



wwPDB EM Validation Summary Report ⓘ

Jun 18, 2026 – 11:29 am BST

PDB ID : 8QK7 / pdb_00008qk7
EMDB ID : EMD-18458
Title : E167K RF2 on E. coli 70S release complex with UAA
Authors : Pundir, S.; Larsson, D.S.D.; Selmer, M.; Sanyal, S.
Deposited on : 2023-09-14
Resolution : 2.77 Å(reported)
Based on initial models : 7K00, 8B0X, 1GQE, 5MDV

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

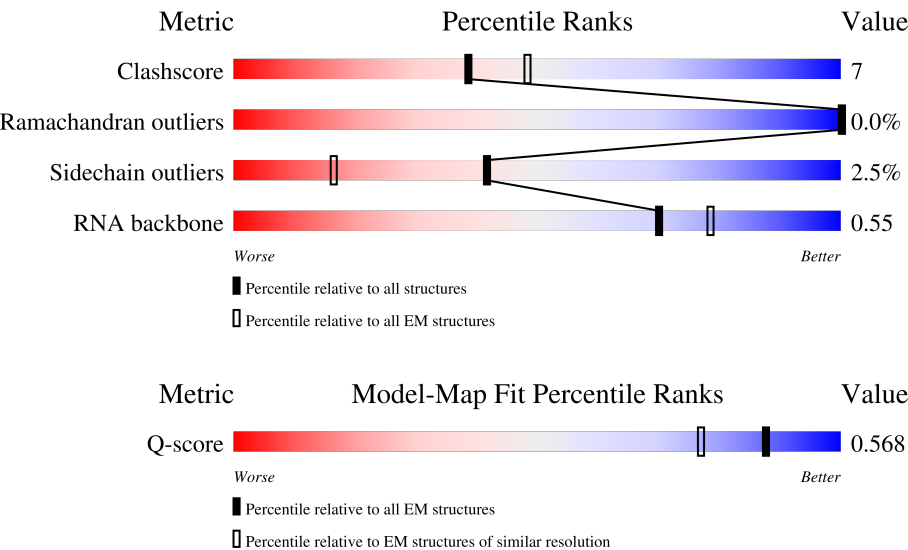
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.77 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.



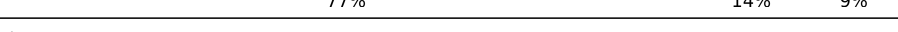
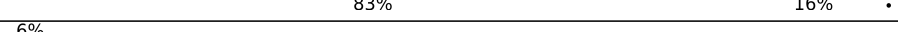
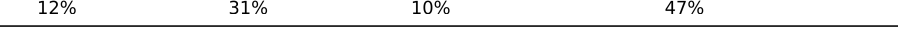
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10695 (2.27 - 3.27)

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	2	1542	
2	g	241	
3	h	233	

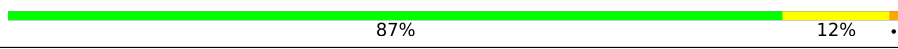
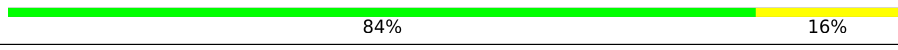
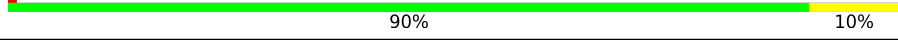
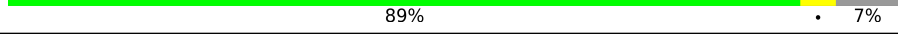
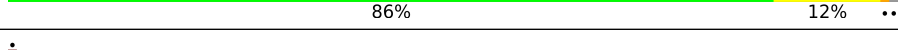
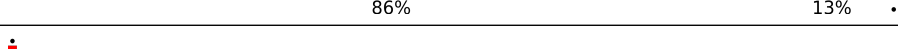
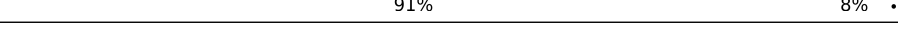
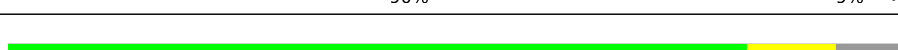
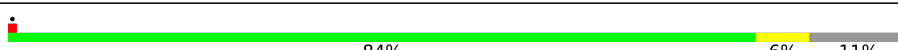
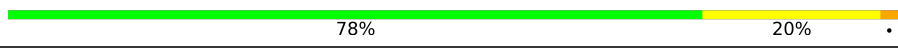
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Mol	Chain	Length	Quality of chain
4	i	206	
5	j	167	
6	k	135	
7	l	179	
8	m	130	
9	n	130	
10	o	103	
11	p	129	
12	q	124	
13	r	118	
14	s	101	
15	t	89	
16	u	82	
17	v	84	
18	w	75	
19	x	92	
20	y	87	
21	z	71	
22	4	49	
23	5	76	
24	1	2904	
25	3	120	
26	B	273	
27	C	209	
28	D	201	

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Mol	Chain	Length	Quality of chain
29	E	179	
30	F	177	
31	J	142	
32	K	123	
33	L	144	
34	M	136	
35	N	127	
36	O	117	
37	P	115	
38	Q	118	
39	R	103	
40	S	110	
41	T	100	
42	U	104	
43	V	94	
44	W	85	
45	X	78	
46	Y	63	
47	Z	59	
48	b	57	
49	c	55	
50	d	46	
51	e	65	
52	f	38	
53	a	70	

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Mol	Chain	Length	Quality of chain
54	I	142	32%37%10%52% .
55	6	365	8%74%23% ..
56	G	149	70%78%20% .

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 148642 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 RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	1536	Total	C	N	O	P	0	0
			32966	14711	6044	10675	1536		

- Molecule 2 is a protein called Small ribosomal subunit protein uS2.

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

- Molecule 3 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	h	210	Total	C	N	O	S	0	0
			1648	1043	309	292	4		

- Molecule 4 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 5 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 6 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 7 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	l	154	Total	C	N	O	S	0	0
			1214	756	235	219	4		

- Molecule 8 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	p	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
p	119	IAS	ASN	variant	UNP P0A7R9

- Molecule 12 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 16 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 18 is a protein called Small ribosomal subunit protein bS18.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 20 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS21.

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

- Molecule 22 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	4	26	Total	C	N	O	P	0	0
			560	251	104	179	26		

- Molecule 23 is a RNA chain called tRNA(fMet).

Mol	Chain	Residues	Atoms					AltConf	Trace
23	5	76	Total	C	N	O	P	2	0
			1665	742	302	543	78		

- Molecule 24 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 25 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	3	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 26 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 27 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 29 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 31 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 32 is a protein called 50S ribosomal protein L14.

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

- Molecule 33 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 34 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	82	MS6	MET	variant	UNP P0ADY7

- Molecule 35 is a protein called 50S ribosomal protein L17.

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

- Molecule 36 is a protein called 50S ribosomal protein L18.

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

- Molecule 37 is a protein called 50S ribosomal protein L19.

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

- Molecule 38 is a protein called 50S ribosomal protein L20.

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

- Molecule 39 is a protein called 50S ribosomal protein L21.

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

- Molecule 40 is a protein called 50S ribosomal protein L22.

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

- Molecule 41 is a protein called 50S ribosomal protein L23.

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

- Molecule 42 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	U	102	Total	C	N	O	S	0	0
			779	492	146	141			

- Molecule 43 is a protein called 50S ribosomal protein L25.

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

- Molecule 44 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	W	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 45 is a protein called 50S ribosomal protein L28.

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

- Molecule 46 is a protein called 50S ribosomal protein L29.

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

- Molecule 47 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	Z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 48 is a protein called 50S ribosomal protein L32.

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

- Molecule 49 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	c	51	Total	C	N	O	S	0	0
			417	269	76	72			

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

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

- Molecule 51 is a protein called 50S ribosomal protein L35.

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

- Molecule 52 is a protein called 50S ribosomal protein L36.

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

- Molecule 53 is a protein called Large ribosomal subunit protein bL31A.

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

- Molecule 54 is a protein called Large ribosomal subunit protein uL11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	I	68	Total	C	N	O	S	0	0
			484	298	89	94	3		

- Molecule 55 is a protein called Peptide chain release factor RF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	6	361	Total	C	N	O	S	0	0
			2855	1757	501	587	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
6	167	LYS	GLU	engineered mutation	UNP P07012

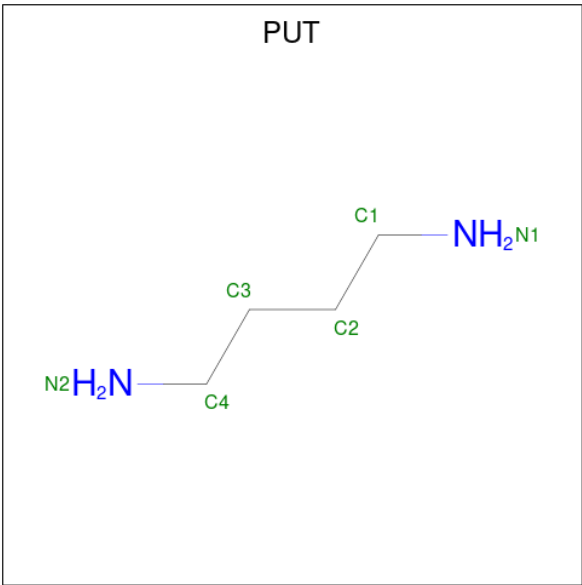
- Molecule 56 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	G	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	2	90	Total	Mg	0
			90	90	
57	5	2	Total	Mg	0
			2	2	
57	1	232	Total	Mg	0
			232	232	
57	3	5	Total	Mg	0
			5	5	
57	C	1	Total	Mg	0
			1	1	
57	Q	1	Total	Mg	0
			1	1	
57	b	1	Total	Mg	0
			1	1	

- Molecule 58 is 1,4-DIAMINOBUTANE (CCD ID: PUT) (formula: C₄H₁₂N₂).



Mol	Chain	Residues	Atoms			AltConf
58	2	1	Total	C	N	0
			6	4	2	
58	2	1	Total	C	N	0
			6	4	2	
58	2	1	Total	C	N	0
			6	4	2	
58	2	1	Total	C	N	0
			6	4	2	
58	2	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	

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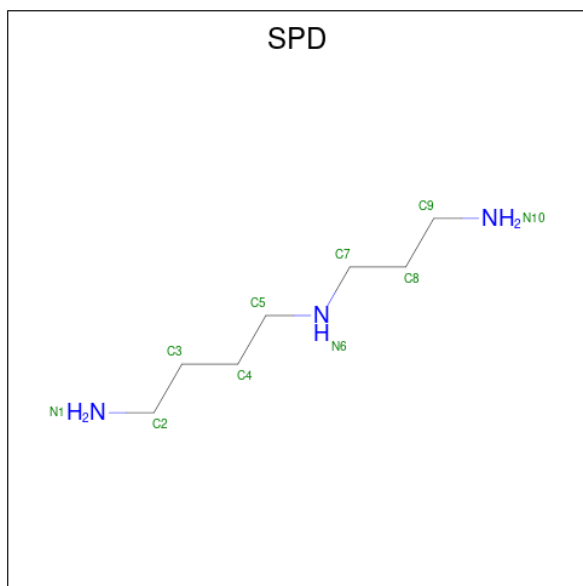
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Mol	Chain	Residues	Atoms			AltConf
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	1	1	Total	C	N	0
			6	4	2	
58	C	1	Total	C	N	0
			6	4	2	

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

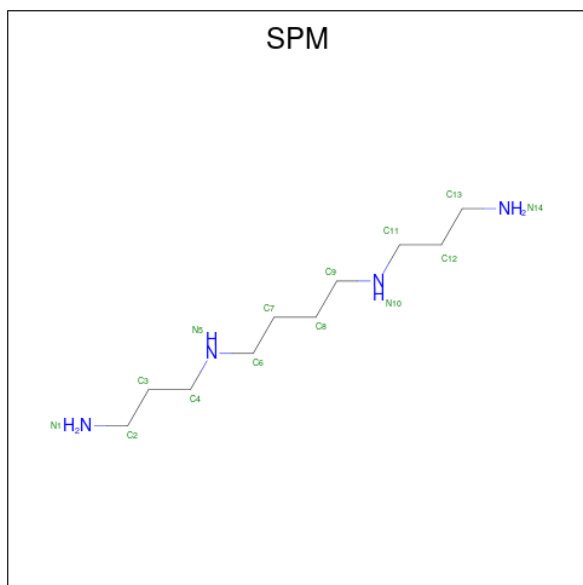
Mol	Chain	Residues	Atoms		AltConf
59	2	34	Total	K	0
			34	34	
59	1	92	Total	K	0
			92	92	

- Molecule 60 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	
60	1	1	Total	C	N	0
			10	7	3	

- Molecule 61 is SPERMINE (CCD ID: SPM) (formula: $C_{10}H_{26}N_4$).



Mol	Chain	Residues	Atoms			AltConf
61	1	1	Total	C	N	0
			14	10	4	
61	1	1	Total	C	N	0
			14	10	4	

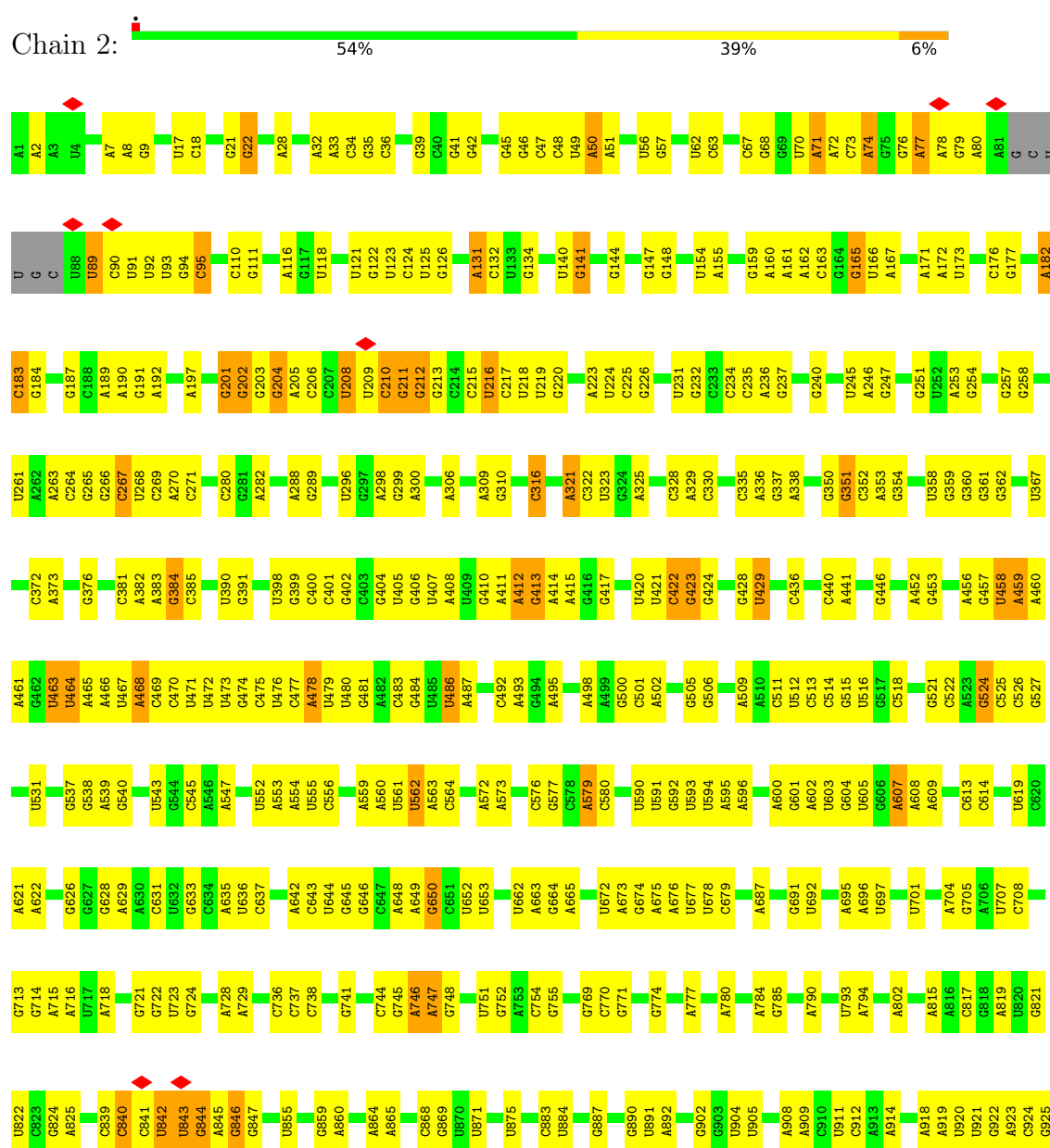
- Molecule 62 is ZINC ION (CCD ID: ZN) (formula: Zn).

