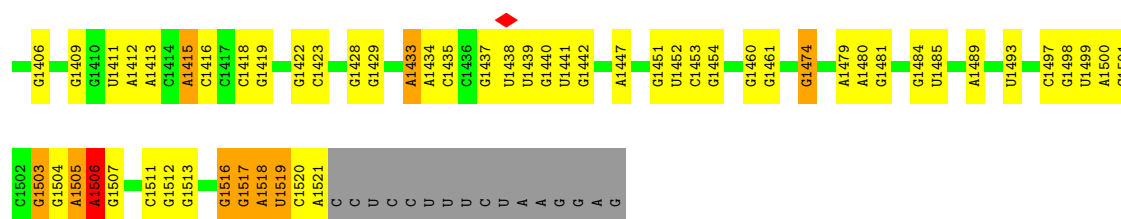
- Molecule 5: 50S ribosomal protein L31



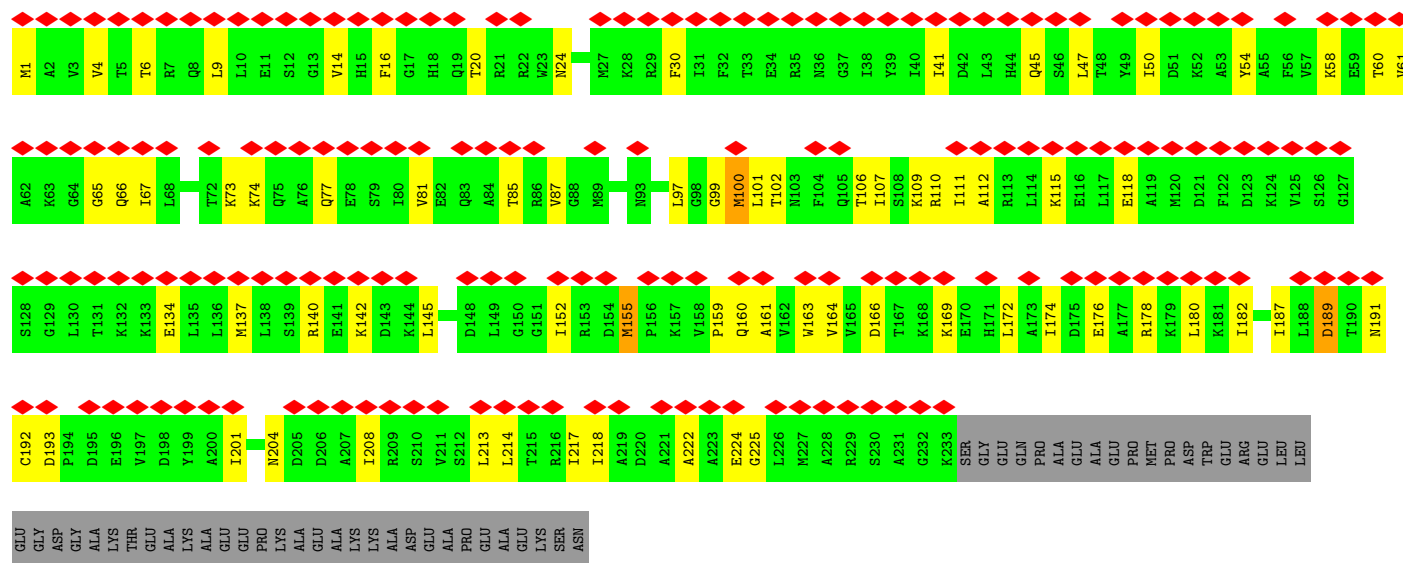
- Molecule 6: 16S rRNA

Response	Percentage
Yes, the U.S. is a democracy	56%
No, the U.S. is not a democracy	36%
Don't know	6%

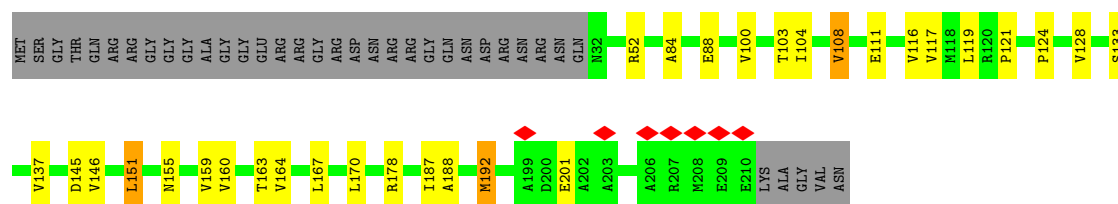




• Molecule 7: 30S ribosomal protein S2

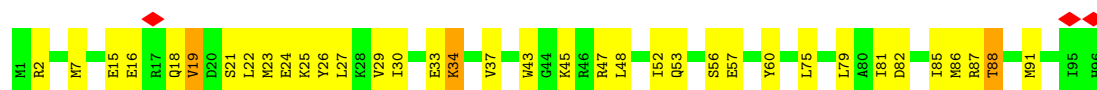


Chain E: 



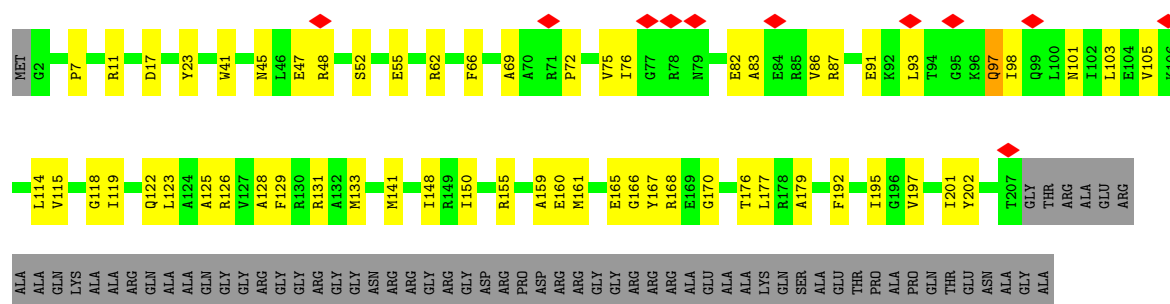
- Molecule 11: 30S ribosomal protein S6

Chain F: 



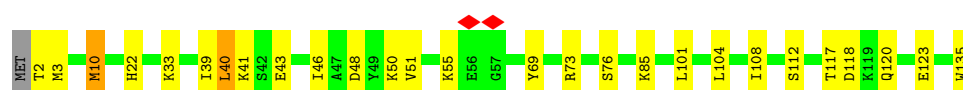
- Molecule 12: 30S ribosomal protein S3

Chain G: 



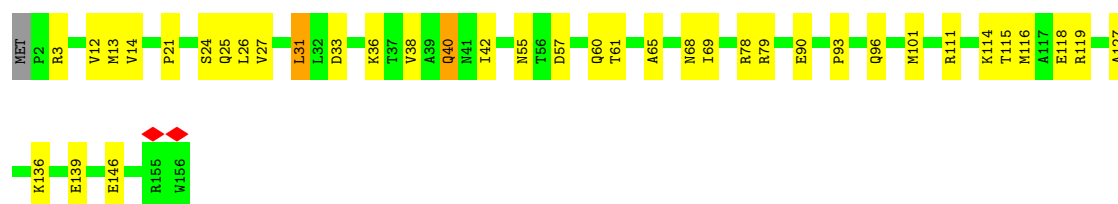
- Molecule 13: 30S ribosomal protein S8

Chain H: 

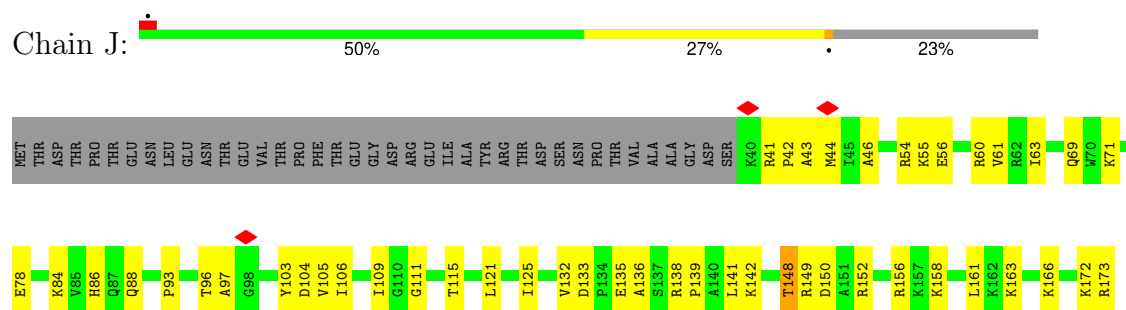


- Molecule 14: 30S ribosomal protein S7

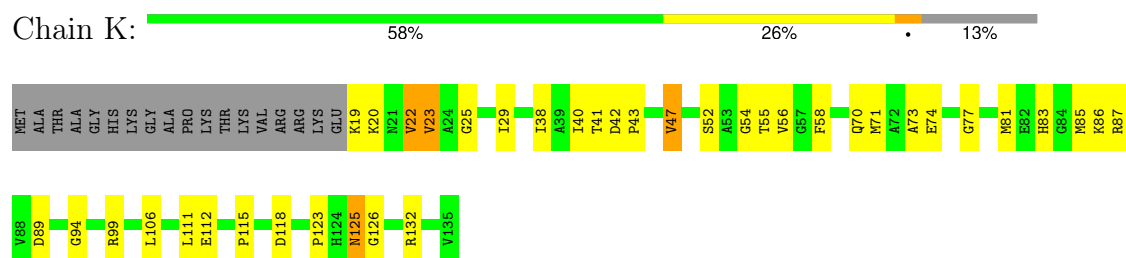
Chain I: 



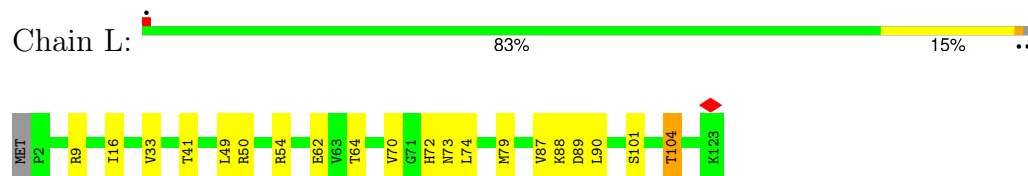
- Molecule 15: 30S ribosomal protein S9



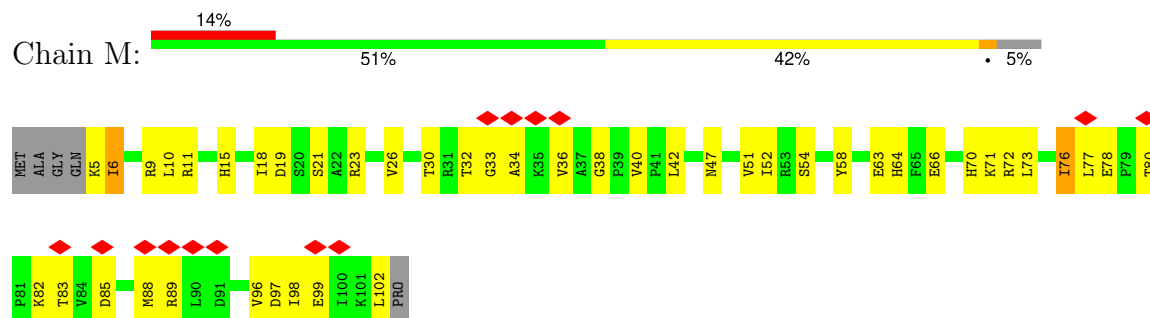
- Molecule 16: 30S ribosomal protein S11



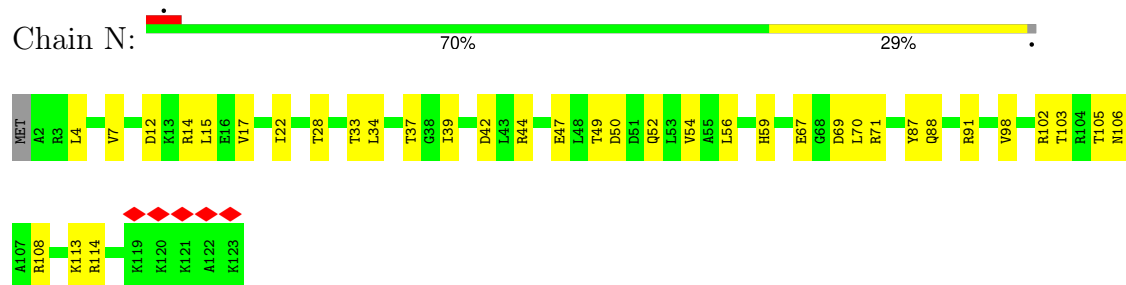
- Molecule 17: 30S ribosomal protein S12



- Molecule 18: Small ribosomal subunit protein uS10



- Molecule 19: 30S ribosomal protein S13



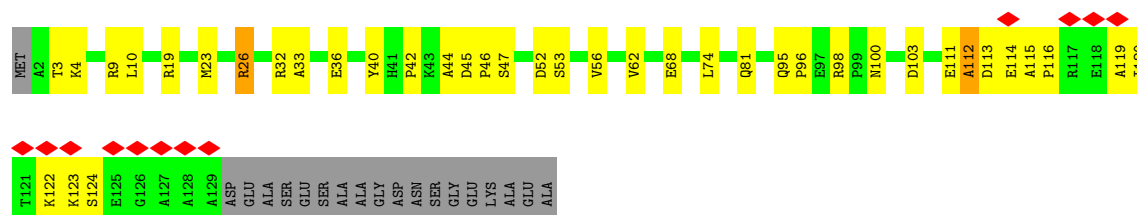
- Molecule 20: 30S ribosomal protein S15

Chain O:  75% 25%



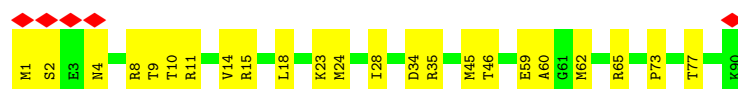
- Molecule 21: 30S ribosomal protein S16

Chain P:  8% 61% 25% 13%



- Molecule 22: 30S ribosomal protein S17

Chain Q:  6% 74% 26%



- Molecule 23: 30S ribosomal protein S18

Chain R:  9% 63% 19% 15%



- Molecule 24: 30S ribosomal protein S14 type Z

Chain S:  74% 23% ..



- Molecule 25: 30S ribosomal protein S20

Chain T:  74% 25% .



- Molecule 26: 30S ribosomal protein S19

Chain U:  68% 22% . 10%



- Molecule 27: 50S ribosomal protein bL37

Chain V: 75% 21% .



- Molecule 28: AURKAIP1/COX24 domain-containing protein

Chain X: 70% 27% .



