



## wwPDB EM Validation Summary Report ⓘ

May 4, 2026 – 11:26 AM 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](mailto: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>.

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

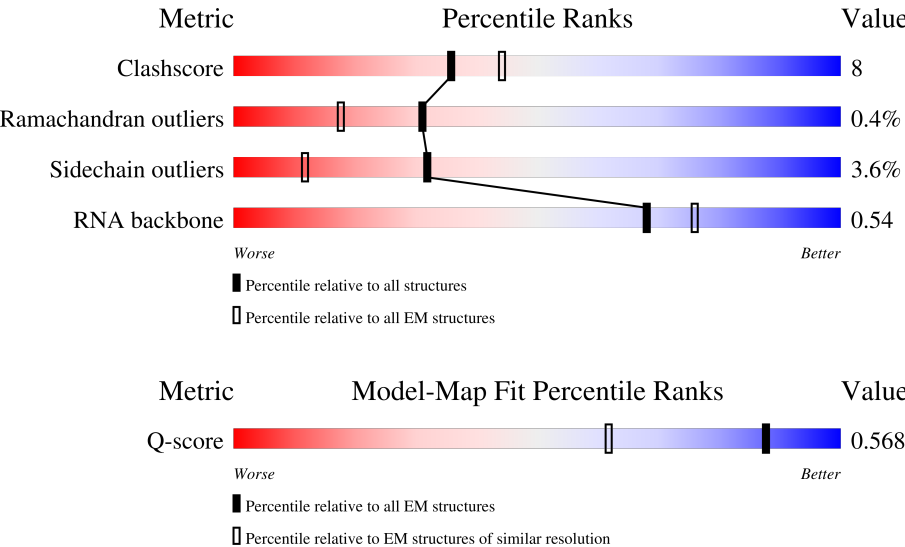
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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) : 2.49

# 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 2.50 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.























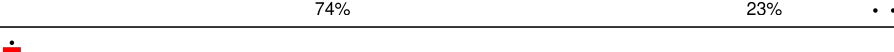


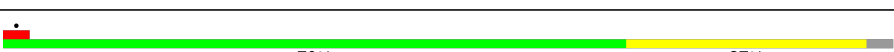

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7115 ( 2.00 - 3.00 )

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  $\geq 3$ , 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	<div><div></div><div>78%</div><div>21%</div><div></div></div>

## 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: C<sub>24</sub>H<sub>29</sub>N<sub>3</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



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

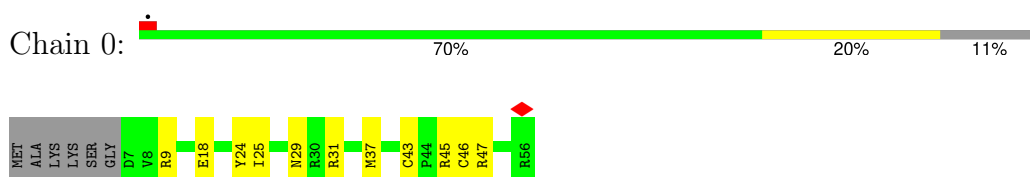
- Molecule 58 is water.

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

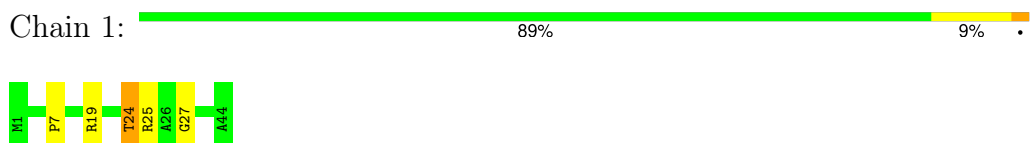
### 3 Residue-property plots [i](#)

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

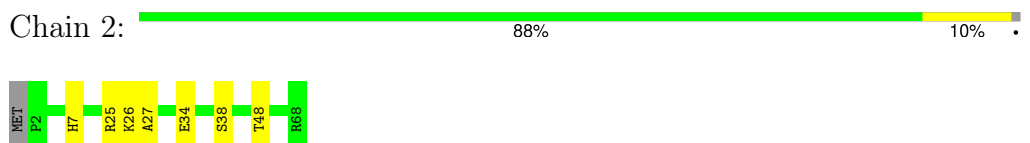
- Molecule 1: 50S ribosomal protein L33



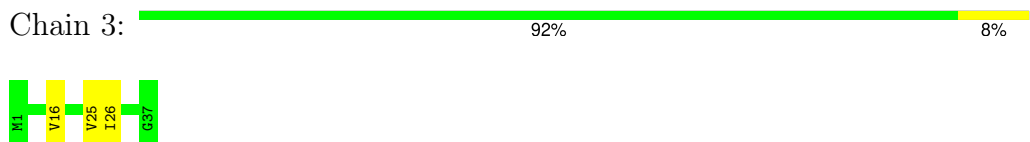
- Molecule 2: 50S ribosomal protein L34



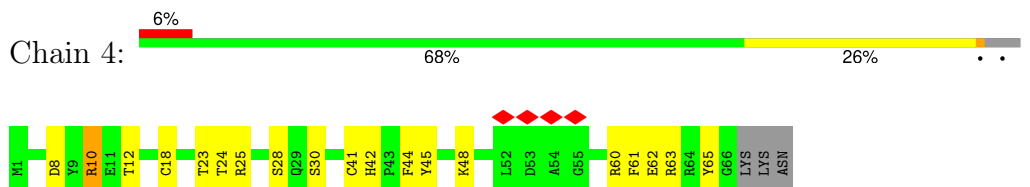
- Molecule 3: Large ribosomal subunit protein bL35



- Molecule 4: 50S ribosomal protein L36



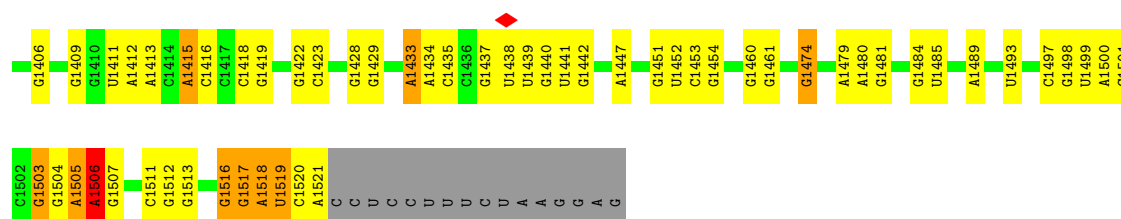
- Molecule 5: 50S ribosomal protein L31



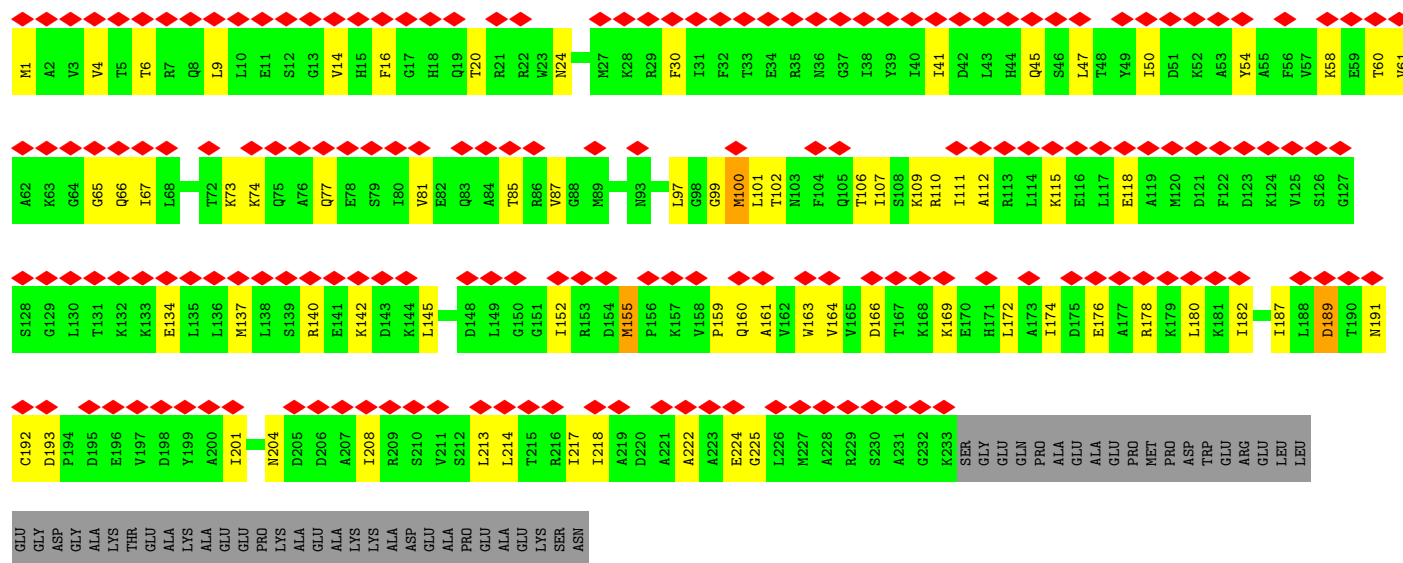
- Molecule 6: 16S rRNA



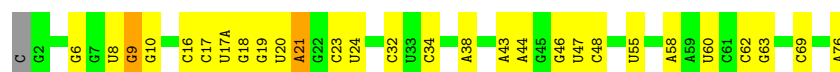




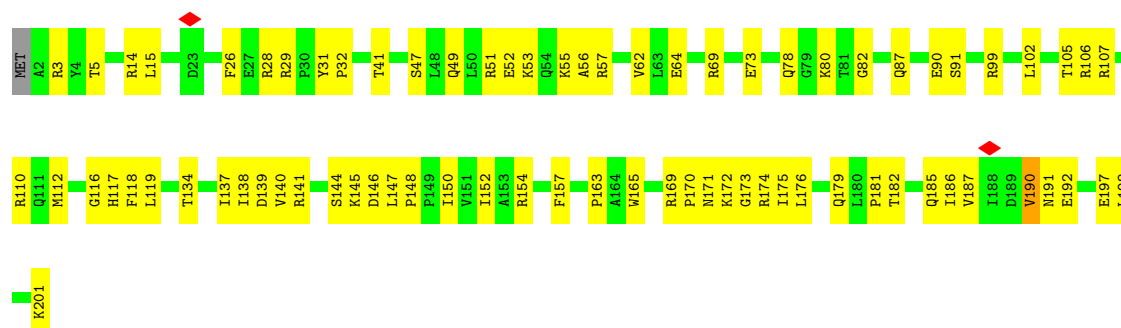
• Molecule 7: 30S ribosomal protein S2



• Molecule 8: initiator tRNA Met (76-MER)

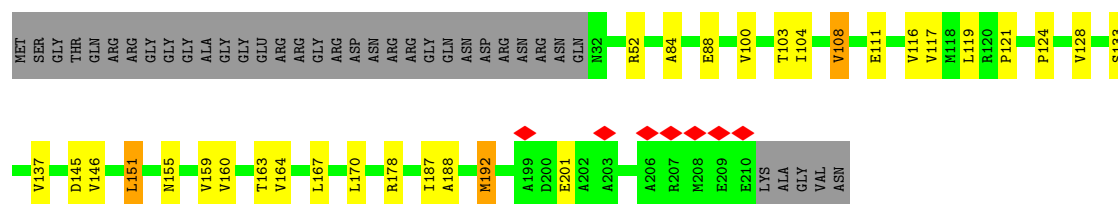


• Molecule 9: 30S ribosomal protein S4



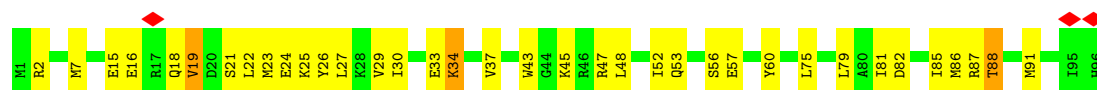
• Molecule 10: Small ribosomal subunit protein uS5

Chain E: 



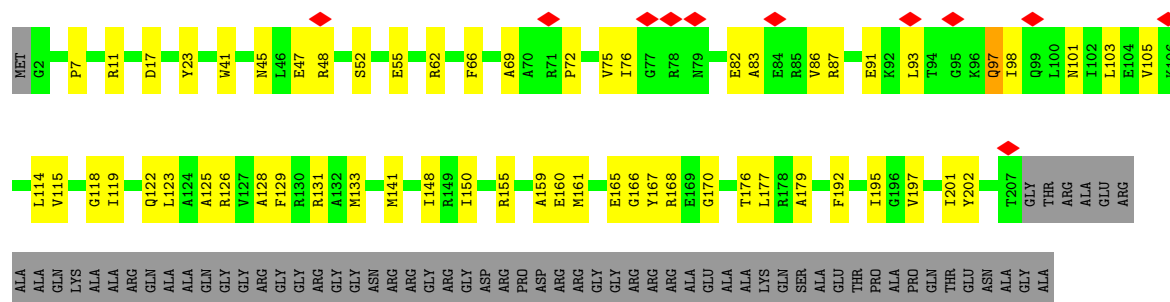
- Molecule 11: 30S ribosomal protein S6

Chain F: 




- Molecule 12: 30S ribosomal protein S3

Chain G: 



- Molecule 13: 30S ribosomal protein S8

Chain H: 