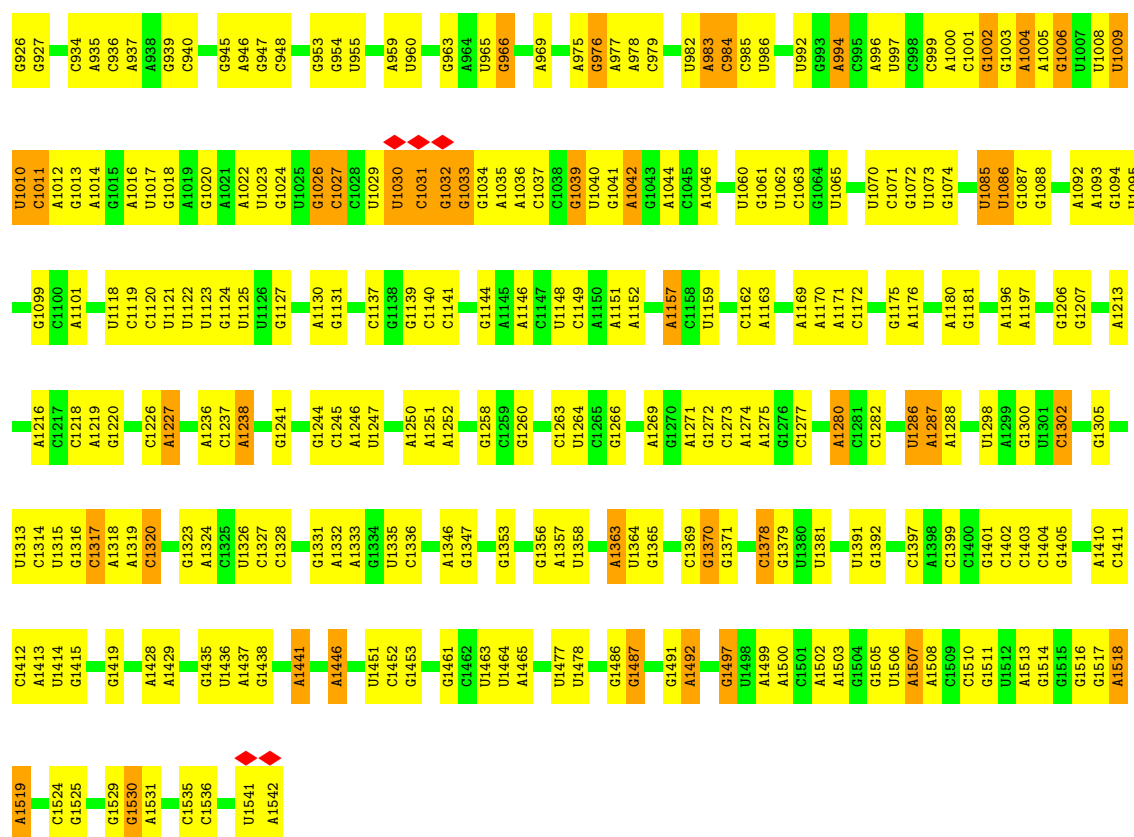
Mol	Chain	Residues	Atoms		AltConf
62	f	1	Total 1	Zn 1	0
62	a	1	Total 1	Zn 1	0

3 Residue-property plots

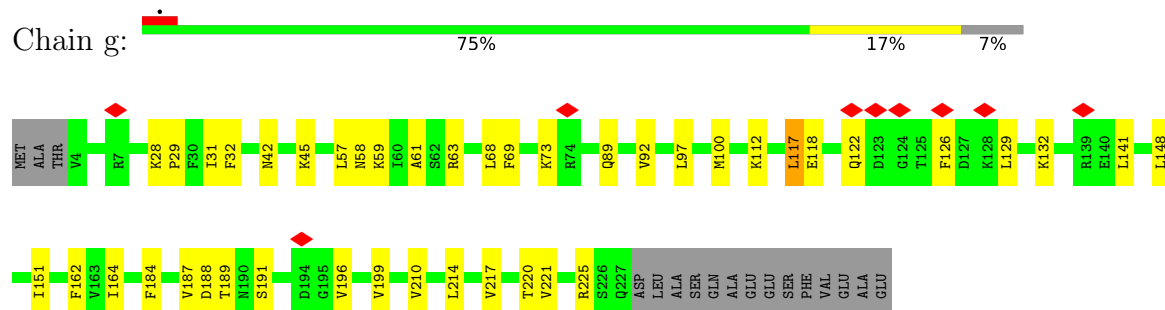
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: 16S rRNA

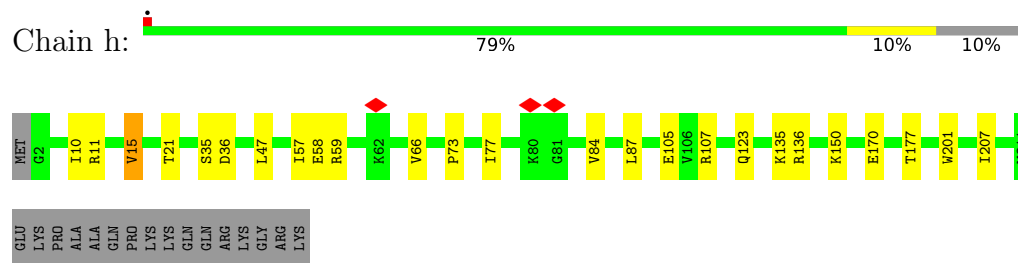




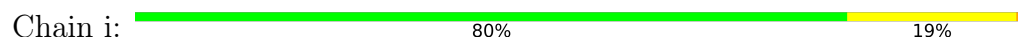
• Molecule 2: Small ribosomal subunit protein uS2

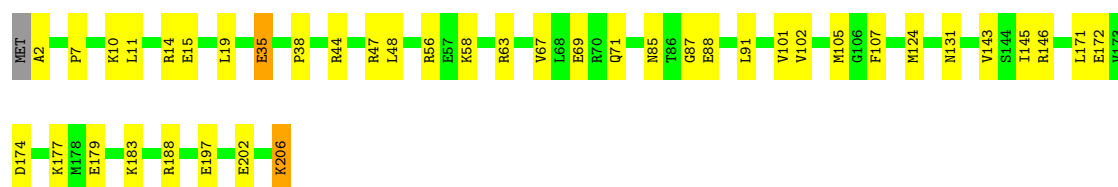


• Molecule 3: Small ribosomal subunit protein uS3

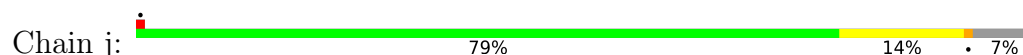


• Molecule 4: Small ribosomal subunit protein uS4

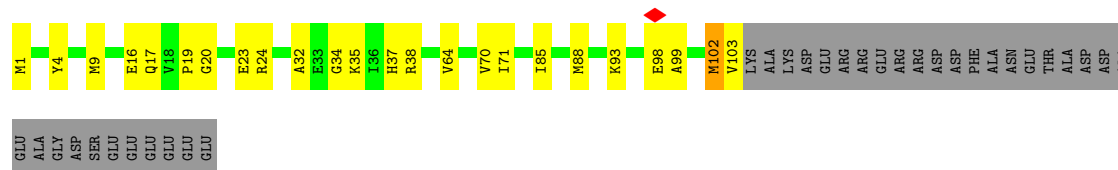




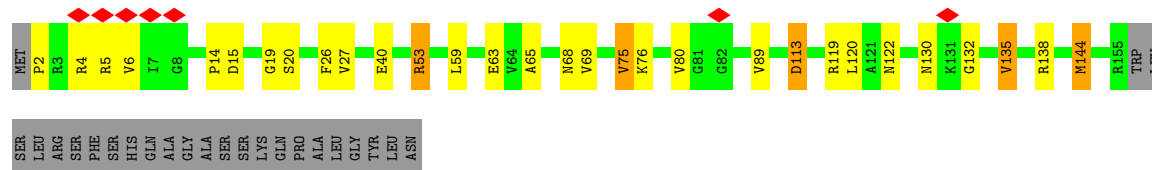
- Molecule 5: Small ribosomal subunit protein uS5



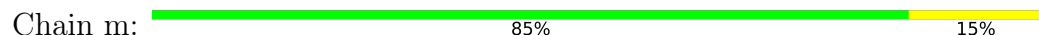
- Molecule 6: Small ribosomal subunit protein bS6, fully modified isoform



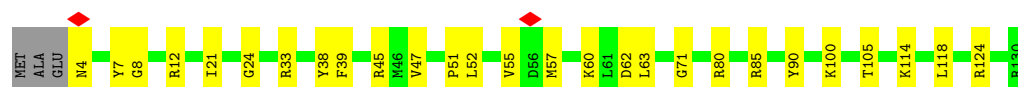
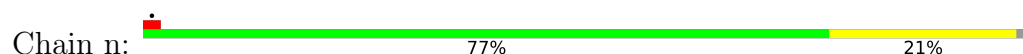
- Molecule 7: Small ribosomal subunit protein uS7



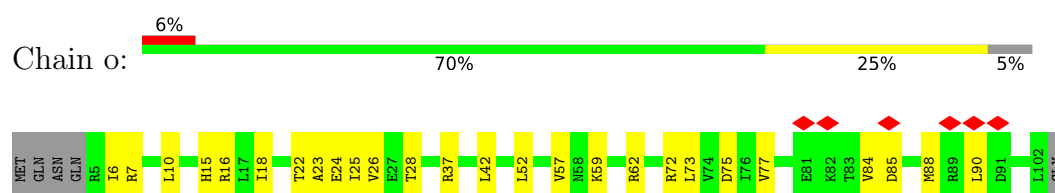
- Molecule 8: Small ribosomal subunit protein uS8



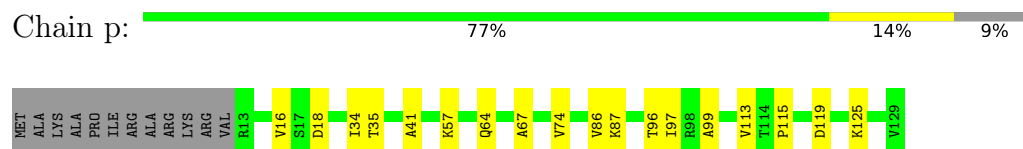
- Molecule 9: Small ribosomal subunit protein uS9



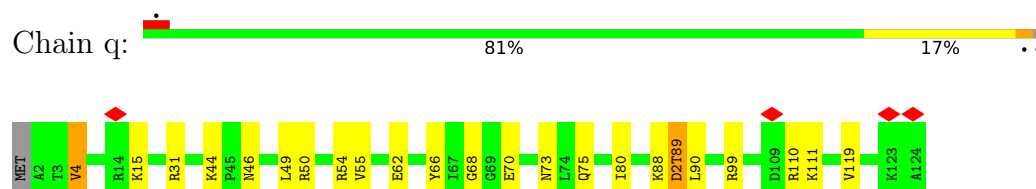
- Molecule 10: Small ribosomal subunit protein uS10



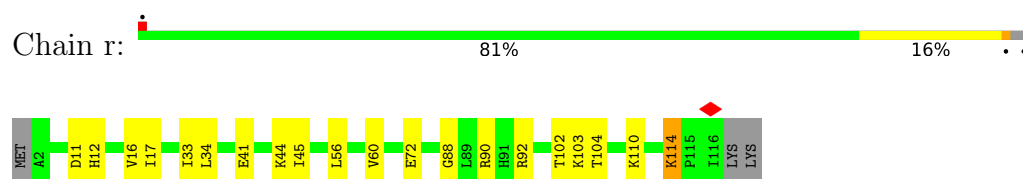
- Molecule 11: Small ribosomal subunit protein uS11



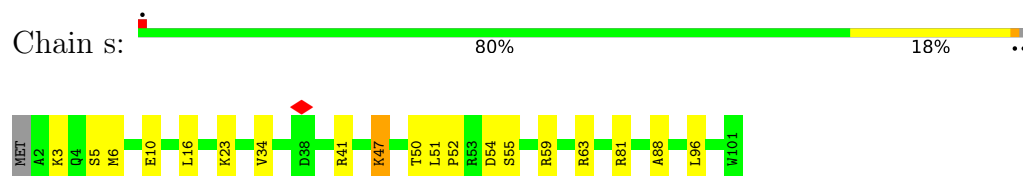
- Molecule 12: Small ribosomal subunit protein uS12



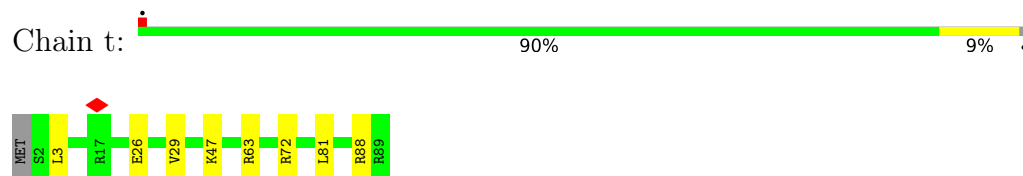
- Molecule 13: Small ribosomal subunit protein uS13



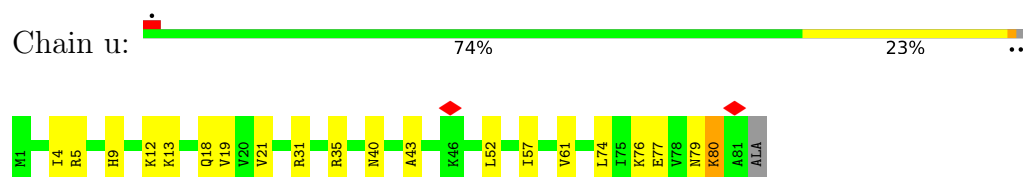
- Molecule 14: Small ribosomal subunit protein uS14



