



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 08:06 PM UTC

PDB ID : 8VV4 / pdb_00008vv4
EMDB ID : EMD-43549
Title : E. coli 70S ribosome with unmodified Lys-tRNA^{Pro}(GGG) in the P/P conformation on a slippery CCC-C codon
Authors : Kimbrough, E.M.; Dunham, C.M.; Nguyen, H.A.
Deposited on : 2024-01-30
Resolution : 3.40 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
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

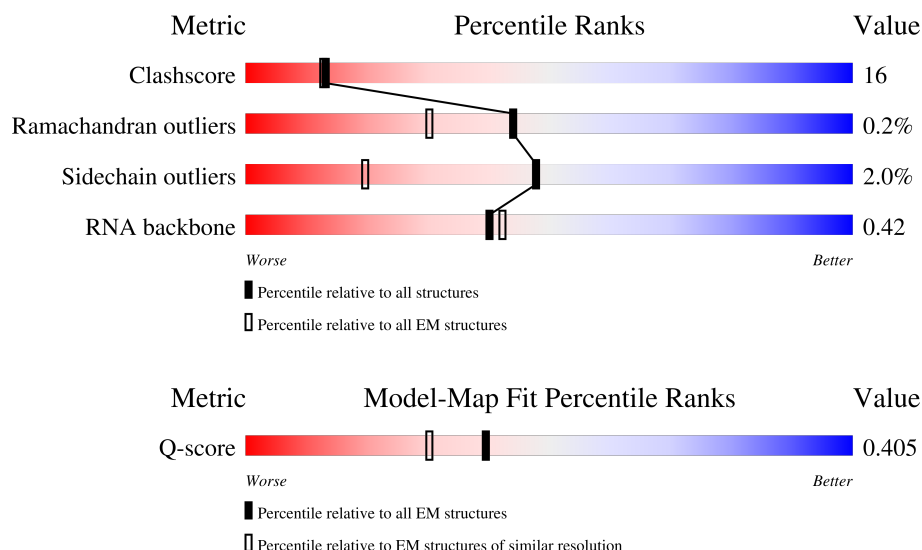
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 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.



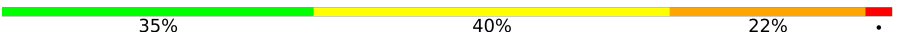
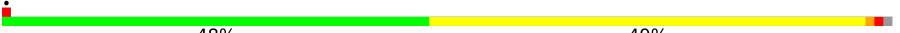
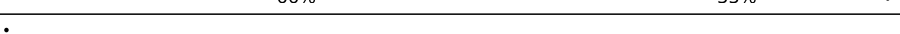
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

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	1	2903	
2	2	1540	
3	3	120	

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Mol	Chain	Length	Quality of chain
4	4	18	
5	5	77	
6	B	273	
7	C	209	
8	D	201	
9	E	179	
10	F	177	
11	G	149	
12	J	142	
13	K	123	
14	L	144	
15	M	136	
16	N	127	
17	O	117	
18	P	115	
19	Q	118	
20	R	103	
21	S	110	
22	T	100	
23	U	104	
24	V	94	
25	W	84	
26	X	78	
27	Y	63	
28	Z	59	

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Mol	Chain	Length	Quality of chain
29	a	70	
30	b	57	
31	c	55	
32	d	46	
33	e	65	
34	f	38	
35	g	241	
36	h	233	
37	i	206	
38	j	167	
39	k	135	
40	l	179	
41	m	130	
42	n	130	
43	o	103	
44	p	129	
45	q	124	
46	r	118	
47	s	101	
48	t	89	
49	u	82	
50	v	84	
51	w	75	
52	x	92	
53	y	87	

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Mol	Chain	Length	Quality of chain
54	z	71	18% 59% 38% ..

2 Entry composition [i](#)

There are 57 unique types of molecules in this entry. The entry contains 143506 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2821	Total	C	N	O	P	0	0
			60570	27020	11157	19572	2821		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1914786293
1	887	A	U	conflict	GB 1914786293
1	1847	G	A	conflict	GB 1914786293
1	2069	A	G	conflict	GB 1914786293
1	?	-	C	deletion	GB 1914786293

- Molecule 2 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	1534	Total	C	N	O	P	0	0
			32929	14693	6041	10661	1534		

- Molecule 3 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	120	Total	C	N	O	P	0	0
			2569	1144	468	837	120		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	7	Total	C	N	O	P	0	0
			145	65	24	49	7		

- Molecule 5 is a RNA chain called tRNA^{Pro}L (GGG).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	77	Total	C	N	O	P	0	0
			1648	733	297	541	77		

- Molecule 6 is a protein called 50S ribosomal protein L2.

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

- Molecule 7 is a protein called 50S ribosomal protein L3.

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

- Molecule 8 is a protein called 50S ribosomal protein L4.

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

- Molecule 9 is a protein called 50S ribosomal protein L5.

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

- Molecule 10 is a protein called 50S ribosomal protein L6.

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

- Molecule 11 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 12 is a protein called 50S ribosomal protein L13.

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

- Molecule 13 is a protein called 50S ribosomal protein L14.

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

- Molecule 14 is a protein called 50S ribosomal protein L15.

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

- Molecule 15 is a protein called 50S ribosomal protein L16.

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

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 17 is a protein called 50S ribosomal protein L18.

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

- Molecule 18 is a protein called 50S ribosomal protein L19.

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

- Molecule 19 is a protein called 50S ribosomal protein L20.

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

- Molecule 20 is a protein called Ribosomal protein L21.

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

- Molecule 21 is a protein called 50S ribosomal protein L22.

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

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	94	Total	C	N	O	S	0	0
			746	470	140	134	2		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	103	Total	C	N	O	0	0
			788	498	148	142		

- Molecule 24 is a protein called 50S ribosomal protein L25.

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

- Molecule 25 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 26 is a protein called 50S ribosomal protein L28.

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

- Molecule 27 is a protein called 50S ribosomal protein L29.

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

- Molecule 28 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	58	Total	C	N	O	S	0	0
			448	281	87	78	2		

- Molecule 29 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 30 is a protein called 50S ribosomal protein L32.

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

- Molecule 31 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	c	52	Total	C	N	O	0	0
			426	275	78	73		

- Molecule 32 is a protein called 50S ribosomal protein L34.

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

- Molecule 33 is a protein called 50S ribosomal protein L35.

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

- Molecule 34 is a protein called 50S ribosomal protein L36.

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

- Molecule 35 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	225	Total	C	N	O	S	0	0
			1760	1113	316	323	8		

- Molecule 36 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	208	Total	C	N	O	S	0	0
			1636	1036	307	290	3		

- Molecule 37 is a protein called 30S ribosomal protein S4.

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

- Molecule 38 is a protein called 30S ribosomal protein S5.

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

- Molecule 39 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	104	Total	C	N	O	S	0	0
			848	536	153	152	7		

- Molecule 40 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

- Molecule 41 is a protein called 30S ribosomal protein S8.

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

- Molecule 42 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	99	Total	C	N	O	S	0	0
			790	495	151	143	1		

- Molecule 44 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 45 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 46 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	116	Total	C	N	O	S	0	0
			900	558	181	158	3		

- Molecule 47 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 48 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 49 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	82	Total	C	N	O	S	0	0
			649	406	128	114	1		

- Molecule 50 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

- Molecule 51 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	66	Total	C	N	O	S	0	0
			544	344	102	97	1		

- Molecule 52 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	y	86	Total	C	N	O	S	0	0
			669	414	138	114	3		

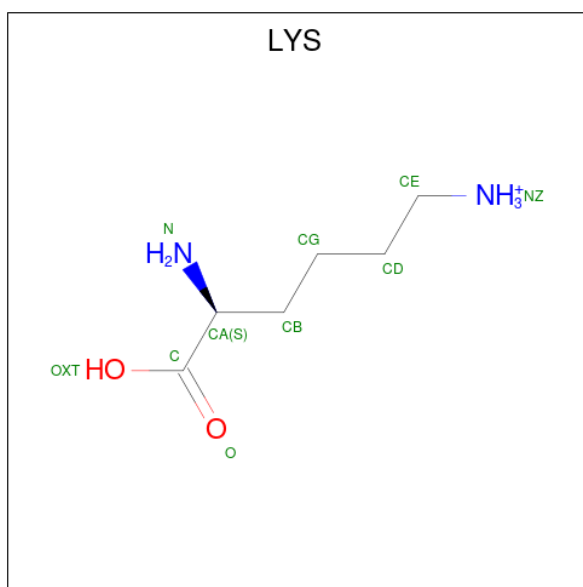
- Molecule 54 is a protein called 30S ribosomal protein S21.

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

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	1	295	Total	Mg	0
			295	295	
55	2	104	Total	Mg	0
			104	104	
55	3	8	Total	Mg	0
			8	8	
55	B	1	Total	Mg	0
			1	1	
55	D	4	Total	Mg	0
			4	4	
55	M	1	Total	Mg	0
			1	1	
55	P	1	Total	Mg	0
			1	1	
55	Q	1	Total	Mg	0
			1	1	
55	R	1	Total	Mg	0
			1	1	
55	T	1	Total	Mg	0
			1	1	
55	X	1	Total	Mg	0
			1	1	
55	Z	1	Total	Mg	0
			1	1	
55	b	1	Total	Mg	0
			1	1	
55	e	3	Total	Mg	0
			3	3	
55	z	1	Total	Mg	0
			1	1	

- Molecule 56 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				AltConf
56	5	1	Total	C	N	O	0
			9	6	2	1	

- Molecule 57 is water.

Mol	Chain	Residues	Atoms		AltConf
57	1	143	Total	O	0
			143	143	
57	2	102	Total	O	0
			102	102	
57	3	5	Total	O	0
			5	5	
57	4	1	Total	O	0
			1	1	
57	5	14	Total	O	0
			14	14	
57	B	2	Total	O	0
			2	2	
57	C	6	Total	O	0
			6	6	
57	D	7	Total	O	0
			7	7	
57	E	8	Total	O	0
			8	8	
57	F	11	Total	O	0
			11	11	
57	G	18	Total	O	0
			18	18	

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Mol	Chain	Residues	Atoms		AltConf
57	J	2	Total 2	O 2	0
57	K	4	Total 4	O 4	0
57	L	6	Total 6	O 6	0
57	M	5	Total 5	O 5	0
57	N	4	Total 4	O 4	0
57	O	4	Total 4	O 4	0
57	P	1	Total 1	O 1	0
57	R	7	Total 7	O 7	0
57	S	3	Total 3	O 3	0
57	T	2	Total 2	O 2	0
57	U	1	Total 1	O 1	0
57	V	4	Total 4	O 4	0
57	W	1	Total 1	O 1	0
57	Y	4	Total 4	O 4	0
57	a	30	Total 30	O 30	0
57	b	1	Total 1	O 1	0
57	c	3	Total 3	O 3	0
57	g	33	Total 33	O 33	0
57	h	13	Total 13	O 13	0
57	i	4	Total 4	O 4	0
57	j	7	Total 7	O 7	0

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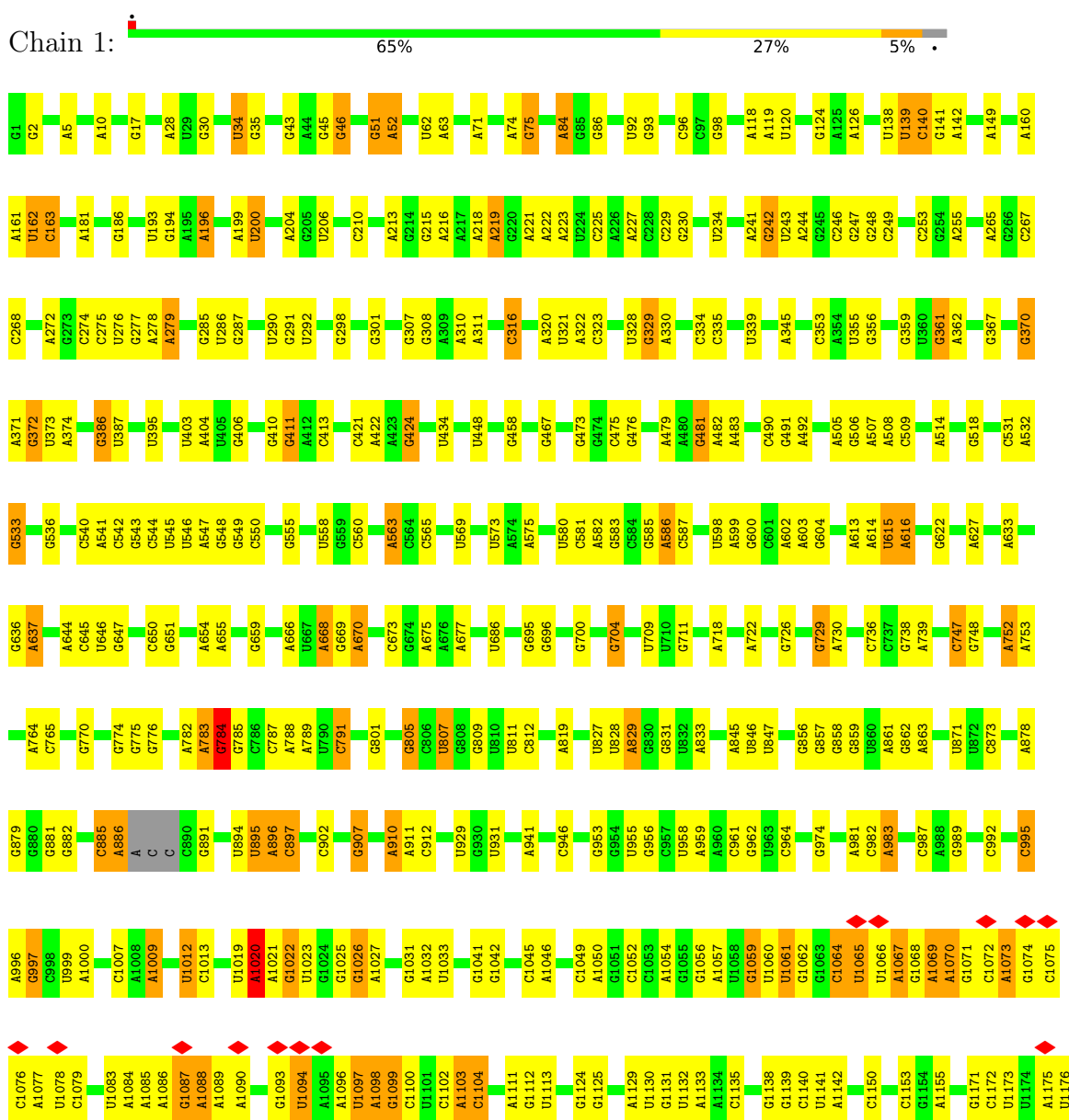
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Mol	Chain	Residues	Atoms		AltConf
57	k	8	Total 8	O 8	0
57	l	12	Total 12	O 12	0
57	m	9	Total 9	O 9	0
57	n	5	Total 5	O 5	0
57	o	11	Total 11	O 11	0
57	p	5	Total 5	O 5	0
57	q	5	Total 5	O 5	0
57	r	8	Total 8	O 8	0
57	s	5	Total 5	O 5	0
57	t	4	Total 4	O 4	0
57	u	5	Total 5	O 5	0
57	v	2	Total 2	O 2	0
57	w	9	Total 9	O 9	0
57	x	1	Total 1	O 1	0
57	y	1	Total 1	O 1	0
57	z	14	Total 14	O 14	0

