



wwPDB EM Validation Summary Report ⓘ

May 18, 2024 – 12:58 PM EDT

PDB ID : 7K53
EMDB ID : EMD-22672
Title : Pre-translocation +1-frameshifting(CCC-A) complex (Structure I-FS)
Authors : Demo, G.; Loveland, A.B.; Svidritskiy, E.; Gamper, H.B.; Hou, Y.M.; Korostelev, A.A.
Deposited on : 2020-09-16
Resolution : 3.20 Å(reported)
Based on initial models : 6ENJ, 5UYM

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.dev92
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36.2

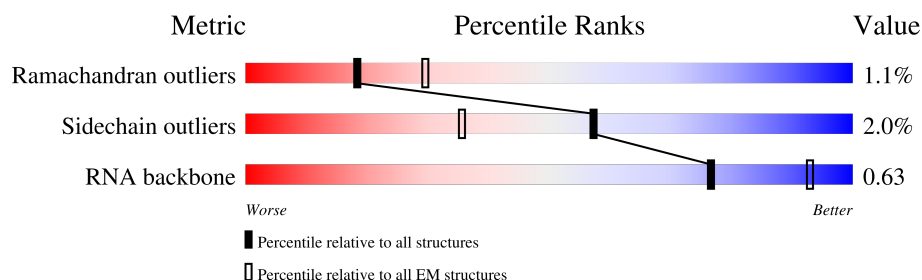
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



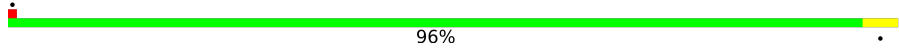
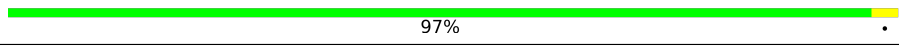
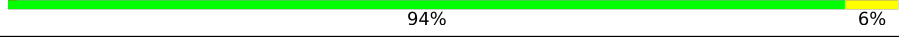
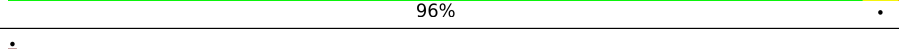
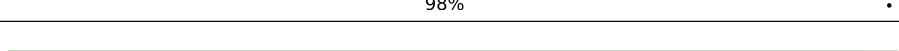
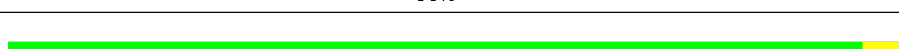
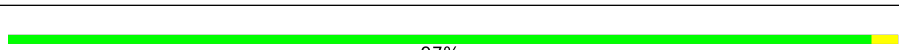

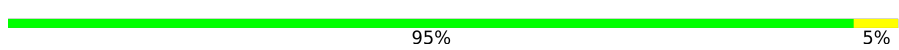
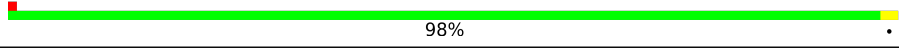
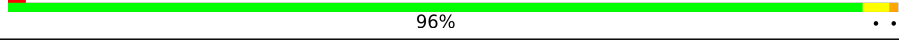
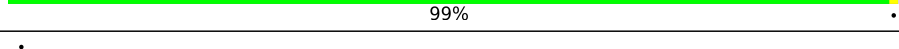
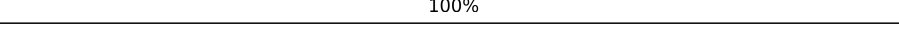
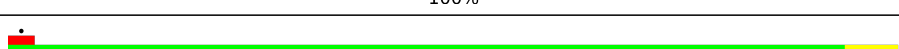
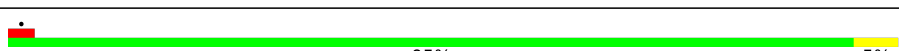
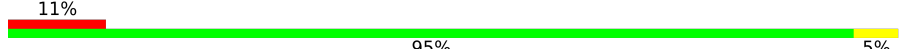
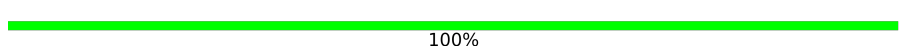
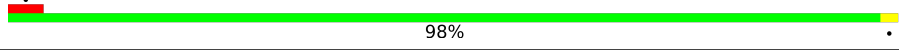
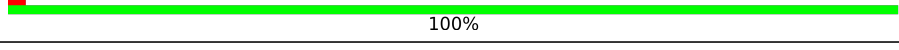
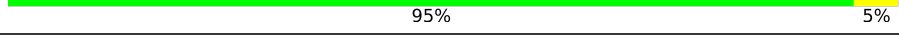
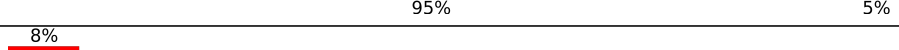
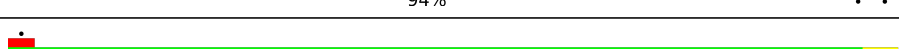



