



wwPDB EM Validation Summary Report ⓘ

Jun 26, 2026 – 06:59 AM EDT

PDB ID : 9PII / pdb_00009pii
EMDB ID : EMD-71668
Title : E. coli 70S ribosome bound to Sarecycline
Authors : Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on : 2025-07-10
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

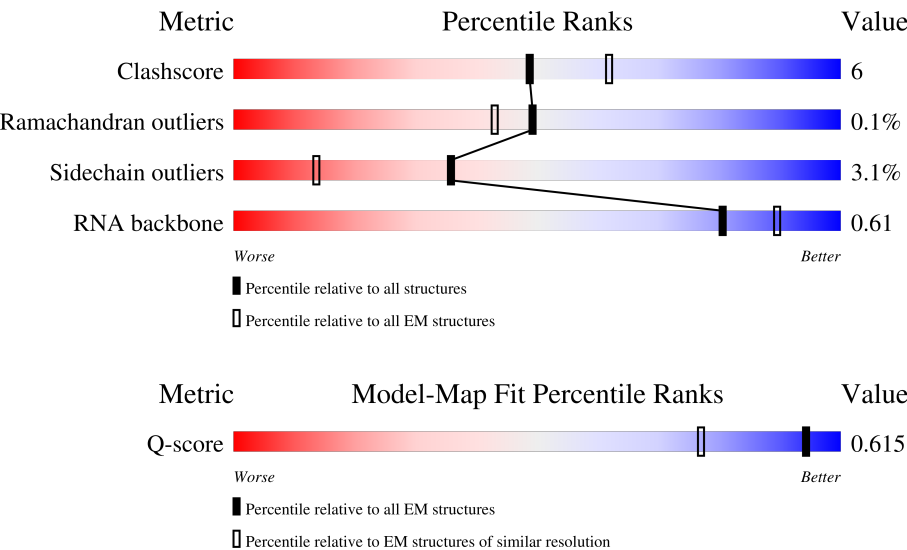
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 2.40 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.



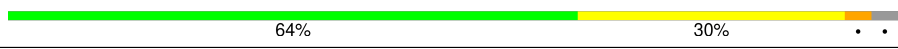
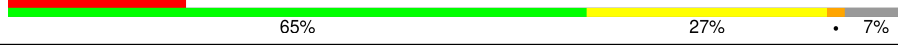
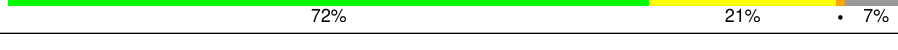
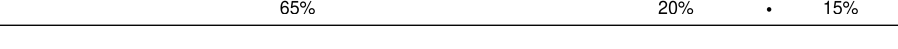
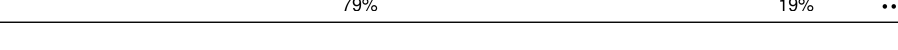
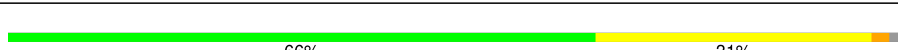
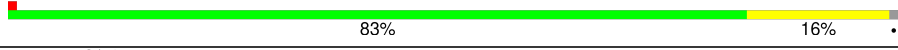
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	55	
2	1	46	
3	2	65	

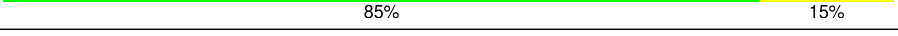
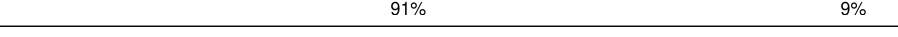
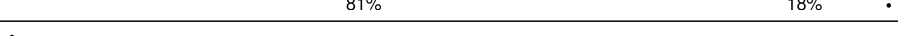
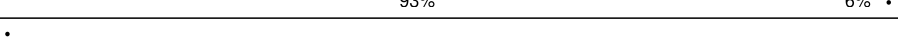
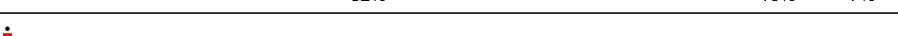
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	22	
28	Z	75	

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Mol	Chain	Length	Quality of chain
29	a	2904	
30	b	120	
31	c	273	
32	d	209	
33	e	201	
34	f	179	
35	g	177	
36	h	149	
37	i	142	
38	j	123	
39	k	144	
40	l	136	
41	m	127	
42	n	117	
43	o	115	
44	p	118	
45	q	103	
46	r	110	
47	s	100	
48	t	104	
49	u	94	
50	v	85	
51	w	78	
52	x	63	
53	y	59	

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Mol	Chain	Length	Quality of chain
54	z	57	 A horizontal bar chart showing the quality of chain 54. The bar is green for 93% and yellow for 5%. A small red square is at the start, and a small black dot is at the end. The text '93%' is centered below the green portion, and '5%' is centered below the yellow portion.

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 141212 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	51	Total	C	N	O	0	0
			417	269	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1500	Total	C	N	O	P	0	0
			32211	14373	5919	10419	1500		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- 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
			877	540	174	160	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 27 is a RNA chain called mRNA.

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

- Molecule 28 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	75	Total	C	N	O	P	S	
			1605	716	291	522	75	1	
								0	0

- Molecule 29 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2753	Total	C	N	O	P		
			59130	26384	10897	19096	2753		
								0	0

- Molecule 30 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	119	Total	C	N	O	P		
			2549	1135	466	829	119		
								0	0

- Molecule 31 is a protein called 50S ribosomal protein L2.

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

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	209	Total	C	N	O	S		
			1566	980	288	294	4		
								0	0

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 37 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	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
			1075	686	205	178	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 42 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

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

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

- Molecule 45 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

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

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called Large ribosomal subunit protein bL25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

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

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- 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
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

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

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	Zn	0
			1	1	

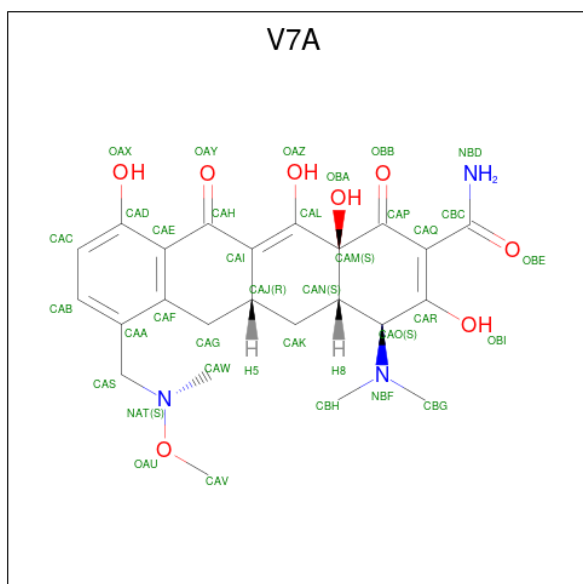
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	62	Total	Mg	0
			62	62	
56	a	211	Total	Mg	0
			211	211	
56	b	5	Total	Mg	0
			5	5	
56	m	1	Total	Mg	0
			1	1	
56	p	2	Total	Mg	0
			2	2	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	24	Total	K	0
			24	24	
57	a	75	Total	K	0
			75	75	
57	b	1	Total	K	0
			1	1	

- Molecule 58 is Sarecycline (CCD ID: V7A) (formula: C₂₄H₂₉N₃O₈) (labeled as "Ligand of Interest" by depositor).



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

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

- Molecule 59 is water.

Mol	Chain	Residues	Atoms				AltConf
59	0	1	Total	O			0
			1	1			
59	1	3	Total	O			0
			3	3			
59	2	3	Total	O			0
			3	3			
59	3	1	Total	O			0
			1	1			
59	A	123	Total	O			0
			123	123			
59	O	1	Total	O			0
			1	1			
59	U	1	Total	O			0
			1	1			
59	a	1091	Total	O			0
			1091	1091			
59	b	14	Total	O			0
			14	14			
59	c	6	Total	O			0
			6	6			
59	d	5	Total	O			0
			5	5			
59	e	5	Total	O			0
			5	5			
59	i	2	Total	O			0
			2	2			
59	k	2	Total	O			0
			2	2			
59	l	1	Total	O			0
			1	1			
59	m	5	Total	O			0
			5	5			
59	o	1	Total	O			0
			1	1			
59	p	4	Total	O			0
			4	4			

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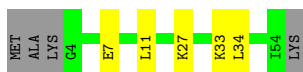
Mol	Chain	Residues	Atoms		AltConf
59	q	7	Total 7	O 7	0
59	r	2	Total 2	O 2	0
59	s	2	Total 2	O 2	0
59	v	1	Total 1	O 1	0
59	y	2	Total 2	O 2	0
59	z	3	Total 3	O 3	0

3 Residue-property plots [i](#)

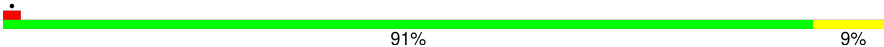
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain 0: 



- Molecule 2: 50S ribosomal protein L34

Chain 1: 



- Molecule 3: 50S ribosomal protein L35

Chain 2: 



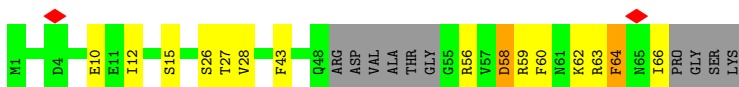
- Molecule 4: 50S ribosomal protein L36

Chain 3: 



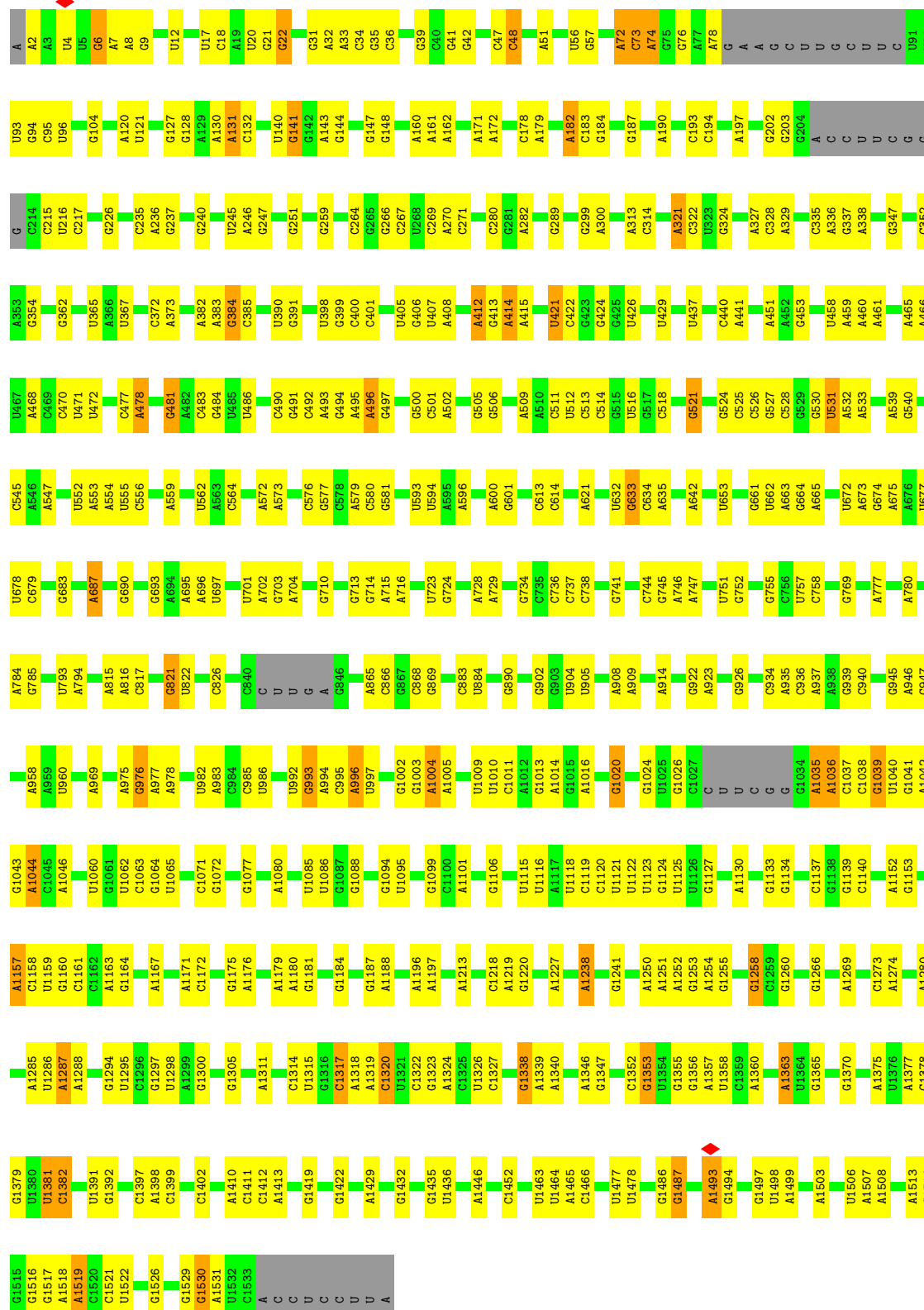
- Molecule 5: 50S ribosomal protein L31

Chain 4: 