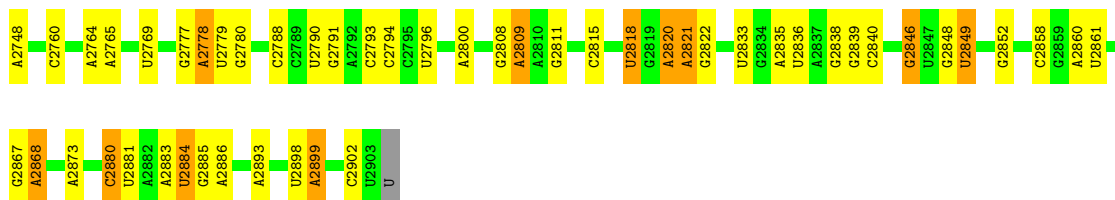
3 Residue-property plots

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: 23S ribosomal RNA

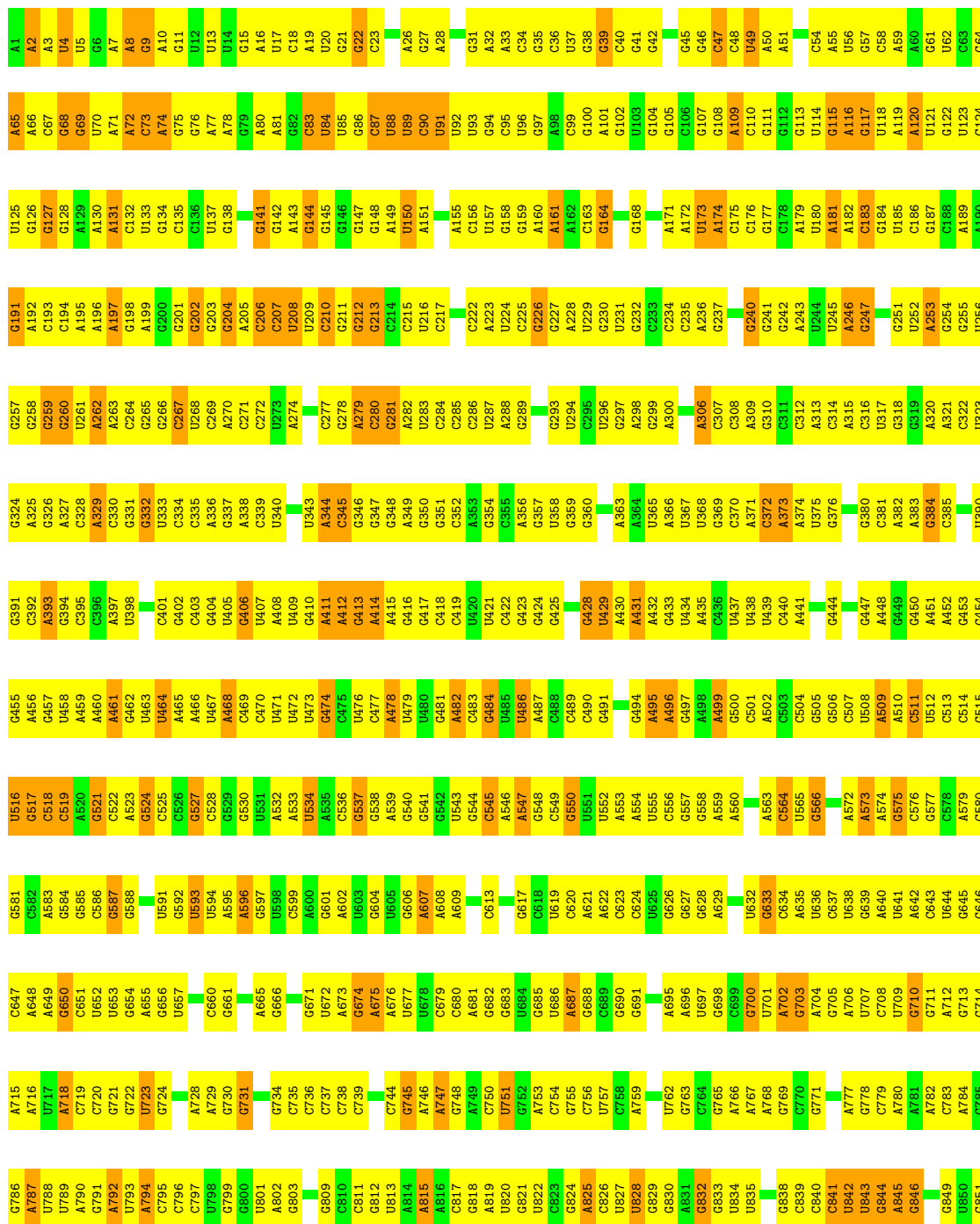


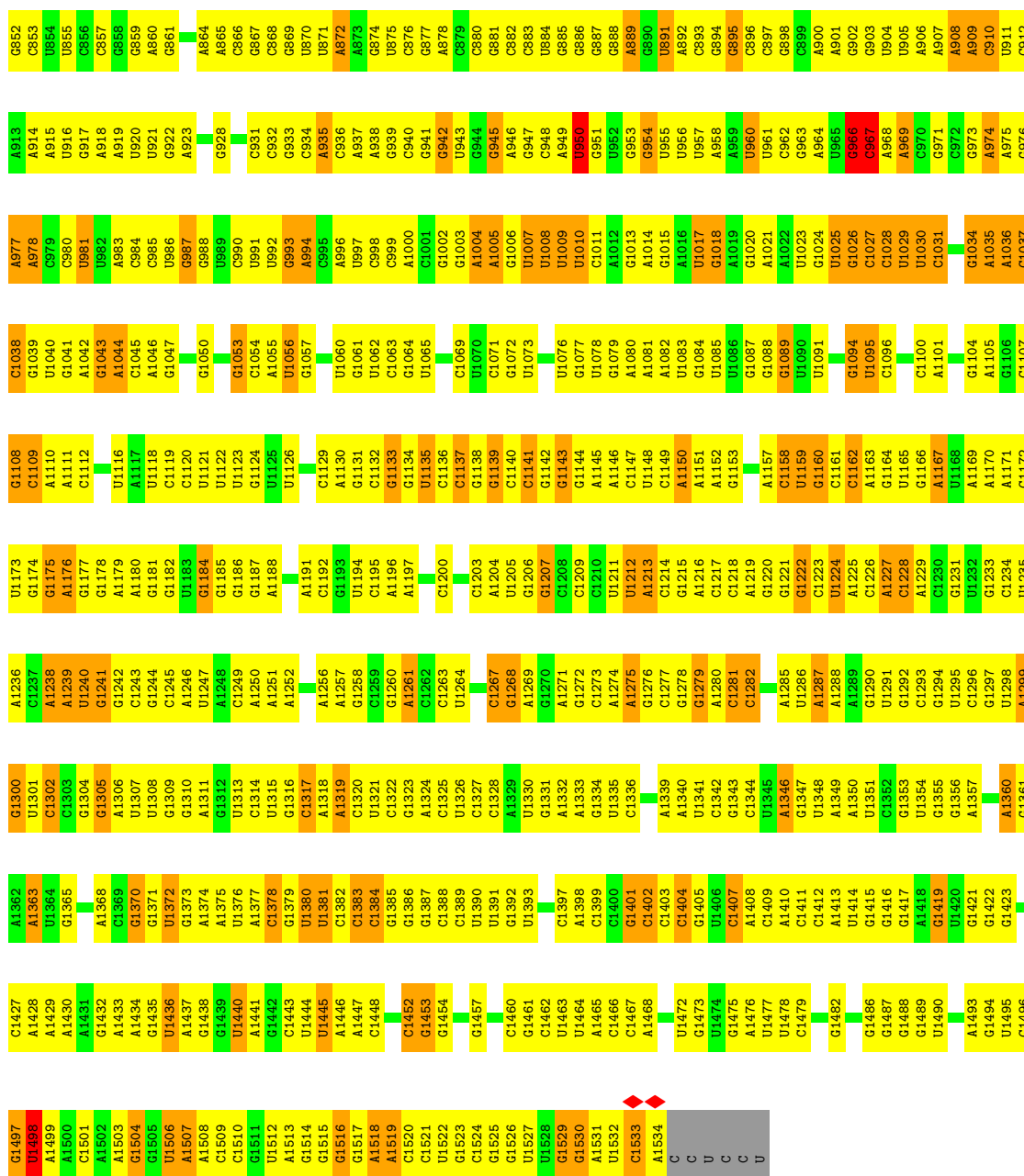




• Molecule 2: 16S ribosomal RNA

Chain 2: 21% 61% 17%

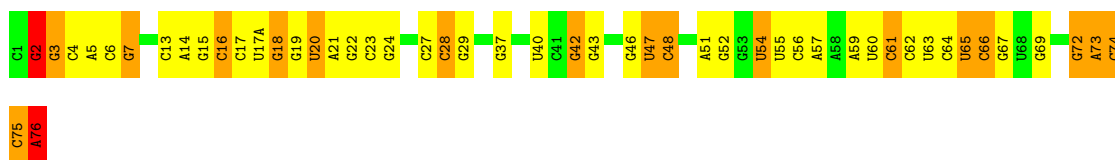






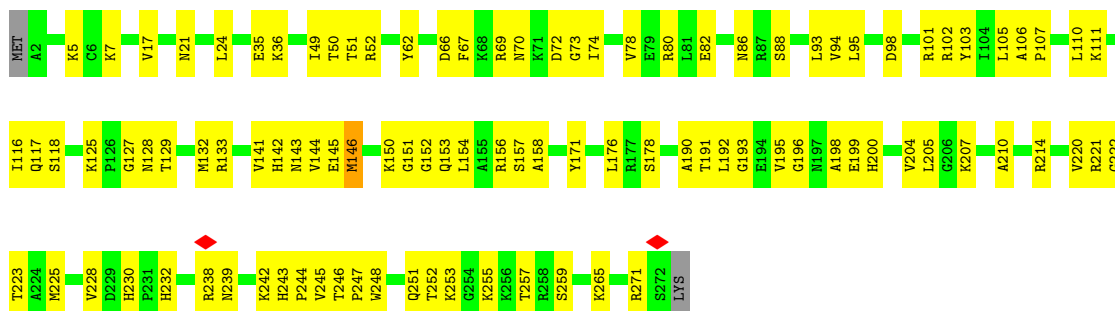
• Molecule 5: tRNA^{Pro}L (GGG)