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	b	271	
2	c	209	
3	d	201	
4	e	177	
5	f	176	
6	g	149	
7	h	131	
8	i	141	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	j	142	 96%
10	k	122	 97%
11	l	143	 94%6%
12	m	136	 96%.
13	n	120	 98%.
14	o	116	 96%.
15	p	114	 96%.
16	q	117	 97%.
17	r	103	 96%.
18	s	110	 95%5%
19	t	93	 98%.
20	u	102	 96%.
21	v	94	 99%.
22	w	75	 100%
23	x	77	 100%
24	y	63	 94%6%
25	z	58	 95%5%
26	A	66	 11%95%5%
27	B	56	 100%
28	C	50	 98%.
29	D	46	 100%
30	E	64	 95%5%
31	F	38	 95%5%
32	G	225	 8%94%.
33	H	206	 96%.

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	I	205	
35	J	157	
36	K	100	
37	L	151	
38	M	129	
39	N	127	
40	O	98	
41	P	116	
42	Q	123	
43	R	114	
44	S	100	
45	T	88	
46	U	82	
47	V	80	
48	W	65	
49	X	79	
50	Y	85	
51	Z	65	
52	a	223	
53	3	1539	
54	1	2903	
55	2	120	
56	5	77	
56	6	77	
57	4	18	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
58	7	77	<div><div>8%</div><div>82%</div><div>18%</div></div>

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 149698 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

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

- Molecule 3 is a protein called 50S ribosomal protein L4.

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

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

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

- Molecule 6 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	g	125	Total	C	N	O	S	0	0
			936	590	166	179	1		

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	84	Total	C	N	O	S	0	0
			633	397	114	118	4		

- Molecule 8 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	i	74	Total	C	N	O	S	0	0
			551	358	91	99	3		

- Molecule 9 is a protein called 50S ribosomal protein L13.

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

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

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

- Molecule 17 is a protein called 50S ribosomal protein L21.

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

- Molecule 18 is a protein called 50S ribosomal protein L22.

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

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	t	93	Total	C	N	O	S	0
			739	466	139	132	2	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	102	Total	C	N	O		0
			780	492	146	142		0

- Molecule 21 is a protein called 50S ribosomal protein L25.

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

- Molecule 22 is a protein called 50S ribosomal protein L27.

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

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

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

- Molecule 26 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	A	66	Total	C	N	O	S	0	0
			523	323	99	95	6		

- Molecule 27 is a protein called 50S ribosomal protein L32.

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

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

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

- Molecule 30 is a protein called 50S ribosomal protein L35.

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

- Molecule 31 is a protein called 50S ribosomal protein L36.

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

- Molecule 32 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	G	218	Total	C	N	O	S	0	0
			1705	1081	305	312	7		

- Molecule 33 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 34 is a protein called 30S ribosomal protein S4.

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

- Molecule 35 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 36 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 37 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 38 is a protein called 30S ribosomal protein S8.

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

- Molecule 39 is a protein called 30S ribosomal protein S9.

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

- Molecule 40 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 41 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 42 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 43 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 44 is a protein called 30S ribosomal protein S14.

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

- Molecule 45 is a protein called 30S ribosomal protein S15.

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

- Molecule 46 is a protein called 30S ribosomal protein S16.