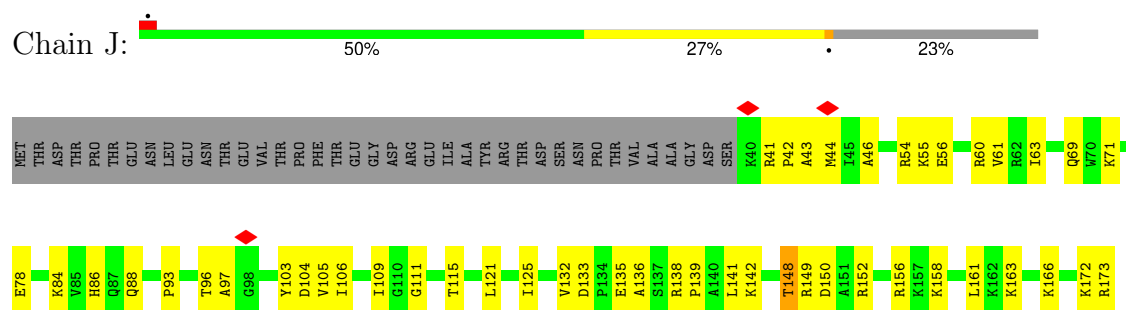


- Molecule 14: 30S ribosomal protein S7

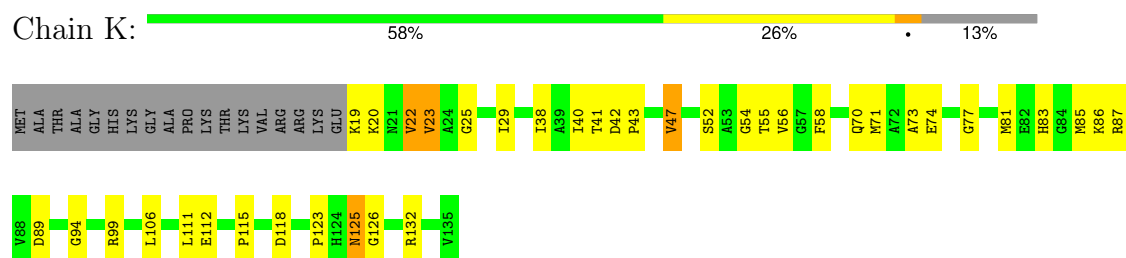
Chain I: 



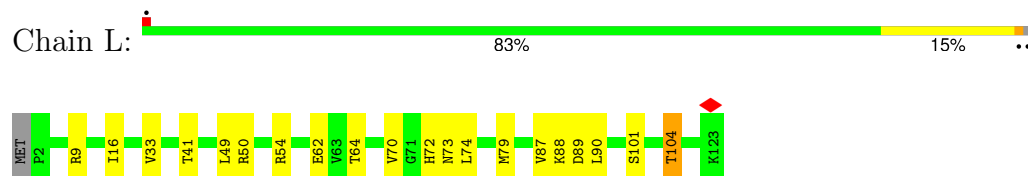
- Molecule 15: 30S ribosomal protein S9



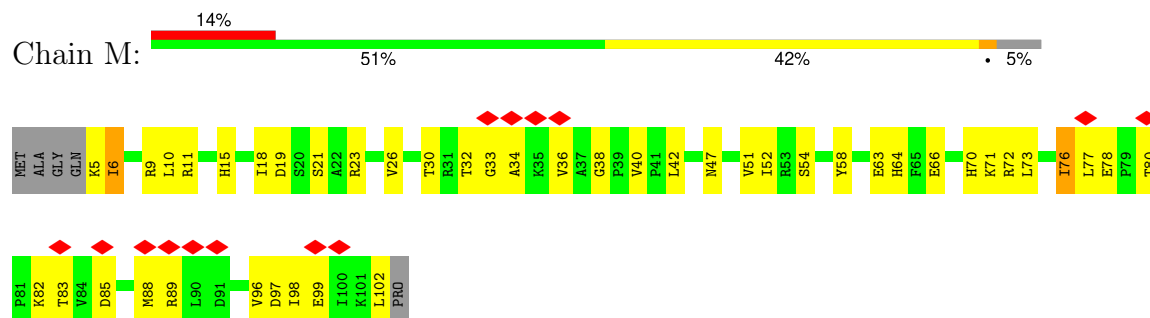
- Molecule 16: 30S ribosomal protein S11



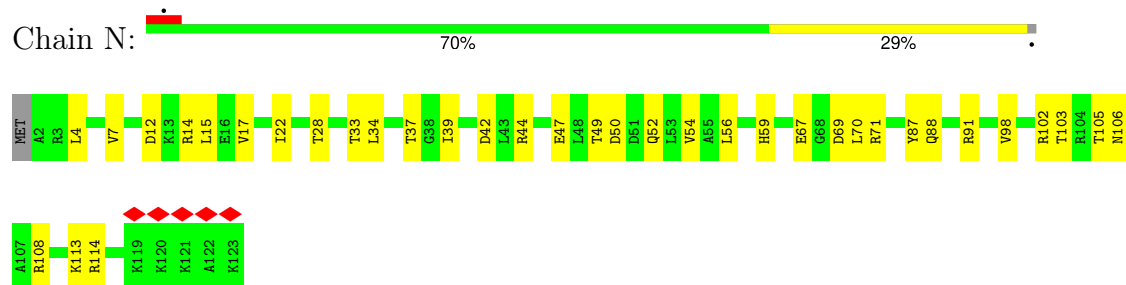
- Molecule 17: 30S ribosomal protein S12



- Molecule 18: Small ribosomal subunit protein uS10



- Molecule 19: 30S ribosomal protein S13



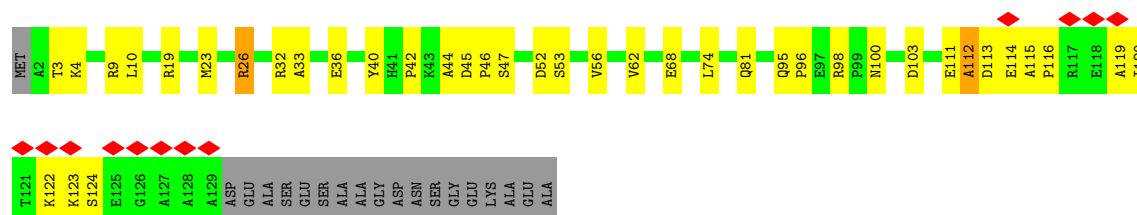
- Molecule 20: 30S ribosomal protein S15

Chain O:  75% 25%




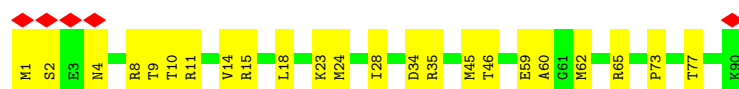
- Molecule 21: 30S ribosomal protein S16

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%



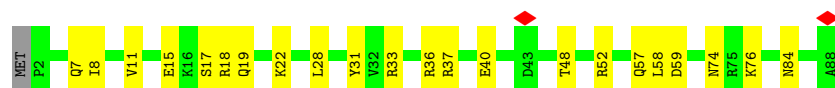
- Molecule 24: 30S ribosomal protein S14 type Z

Chain S:  74% 23%



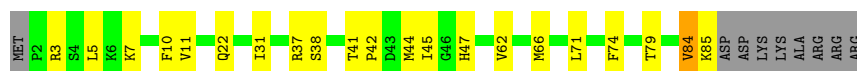
- Molecule 25: 30S ribosomal protein S20

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% .



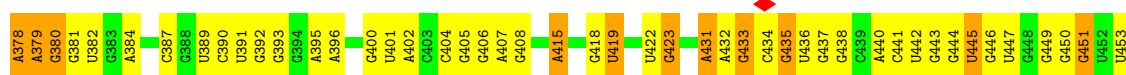
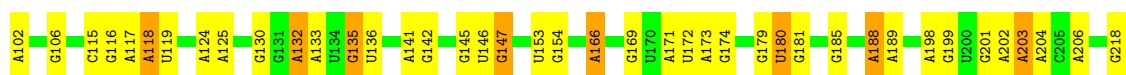
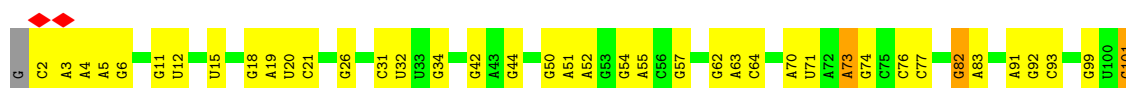
- Molecule 29: mRNA 32MF