Chain 5: 35% 40% 22%



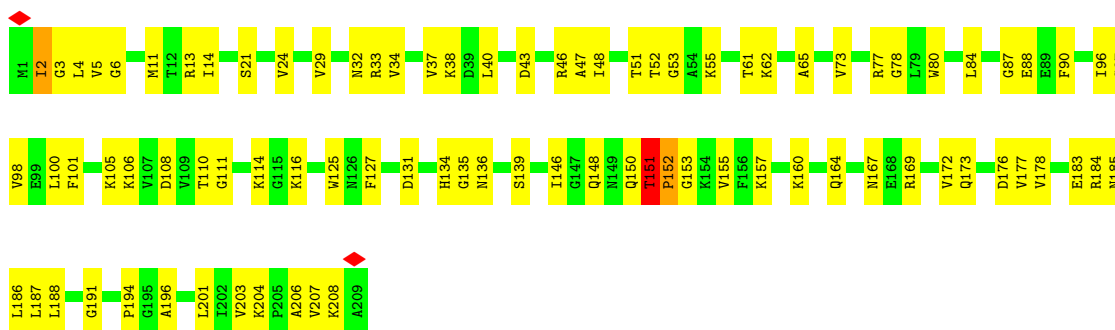
• Molecule 6: 50S ribosomal protein L2

Chain B: 62% 37%



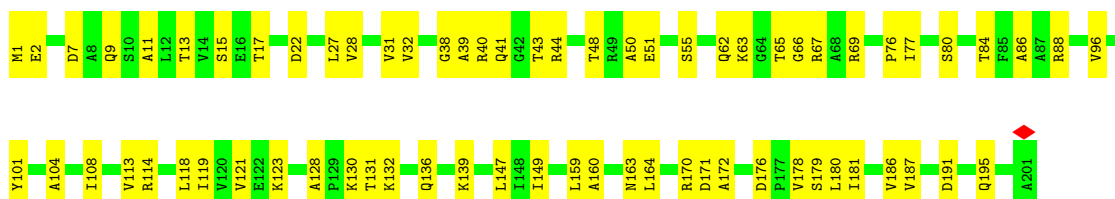
• Molecule 7: 50S ribosomal protein L3

Chain C: 58% 40%

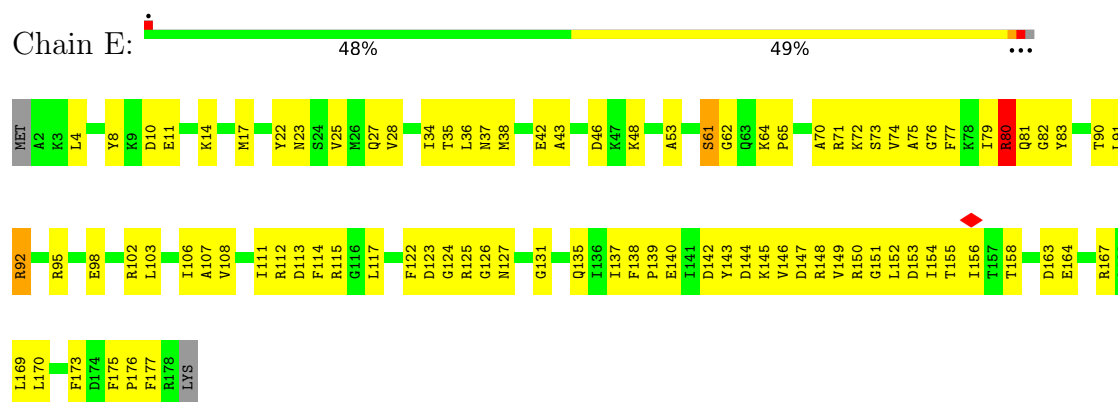


• Molecule 8: 50S ribosomal protein L4

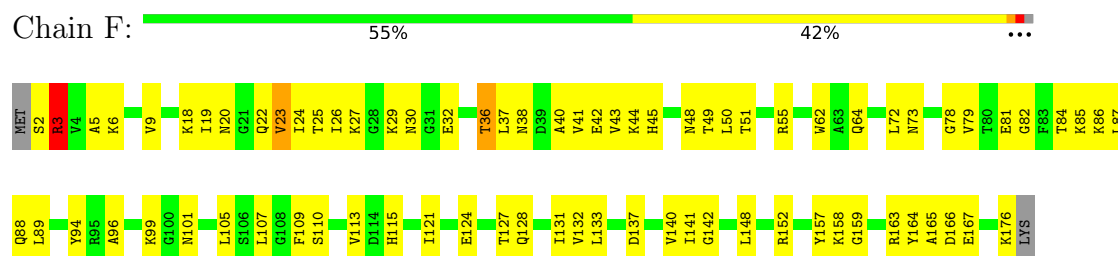
Chain D: 66% 34%



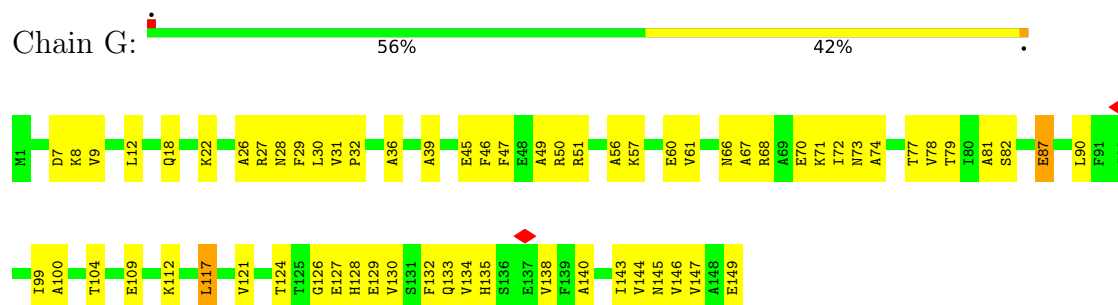
- Molecule 9: 50S ribosomal protein L5



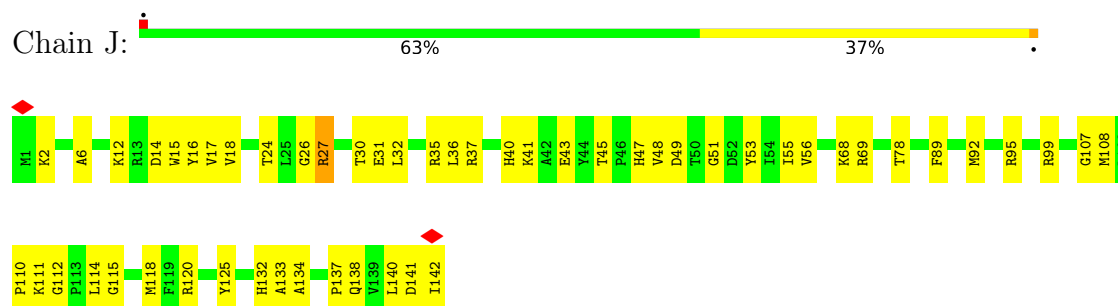
- Molecule 10: 50S ribosomal protein L6



- Molecule 11: Large ribosomal subunit protein bL9

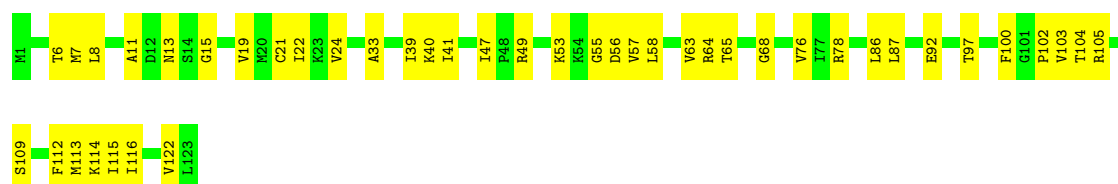


- Molecule 12: 50S ribosomal protein L13

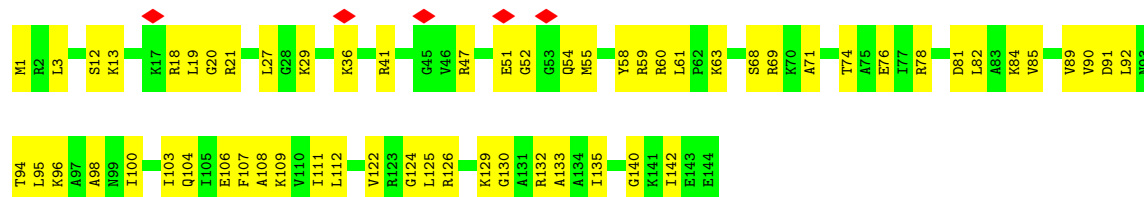


- Molecule 13: 50S ribosomal protein L14

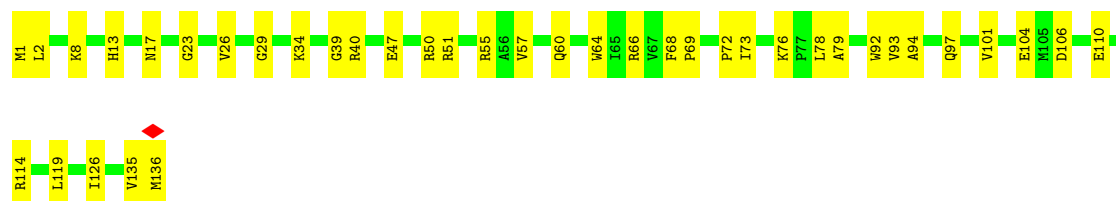




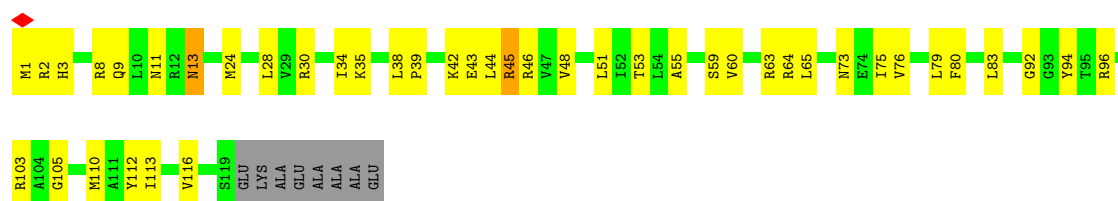
- Molecule 14: 50S ribosomal protein L15



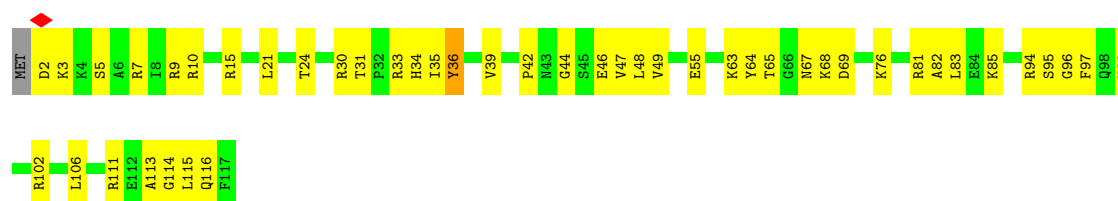
- Molecule 15: 50S ribosomal protein L16



- Molecule 16: Large ribosomal subunit protein bL17



- Molecule 17: 50S ribosomal protein L18



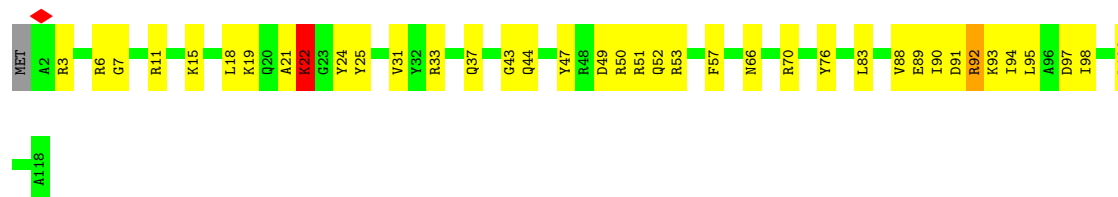
- Molecule 18: 50S ribosomal protein L19

Chain P:  66% 33%



- Molecule 19: 50S ribosomal protein L20

Chain Q:  67% 31%



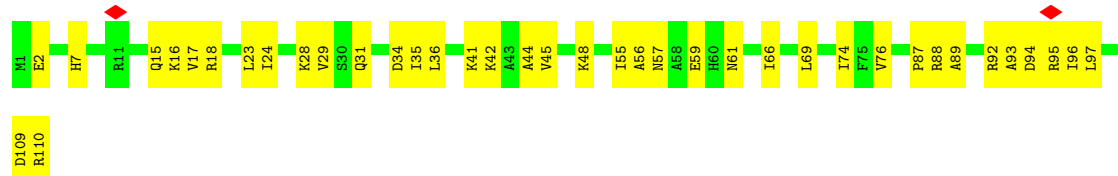
- Molecule 20: Ribosomal protein L21

Chain R:  75% 24%



- Molecule 21: 50S ribosomal protein L22

Chain S:  64% 36%



- Molecule 22: 50S ribosomal protein L23

Chain T:  63% 31% 6%



- Molecule 23: 50S ribosomal protein L24

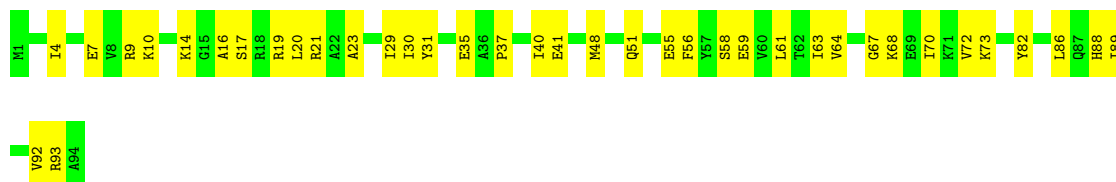
Chain U:  62% 37%





- Molecule 24: 50S ribosomal protein L25

Chain V:



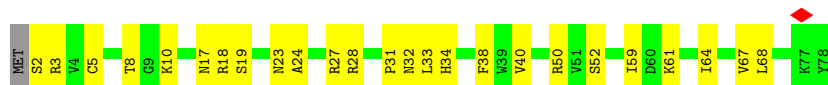
- Molecule 25: Large ribosomal subunit protein bL27

Chain W:



- Molecule 26: 50S ribosomal protein L28

Chain X:



- Molecule 27: 50S ribosomal protein L29

Chain Y:



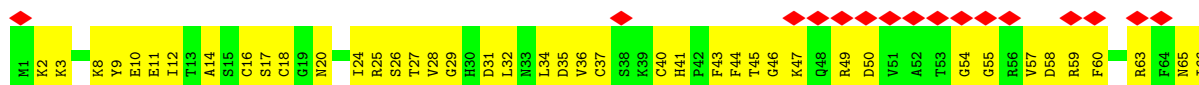
- Molecule 28: Large ribosomal subunit protein uL30

Chain Z:



- Molecule 29: 50S ribosomal protein L31

Chain a:



PRO
GLY
SER
LYS

- Molecule 30: 50S ribosomal protein L32

Chain b: 



- Molecule 31: Large ribosomal subunit protein bL33

Chain c: 



- Molecule 32: 50S ribosomal protein L34

Chain d: 



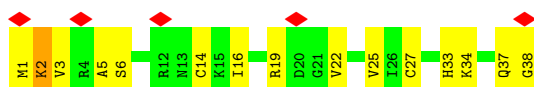
- Molecule 33: 50S ribosomal protein L35

Chain e: 



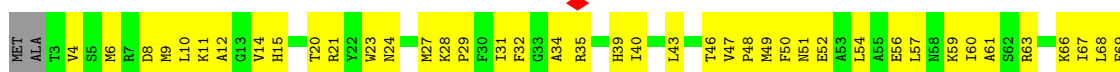
- Molecule 34: 50S ribosomal protein L36

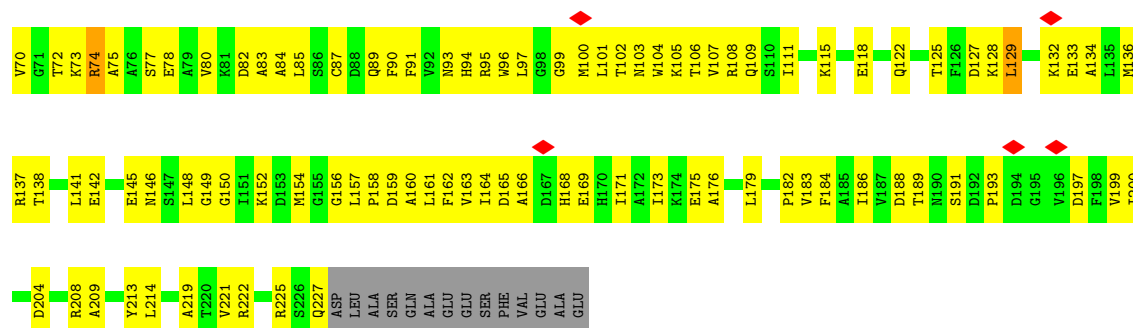
Chain f: 



- Molecule 35: 30S ribosomal protein S2

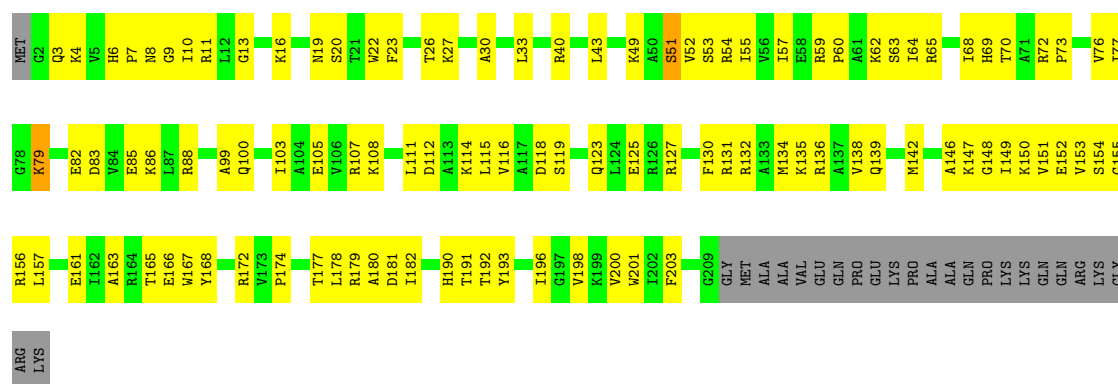
Chain g: 