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

- Molecule 47 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 48 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 49 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 50 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Y	85	Total	C	N	O	S	0	0
			665	411	137	114	3		

- Molecule 51 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 52 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 53 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 54 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 802133627

- Molecule 55 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1266961702

- Molecule 56 is a RNA chain called tRNAfMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
56	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

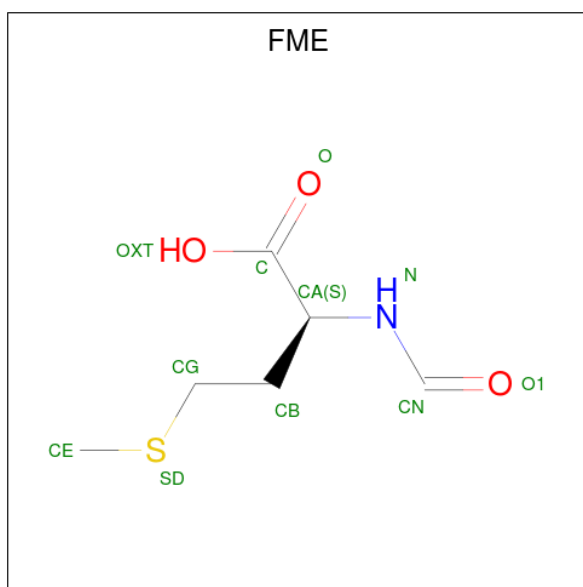
- Molecule 57 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	4	18	Total	C	N	O	P	0	0
			388	175	78	118	17		

- Molecule 58 is a RNA chain called tRNAPro.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	7	77	Total	C	N	O	P	0	0
			1647	733	295	542	77		

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
59	5	1	10	6	1	2	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: 50S ribosomal protein L2

Chain b:  94% 6%



- Molecule 2: 50S ribosomal protein L3

Chain c:  98% .



- Molecule 3: 50S ribosomal protein L4

Chain d:  97% .



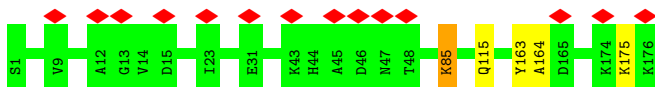
- Molecule 4: 50S ribosomal protein L5

Chain e:  97% .

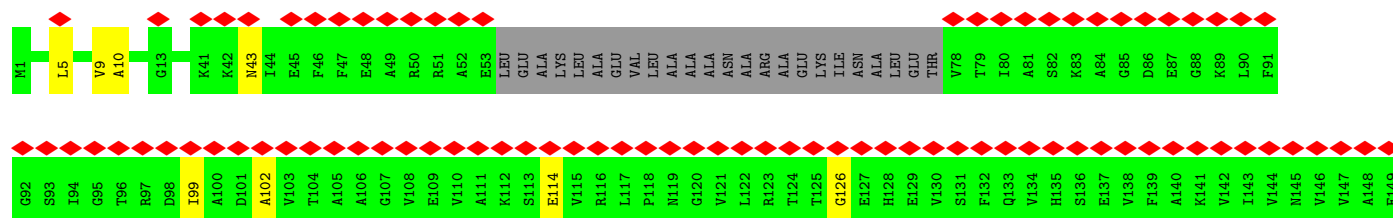
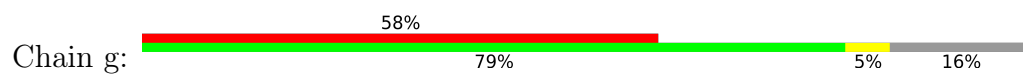


- Molecule 5: 50S ribosomal protein L6

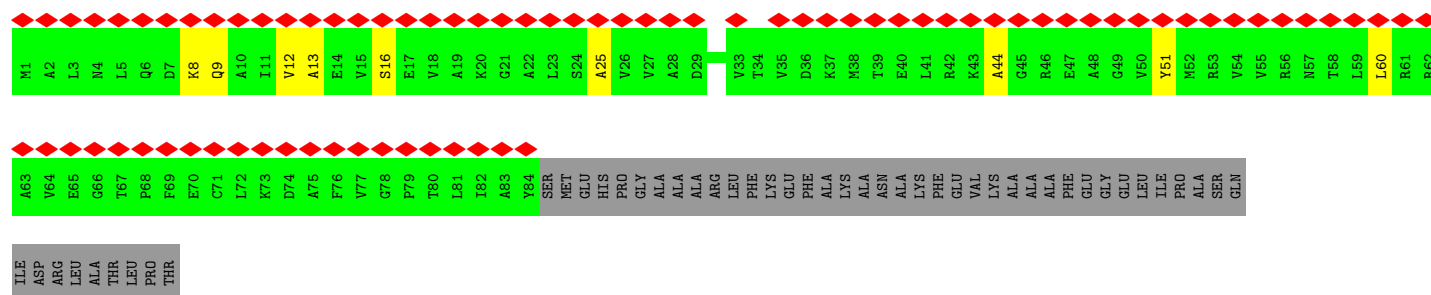
Chain f:  8% 97% ..