- Molecule 15: Small ribosomal subunit protein uS15



- Molecule 16: Small ribosomal subunit protein bS16



- Molecule 17: Small ribosomal subunit protein uS17

Chain v:  70% 21% 6%



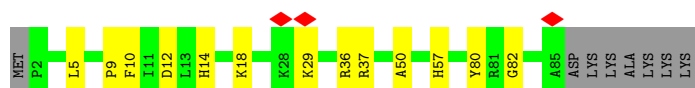
- Molecule 18: Small ribosomal subunit protein bS18

Chain w:  79% 9% 12%



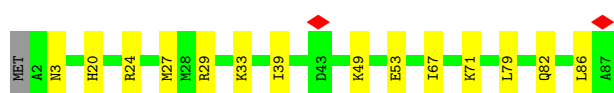
- Molecule 19: Small ribosomal subunit protein uS19

Chain x:  77% 14% 9%



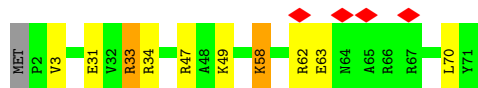
- Molecule 20: Small ribosomal subunit protein bS20

Chain y:  83% 16% 1%

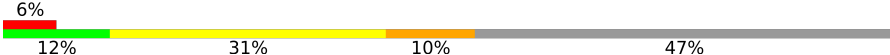


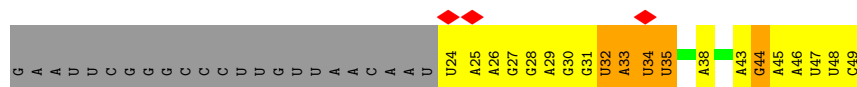
- Molecule 21: Small ribosomal subunit protein bS21

Chain z:  6% 85% 11%



- Molecule 22: mRNA

Chain 4:  6% 12% 31% 10% 47%



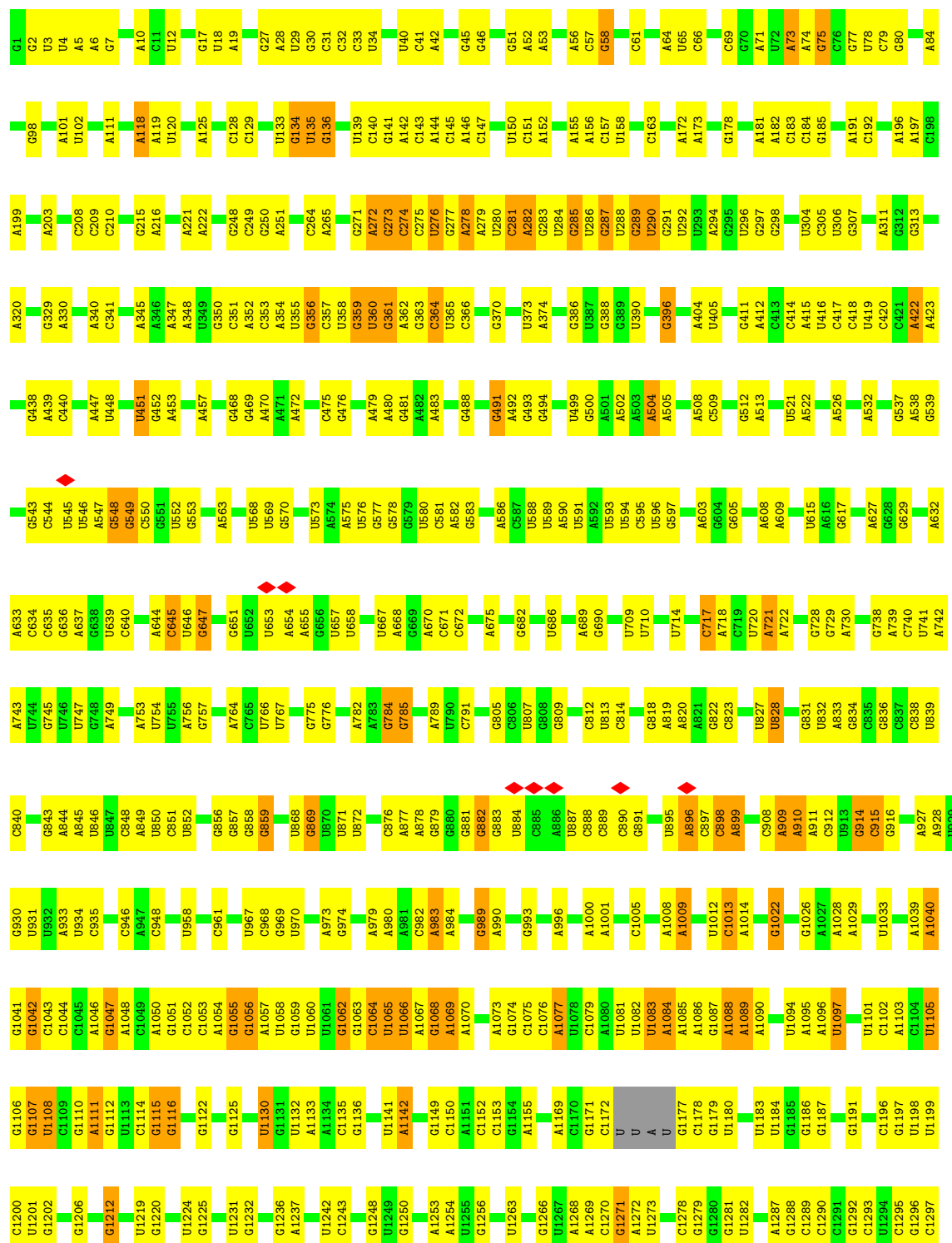
- Molecule 23: tRNA(fMet)

Chain 5:  50% 46% 4%

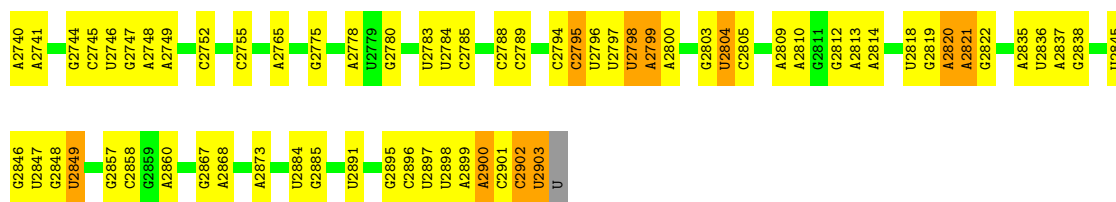


• Molecule 24: 23S rRNA

Chain 1: 59% 36% 5%

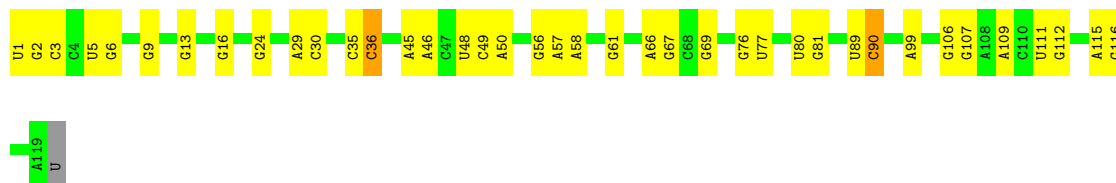


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U2615	U2519	U2402	G2294	A2199	G2136	A1938	G1813	U1716	U1590	C1499	A1413	A1301
C2626	C2520	A2406	A2298	A2204	U2137	U1939	U1816	A1717	A1591	G1500	U1415	C1306
U2629	G2525	A2406	U2299	G2206	G2138	U1946	G1817	U1720	U1594	U1507	G1416	A1307
C2636	G2529	G2410	G2303	A2211	U2139	U1947	U1818	G1721	C1595	A1508	A1419	A1306
U2637	G2532	A2411	G2304	A2212	G2140	C1947	G1824	C1726	A1596	G1509	A1420	C1315
G2638	G2533	A2412	U2305	G2215	G2141	C1965	U1828	C1727	A1597	G1510	U1317	U1316
A2639	G2537	U2419	G2307	G2216	A2142	A1966	A1829	U1729	U1599	A1509	U1318	G1317
G2640	A2534	A2425	G2308	G2217	G2143	C1967	U1839	C1730	G1601	G1513	C1319	C1320
G2641	U2537	A2425	U2312	G2217	U2144	U1970	G1840	G1731	U1602	A1515	G1423	A1321
C2646	C2538	G2429	U2313	A2225	C2145	U1971	U1841	C1732	A1603	C1526	A1430	A1322
G2648	G2543	A2430	A2314	G2226	G2146	U1972	G1842	G1733	C1607	G1527	A1431	C1323
C2649	G2544	A2435	G2315	A2227	A2147	U1991	C1843	U1735	U1608	A1528	A1434	U1329
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A2657	U2548	C2442	A2322	G2230	C2150	U1993	A1847	G1737	A1614	G1531	U1438	U1352
G2661	U2554	C2443	U2323	U2233	U2151	G2012	A1853	A1738	A1614	A1532	A1439	A1353
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U2688	G2566	G2458	A2333	U2244	A2158	C2025	G1869	C1760	C1646	C1541	G1448	C1362
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U2690	U2571	U2460	A2335	G2246	C2160	G2027	A1871	C1764	U1648	A1543	A1463	A1366
U2698	C2572	C2462	A2336	A2247	G2161	U2028	A1872	G1771	G1649	A1545	U1468	G1370
C2699	A2573	A2469	G2339	G2250	G2162	G2029	C1873	A1772	C1656	C1547	U1459	G1371
U2701	G2574	G2470	A2340	G2251	A2163	A2030	C1874	A1773	U1657	A1548	U1460	U1375
C2710	C2575	A2476	G2345	U2259	C2164	G2032	G1875	U1789	A1688	U1549	G1464	A1378
G2714	U2580	U2477	A2346	A2266	G2165	A2033	C1881	U1782	C1674	U1554	G1465	U1379
C2715	G2581	A2478	C2347	A2267	U2166	C2036	U1882	C1675	C1558	C1558	A1469	A1383
C2717	G2582	C2483	C2350	A2268	U2167	A2037	U1883	A1676	U1559	A1569	A1470	A1384
G2718	U2583	U2491	G2361	A2273	G2168	U2039	G1884	A1677	A1677	G1560	G1471	A1385
C2723	U2584	G2494	G2372	A2274	A2169	G2040	A1889	C1790	A1678	U1563	G1475	C1386
A2725	U2585	G2495	U2377	A2279	A2170	C2043	A1890	A1791	G1682	C1564	G1478	G1388
A2726	G2590	C2496	A2381	G2283	U2172	G2049	G1906	A1794	U1683	C1566	G1482	A1392
A2727	C2591	C2496	G2382	A2284	A2173	C2050	G1907	C1795	U1684	A1569	G1483	A1393
U2728	G2592	G2502	A2383	A2285	C2175	A2051	G1910	U1796	C1685	A1570	U1484	A1394
G2729	A2600	U2504	G2384	G2286	A2176	C2056	A1913	U1797	G1703	A1571	U1485	A1395
G2732	G2603	U2506	U2384	A2287	C2177	G2056	A1914	G1799	C1704	A1572	U1486	C1399
A2733	U2609	C2507	G2385	G2288	G2178	A2060	G1920	A1801	U1709	U1578	C1493	U1405
	U2613	U2514	A2386	G2290	C2179	G2061	G1929	A1802	A1711	A1583	A1494	U1406
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					U2182							
					A2183							
					A2184							
					U2185							
					G2186							
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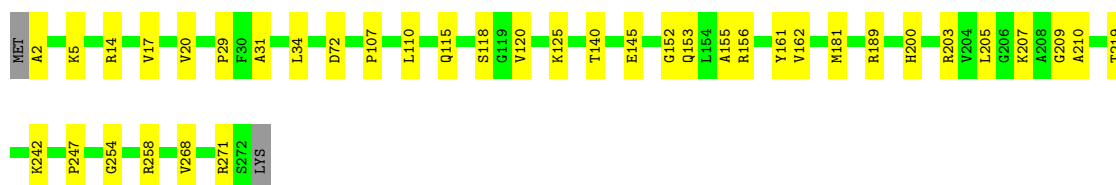
• Molecule 25: 5S rRNA

Chain 3: 67% 31% ..



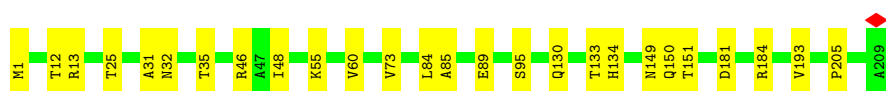
• Molecule 26: Large ribosomal subunit protein uL2

Chain B: 85% 14% .



• Molecule 27: Large ribosomal subunit protein uL3

Chain C: 88% 12%



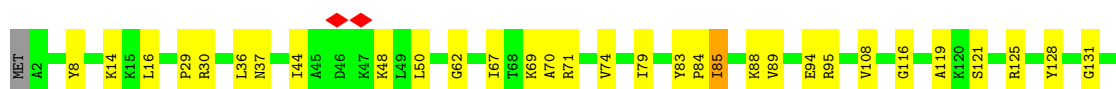
• Molecule 28: Large ribosomal subunit protein uL4

Chain D: 87% 13%



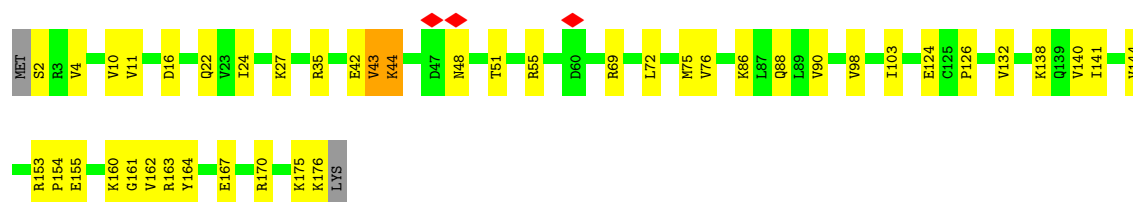
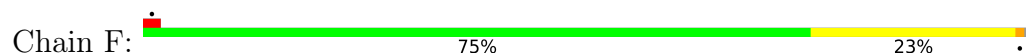
• Molecule 29: Large ribosomal subunit protein uL5

Chain E: 73% 25% ..

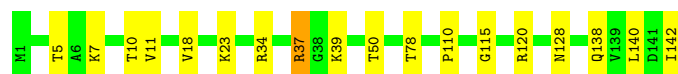
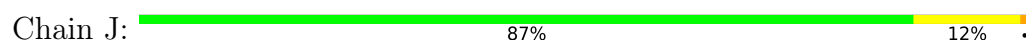




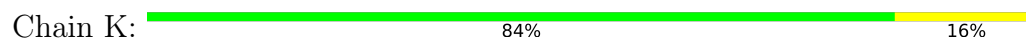
- Molecule 30: Large ribosomal subunit protein uL6



- Molecule 31: Large ribosomal subunit protein uL13



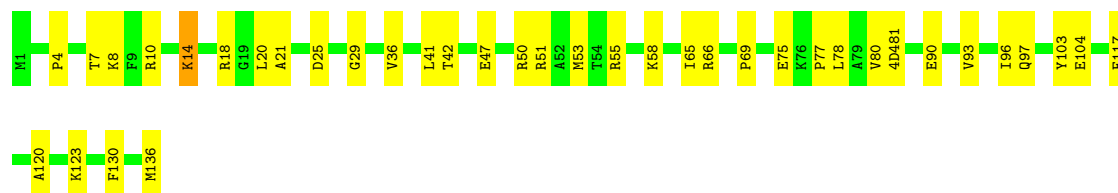
- Molecule 32: 50S ribosomal protein L14



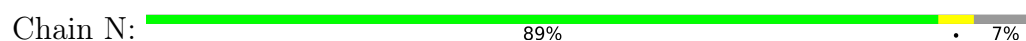
- Molecule 33: 50S ribosomal protein L15



- Molecule 34: Large ribosomal subunit protein uL16



- Molecule 35: 50S ribosomal protein L17





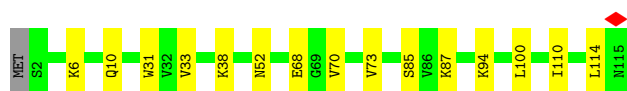
- Molecule 36: 50S ribosomal protein L18

Chain O: 86% 12% ..