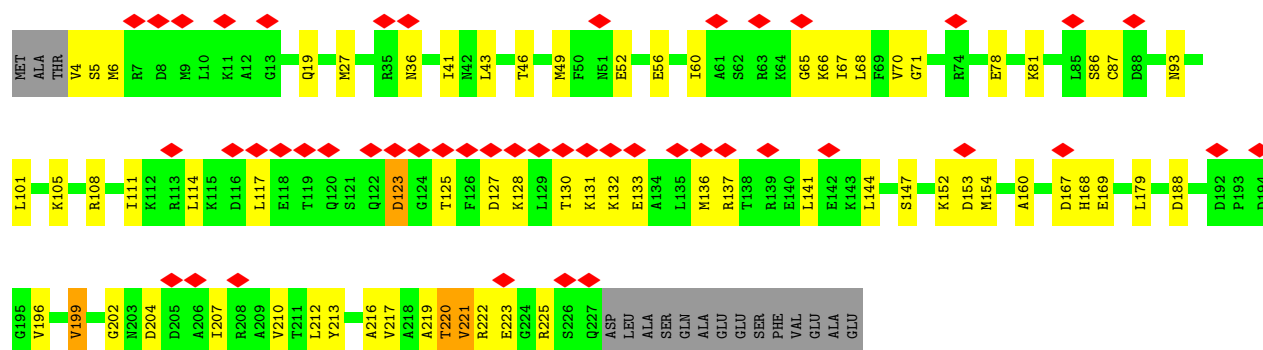


- Molecule 6: 16S rRNA

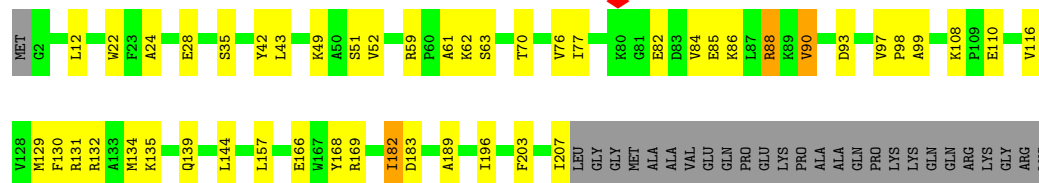
Chain A:  64% 30%



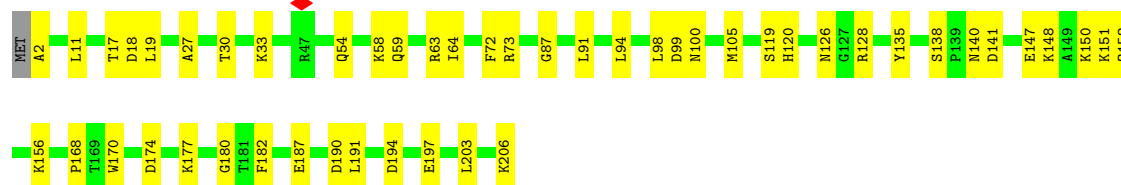
• Molecule 7: 30S ribosomal protein S2



- Molecule 8: Small ribosomal subunit protein uS3



- Molecule 9: Small ribosomal subunit protein uS4

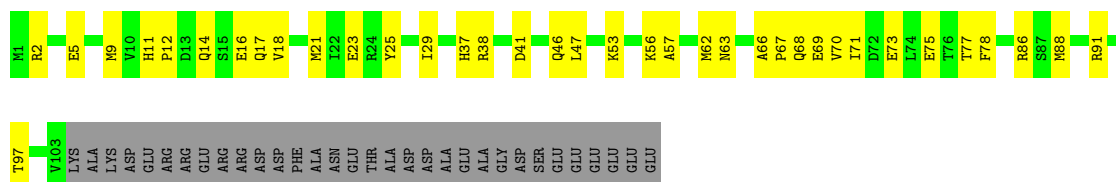


- Molecule 10: Small ribosomal subunit protein uS5

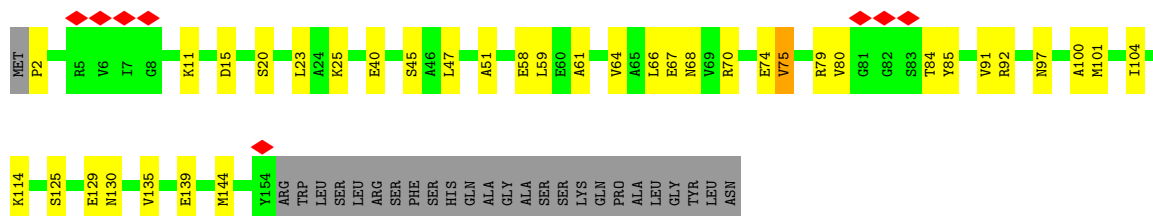


- Molecule 11: Small ribosomal subunit protein bS6

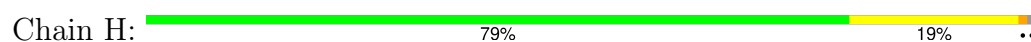




- Molecule 12: Small ribosomal subunit protein uS7



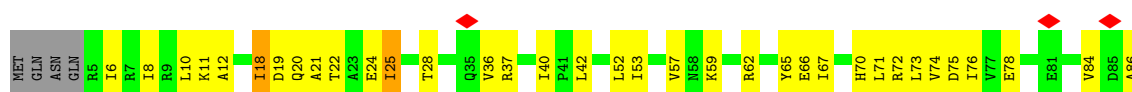
- Molecule 13: Small ribosomal subunit protein uS8



- Molecule 14: Small ribosomal subunit protein uS9

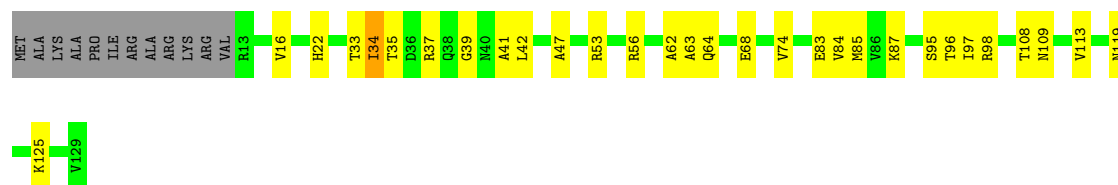


- Molecule 15: Small ribosomal subunit protein uS10

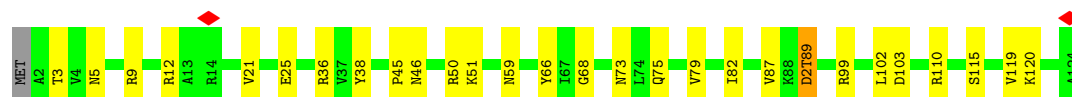
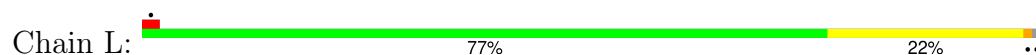


- Molecule 16: 30S ribosomal protein S11

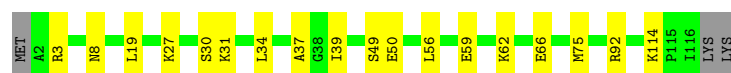
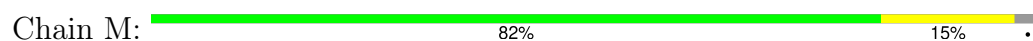




- Molecule 17: Small ribosomal subunit protein uS12



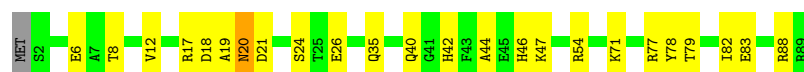
- Molecule 18: Small ribosomal subunit protein uS13



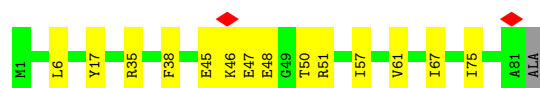
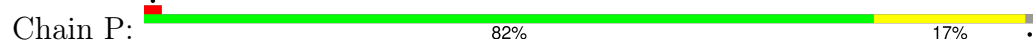
- Molecule 19: Small ribosomal subunit protein uS14



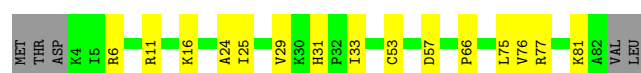
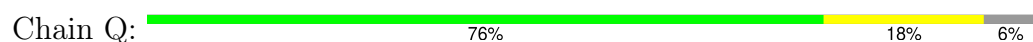
- Molecule 20: Small ribosomal subunit protein uS15



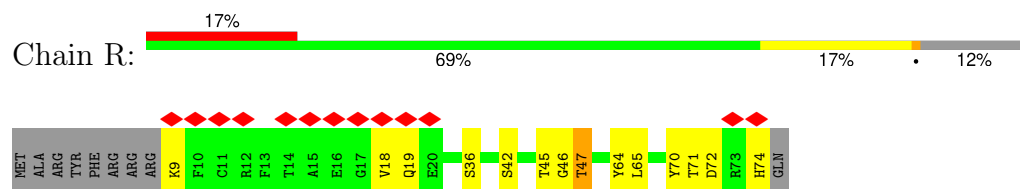
- Molecule 21: Small ribosomal subunit protein bS16



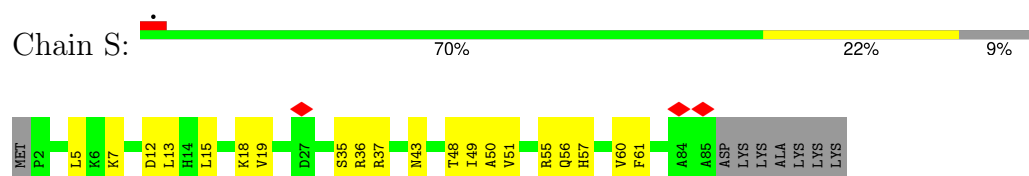
- Molecule 22: Small ribosomal subunit protein uS17



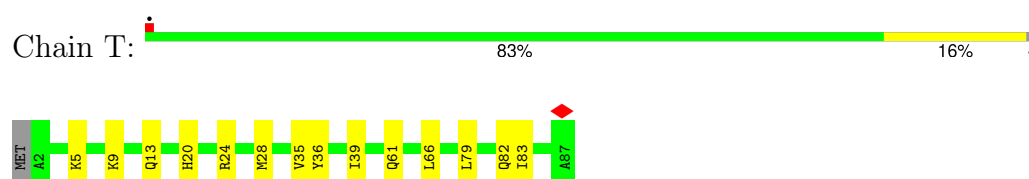
- Molecule 23: Small ribosomal subunit protein bS18



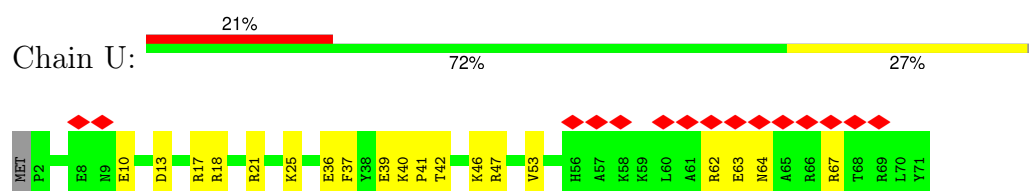
- Molecule 24: Small ribosomal subunit protein uS19



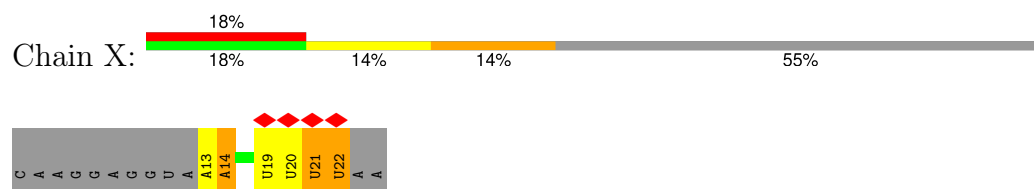
- Molecule 25: Small ribosomal subunit protein bS20



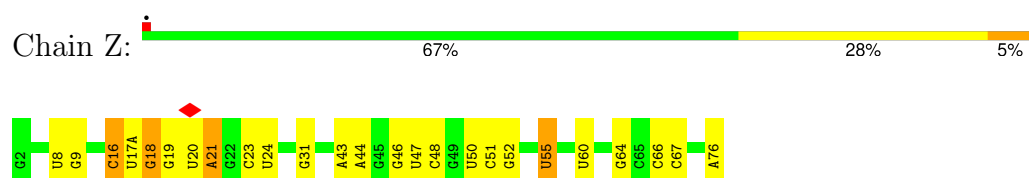
- Molecule 26: Small ribosomal subunit protein bS21