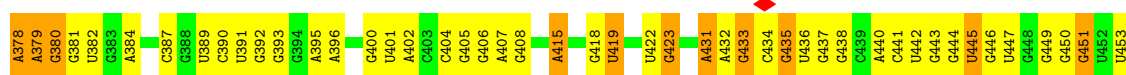
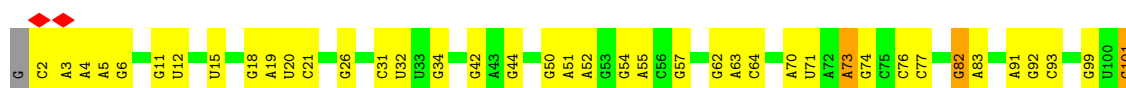
- Molecule 29: mRNA 32MF

Chain Y: 5% 23% 14% 9% 55%

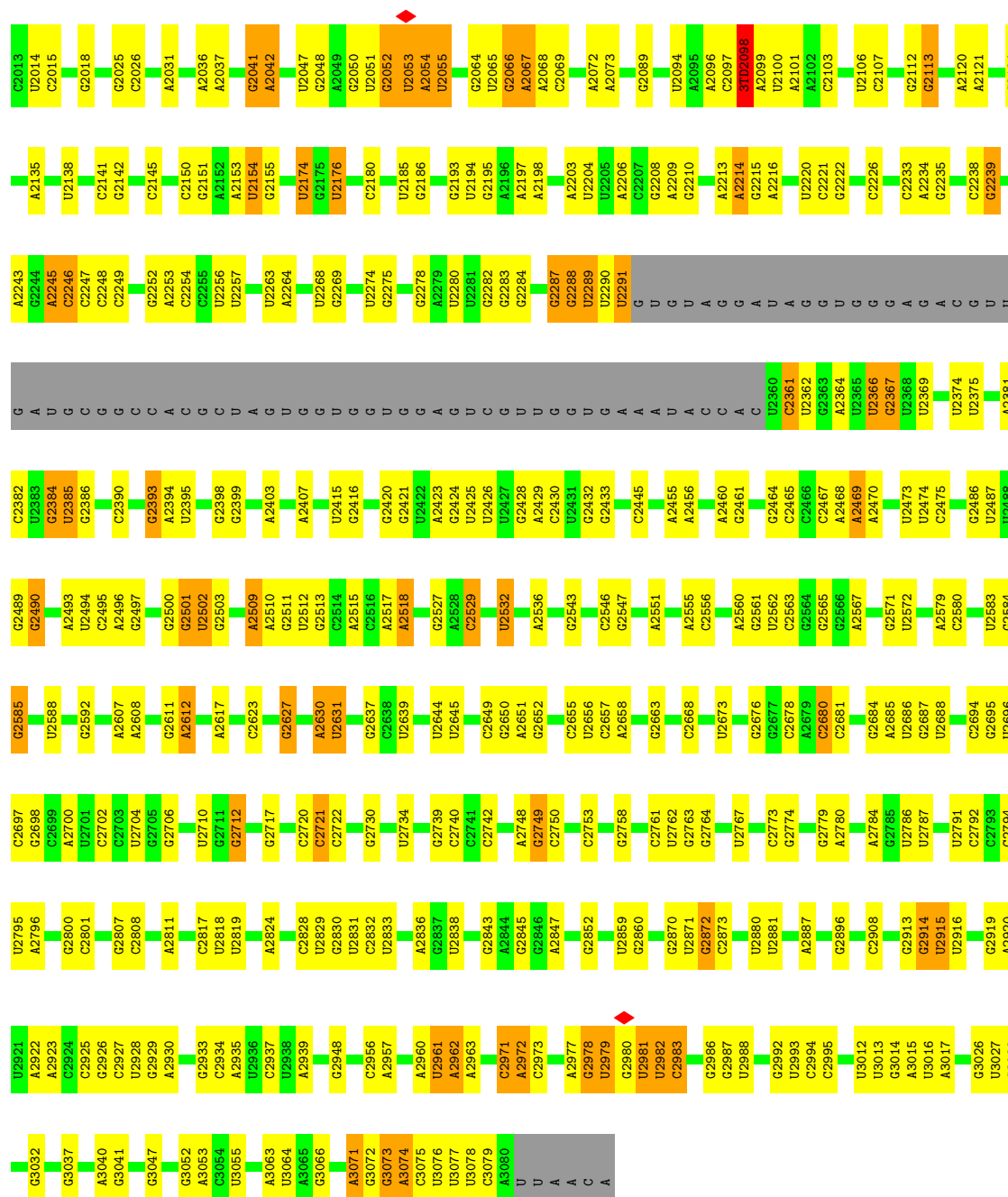


- Molecule 30: 23S rRNA

Chain a: 57% 31% 6% 6%

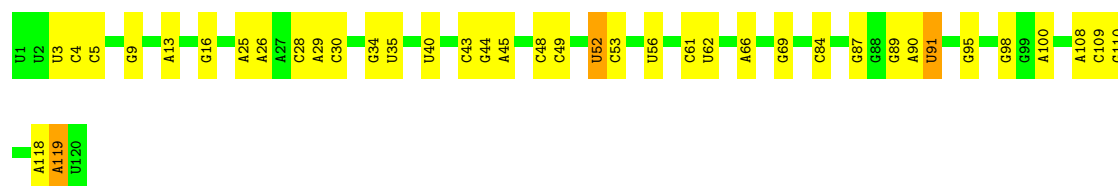


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G1905	U1762	A1676	U	U	U1455	G1327	U1191	A1011	A905	G797	U683	G587	G588
A1907	G1763	G1685	A	G	A1460	A1328	A1192	G1014	U911	G798	G686	A589	A590
C1908	C1686	C1687	G	U	A1461	A1331	A1193	U1015	U912	G799	A687	G592	A593
C1909	G1767	G1688	C	U	C1462	U1332	G1195	A1028	U913	A800	A692	G596	U599
A1910	A1768	U1688	U	U	C1463	G1333	U1196	G1029	G916	A801	A693	U600	U608
G1911	G1769	G1689	U	U	C1464	G1337	U1199	A1030	U917	G802	U698	G609	G618
U1912	U1770	A1690	G	G	A1465	G1337	U1200	C1031	G918	U806	G699	G704	G619
G1913	U1771	A1691	G	G	U1466	G1348	A1211	U1038	G921	C807	U700	U709	C620
C1914	G1772	G1692	G	G	U1466	U1349	U1215	A1042	G930	G814	U701	G710	C621
G1915	G1773	U1693	A	A	A1471	U1350	U1216	A1043	G931	U815	G704	G711	C622
U1916	U1774	A1697	C	U	U1472	G1350	A1217	G1044	G935	C816	G704	G712	C623
G1917	G1775	C1608	U	U	C1481	U1351	U1218	U1047	U936	G817	U709	G713	C624
U1918	G1776	G1609	G	G	G1482	U1358	U1219	U1048	U937	G818	U710	G714	C625
G1919	C1780	A1611	U	U	U1486	G1359	U1220	U1049	U938	A824	U711	G715	C626
U1920	G1781	G1612	U	U	U1487	G1360	U1221	U1050	U939	C825	U712	G716	C627
G1921	U1782	U1613	U	U	U1488	G1361	U1222	U1051	U940	C826	U713	G717	C628
U1922	A1703	U1614	U	U	C1489	G1362	U1223	U1052	G941	A825	U714	G718	C629
G1923	A1704	G1615	U	U	C1490	G1363	U1224	U1053	A942	C826	U715	G719	C630
U1924	U1705	U1616	U	U	C1491	G1364	U1225	U1054	G943	U832	U720	G720	C631
A1925	G1706	G1617	G	G	C1492	U1365	U1226	U1055	G944	U833	U721	G721	C632
G1926	G1707	U1618	A	A	U1493	U1366	U1227	U1056	G945	G834	U722	G722	C633
U1927	G1708	U1619	U	U	U1494	U1367	U1228	U1057	A951	A849	U723	G723	C634
G1928	G1709	A1620	C	C	U1495	A1377	U1229	U1058	U960	U853	U724	G724	C635
U1929	A1710	G1621	G	G	G1496	U1378	U1230	U1059	U961	U854	U725	G725	C636
G1930	G1711	U1622	U	U	U1497	U1379	U1231	U1060	U962	U855	U726	G726	C637
U1931	G1712	C1623	U	U	U1498	U1380	U1232	U1061	U963	U856	U727	G727	C638
A1932	C1713	A1624	C	C	U1499	U1381	U1233	U1062	U964	U857	U728	G728	C639
U1933	G1714	U1625	U	U	U1500	U1382	U1234	U1063	U965	U858	U729	G729	C640
G1934	A1715	C1626	G	G	U1501	U1383	U1235	U1064	U966	U859	U730	G730	C641
U1935	U1716	G1627	U	U	U1502	U1384	U1236	U1065	U967	U860	U731	G731	C642
G1936	G1717	U1628	G	G	U1503	C1391	U1237	U1066	U968	U861	U732	G732	C643
U1937	U1718	C1629	U	U	U1504	A1392	U1238	U1067	U969	U862	U733	G733	C644
G1938	U1719	G1630	U	U	U1505	U1393	U1239	U1068	U970	U863	U734	G734	C645
U1939	U1720	U1631	G	G	U1506	U1394	U1240	U1069	U971	U864	U735	G735	C646
A1940	G1721	U1632	G	G	U1507	U1395	U1241	U1070	U972	U865	U736	G736	C647
G1941	U1722	U1633	U	U	U1508	U1396	U1242	U1071	U973	U866	U737	G737	C648
U1942	U1723	G1634	U	U	U1509	U1397	U1243	U1072	U974	U867	U738	G738	C649
G1943	U1724	U1635	G	G	U1510	U1402	U1244	U1073	U975	U868	U739	G739	C650
U1944	G1725	U1636	U	U	U1511	U1403	U1245	U1074	U976	U869	U740	G740	C651
G1945	U1726	G1637	A	A	U1512	G1404	U1246	U1075	U977	U870	U741	G741	C652
U1946	U1727	U1638	U	U	U1513	U1405	U1247	U1076	U978	U871	U742	G742	C653
G1947	G1728	U1639	U	U	U1514	U1406	U1248	U1077	U979	U872	U743	G743	C654
U1948	U1729	U1640	G	G	U1515	U1416	U1249	U1078	U980	U873	U744	G744	C655
G1949	G1730	U1641	U	U	U1516	G1417	U1250	U1079	U981	U874	U745	G745	C656
U1950	U1731	U1642	U	U	U1517	U1418	U1251	U1080	U982	U875	U746	G746	C657
G1951	G1732	G1643	G	G	U1518	U1419	U1252	U1081	U983	U876	U747	G747	C658
U1952	U1733	U1644	U	U	U1519	U1420	U1253	U1082	U984	U877	U748	G748	C659
G1953	U1734	G1645	U	U	U1520	U1421	U1254	U1083	U985	U878	U749	G749	C660
U1954	U1735	U1646	A	A	U1521	U1422	U1255	U1084	U986	U879	U750	G750	C661
A1955	U1736	A1650	U	U	U1522	U1423	U1256	U1085	U987	U880	U751	G751	C662
U1956	U1737	U1651	U	U	U1523	U1424	U1257	U1086	U988	U881	U752	G752	C663
A1957	U1738	C1661	C	C	U1524	U1425	U1258	U1087	U989	U882	U753	G753	C664
G1958	U1739	U1662	A	A	U1525	U1426	U1259	U1088	U990	U883	U754	G754	C665
U1959	U1740	G1663	G	G	U1526	U1427	U1260	U1089	U991	U884	U755	G755	C666
G1960	A1743	U1664	U	U	U1527	U1428	U1261	U1090	U992	U885	U756	G756	C667
U1961	G1744	U1665	A	A	U1528	U1429	U1262	U1091	U993	U886	U757	G757	C668
G1962	U1745	C1666	U	U	U1529	U1430	U1263	U1092	U994	U887	U758	G758	C669
U1963	U1746	U1667	C	C	U1530	U1431	U1264	U1093	U995	U888	U759	G759	C670
G1964	U1747	G1668	U	U	U1531	U1432	U1265	U1094	U996	U889	U760	G760	C671
U1965	U1748	U1669	A	A	U1532	U1433	U1266	U1095	U997	U890	U761	G761	C672
A1966	U1749	C1669	U	U	U1533	U1434	U1267	U1096	U998	U891	U762	G762	C673
G1967	U1750	U1670	U	U	U1534	U1435	U1268	U1097	U999	U892	U763	G763	C674
U1968	U1751	G1671	C	C	U1535	U1436	U1269	U1098	U1000	U893	U764	G764	C675
G1969	U1752	U1672	A	A	U1536	U1437	U1270	U1099	U1001	U894	U765	G765	C676
U1970	A1753	C1673	U	U	U1537	U1438	U1271	U1100	U1002	U895	U766	G766	C677
G1971	U1754	U1674	U	U	U1538	U1439	U1272	U1101	U1003	U896	U767	G767	C678
U1972	U1755	G1675	C	C	U1539	U1440	U1273	U1102	U1004	U897	U768	G768	C679
G1973	U1756	U1676	U	U	U1540	U1441	U1274	U1103	U1005	U898	U769	G769	C680
U1974	U1757	C1677	A	A	U1541	U1442	U1275	U1104	U1006	U899	U770	G770	C681
G1975	U1758	U1678	U	U	U1542	U1443	U1276	U1105	U1007	U900	U771	G771	C682
U1976	U1759	G1679	C	C	U1543	U1444	U1277	U1106	U1008	U901	U772	G772	C683
G1977	U1760	U1680	U	U	U1544	U1445	U1278	U1107	U1009	U902	U773	G773	C684
U1978	U1761	C1681	A	A	U1545	U1446	U1279	U1108	U1010	U903	U774	G774	C685
G1979	U1762	U1682	U	U	U1546	U1447	U1280	U1109	U1011	U904	U775	G775	C686
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G1981	A1861	U1684	U	U	U1548	U1449	U1282	U1111	U1013	U906	U777	G777	C688
U1982	U1862	U1685	A	A	U1549	U1450	U1283	U1112	U1014	U907	U778	G778	C689
G1983	A1863	C1686	U	U	U1550	U1451	U1284	U1113	U1015	U908	U779	G779	C690
U1984	C1866	U1687	C	C	U1551	U1452	U1285	U1114	U1016	U909	U780	G780	C691
G1985	C1867	U1688	U	U	U1552	U1453	U1286	U1115	U1017	U910	U781	G781	C692
A1986	U1881	U1689	U	U	U1553	U1454	U1287	U1116	U1018	U911	U782	G782	C693
U1987	U1882	C1690	A	A	U1554	U1455	U1288	U1117	U1019	U912	U783	G783	C694
G1988	U1883	U1691	C	C	U1555	U1456	U1289	U1118	U1020	U913	U784	G784	C695
U1989	U1884	G1692	G	G	U1556	U1457	U1290	U1119	U1021	U914	U785	G785	C696
G1990	C1895	U1693	U	U	U1557	U1458	U1291	U1120	U1022	U915	U786	G786	C697
U1991	A1896	C1694	A	A	U1558	U1459	U1292	U1121	U1023	U916	U787	G787	C698
G1992	U1897	U1695	U	U	U1559	U1460	U1293	U1122	U1024	U917	U788	G788	C699
U1993	C1898	U1696	C	C	U1560	U1461	U1294	U1123	U1025	U918	U789	G789	C700
G1994	U1899	G1697	U	U	U1561	U1462	U1295	U1124	U1026	U919	U790	G790	C701
U1995	U1901	U1698	A	A	U1562	U1463	U1296	U1125	U1027	U920	U791	G791	C702
G1996	C1902	C1699	U	U	U1563	U1464	U1297	U1126	U1028	U921	U792	G792	C703
U1997	U1903	U1700	C	C	U1564	U1465	U1298	U1127	U1029	U922	U793	G793	C704
G1998	U1904	G1701	U	U	U1565	U1466	U1299	U1128	U1030	U923	U794	G794	C705
U1999	A1905	U1702	A	A	U1566	U1467	U1300	U1129	U1031	U924	U795	G795	C706
G2000	C1906	C1703	G	G	U1567	U1468	U1301	U1130	U1032	U925	U796	G796	C707
U2001	U1907	U1704	U	U	U1568	U1469	U1302	U1131	U1033	U926	U797	G797	C708
G2002	A1908	G170											



• Molecule 31: 5S rRNA

Chain b: 68% 30%



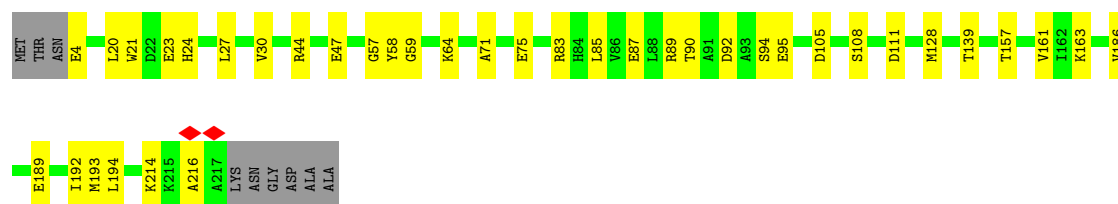
• Molecule 32: 50S ribosomal protein L2

Chain c:  85% 13% ..