- Molecule 37: 50S ribosomal protein L19

Chain P: 86% 13% .



- Molecule 38: 50S ribosomal protein L20

Chain Q: 91% 8% .



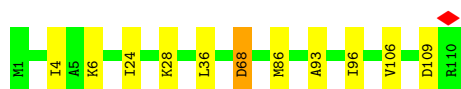
- Molecule 39: 50S ribosomal protein L21

Chain R: 87% 12% .



- Molecule 40: 50S ribosomal protein L22

Chain S: 90% 9% .



- Molecule 41: 50S ribosomal protein L23

Chain T: 83% 10% 7%

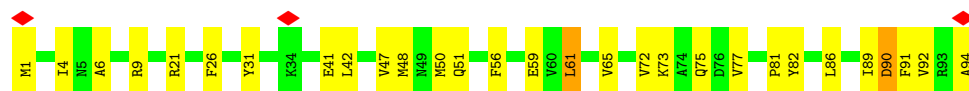


- Molecule 42: 50S ribosomal protein L24

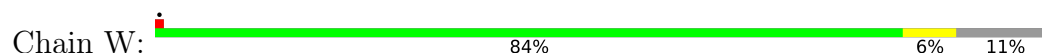
Chain U: 81% 17% .



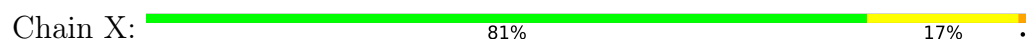
- Molecule 43: 50S ribosomal protein L25



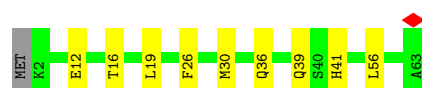
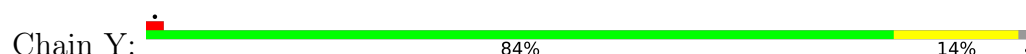
- Molecule 44: 50S ribosomal protein L27



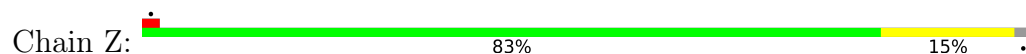
- Molecule 45: 50S ribosomal protein L28



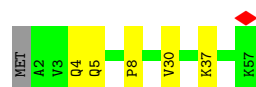
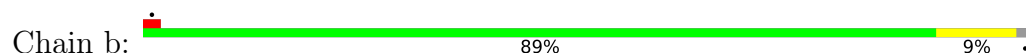
- Molecule 46: 50S ribosomal protein L29



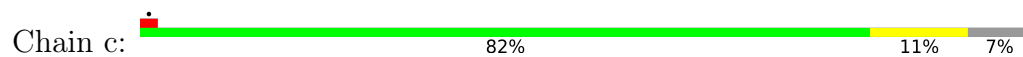
- Molecule 47: 50S ribosomal protein L30



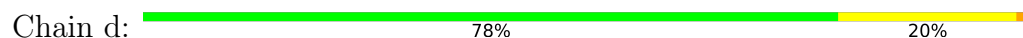
- Molecule 48: 50S ribosomal protein L32



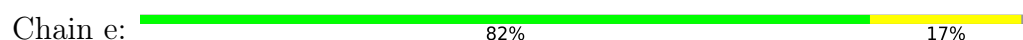
- Molecule 49: 50S ribosomal protein L33



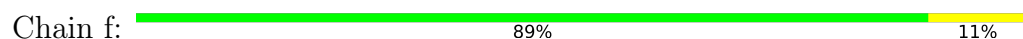
- Molecule 50: 50S ribosomal protein L34



- Molecule 51: 50S ribosomal protein L35



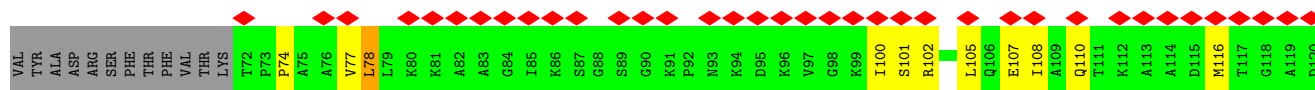
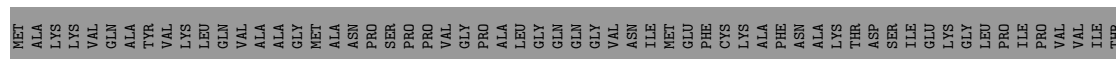
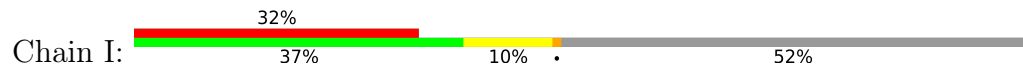
- Molecule 52: 50S ribosomal protein L36



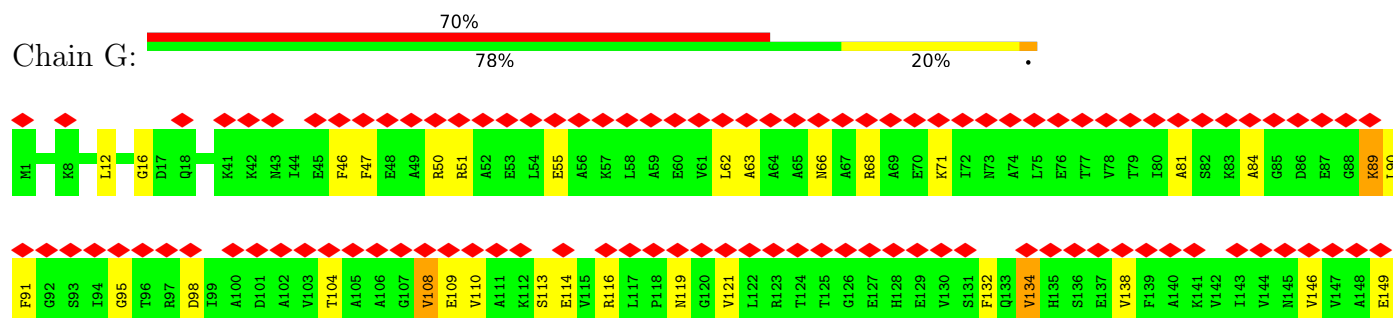
- Molecule 53: Large ribosomal subunit protein bL31A



- Molecule 54: Large ribosomal subunit protein uL11



- Molecule 55: Peptide chain release factor RF2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	100479	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 ($e^-/\text{\AA}^2$)	40.56	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.900	Depositor
Minimum map value	-0.259	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	427.856, 427.856, 427.856	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8228, 0.8228, 0.8228	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H2U, UR3, K, SPD, MEQ, 1MG, OMG, 3TD, SPM, MS6, 6MZ, PSU, 5MU, OMU, 2MA, G7M, MA6, IAS, ZN, D2T, 2MG, PUT, 4OC, 5MC, MG, 4D4, OMC

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	2	0.19	0/36631	0.30	0/57136
2	g	0.16	0/1784	0.36	0/2403
3	h	0.17	0/1675	0.32	0/2256
4	i	0.15	0/1665	0.30	0/2227
5	j	0.18	0/1165	0.38	0/1568
6	k	0.16	0/858	0.31	0/1160
7	l	0.16	0/1230	0.35	0/1649
8	m	0.17	0/989	0.33	0/1326
9	n	0.14	0/1034	0.33	0/1375
10	o	0.18	0/796	0.37	0/1077
11	p	0.18	0/884	0.34	0/1191
12	q	0.17	0/960	0.37	0/1286
13	r	0.15	0/900	0.37	0/1204
14	s	0.17	0/817	0.29	0/1088
15	t	0.16	0/722	0.33	0/964
16	u	0.16	0/653	0.35	0/877
17	v	0.13	0/650	0.32	0/871
18	w	0.16	0/553	0.30	0/742
19	x	0.14	0/685	0.30	0/922
20	y	0.19	0/676	0.29	0/895
21	z	0.16	0/597	0.30	0/792
22	4	0.18	0/628	0.39	0/977
23	5	0.17	0/1859	0.29	0/2894
24	1	0.21	0/69147	0.30	0/107869
25	3	0.16	0/2850	0.26	0/4444
26	B	0.19	0/2121	0.37	0/2852
27	C	0.18	0/1576	0.33	0/2119
28	D	0.19	0/1571	0.33	0/2113
29	E	0.16	0/1434	0.37	0/1926
30	F	0.17	0/1333	0.41	0/1805
31	J	0.17	0/1152	0.29	0/1551

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	K	0.20	0/955	0.36	0/1279
33	L	0.19	0/1062	0.38	0/1413
34	M	0.18	0/1073	0.35	0/1433
35	N	0.21	0/958	0.40	0/1281
36	O	0.15	0/902	0.30	0/1209
37	P	0.19	0/929	0.33	0/1242
38	Q	0.19	0/960	0.32	0/1278
39	R	0.20	0/829	0.40	0/1107
40	S	0.20	0/864	0.33	0/1156
41	T	0.17	0/744	0.40	0/994
42	U	0.14	0/787	0.30	0/1051
43	V	0.17	0/766	0.35	0/1025
44	W	0.19	0/589	0.37	0/779
45	X	0.19	0/635	0.31	0/848
46	Y	0.16	0/502	0.27	0/667
47	Z	0.19	0/453	0.38	0/605
48	b	0.18	0/450	0.32	0/599
49	c	0.16	0/424	0.33	0/565
50	d	0.21	0/380	0.41	0/498
51	e	0.18	0/513	0.35	0/676
52	f	0.20	0/303	0.34	0/397
53	a	0.15	0/488	0.33	0/649
54	I	0.12	0/486	0.32	0/650
55	6	0.19	0/2884	0.36	0/3885
56	G	0.11	0/1122	0.26	0/1515
All	All	0.19	0/159653	0.31	0/238360

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	32966	0	16605	478	0
2	g	1753	0	1780	28	0
3	h	1648	0	1722	14	0
4	i	1643	0	1707	29	0
5	j	1152	0	1196	17	0
6	k	839	0	833	15	0
7	l	1214	0	1267	18	0
8	m	979	0	1031	14	0
9	n	1022	0	1070	19	0
10	o	786	0	828	14	0
11	p	877	0	884	10	0
12	q	957	0	1017	16	0
13	r	891	0	952	14	0
14	s	805	0	844	11	0
15	t	714	0	734	4	0
16	u	643	0	661	11	0
17	v	641	0	682	15	0
18	w	544	0	565	5	0
19	x	668	0	693	15	0
20	y	670	0	719	9	0
21	z	589	0	629	4	0
22	4	560	0	279	19	0
23	5	1665	0	848	10	0
24	1	62252	0	31316	723	0
25	3	2549	0	1291	22	0
26	B	2082	0	2154	27	0
27	C	1566	0	1617	18	0
28	D	1552	0	1619	18	0
29	E	1410	0	1444	32	0
30	F	1313	0	1358	26	0
31	J	1129	0	1162	13	0
32	K	946	0	1023	14	0
33	L	1053	0	1129	9	0
34	M	1075	0	1145	24	0
35	N	945	0	989	2	0
36	O	892	0	923	10	0
37	P	917	0	962	11	0
38	Q	947	0	1019	8	0
39	R	816	0	839	6	0
40	S	857	0	922	7	0
41	T	738	0	807	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	U	779	0	830	11	0
43	V	753	0	780	20	0
44	W	582	0	599	5	0
45	X	625	0	652	12	0
46	Y	501	0	531	6	0
47	Z	449	0	488	6	0
48	b	444	0	458	5	0
49	c	417	0	451	4	0
50	d	377	0	418	10	0
51	e	504	0	572	7	0
52	f	302	0	340	2	0
53	a	480	0	478	15	0
54	I	484	0	521	9	0
55	6	2855	0	2756	63	0
56	G	1111	0	1148	18	0
57	1	232	0	0	0	0
57	2	90	0	0	0	0
57	3	5	0	0	0	0
57	5	2	0	0	0	0
57	C	1	0	0	0	0
57	Q	1	0	0	0	0
57	b	1	0	0	0	0
58	1	90	0	180	6	0
58	2	30	0	60	5	0
58	C	6	0	12	0	0
59	1	92	0	0	0	0
59	2	34	0	0	0	0
60	1	100	0	190	2	0
61	1	28	0	52	2	0
62	a	1	0	0	0	0
62	f	1	0	0	0	0
All	All	148642	0	100781	1788	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 7.