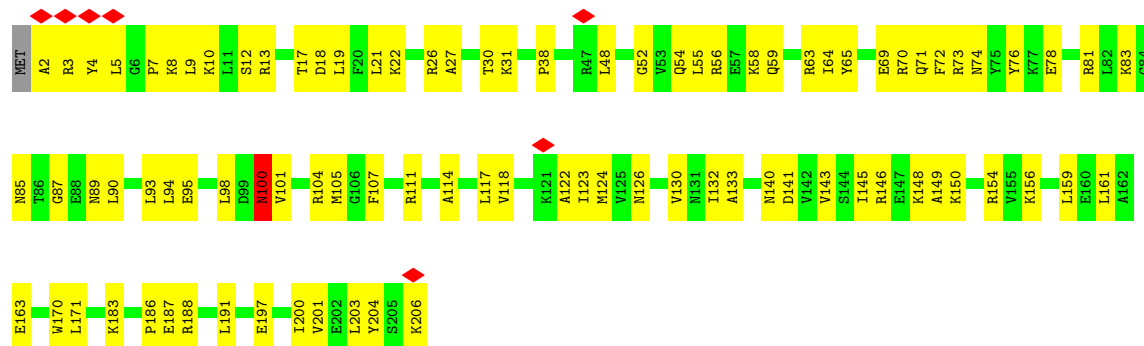
• Molecule 36: 30S ribosomal protein S3

Chain h: 44% 45% 11%



• Molecule 37: 30S ribosomal protein S4

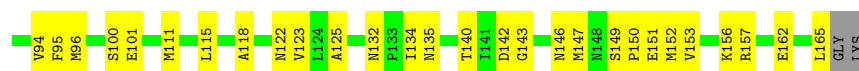
Chain i: 56% 43%



• Molecule 38: 30S ribosomal protein S5

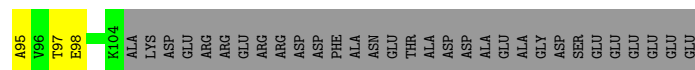
Chain j: 56% 37% 7%





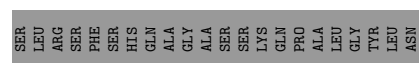
- Molecule 39: 30S ribosomal protein S6

Chain k: 45% 31% 23%



- Molecule 40: 30S ribosomal protein S7

Chain l: 47% 33% 16%



- Molecule 41: 30S ribosomal protein S8

Chain m: 58% 40% 2%



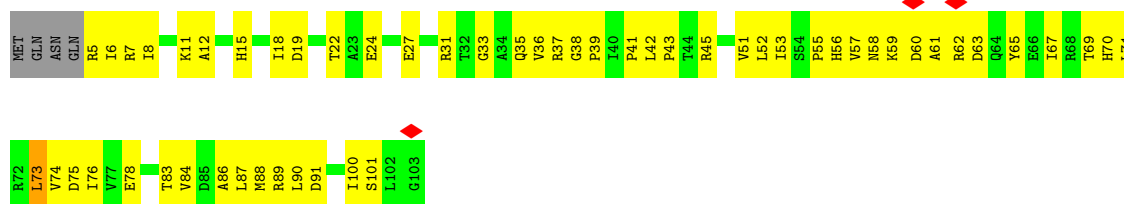
- Molecule 42: Small ribosomal subunit protein uS9

Chain n: 48% 49% 3%



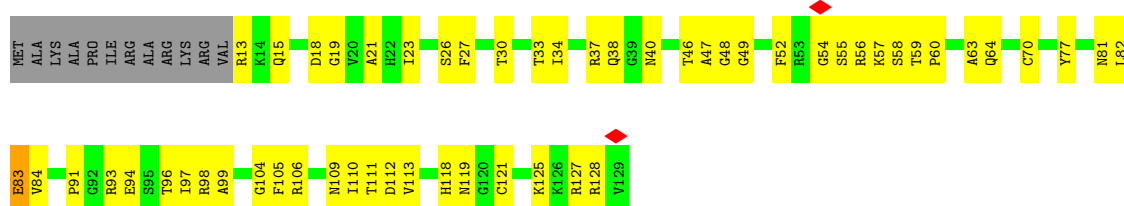
- Molecule 43: 30S ribosomal protein S10

Chain o: 



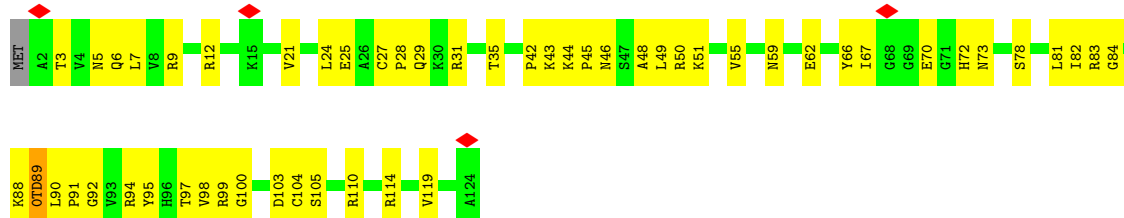
- Molecule 44: 30S ribosomal protein S11

Chain p: 



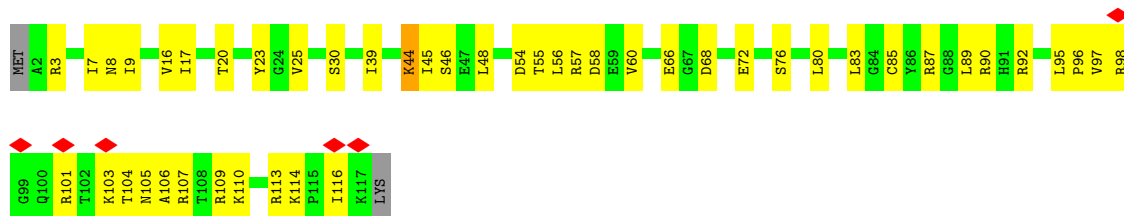
- Molecule 45: Small ribosomal subunit protein uS12

Chain q: 



- Molecule 46: 30S ribosomal protein S13

Chain r: 



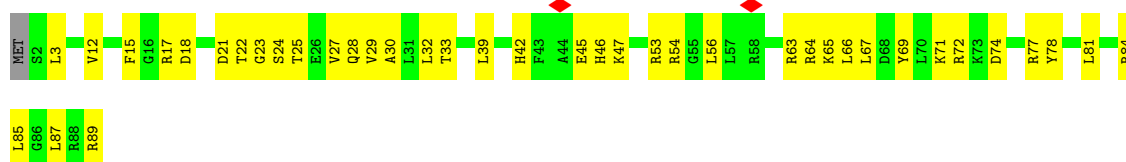
- Molecule 47: Small ribosomal subunit protein uS14

Chain s: 

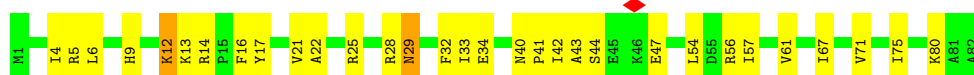




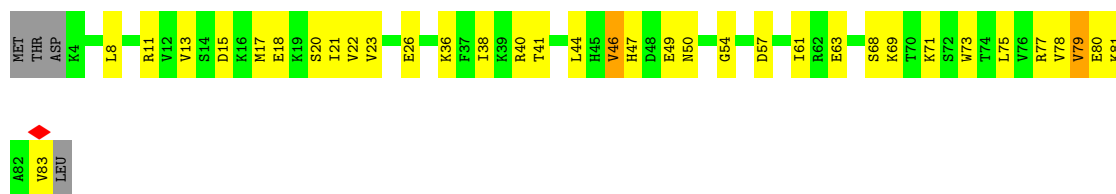
- Molecule 48: Small ribosomal subunit protein uS15



- Molecule 49: 30S ribosomal protein S16



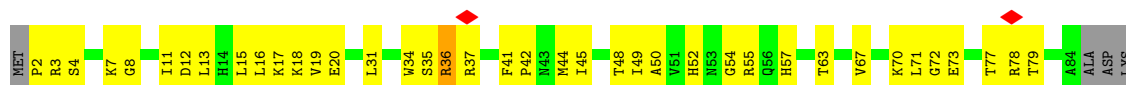
- Molecule 50: Small ribosomal subunit protein uS17



- Molecule 51: 30S ribosomal protein S18

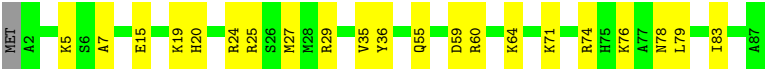


- Molecule 52: 30S ribosomal protein S19

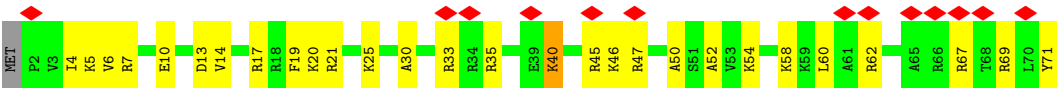


LYS
ALA
LYS
LYS
LYS

- Molecule 53: 30S ribosomal protein S20



- Molecule 54: 30S ribosomal protein S21



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29634	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	56.07	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.026	Depositor
Minimum map value	-0.015	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00281	Depositor
Map size ($\text{\AA}$)	547.3792, 547.3792, 547.3792	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0691, 1.0691, 1.0691	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 2MG, G7M, 4OC, PSU, 0TD, MG, MA6, 5MC, UR3

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	1	0.40	0/67839	0.45	13/105827 (0.0%)
2	2	0.42	0/36590	0.46	3/57074 (0.0%)
3	3	0.45	0/2872	0.49	0/4478
4	4	0.39	0/160	0.81	0/246
5	5	0.40	1/1841 (0.1%)	0.72	3/2870 (0.1%)
6	B	0.45	1/2121 (0.0%)	0.56	0/2852
7	C	0.74	0/1586	0.83	3/2134 (0.1%)
8	D	0.49	0/1571	0.64	1/2113 (0.0%)
9	E	0.46	0/1434	0.69	1/1926 (0.1%)
10	F	0.63	0/1333	0.71	0/1805
11	G	0.36	0/1122	0.66	0/1515
12	J	0.52	0/1152	0.62	0/1551
13	K	0.44	0/955	0.55	0/1279
14	L	0.67	0/1062	0.79	1/1413 (0.1%)
15	M	0.45	0/1093	0.53	0/1460
16	N	0.54	0/964	0.68	0/1289
17	O	0.45	0/902	0.65	0/1209
18	P	0.44	0/929	0.61	0/1242
19	Q	0.47	0/960	0.63	1/1278 (0.1%)
20	R	0.62	0/829	0.75	0/1107
21	S	0.67	0/864	0.74	0/1156
22	T	0.41	0/752	0.55	0/1005
23	U	0.57	0/796	0.64	0/1062
24	V	0.50	0/766	0.61	0/1025
25	W	0.69	0/582	0.72	0/769
26	X	0.47	0/635	0.58	0/848
27	Y	0.62	0/502	0.83	2/667 (0.3%)
28	Z	0.97	0/452	0.98	0/605
29	a	0.34	0/531	0.64	0/709
30	b	0.57	0/450	0.62	0/599
31	c	0.45	0/433	0.68	1/576 (0.2%)
32	d	0.35	0/380	0.54	0/498

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	e	0.42	0/513	0.63	0/676
34	f	0.44	0/303	0.67	0/397
35	g	0.42	0/1791	0.68	1/2413 (0.0%)
36	h	0.46	0/1663	0.69	0/2241
37	i	0.49	0/1665	0.67	1/2227 (0.0%)
38	j	0.44	0/1165	0.63	0/1568
39	k	0.54	0/867	0.78	1/1171 (0.1%)
40	l	0.48	0/1195	0.81	4/1602 (0.2%)
41	m	0.57	0/989	0.78	1/1326 (0.1%)
42	n	0.45	0/1034	0.67	0/1375
43	o	0.43	0/800	0.73	2/1082 (0.2%)
44	p	0.46	0/893	0.68	1/1205 (0.1%)
45	q	0.55	0/960	0.72	0/1286
46	r	0.43	0/909	0.61	0/1215
47	s	0.36	0/817	0.54	0/1088
48	t	0.43	0/722	0.65	0/964
49	u	0.41	0/659	0.61	0/884
50	v	0.44	0/657	0.65	0/881
51	w	0.58	0/553	0.67	0/743
52	x	0.44	0/680	0.61	0/915
53	y	0.41	0/675	0.56	0/895
54	z	0.42	0/597	0.78	0/792
All	All	0.44	2/154565 (0.0%)	0.52	40/231133 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
7	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	146	MET	C-N	-6.26	1.23	1.33
5	5	76	A	C3'-O3'	5.09	1.49	1.42

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	784	G	C2'-C3'-O3'	-11.94	95.79	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1	79	ARG	N-CA-C	10.56	124.02	108.60
1	1	1378	A	C2'-C3'-O3'	-10.23	94.16	109.50
14	L	36	LYS	N-CA-C	9.50	124.25	112.47
1	1	1930	G	C4'-C3'-O3'	8.66	122.40	109.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	151	THR	Peptide