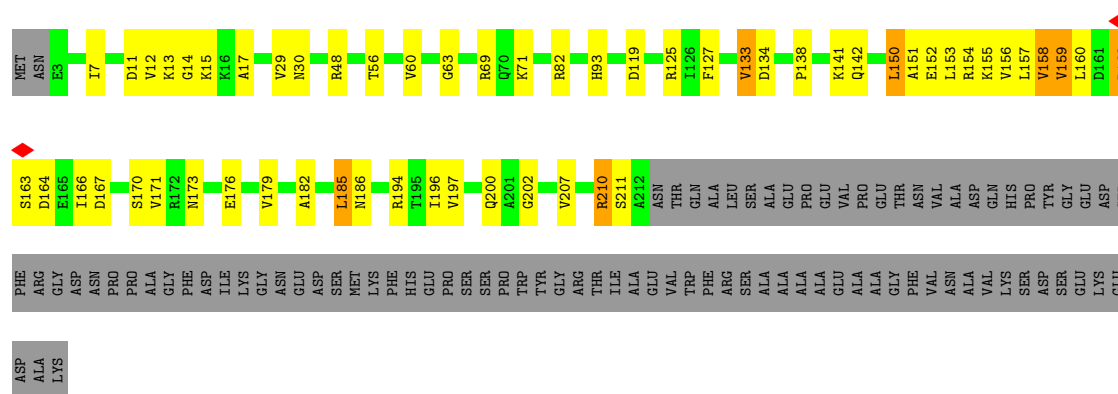
- Molecule 33: 50S ribosomal protein L3

Chain d:  79% 17% .



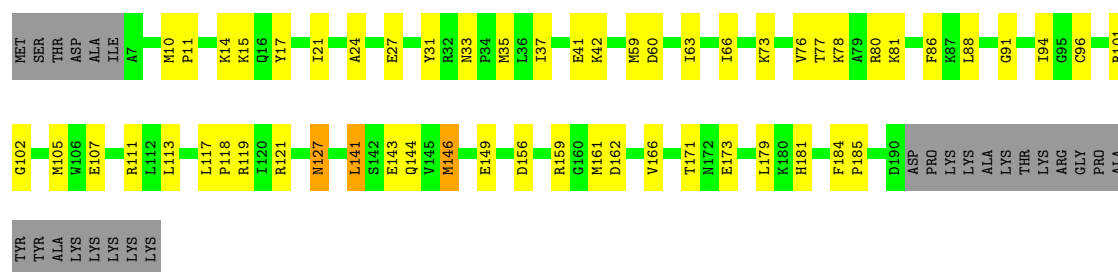
- Molecule 34: 50S ribosomal protein L4

Chain e:  51% 17% . 30%

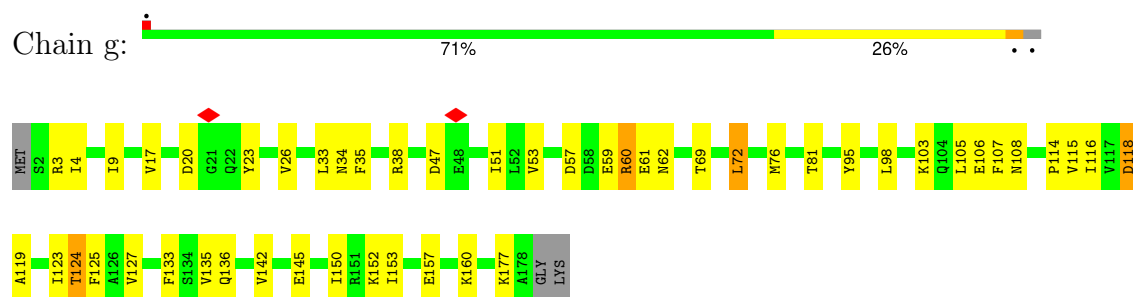


- Molecule 35: 50S ribosomal protein L5

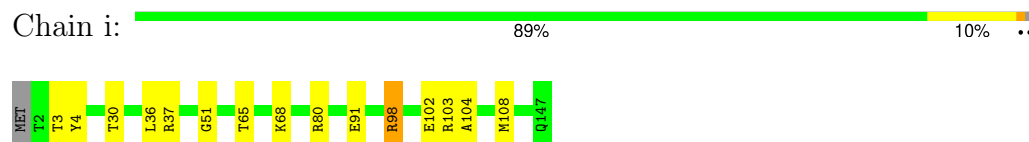
Chain f:  61% 25% . 12%



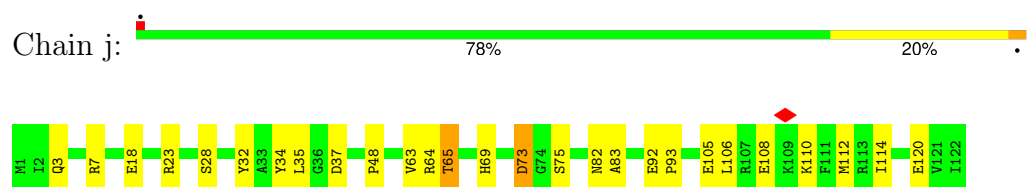
- Molecule 36: 50S ribosomal protein L6



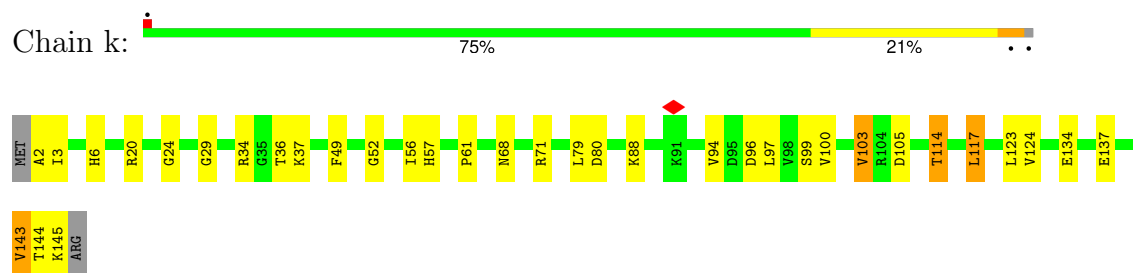
- Molecule 37: 50S ribosomal protein L13



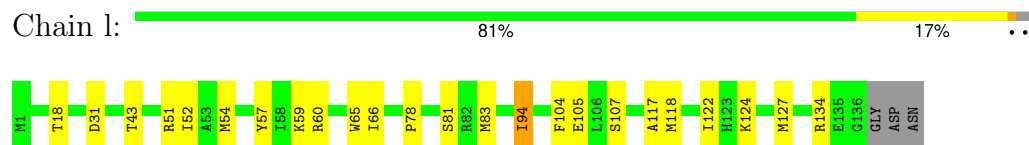
- Molecule 38: 50S ribosomal protein L14



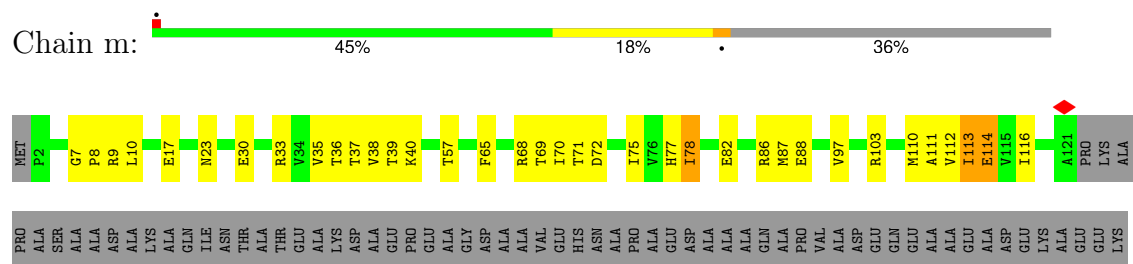
- Molecule 39: 50S ribosomal protein L15



- Molecule 40: 50S ribosomal protein L16



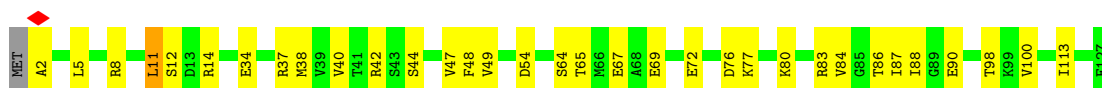
- Molecule 41: Large ribosomal subunit protein bL17



PRO
GLU
ALA

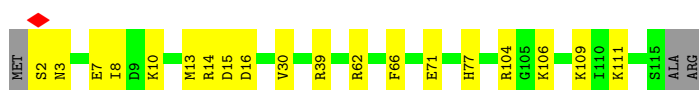
- Molecule 42: 50S ribosomal protein L18

Chain n:  73% 25%



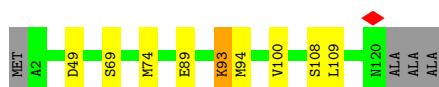
- Molecule 43: 50S ribosomal protein L19

Chain o:  81% 16%



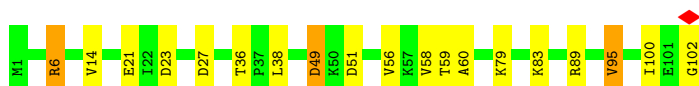
- Molecule 44: 50S ribosomal protein L20

Chain p:  89% 7%



- Molecule 45: Large ribosomal subunit protein bL21

Chain q:  81% 16%



- Molecule 46: 50S ribosomal protein L22

Chain r:  69% 17% 14%



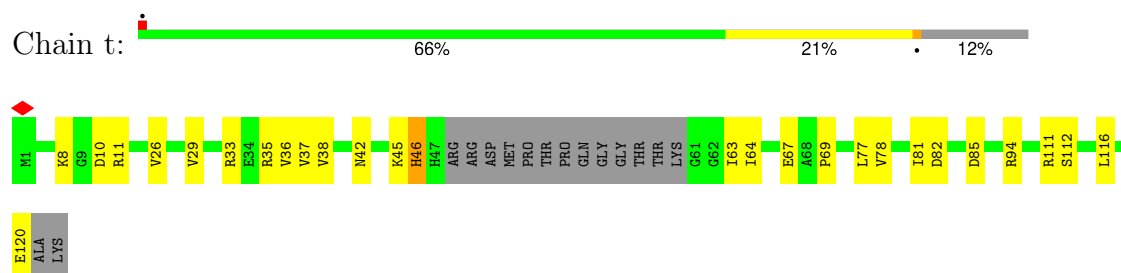
ALA
ALA
LYS
SER
GLU
THR
GLY
GLY
ALA

- Molecule 47: 50S ribosomal protein L23

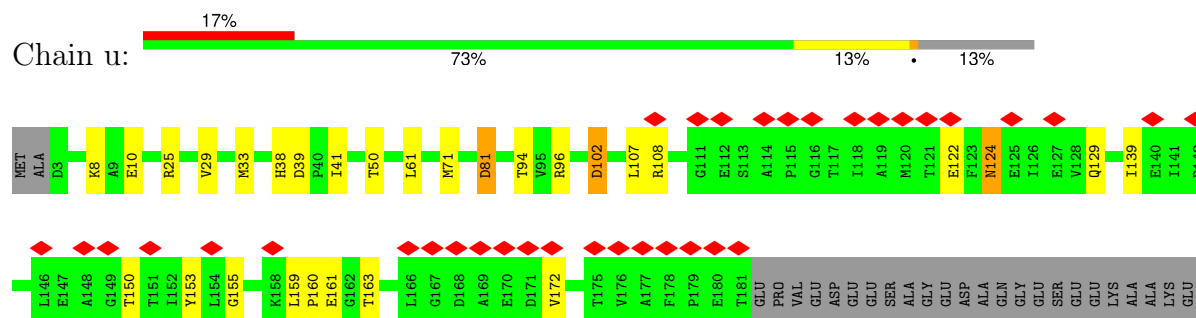
Chain s:  67% 26% 7%



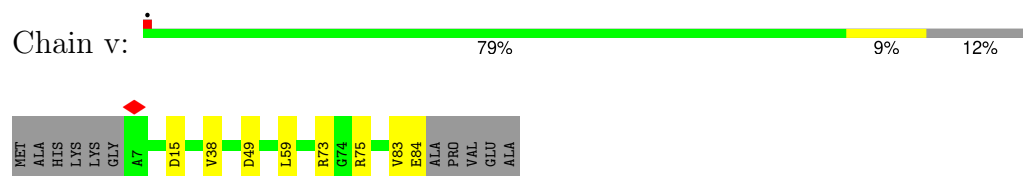
- Molecule 48: Large ribosomal subunit protein uL24



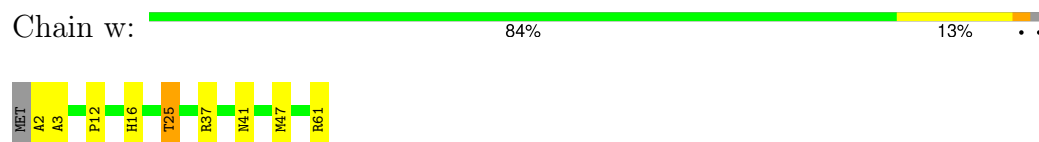
- Molecule 49: 50S ribosomal protein L25



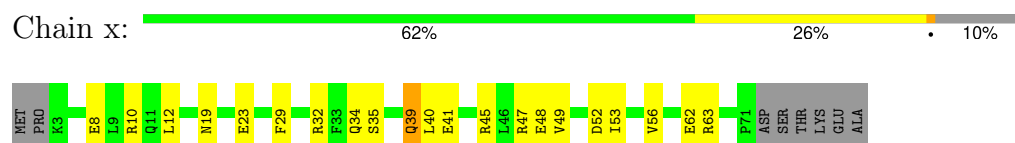
- Molecule 50: 50S ribosomal protein L27



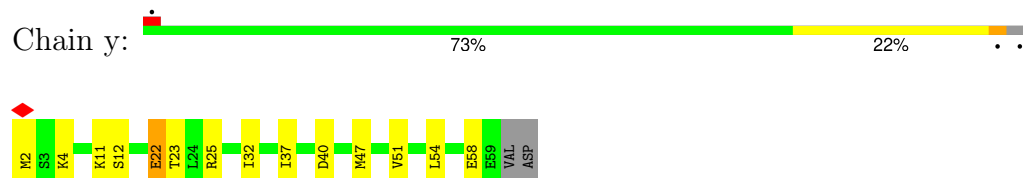
- Molecule 51: 50S ribosomal protein L28



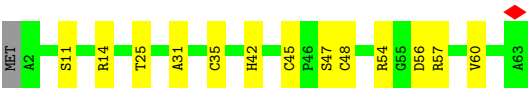
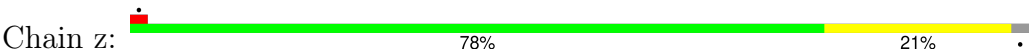
- Molecule 52: 50S ribosomal protein L29