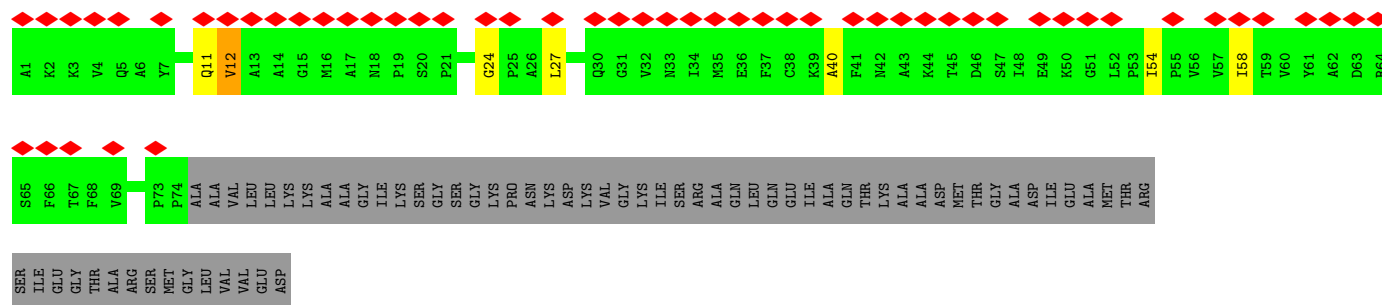
- Molecule 6: 50S ribosomal protein L9



• Molecule 7: 50S ribosomal protein L10



• Molecule 8: 50S ribosomal protein L11



• Molecule 9: 50S ribosomal protein L13



• Molecule 10: 50S ribosomal protein L14

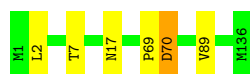




- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16



- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



- Molecule 15: 50S ribosomal protein L19



- Molecule 16: 50S ribosomal protein L20



- Molecule 17: 50S ribosomal protein L21





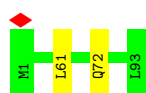
- Molecule 18: 50S ribosomal protein L22

Chain s: 95% 5%



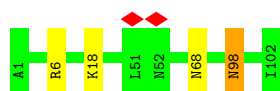
- Molecule 19: 50S ribosomal protein L23

Chain t: 98% .



- Molecule 20: 50S ribosomal protein L24

Chain u: 96% ..



- Molecule 21: 50S ribosomal protein L25

Chain v: 99% .



- Molecule 22: 50S ribosomal protein L27

Chain w: 100%



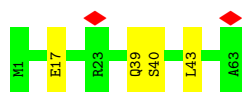
- Molecule 23: 50S ribosomal protein L28

Chain x: 100%

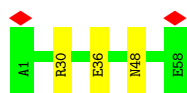
There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L29

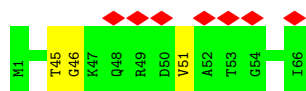
Chain y: 94% 6%



- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31



- Molecule 27: 50S ribosomal protein L32



There are no outlier residues recorded for this chain.

- Molecule 28: 50S ribosomal protein L33



- Molecule 29: 50S ribosomal protein L34

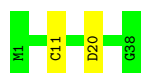


- Molecule 30: 50S ribosomal protein L35

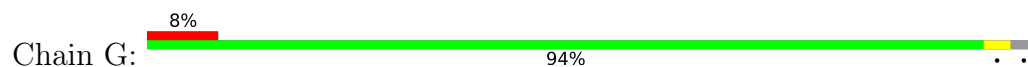


- Molecule 31: 50S ribosomal protein L36

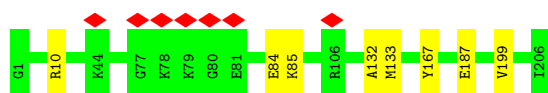




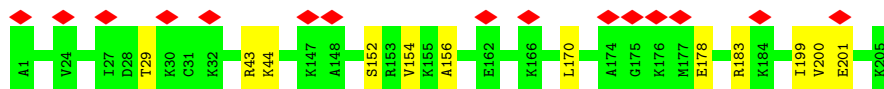
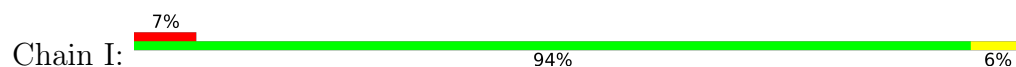
- Molecule 32: 30S ribosomal protein S2