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	1	60570	0	30467	575	0
2	2	32929	0	16587	1373	0
3	3	2569	0	1301	117	0
4	4	145	0	77	5	0
5	5	1648	0	833	22	0
6	B	2082	0	2154	92	0
7	C	1565	0	1616	80	0
8	D	1552	0	1619	73	0
9	E	1410	0	1444	85	0
10	F	1313	0	1358	71	0
11	G	1111	0	1148	63	0
12	J	1129	0	1162	47	0
13	K	946	0	1023	33	0
14	L	1053	0	1129	74	0
15	M	1074	0	1157	42	0
16	N	951	0	994	42	0
17	O	892	0	923	42	0
18	P	917	0	962	36	0
19	Q	947	0	1019	47	0
20	R	816	0	839	21	0
21	S	857	0	922	44	0
22	T	746	0	811	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	U	788	0	844	29	0
24	V	753	0	780	29	0
25	W	575	0	592	34	0
26	X	625	0	652	23	0
27	Y	501	0	531	16	0
28	Z	448	0	488	30	0
29	a	522	0	524	42	0
30	b	444	0	458	33	0
31	c	426	0	464	16	0
32	d	377	0	418	27	0
33	e	504	0	572	30	0
34	f	302	0	343	17	0
35	g	1760	0	1787	131	0
36	h	1636	0	1710	105	0
37	i	1643	0	1707	87	0
38	j	1152	0	1196	55	0
39	k	848	0	846	42	0
40	l	1181	0	1238	60	0
41	m	979	0	1031	47	0
42	n	1022	0	1070	60	0
43	o	790	0	831	62	0
44	p	877	0	887	54	0
45	q	957	0	1017	50	0
46	r	900	0	965	53	0
47	s	805	0	844	57	0
48	t	714	0	734	37	0
49	u	649	0	666	27	0
50	v	648	0	691	28	0
51	w	544	0	560	44	0
52	x	663	0	688	41	0
53	y	669	0	719	23	0
54	z	589	0	629	33	0
55	1	295	0	0	0	0
55	2	104	0	0	0	0
55	3	8	0	0	0	0
55	B	1	0	0	0	0
55	D	4	0	0	0	0
55	M	1	0	0	0	0
55	P	1	0	0	0	0
55	Q	1	0	0	0	0
55	R	1	0	0	0	0
55	T	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
55	X	1	0	0	0	0
55	Z	1	0	0	0	0
55	b	1	0	0	0	0
55	e	3	0	0	0	0
55	z	1	0	0	0	0
56	5	9	0	12	0	0
57	1	143	0	0	38	0
57	2	102	0	0	24	0
57	3	5	0	0	2	0
57	4	1	0	0	1	0
57	5	14	0	0	4	0
57	B	2	0	0	2	0
57	C	6	0	0	1	0
57	D	7	0	0	6	0
57	E	8	0	0	1	0
57	F	11	0	0	4	0
57	G	18	0	0	8	0
57	J	2	0	0	0	0
57	K	4	0	0	5	0
57	L	6	0	0	2	0
57	M	5	0	0	2	0
57	N	4	0	0	0	0
57	O	4	0	0	0	0
57	P	1	0	0	0	0
57	R	7	0	0	0	0
57	S	3	0	0	1	0
57	T	2	0	0	0	0
57	U	1	0	0	0	0
57	V	4	0	0	1	0
57	W	1	0	0	0	0
57	Y	4	0	0	1	0
57	a	30	0	0	13	0
57	b	1	0	0	0	0
57	c	3	0	0	3	0
57	g	33	0	0	20	0
57	h	13	0	0	8	0
57	i	4	0	0	0	0
57	j	7	0	0	4	0
57	k	8	0	0	2	0
57	l	12	0	0	5	0
57	m	9	0	0	2	0
57	n	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	o	11	0	0	9	0
57	p	5	0	0	2	0
57	q	5	0	0	1	0
57	r	8	0	0	1	0
57	s	5	0	0	0	0
57	t	4	0	0	1	0
57	u	5	0	0	3	0
57	v	2	0	0	1	0
57	w	9	0	0	6	0
57	x	1	0	0	0	0
57	y	1	0	0	0	0
57	z	14	0	0	4	0
All	All	143506	0	96039	3784	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 16.

The worst 5 of 3784 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)
51:w:18:VAL:HB	57:w:102:HOH:O	1.27	1.31
1:l:1460:U:H5''	57:l:3417:HOH:O	1.32	1.28
35:g:115:LYS:HD2	57:g:329:HOH:O	1.42	1.17
35:g:74:ARG:HD2	57:g:313:HOH:O	1.44	1.16
54:z:67:ARG:HB3	57:z:202:HOH:O	1.44	1.16

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	
6	B	269/273 (98%)	241 (90%)	28 (10%)	0	100	100
7	C	207/209 (99%)	176 (85%)	29 (14%)	2 (1%)	12	40
8	D	199/201 (99%)	192 (96%)	7 (4%)	0	100	100
9	E	175/179 (98%)	154 (88%)	21 (12%)	0	100	100
10	F	173/177 (98%)	153 (88%)	19 (11%)	1 (1%)	21	50
11	G	147/149 (99%)	129 (88%)	18 (12%)	0	100	100
12	J	140/142 (99%)	133 (95%)	6 (4%)	1 (1%)	18	47
13	K	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
14	L	142/144 (99%)	116 (82%)	26 (18%)	0	100	100
15	M	134/136 (98%)	117 (87%)	17 (13%)	0	100	100
16	N	117/127 (92%)	104 (89%)	13 (11%)	0	100	100
17	O	114/117 (97%)	108 (95%)	6 (5%)	0	100	100
18	P	112/115 (97%)	104 (93%)	8 (7%)	0	100	100
19	Q	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
20	R	101/103 (98%)	85 (84%)	16 (16%)	0	100	100
21	S	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
22	T	92/100 (92%)	88 (96%)	4 (4%)	0	100	100
23	U	101/104 (97%)	88 (87%)	13 (13%)	0	100	100
24	V	92/94 (98%)	84 (91%)	8 (9%)	0	100	100
25	W	73/84 (87%)	62 (85%)	11 (15%)	0	100	100
26	X	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
27	Y	60/63 (95%)	58 (97%)	2 (3%)	0	100	100
28	Z	56/59 (95%)	47 (84%)	8 (14%)	1 (2%)	6	26
29	a	64/70 (91%)	60 (94%)	4 (6%)	0	100	100
30	b	54/57 (95%)	48 (89%)	6 (11%)	0	100	100
31	c	50/55 (91%)	49 (98%)	1 (2%)	0	100	100
32	d	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
33	e	62/65 (95%)	55 (89%)	6 (10%)	1 (2%)	7	29
34	f	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
35	g	223/241 (92%)	195 (87%)	27 (12%)	1 (0%)	30	59
36	h	206/233 (88%)	186 (90%)	19 (9%)	1 (0%)	24	54
37	i	203/206 (98%)	178 (88%)	25 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	j	154/167 (92%)	140 (91%)	14 (9%)	0	100	100
39	k	102/135 (76%)	89 (87%)	12 (12%)	1 (1%)	12	40
40	l	149/179 (83%)	134 (90%)	12 (8%)	3 (2%)	6	25
41	m	127/130 (98%)	112 (88%)	15 (12%)	0	100	100
42	n	125/130 (96%)	113 (90%)	12 (10%)	0	100	100
43	o	97/103 (94%)	84 (87%)	13 (13%)	0	100	100
44	p	115/129 (89%)	102 (89%)	13 (11%)	0	100	100
45	q	120/124 (97%)	105 (88%)	15 (12%)	0	100	100
46	r	114/118 (97%)	100 (88%)	14 (12%)	0	100	100
47	s	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
48	t	86/89 (97%)	82 (95%)	4 (5%)	0	100	100
49	u	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	9	33
50	v	78/84 (93%)	70 (90%)	7 (9%)	1 (1%)	9	33
51	w	64/75 (85%)	58 (91%)	6 (9%)	0	100	100
52	x	81/92 (88%)	70 (86%)	11 (14%)	0	100	100
53	y	84/87 (97%)	82 (98%)	2 (2%)	0	100	100
54	z	68/71 (96%)	63 (93%)	5 (7%)	0	100	100
All	All	5607/5912 (95%)	5038 (90%)	555 (10%)	14 (0%)	44	71

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	C	152	PRO
40	l	84	THR
35	g	128	LYS
36	h	51	SER
39	k	41	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	
6	B	216/218 (99%)	214 (99%)	2 (1%)	70	76
7	C	164/164 (100%)	160 (98%)	4 (2%)	43	62
8	D	165/165 (100%)	163 (99%)	2 (1%)	63	72
9	E	148/150 (99%)	142 (96%)	6 (4%)	27	52
10	F	136/138 (99%)	133 (98%)	3 (2%)	45	63
11	G	114/114 (100%)	112 (98%)	2 (2%)	51	67
12	J	116/116 (100%)	115 (99%)	1 (1%)	70	76
13	K	104/104 (100%)	104 (100%)	0	100	100
14	L	103/103 (100%)	100 (97%)	3 (3%)	37	60
15	M	109/109 (100%)	109 (100%)	0	100	100
16	N	99/103 (96%)	96 (97%)	3 (3%)	36	59
17	O	86/87 (99%)	85 (99%)	1 (1%)	63	72
18	P	99/100 (99%)	99 (100%)	0	100	100
19	Q	89/90 (99%)	87 (98%)	2 (2%)	45	63
20	R	84/84 (100%)	80 (95%)	4 (5%)	23	50
21	S	93/93 (100%)	91 (98%)	2 (2%)	45	63
22	T	81/84 (96%)	80 (99%)	1 (1%)	63	72
23	U	84/85 (99%)	84 (100%)	0	100	100
24	V	78/78 (100%)	78 (100%)	0	100	100
25	W	57/62 (92%)	55 (96%)	2 (4%)	32	56
26	X	67/68 (98%)	66 (98%)	1 (2%)	57	69
27	Y	54/55 (98%)	49 (91%)	5 (9%)	8	29
28	Z	48/49 (98%)	48 (100%)	0	100	100
29	a	59/62 (95%)	59 (100%)	0	100	100
30	b	47/48 (98%)	44 (94%)	3 (6%)	16	42
31	c	47/49 (96%)	47 (100%)	0	100	100
32	d	38/38 (100%)	38 (100%)	0	100	100
33	e	51/52 (98%)	48 (94%)	3 (6%)	18	44
34	f	34/34 (100%)	33 (97%)	1 (3%)	37	60
35	g	187/199 (94%)	185 (99%)	2 (1%)	65	74
36	h	171/190 (90%)	166 (97%)	5 (3%)	37	60
37	i	172/173 (99%)	171 (99%)	1 (1%)	78	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	j	119/126 (94%)	119 (100%)	0	100	100
39	k	91/116 (78%)	90 (99%)	1 (1%)	65	74
40	l	124/147 (84%)	117 (94%)	7 (6%)	19	46
41	m	104/105 (99%)	103 (99%)	1 (1%)	68	75
42	n	105/107 (98%)	103 (98%)	2 (2%)	50	66
43	o	86/90 (96%)	85 (99%)	1 (1%)	63	72
44	p	90/99 (91%)	88 (98%)	2 (2%)	45	63
45	q	102/103 (99%)	101 (99%)	1 (1%)	68	75
46	r	94/96 (98%)	91 (97%)	3 (3%)	34	58
47	s	83/84 (99%)	83 (100%)	0	100	100
48	t	76/77 (99%)	76 (100%)	0	100	100
49	u	65/65 (100%)	63 (97%)	2 (3%)	35	59
50	v	74/78 (95%)	68 (92%)	6 (8%)	11	36
51	w	57/65 (88%)	55 (96%)	2 (4%)	32	56
52	x	72/79 (91%)	69 (96%)	3 (4%)	26	52
53	y	65/66 (98%)	65 (100%)	0	100	100
54	z	60/61 (98%)	59 (98%)	1 (2%)	53	67
All	All	4667/4828 (97%)	4576 (98%)	91 (2%)	48	66

5 of 91 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	h	190	HIS
44	p	83	GLU
39	k	14	GLN
40	l	86	GLN
46	r	45	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 99 such sidechains are listed below:

Mol	Chain	Res	Type
35	g	190	ASN
39	k	63	ASN
36	h	6	HIS
37	i	74	ASN

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Mol	Chain	Res	Type
41	m	21	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2817/2903 (97%)	595 (21%)	23 (0%)
2	2	1532/1540 (99%)	361 (23%)	9 (0%)
3	3	119/120 (99%)	32 (26%)	0
4	4	6/18 (33%)	3 (50%)	1 (16%)
5	5	76/77 (98%)	37 (48%)	5 (6%)
All	All	4550/4658 (97%)	1028 (22%)	38 (0%)

5 of 1028 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	2	G
1	1	5	A
1	1	10	A
1	1	34	U
1	1	35	G

5 of 38 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	1109	C
5	5	60	U
2	2	1299	A
4	4	14	G
5	5	74	C

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

12 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
2	2MG	2	966	2	23,26,27	2.82	9 (39%)	33,38,41	2.24	11 (33%)
2	5MC	2	967	2	19,22,23	3.91	8 (42%)	26,32,35	1.02	2 (7%)
2	5MC	2	1407	2	19,22,23	3.59	8 (42%)	26,32,35	1.07	1 (3%)
2	2MG	2	1516	2	23,26,27	2.87	9 (39%)	33,38,41	2.10	11 (33%)
2	MA6	2	1518	2	23,26,27	1.54	4 (17%)	33,38,41	2.45	16 (48%)
2	PSU	2	516	2	18,21,22	1.55	3 (16%)	21,30,33	2.33	7 (33%)
2	UR3	2	1498	2	19,22,23	2.76	7 (36%)	26,32,35	1.54	4 (15%)
2	MA6	2	1519	2	23,26,27	1.53	5 (21%)	33,38,41	2.50	14 (42%)
2	G7M	2	527	2	23,26,27	3.58	12 (52%)	34,39,42	1.65	7 (20%)
2	4OC	2	1402	2	20,23,24	3.09	8 (40%)	25,32,35	0.88	2 (8%)
2	2MG	2	1207	2	23,26,27	2.86	8 (34%)	33,38,41	2.28	10 (30%)
45	0TD	q	89	45	8,9,10	2.10	3 (37%)	6,11,13	2.58	3 (50%)

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
2	2MG	2	966	2	-	1/9/27/28	0/3/3/3
2	5MC	2	967	2	-	2/7/25/26	0/2/2/2
2	5MC	2	1407	2	-	0/7/25/26	0/2/2/2
2	2MG	2	1516	2	-	0/9/27/28	0/3/3/3
2	MA6	2	1518	2	-	1/11/29/30	0/3/3/3
2	PSU	2	516	2	-	2/7/25/26	0/2/2/2
2	UR3	2	1498	2	-	3/7/25/26	0/2/2/2
2	MA6	2	1519	2	-	5/11/29/30	0/3/3/3
2	G7M	2	527	2	-	3/7/25/26	0/3/3/3
2	4OC	2	1402	2	-	1/9/29/30	0/2/2/2
2	2MG	2	1207	2	-	0/9/27/28	0/3/3/3
45	0TD	q	89	45	-	3/7/12/14	-

The worst 5 of 84 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	527	G7M	C8-N7	10.62	1.51	1.33
2	2	967	5MC	C6-C5	9.25	1.49	1.34
2	2	1407	5MC	C6-C5	8.82	1.49	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	1207	2MG	C2-N3	7.56	1.46	1.32
2	2	1516	2MG	C2-N3	7.40	1.46	1.32

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	516	PSU	N1-C2-N3	7.07	122.63	115.17
2	2	1207	2MG	C2-N3-C4	6.91	120.64	112.00
2	2	966	2MG	C2-N3-C4	6.24	119.80	112.00
2	2	1516	2MG	C2-N3-C4	6.19	119.75	112.00
2	2	1519	MA6	C5-C4-N3	-5.92	118.57	126.72

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	2	516	PSU	O4'-C1'-C5-C4
2	2	516	PSU	O4'-C1'-C5-C6
2	2	967	5MC	O4'-C4'-C5'-O5'
2	2	1402	4OC	C1'-C2'-O2'-CM2
2	2	1498	UR3	O4'-C4'-C5'-O5'

There are no ring outliers.