- Molecule 53: 50S ribosomal protein L30



● Molecule 54: 50S ribosomal protein L32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	80548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.654	Depositor
Minimum map value	-0.221	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 4SU, OMC, OMU, UR3, H2U, V7A, 4OC, OMG, 3TD, PSU, ZN, MG, MA6, G7M, 2MA, 2MG, 5MU, 5MC

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	0.21	0/429	0.42	0/569
2	1	0.20	0/365	0.26	0/478
3	2	0.20	0/519	0.30	0/682
4	3	0.18	0/305	0.31	0/401
5	4	0.28	0/521	0.46	0/700
6	A	0.21	0/35898	0.30	0/56012
7	B	0.14	0/1864	0.40	1/2509 (0.0%)
8	C	0.27	0/1725	0.35	0/2689
9	D	0.25	0/1662	0.45	0/2239
10	E	0.16	0/1325	0.34	0/1789
11	F	0.20	0/794	0.56	1/1069 (0.1%)
12	G	0.17	0/1638	0.41	0/2201
13	H	0.20	0/1036	0.44	0/1395
14	I	0.17	0/1246	0.43	0/1679
15	J	0.19	0/1027	0.45	0/1376
16	K	0.20	0/874	0.46	0/1177
17	L	0.26	0/960	0.44	0/1283
18	M	0.20	0/800	0.55	0/1080
19	N	0.17	0/985	0.39	0/1317
20	O	0.20	0/718	0.44	0/959
21	P	0.38	0/1013	0.59	0/1370
22	Q	0.18	0/734	0.41	0/978
23	R	0.21	0/532	0.41	0/713
24	S	0.62	0/484	0.88	1/644 (0.2%)
25	T	0.19	0/676	0.30	0/897
26	U	0.19	0/675	0.47	0/908
27	V	0.21	0/184	0.30	0/236
28	X	0.19	0/277	0.36	0/355
29	Y	0.50	0/235	0.64	0/363
30	a	0.26	0/69472	0.35	3/108408 (0.0%)
31	b	0.22	0/2871	0.29	0/4475

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.22	0/2132	0.38	1/2871 (0.0%)
33	d	0.22	0/1611	0.41	0/2172
34	e	0.30	0/1600	0.56	0/2165
35	f	0.20	0/1493	0.44	0/2001
36	g	0.16	0/1398	0.38	0/1884
37	i	0.29	0/1164	0.48	0/1574
38	j	0.21	0/957	0.37	0/1282
39	k	0.31	0/1090	0.57	0/1465
40	l	0.22	0/1108	0.40	0/1488
41	m	0.42	0/949	0.63	1/1277 (0.1%)
42	n	0.21	0/959	0.44	0/1281
43	o	0.20	0/909	0.31	0/1216
44	p	0.22	0/969	0.28	0/1292
45	q	0.20	0/785	0.42	0/1050
46	r	0.20	0/1028	0.33	0/1379
47	s	0.22	0/759	0.42	0/1022
48	t	0.19	0/840	0.43	0/1123
49	u	0.17	0/1396	0.39	0/1896
50	v	0.20	0/598	0.35	0/800
51	w	0.22	0/483	0.34	0/648
52	x	0.20	0/567	0.38	0/759
53	y	0.18	0/471	0.31	0/627
54	z	0.20	0/487	0.29	0/654
All	All	0.24	0/155597	0.36	8/232877 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
21	P	0	1
24	S	0	2
34	e	0	1
37	i	0	2
All	All	0	6

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	152	ILE	N-CA-C	-6.23	106.70	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1898	C	O3'-P-O5'	-6.21	94.69	104.00
32	c	274	SER	CB-CA-C	-5.51	110.20	116.54
30	a	739	G	C4'-C3'-O3'	5.20	117.19	109.40
30	a	2961	U	O3'-P-O5'	5.18	111.78	104.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
21	P	26	ARG	Sidechain
24	S	23	ARG	Sidechain
24	S	45	ARG	Sidechain
34	e	162	ARG	Sidechain
37	i	98	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	423	0	429	9	0
2	1	362	0	388	4	0
3	2	513	0	565	5	0
4	3	302	0	330	2	0
5	4	512	0	499	14	0
6	A	32340	0	16267	392	0
7	B	1836	0	1902	46	0
8	C	1625	0	829	8	0
9	D	1632	0	1663	55	0
10	E	1309	0	1349	22	0
11	F	785	0	818	27	0
12	G	1613	0	1626	41	0
13	H	1021	0	1059	17	0
14	I	1225	0	1275	26	0
15	J	1012	0	1069	34	0
16	K	858	0	884	27	0
17	L	948	0	1031	14	0
18	M	786	0	823	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	976	0	1031	26	0
20	O	708	0	737	23	0
21	P	994	0	1008	29	0
22	Q	728	0	772	14	0
23	R	527	0	580	11	0
24	S	474	0	499	11	0
25	T	673	0	726	14	0
26	U	658	0	671	15	0
27	V	183	0	202	5	0
28	X	277	0	338	5	0
29	Y	211	0	106	4	0
30	a	62432	0	31308	621	0
31	b	2567	0	1297	23	0
32	c	2091	0	2150	24	0
33	d	1586	0	1634	31	0
34	e	1577	0	1619	51	0
35	f	1468	0	1487	43	0
36	g	1376	0	1421	34	0
37	i	1139	0	1163	8	0
38	j	946	0	1011	16	0
39	k	1072	0	1106	30	0
40	l	1082	0	1117	16	0
41	m	936	0	997	22	0
42	n	952	0	995	21	0
43	o	896	0	928	15	0
44	p	958	0	986	6	0
45	q	778	0	824	9	0
46	r	1017	0	1070	14	0
47	s	751	0	803	20	0
48	t	833	0	883	15	0
49	u	1376	0	1397	19	0
50	v	591	0	581	4	0
51	w	474	0	487	5	0
52	x	564	0	582	15	0
53	y	467	0	504	8	0
54	z	477	0	479	11	0
55	0	1	0	0	0	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
55	S	1	0	0	0	0
55	w	1	0	0	0	0
55	z	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	A	63	0	0	0	0
56	a	233	0	0	0	0
56	b	2	0	0	0	0
56	c	1	0	0	0	0
56	d	1	0	0	0	0
56	k	1	0	0	0	0
57	A	35	0	0	0	0
57	a	35	0	0	0	0
58	A	11	0	0	0	0
58	a	108	0	0	0	0
58	b	1	0	0	0	0
58	c	1	0	0	0	0
All	All	144415	0	96305	1820	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 8.

The worst 5 of 1820 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)
11:F:22:LEU:HA	11:F:25:LYS:HE3	1.52	0.90
35:f:21:ILE:HD12	35:f:181:HIS:HB3	1.58	0.86
30:a:669:A:H62	30:a:1328:A:H2	1.23	0.84
34:e:133:VAL:HG23	34:e:141:LYS:HD3	1.60	0.81
9:D:90:GLU:HG3	9:D:186:ILE:HG12	1.65	0.79

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	48/56 (86%)	46 (96%)	2 (4%)	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	65/68 (96%)	65 (100%)	0	0	100	100
4	3	35/37 (95%)	35 (100%)	0	0	100	100
5	4	64/69 (93%)	57 (89%)	7 (11%)	0	100	100
7	B	231/283 (82%)	214 (93%)	15 (6%)	2 (1%)	14	27
9	D	198/201 (98%)	184 (93%)	14 (7%)	0	100	100
10	E	177/215 (82%)	174 (98%)	3 (2%)	0	100	100
11	F	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
12	G	204/269 (76%)	198 (97%)	6 (3%)	0	100	100
13	H	132/135 (98%)	129 (98%)	3 (2%)	0	100	100
14	I	153/156 (98%)	147 (96%)	6 (4%)	0	100	100
15	J	132/173 (76%)	120 (91%)	11 (8%)	1 (1%)	16	31
16	K	115/135 (85%)	105 (91%)	9 (8%)	1 (1%)	14	27
17	L	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
18	M	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	24
19	N	120/123 (98%)	110 (92%)	10 (8%)	0	100	100
20	O	85/87 (98%)	84 (99%)	1 (1%)	0	100	100
21	P	126/147 (86%)	112 (89%)	13 (10%)	1 (1%)	16	31
22	Q	88/90 (98%)	78 (89%)	9 (10%)	1 (1%)	11	22
23	R	65/79 (82%)	60 (92%)	4 (6%)	1 (2%)	8	16
24	S	58/61 (95%)	55 (95%)	2 (3%)	1 (2%)	7	13
25	T	85/88 (97%)	85 (100%)	0	0	100	100
26	U	82/93 (88%)	75 (92%)	6 (7%)	1 (1%)	10	20
27	V	21/24 (88%)	20 (95%)	1 (5%)	0	100	100
28	X	30/33 (91%)	29 (97%)	0	1 (3%)	3	4
32	c	272/278 (98%)	260 (96%)	11 (4%)	1 (0%)	30	49
33	d	212/223 (95%)	204 (96%)	8 (4%)	0	100	100
34	e	208/301 (69%)	178 (86%)	26 (12%)	4 (2%)	6	11
35	f	182/210 (87%)	169 (93%)	13 (7%)	0	100	100
36	g	175/180 (97%)	168 (96%)	7 (4%)	0	100	100
37	i	144/147 (98%)	141 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	j	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
39	k	142/146 (97%)	124 (87%)	17 (12%)	1 (1%)	18	34
40	l	134/139 (96%)	125 (93%)	9 (7%)	0	100	100
41	m	118/187 (63%)	110 (93%)	7 (6%)	1 (1%)	16	31
42	n	124/127 (98%)	120 (97%)	4 (3%)	0	100	100
43	o	112/117 (96%)	110 (98%)	2 (2%)	0	100	100
44	p	117/123 (95%)	116 (99%)	1 (1%)	0	100	100
45	q	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
46	r	130/153 (85%)	125 (96%)	5 (4%)	0	100	100
47	s	93/102 (91%)	85 (91%)	7 (8%)	1 (1%)	11	22
48	t	103/122 (84%)	94 (91%)	8 (8%)	1 (1%)	12	24
49	u	177/205 (86%)	168 (95%)	9 (5%)	0	100	100
50	v	76/89 (85%)	74 (97%)	1 (1%)	1 (1%)	9	18
51	w	58/61 (95%)	53 (91%)	4 (7%)	1 (2%)	7	13
52	x	67/77 (87%)	62 (92%)	5 (8%)	0	100	100
53	y	56/60 (93%)	53 (95%)	3 (5%)	0	100	100
54	z	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
All	All	5646/6322 (89%)	5320 (94%)	304 (5%)	22 (0%)	31	49

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	B	100	MET
22	Q	9	THR
24	S	27	CYS
26	U	84	VAL
28	X	4	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/51 (92%)	47 (100%)	0	100	100
2	1	36/36 (100%)	35 (97%)	1 (3%)	38	66
3	2	54/55 (98%)	53 (98%)	1 (2%)	50	76
4	3	35/35 (100%)	35 (100%)	0	100	100
5	4	56/59 (95%)	52 (93%)	4 (7%)	13	29
7	B	197/234 (84%)	189 (96%)	8 (4%)	27	53
9	D	175/176 (99%)	169 (97%)	6 (3%)	32	60
10	E	130/155 (84%)	125 (96%)	5 (4%)	29	56
11	F	89/89 (100%)	87 (98%)	2 (2%)	45	73
12	G	160/200 (80%)	155 (97%)	5 (3%)	35	62
13	H	108/109 (99%)	104 (96%)	4 (4%)	30	57
14	I	132/133 (99%)	125 (95%)	7 (5%)	20	42
15	J	97/131 (74%)	94 (97%)	3 (3%)	35	62
16	K	88/101 (87%)	83 (94%)	5 (6%)	18	39
17	L	103/104 (99%)	99 (96%)	4 (4%)	28	55
18	M	89/93 (96%)	87 (98%)	2 (2%)	45	73
19	N	99/100 (99%)	97 (98%)	2 (2%)	48	75
20	O	74/74 (100%)	73 (99%)	1 (1%)	59	81
21	P	103/115 (90%)	99 (96%)	4 (4%)	28	55
22	Q	81/81 (100%)	78 (96%)	3 (4%)	30	57
23	R	55/65 (85%)	53 (96%)	2 (4%)	31	58
24	S	48/49 (98%)	47 (98%)	1 (2%)	47	74
25	T	68/69 (99%)	64 (94%)	4 (6%)	18	37
26	U	72/80 (90%)	69 (96%)	3 (4%)	26	52
27	V	16/17 (94%)	16 (100%)	0	100	100
28	X	28/29 (97%)	27 (96%)	1 (4%)	31	58
32	c	216/220 (98%)	209 (97%)	7 (3%)	34	62
33	d	166/172 (96%)	165 (99%)	1 (1%)	78	91
34	e	165/237 (70%)	157 (95%)	8 (5%)	23	46
35	f	154/175 (88%)	146 (95%)	8 (5%)	21	42
36	g	150/152 (99%)	144 (96%)	6 (4%)	28	54
37	i	118/120 (98%)	114 (97%)	4 (3%)	32	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	j	101/101 (100%)	98 (97%)	3 (3%)	36	64
39	k	111/113 (98%)	107 (96%)	4 (4%)	31	58
40	l	108/110 (98%)	105 (97%)	3 (3%)	38	66
41	m	100/142 (70%)	96 (96%)	4 (4%)	28	54
42	n	95/96 (99%)	92 (97%)	3 (3%)	34	62
43	o	97/99 (98%)	96 (99%)	1 (1%)	68	86
44	p	98/99 (99%)	96 (98%)	2 (2%)	48	75
45	q	84/84 (100%)	74 (88%)	10 (12%)	5	11
46	r	105/118 (89%)	100 (95%)	5 (5%)	23	46
47	s	84/89 (94%)	83 (99%)	1 (1%)	63	83
48	t	91/103 (88%)	87 (96%)	4 (4%)	25	50
49	u	149/168 (89%)	143 (96%)	6 (4%)	28	54
50	v	60/67 (90%)	57 (95%)	3 (5%)	22	44
51	w	52/53 (98%)	50 (96%)	2 (4%)	29	56
52	x	61/68 (90%)	59 (97%)	2 (3%)	33	61
53	y	53/55 (96%)	51 (96%)	2 (4%)	29	56
54	z	51/52 (98%)	49 (96%)	2 (4%)	28	55
All	All	4709/5133 (92%)	4540 (96%)	169 (4%)	32	58

5 of 169 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
39	k	103	VAL
46	r	3	LYS
40	l	18	THR
44	p	93	LYS
48	t	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
41	m	62	ASN
49	u	134	ASN
15	J	88	GLN
13	H	22	HIS

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Mol	Chain	Res	Type
51	w	48	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	Y	9/22 (40%)	4 (44%)	0
30	a	2891/3086 (93%)	518 (17%)	0
31	b	117/120 (97%)	11 (9%)	0
6	A	1503/1537 (97%)	253 (16%)	17 (1%)
8	C	75/77 (97%)	13 (17%)	1 (1%)
All	All	4595/4842 (94%)	799 (17%)	18 (0%)

5 of 799 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	7	A
6	A	9	U
6	A	10	G
6	A	13	G
6	A	36	A

5 of 18 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1479	A
8	C	17(A)	U
6	A	1520	C
6	A	1130	G
6	A	1384	C