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

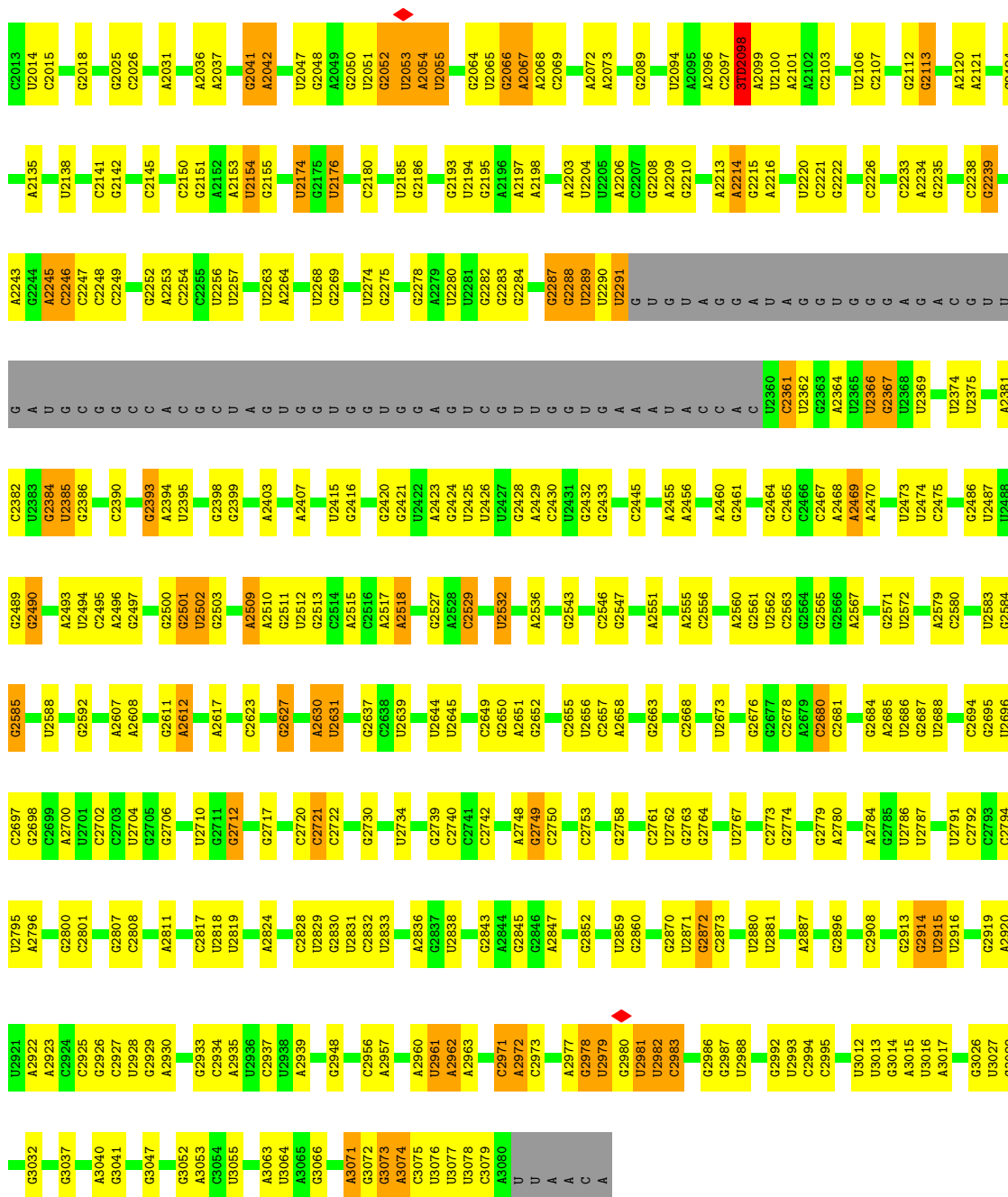


- Molecule 30: 23S rRNA

Chain a: 57% 31% 6% 6%

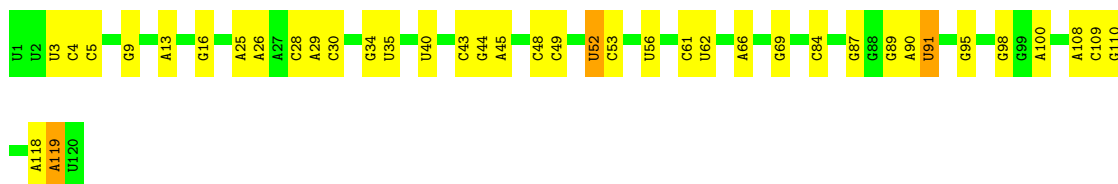


U1904	G581	A1010	G1324	G1190	G1318	A1441	G	A1675	G1761	U1904
G1905	U682	A1011	A905	U1191	U1124	U	U	A1676	G1762	G1905
C1906	G683	G1014	U911	C1192	U1128	U1455	A	G1685	U1763	C1906
A1907	G686	U1015	U912	A1193	A1129	A1328	G	C1686	G1764	A1907
C1908	A687	U1016	U913	G1194	G1130	A1329	G	C1687	U1765	C1908
U1909	U688	A1017	G916	U1195	C1135	A1331	U	U1688	A1766	U1909
G1910	A692	G1018	U917	U1196	C1136	U1332	U	C1689	U1767	G1910
G1911	A693	G1019	G918	U1197	C1137	G1333	G	G1690	G1768	G1911
U1912	U698	A1020	G921	U1198	U1138	G1334	U	A1691	U1769	U1912
C1913	G699	G1021	G930	U1199	G1139	U1335	G	C1692	G1770	C1913
G1914	G700	C1031	G931	U1200	A1140	G1336	G	U1693	U1771	G1914
U1915	U701	U1032	U935	U1201	G1141	U1337	G	C1694	G1772	U1915
G1916	G704	G1033	G942	U1202	U1142	G1338	U	A1695	U1773	G1916
U1917	U709	A1034	G943	U1203	U1143	U1339	A	U1696	G1774	U1917
C1918	C710	G1035	G944	U1204	G1144	U1340	U	A1697	G1775	C1918
U1919	G711	U1036	U945	U1205	U1145	G1341	U	C1698	U1776	U1919
G1920	C712	G1037	U946	U1206	G1146	U1342	U	A1699	G1777	G1920
U1921	A713	U1038	U947	U1207	C1147	U1343	G	C1700	U1778	U1921
G1922	C714	G1039	U948	U1208	U1148	U1344	U	U1701	G1779	G1922
U1923	G715	U1040	U949	U1209	U1149	U1345	U	A1702	U1780	U1923
C1924	C716	G1041	U950	U1210	G1150	U1346	U	C1703	G1781	C1924
U1925	U717	U1042	U951	U1211	G1151	G1347	U	U1704	U1782	U1925
G1926	C718	A1043	U952	U1212	U1152	U1348	U	A1705	U1783	G1926
U1927	A719	G1044	U953	U1213	G1153	U1349	U	C1706	U1784	U1927
C1928	C720	U1045	U954	U1214	U1154	U1350	U	U1707	U1785	C1928
U1929	G721	G1046	U955	U1215	C1155	U1351	U	G1708	U1786	U1929
G1930	A722	U1047	U956	U1216	U1156	U1352	U	C1709	U1787	G1930
U1931	C723	G1048	U957	U1217	G1157	U1353	U	U1710	U1788	U1931
C1932	G724	U1049	U958	U1218	C1158	U1354	U	A1711	U1789	C1932
U1933	U725	A1050	U959	U1219	U1159	U1355	U	C1712	U1790	U1933
G1934	C726	G1051	U960	U1220	U1160	U1356	U	U1713	U1791	G1934
U1935	G727	U1052	U961	U1221	C1161	U1357	U	G1714	U1792	U1935
C1936	A728	G1053	U962	U1222	U1162	U1358	U	U1715	U1793	C1936
U1937	C729	U1054	U963	U1223	U1163	U1359	U	A1716	U1794	U1937
G1938	U730	G1055	U964	U1224	C1164	U1360	U	C1717	U1795	G1938
U1939	G731	U1056	U965	U1225	U1165	U1361	U	U1718	U1796	U1939
C1940	A732	G1057	U966	U1226	U1166	U1362	U	G1719	U1797	C1940
U1941	C733	U1058	U967	U1227	U1167	U1363	U	U1720	U1798	U1941
G1942	U734	A1059	U968	U1228	U1168	U1364	U	A1721	U1799	G1942
U1943	G735	G1060	U969	U1229	U1169	U1365	U	C1722	U1800	U1943
C1944	A736	U1061	U970	U1230	C1169	U1366	U	U1723	U1801	C1944
U1945	C737	G1062	U971	U1231	U1170	U1367	U	G1724	U1802	U1945
G1946	U738	U1063	U972	U1232	U1171	U1368	U	U1725	U1803	G1946
U1947	A739	A1064	U973	U1233	U1172	U1369	U	C1726	U1804	U1947
C1948	C739	G1065	U974	U1234	U1173	U1370	U	U1727	U1805	C1948
U1949	G740	U1066	U975	U1235	U1174	U1371	U	G1728	U1806	U1949
G1950	A741	G1067	U976	U1236	U1175	U1372	U	U1729	U1807	G1950
U1951	C742	U1068	U977	U1237	U1176	U1373	U	A1730	U1808	U1951
C1952	U743	A1069	U978	U1238	U1177	U1374	U	C1731	U1809	C1952
U1953	G744	G1070	U979	U1239	U1178	U1375	U	U1732	U1810	U1953
G1954	A745	U1071	U980	U1240	U1179	U1376	U	G1733	U1811	G1954
U1955	C746	A1072	U981	U1241	U1180	U1377	U	U1734	U1812	U1955
C1956	U747	G1073	U982	U1242	U1181	U1378	U	A1735	U1813	C1956
U1957	A748	U1074	U983	U1243	U1182	U1379	U	C1736	U1814	U1957
G1958	C749	G1075	U984	U1244	U1183	U1380	U	U1737	U1815	G1958
U1959	G750	U1076	U985	U1245	U1184	U1381	U	A1738	U1816	U1959
C1960	A751	G1077	U986	U1246	U1185	U1382	U	C1739	U1817	C1960
U1961	C752	U1078	U987	U1247	U1186	U1383	U	U1740	U1818	U1961
G1962	U753	A1079	U988	U1248	U1187	U1384	U	G1741	U1819	G1962
U1963	G754	G1080	U989	U1249	U1188	U1385	U	U1742	U1820	U1963
C1964	A755	U1081	U990	U1250	U1189	U1386	U	A1743	U1821	C1964
U1965	C756	G1082	U991	U1251	U1190	U1387	U	C1744	U1822	U1965
G1966	U757	A1083	U992	U1252	U1191	U1388	U	U1745	U1823	G1966
U1967	A758	U1084	U993	U1253	U1192	U1389	U	G1746	U1824	U1967
C1968	C759	G1085	U994	U1254	U1193	U1390	U	A1747	U1825	C1968
U1969	G760	U1086	U995	U1255	U1194	U1391	U	C1748	U1826	U1969
G1970	A761	A1087	U996	U1256	U1195	U1392	U	U1749	U1827	G1970
U1971	C762	G1088	U997	U1257	U1196	U1393	U	G1750	U1828	U1971
C1972	U763	U1089	U998	U1258	U1197	U1394	U	U1751	U1829	C1972
U1973	G764	G1090	U999	U1259	U1198	U1395	U	A1752	U1830	U1973
G1974	A765	U1091	U1000	U1260	U1199	U1396	U	C1753	U1831	G1974
C1975	C766	A1092	U1001	U1261	U1200	U1397	U	U1754	U1832	C1975
U1976	U767	G1093	U1002	U1262	U1201	U1398	U	G1755	U1833	U1976
G1977	A768	U1094	U1003	U1263	U1202	U1399	U	U1756	U1834	G1977
U1978	C769	G1095	U1004	U1264	U1203	U1400	U	A1757	U1835	U1978
C1979	U769	A1096	U1005	U1265	U1204	U1401	U	C1758	U1836	C1979
U1980	G770	G1097	U1006	U1266	U1205	U1402	U	U1759	U1837	U1980
G1981	A771	U1098	U1007	U1267	U1206	U1403	U	G1760	U1838	G1981
U1982	C772	G1099	U1008	U1268	U1207	U1404	U	U1761	U1839	U1982
C1983	U773	A1100	U1009	U1269	U1208	U1405	U	A1762	U1840	C1983
U1984	G774	U1101	U1010	U1270	U1209	U1406	U	C1763	U1841	U1984
G1985	A775	G1102	U1011	U1271	U1210	U1407	U	U1764	U1842	G1985
U1986	C775	A1103	U1012	U1272	U1211	U1408	U	G1765	U1843	U1986
C1987	U776	G1104	U1013	U1273	U1212	U1409	U	U1766	U1844	C1987
U1988	A777	U1105	U1014	U1274	U1213	U1410	U	A1767	U1845	U1988
G1989	C778	G1106	U1015	U1275	U1214	U1411	U	C1768	U1846	G1989
U1990	G779	A1107	U1016	U1276	U1215	U1412	U	U1769	U1847	U1990
C1991	U780	U1108	U1017	U1277	U1216	U1413	U	G1770	U1848	C1991
U1992	A781	G1109	U1018	U1278	U1217	U1414	U	U1771	U1849	U1992
G1993	C782	A1110	U1019	U1279	U1218	U1415	U	A1772	U1850	G1993
U1994	G783	U1111	U1020	U1280	U1219	U1416	U	C1773	U1851	U1994
C1995	U784	G1112	U1021	U1281	U1220	U1417	U	U1774	U1852	C1995
U1996	A785	A1113	U1022	U1282	U1221	U1418	U	G1775	U1853	U1996
G1997	C785	U1114	U1023	U1283	U1222	U1419	U	A1776	U1854	G1997
U1998	G786	G1115	U1024	U1284	U1223	U1420	U	C1777	U1855	U1998
C1999	U787	A1116	U1025	U1285	U1224	U1421	U	U1778	U1856	C1999
U2000	A788	U1117	U1026	U1286	U1225	U1422	U	G1779	U1857	U2000
G2001	C788	G1118	U1027	U1287	U1226	U1423	U	U1780	U1858	G2001
U2002	G789	U1119	U1028	U1288	U1227	U1424	U	A1781	U1859	U2002
C2003	U790	A1120	U1029	U1289	U1228	U1425	U	C1782	U1860	C2003
U2004	A791	U1121	U1030	U1290	U1229	U1426	U	U1783	U1861	U2004
G2005	C792	G1122	U1031	U1291	U1230	U1427	U	G1784	U1862	G2005
U2006	G793	A1123	U1032	U1292	U1231	U1428	U	U1785	U1863	U2006
C2007	U794	U1124	U1033	U1293	U1232	U1429	U	A1786	U1864	C2007
U2008	A795	G1125	U1034	U1294	U1233	U1430	U	C1787	U1865	U2008
G2009	C795	U1126	U1035	U1295	U1234	U1431	U	U1788	U1866	G2009
U2010	G796	A1127	U1036	U1296	U1235	U1432	U	G1789	U1867	U2010
C2011	U797	G1128	U1037	U1297	U1236	U1433	U	A1790	U1868	C2011
U2012	A798	U1129	U1038	U1298	U1237	U1434	U	C1791	U1869	U2012
G2013	C798	A1130	U1039	U1299	U1238	U1435	U	U1792	U1870	G2013
U2014	G799	U1131	U1040	U1300	U1239	U1436	U	G1793	U1871	U2014
C2015	U800	G1132	U1041	U1301	U1240	U1437	U	A1794	U1872	C2015
U2016	A801	A1133	U1042	U1302	U1241	U1438	U	C1795	U1873	U2016
G2017	C802	U1134	A1043	U1303	U1242	U1439	U	U1796	U1874	G2017
U2018	G803	G1135	G1044	U1304	U1243	U1440	U	G1797	U1875	U2018
C2019	U804	U1136	U1045	U1305	U1244	U1441	U	A1798	U1876	C2019
U2020	A805	A1137	U1046	U1306	U1245	U1442	U	C1799	U1877	U2020




# Molecule 31: 5S rRNA

Chain b: 68% 30%




# Molecule 32: 50S ribosomal protein L2

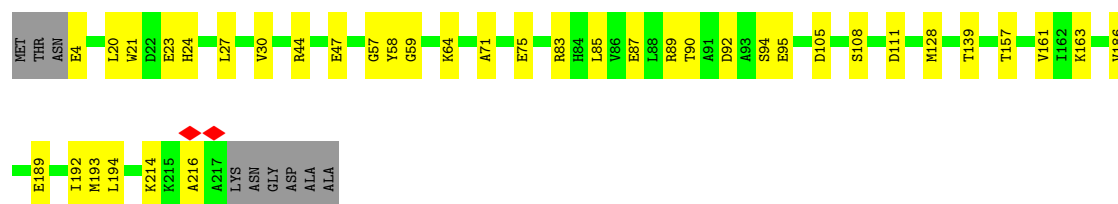


Chain c:  85% 13% ..



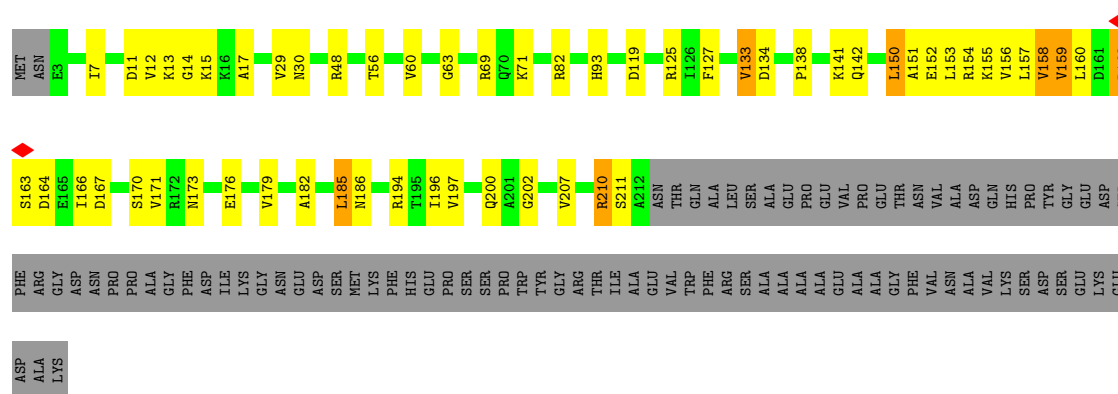
- Molecule 33: 50S ribosomal protein L3

Chain d:  79% 17% .