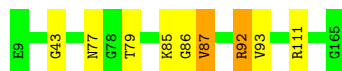
- Molecule 33: 30S ribosomal protein S3



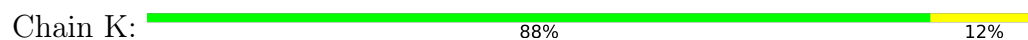
- Molecule 34: 30S ribosomal protein S4



- Molecule 35: 30S ribosomal protein S5



- Molecule 36: 30S ribosomal protein S6



- Molecule 37: 30S ribosomal protein S7

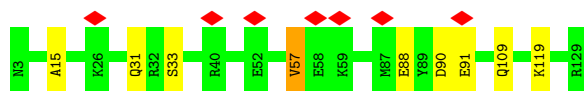
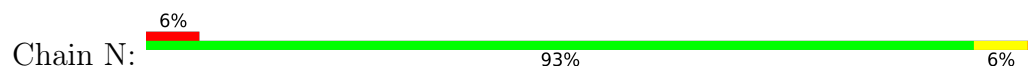


- Molecule 38: 30S ribosomal protein S8

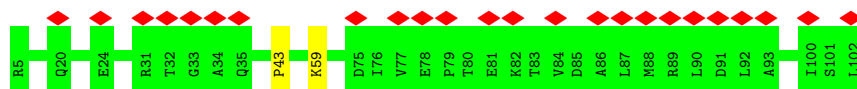




- Molecule 39: 30S ribosomal protein S9



- Molecule 40: 30S ribosomal protein S10



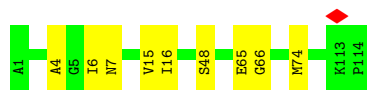
- Molecule 41: 30S ribosomal protein S11



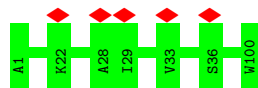
- Molecule 42: 30S ribosomal protein S12



- Molecule 43: 30S ribosomal protein S13

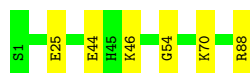


- Molecule 44: 30S ribosomal protein S14



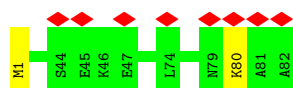
- Molecule 45: 30S ribosomal protein S15

Chain T:  93% 7%



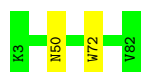
- Molecule 46: 30S ribosomal protein S16

Chain U:  10% 98% .



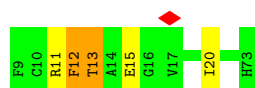
- Molecule 47: 30S ribosomal protein S17

Chain V:  98% .



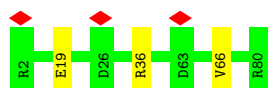
- Molecule 48: 30S ribosomal protein S18

Chain W:  92% 5% .



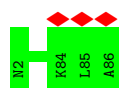
- Molecule 49: 30S ribosomal protein S19

Chain X:  96% .




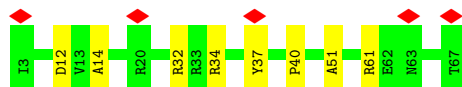
- Molecule 50: 30S ribosomal protein S20