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

34 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
6	2MG	A	1503	6	23,26,27	3.05	8 (34%)	33,38,41	2.62	12 (36%)
6	MA6	A	1506	6	23,26,27	1.41	4 (17%)	33,38,41	3.15	13 (39%)
30	5MU	a	2122	30	19,22,23	0.30	0	27,32,35	0.41	0
30	OMU	a	2734	30	19,22,23	2.90	6 (31%)	25,31,34	1.89	5 (20%)
30	PSU	a	1038	30	18,21,22	0.91	1 (5%)	21,30,33	0.88	0
30	2MG	a	2018	30	23,26,27	3.04	8 (34%)	33,38,41	2.62	12 (36%)
30	OMC	a	2680	56,30	19,22,23	3.16	8 (42%)	25,31,34	0.89	0
6	5MC	A	951	6	19,22,23	4.50	8 (42%)	26,32,35	0.99	1 (3%)
6	5MC	A	1391	6	19,22,23	4.40	8 (42%)	26,32,35	0.96	2 (7%)
6	G7M	A	509	6	23,26,27	2.61	9 (39%)	34,39,42	1.72	7 (20%)
30	PSU	a	2686	30	18,21,22	0.92	1 (5%)	21,30,33	0.74	0
8	5MC	C	32	8	19,22,23	4.42	8 (42%)	26,32,35	1.01	1 (3%)
6	PSU	A	498	56,6	18,21,22	0.93	1 (5%)	21,30,33	0.69	0
30	5MC	a	2145	30	19,22,23	4.36	8 (42%)	26,32,35	1.08	2 (7%)
6	4OC	A	1389	6	20,23,24	3.10	8 (40%)	25,32,35	0.92	1 (4%)
6	UR3	A	1485	6	19,22,23	2.70	8 (42%)	26,32,35	1.63	2 (7%)
30	PSU	a	2787	30	18,21,22	0.94	1 (5%)	21,30,33	0.77	0
6	5MC	A	1387	6	19,22,23	4.48	8 (42%)	26,32,35	1.07	1 (3%)
8	PSU	C	55	8	18,21,22	0.93	1 (5%)	21,30,33	0.71	0
30	PSU	a	2094	30	18,21,22	0.92	1 (5%)	21,30,33	0.67	0
30	3TD	a	2098	30	19,22,23	4.13	7 (36%)	23,32,35	1.86	5 (21%)
30	2MA	a	2685	56,30	22,25,26	0.85	1 (4%)	32,37,40	1.20	5 (15%)
8	4SU	C	8	8	18,21,22	3.75	7 (38%)	25,30,33	2.31	4 (16%)
30	PSU	a	2786	30	18,21,22	0.91	1 (5%)	21,30,33	0.77	0
6	2MG	A	950	6	23,26,27	3.12	8 (34%)	33,38,41	2.51	12 (36%)
30	PSU	a	2100	30	18,21,22	0.90	1 (5%)	21,30,33	0.66	0
8	5MU	C	54	8	19,22,23	0.25	0	27,32,35	0.42	0
30	H2U	a	2631	30	18,21,22	3.06	5 (27%)	19,30,33	1.49	4 (21%)
30	PSU	a	2762	30	18,21,22	0.95	1 (5%)	21,30,33	0.90	1 (4%)
30	OMG	a	2433	8,30	23,26,27	2.53	9 (39%)	32,38,41	2.41	11 (34%)
6	5MC	A	1394	6	19,22,23	4.37	8 (42%)	26,32,35	1.03	2 (7%)
30	PSU	a	2639	30	18,21,22	0.92	1 (5%)	21,30,33	0.74	0
30	2MG	a	2627	30	23,26,27	3.03	8 (34%)	33,38,41	2.46	12 (36%)
6	MA6	A	1505	6	23,26,27	1.38	4 (17%)	33,38,41	3.02	12 (36%)

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
6	2MG	A	1503	6	-	0/9/27/28	0/3/3/3
6	MA6	A	1506	6	-	2/11/29/30	0/3/3/3
30	5MU	a	2122	30	-	0/7/25/26	0/2/2/2
30	OMU	a	2734	30	-	0/9/27/28	0/2/2/2
30	PSU	a	1038	30	-	0/7/25/26	0/2/2/2
30	2MG	a	2018	30	-	2/9/27/28	0/3/3/3
30	OMC	a	2680	56,30	-	0/9/27/28	0/2/2/2
6	5MC	A	951	6	-	0/7/25/26	0/2/2/2
6	5MC	A	1391	6	-	0/7/25/26	0/2/2/2
6	G7M	A	509	6	-	3/7/25/26	0/3/3/3
30	PSU	a	2686	30	-	1/7/25/26	0/2/2/2
8	5MC	C	32	8	-	0/7/25/26	0/2/2/2
6	PSU	A	498	56,6	-	0/7/25/26	0/2/2/2
30	5MC	a	2145	30	-	0/7/25/26	0/2/2/2
6	4OC	A	1389	6	-	1/9/29/30	0/2/2/2
6	UR3	A	1485	6	-	0/7/25/26	0/2/2/2
30	PSU	a	2787	30	-	0/7/25/26	0/2/2/2
6	5MC	A	1387	6	-	2/7/25/26	0/2/2/2
8	PSU	C	55	8	-	0/7/25/26	0/2/2/2
30	PSU	a	2094	30	-	0/7/25/26	0/2/2/2
30	3TD	a	2098	30	-	2/7/25/26	0/2/2/2
30	2MA	a	2685	56,30	-	1/7/25/26	0/3/3/3
8	4SU	C	8	8	-	0/7/25/26	0/2/2/2
30	PSU	a	2786	30	-	0/7/25/26	0/2/2/2
6	2MG	A	950	6	-	0/9/27/28	0/3/3/3
30	PSU	a	2100	30	-	0/7/25/26	0/2/2/2
8	5MU	C	54	8	-	0/7/25/26	0/2/2/2
30	H2U	a	2631	30	-	0/7/38/39	0/2/2/2
30	PSU	a	2762	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2433	8,30	-	1/9/27/28	0/3/3/3
6	5MC	A	1394	6	-	0/7/25/26	0/2/2/2
30	PSU	a	2639	30	-	0/7/25/26	0/2/2/2
30	2MG	a	2627	30	-	2/9/27/28	0/3/3/3
6	MA6	A	1505	6	-	0/11/29/30	0/3/3/3

The worst 5 of 166 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2098	3TD	C6-C5	12.83	1.49	1.35
6	A	951	5MC	C6-C5	9.70	1.50	1.34
6	A	1387	5MC	C6-C5	9.61	1.50	1.34
6	A	1394	5MC	C6-C5	9.53	1.50	1.34
8	C	32	5MC	C6-C5	9.53	1.50	1.34

The worst 5 of 127 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1506	MA6	N1-C6-N6	-11.15	103.27	116.86
6	A	1505	MA6	N1-C6-N6	-10.56	103.99	116.86
8	C	8	4SU	C4-N3-C2	-7.90	119.74	127.31
30	a	2018	2MG	C2-N3-C4	7.36	121.21	112.00
6	A	1506	MA6	C5-C6-N6	7.19	136.72	125.33

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1506	MA6	O4'-C4'-C5'-O5'
30	a	2098	3TD	O4'-C4'-C5'-O5'
6	A	509	G7M	C3'-C4'-C5'-O5'
30	a	2098	3TD	C3'-C4'-C5'-O5'
30	a	2627	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1503	2MG	2	0
6	A	1506	MA6	2	0
6	A	1389	4OC	1	0
30	a	2098	3TD	2	0
6	A	950	2MG	1	0
30	a	2631	H2U	1	0
6	A	1505	MA6	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 309 ligands modelled in this entry, 307 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	V7A	A	1602	56	37,38,38	1.11	2 (5%)	43,60,60	1.02	3 (6%)
57	V7A	a	3145	56	37,38,38	1.09	2 (5%)	43,60,60	0.92	1 (2%)

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
57	V7A	A	1602	56	-	5/13/72/72	0/4/4/4
57	V7A	a	3145	56	-	8/13/72/72	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	A	1602	V7A	CBC-NBD	5.10	1.48	1.33
57	a	3145	V7A	CBC-NBD	5.01	1.47	1.33
57	a	3145	V7A	OAY-CAH	2.23	1.27	1.23
57	A	1602	V7A	OAY-CAH	2.12	1.27	1.23

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	1602	V7A	CAH-CAI-CAL	2.93	121.12	118.80
57	A	1602	V7A	OBA-CAM-CAL	-2.41	106.29	110.14
57	a	3145	V7A	CAM-CAP-CAQ	2.39	119.55	115.75
57	A	1602	V7A	OAZ-CAL-CAM	2.28	116.67	113.37

There are no chirality outliers.

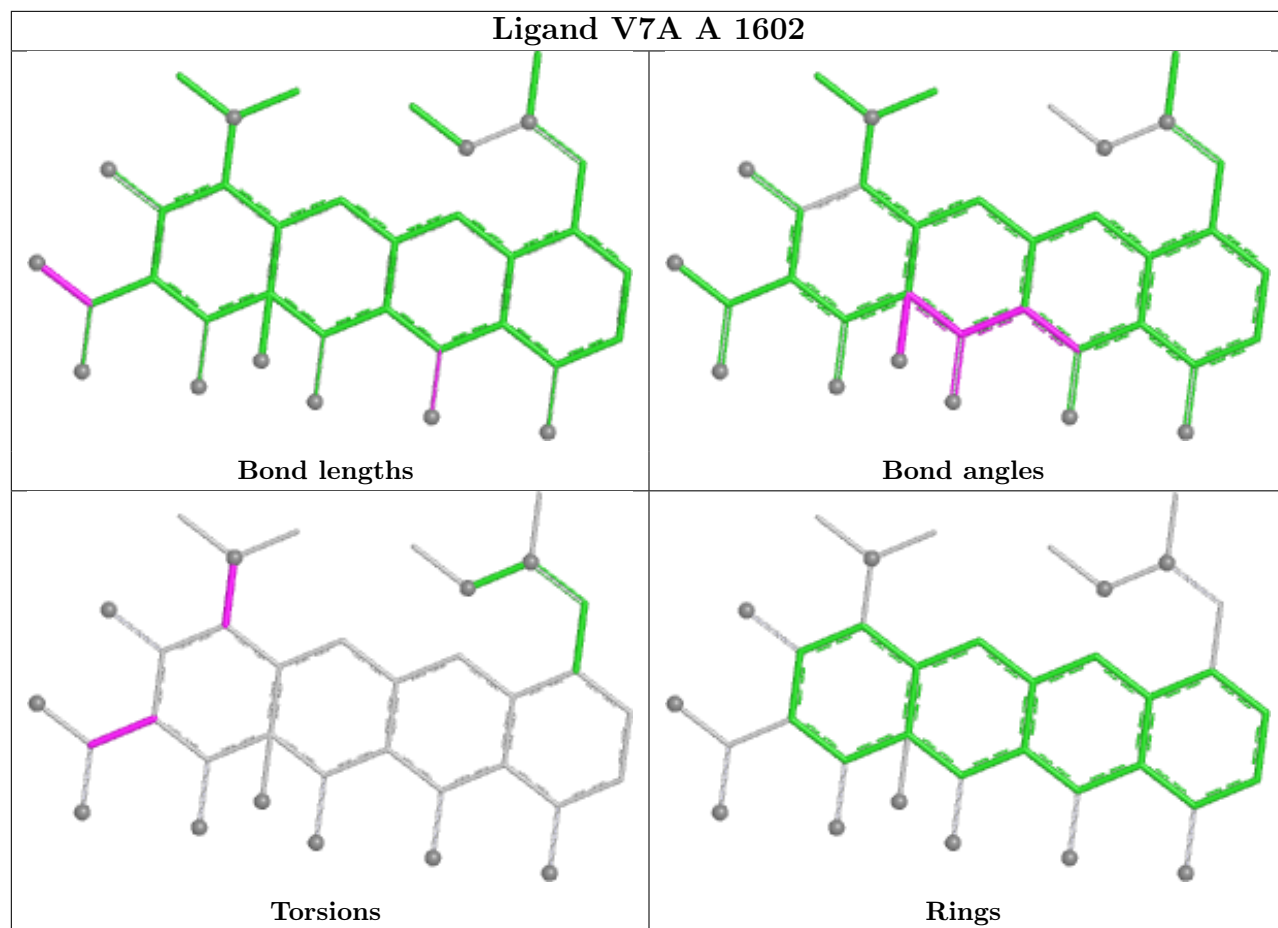
5 of 13 torsion outliers are listed below:

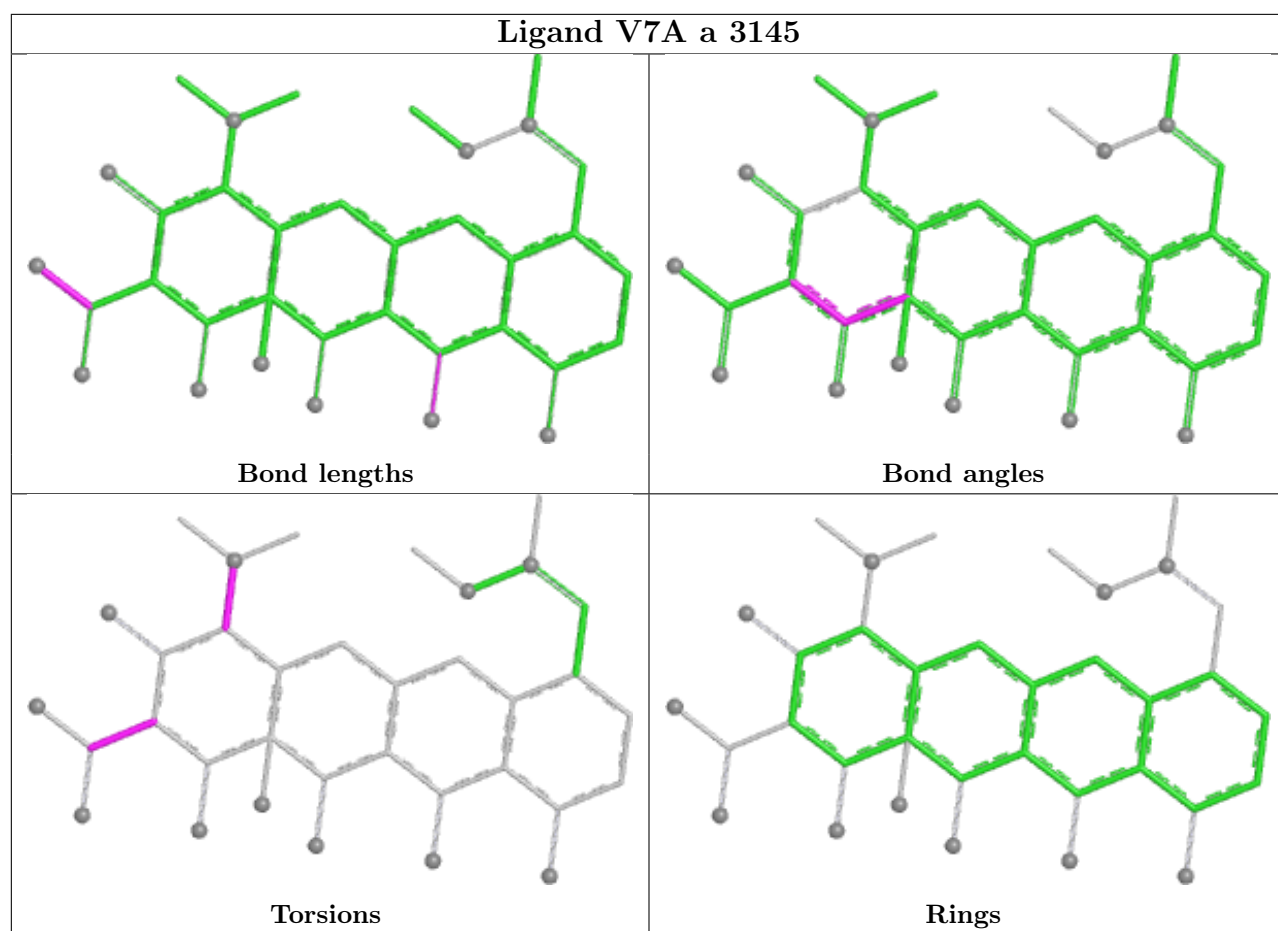
Mol	Chain	Res	Type	Atoms
57	A	1602	V7A	CAN-CAO-NBF-CBG
57	A	1602	V7A	CAP-CAQ-CBC-NBD
57	A	1602	V7A	CAP-CAQ-CBC-OBE
57	a	3145	V7A	CAR-CAO-NBF-CBG
57	a	3145	V7A	CAR-CAO-NBF-CBH

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

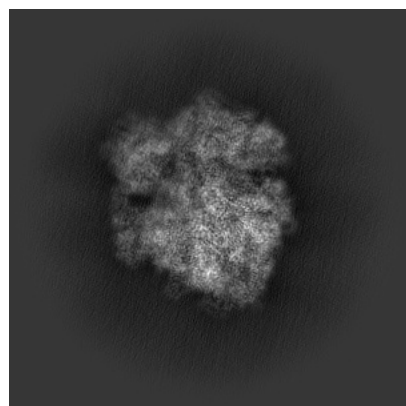
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71683. These allow visual inspection of the internal detail of the map and identification of artifacts.