The worst 5 of 1788 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)
24:1:2100:G:H1	24:1:2189:U:H3	1.19	0.88
1:2:673:A:H2'	1:2:674:G:C8	2.17	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:568:U:H1'	24:1:2030:6MZ:H9C1	1.63	0.78
1:2:946:A:H2'	1:2:947:G:C8	2.19	0.77
1:2:73:C:HO2'	1:2:74:A:H8	1.33	0.77

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	
2	g	222/241 (92%)	213 (96%)	9 (4%)	0	100	100
3	h	208/233 (89%)	202 (97%)	6 (3%)	0	100	100
4	i	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
5	j	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
6	k	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
7	l	152/179 (85%)	148 (97%)	4 (3%)	0	100	100
8	m	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	n	125/130 (96%)	123 (98%)	2 (2%)	0	100	100
10	o	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	35
11	p	113/129 (88%)	109 (96%)	4 (4%)	0	100	100
12	q	120/124 (97%)	115 (96%)	5 (4%)	0	100	100
13	r	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
14	s	98/101 (97%)	98 (100%)	0	0	100	100
15	t	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
16	u	79/82 (96%)	75 (95%)	3 (4%)	1 (1%)	9	28
17	v	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
18	w	64/75 (85%)	64 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	x	82/92 (89%)	82 (100%)	0	0	100	100
20	y	84/87 (97%)	83 (99%)	1 (1%)	0	100	100
21	z	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
26	B	269/273 (98%)	266 (99%)	3 (1%)	0	100	100
27	C	206/209 (99%)	201 (98%)	5 (2%)	0	100	100
28	D	199/201 (99%)	198 (100%)	1 (0%)	0	100	100
29	E	175/179 (98%)	169 (97%)	6 (3%)	0	100	100
30	F	173/177 (98%)	169 (98%)	4 (2%)	0	100	100
31	J	140/142 (99%)	140 (100%)	0	0	100	100
32	K	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
33	L	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
34	M	132/136 (97%)	131 (99%)	1 (1%)	0	100	100
35	N	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
36	O	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
37	P	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
38	Q	115/118 (98%)	115 (100%)	0	0	100	100
39	R	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
40	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
41	T	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
42	U	100/104 (96%)	97 (97%)	3 (3%)	0	100	100
43	V	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
44	W	74/85 (87%)	71 (96%)	3 (4%)	0	100	100
45	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
46	Y	60/63 (95%)	60 (100%)	0	0	100	100
47	Z	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
48	b	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
49	c	49/55 (89%)	49 (100%)	0	0	100	100
50	d	44/46 (96%)	42 (96%)	2 (4%)	0	100	100
51	e	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
52	f	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
53	a	56/70 (80%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	I	66/142 (46%)	64 (97%)	2 (3%)	0	100	100
55	6	358/365 (98%)	352 (98%)	6 (2%)	0	100	100
56	G	147/149 (99%)	139 (95%)	8 (5%)	0	100	100
All	All	6015/6420 (94%)	5880 (98%)	133 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	o	57	VAL
16	u	80	LYS

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	
2	g	186/199 (94%)	184 (99%)	2 (1%)	65	85
3	h	172/190 (90%)	169 (98%)	3 (2%)	53	80
4	i	172/173 (99%)	168 (98%)	4 (2%)	44	75
5	j	119/126 (94%)	116 (98%)	3 (2%)	42	73
6	k	90/116 (78%)	87 (97%)	3 (3%)	33	66
7	l	127/147 (86%)	119 (94%)	8 (6%)	16	41
8	m	104/105 (99%)	103 (99%)	1 (1%)	68	86
9	n	105/107 (98%)	104 (99%)	1 (1%)	68	86
10	o	86/90 (96%)	83 (96%)	3 (4%)	32	64
11	p	89/98 (91%)	89 (100%)	0	100	100
12	q	102/103 (99%)	100 (98%)	2 (2%)	48	77
13	r	93/96 (97%)	90 (97%)	3 (3%)	34	67
14	s	83/84 (99%)	82 (99%)	1 (1%)	63	84
15	t	76/77 (99%)	74 (97%)	2 (3%)	40	72
16	u	65/65 (100%)	64 (98%)	1 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	v	73/78 (94%)	71 (97%)	2 (3%)	39	71
18	w	57/65 (88%)	57 (100%)	0	100	100
19	x	72/79 (91%)	72 (100%)	0	100	100
20	y	65/66 (98%)	61 (94%)	4 (6%)	16	42
21	z	60/61 (98%)	54 (90%)	6 (10%)	7	21
26	B	216/218 (99%)	216 (100%)	0	100	100
27	C	163/163 (100%)	162 (99%)	1 (1%)	78	91
28	D	165/165 (100%)	161 (98%)	4 (2%)	43	74
29	E	148/150 (99%)	145 (98%)	3 (2%)	48	77
30	F	136/138 (99%)	131 (96%)	5 (4%)	30	62
31	J	116/116 (100%)	114 (98%)	2 (2%)	53	80
32	K	104/104 (100%)	102 (98%)	2 (2%)	50	78
33	L	103/103 (100%)	100 (97%)	3 (3%)	37	70
34	M	107/107 (100%)	103 (96%)	4 (4%)	30	62
35	N	98/103 (95%)	96 (98%)	2 (2%)	48	77
36	O	86/87 (99%)	83 (96%)	3 (4%)	32	64
37	P	99/100 (99%)	99 (100%)	0	100	100
38	Q	89/90 (99%)	89 (100%)	0	100	100
39	R	84/84 (100%)	79 (94%)	5 (6%)	17	43
40	S	93/93 (100%)	91 (98%)	2 (2%)	45	75
41	T	80/84 (95%)	78 (98%)	2 (2%)	42	73
42	U	83/85 (98%)	83 (100%)	0	100	100
43	V	78/78 (100%)	75 (96%)	3 (4%)	29	61
44	W	58/63 (92%)	58 (100%)	0	100	100
45	X	67/68 (98%)	66 (98%)	1 (2%)	57	81
46	Y	54/55 (98%)	53 (98%)	1 (2%)	50	78
47	Z	48/49 (98%)	48 (100%)	0	100	100
48	b	47/48 (98%)	47 (100%)	0	100	100
49	c	46/49 (94%)	45 (98%)	1 (2%)	45	75
50	d	38/38 (100%)	37 (97%)	1 (3%)	40	72
51	e	51/52 (98%)	49 (96%)	2 (4%)	28	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
52	f	34/34 (100%)	34 (100%)	0	100	100
53	a	55/62 (89%)	52 (94%)	3 (6%)	19	47
54	I	50/110 (46%)	48 (96%)	2 (4%)	28	60
55	6	305/310 (98%)	290 (95%)	15 (5%)	22	52
56	G	114/114 (100%)	107 (94%)	7 (6%)	17	43
All	All	5011/5245 (96%)	4888 (98%)	123 (2%)	42	73

5 of 123 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
30	F	10	VAL
55	6	234	ILE
34	M	14	LYS
55	6	200	ARG
56	G	108	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
40	S	40	ASN
53	a	61	ASN
42	U	74	ASN
46	Y	27	ASN
55	6	290	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	1534/1542 (99%)	230 (14%)	6 (0%)
22	4	25/49 (51%)	8 (32%)	1 (4%)
23	5	73/76 (96%)	28 (38%)	0
24	1	2897/2904 (99%)	439 (15%)	8 (0%)
25	3	118/120 (98%)	13 (11%)	0
All	All	4647/4691 (99%)	718 (15%)	15 (0%)

5 of 718 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	2	A
1	2	7	A
1	2	9	G
1	2	22	G
1	2	32	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
24	1	277	G
24	1	2162	G
24	1	404	A
24	1	2884	U
24	1	784	G

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

41 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	$\# Z > 2$
12	D2T	q	89	12	7,9,10	0.88	0	6,11,13	1.77	2 (33%)
24	6MZ	1	2030	24	22,25,26	0.31	0	30,36,39	0.43	0
24	2MG	1	1835	24	23,26,27	0.30	0	32,38,41	0.31	0
1	UR3	2	1498	1	19,22,23	0.31	0	26,32,35	0.34	0
24	PSU	1	746	24,57	18,21,22	0.62	0	22,30,33	0.36	0
24	PSU	1	955	24	18,21,22	0.55	0	22,30,33	0.57	0
1	5MC	2	1407	1	18,22,23	0.33	0	26,32,35	0.46	0
24	PSU	1	1911	24	18,21,22	0.51	0	22,30,33	0.57	0
1	2MG	2	1207	59,1	23,26,27	0.31	0	32,38,41	0.32	0
24	OMU	1	2552	24,57	19,22,23	0.30	0	26,31,34	0.43	0
1	G7M	2	527	59,1	23,26,27	0.35	0	35,39,42	0.50	0
24	1MG	1	745	24	22,26,27	0.35	0	33,39,42	0.60	1 (3%)
24	H2U	1	2449	24	18,21,22	0.31	0	21,30,33	0.45	0
24	PSU	1	1917	24	18,21,22	0.53	0	22,30,33	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MA6	2	1518	1	23,26,27	0.30	0	34,38,41	0.66	1 (2%)
1	PSU	2	516	1,57	18,21,22	0.53	0	22,30,33	0.61	1 (4%)
24	2MG	1	2445	24	23,26,27	0.35	0	32,38,41	0.29	0
24	3TD	1	1915	24,57	19,22,23	0.53	0	21,32,35	0.64	0
24	OMC	1	2498	24,57	19,22,23	0.34	0	26,31,34	0.45	0
24	PSU	1	2457	24	18,21,22	0.56	0	22,30,33	0.59	1 (4%)
24	PSU	1	2504	24,59	18,21,22	0.54	0	22,30,33	0.63	0
1	4OC	2	1402	1,57	20,23,24	0.31	0	26,32,35	0.50	0
11	IAS	p	119	11	6,7,8	0.96	0	6,8,10	1.24	1 (16%)
27	MEQ	C	150	27	8,9,10	0.84	0	5,10,12	0.17	0
24	2MA	1	2503	24,57,59	22,25,26	0.97	1 (4%)	33,37,40	1.32	3 (9%)
1	2MG	2	966	1	23,26,27	0.31	0	32,38,41	0.35	0
34	MS6	M	82	34	5,7,8	0.26	0	2,7,9	0.09	0
34	4D4	M	81	34	9,11,12	0.72	0	8,13,15	1.98	3 (37%)
24	5MC	1	1962	24,59	18,22,23	0.30	0	26,32,35	0.43	0
55	MEQ	6	252	55	8,9,10	0.91	0	5,10,12	0.50	0
1	MA6	2	1519	1	23,26,27	0.31	0	34,38,41	0.68	1 (2%)
24	5MU	1	747	24	19,22,23	0.32	0	28,32,35	0.32	0
24	PSU	1	2605	24	18,21,22	0.51	0	22,30,33	0.65	0
24	G7M	1	2069	24,59	23,26,27	0.35	0	35,39,42	0.47	0
1	2MG	2	1516	1	23,26,27	0.32	0	32,38,41	0.44	0
24	PSU	1	2580	24	18,21,22	0.60	1 (5%)	22,30,33	0.67	1 (4%)
24	PSU	1	2604	24	18,21,22	0.50	0	22,30,33	0.64	0
1	5MC	2	967	1	18,22,23	0.31	0	26,32,35	0.43	0
24	5MU	1	1939	24,59	19,22,23	0.32	0	28,32,35	0.42	0
24	OMG	1	2251	24,23,59	23,26,27	0.32	0	33,38,41	0.34	0
24	6MZ	1	1618	24	22,25,26	0.30	0	30,36,39	0.42	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
12	D2T	q	89	12	-	4/7/12/14	-
24	6MZ	1	2030	24	-	2/9/27/28	0/3/3/3
24	2MG	1	1835	24	-	0/9/27/28	0/3/3/3
1	UR3	2	1498	1	-	0/7/25/26	0/2/2/2
24	PSU	1	746	24,57	-	1/7/25/26	0/2/2/2
24	PSU	1	955	24	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	2	1407	1	-	0/7/25/26	0/2/2/2
24	PSU	1	1911	24	-	0/7/25/26	0/2/2/2
1	2MG	2	1207	59,1	-	0/9/27/28	0/3/3/3
24	OMU	1	2552	24,57	-	0/9/27/28	0/2/2/2
1	G7M	2	527	59,1	-	3/7/25/26	0/3/3/3
24	1MG	1	745	24	-	0/7/25/26	0/3/3/3
24	H2U	1	2449	24	-	0/7/38/39	0/2/2/2
24	PSU	1	1917	24	-	0/7/25/26	0/2/2/2
1	MA6	2	1518	1	-	0/11/29/30	0/3/3/3
1	PSU	2	516	1,57	-	0/7/25/26	0/2/2/2
24	2MG	1	2445	24	-	2/9/27/28	0/3/3/3
24	3TD	1	1915	24,57	-	0/7/25/26	0/2/2/2
24	OMC	1	2498	24,57	-	0/9/27/28	0/2/2/2
24	PSU	1	2457	24	-	0/7/25/26	0/2/2/2
24	PSU	1	2504	24,59	-	0/7/25/26	0/2/2/2
1	4OC	2	1402	1,57	-	1/9/29/30	0/2/2/2
11	IAS	p	119	11	-	1/7/7/8	-
27	MEQ	C	150	27	-	3/8/9/11	-
24	2MA	1	2503	24,57,59	-	2/7/25/26	0/3/3/3
1	2MG	2	966	1	-	2/9/27/28	0/3/3/3
34	MS6	M	82	34	-	1/4/6/8	-
34	4D4	M	81	34	-	1/11/12/14	-
24	5MC	1	1962	24,59	-	0/7/25/26	0/2/2/2
55	MEQ	6	252	55	-	3/8/9/11	-
1	MA6	2	1519	1	-	1/11/29/30	0/3/3/3
24	5MU	1	747	24	-	0/7/25/26	0/2/2/2
24	PSU	1	2605	24	-	0/7/25/26	0/2/2/2
24	G7M	1	2069	24,59	-	2/7/25/26	0/3/3/3
1	2MG	2	1516	1	-	0/9/27/28	0/3/3/3
24	PSU	1	2580	24	-	0/7/25/26	0/2/2/2
24	PSU	1	2604	24	-	0/7/25/26	0/2/2/2
1	5MC	2	967	1	-	0/7/25/26	0/2/2/2
24	5MU	1	1939	24,59	-	0/7/25/26	0/2/2/2
24	OMG	1	2251	24,23,59	-	1/9/27/28	0/3/3/3
24	6MZ	1	1618	24	-	0/9/27/28	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	2503	2MA	C6-N6	-3.39	1.25	1.34
24	1	2580	PSU	O4'-C1'	-2.08	1.41	1.43

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	2503	2MA	N6-C6-N1	4.57	123.49	117.03
34	M	81	4D4	NE-CZ-NH2	3.82	127.42	120.70
24	1	2503	2MA	C2-N1-C6	3.79	124.00	118.08
24	1	2503	2MA	C5-C6-N1	-3.47	113.03	119.01
34	M	81	4D4	O-C-CA	-3.04	116.82	124.78

There are no chirality outliers.

5 of 30 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	2	966	2MG	C3'-C4'-C5'-O5'
12	q	89	D2T	CA-CB-CG-OD1
12	q	89	D2T	CA-CB-CG-OD2
27	C	150	MEQ	N-CA-CB-CG
27	C	150	MEQ	C-CA-CB-CG

There are no ring outliers.