Chain Y:  100%

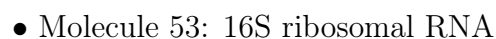


- Molecule 51: 30S ribosomal protein S21

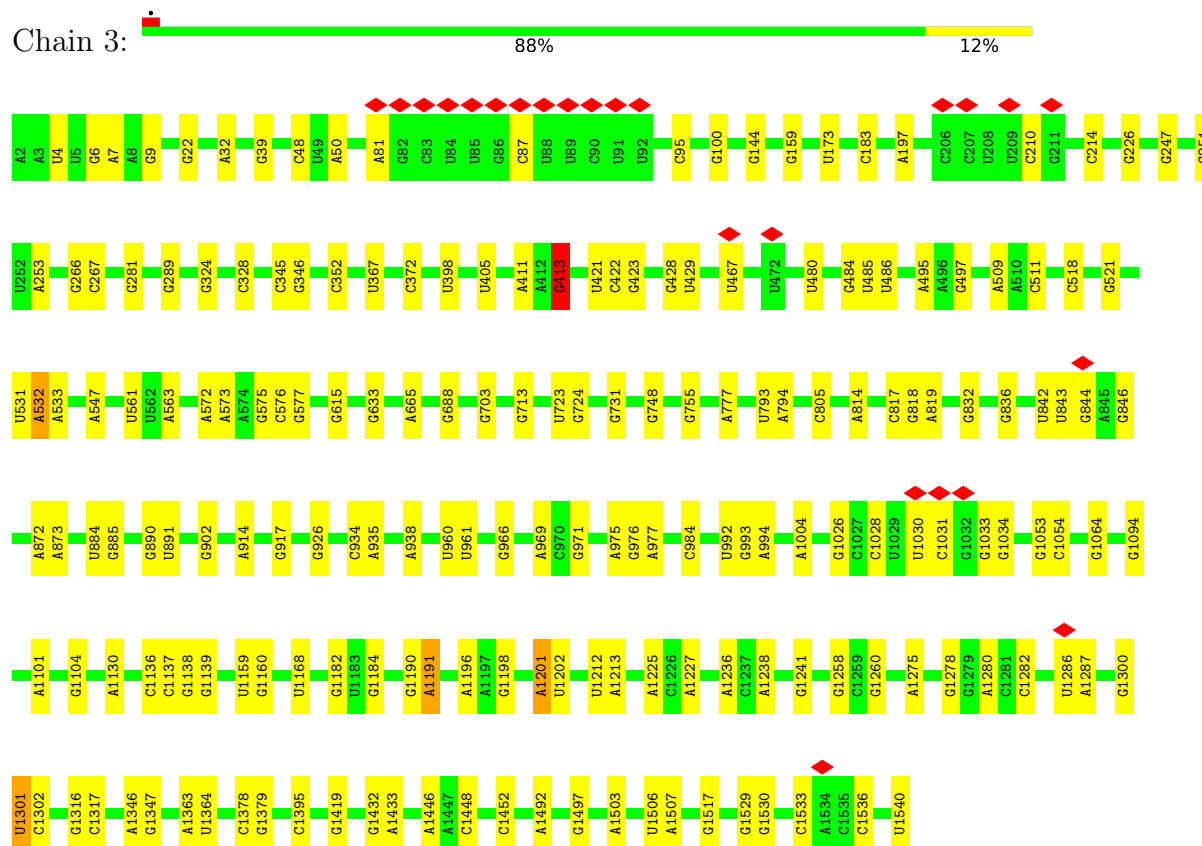
Chain Z:  8% 88% 12%



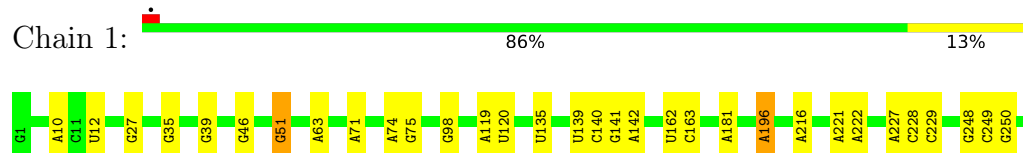
Chain a:

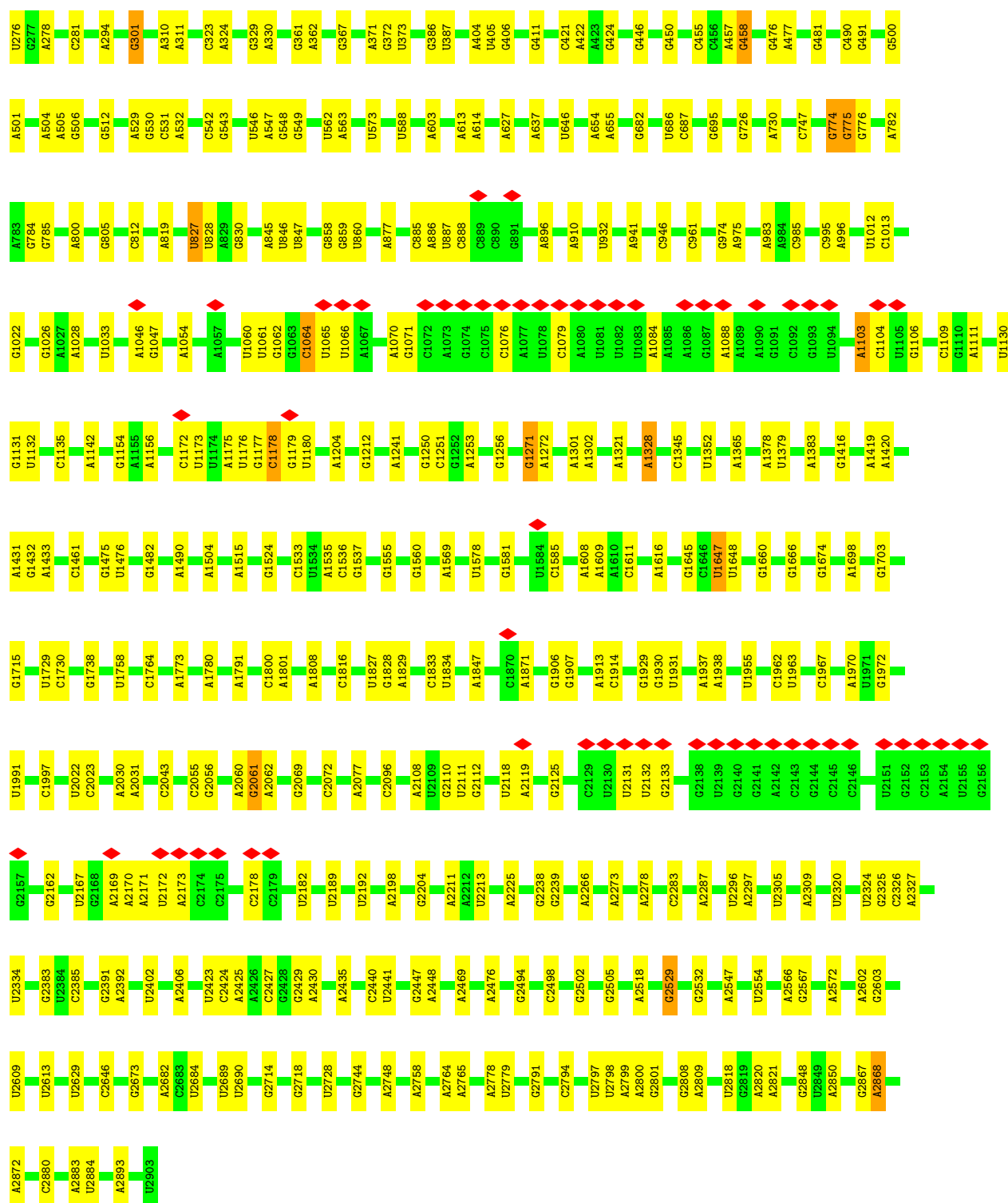


Chain 3:



Chain 1:






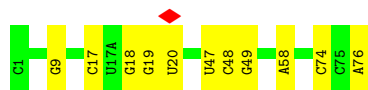
• Molecule 55: 5S ribosomal RNA


Chain 2:

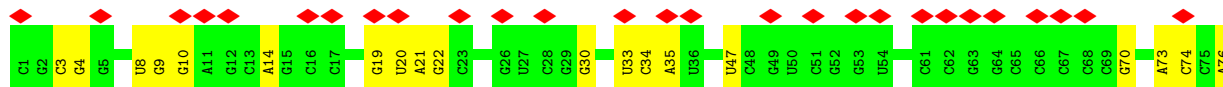


● Molecule 56: tRNA^{fMet}

Chain 5:  86% 14%

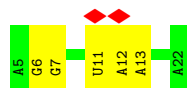
● Molecule 56: tRNA^{fMet}


Chain 6:  35% 75% 25%



● Molecule 57: mRNA

Chain 4:  11% 72% 28%

● Molecule 58: tRNA^{Pro}

Chain 7:  8% 82% 18%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12108	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	47.5	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	24.420	Depositor
Minimum map value	-6.345	Depositor
Average map value	0.018	Depositor
Map value standard deviation	1.346	Depositor
Recommended contour level	3.7	Depositor
Map size (Å)	419.99997, 419.99997, 419.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FME