- Molecule 27: mRNA



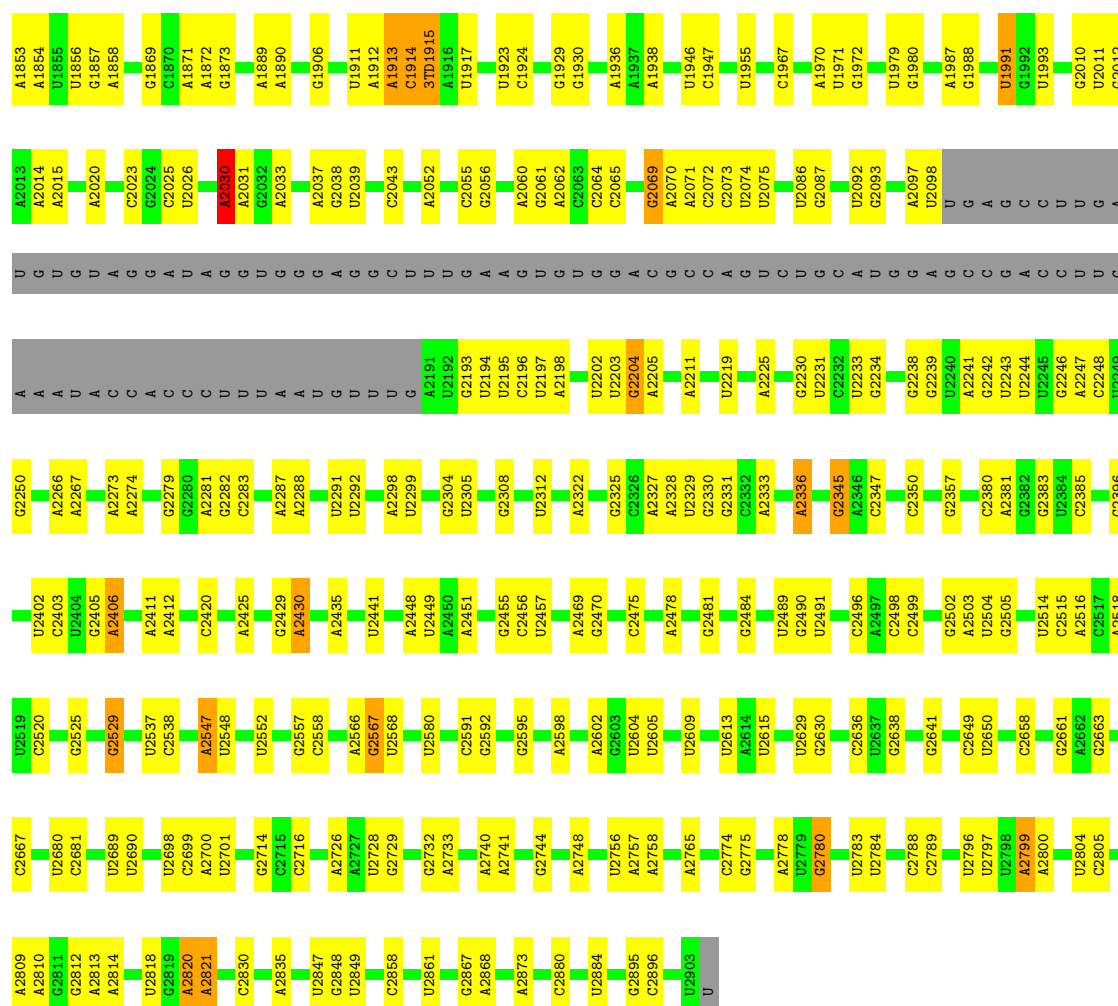
- Molecule 28: P-site tRNA



- Molecule 29: 23S rRNA

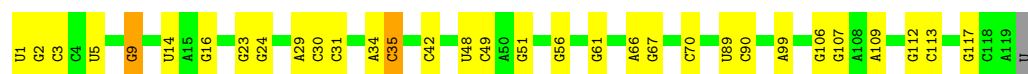


G1703	G1704	A1705	G1710	G1715	U1720	G1721	C1727	C1728	U1729	C1730	G1731	G1732	G1733	G1734	U1735	U1736	U1599	G1737	G1738	A1746	U1747	C1748	U1751	C1752	C1764	A1773	A1786	C1790	A1791	A1794	C1795	U1796	G1797	C1800	A1801	A1802	A1803	G1807	A1808	A1809	C1816	A1829	A1848				
U1570	A1571	G1572	G1573	U1578	A1583	U1584	C1585	A1586	A1590	A1591	U1594	C1595	A1596	A1597	U1598	U1599	C1600	C1607	A1608	A1609	A1614	A1618	U1636	A1637	A1641	G1642	U1647	U1648	A1654	A1655	C1656	U1657	G1667	G1674	A1677	A1678	U1680	G1681	G1682	U1683	U1563	C1564	A1566	A1569			
A1434	G1435	G1441	U1442	U1443	U1444	G1445	C1447	G1448	G1452	A1469	A1470	G1482	U1485	U1486	U1487	C1493	A1494	A1495	U1496	U1497	C1498	U1506	C1507	A1508	U1509	G1510	A1515	G1524	G1527	U1534	A1535	C1536	G1537	U1542	G1543	A1544	A1548	A1549	U1563	C1564	A1566	A1569					
G1281	U1282	G1283	G1292	C1293	G1300	A1301	A1321	U1326	A1327	A1328	U1329	U1340	U1352	A1353	A1354	C1357	G1358	G1361	C1362	A1365	A1378	U1379	G1380	A1383	C1386	A1387	G1388	A1392	A1393	U1394	A1395	U1405	U1406	G1410	U1411	G1416	U1428	G1429	G1430	A1431	G1432	A1433					
G1131	U1132	A1133	C1135	U1141	A1142	G1149	C1150	G1168	A1169	C1172	U1177	A1178	U1180	U1181	G1182	U1183	U1184	U1188	G1197	U1198	U1199	C1200	G1212	G1225	A1226	G1236	G1248	U1249	G1250	A1253	G1256	G1266	G1271	U1272	U1273	C1278	G1279	G1280									
U	U	G	C	U	A	G	A	C	A	C	U	A	U	A	A	G	A	A	A	C	U	G	A	A	U	C	U	C	A	C	U	G	G1107	U1108	C1109	G1110	A1111	G1112	G1115	G1116	G1128	A1129	U1130				
G904	A910	A911	G930	U931	C946	U955	A959	A960	C961	C964	G969	U970	A973	G974	C981	A983	A984	G993	A996	A1000	A1001	A1009	U1012	C1013	A1014	G1026	A1027	A1028	A1029	U1033	C1045	A1046	G1047	A1048	C1052	C	A	G	A	U	G						
G805	C806	U807	C812	U813	C814	U827	U828	U832	A833	G834	U839	C840	U846	U847	C848	A849	U850	C851	U852	G856	G857	G858	G859	G869	U870	U871	U872	C876	A877	A878	G880	G881	G882	C885	C888	C889	C890	G891	A892	C893	U894	U895	A896	C897	C898	A899	C903
U658	U667	A668	G669	A670	G682	A685	U686	A693	U694	G708	U709	U710	A716	U720	A721	U722	C723	U724	G729	A730	A739	C740	A742	U744	G745	U746	U747	A752	A753	U754	U755	A756	G757	A764	A782	A783	U784	G785	C796	G797							
G548	G549	C550	A563	U568	U569	G570	U573	A574	A575	G579	U580	A582	G583	U588	U589	U593	U594	C595	U596	G597	U598	A599	A603	A608	A609	A614	U615	A627	A632	A633	C634	C635	G636	A637	G638	U639	C640	A644	C645	U646	G647	A654	G655	G656	U657		
G411	C414	A415	U419	C420	G425	C445	C446	C475	G476	A479	A480	G481	G491	A492	G493	G494	G495	U499	G500	A503	A504	A505	A508	C509	A510	U511	G512	G518	U519	A522	C523	A529	G530	C531	A532	G533	U534	A538	C542	G543	C544	U545	U546	A547			
A272	G273	A278	U280	C281	U284	G285	U287	U288	G289	U296	C297	G298	A299	C302	G303	U304	C305	U306	G307	G308	A309	A310	A311	G319	G329	A330	A347	A348	C353	G356	G359	U360	A361	G362	G363	C364	U365	C366	G367	G386	G396	U397	U405				
U120	A126	G136	U137	U138	U139	C140	A142	A146	C147	U150	C151	A152	A155	A156	C157	U158	G163	A172	A173	A181	A182	C183	G189	A190	A191	C192	A196	A197	A199	C210	G215	G216	A219	A222	A233	U234	G248	G249	A251								



• Molecule 30: 5S rRNA

Chain b: 72% 25%



• Molecule 31: 50S ribosomal protein L2

Chain c: 89% 11%



• Molecule 32: 50S ribosomal protein L3

Chain d: 85% 15%

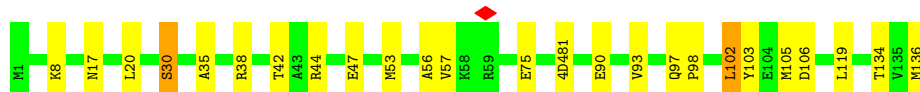
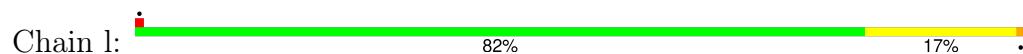




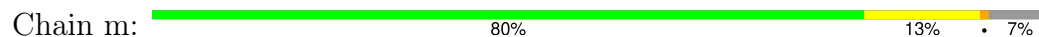
- Molecule 39: Large ribosomal subunit protein uL15



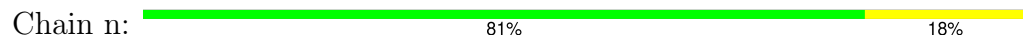
- Molecule 40: 50S ribosomal protein L16



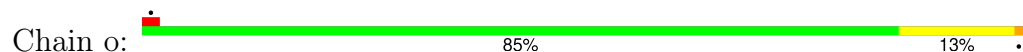
- Molecule 41: Large ribosomal subunit protein bL17



- Molecule 42: Large ribosomal subunit protein uL18



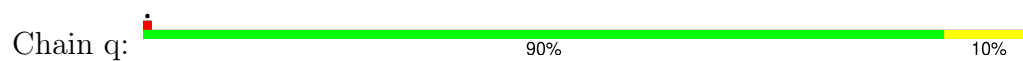
- Molecule 43: Large ribosomal subunit protein bL19



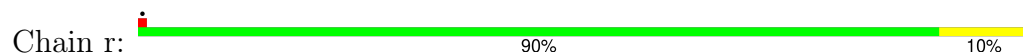
- Molecule 44: 50S ribosomal protein L20



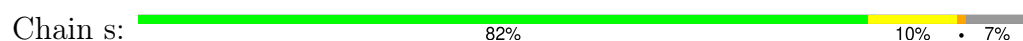
- Molecule 45: Ribosomal protein L21



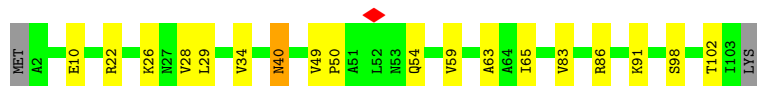
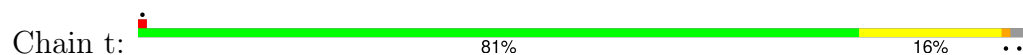
- Molecule 46: 50S ribosomal protein L22



- Molecule 47: 50S ribosomal protein L23



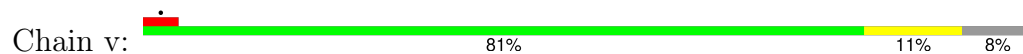
- Molecule 48: 50S ribosomal protein L24



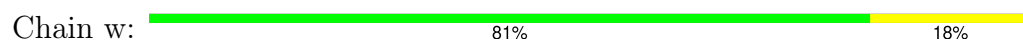
- Molecule 49: Large ribosomal subunit protein bL25



- Molecule 50: 50S ribosomal protein L27

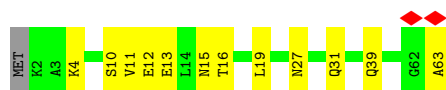


- Molecule 51: 50S ribosomal protein L28



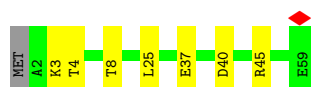
- Molecule 52: Large ribosomal subunit protein uL29

Chain x:  79% 19%



- Molecule 53: 50S ribosomal protein L30

Chain y:  86% 12%



- Molecule 54: 50S ribosomal protein L32

Chain z:  93% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	234706	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	0.743	Depositor
Minimum map value	-0.230	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.07	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: D2T, K, MG, 4OC, H2U, OMU, OMC, V7A, ZN, 2MA, PSU, 5MC, 1MG, G7M, UR3, MA6, 4D4, 4SU, OMG, 5MU, MEQ, 6MZ, 2MG, 3TD

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	0.20	0/424	0.38	0/565
2	1	0.24	0/380	0.29	0/498
3	2	0.22	0/513	0.29	0/676
4	3	0.22	0/303	0.25	0/397
5	4	0.17	0/488	0.38	0/649
6	A	0.22	0/35787	0.28	0/55816
7	B	0.16	0/1784	0.39	0/2403
8	C	0.16	0/1651	0.32	0/2225
9	D	0.16	0/1665	0.27	0/2227
10	E	0.20	0/1165	0.35	0/1568
11	F	0.22	0/858	0.44	0/1160
12	G	0.17	0/1219	0.34	0/1635
13	H	0.20	0/989	0.38	0/1326
14	I	0.17	0/1034	0.36	0/1375
15	J	0.21	0/796	0.47	0/1077
16	K	0.19	0/893	0.34	0/1205
17	L	0.24	0/960	0.40	0/1286
18	M	0.18	0/900	0.38	0/1204
19	N	0.28	0/817	0.48	0/1088
20	O	0.20	0/722	0.39	0/964
21	P	0.19	0/653	0.35	0/877
22	Q	0.18	0/650	0.32	0/871
23	R	0.19	0/553	0.34	0/742
24	S	0.18	0/685	0.39	0/922
25	T	0.21	0/676	0.33	0/895
26	U	0.15	0/597	0.29	0/792
27	X	0.17	0/235	0.24	0/363
28	Z	0.23	0/1703	0.32	0/2655
29	a	0.29	0/65651	0.33	0/102413
30	b	0.21	0/2850	0.24	0/4444
31	c	0.26	0/2121	0.37	1/2852 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	d	0.23	0/1576	0.30	0/2119
33	e	0.21	0/1571	0.29	0/2113
34	f	0.16	0/1434	0.31	0/1926
35	g	0.23	0/1343	0.44	0/1816
36	h	0.18	0/306	0.53	0/413
37	i	0.22	0/1152	0.31	0/1551
38	j	0.23	0/955	0.31	0/1279
39	k	0.21	0/1062	0.27	0/1413
40	l	0.25	0/1081	0.36	0/1443
41	m	0.24	0/958	0.35	0/1281
42	n	0.18	0/902	0.33	0/1209
43	o	0.23	0/929	0.34	0/1242
44	p	0.24	0/960	0.30	0/1278
45	q	0.24	0/829	0.47	0/1107
46	r	0.22	0/864	0.33	0/1156
47	s	0.22	0/744	0.42	0/994
48	t	0.21	0/787	0.42	0/1051
49	u	0.20	0/766	0.32	0/1025
50	v	0.21	0/593	0.29	0/785
51	w	0.23	0/635	0.29	0/848
52	x	0.23	0/502	0.49	0/667
53	y	0.20	0/453	0.30	0/605
54	z	0.22	0/450	0.31	0/599
All	All	0.25	0/150574	0.32	1/225090 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	146	MET	N-CA-C	-5.39	107.25	113.88