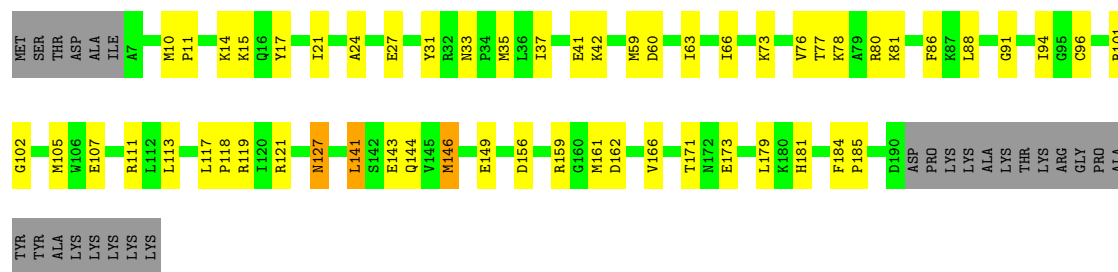
- Molecule 34: 50S ribosomal protein L4

Chain e:  51% 17% . 30%

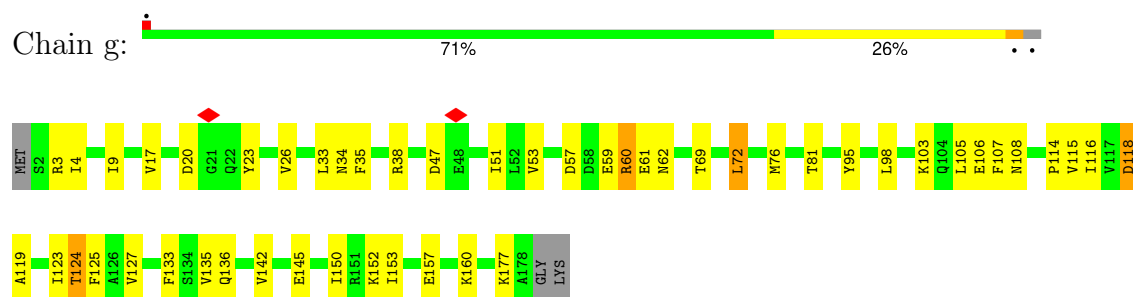


- Molecule 35: 50S ribosomal protein L5

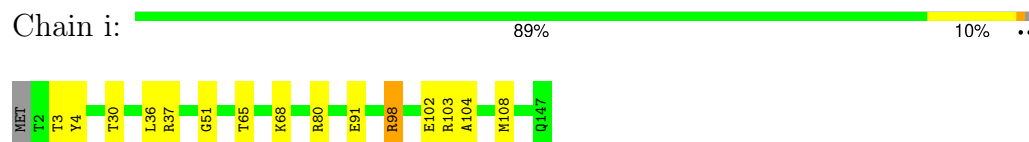
Chain f:  61% 25% . 12%



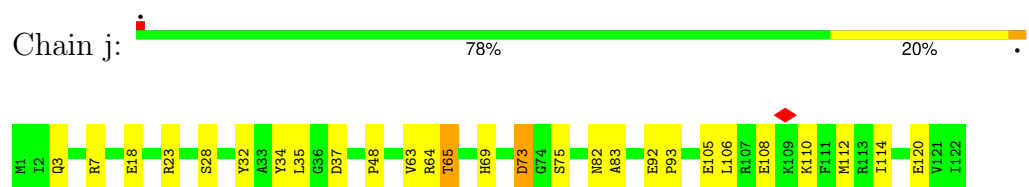
- Molecule 36: 50S ribosomal protein L6



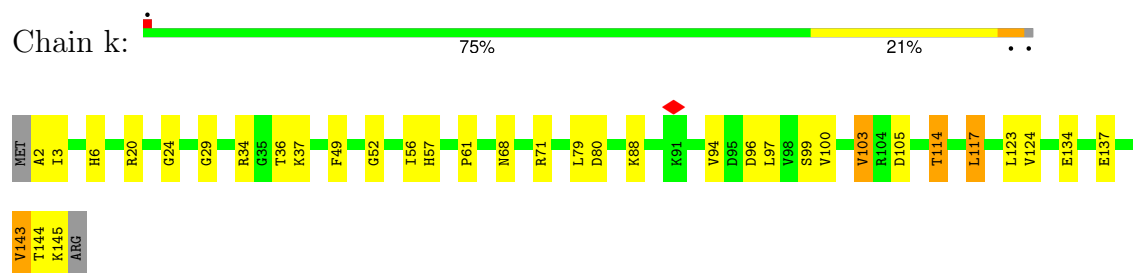
- Molecule 37: 50S ribosomal protein L13



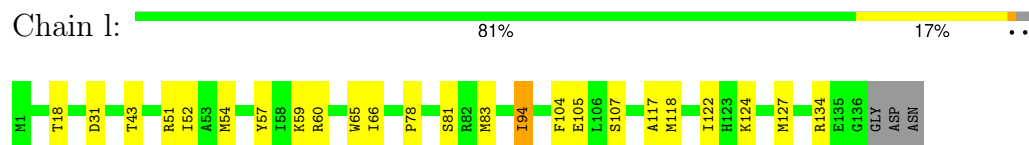
- Molecule 38: 50S ribosomal protein L14



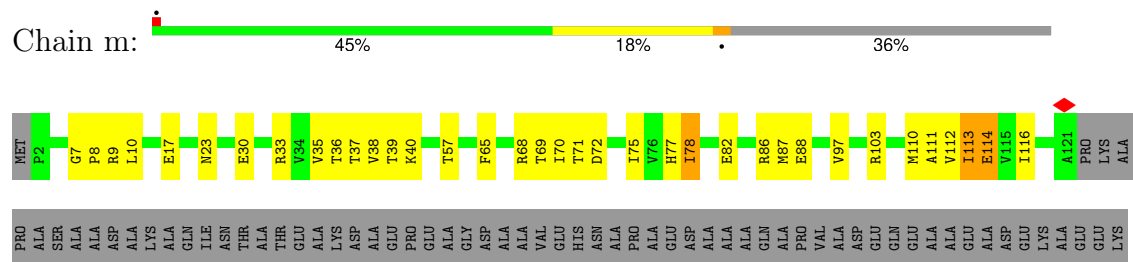
- Molecule 39: 50S ribosomal protein L15



- Molecule 40: 50S ribosomal protein L16



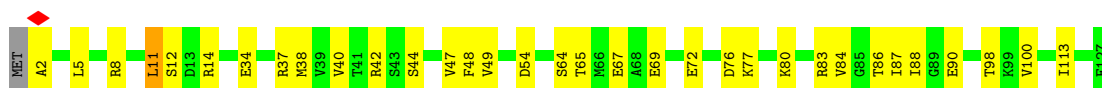
- Molecule 41: Large ribosomal subunit protein bL17




PRO  
GLU  
ALA

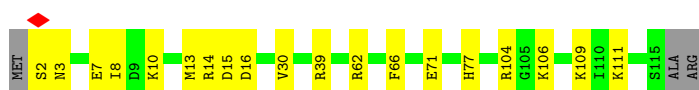
- Molecule 42: 50S ribosomal protein L18

Chain n:  73% 25% ..



- Molecule 43: 50S ribosomal protein L19

Chain o:  81% 16% .




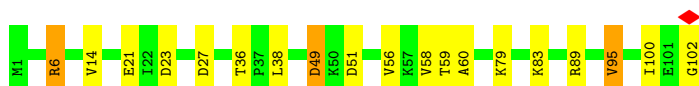
- Molecule 44: 50S ribosomal protein L20

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%



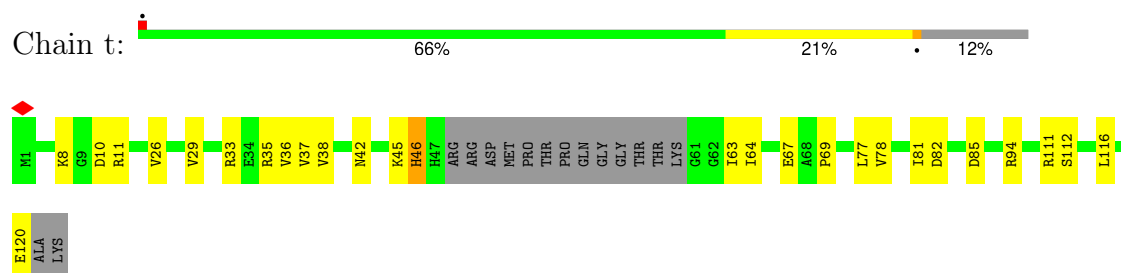
ALA  
ALA  
LYS  
SER  
GLU  
THR  
GLY  
LYS  
GLY  
ALA

- Molecule 47: 50S ribosomal protein L23

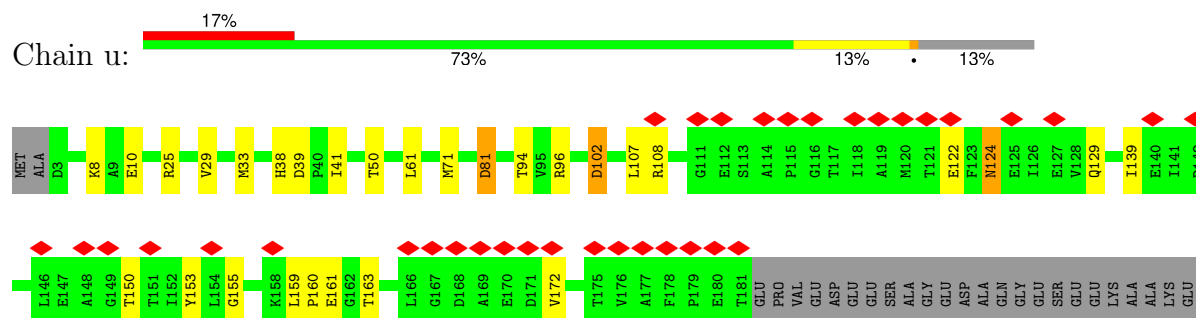
Chain s:  67% 26% 7%



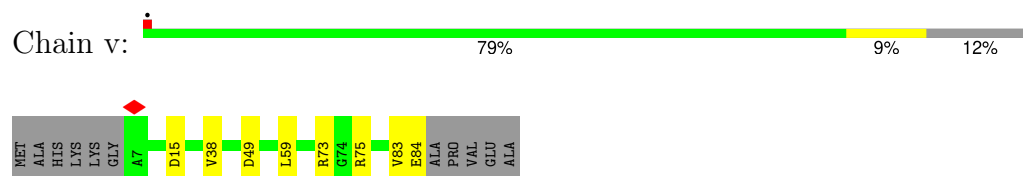
- Molecule 48: Large ribosomal subunit protein uL24



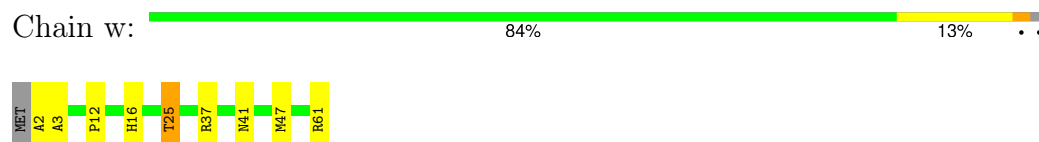
- Molecule 49: 50S ribosomal protein L25



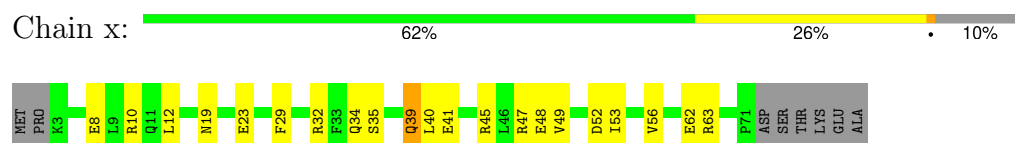
- Molecule 50: 50S ribosomal protein L27



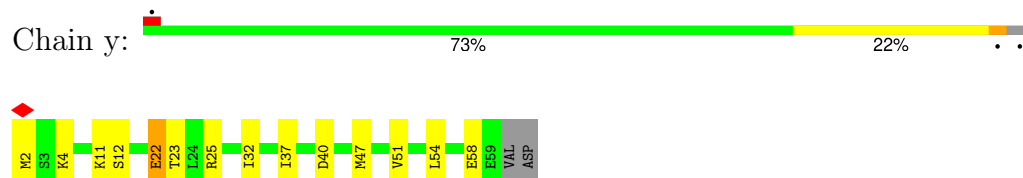
- Molecule 51: 50S ribosomal protein L28



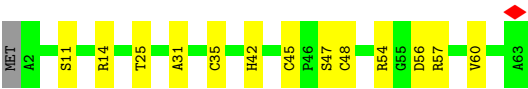
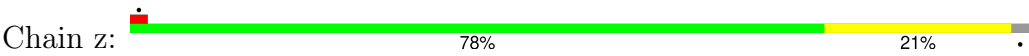
- Molecule 52: 50S ribosomal protein L29



- 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: OMC, 5MU, 3TD, UR3, 2MA, 2MG, 5MC, V7A, 4OC, H2U, MA6, PSU, OMU, MG, ZN, OMG, 4SU, G7M

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

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

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

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
30	a	2098	3TD	2	0
6	A	950	2MG	1	0
30	a	2631	H2U	1	0
6	A	1503	2MG	2	0
6	A	1505	MA6	1	0
6	A	1389	4OC	1	0
6	A	1506	MA6	2	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.