11 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	q	89	D2T	1	0
24	1	2030	6MZ	2	0
1	2	1207	2MG	1	0
1	2	1518	MA6	1	0
1	2	1402	4OC	2	0
27	C	150	MEQ	2	0
1	2	966	2MG	1	0
1	2	1519	MA6	2	0
1	2	1516	2MG	2	0
24	1	1939	5MU	1	0
24	1	2251	OMG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 493 ligands modelled in this entry, 460 are monoatomic - leaving 33 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	PUT	2	1685	-	5,5,5	0.13	0	4,4,4	0.15	0
58	PUT	2	1686	-	5,5,5	0.12	0	4,4,4	0.17	0
60	SPD	1	3207	-	9,9,9	0.09	0	8,8,8	0.20	0
58	PUT	1	3332	-	5,5,5	0.12	0	4,4,4	0.17	0
58	PUT	2	1726	-	5,5,5	0.12	0	4,4,4	0.15	0
60	SPD	1	3206	-	9,9,9	0.10	0	8,8,8	0.12	0
58	PUT	1	3333	-	5,5,5	0.12	0	4,4,4	0.17	0
58	PUT	2	1728	-	5,5,5	0.11	0	4,4,4	0.19	0
58	PUT	1	3326	-	5,5,5	0.08	0	4,4,4	0.20	0
58	PUT	1	3344	-	5,5,5	0.12	0	4,4,4	0.15	0
58	PUT	1	3337	-	5,5,5	0.08	0	4,4,4	0.18	0
58	PUT	1	3330	-	5,5,5	0.11	0	4,4,4	0.17	0
60	SPD	1	3213	-	9,9,9	0.08	0	8,8,8	0.13	0
60	SPD	1	3209	-	9,9,9	0.09	0	8,8,8	0.16	0
58	PUT	1	3338	-	5,5,5	0.11	0	4,4,4	0.20	0
58	PUT	1	3329	-	5,5,5	0.10	0	4,4,4	0.16	0
61	SPM	1	3349	-	13,13,13	0.35	0	12,12,12	0.87	0
58	PUT	C	301	-	5,5,5	0.12	0	4,4,4	0.17	0
58	PUT	2	1725	-	5,5,5	0.12	0	4,4,4	0.17	0
58	PUT	1	3351	-	5,5,5	0.09	0	4,4,4	0.18	0
60	SPD	1	3214	-	9,9,9	0.08	0	8,8,8	0.15	0
60	SPD	1	3210	-	9,9,9	0.09	0	8,8,8	0.12	0
58	PUT	1	3327	-	5,5,5	0.11	0	4,4,4	0.16	0
58	PUT	1	3328	-	5,5,5	0.09	0	4,4,4	0.19	0
61	SPM	1	3216	-	13,13,13	0.35	0	12,12,12	0.86	0
58	PUT	1	3334	-	5,5,5	0.11	0	4,4,4	0.16	0
58	PUT	1	3339	-	5,5,5	0.09	0	4,4,4	0.15	0
60	SPD	1	3208	-	9,9,9	0.12	0	8,8,8	0.11	0
60	SPD	1	3215	-	9,9,9	0.11	0	8,8,8	0.09	0
60	SPD	1	3335	-	9,9,9	0.11	0	8,8,8	0.12	0
58	PUT	1	3212	-	5,5,5	0.10	0	4,4,4	0.15	0
58	PUT	1	3331	-	5,5,5	0.12	0	4,4,4	0.19	0
60	SPD	1	3211	-	9,9,9	0.09	0	8,8,8	0.16	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
58	PUT	2	1685	-	-	2/3/3/3	-
58	PUT	2	1686	-	-	1/3/3/3	-
60	SPD	1	3207	-	-	3/7/7/7	-
58	PUT	1	3332	-	-	1/3/3/3	-
58	PUT	2	1726	-	-	3/3/3/3	-
60	SPD	1	3206	-	-	1/7/7/7	-
58	PUT	1	3333	-	-	0/3/3/3	-
58	PUT	2	1728	-	-	1/3/3/3	-
58	PUT	1	3326	-	-	1/3/3/3	-
58	PUT	1	3344	-	-	0/3/3/3	-
58	PUT	1	3337	-	-	0/3/3/3	-
58	PUT	1	3330	-	-	0/3/3/3	-
60	SPD	1	3213	-	-	3/7/7/7	-
60	SPD	1	3209	-	-	2/7/7/7	-
58	PUT	1	3338	-	-	1/3/3/3	-
58	PUT	1	3329	-	-	1/3/3/3	-
61	SPM	1	3349	-	-	6/11/11/11	-
58	PUT	C	301	-	-	1/3/3/3	-
58	PUT	2	1725	-	-	0/3/3/3	-
58	PUT	1	3351	-	-	3/3/3/3	-
60	SPD	1	3214	-	-	0/7/7/7	-
60	SPD	1	3210	-	-	5/7/7/7	-
58	PUT	1	3327	-	-	3/3/3/3	-
58	PUT	1	3328	-	-	2/3/3/3	-
61	SPM	1	3216	-	-	7/11/11/11	-
58	PUT	1	3334	-	-	2/3/3/3	-
58	PUT	1	3339	-	-	1/3/3/3	-
60	SPD	1	3208	-	-	4/7/7/7	-
60	SPD	1	3215	-	-	5/7/7/7	-
60	SPD	1	3335	-	-	3/7/7/7	-
58	PUT	1	3212	-	-	1/3/3/3	-
58	PUT	1	3331	-	-	1/3/3/3	-
60	SPD	1	3211	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	C	301	PUT	C1-C2-C3-C4
61	1	3349	SPM	N5-C6-C7-C8
60	1	3211	SPD	N6-C7-C8-C9
60	1	3215	SPD	C3-C4-C5-N6
61	1	3216	SPM	C7-C8-C9-N10

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	2	1685	PUT	1	0
58	2	1686	PUT	1	0
58	2	1726	PUT	2	0
58	2	1728	PUT	1	0
58	1	3330	PUT	1	0
61	1	3349	SPM	2	0
58	1	3334	PUT	1	0
58	1	3339	PUT	1	0
60	1	3335	SPD	1	0
58	1	3212	PUT	2	0
58	1	3331	PUT	1	0
60	1	3211	SPD	1	0

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.

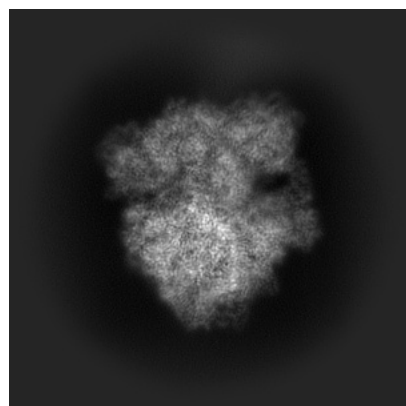
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18458. These allow visual inspection of the internal detail of the map and identification of artifacts.

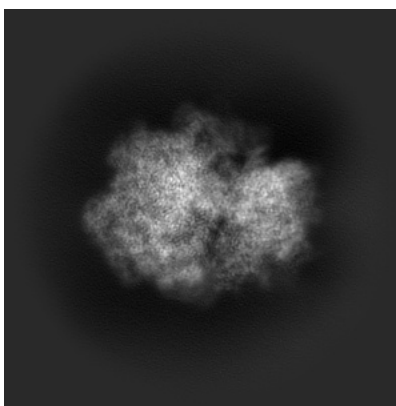
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

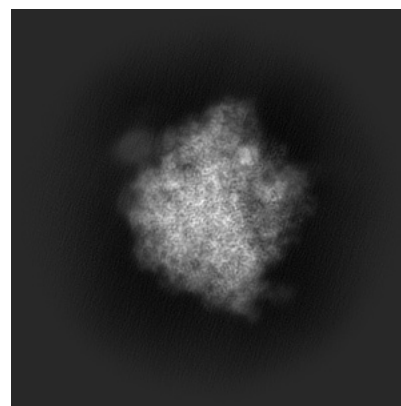
6.1.1 Primary map



X

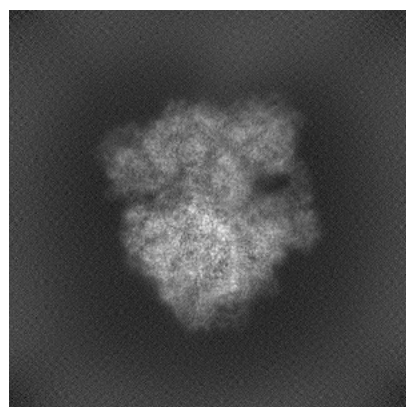


Y

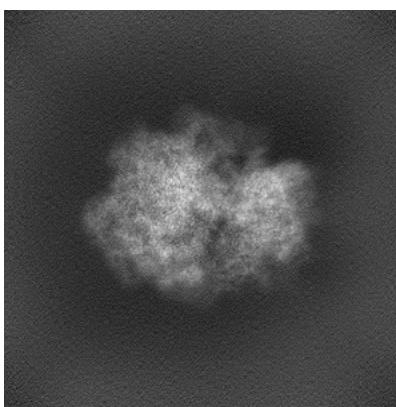


Z

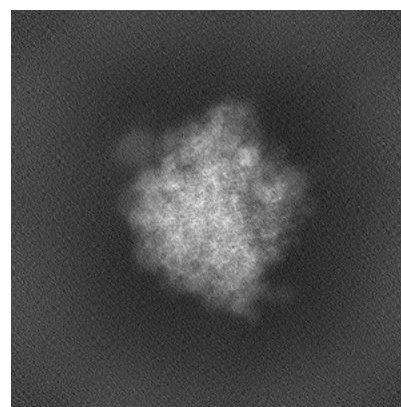
6.1.2 Raw map



X



Y

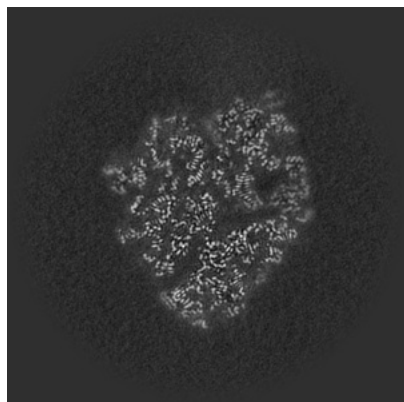


Z

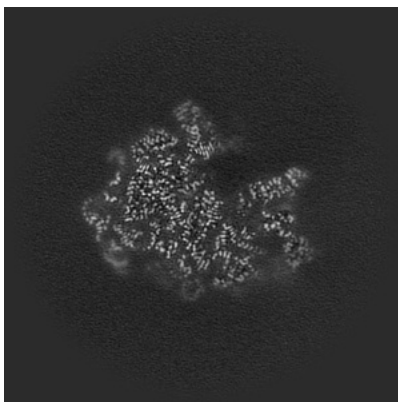
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

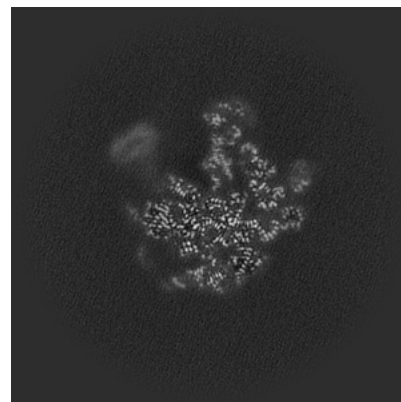
6.2.1 Primary map



X Index: 260

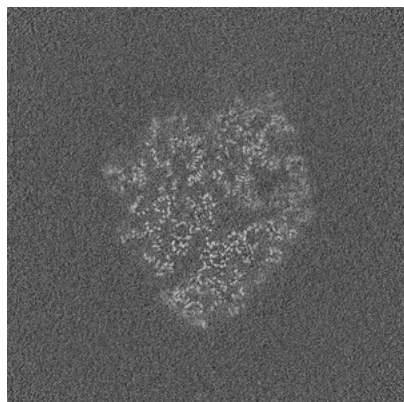


Y Index: 260

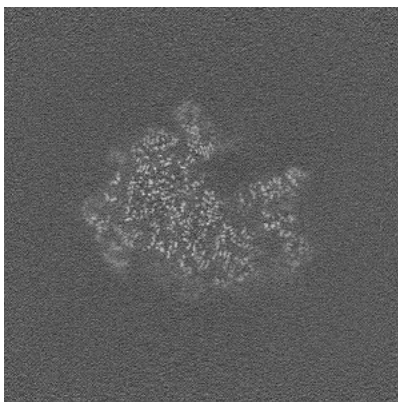


Z Index: 260

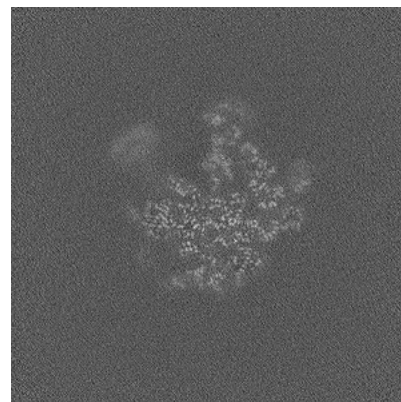
6.2.2 Raw map



X Index: 260



Y Index: 260

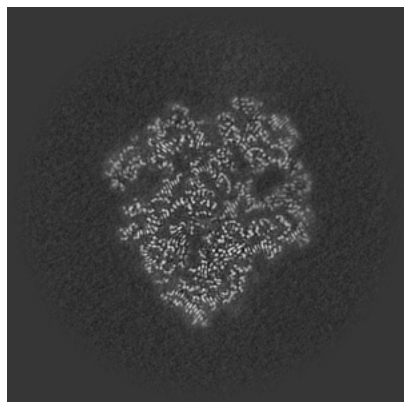


Z Index: 260

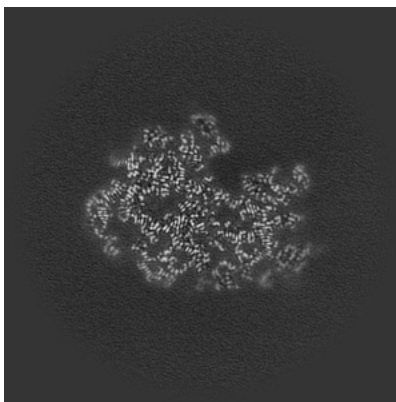
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

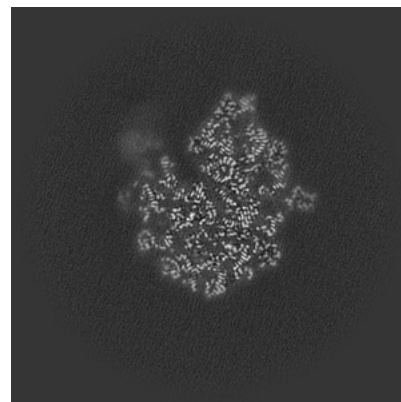
6.3.1 Primary map



X Index: 267

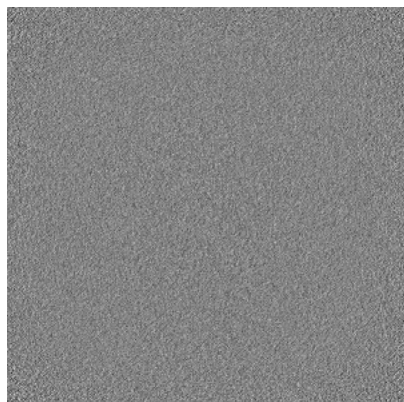


Y Index: 246

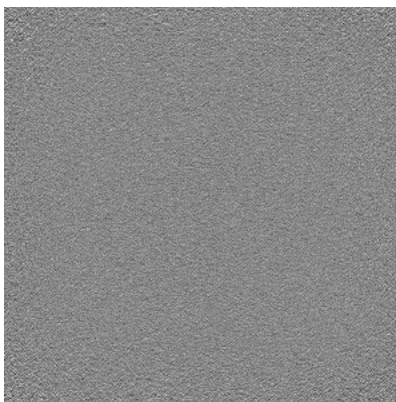


Z Index: 230

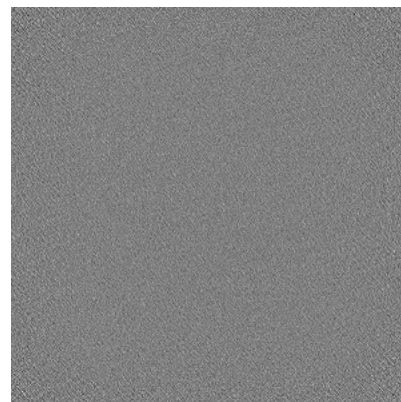
6.3.2 Raw map



X Index: 0



Y Index: 0

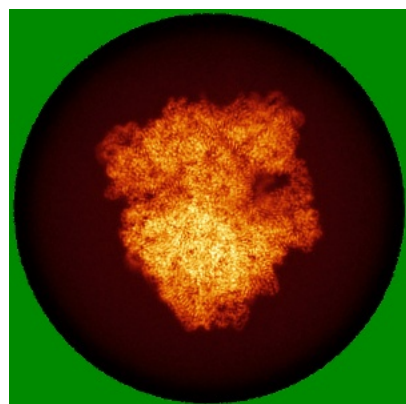


Z Index: 0

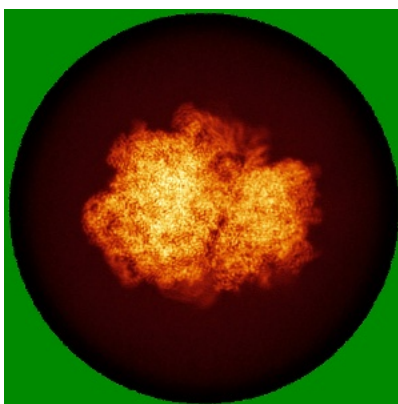
The images above show the largest variance slices of the map in three orthogonal directions.