9 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	966	2MG	3	0
2	2	967	5MC	3	0
2	2	1407	5MC	1	0
2	2	1516	2MG	1	0
2	2	1518	MA6	2	0
2	2	1498	UR3	1	0
2	2	1402	4OC	5	0
2	2	1207	2MG	3	0
45	q	89	0TD	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 425 ligands modelled in this entry, 424 are monoatomic - leaving 1 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	$\# Z > 2$
56	LYS	5	101	5	7,8,9	0.64	0	3,8,10	0.32	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
56	LYS	5	101	5	-	2/6/7/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	5	101	LYS	CE-CD-CG-CB
56	5	101	LYS	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

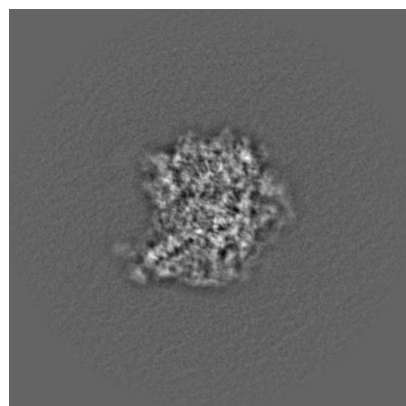
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43549. These allow visual inspection of the internal detail of the map and identification of artifacts.

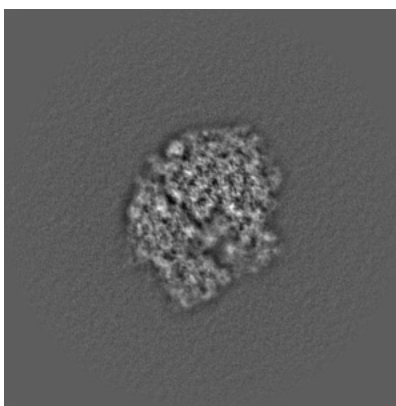
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

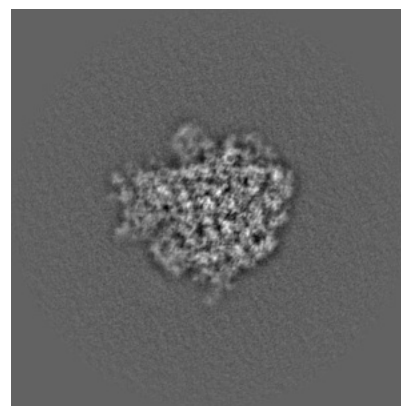
6.1.1 Primary map



X

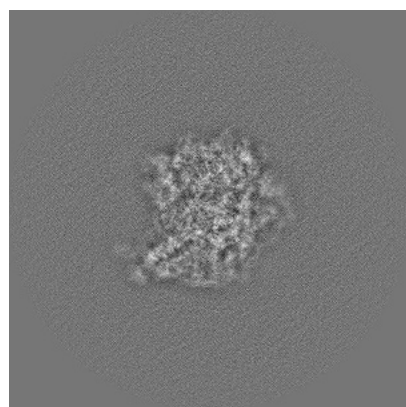


Y

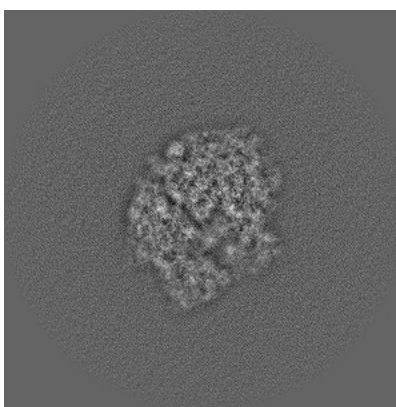


Z

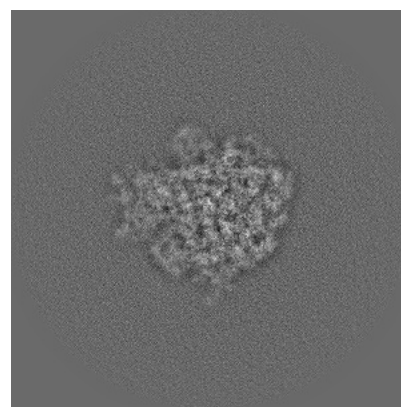
6.1.2 Raw map



X



Y

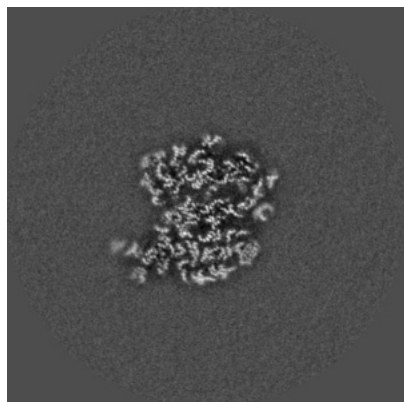


Z

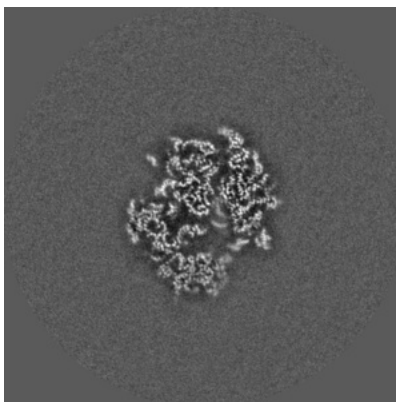
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

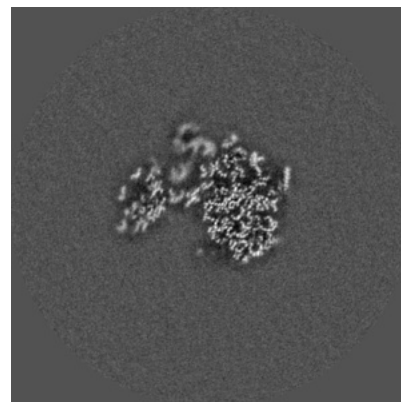
6.2.1 Primary map



X Index: 256

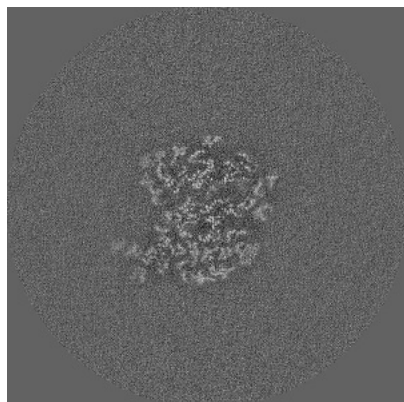


Y Index: 256

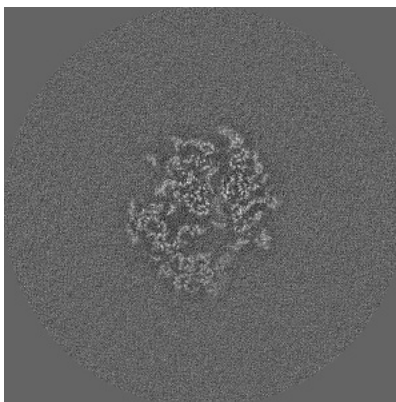


Z Index: 256

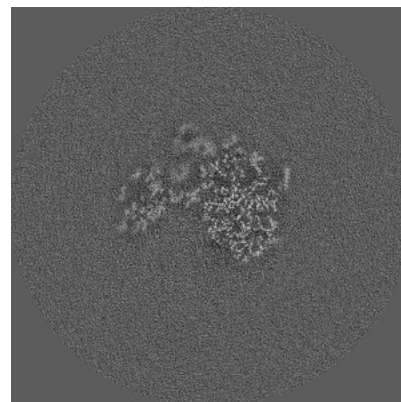
6.2.2 Raw map



X Index: 256



Y Index: 256

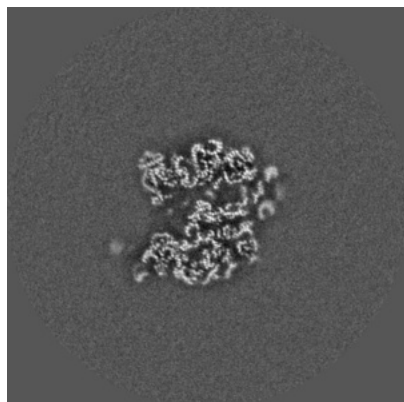


Z Index: 256

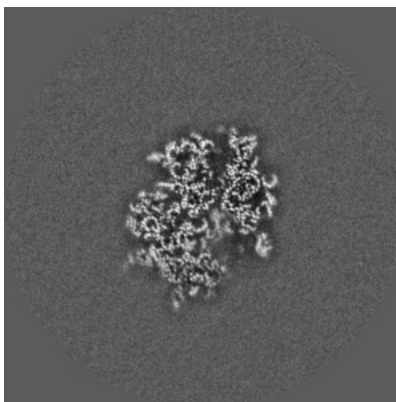
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

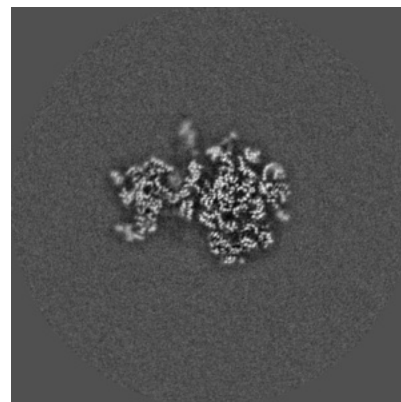
6.3.1 Primary map



X Index: 250

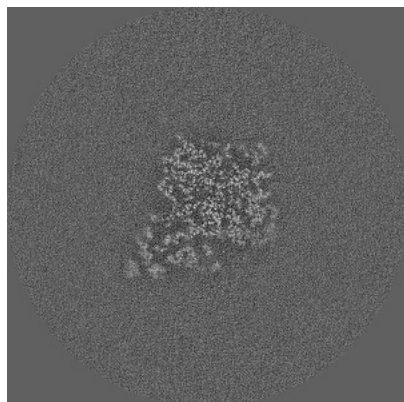


Y Index: 263

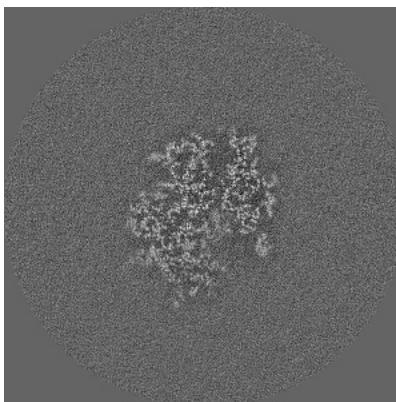


Z Index: 241

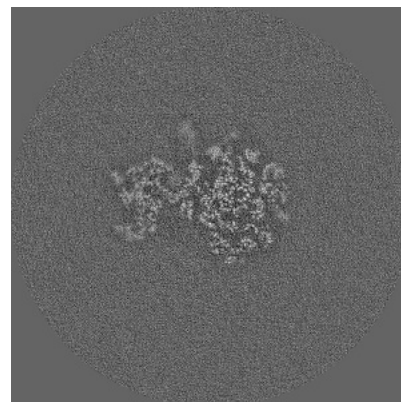
6.3.2 Raw map



X Index: 275



Y Index: 263

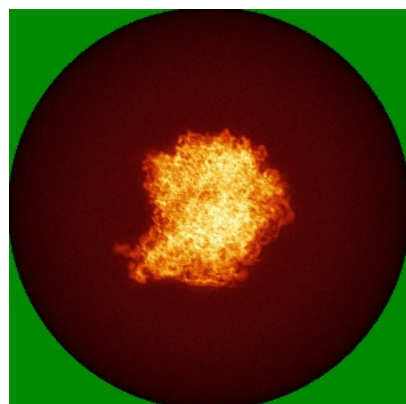


Z Index: 241

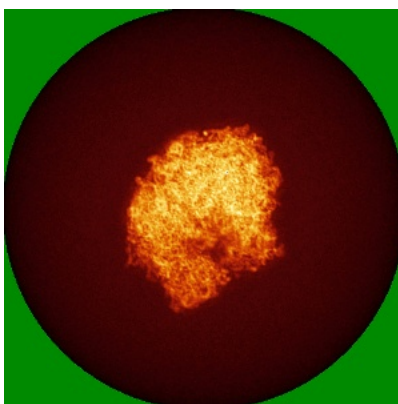
The images above show the largest variance slices of the map in three orthogonal directions.