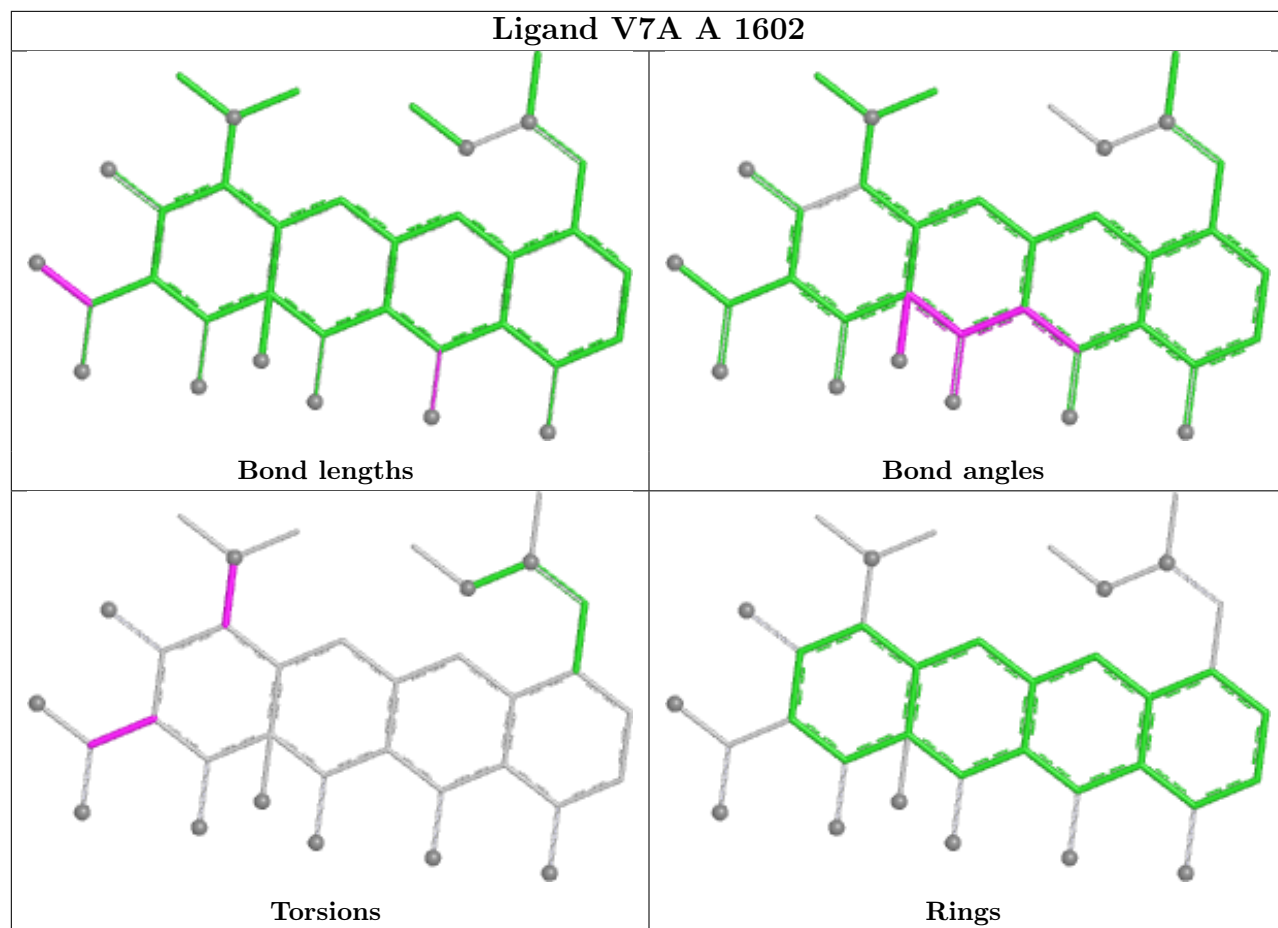
5 of 13 torsion outliers are listed below:

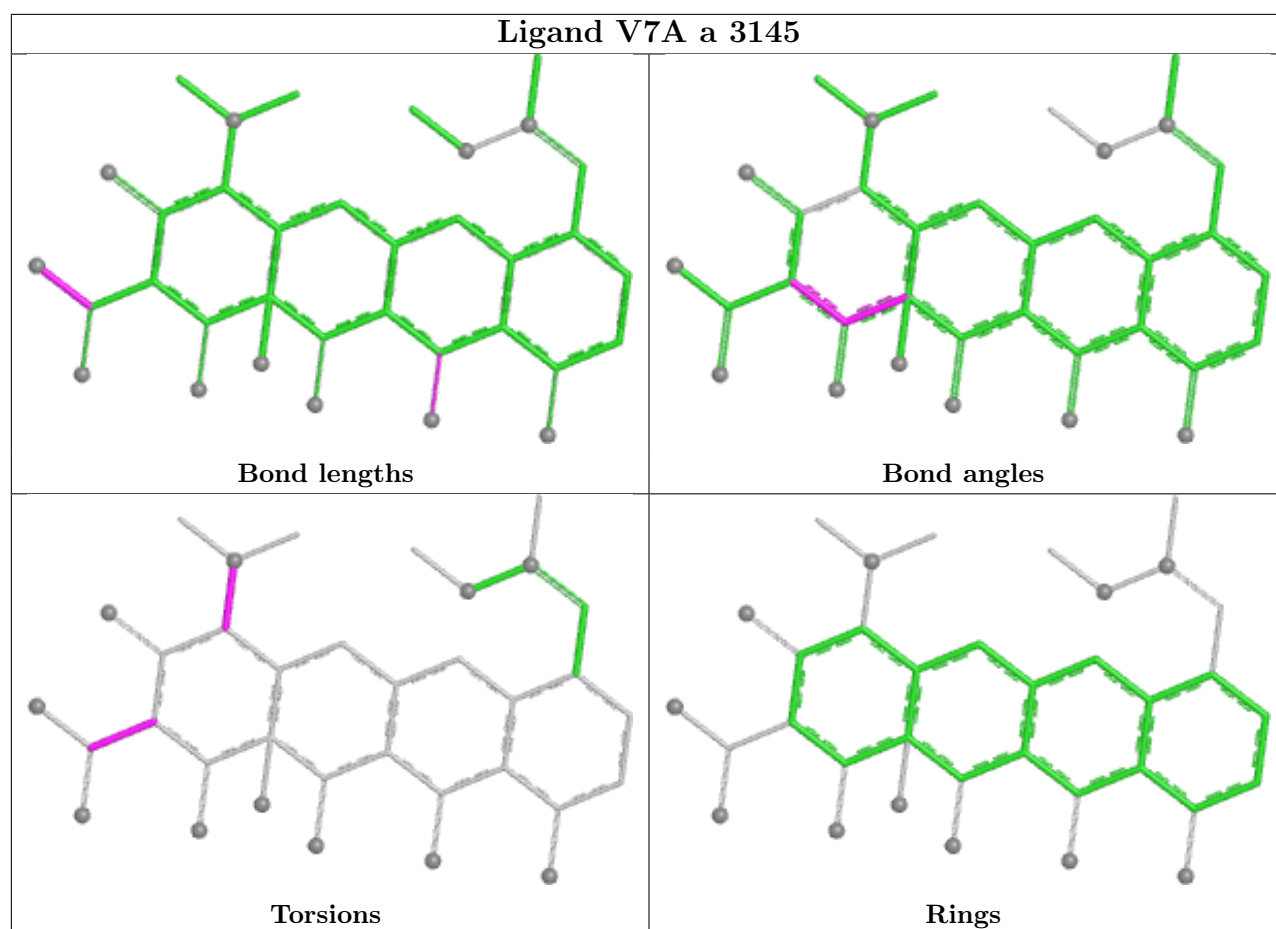
Mol	Chain	Res	Type	Atoms
57	A	1602	V7A	CAN-CAO-NBF-CBG
57	A	1602	V7A	CAP-CAQ-CBC-NBD
57	A	1602	V7A	CAP-CAQ-CBC-OBE
57	a	3145	V7A	CAR-CAO-NBF-CBG
57	a	3145	V7A	CAR-CAO-NBF-CBH

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.



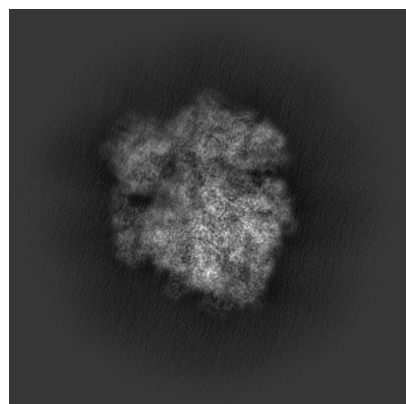
## 6 Map visualisation [i](#)

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.

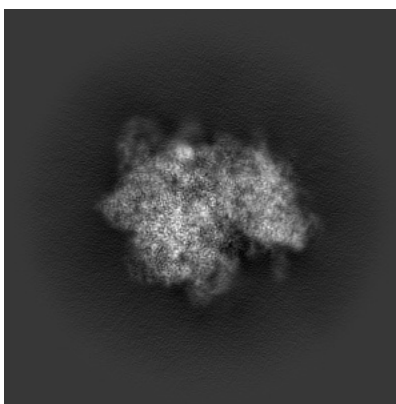
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