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	417	0	451	3	0
2	1	377	0	418	3	0
3	2	504	0	572	8	0
4	3	302	0	340	3	0
5	4	480	0	482	11	0
6	A	32211	0	16225	283	0
7	B	1753	0	1780	42	0
8	C	1624	0	1696	34	0
9	D	1643	0	1707	29	0
10	E	1152	0	1196	24	0
11	F	839	0	833	29	0
12	G	1203	0	1254	28	0
13	H	979	0	1031	14	0
14	I	1022	0	1070	30	0
15	J	786	0	828	32	0
16	K	877	0	887	20	0
17	L	957	0	1017	18	0
18	M	891	0	952	12	0
19	N	805	0	844	30	0
20	O	714	0	734	19	0
21	P	643	0	661	10	0
22	Q	641	0	682	9	0
23	R	544	0	565	10	0
24	S	668	0	693	17	0
25	T	670	0	719	11	0
26	U	589	0	629	12	0
27	X	211	0	106	5	0
28	Z	1605	0	818	11	0
29	a	59130	0	29757	404	0
30	b	2549	0	1288	20	0
31	c	2082	0	2154	17	0
32	d	1566	0	1618	19	0
33	e	1552	0	1619	7	0
34	f	1410	0	1444	18	0
35	g	1323	0	1371	32	0
36	h	303	0	327	9	0
37	i	1129	0	1162	16	0
38	j	946	0	1023	7	0
39	k	1053	0	1129	7	0
40	l	1075	0	1154	14	0
41	m	945	0	989	10	0
42	n	892	0	923	13	0
43	o	917	0	962	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	p	947	0	1019	4	0
45	q	816	0	839	2	0
46	r	857	0	922	6	0
47	s	738	0	807	10	0
48	t	779	0	831	9	0
49	u	753	0	780	19	0
50	v	586	0	596	5	0
51	w	625	0	652	7	0
52	x	501	0	531	10	0
53	y	449	0	488	4	0
54	z	444	0	458	2	0
55	3	1	0	0	0	0
56	A	62	0	0	0	0
56	a	211	0	0	0	0
56	b	5	0	0	0	0
56	m	1	0	0	0	0
56	p	2	0	0	0	0
57	A	24	0	0	0	0
57	a	75	0	0	0	0
57	b	1	0	0	0	0
58	A	35	0	0	0	0
58	a	35	0	0	1	0
59	0	1	0	0	0	0
59	1	3	0	0	0	0
59	2	3	0	0	1	0
59	3	1	0	0	0	0
59	A	123	0	0	0	0
59	O	1	0	0	0	0
59	U	1	0	0	0	0
59	a	1091	0	0	0	0
59	b	14	0	0	0	0
59	c	6	0	0	0	0
59	d	5	0	0	0	0
59	e	5	0	0	0	0
59	i	2	0	0	0	0
59	k	2	0	0	0	0
59	l	1	0	0	0	0
59	m	5	0	0	0	0
59	o	1	0	0	0	0
59	p	4	0	0	0	0
59	q	7	0	0	0	0
59	r	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	s	2	0	0	0	0
59	v	1	0	0	0	0
59	y	2	0	0	0	0
59	z	3	0	0	0	0
All	All	141212	0	94033	1323	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1323 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)
29:a:881:G:H1	29:a:895:U:H3	1.09	0.97
6:A:1086:U:H3	6:A:1099:G:H22	1.21	0.88
5:4:60:PHE:O	5:4:64:PHE:HB2	1.76	0.85
5:4:59:ARG:HA	5:4:62:LYS:HD3	1.59	0.82
29:a:1047:G:HO2'	29:a:1110:G:H1	1.26	0.82

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	49/55 (89%)	49 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	52 (93%)	4 (7%)	0	100	100
7	B	222/241 (92%)	209 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	C	204/233 (88%)	193 (95%)	11 (5%)	0	100	100
9	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
10	E	154/167 (92%)	148 (96%)	6 (4%)	0	100	100
11	F	101/135 (75%)	97 (96%)	4 (4%)	0	100	100
12	G	151/179 (84%)	140 (93%)	11 (7%)	0	100	100
13	H	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
14	I	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
15	J	96/103 (93%)	91 (95%)	4 (4%)	1 (1%)	12	20
16	K	115/129 (89%)	110 (96%)	5 (4%)	0	100	100
17	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
18	M	113/118 (96%)	109 (96%)	4 (4%)	0	100	100
19	N	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	12	20
20	O	86/89 (97%)	81 (94%)	5 (6%)	0	100	100
21	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
22	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
23	R	64/75 (85%)	61 (95%)	3 (5%)	0	100	100
24	S	82/92 (89%)	79 (96%)	3 (4%)	0	100	100
25	T	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
26	U	68/71 (96%)	68 (100%)	0	0	100	100
31	c	269/273 (98%)	264 (98%)	5 (2%)	0	100	100
32	d	206/209 (99%)	201 (98%)	4 (2%)	1 (0%)	24	37
33	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
34	f	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
35	g	174/177 (98%)	163 (94%)	10 (6%)	1 (1%)	21	32
36	h	39/149 (26%)	32 (82%)	7 (18%)	0	100	100
37	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
38	j	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
39	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
40	l	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
41	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
42	n	114/117 (97%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
44	p	115/118 (98%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
46	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
48	t	100/104 (96%)	94 (94%)	6 (6%)	0	100	100
49	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
50	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
51	w	75/78 (96%)	75 (100%)	0	0	100	100
52	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
53	y	56/59 (95%)	53 (95%)	3 (5%)	0	100	100
54	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
All	All	5484/5913 (93%)	5294 (96%)	186 (3%)	4 (0%)	49	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	J	57	VAL
32	d	149	ASN
35	g	46	ALA
19	N	33	ASP

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	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	63
3	2	51/52 (98%)	49 (96%)	2 (4%)	28	48
4	3	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	4	55/62 (89%)	50 (91%)	5 (9%)	9	14
7	B	186/199 (94%)	178 (96%)	8 (4%)	26	44
8	C	170/190 (90%)	163 (96%)	7 (4%)	27	46
9	D	172/173 (99%)	168 (98%)	4 (2%)	44	66
10	E	119/126 (94%)	115 (97%)	4 (3%)	32	54
11	F	90/116 (78%)	88 (98%)	2 (2%)	45	67
12	G	126/147 (86%)	123 (98%)	3 (2%)	43	65
13	H	104/105 (99%)	98 (94%)	6 (6%)	18	32
14	I	105/107 (98%)	104 (99%)	1 (1%)	68	84
15	J	86/90 (96%)	83 (96%)	3 (4%)	32	53
16	K	90/99 (91%)	85 (94%)	5 (6%)	19	33
17	L	102/103 (99%)	99 (97%)	3 (3%)	37	60
18	M	93/96 (97%)	92 (99%)	1 (1%)	65	82
19	N	83/84 (99%)	80 (96%)	3 (4%)	31	52
20	O	76/77 (99%)	75 (99%)	1 (1%)	61	80
21	P	65/65 (100%)	64 (98%)	1 (2%)	57	77
22	Q	73/78 (94%)	72 (99%)	1 (1%)	59	79
23	R	57/65 (88%)	53 (93%)	4 (7%)	14	24
24	S	72/79 (91%)	71 (99%)	1 (1%)	59	79
25	T	65/66 (98%)	65 (100%)	0	100	100
26	U	60/61 (98%)	59 (98%)	1 (2%)	53	74
31	c	216/218 (99%)	214 (99%)	2 (1%)	70	85
32	d	163/163 (100%)	160 (98%)	3 (2%)	51	73
33	e	165/165 (100%)	156 (94%)	9 (6%)	19	34
34	f	148/150 (99%)	139 (94%)	9 (6%)	17	30
35	g	137/138 (99%)	124 (90%)	13 (10%)	8	13
36	h	32/114 (28%)	31 (97%)	1 (3%)	35	57
37	i	116/116 (100%)	113 (97%)	3 (3%)	40	63
38	j	104/104 (100%)	103 (99%)	1 (1%)	68	84
39	k	103/103 (100%)	100 (97%)	3 (3%)	37	60
40	l	108/108 (100%)	105 (97%)	3 (3%)	38	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	m	98/103 (95%)	96 (98%)	2 (2%)	48	70
42	n	86/87 (99%)	84 (98%)	2 (2%)	44	66
43	o	99/100 (99%)	98 (99%)	1 (1%)	68	84
44	p	89/90 (99%)	88 (99%)	1 (1%)	65	82
45	q	84/84 (100%)	78 (93%)	6 (7%)	13	23
46	r	93/93 (100%)	91 (98%)	2 (2%)	45	67
47	s	80/84 (95%)	79 (99%)	1 (1%)	61	80
48	t	83/85 (98%)	77 (93%)	6 (7%)	13	23
49	u	78/78 (100%)	75 (96%)	3 (4%)	29	49
50	v	58/63 (92%)	57 (98%)	1 (2%)	53	74
51	w	67/68 (98%)	64 (96%)	3 (4%)	24	42
52	x	54/55 (98%)	54 (100%)	0	100	100
53	y	48/49 (98%)	47 (98%)	1 (2%)	47	69
54	z	47/48 (98%)	47 (100%)	0	100	100
All	All	4574/4827 (95%)	4431 (97%)	143 (3%)	36	57

5 of 143 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	m	65	LEU
44	p	13	ARG
48	t	40	ASN
16	K	95	SER
16	K	34	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
35	g	48	ASN
49	u	12	GLN
36	h	20	ASN
45	q	82	HIS
19	N	35	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	9/22 (40%)	5 (55%)	0
28	Z	74/75 (98%)	11 (14%)	2 (2%)
29	a	2749/2904 (94%)	283 (10%)	0
30	b	118/120 (98%)	9 (7%)	0
6	A	1495/1542 (96%)	177 (11%)	2 (0%)
All	All	4445/4663 (95%)	485 (10%)	4 (0%)

5 of 485 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	6	G
6	A	9	G
6	A	22	G
6	A	32	A

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	182	A
6	A	1035	A
28	Z	16	C
28	Z	17(A)	U

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

42 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	$\# Z > 2$
29	PSU	a	2457	29	18,21,22	1.08	2 (11%)	21,30,33	2.01	6 (28%)
6	4OC	A	1402	6	20,23,24	3.19	8 (40%)	25,32,35	0.90	1 (4%)
6	MA6	A	1518	6	23,26,27	0.30	0	33,38,41	0.64	1 (3%)
29	OMC	a	2498	29,56	19,22,23	0.64	0	25,31,34	0.70	0
32	MEQ	d	150	32	8,9,10	0.87	0	5,10,12	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PSU	a	1911	29	18,21,22	1.06	1 (5%)	21,30,33	1.96	5 (23%)
6	G7M	A	527	6	23,26,27	0.73	1 (4%)	34,39,42	0.64	1 (2%)
6	5MC	A	967	6	19,22,23	0.60	0	26,32,35	0.63	0
6	2MG	A	966	6	23,26,27	0.51	0	33,38,41	0.51	0
29	3TD	a	1915	29	19,22,23	4.11	7 (36%)	23,32,35	1.79	3 (13%)
29	PSU	a	2504	57,29	18,21,22	1.12	1 (5%)	21,30,33	1.94	4 (19%)
29	PSU	a	1917	29	18,21,22	1.06	1 (5%)	21,30,33	1.95	4 (19%)
29	5MC	a	1962	57,29	19,22,23	0.66	0	26,32,35	0.68	0
29	PSU	a	746	29,56	18,21,22	1.10	1 (5%)	21,30,33	1.87	3 (14%)
29	PSU	a	955	29	18,21,22	1.07	1 (5%)	21,30,33	2.03	4 (19%)
28	5MU	Z	54	28	19,22,23	0.38	0	27,32,35	0.63	0
29	OMU	a	2552	57,29	19,22,23	2.96	7 (36%)	25,31,34	1.90	5 (20%)
29	2MA	a	2503	57,29,56	22,25,26	0.84	1 (4%)	32,37,40	1.20	4 (12%)
6	MA6	A	1519	6	23,26,27	0.29	0	33,38,41	0.74	1 (3%)
29	5MU	a	1939	57,29	19,22,23	0.57	0	27,32,35	0.47	0
29	G7M	a	2069	57,29	23,26,27	2.61	9 (39%)	34,39,42	2.35	11 (32%)
29	OMG	a	2251	57,29,28	23,26,27	0.56	0	32,38,41	0.44	0
29	2MG	a	2445	29	23,26,27	0.58	0	33,38,41	0.45	0
29	PSU	a	2604	29	18,21,22	1.04	1 (5%)	21,30,33	2.01	5 (23%)
6	2MG	A	1207	6	23,26,27	0.47	0	33,38,41	0.52	0
28	4SU	Z	8	28	18,21,22	3.85	8 (44%)	25,30,33	2.32	5 (20%)
29	1MG	a	745	29	23,26,27	2.85	8 (34%)	33,39,42	1.69	6 (18%)
29	PSU	a	2605	29	18,21,22	1.07	1 (5%)	21,30,33	1.95	4 (19%)
6	UR3	A	1498	6	19,22,23	2.73	8 (42%)	26,32,35	1.63	3 (11%)
6	5MC	A	1407	6	19,22,23	0.65	0	26,32,35	0.68	0
17	D2T	L	89	17	8,9,10	1.56	1 (12%)	6,11,13	1.90	2 (33%)
40	4D4	l	81	40	9,11,12	2.03	2 (22%)	7,13,15	1.88	3 (42%)
28	PSU	Z	55	28	18,21,22	1.10	1 (5%)	21,30,33	1.94	5 (23%)
6	2MG	A	1516	6	23,26,27	0.53	0	33,38,41	0.74	0
29	5MU	a	747	29	19,22,23	0.48	0	27,32,35	0.72	1 (3%)
29	2MG	a	1835	29	23,26,27	0.52	0	33,38,41	0.44	0
29	PSU	a	2580	29	18,21,22	1.11	3 (16%)	21,30,33	1.98	5 (23%)
29	6MZ	a	1618	29	22,25,26	2.24	7 (31%)	29,36,39	2.42	10 (34%)
29	6MZ	a	2030	29	22,25,26	2.29	7 (31%)	29,36,39	2.47	13 (44%)
28	5MC	Z	32	28	19,22,23	0.65	0	26,32,35	0.69	0
29	H2U	a	2449	29	18,21,22	0.54	0	19,30,33	1.13	1 (5%)
6	PSU	A	516	6,56	18,21,22	1.08	1 (5%)	21,30,33	1.91	5 (23%)