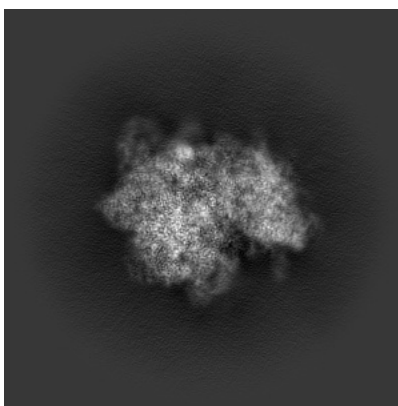
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

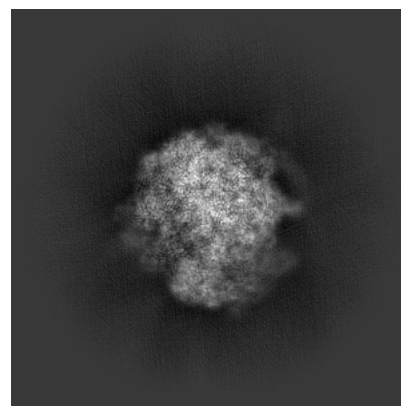
6.1.1 Primary map



X

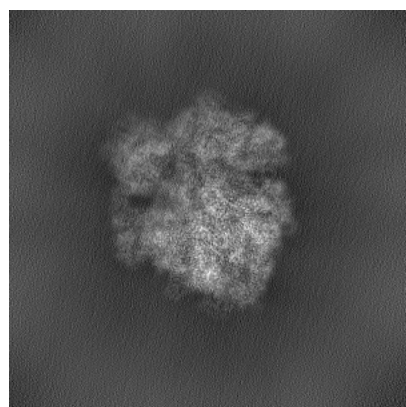


Y

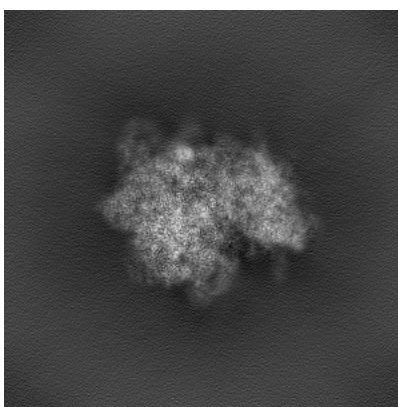


Z

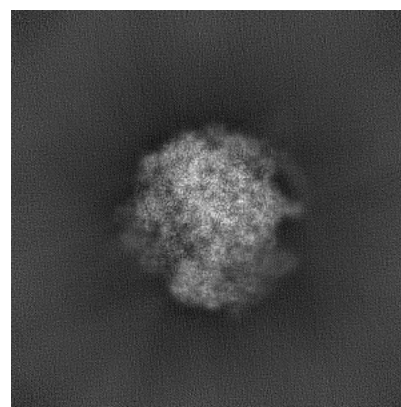
6.1.2 Raw map



X



Y

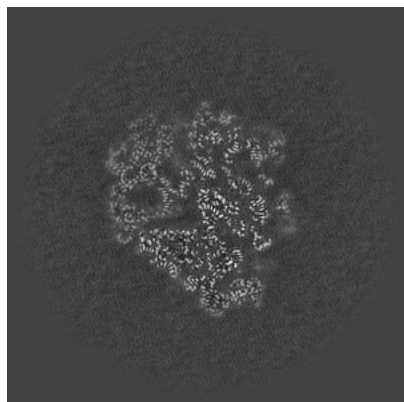


Z

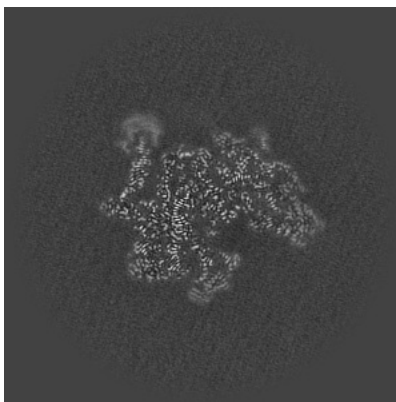
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

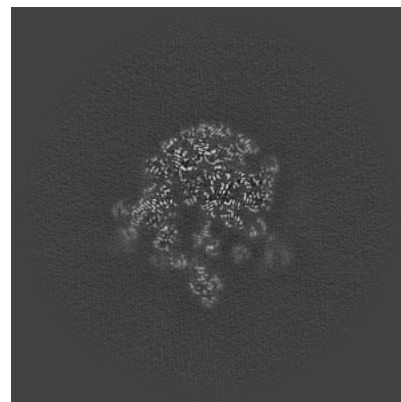
6.2.1 Primary map



X Index: 220

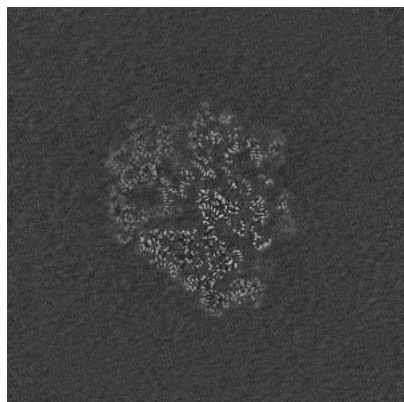


Y Index: 220

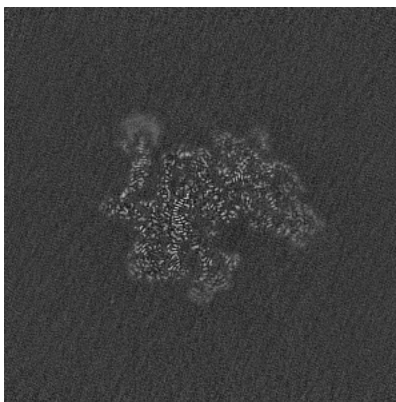


Z Index: 220

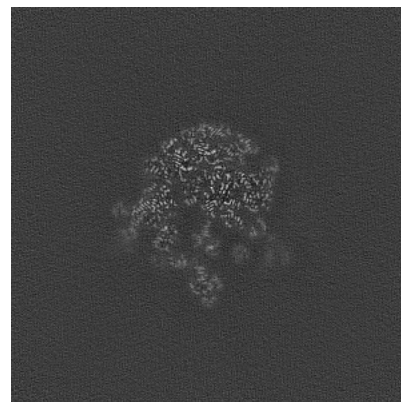
6.2.2 Raw map



X Index: 220



Y Index: 220

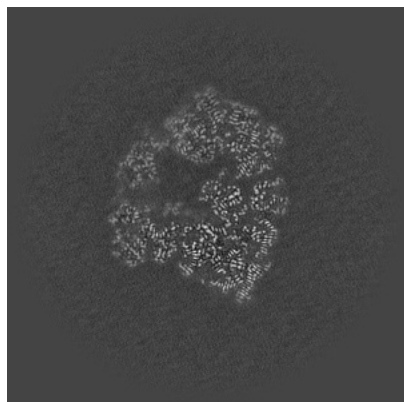


Z Index: 220

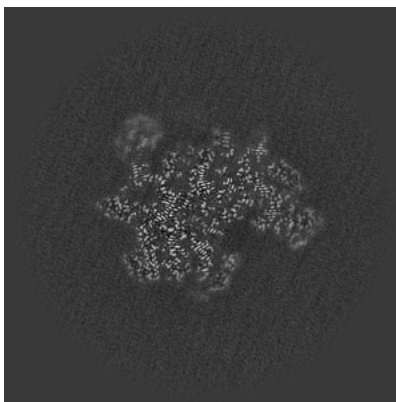
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

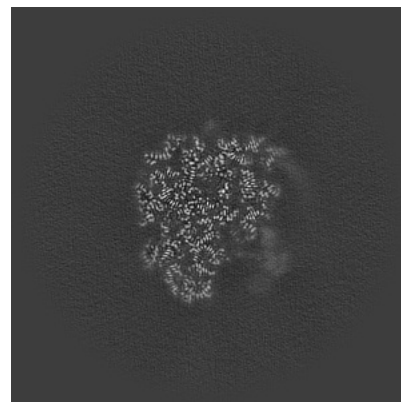
6.3.1 Primary map



X Index: 203

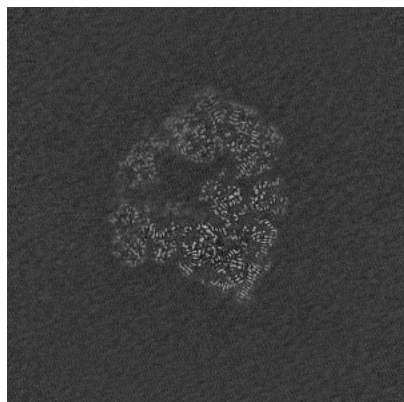


Y Index: 225

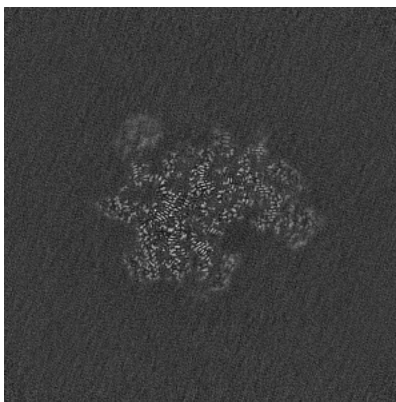


Z Index: 190

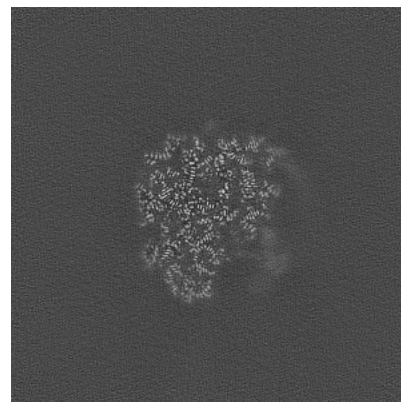
6.3.2 Raw map



X Index: 203



Y Index: 225

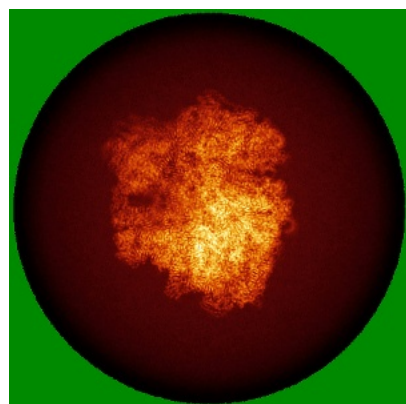


Z Index: 190

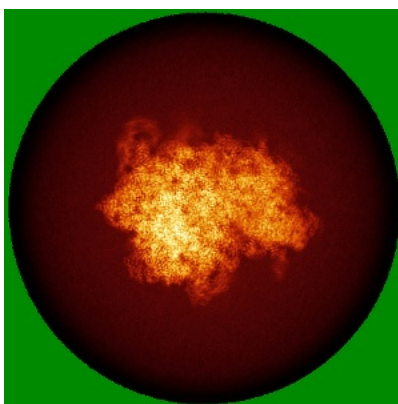
The images above show the largest variance slices of the map in three orthogonal directions.