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

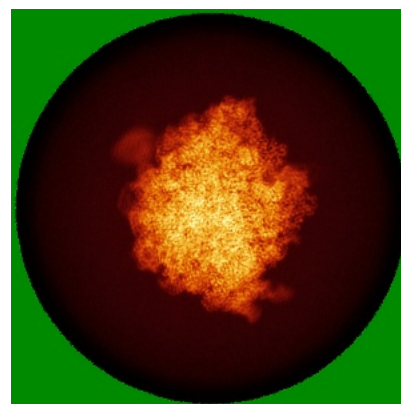
6.4.1 Primary map



X

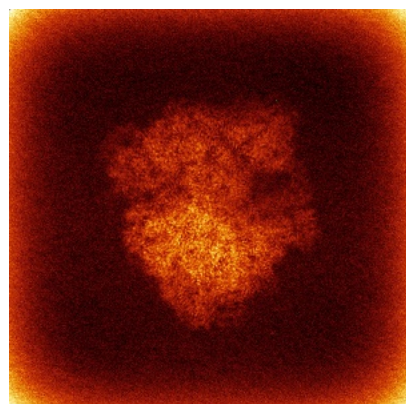


Y

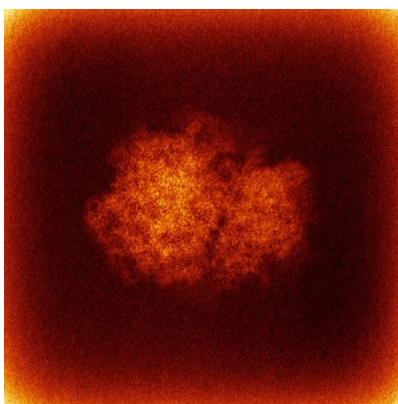


Z

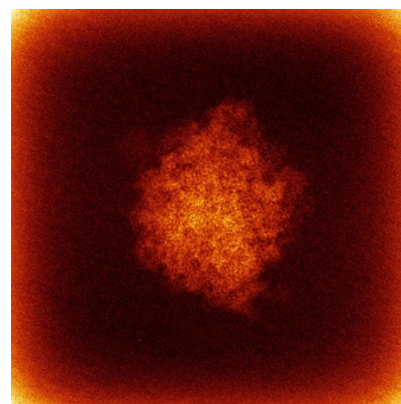
6.4.2 Raw map



X



Y

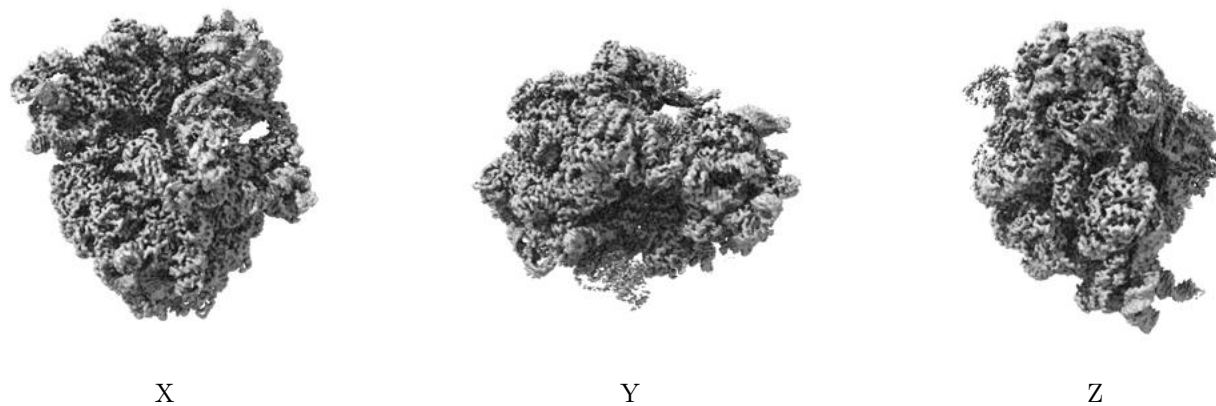


Z

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.

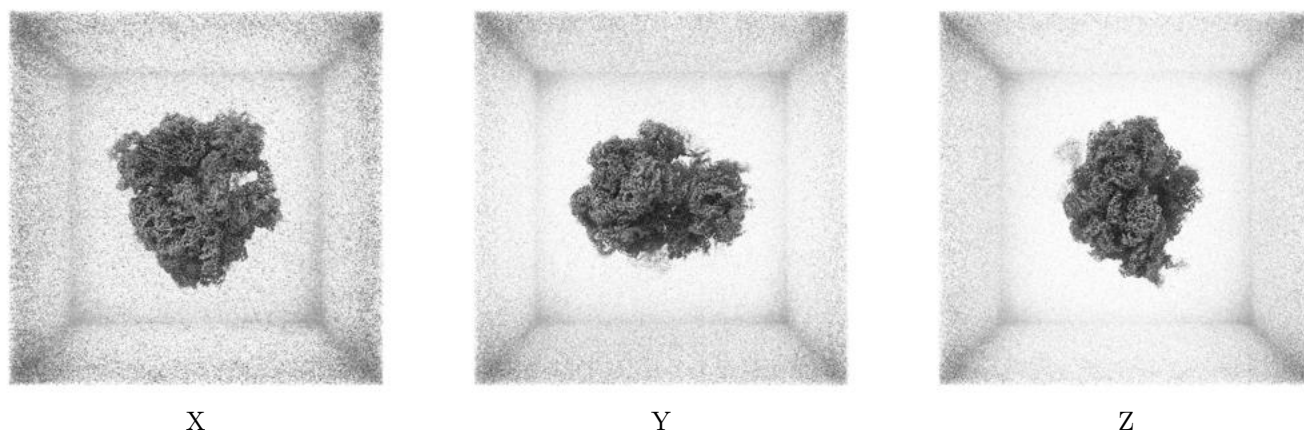
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. 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.

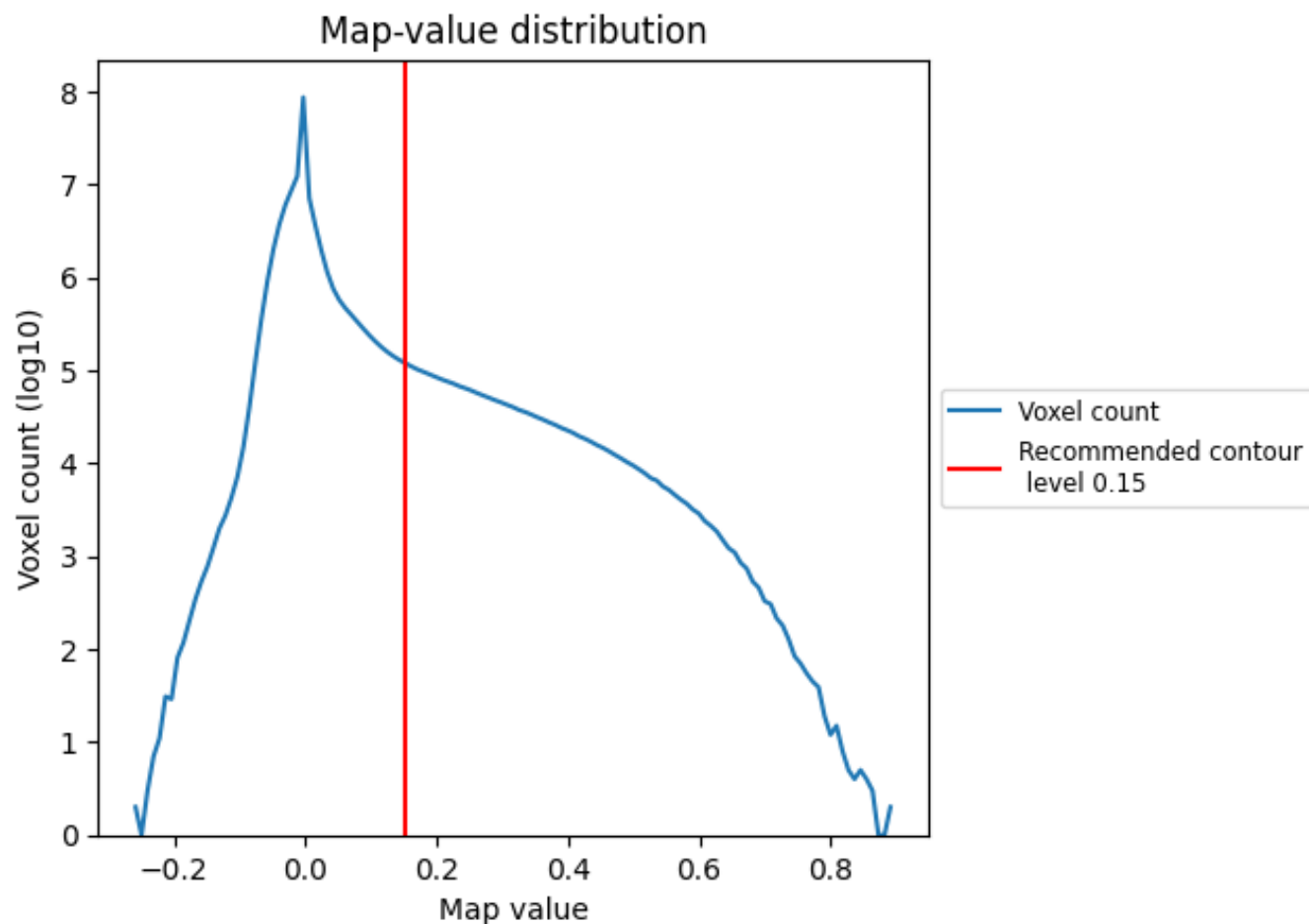
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

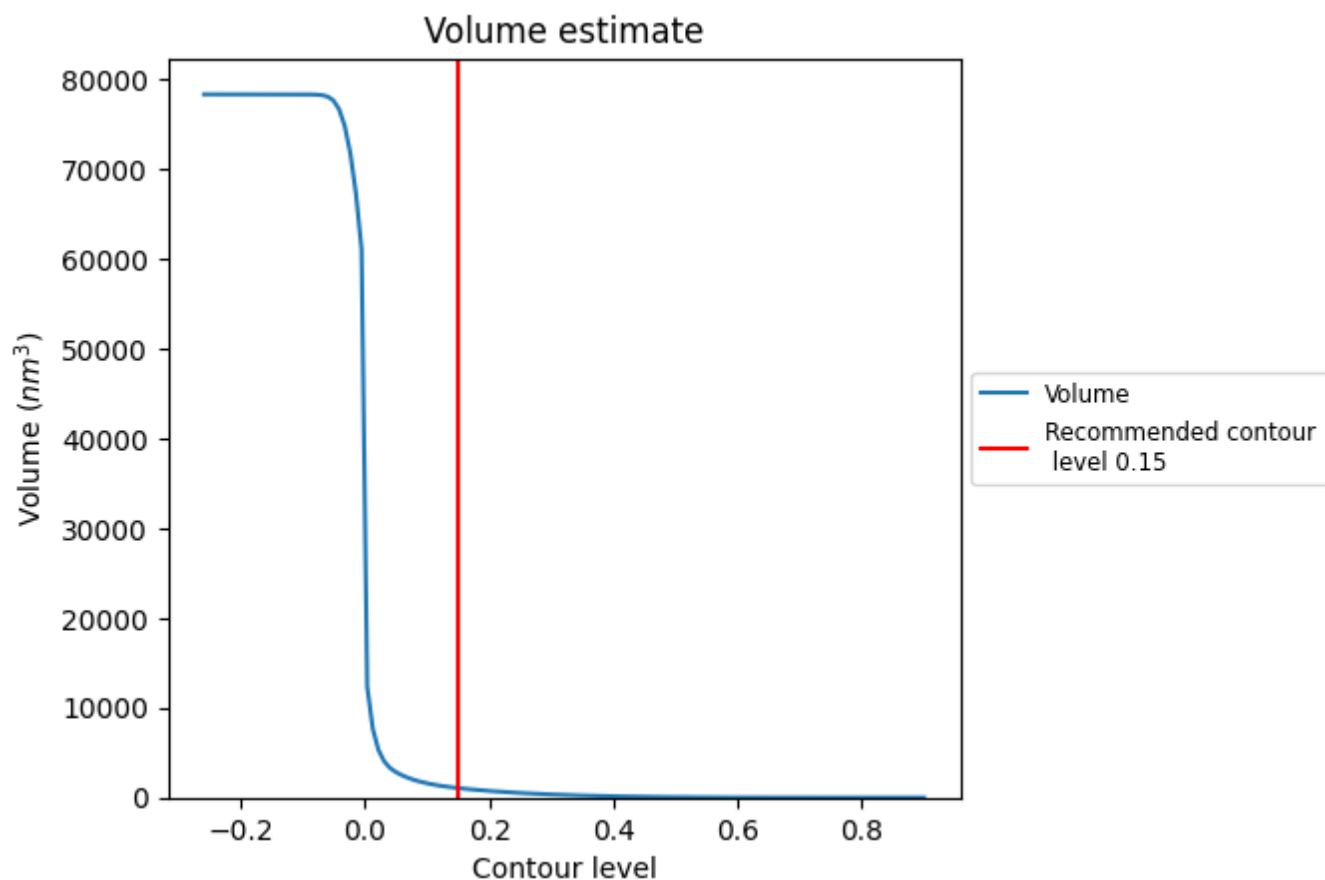
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