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
29	PSU	a	2457	29	-	0/7/25/26	0/2/2/2
6	4OC	A	1402	6	-	1/9/29/30	0/2/2/2
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
29	OMC	a	2498	29,56	-	1/9/27/28	0/2/2/2
32	MEQ	d	150	32	-	2/8/9/11	-
29	PSU	a	1911	29	-	0/7/25/26	0/2/2/2
6	G7M	A	527	6	-	2/7/25/26	0/3/3/3
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
6	2MG	A	966	6	-	0/9/27/28	0/3/3/3
29	3TD	a	1915	29	-	0/7/25/26	0/2/2/2
29	PSU	a	2504	57,29	-	2/7/25/26	0/2/2/2
29	PSU	a	1917	29	-	0/7/25/26	0/2/2/2
29	5MC	a	1962	57,29	-	0/7/25/26	0/2/2/2
29	PSU	a	746	29,56	-	2/7/25/26	0/2/2/2
29	PSU	a	955	29	-	0/7/25/26	0/2/2/2
28	5MU	Z	54	28	-	0/7/25/26	0/2/2/2
29	OMU	a	2552	57,29	-	1/9/27/28	0/2/2/2
29	2MA	a	2503	57,29,56	-	2/7/25/26	0/3/3/3
6	MA6	A	1519	6	-	0/11/29/30	0/3/3/3
29	5MU	a	1939	57,29	-	0/7/25/26	0/2/2/2
29	G7M	a	2069	57,29	-	2/7/25/26	0/3/3/3
29	OMG	a	2251	57,29,28	-	1/9/27/28	0/3/3/3
29	2MG	a	2445	29	-	1/9/27/28	0/3/3/3
29	PSU	a	2604	29	-	0/7/25/26	0/2/2/2
6	2MG	A	1207	6	-	0/9/27/28	0/3/3/3
28	4SU	Z	8	28	-	0/7/25/26	0/2/2/2
29	1MG	a	745	29	-	0/7/25/26	0/3/3/3
29	PSU	a	2605	29	-	0/7/25/26	0/2/2/2
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	4/7/12/14	-
40	4D4	l	81	40	-	4/11/12/14	-
28	PSU	Z	55	28	-	0/7/25/26	0/2/2/2
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
29	5MU	a	747	29	-	0/7/25/26	0/2/2/2
29	2MG	a	1835	29	-	0/9/27/28	0/3/3/3
29	PSU	a	2580	29	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	6MZ	a	1618	29	-	0/9/27/28	0/3/3/3
29	6MZ	a	2030	29	-	2/9/27/28	0/3/3/3
28	5MC	Z	32	28	-	0/7/25/26	0/2/2/2
29	H2U	a	2449	29	-	0/7/38/39	0/2/2/2
6	PSU	A	516	6,56	-	0/7/25/26	0/2/2/2

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	1915	3TD	C6-C5	12.83	1.49	1.35
29	a	1915	3TD	C2-N1	9.11	1.48	1.37
28	Z	8	4SU	C4-N3	8.56	1.46	1.37
29	a	1618	6MZ	C6-N6	7.96	1.43	1.34
29	a	745	1MG	C2-N3	7.80	1.45	1.33

The worst 5 of 121 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	Z	8	4SU	C4-N3-C2	-7.86	119.78	127.31
29	a	2069	G7M	C1'-N9-C4	6.03	144.29	126.49
29	a	2552	OMU	C4-N3-C2	-5.98	119.19	126.61
6	A	1498	UR3	C4-N3-C2	-5.82	119.90	124.58
29	a	1915	3TD	N1-C2-N3	5.69	120.26	116.13

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
40	l	81	4D4	CA-CB-CG-CD
29	a	2504	PSU	O4'-C4'-C5'-O5'
32	d	150	MEQ	OE1-CD-CG-CB

There are no ring outliers.

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	1915	3TD	1	0
6	A	1519	MA6	1	0
17	L	89	D2T	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
28	Z	55	PSU	1	0
6	A	1516	2MG	1	0
29	a	2030	6MZ	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 384 ligands modelled in this entry, 382 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	$\# Z > 2$
58	V7A	A	1674	56	37,38,38	1.10	2 (5%)	43,60,60	0.96	4 (9%)
58	V7A	a	3008	-	37,38,38	1.11	2 (5%)	43,60,60	1.21	5 (11%)

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
58	V7A	A	1674	56	-	2/13/72/72	0/4/4/4
58	V7A	a	3008	-	-	7/13/72/72	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	a	3008	V7A	CBC-NBD	5.03	1.48	1.33
58	A	1674	V7A	CBC-NBD	4.93	1.47	1.33
58	a	3008	V7A	OAY-CAH	2.25	1.28	1.23
58	A	1674	V7A	OAY-CAH	2.25	1.27	1.23

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	a	3008	V7A	CAF-CAG-CAJ	3.58	117.86	113.12
58	a	3008	V7A	CAH-CAI-CAL	2.26	120.59	118.80
58	A	1674	V7A	CAH-CAI-CAL	2.11	120.47	118.80
58	A	1674	V7A	OAZ-CAL-CAM	2.10	116.41	113.37
58	a	3008	V7A	OAZ-CAL-CAI	-2.08	119.49	123.52

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

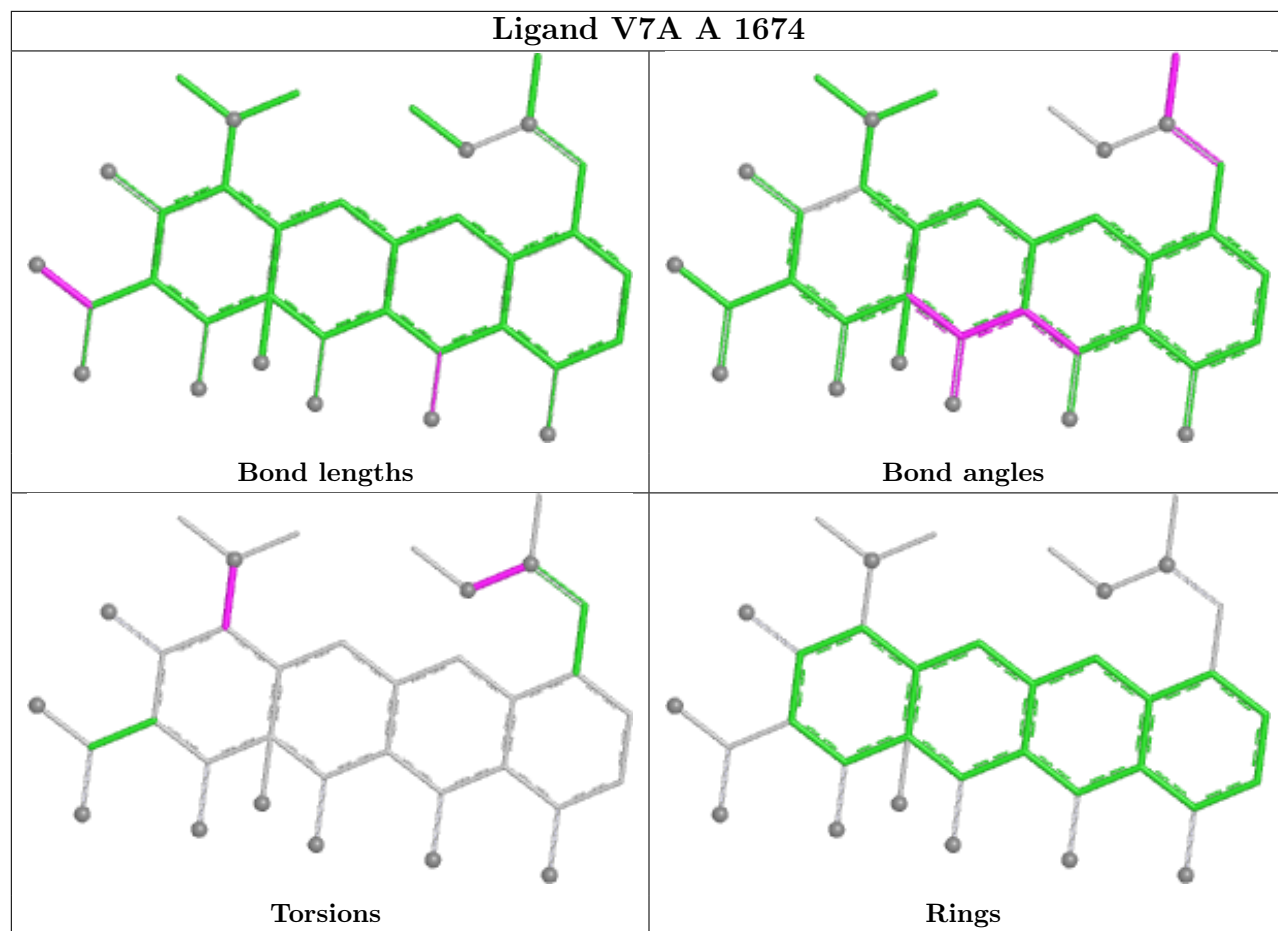
Mol	Chain	Res	Type	Atoms
58	A	1674	V7A	CAN-CAO-NBF-CBG
58	a	3008	V7A	CAF-CAA-CAS-NAT
58	a	3008	V7A	CAN-CAO-NBF-CBG
58	a	3008	V7A	CAR-CAO-NBF-CBG
58	a	3008	V7A	CAR-CAO-NBF-CBH

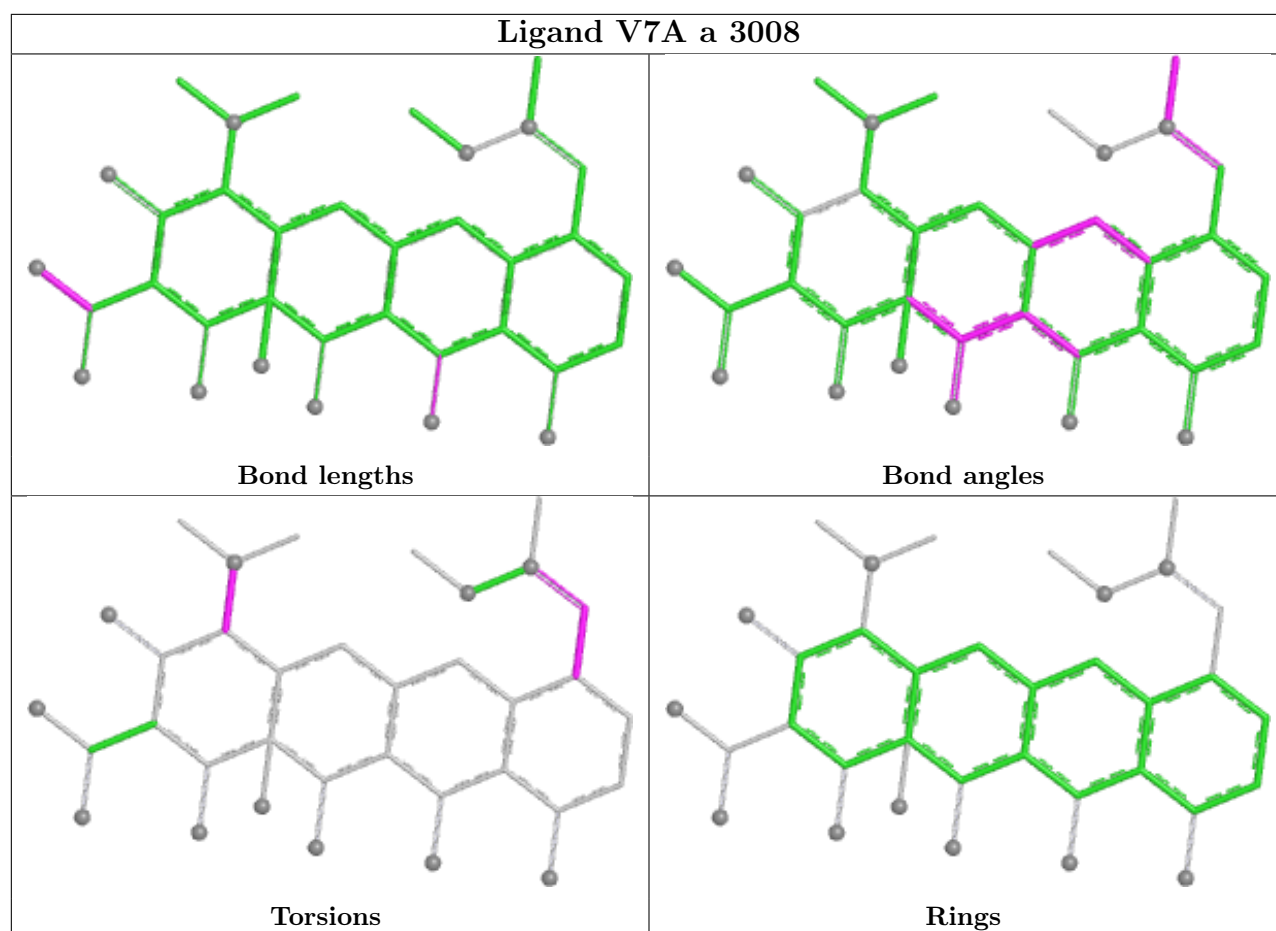
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	a	3008	V7A	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

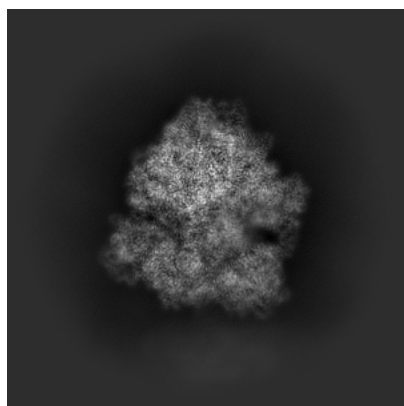
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-71668. These allow visual inspection of the internal detail of the map and identification of artifacts.