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

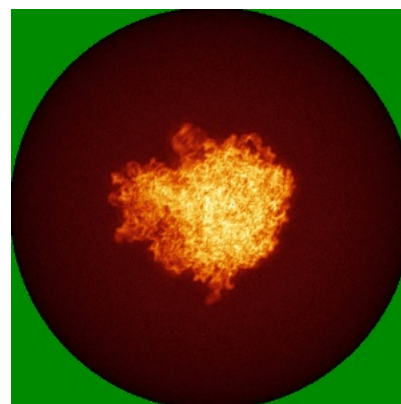
6.4.1 Primary map



X

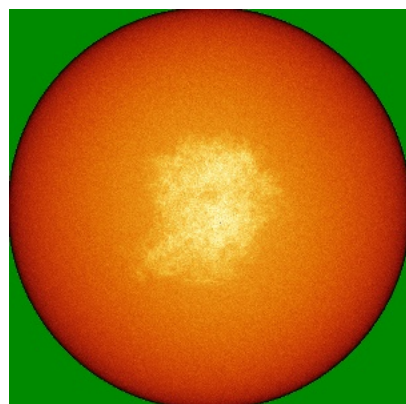


Y

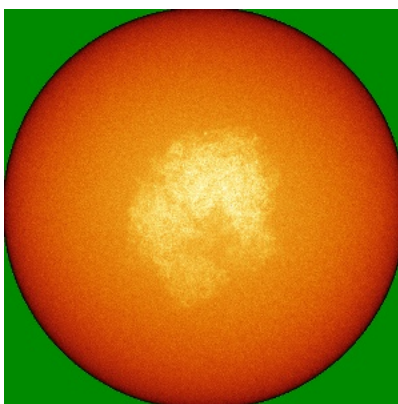


Z

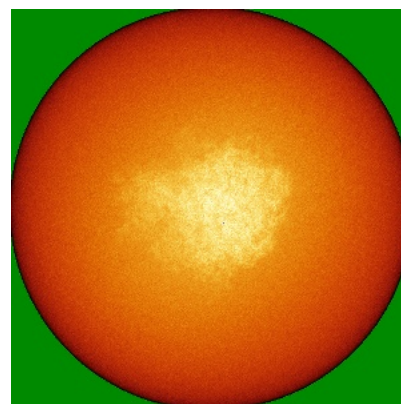
6.4.2 Raw map



X



Y

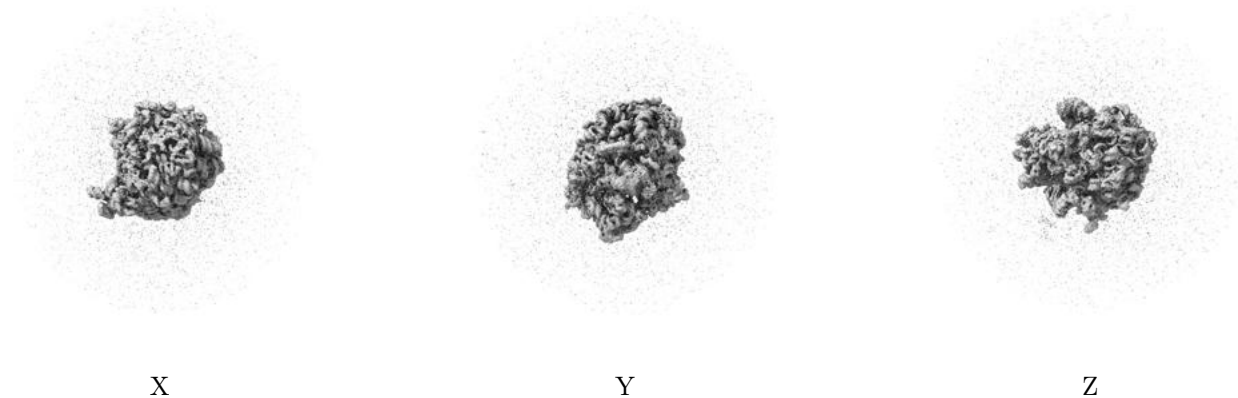


Z

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.

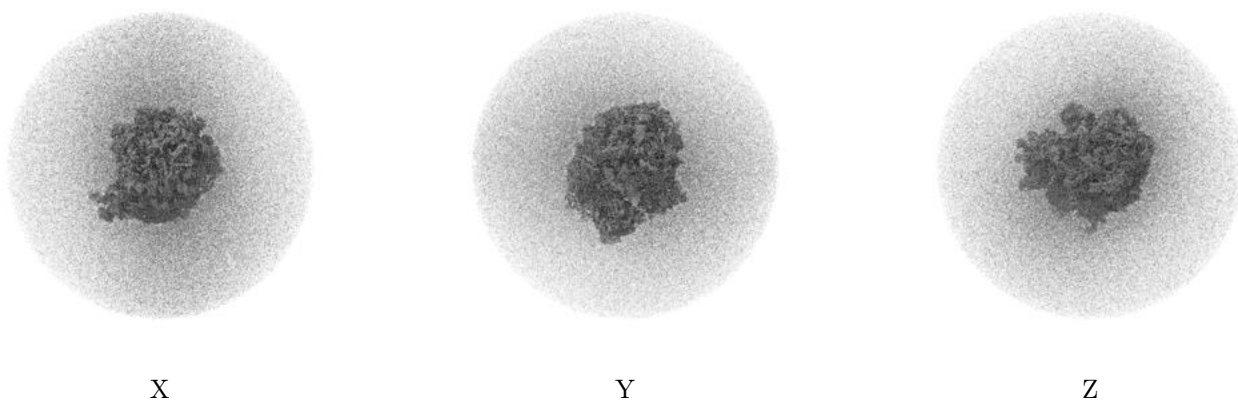
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00281. 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.

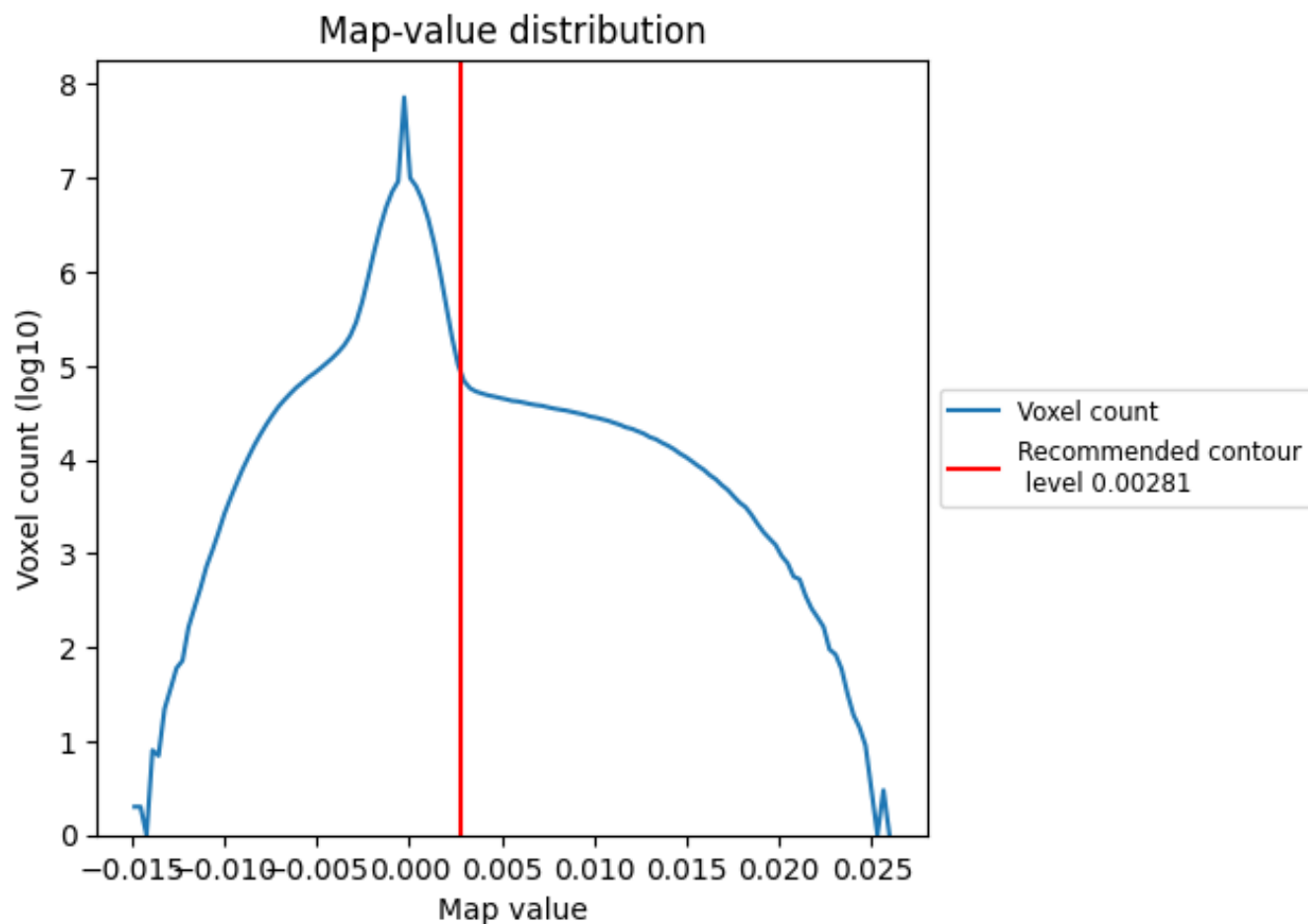
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

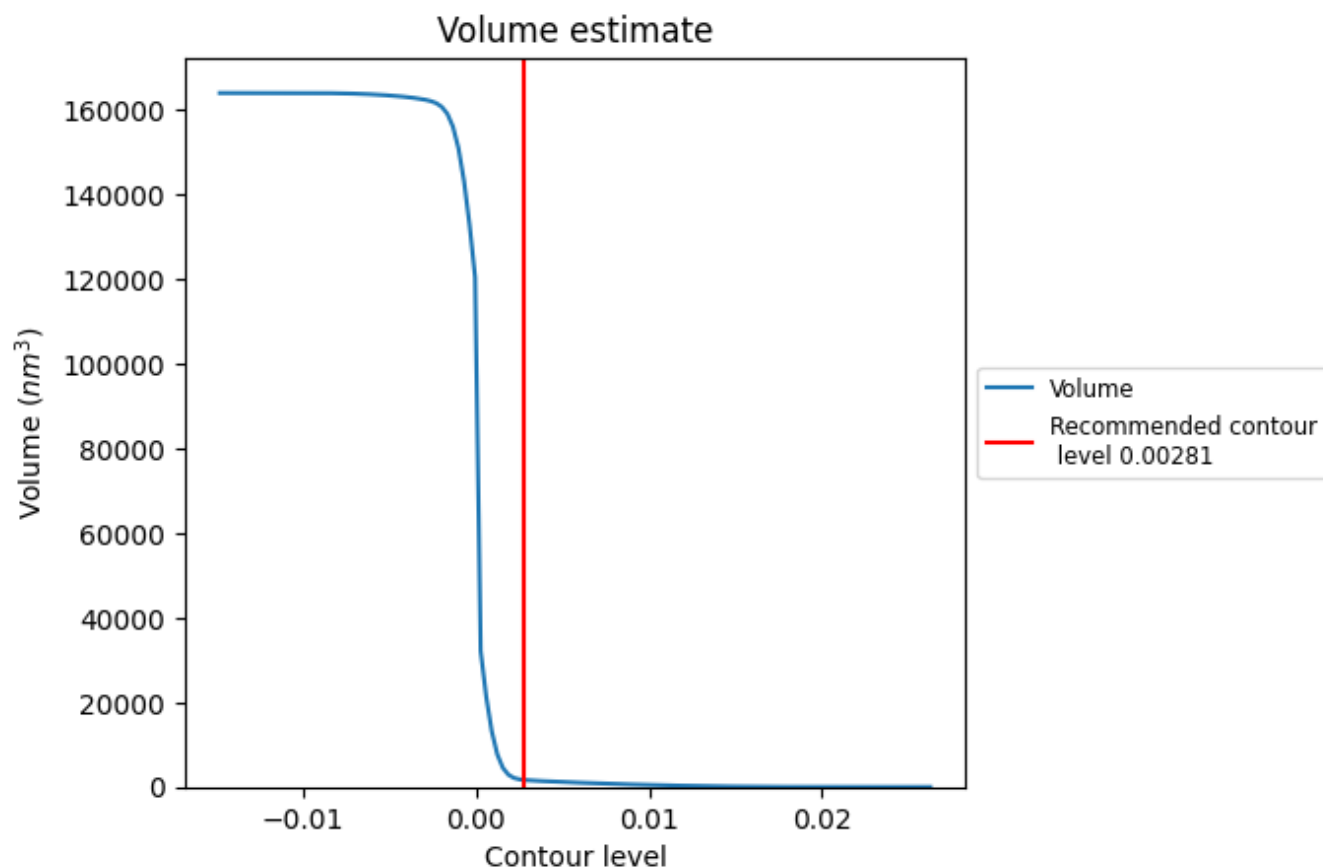
This section contains the results of statistical analysis of the map.

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.

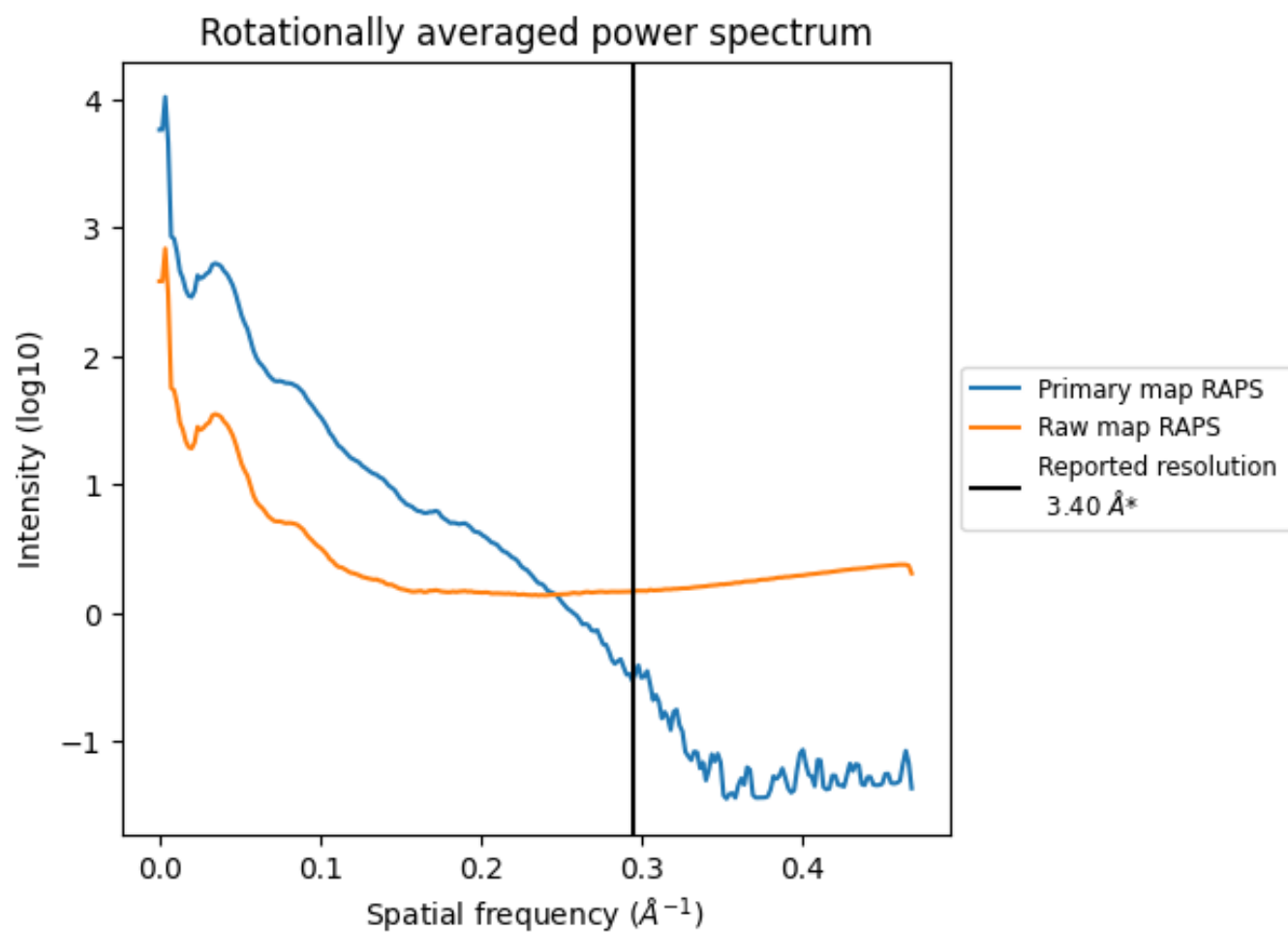
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1643 nm³; this corresponds to an approximate mass of 1485 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 ⓘ