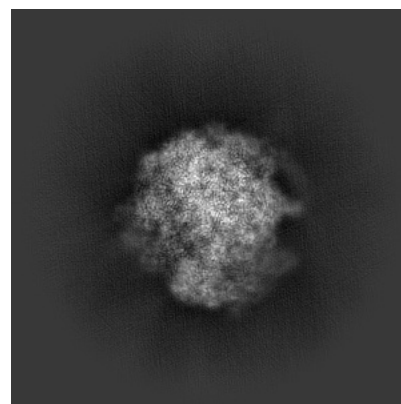
#### 6.1.1 Primary map



X

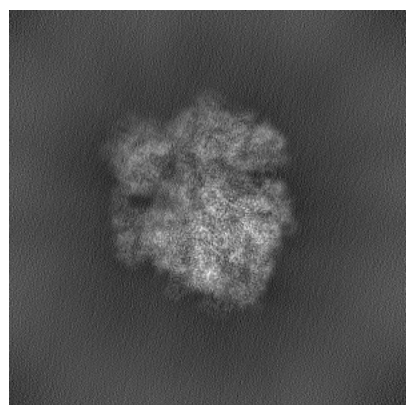


Y

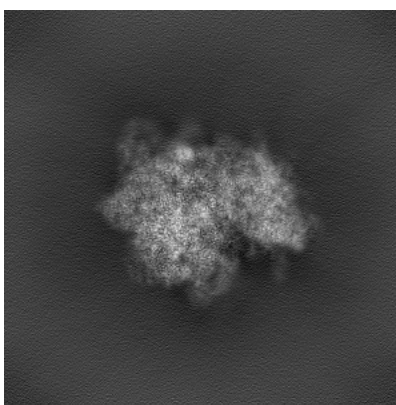


Z

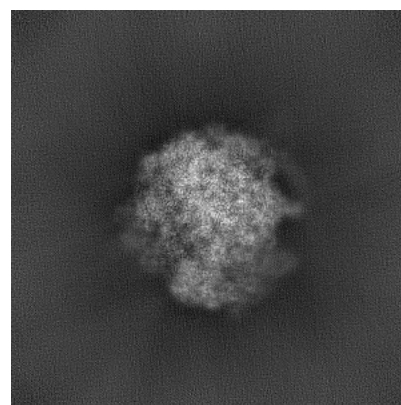
#### 6.1.2 Raw map



X



Y



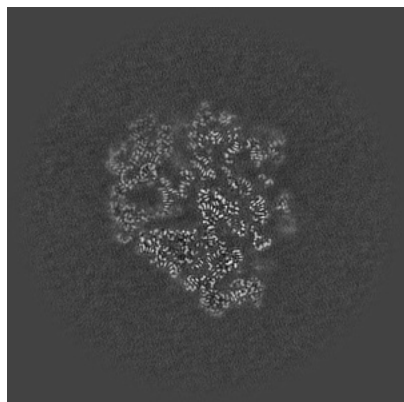
Z

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

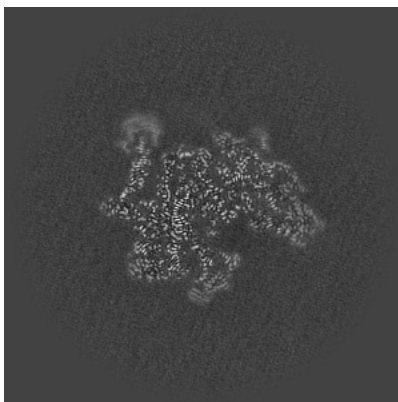


## 6.2 Central slices [i](#)

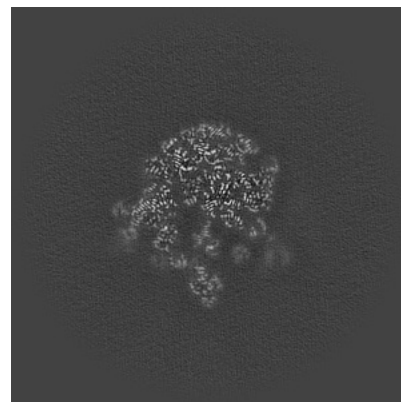
### 6.2.1 Primary map



X Index: 220

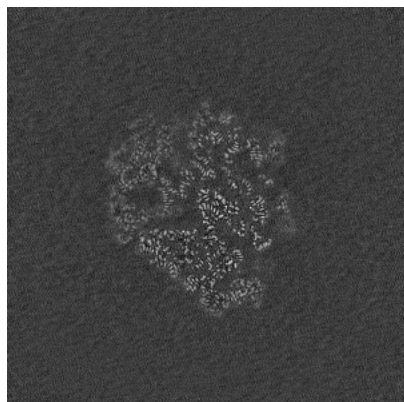


Y Index: 220

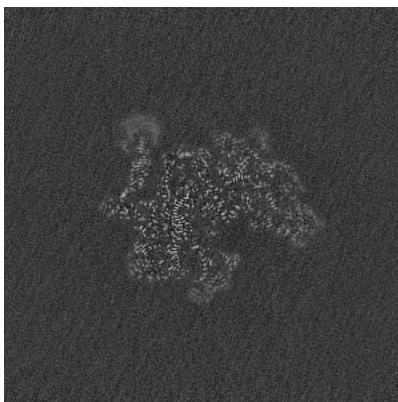


Z Index: 220

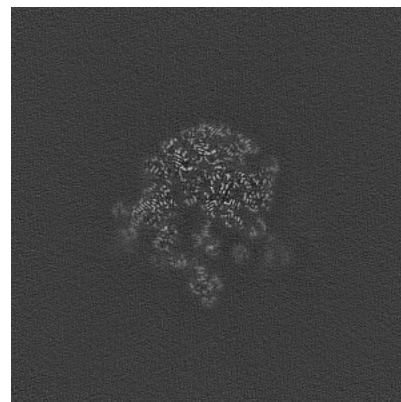
### 6.2.2 Raw map



X Index: 220



Y Index: 220

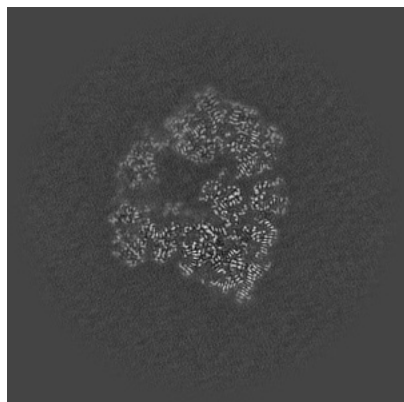


Z Index: 220

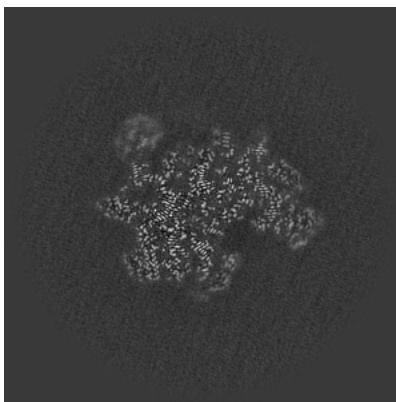
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

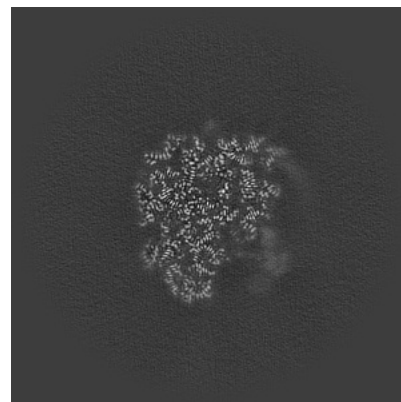
### 6.3.1 Primary map



X Index: 203

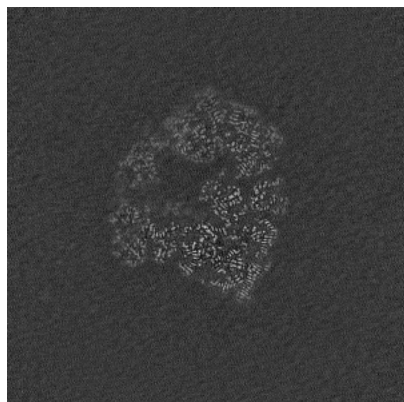


Y Index: 225

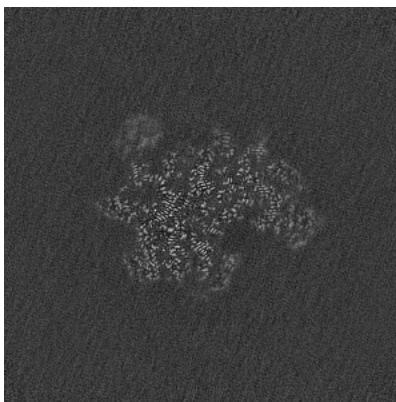


Z Index: 190

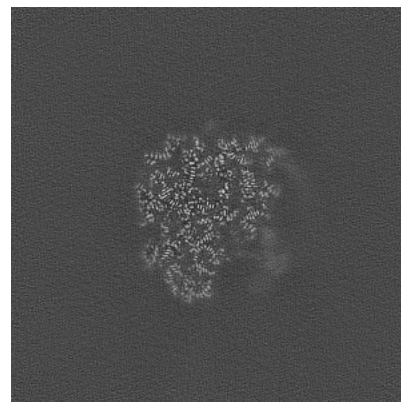
### 6.3.2 Raw map



X Index: 203



Y Index: 225

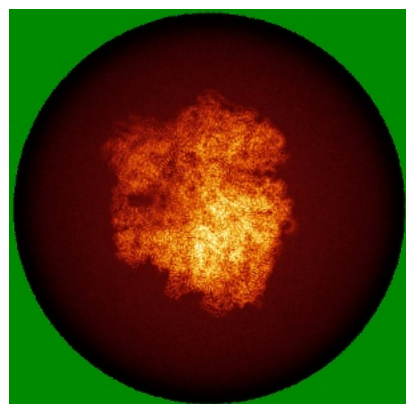


Z Index: 190

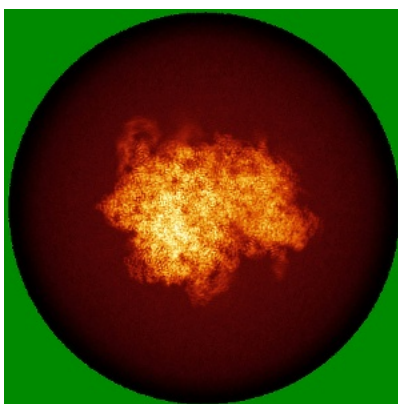
The images above show the largest variance slices of the map in three orthogonal directions.

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

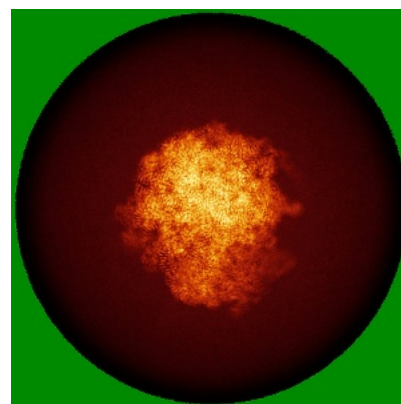
### 6.4.1 Primary map



X

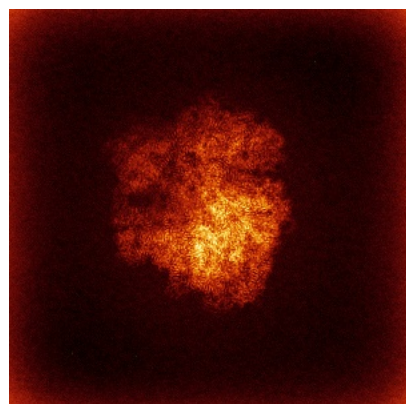


Y

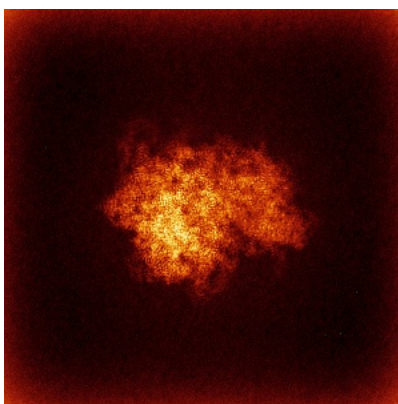


Z

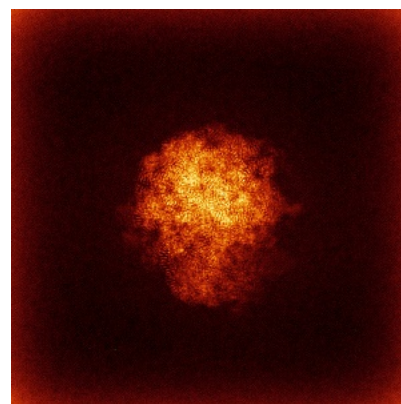
### 6.4.2 Raw map



X



Y



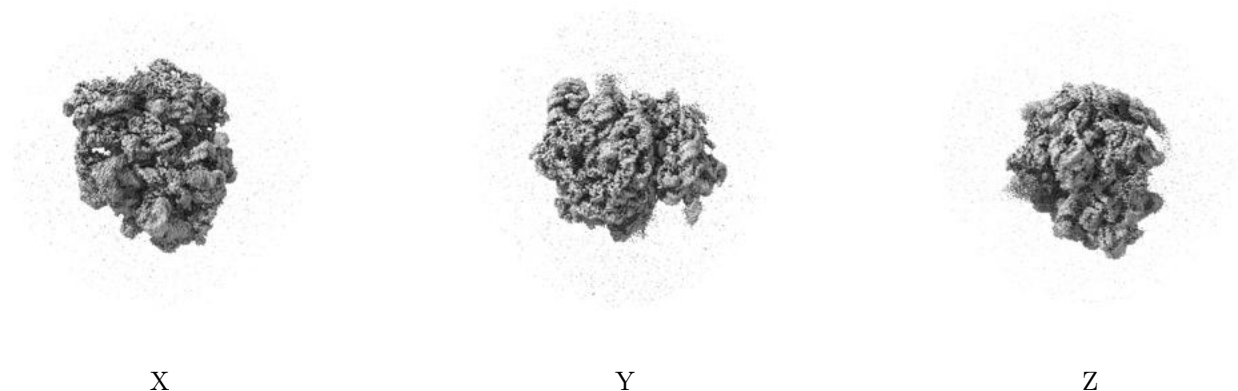
Z

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.



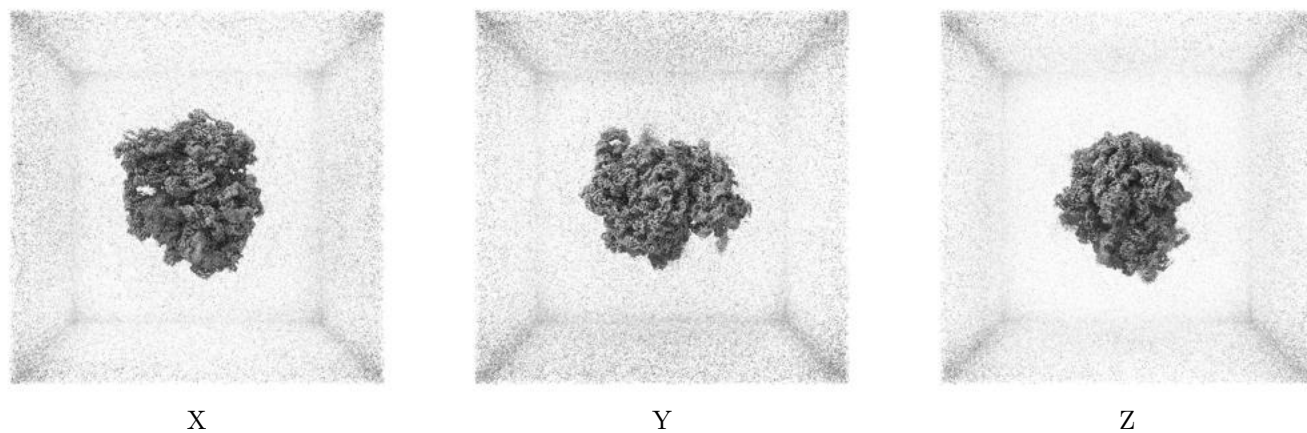
## 6.5 Orthogonal surface views [i](#)