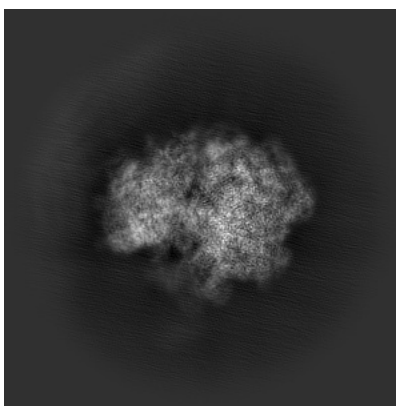
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

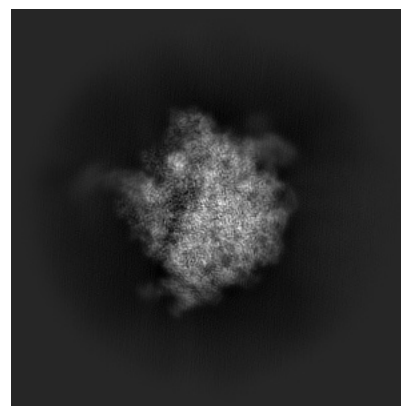
6.1.1 Primary map



X

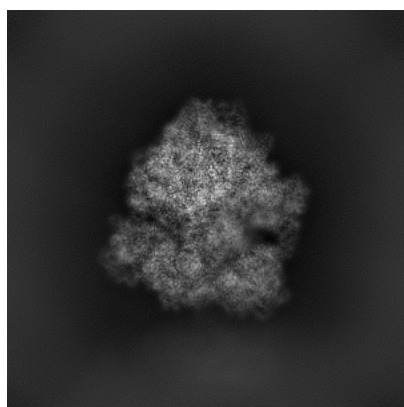


Y

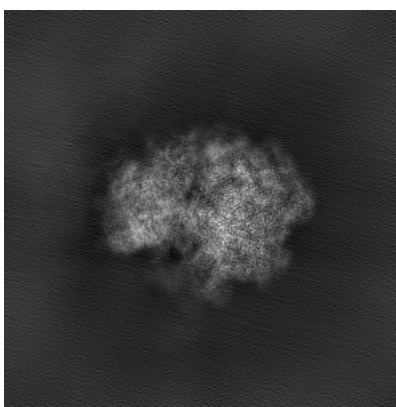


Z

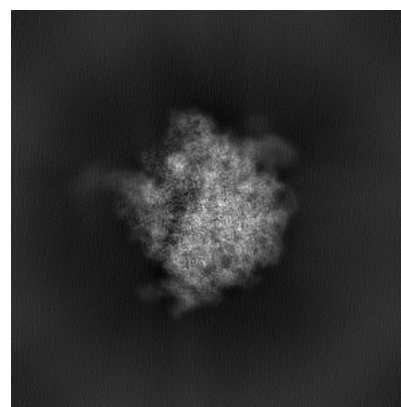
6.1.2 Raw map



X



Y

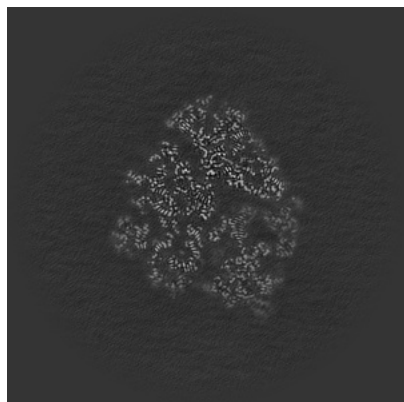


Z

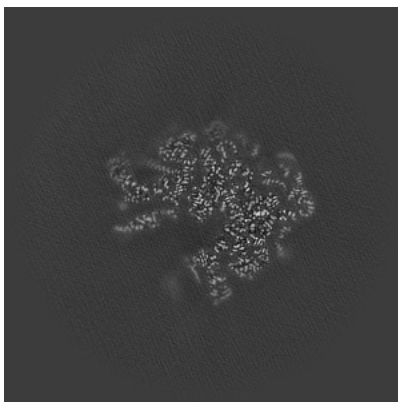
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

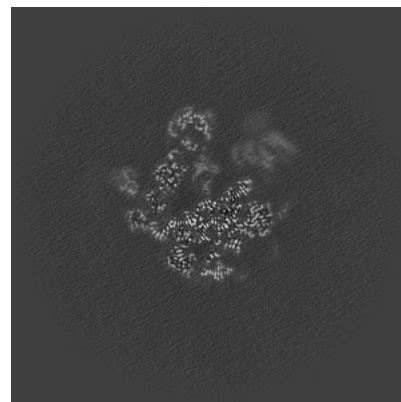
6.2.1 Primary map



X Index: 220

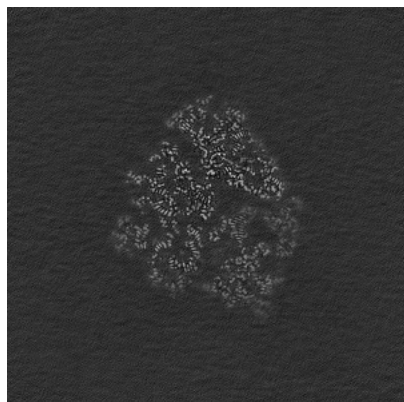


Y Index: 220

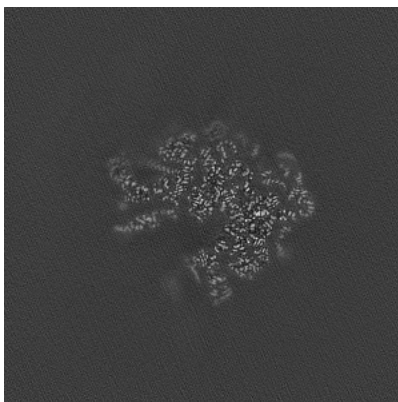


Z Index: 220

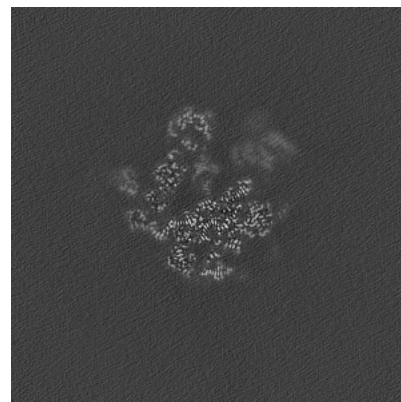
6.2.2 Raw map



X Index: 220



Y Index: 220

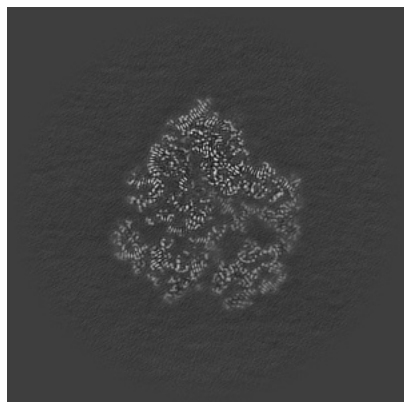


Z Index: 220

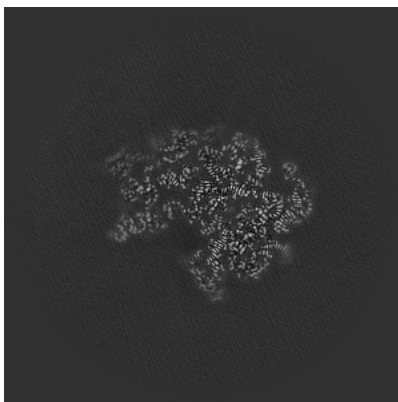
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

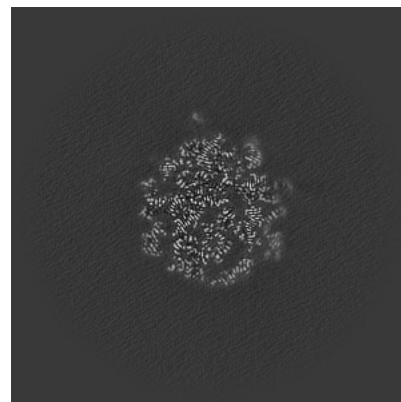
6.3.1 Primary map



X Index: 213

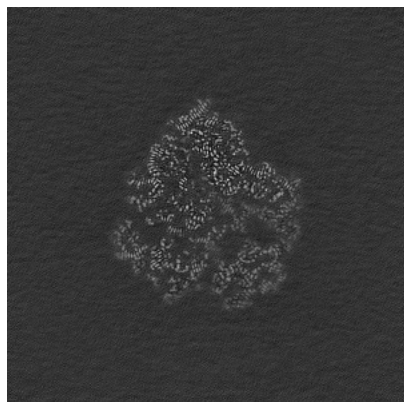


Y Index: 213

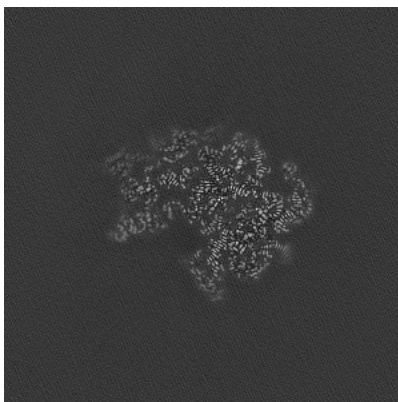


Z Index: 258

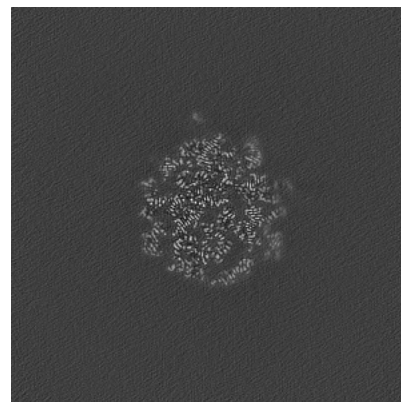
6.3.2 Raw map



X Index: 213



Y Index: 213

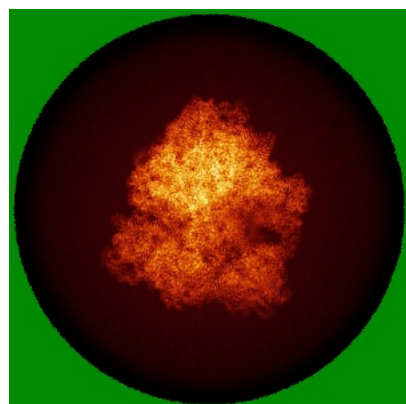


Z Index: 258

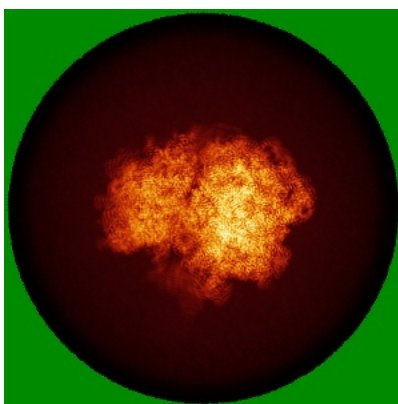
The images above show the largest variance slices of the map in three orthogonal directions.

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

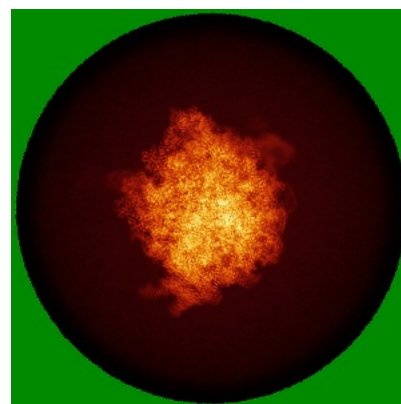
6.4.1 Primary map



X

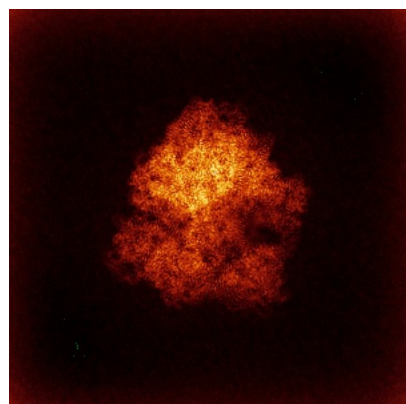


Y

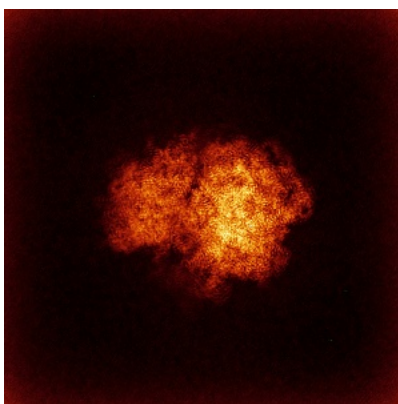


Z

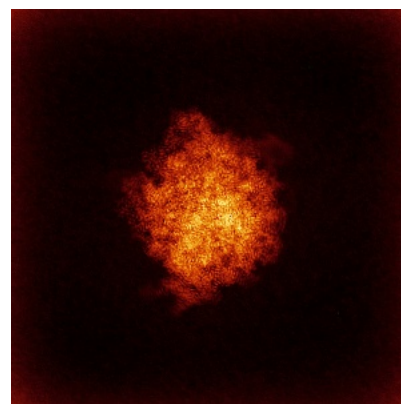
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



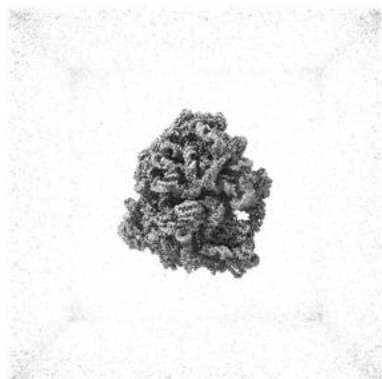
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

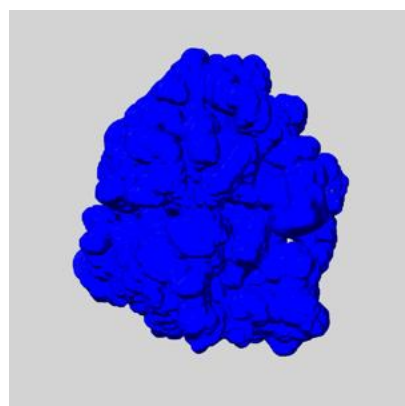
6.6 Mask visualisation [i](#)