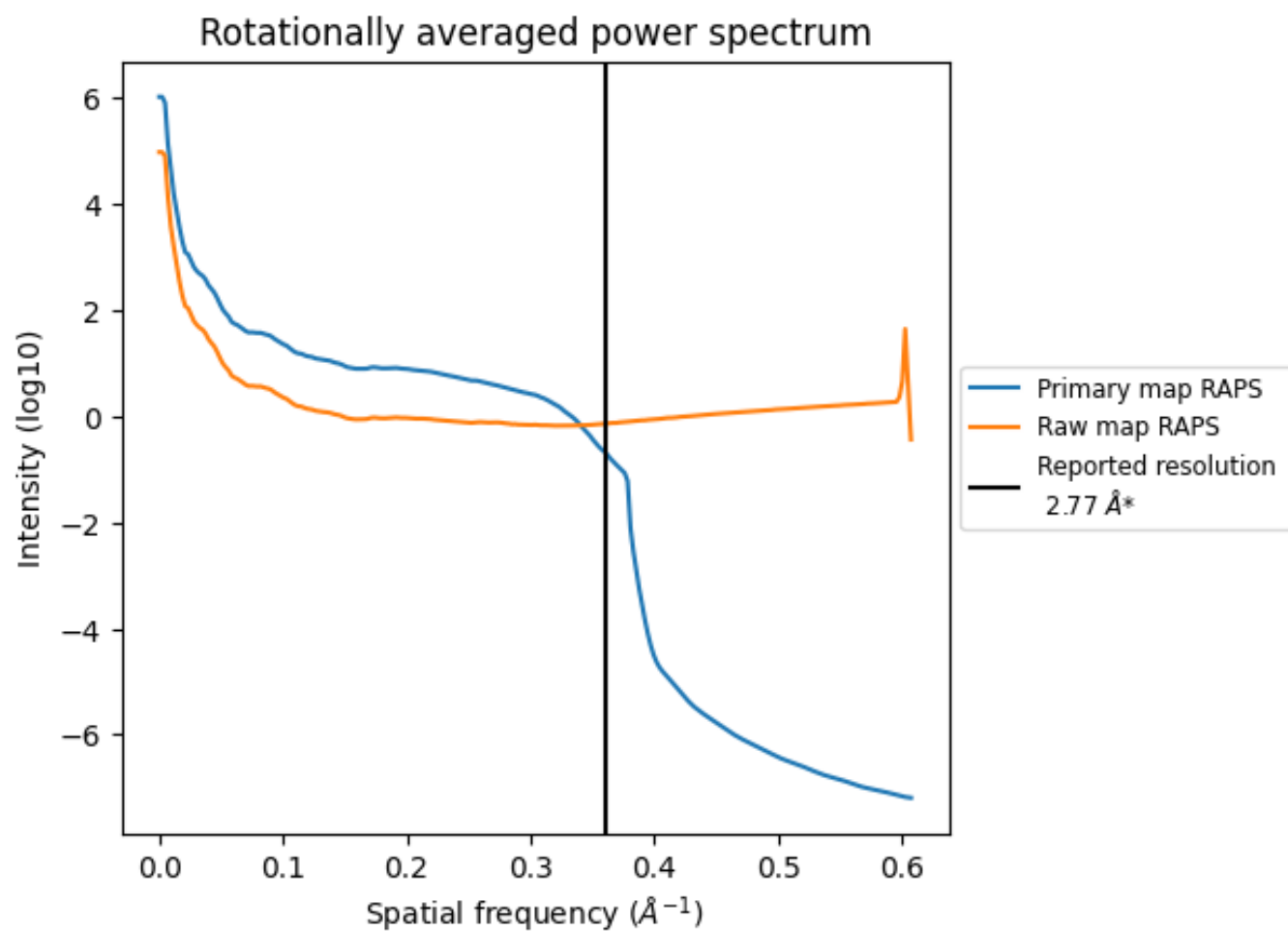
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1055 nm³; this corresponds to an approximate mass of 953 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 ⓘ

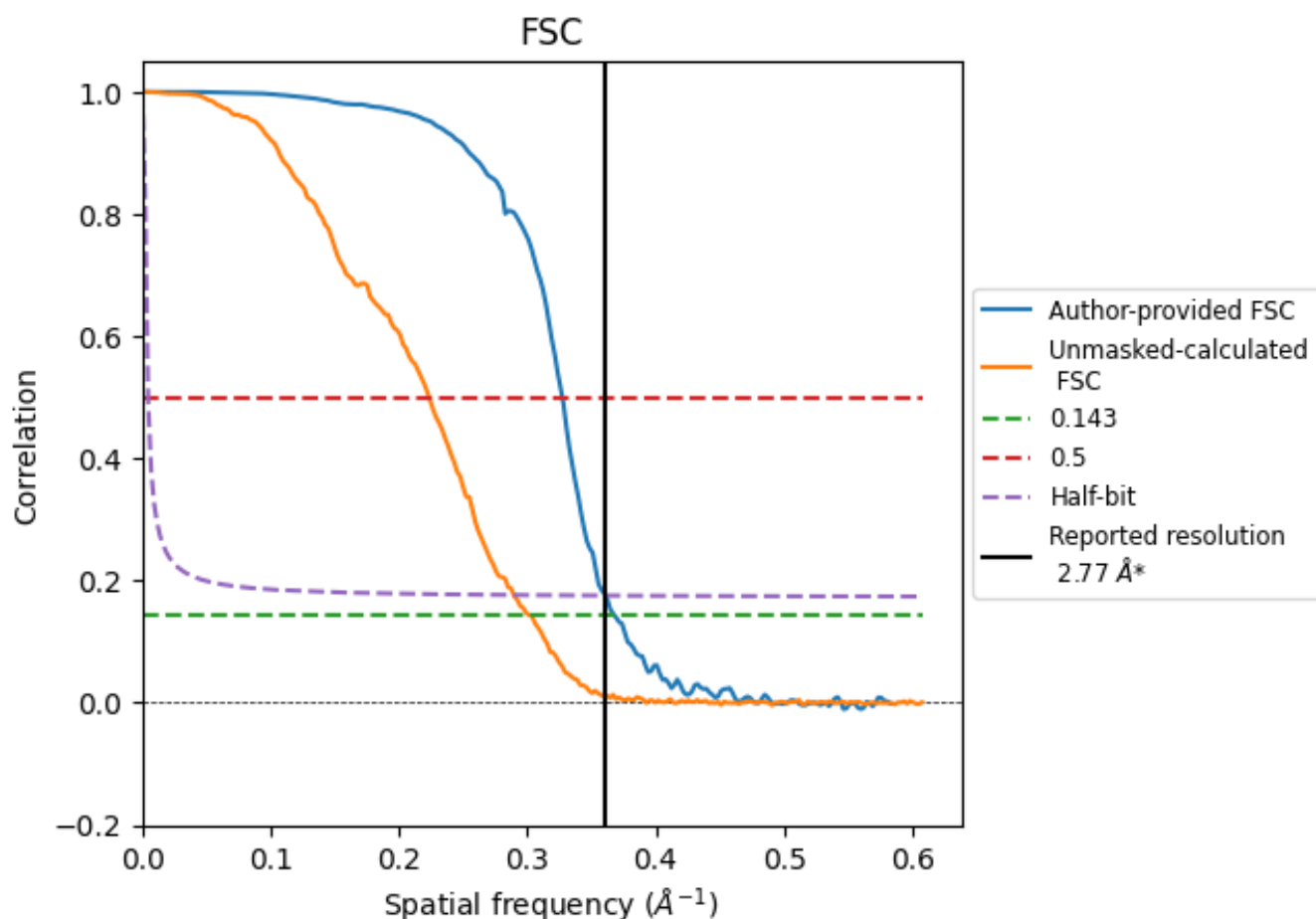


*Reported resolution corresponds to spatial frequency of 0.361 $\text{\AA}^{-1}$

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 0.361 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

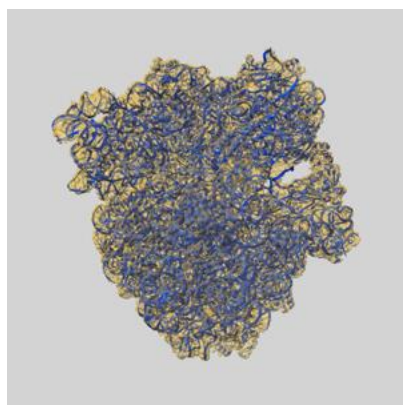
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.77	-	-
Author-provided FSC curve	2.72	3.06	2.77
Unmasked-calculated*	3.31	4.47	3.45

*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 3.31 differs from the reported value 2.77 by more than 10 %

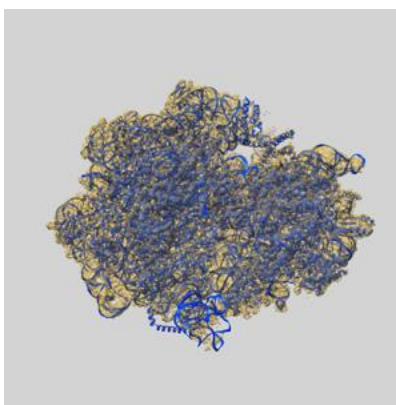
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-18458 and PDB model 8QK7. Per-residue inclusion information can be found in section [3](#) on page [19](#).

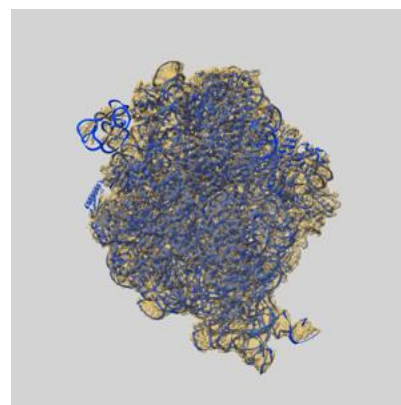
9.1 Map-model overlay [i](#)



X



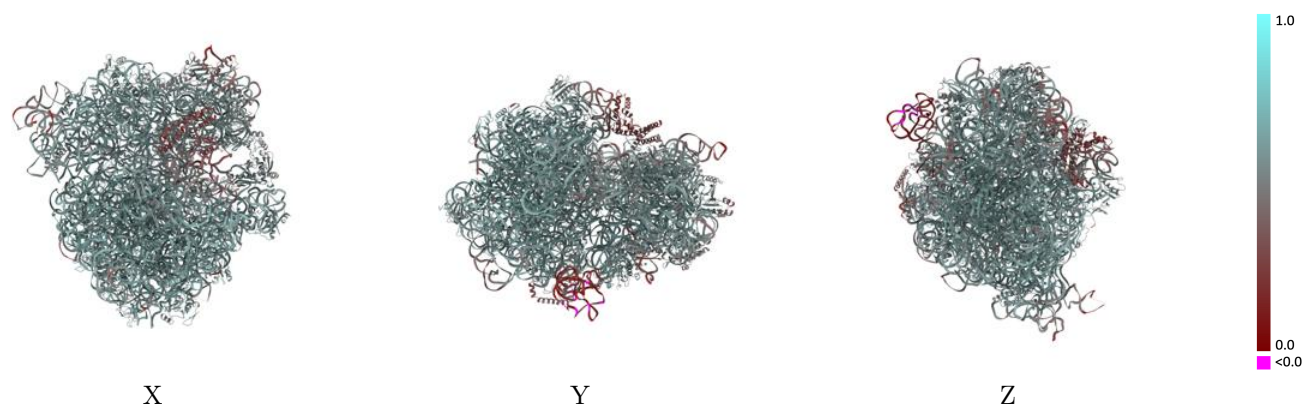
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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](#)



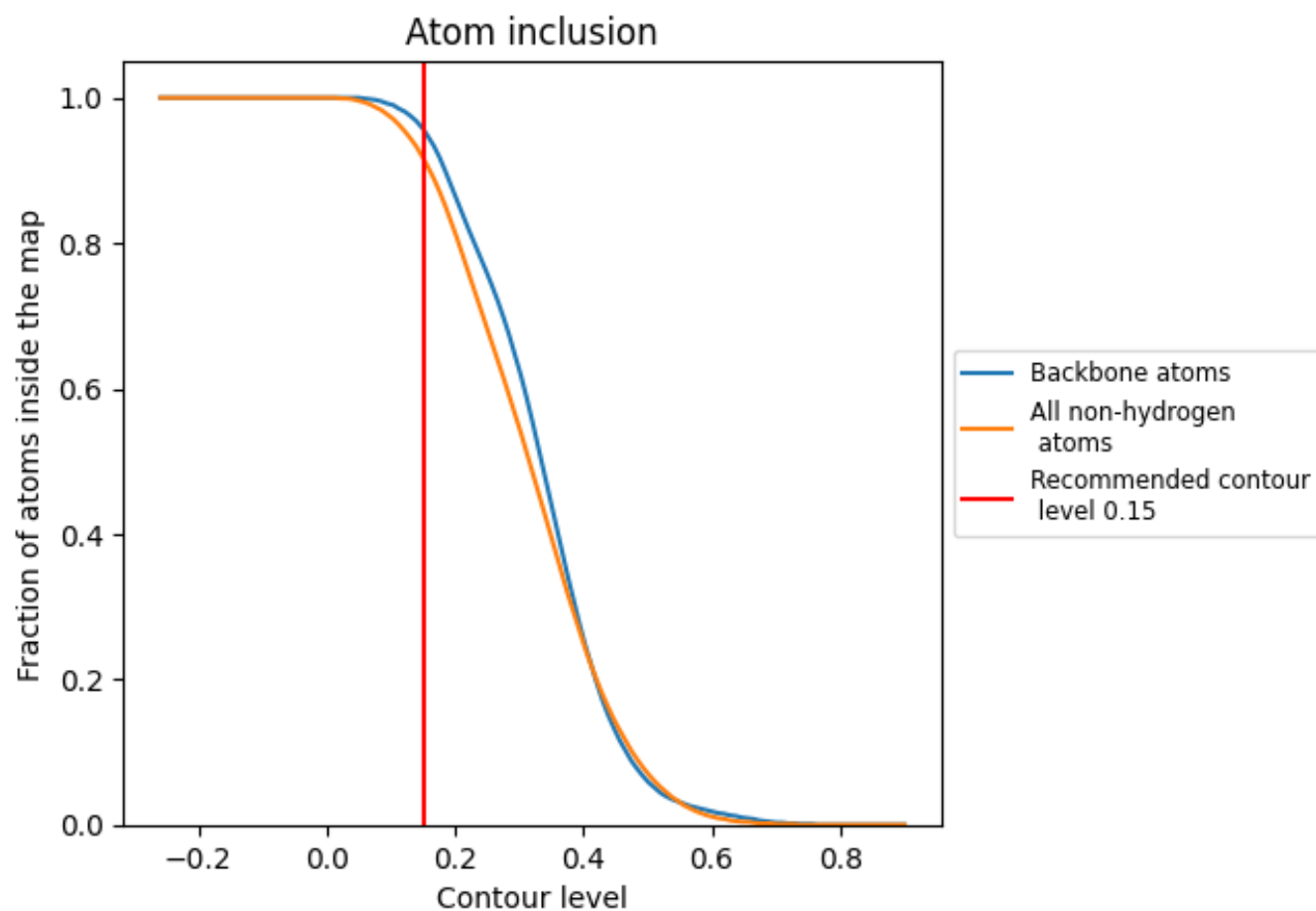
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 92% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9170	 0.5680
1	 0.9550	 0.5780
2	 0.9690	 0.5680
3	 0.9740	 0.5710
4	 0.7380	 0.4030
5	 0.9320	 0.5630
6	 0.6980	 0.4670
B	 0.9200	 0.6110
C	 0.9230	 0.6090
D	 0.8850	 0.5790
E	 0.7550	 0.5190
F	 0.7730	 0.5230
G	 0.2900	 0.3970
I	 0.2640	 0.2390
J	 0.9340	 0.6000
K	 0.8880	 0.6040
L	 0.9180	 0.5970
M	 0.8810	 0.6000
N	 0.9590	 0.6120
O	 0.8790	 0.5650
P	 0.8870	 0.6050
Q	 0.9460	 0.6090
R	 0.8910	 0.5940
S	 0.9090	 0.6000
T	 0.8530	 0.5720
U	 0.8530	 0.5520
V	 0.8330	 0.5690
W	 0.9050	 0.5970
X	 0.9080	 0.6010
Y	 0.8260	 0.5330
Z	 0.8900	 0.5910
a	 0.7310	 0.4970
b	 0.9160	 0.5980
c	 0.8340	 0.5770
d	 0.9610	 0.6210



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Chain	Atom inclusion	Q-score
e	 0.9530	 0.6220
f	 0.9280	 0.6000
g	 0.7320	 0.4980
h	 0.8360	 0.5520
i	 0.8480	 0.5590
j	 0.8840	 0.5790
k	 0.8180	 0.5450
l	 0.7630	 0.5250
m	 0.8780	 0.5750
n	 0.8340	 0.5480
o	 0.7460	 0.5120
p	 0.8640	 0.5720
q	 0.8750	 0.5920
r	 0.8100	 0.5420
s	 0.8610	 0.5500
t	 0.8520	 0.5630
u	 0.8810	 0.5770
v	 0.8160	 0.5550
w	 0.8510	 0.5630
x	 0.7930	 0.5320
y	 0.8750	 0.5560
z	 0.7250	 0.5210