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

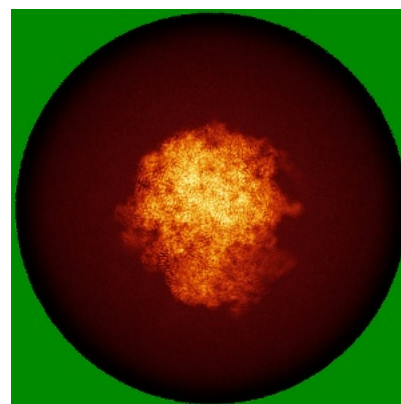
6.4.1 Primary map



X

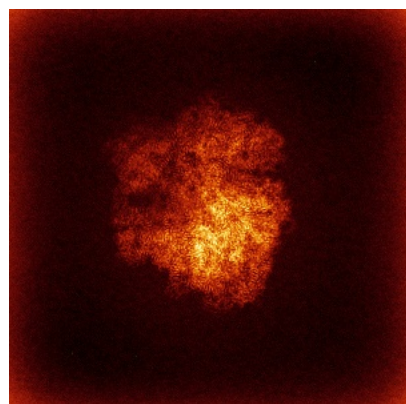


Y

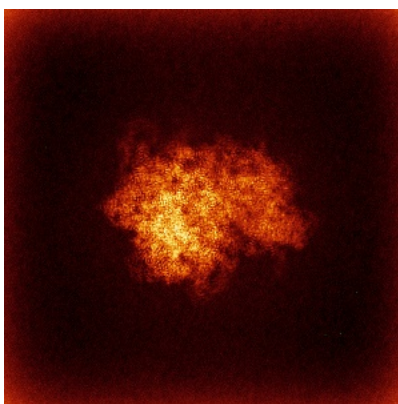


Z

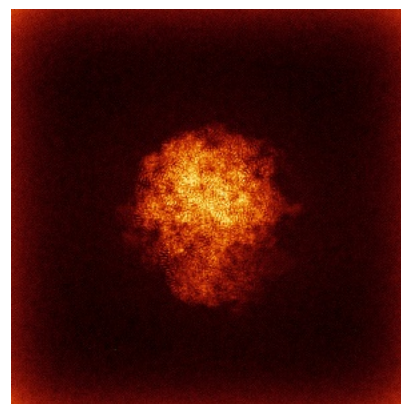
6.4.2 Raw map



X



Y

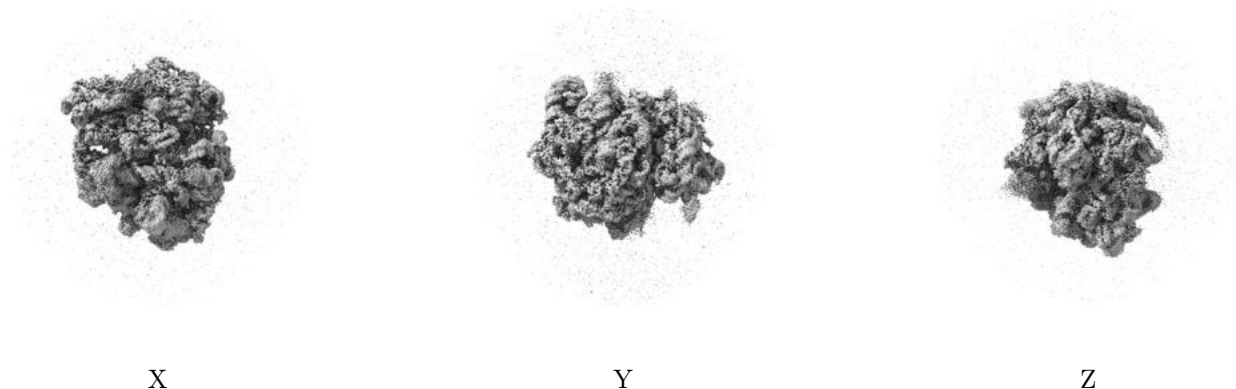


Z

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

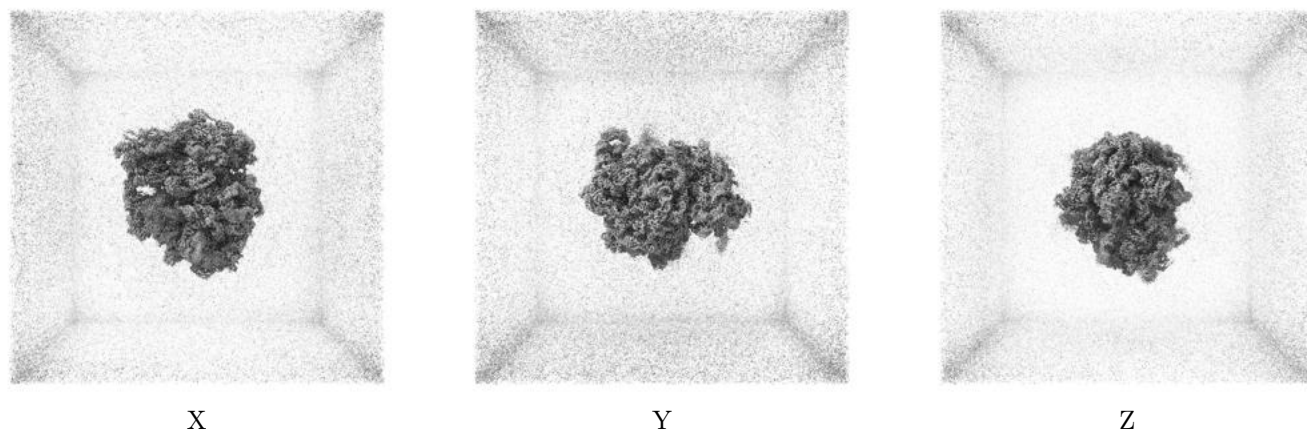
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

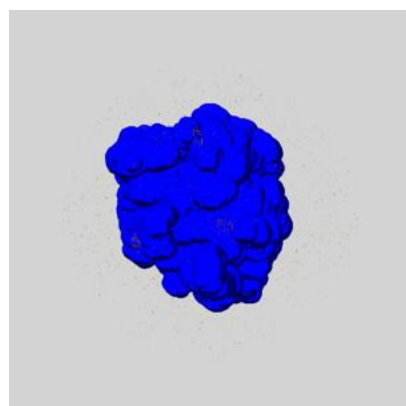
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

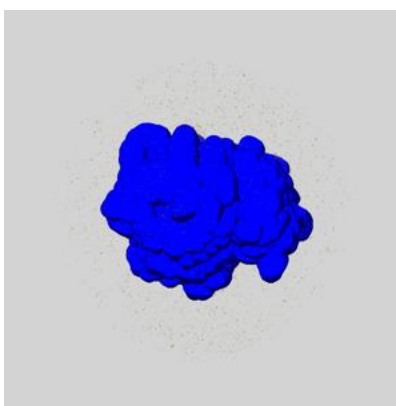
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

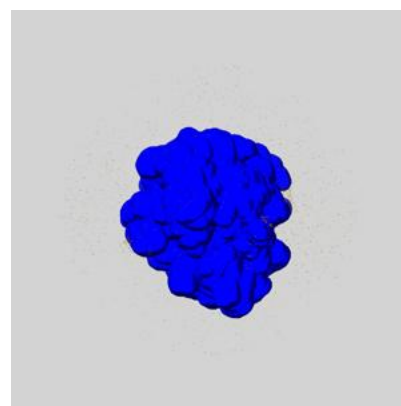
6.6.1 emd_71683_msk_1.map [i](#)



X



Y

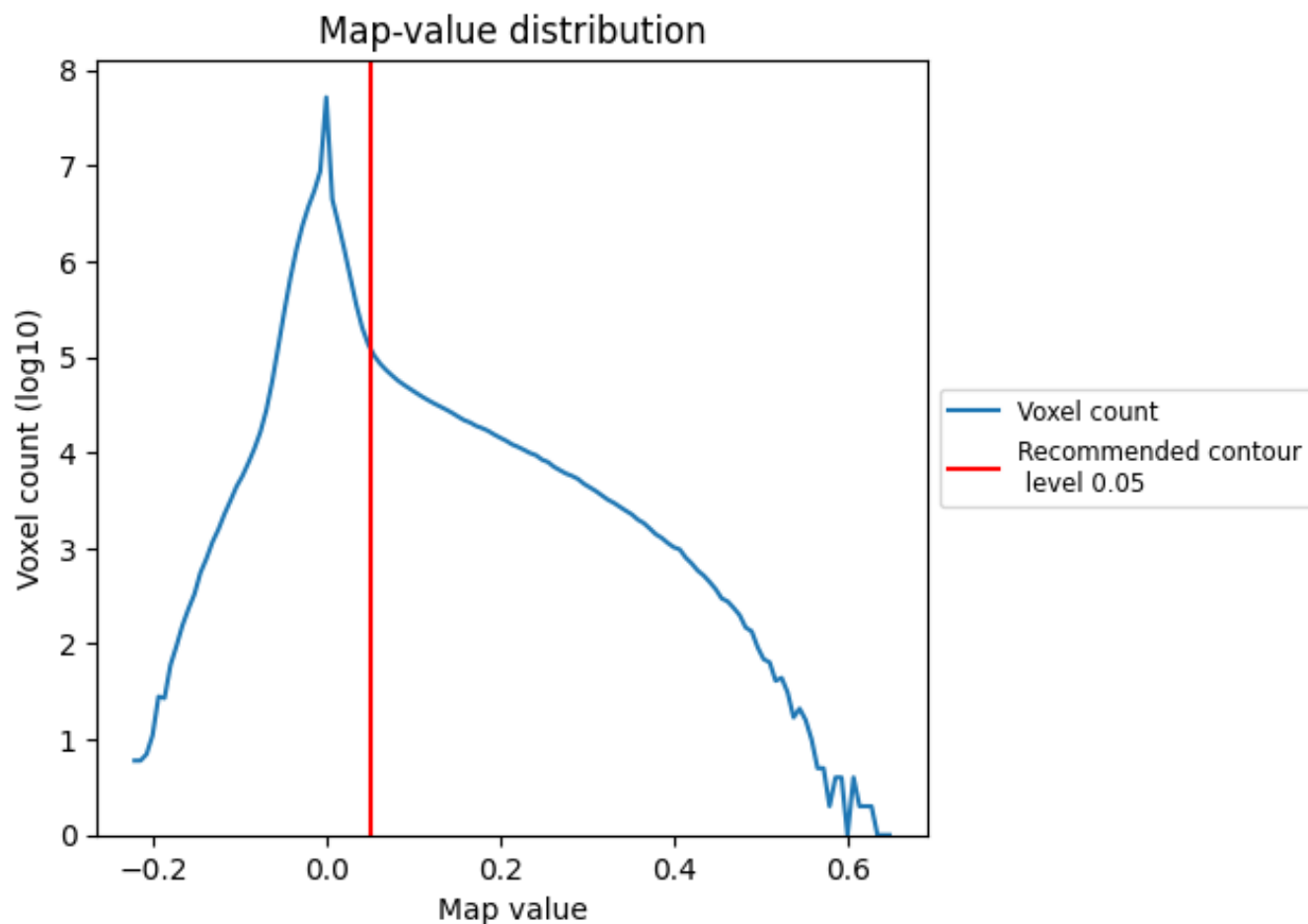


Z

7 Map analysis [i](#)

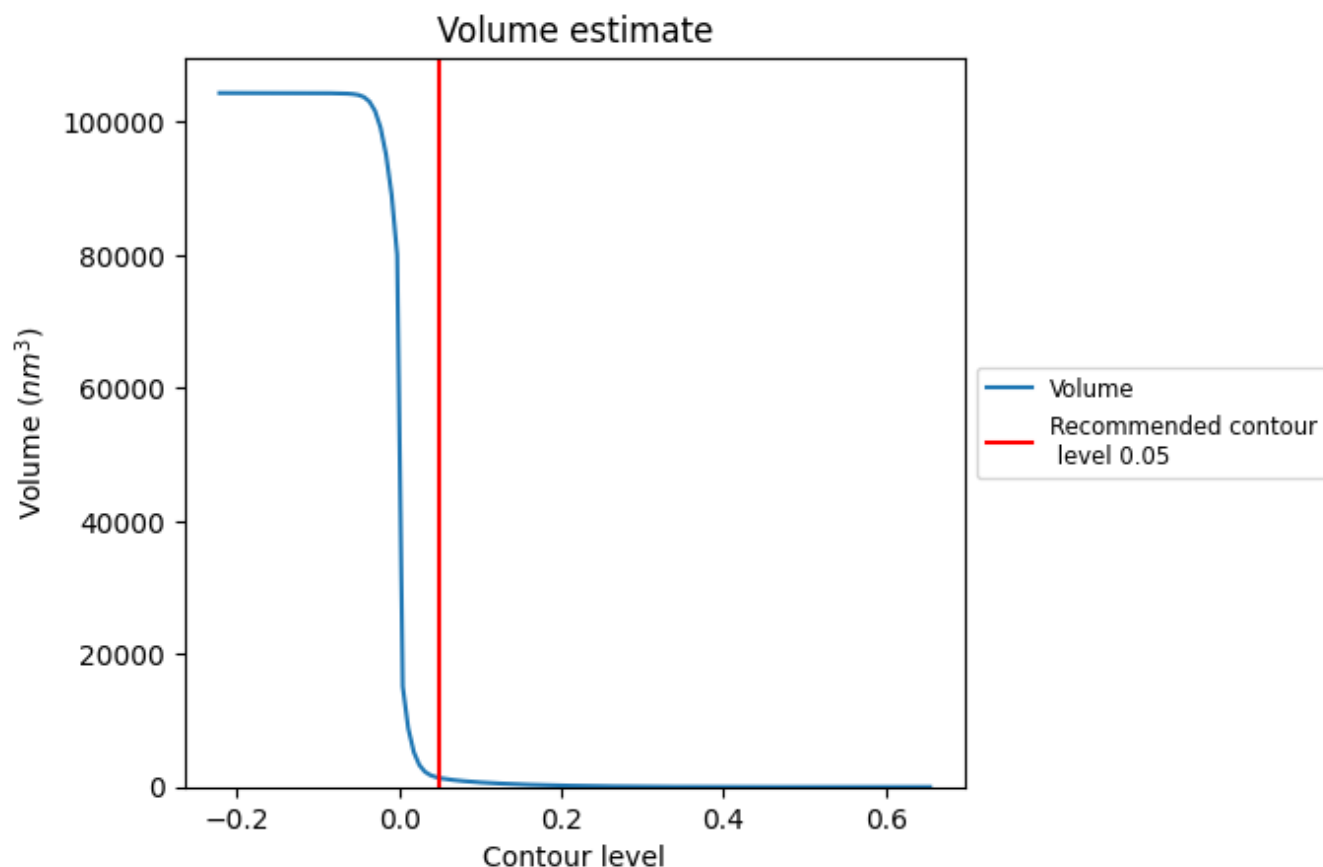
This section contains the results of statistical analysis of the map.

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.

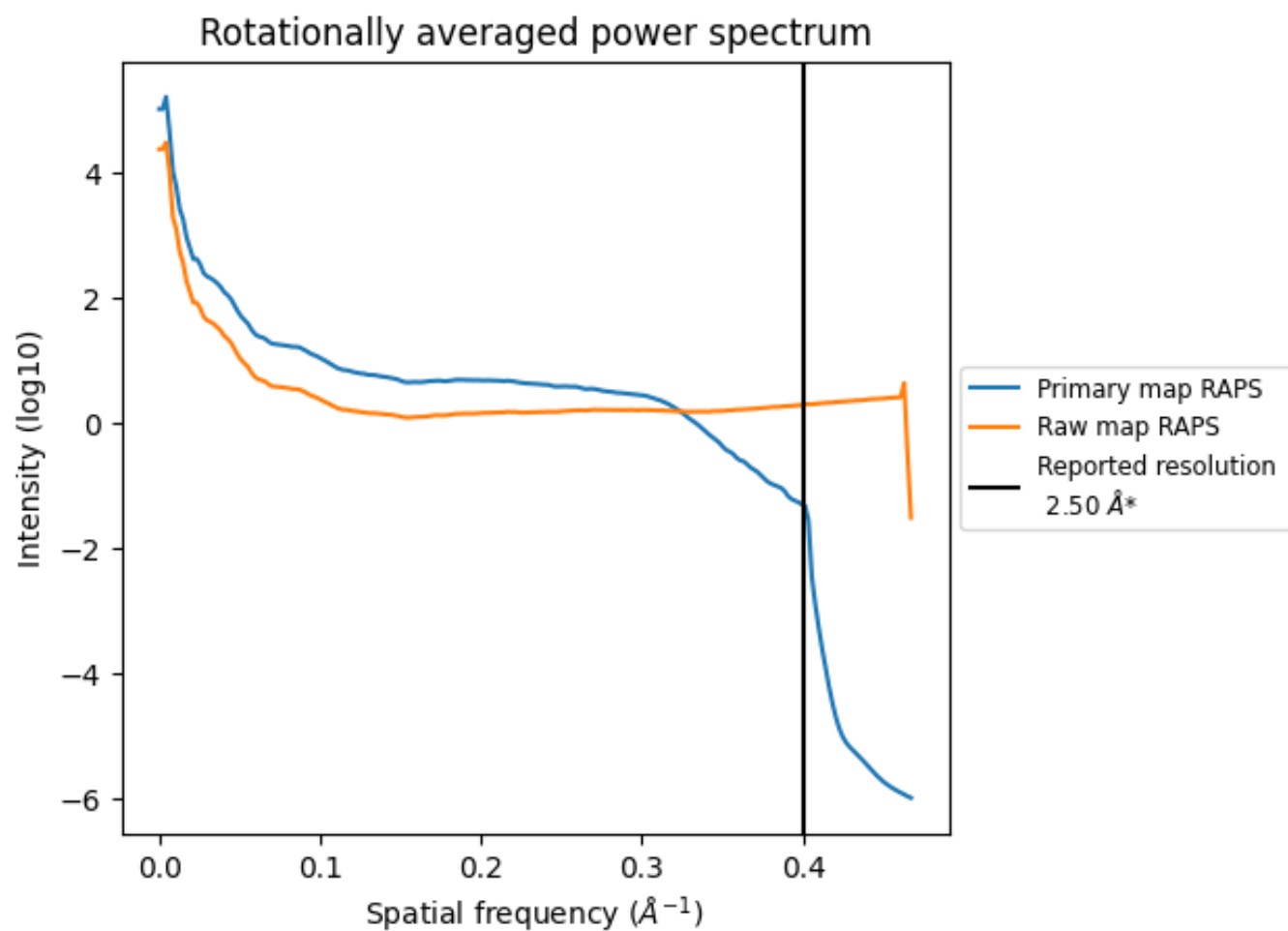
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1360 nm^3 ; this corresponds to an approximate mass of 1229 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 ⓘ