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

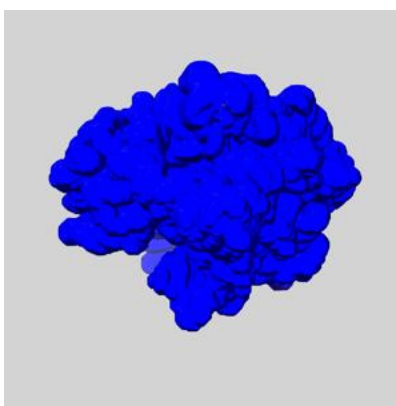
A mask typically either:

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

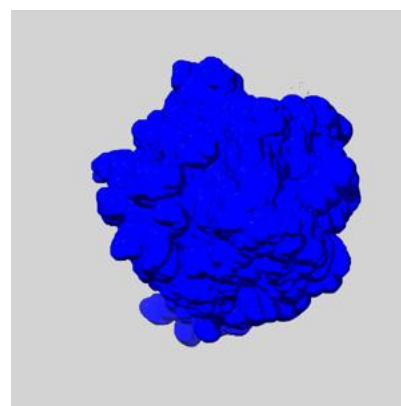
6.6.1 emd_71668_msk_1.map [i](#)



X



Y

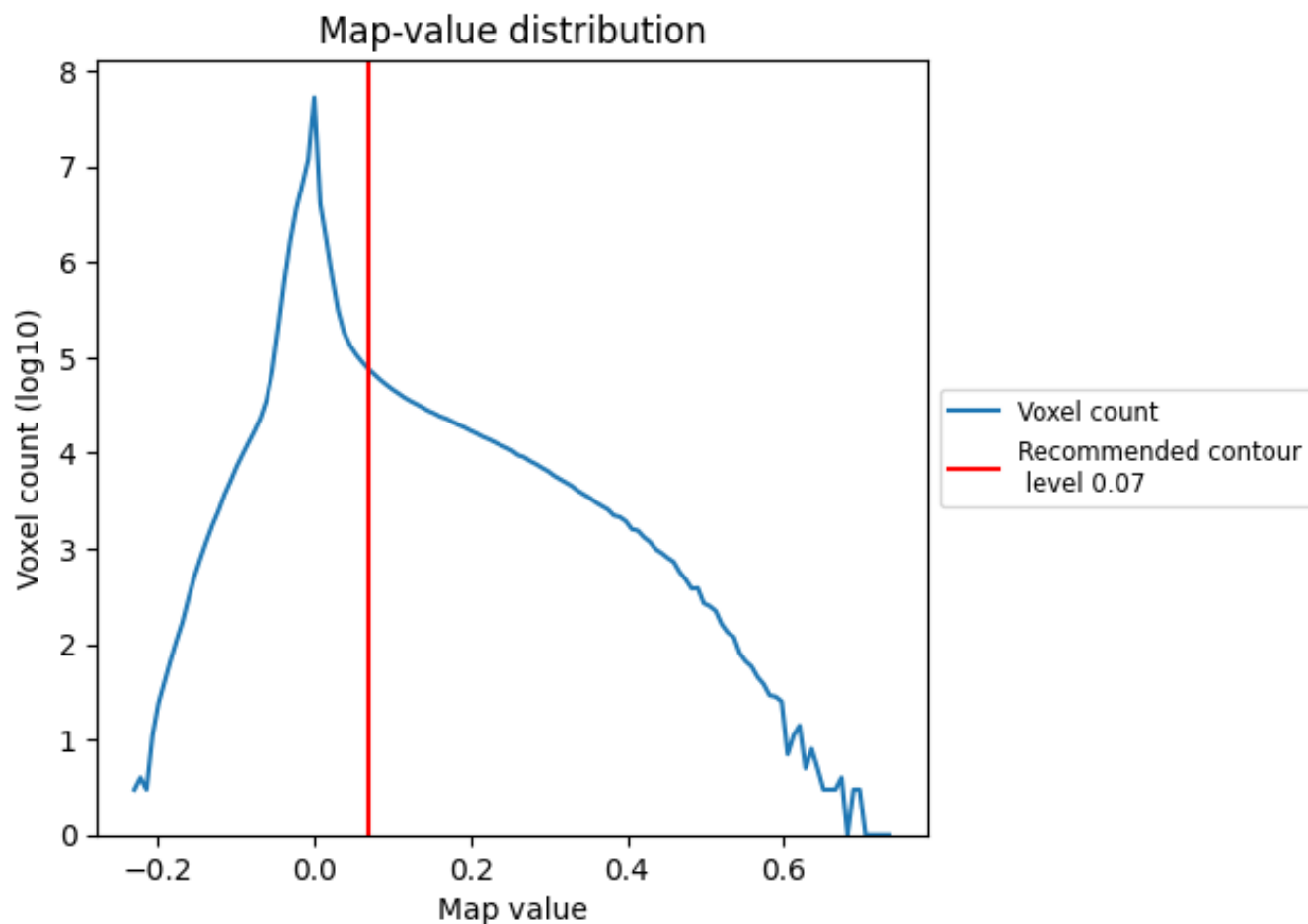


Z

7 Map analysis [i](#)

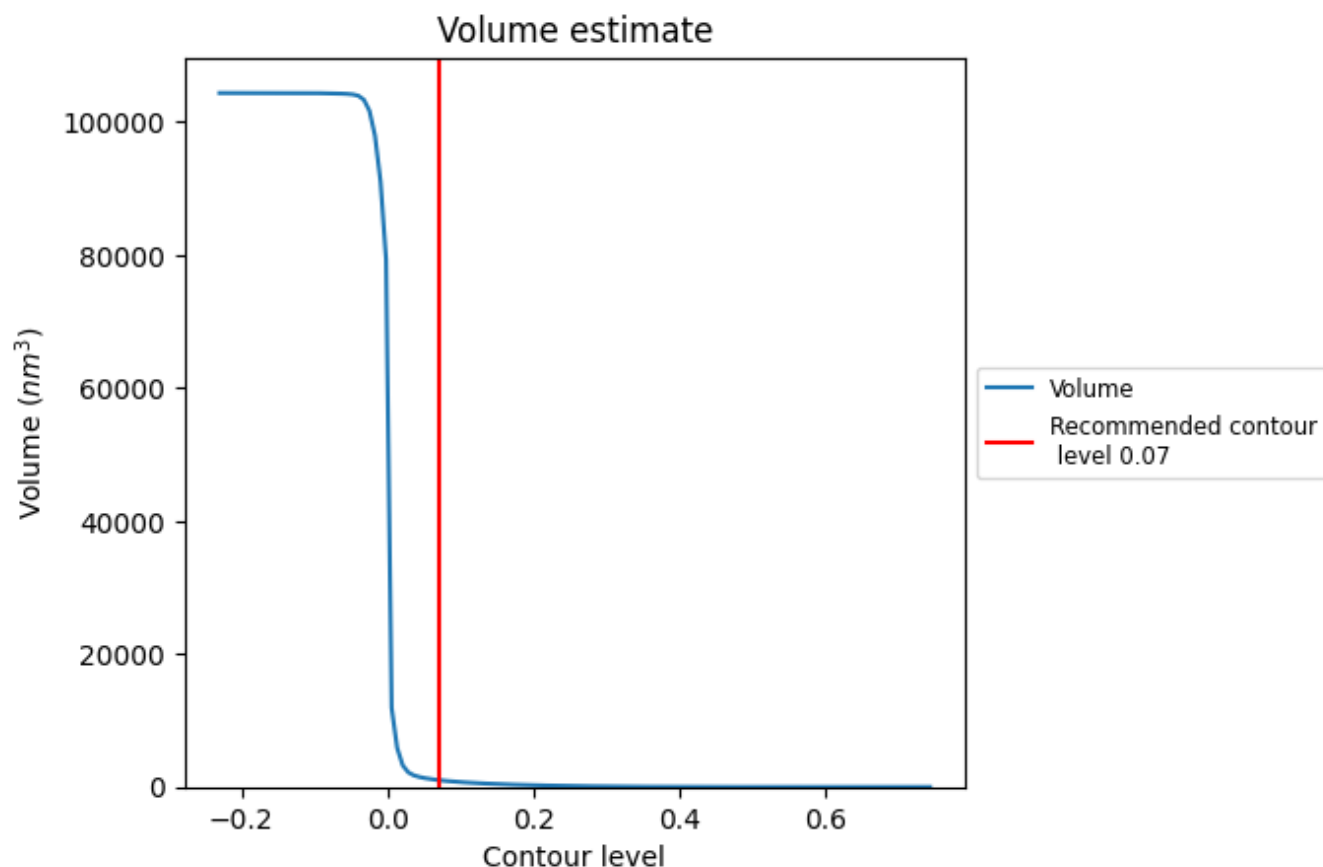
This section contains the results of statistical analysis of the map.

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.

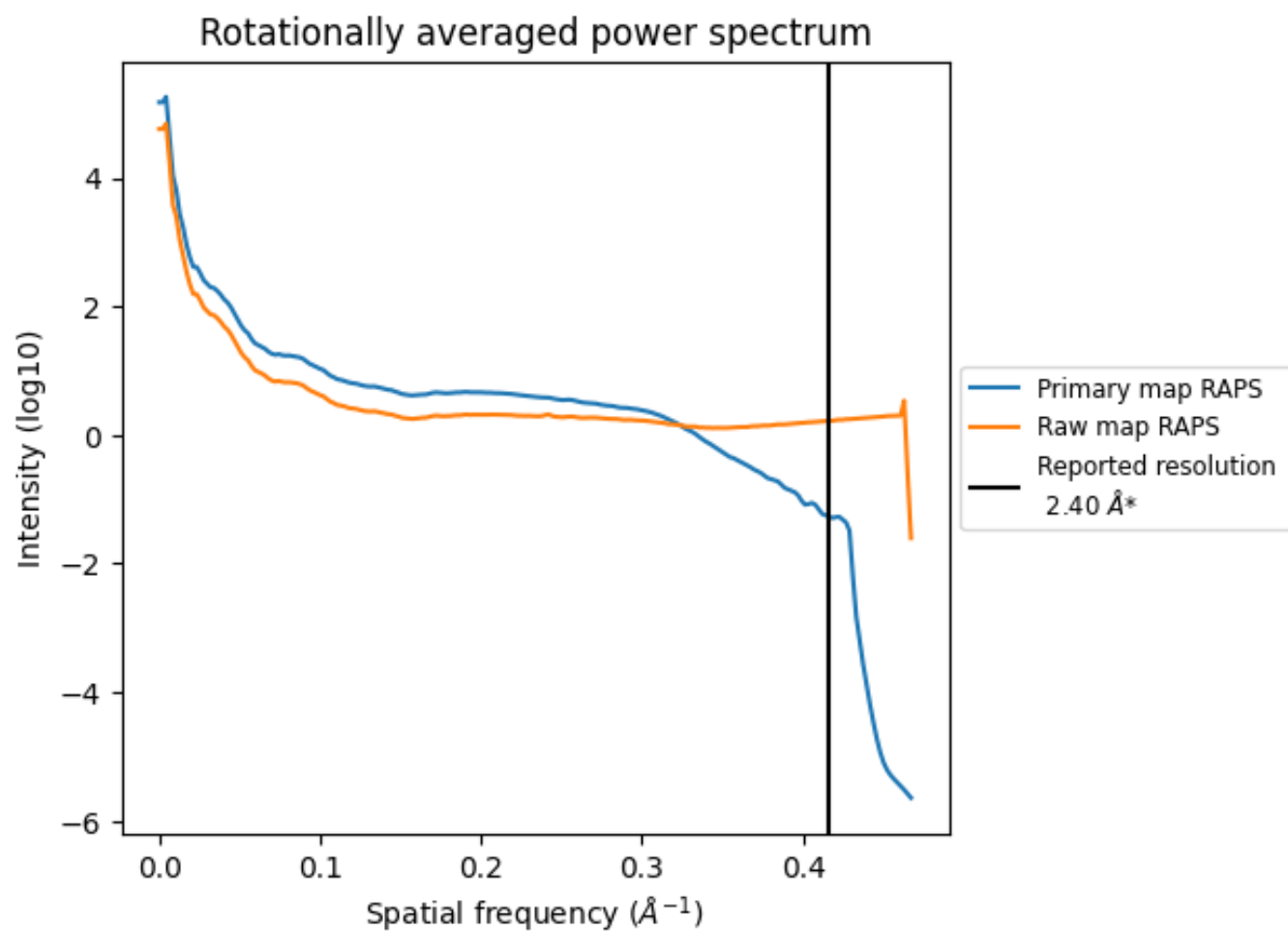
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1031 nm^3 ; this corresponds to an approximate mass of 931 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 ⓘ