### 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.

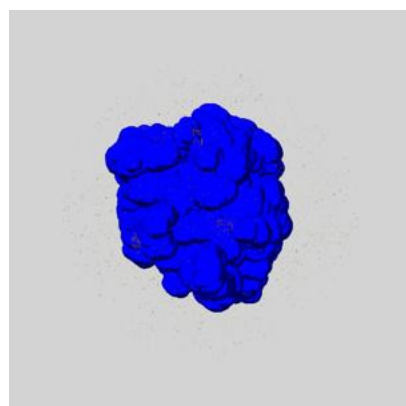
## 6.6 Mask visualisation [i](#)

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

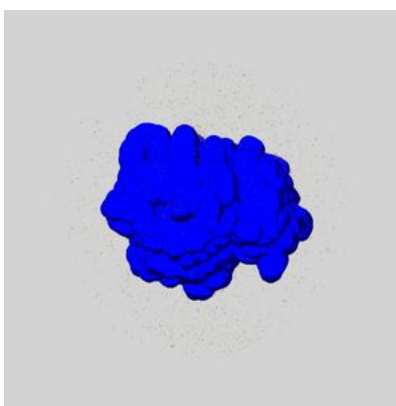
A mask typically either:

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

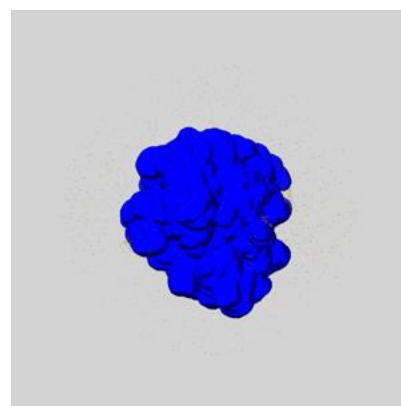
### 6.6.1 emd\_71683\_msk\_1.map [i](#)



X



Y

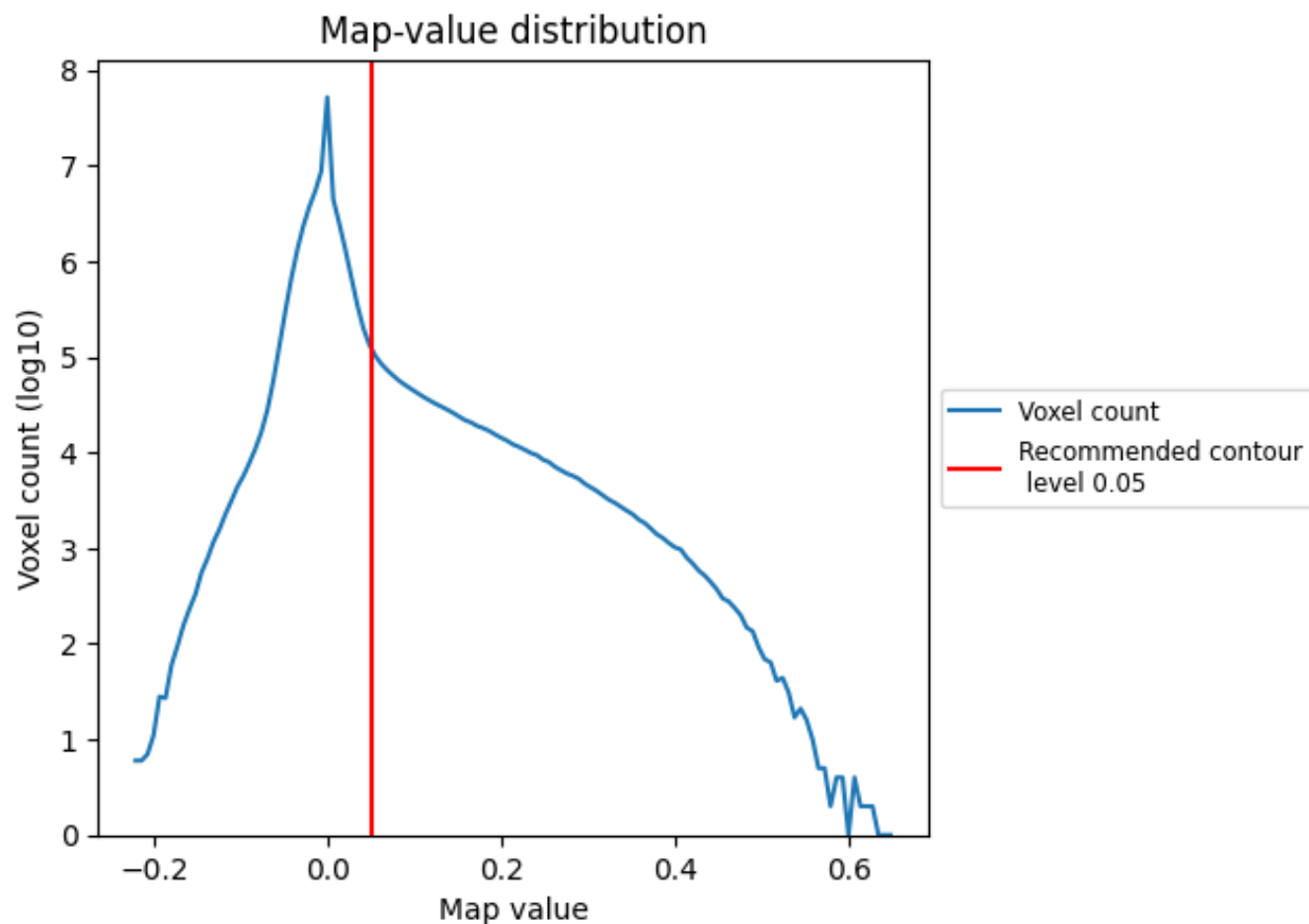


Z

## 7 Map analysis [i](#)

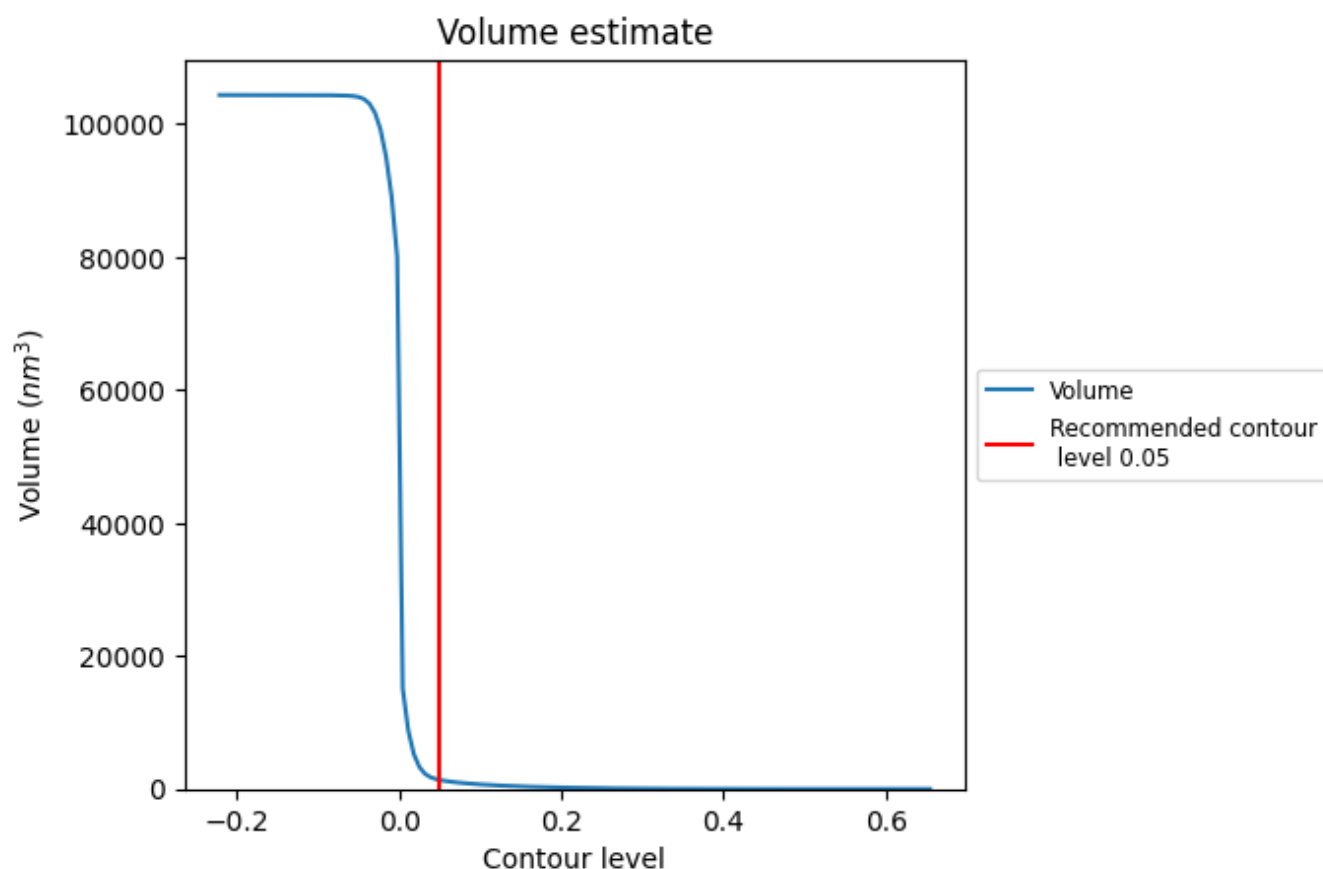
This section contains the results of statistical analysis of the map.

### 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.

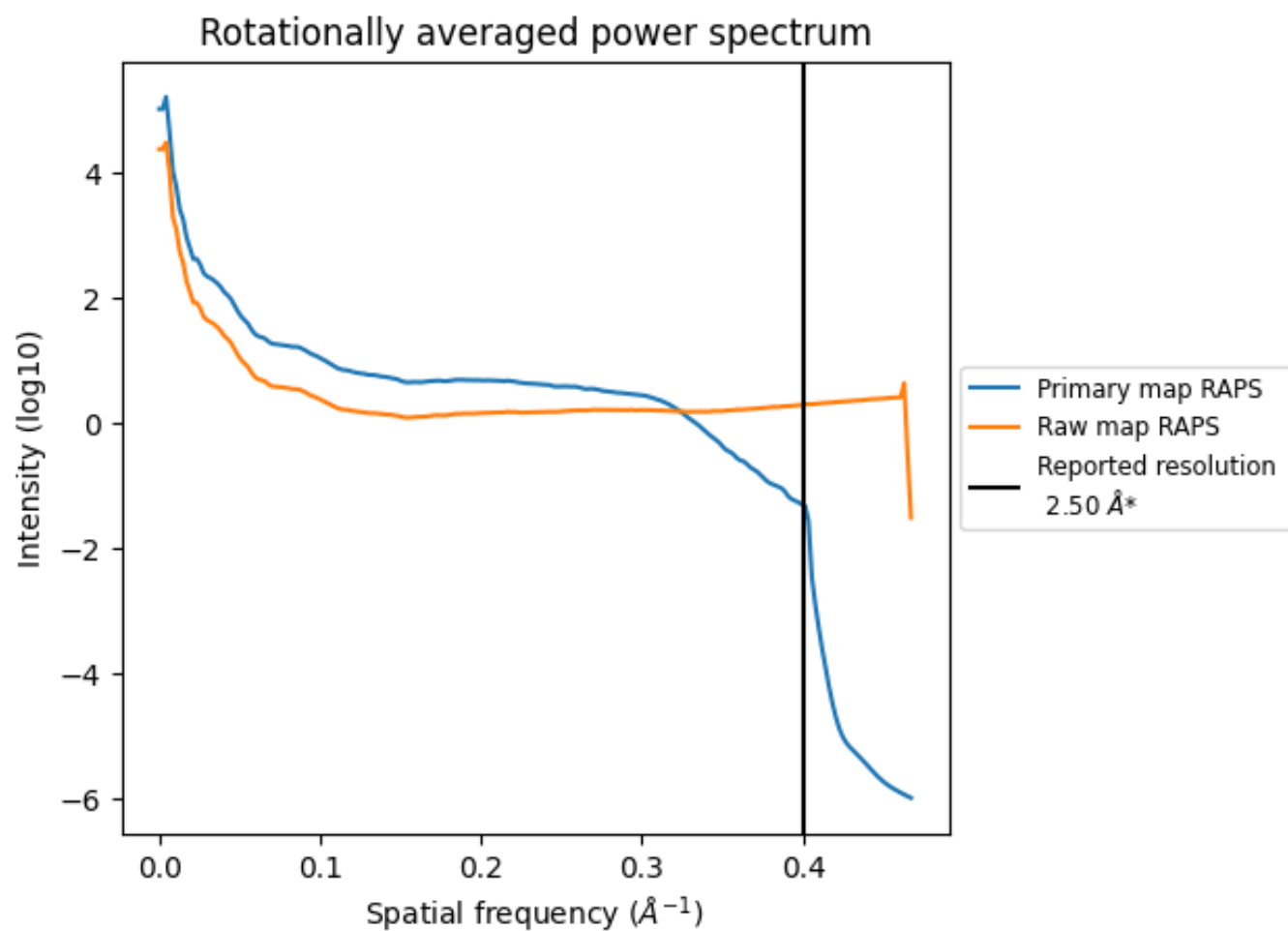
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1360  $\text{nm}^3$ ; 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 ⓘ