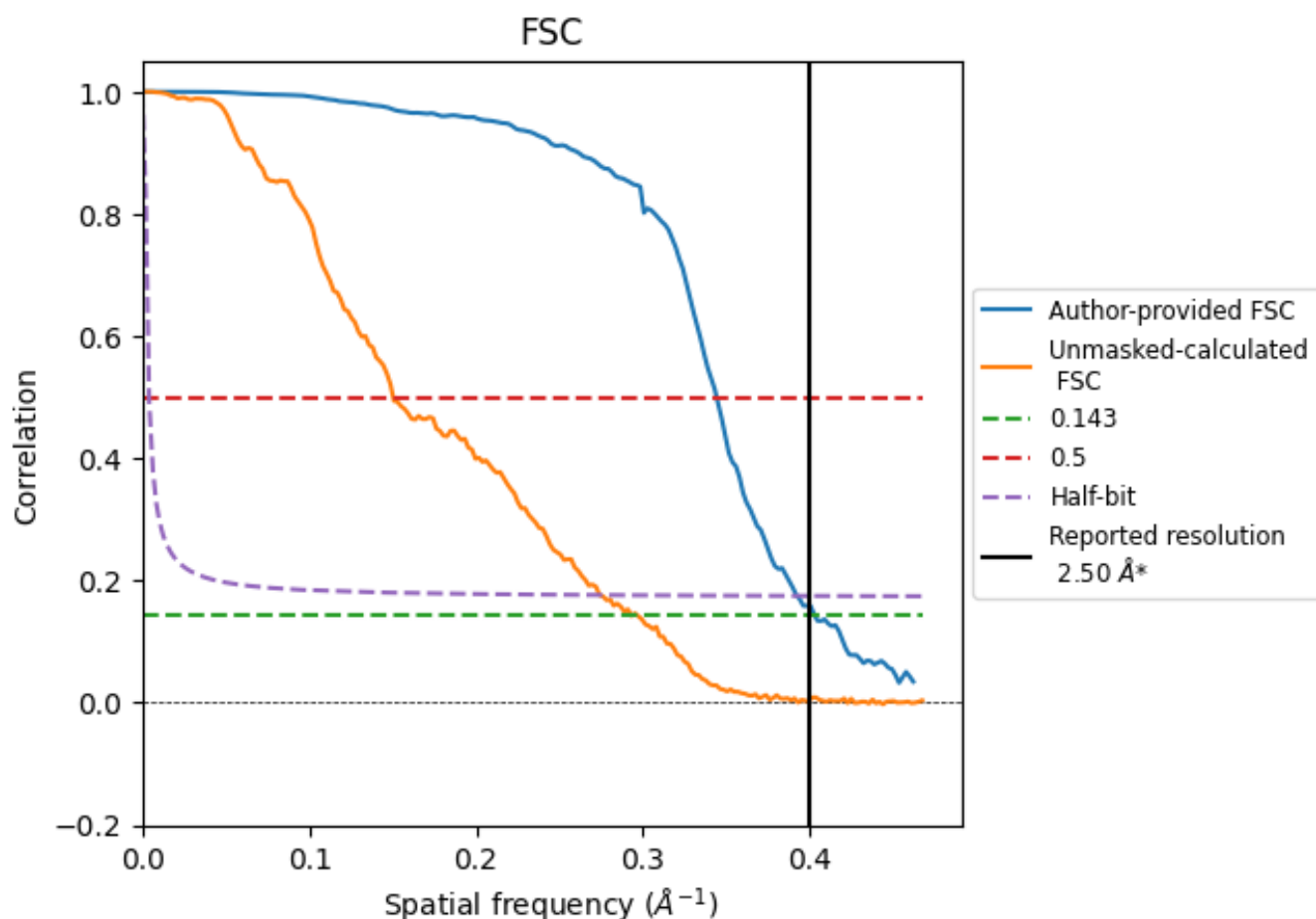


*Reported resolution corresponds to spatial frequency of 0.400 $\text{\AA}^{-1}$

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 0.400 Å⁻¹

8.2 Resolution estimates [i](#)

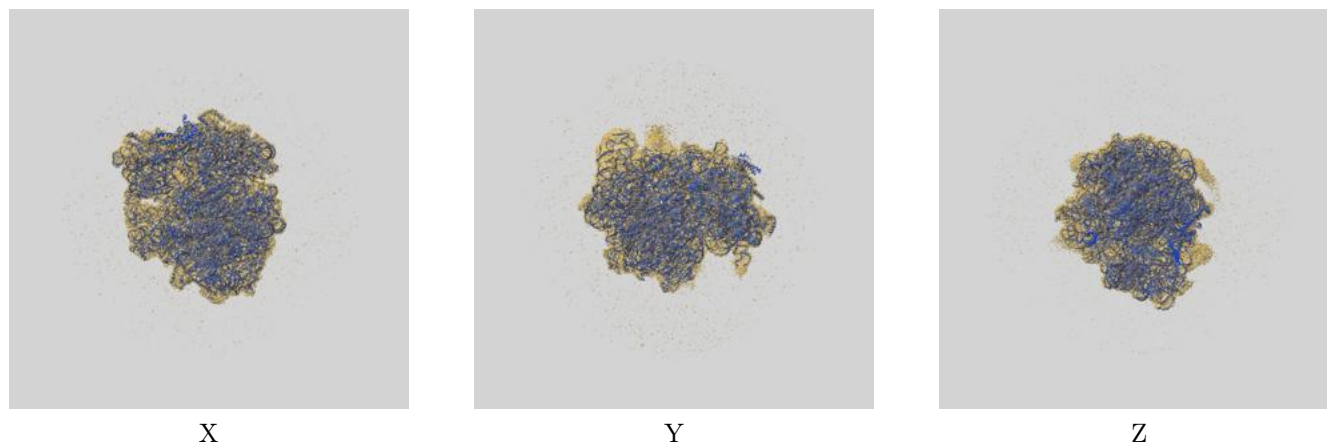
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.48	2.91	2.55
Unmasked-calculated*	3.41	6.65	3.65

*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 3.41 differs from the reported value 2.5 by more than 10 %

9 Map-model fit [i](#)

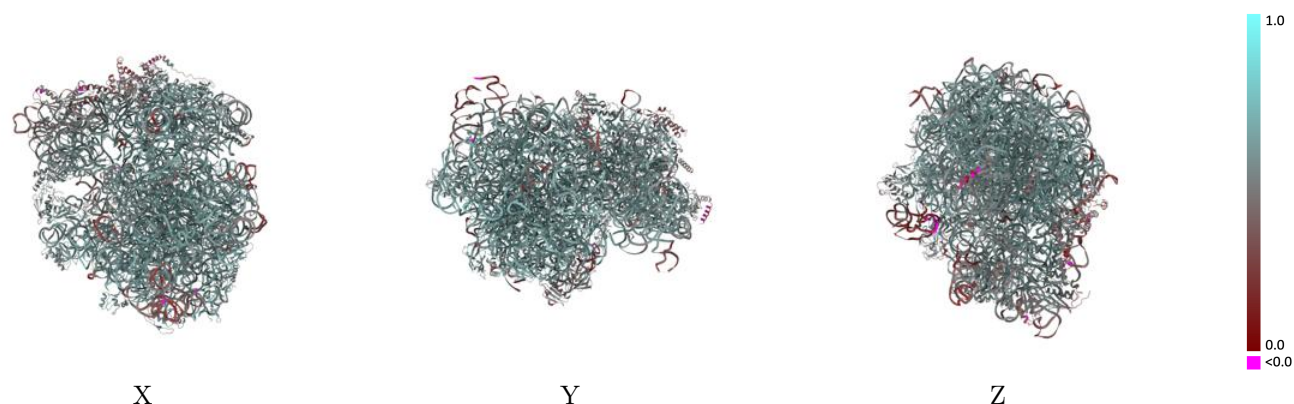
This section contains information regarding the fit between EMDB map EMD-71683 and PDB model 9PJ8. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



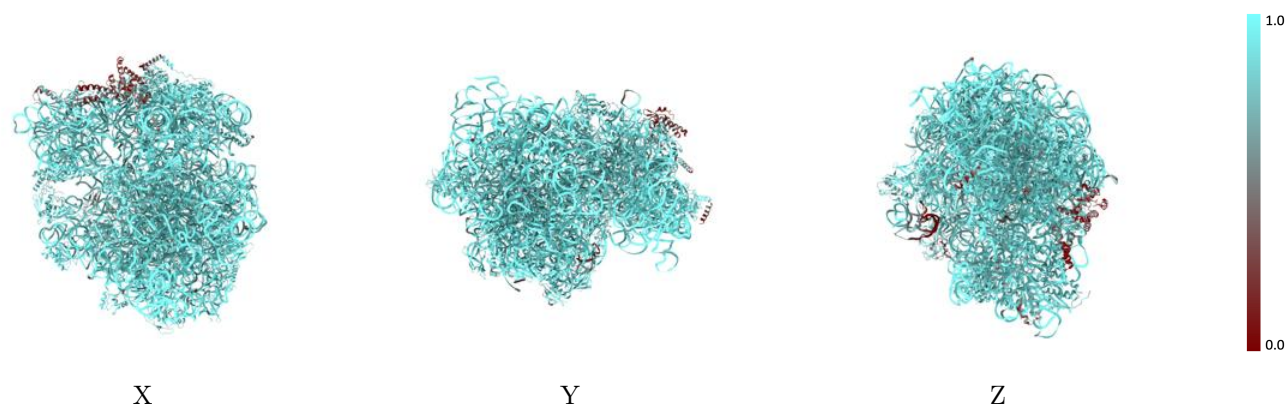
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



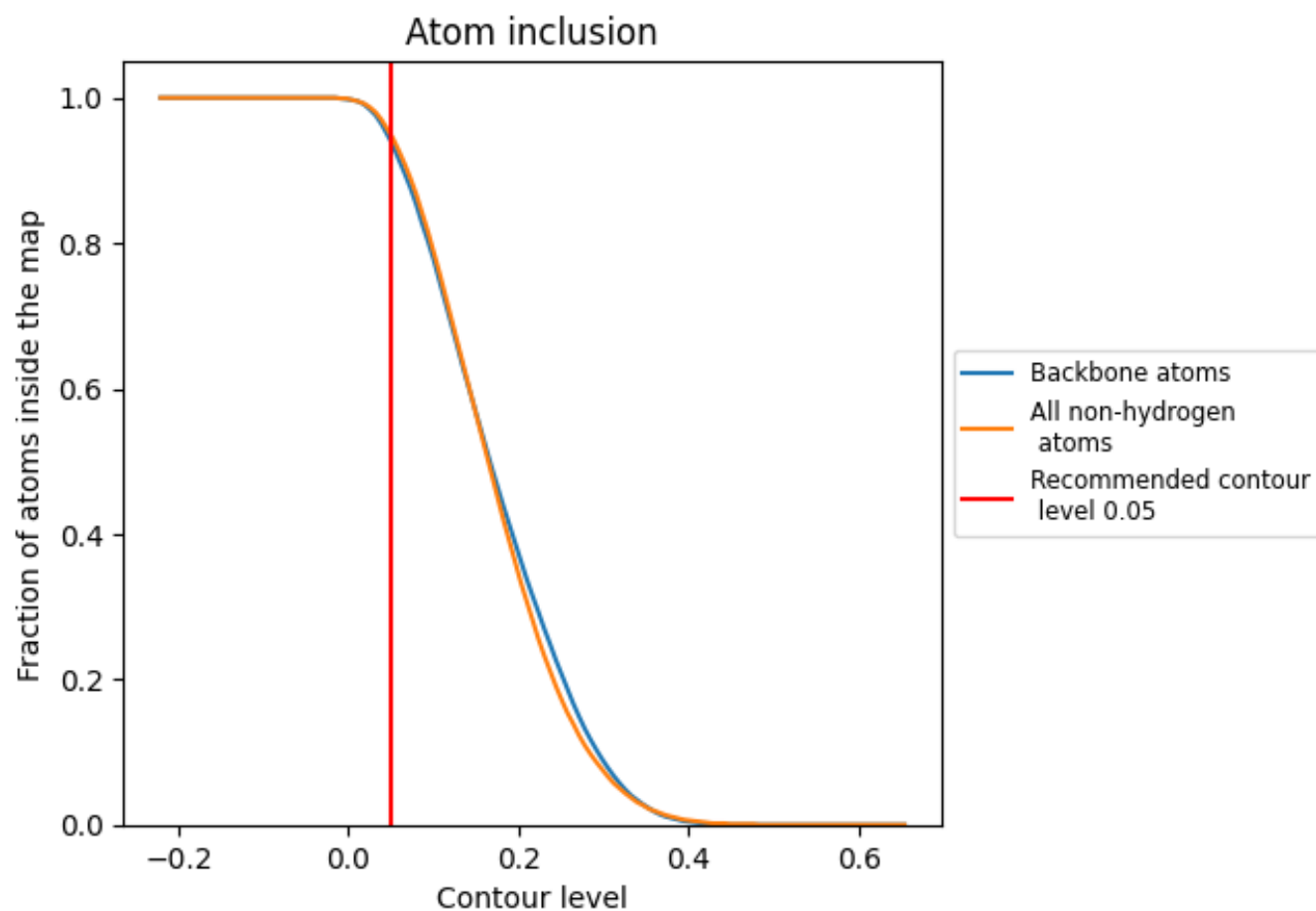
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9490	 0.5680
0	 0.9580	 0.6020
1	 0.9940	 0.6400
2	 0.9680	 0.6250
3	 0.9490	 0.6080
4	 0.8960	 0.5030
A	 0.9830	 0.5610
B	 0.2570	 0.3670
C	 0.9610	 0.5600
D	 0.9060	 0.5040
E	 0.8750	 0.5530
F	 0.8960	 0.5240
G	 0.7980	 0.5000
H	 0.9390	 0.5740
I	 0.9020	 0.5240
J	 0.8970	 0.4760
K	 0.9510	 0.5540
L	 0.9390	 0.5870
M	 0.7200	 0.4460
N	 0.8750	 0.5200
O	 0.9460	 0.5570
P	 0.8710	 0.4960
Q	 0.8920	 0.5490
R	 0.8510	 0.5230
S	 0.8900	 0.5480
T	 0.9310	 0.5590
U	 0.9260	 0.5000
V	 0.9770	 0.6370
X	 0.9110	 0.5860
Y	 0.7390	 0.4520
a	 0.9710	 0.5830
b	 0.9960	 0.5910
c	 0.9670	 0.6220
d	 0.9750	 0.6070
e	 0.9510	 0.5800



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Chain	Atom inclusion	Q-score
f	 0.9440	 0.5440
g	 0.9040	 0.4950
i	 0.9730	 0.6160
j	 0.9390	 0.5990
k	 0.9490	 0.5950
l	 0.9640	 0.6060
m	 0.9690	 0.6070
n	 0.9590	 0.5610
o	 0.9460	 0.6060
p	 0.9620	 0.6130
q	 0.9530	 0.5900
r	 0.9460	 0.6060
s	 0.9590	 0.5900
t	 0.9420	 0.5670
u	 0.7270	 0.4660
v	 0.9630	 0.6220
w	 0.9800	 0.6260
x	 0.9360	 0.5610
y	 0.9510	 0.6100
z	 0.9610	 0.6170