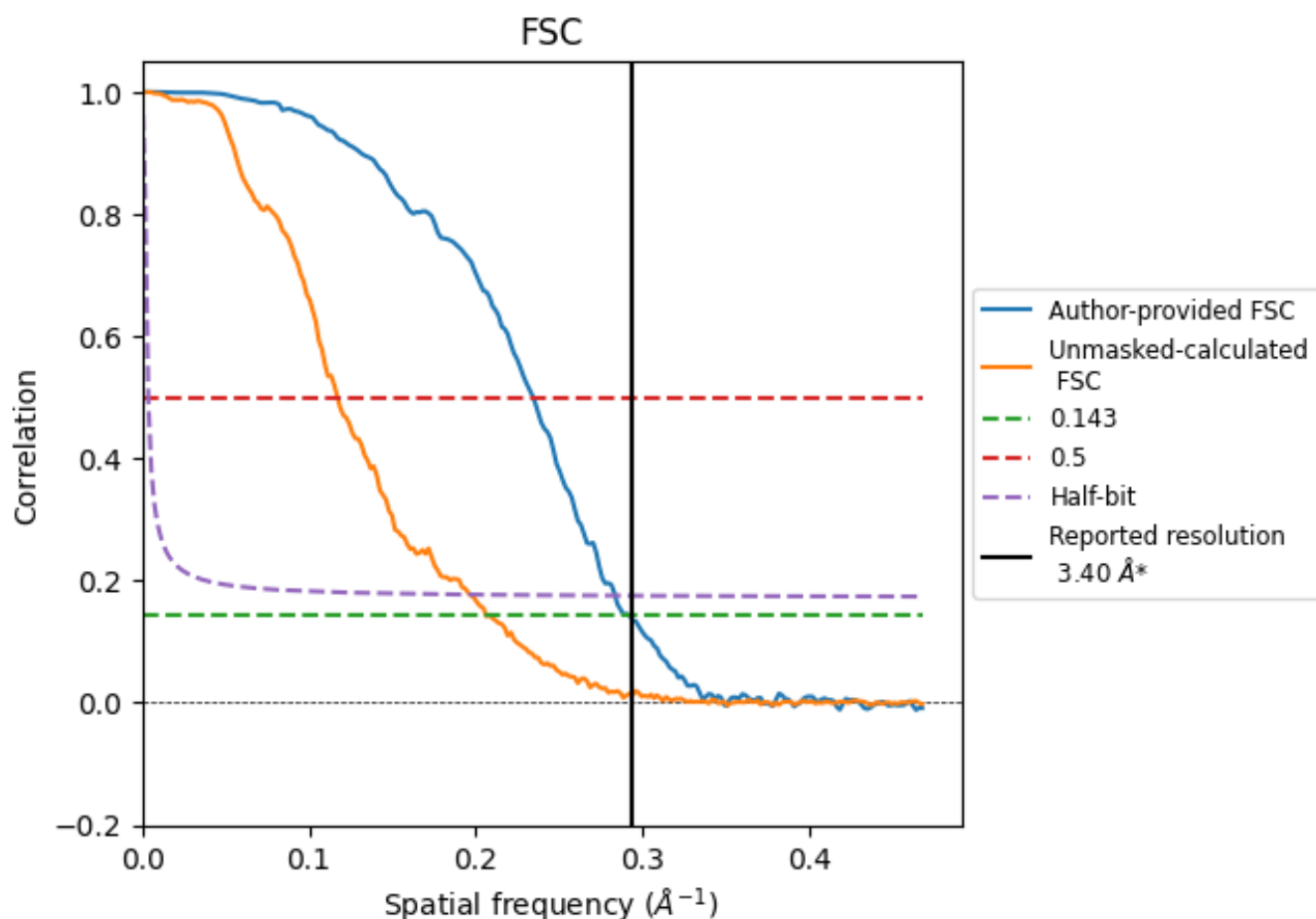


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

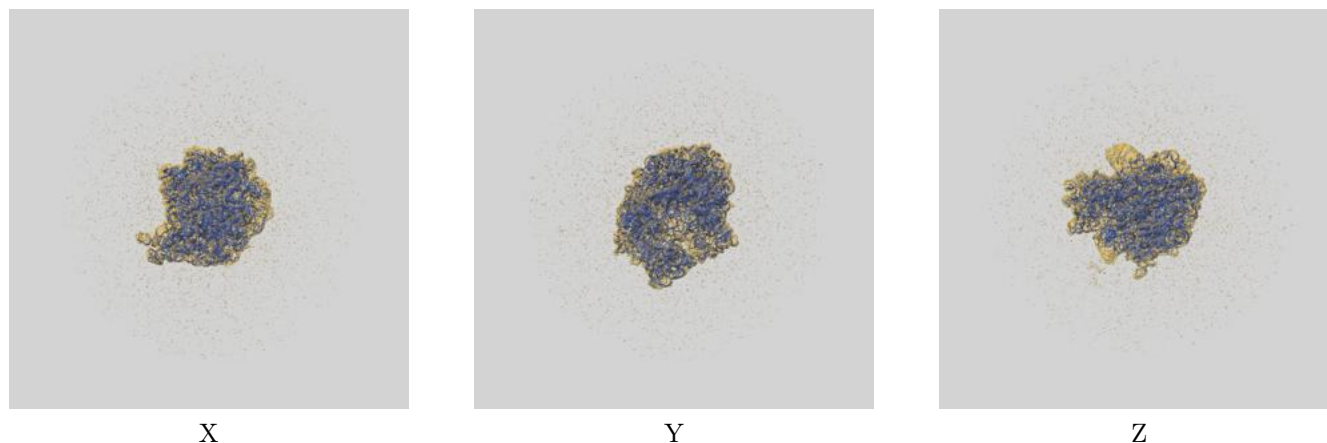
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	4.27	3.53
Unmasked-calculated*	4.85	8.54	5.08

*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 4.85 differs from the reported value 3.4 by more than 10 %

9 Map-model fit [i](#)

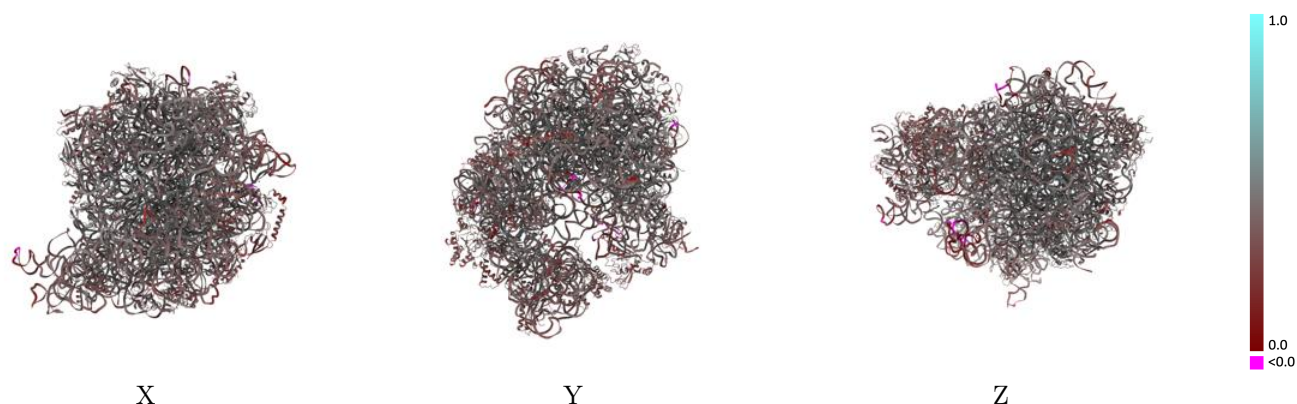
This section contains information regarding the fit between EMDB map EMD-43549 and PDB model 8VV4. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.00281 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](#)

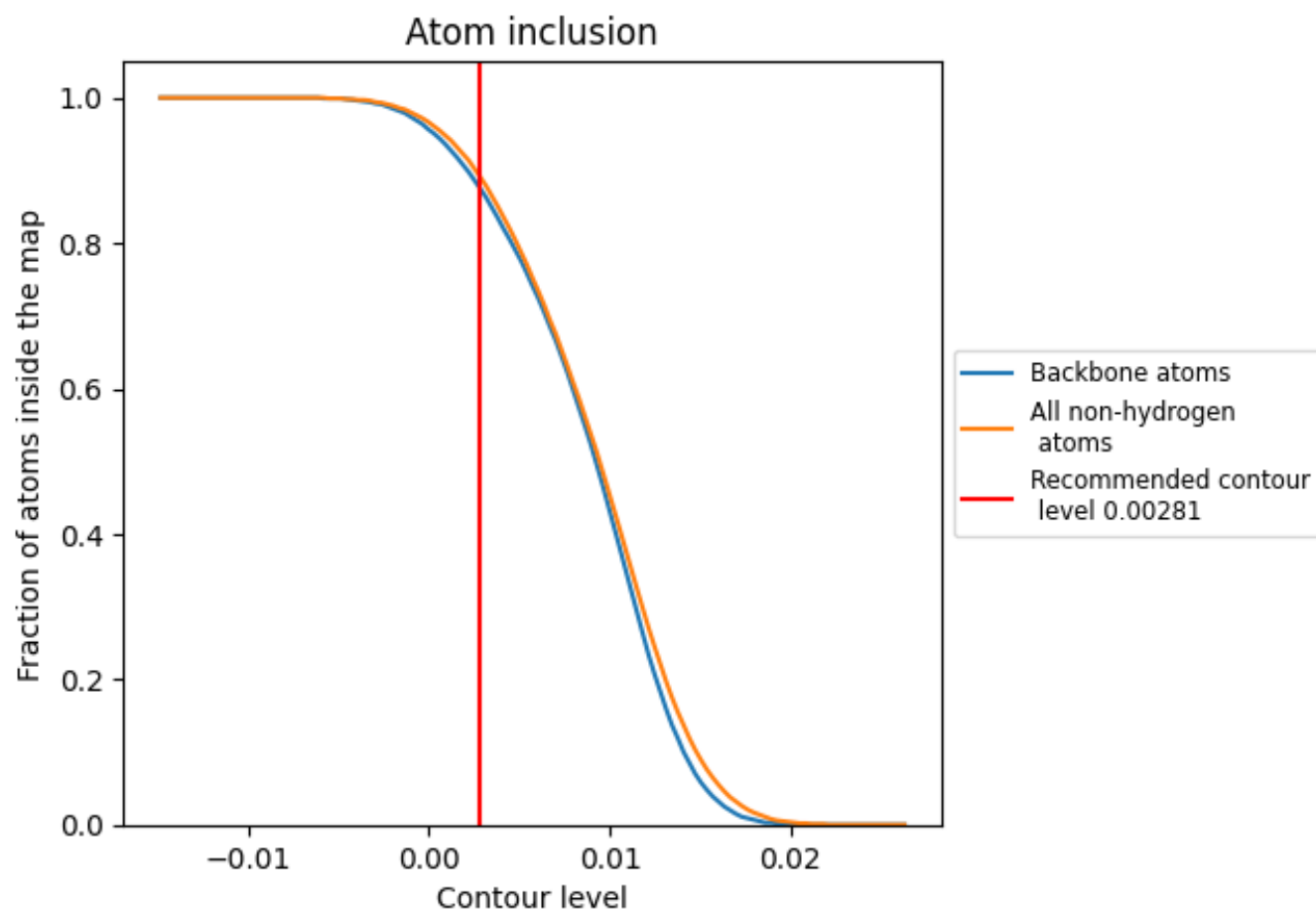


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 89% 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 (0.00281) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8920	 0.4050
1	 0.9430	 0.4200
2	 0.9510	 0.4030
3	 0.9590	 0.3920
4	 0.7170	 0.4050
5	 0.9320	 0.3750
B	 0.7910	 0.4460
C	 0.8210	 0.4420
D	 0.8140	 0.4110
E	 0.8000	 0.3320
F	 0.8700	 0.3860
G	 0.8280	 0.3010
J	 0.8130	 0.4270
K	 0.7980	 0.4430
L	 0.7820	 0.4300
M	 0.7950	 0.4380
N	 0.7960	 0.4360
O	 0.7960	 0.3750
P	 0.8230	 0.4360
Q	 0.7790	 0.4030
R	 0.8380	 0.4320
S	 0.7930	 0.4230
T	 0.7630	 0.4050
U	 0.8180	 0.3980
V	 0.8710	 0.4040
W	 0.7910	 0.4420
X	 0.7840	 0.4190
Y	 0.8080	 0.3520
Z	 0.8400	 0.4290
a	 0.5580	 0.2530
b	 0.7790	 0.4210
c	 0.8330	 0.4050
d	 0.7610	 0.4490
e	 0.7050	 0.4350
f	 0.6850	 0.4090



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Chain	Atom inclusion	Q-score
g	 0.7650	 0.3190
h	 0.8090	 0.3820
i	 0.7320	 0.3500
j	 0.8010	 0.3970
k	 0.8330	 0.3610
l	 0.7740	 0.3470
m	 0.8150	 0.4040
n	 0.7620	 0.3460
o	 0.7330	 0.3510
p	 0.8070	 0.3760
q	 0.7870	 0.3930
r	 0.7800	 0.3380
s	 0.7300	 0.3590
t	 0.8150	 0.3700
u	 0.7690	 0.4140
v	 0.7970	 0.3620
w	 0.6500	 0.3230
x	 0.7790	 0.3400
y	 0.7230	 0.3370
z	 0.5730	 0.2750