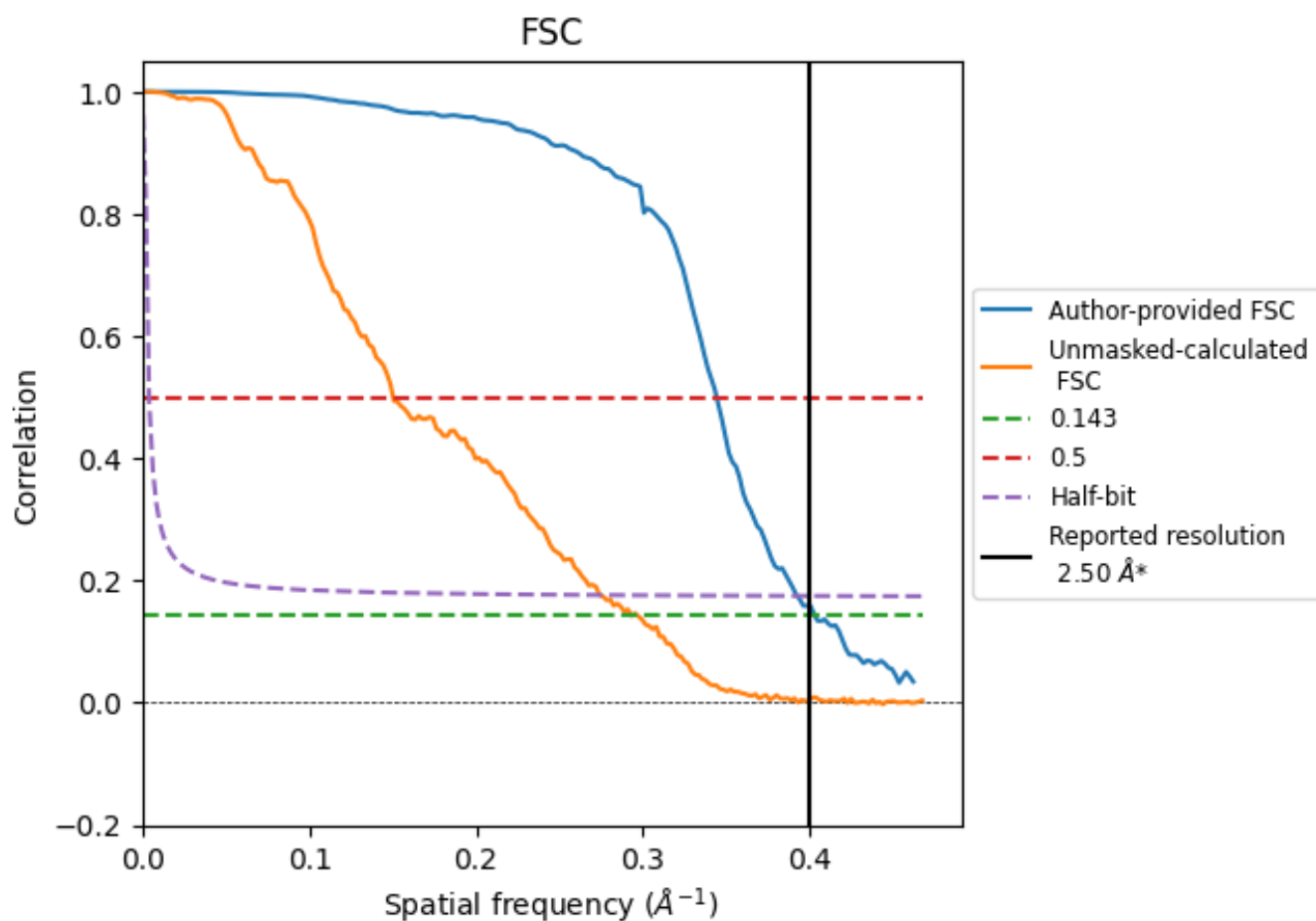
\*Reported resolution corresponds to spatial frequency of 0.400 Å<sup>-1</sup>



## 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  $\text{\AA}^{-1}$

## 8.2 Resolution estimates

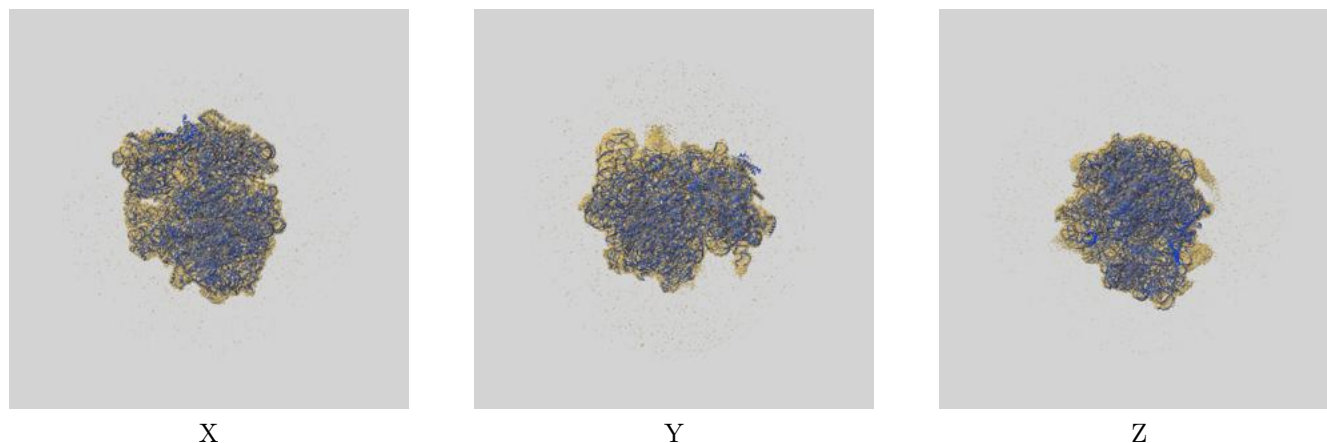
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.50	-	-
Author-provided FSC curve	2.48	2.91	2.55
Unmasked-calculated*	3.41	6.65	3.65

\*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](#)

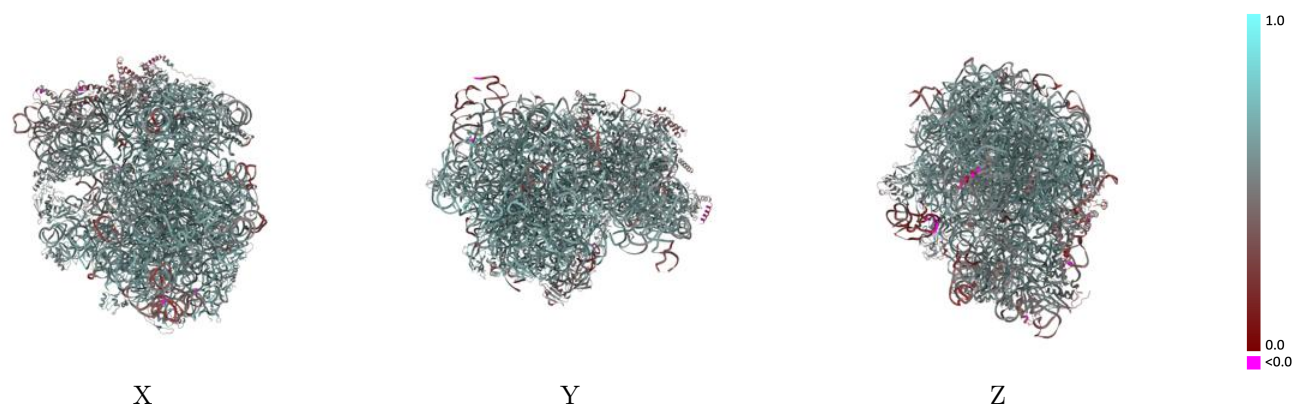
This section contains information regarding the fit between EMDB map EMD-71683 and PDB model 9PJ8. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

### 9.1 Map-model overlay [i](#)



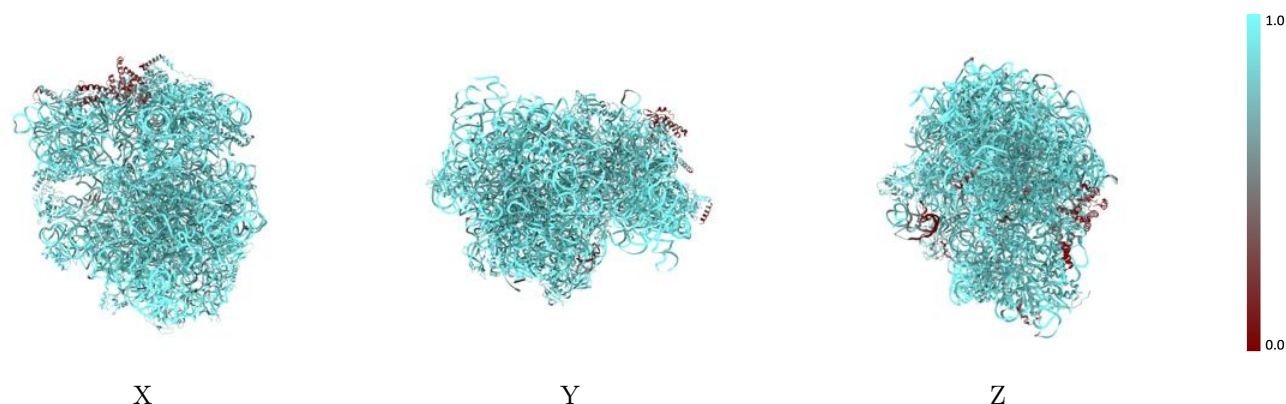
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



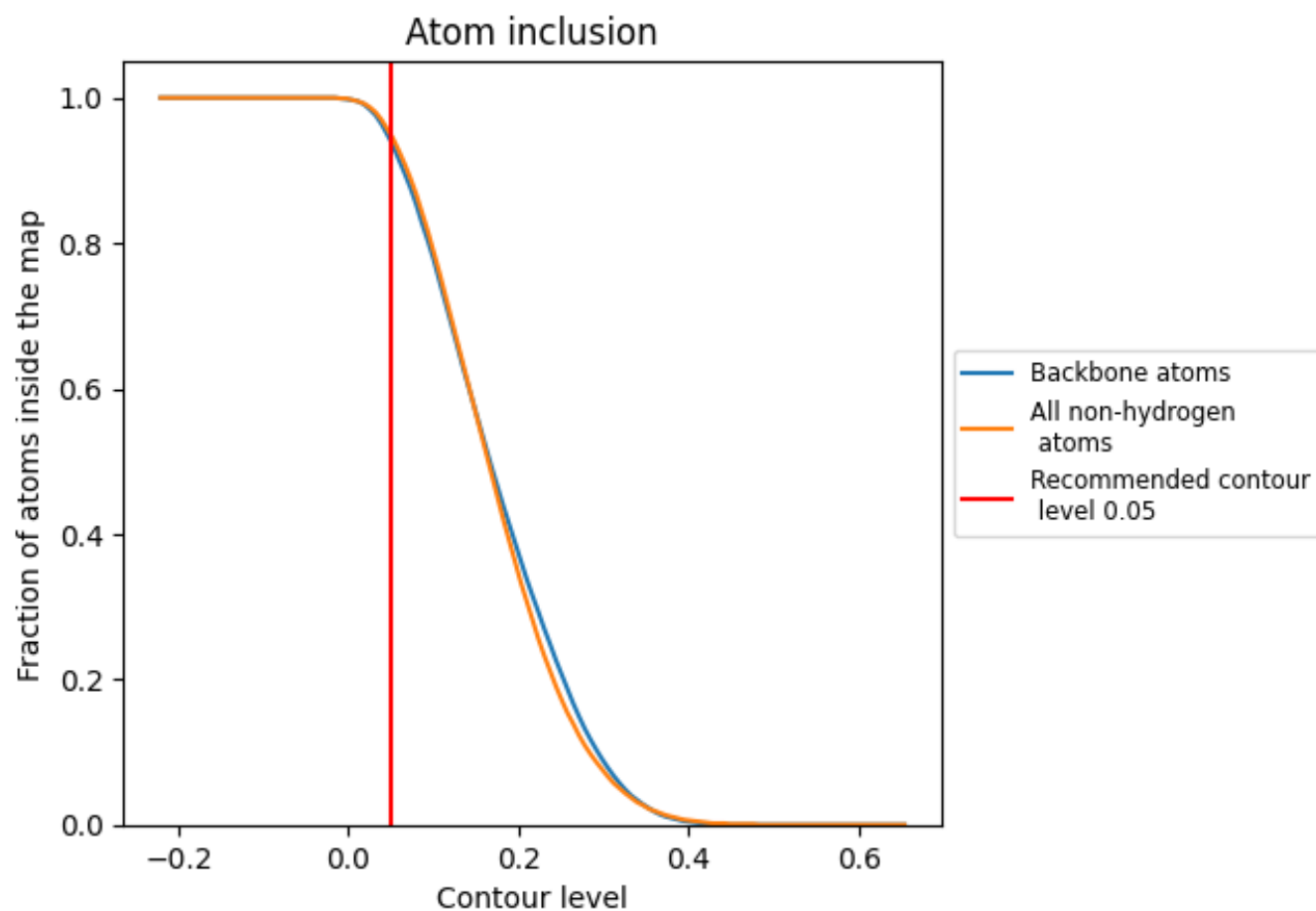
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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







































































## 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