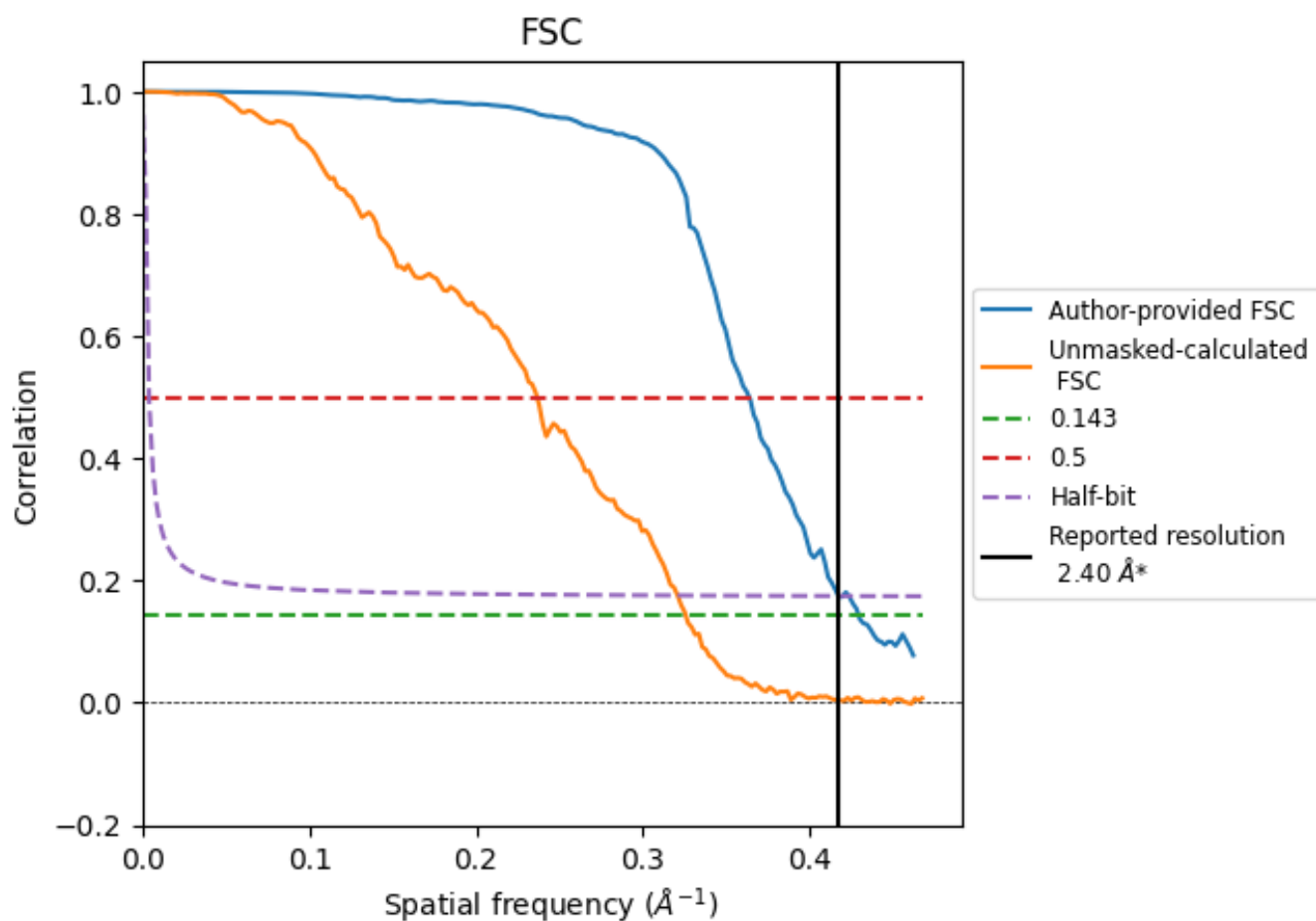


*Reported resolution corresponds to spatial frequency of 0.417 $\text{\AA}^{-1}$

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 0.417 Å⁻¹

8.2 Resolution estimates

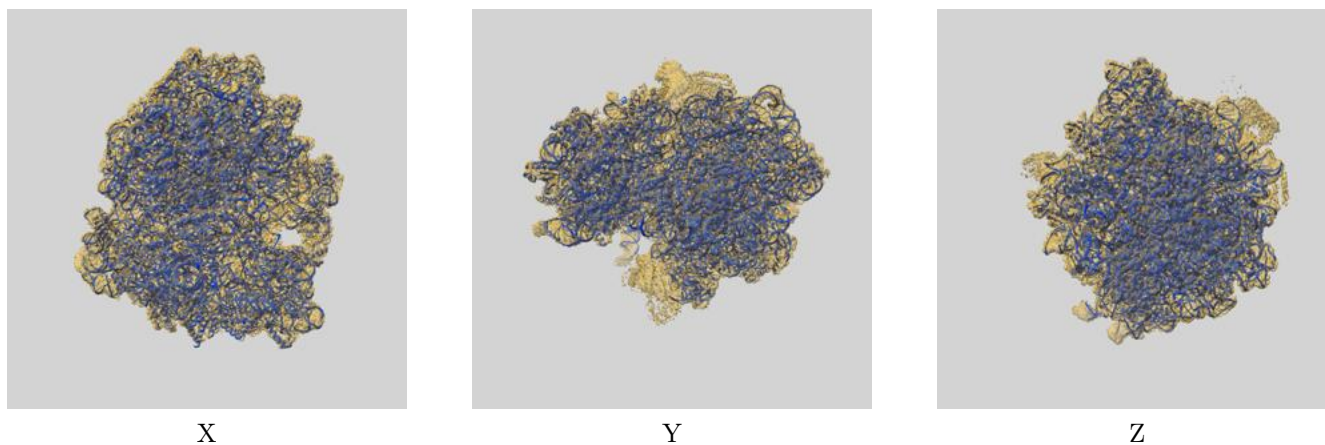
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.33	2.75	2.40
Unmasked-calculated*	3.07	4.23	3.12

*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 3.07 differs from the reported value 2.4 by more than 10 %

9 Map-model fit [i](#)

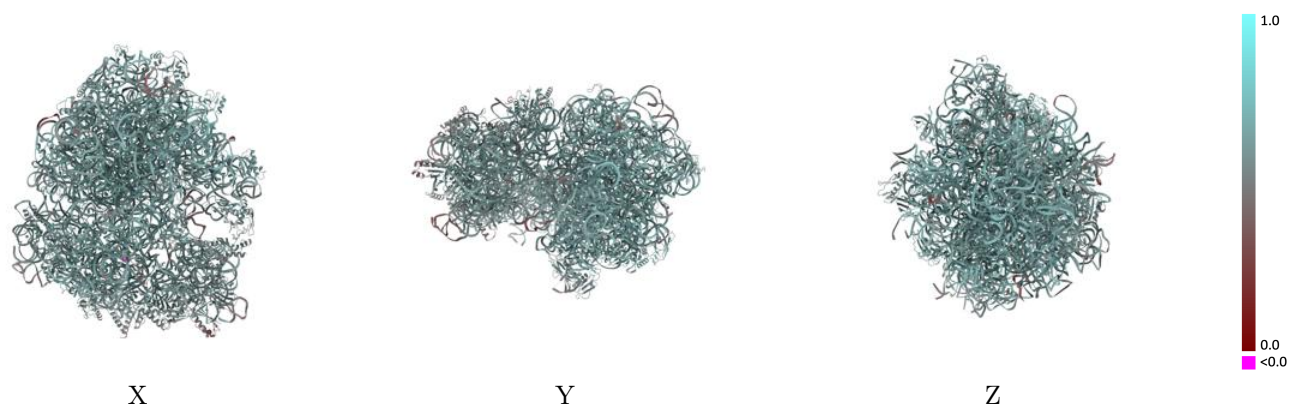
This section contains information regarding the fit between EMDB map EMD-71668 and PDB model 9PII. Per-residue inclusion information can be found in section [3](#) on page [17](#).

9.1 Map-model overlay [i](#)



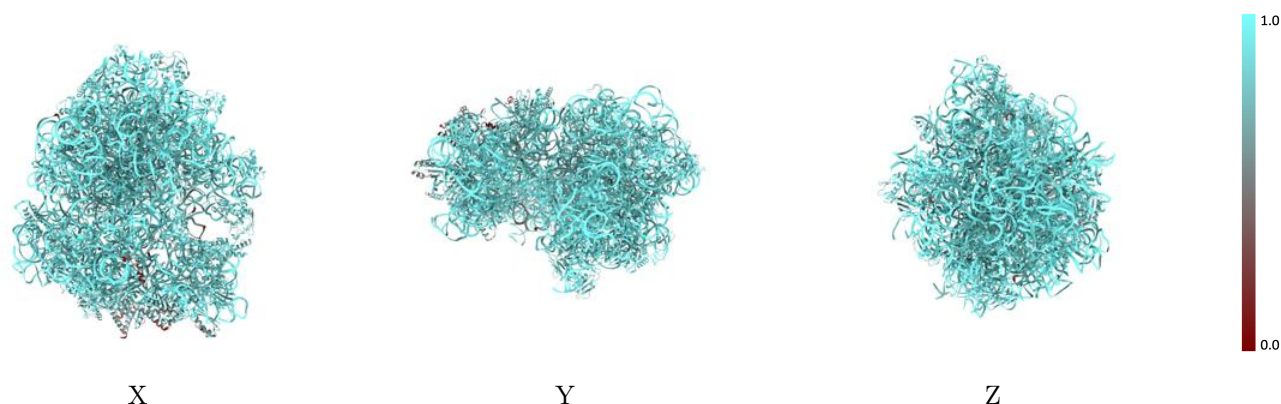
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



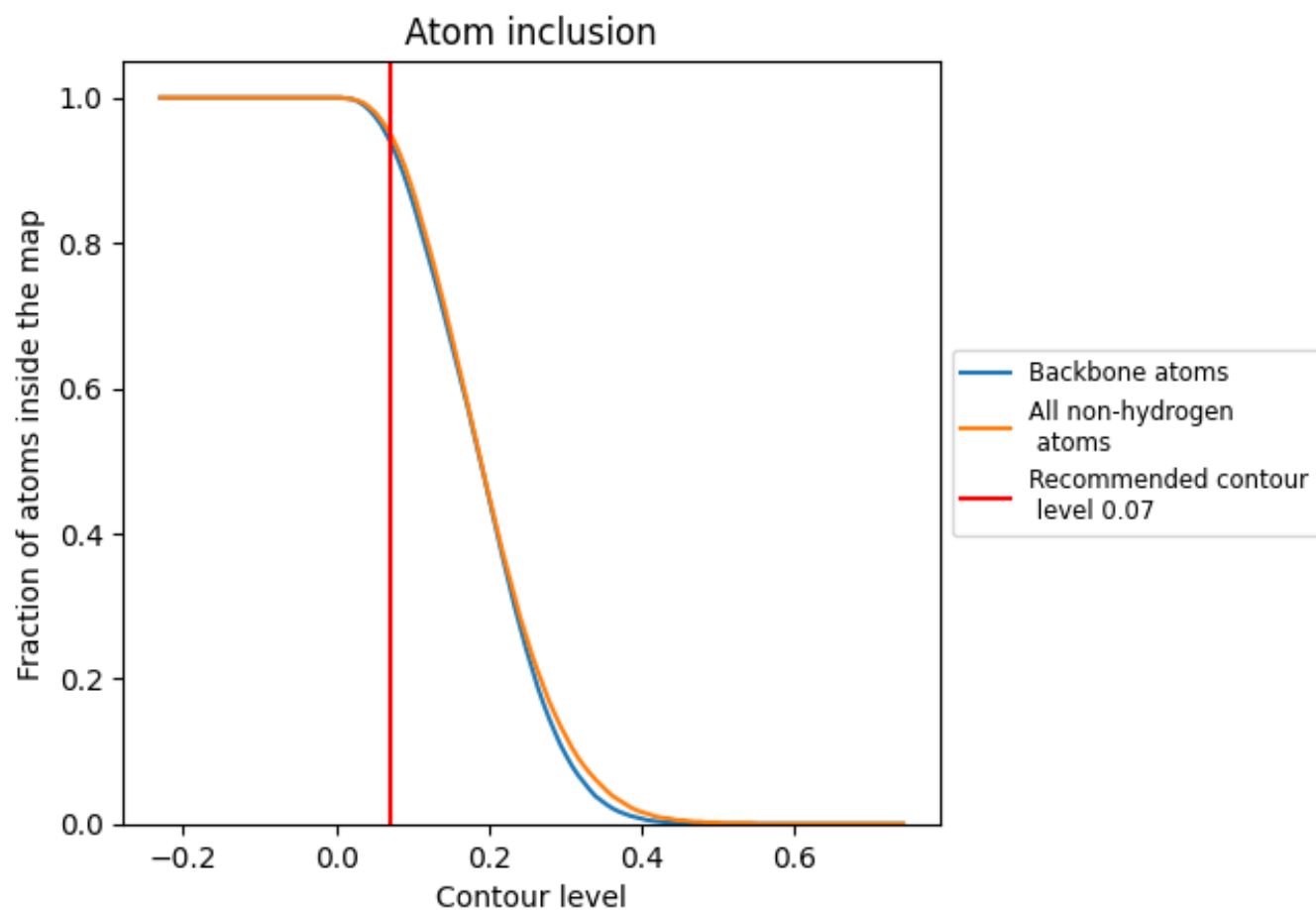
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9530	 0.6150
0	 0.9170	 0.6300
1	 0.9690	 0.6570
2	 0.9650	 0.6580
3	 0.9320	 0.6400
4	 0.7920	 0.5290
A	 0.9840	 0.6010
B	 0.6030	 0.5340
C	 0.8560	 0.5800
D	 0.8790	 0.5860
E	 0.9140	 0.6160
F	 0.8670	 0.5700
G	 0.8110	 0.5540
H	 0.9200	 0.6150
I	 0.8970	 0.5670
J	 0.7570	 0.5270
K	 0.8900	 0.5960
L	 0.9070	 0.6190
M	 0.8780	 0.5760
N	 0.8710	 0.5730
O	 0.9230	 0.5970
P	 0.9370	 0.6030
Q	 0.8990	 0.6080
R	 0.7630	 0.5610
S	 0.8240	 0.5520
T	 0.9050	 0.5970
U	 0.6560	 0.5430
X	 0.6020	 0.4460
Z	 0.8620	 0.5670
a	 0.9870	 0.6320
b	 0.9830	 0.6050
c	 0.9610	 0.6560
d	 0.9570	 0.6480
e	 0.9260	 0.6240
f	 0.8730	 0.5690



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	 0.8640	 0.5650
h	 0.8030	 0.5640
i	 0.9520	 0.6430
j	 0.9290	 0.6410
k	 0.9440	 0.6380
l	 0.9360	 0.6360
m	 0.9700	 0.6490
n	 0.9370	 0.6090
o	 0.9170	 0.6340
p	 0.9700	 0.6530
q	 0.9400	 0.6300
r	 0.9410	 0.6410
s	 0.9150	 0.6130
t	 0.9150	 0.5940
u	 0.9130	 0.6100
v	 0.9390	 0.6460
w	 0.9450	 0.6410
x	 0.9040	 0.5820
y	 0.9220	 0.6340
z	 0.9390	 0.6420