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	b	0.56	1/2122 (0.0%)	0.72	2/2852 (0.1%)
2	c	0.57	1/1586 (0.1%)	0.71	0/2134
3	d	0.58	1/1571 (0.1%)	0.69	1/2113 (0.0%)
4	e	0.64	2/1435 (0.1%)	0.69	1/1926 (0.1%)
5	f	0.70	2/1343 (0.1%)	0.75	1/1816 (0.1%)
6	g	0.85	4/946 (0.4%)	0.79	0/1275
7	h	1.21	4/638 (0.6%)	1.04	3/860 (0.3%)
8	i	1.03	4/564 (0.7%)	0.86	0/768
9	j	0.53	1/1152 (0.1%)	0.67	2/1551 (0.1%)
10	k	0.62	0/948	0.76	0/1268
11	l	0.54	0/1054	0.73	0/1403
12	m	0.64	0/1093	0.74	0/1460
13	n	0.56	1/974 (0.1%)	0.65	0/1301
14	o	0.76	4/902 (0.4%)	0.70	0/1209
15	p	0.57	1/929 (0.1%)	0.70	0/1242
16	q	0.63	0/960	0.65	0/1278
17	r	0.58	0/829	0.73	0/1107
18	s	0.74	4/864 (0.5%)	0.76	0/1156
19	t	0.56	0/745	0.68	0/994
20	u	0.54	0/788	0.69	0/1051
21	v	0.51	0/766	0.62	0/1025
22	w	0.57	0/582	0.68	0/769
23	x	0.49	0/635	0.64	0/848
24	y	0.79	2/510 (0.4%)	0.79	0/677
25	z	0.55	0/453	0.67	0/605
26	A	0.78	2/532 (0.4%)	0.70	0/709
27	B	0.48	0/450	0.63	0/599
28	C	0.58	1/417 (0.2%)	0.61	0/554
29	D	0.52	0/380	0.64	0/498
30	E	0.52	0/513	0.64	0/676
31	F	0.55	0/303	0.72	1/397 (0.3%)
32	G	0.66	3/1736 (0.2%)	0.71	1/2338 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	H	0.67	3/1652 (0.2%)	0.66	0/2225
34	I	0.65	5/1665 (0.3%)	0.69	2/2227 (0.1%)
35	J	0.70	2/1170 (0.2%)	0.82	4/1573 (0.3%)
36	K	1.03	8/836 (1.0%)	0.85	2/1128 (0.2%)
37	L	0.64	2/1196 (0.2%)	0.67	0/1602
38	M	0.66	1/989 (0.1%)	0.71	1/1326 (0.1%)
39	N	0.66	2/1034 (0.2%)	0.74	2/1375 (0.1%)
40	O	0.60	0/797	0.69	0/1077
41	P	0.58	1/886 (0.1%)	0.68	0/1195
42	Q	0.66	0/969	0.77	0/1300
43	R	0.71	4/893 (0.4%)	0.75	0/1193
44	S	0.59	0/817	0.63	0/1088
45	T	0.63	3/722 (0.4%)	0.66	0/964
46	U	0.61	1/659 (0.2%)	0.64	0/884
47	V	0.60	1/658 (0.2%)	0.68	0/881
48	W	0.59	1/545 (0.2%)	0.68	1/731 (0.1%)
49	X	0.75	2/653 (0.3%)	0.77	0/877
50	Y	0.76	0/671	0.68	0/888
51	Z	0.68	1/551 (0.2%)	0.76	0/728
52	a	0.93	5/1034 (0.5%)	0.88	1/1387 (0.1%)
53	3	0.53	0/36963	0.67	6/57662 (0.0%)
54	1	0.48	0/69796	0.67	8/108888 (0.0%)
55	2	0.46	0/2872	0.67	0/4479
56	5	0.41	0/1832	0.67	0/2855
56	6	0.53	0/1832	0.69	0/2855
57	4	0.49	0/436	0.68	0/679
58	7	0.50	0/1840	0.73	1/2868 (0.0%)
All	All	0.55	80/162688 (0.0%)	0.68	40/243394 (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
35	J	0	2
53	3	0	14
54	1	0	45
55	2	0	3
All	All	0	64

The worst 5 of 80 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	K	13	ASP	C-O	11.51	1.45	1.23
7	h	44	ALA	C-O	11.26	1.44	1.23
7	h	12	VAL	C-O	10.25	1.42	1.23
6	g	114	GLU	C-O	10.16	1.42	1.23
26	A	46	GLY	C-O	9.63	1.39	1.23

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	J	85	LYS	C-N-CA	-7.77	105.97	122.30
35	J	92	ARG	O-C-N	-7.38	110.89	122.70
39	N	31	GLN	O-C-N	-6.98	111.53	122.70
34	I	154	VAL	C-N-CA	-6.89	104.47	121.70
7	h	8	LYS	C-N-CA	-6.67	105.04	121.70

There are no chirality outliers.

5 of 64 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
53	3	159	G	Sidechain
53	3	324	G	Sidechain
53	3	405	U	Sidechain
35	J	86	GLY	Mainchain
35	J	92	ARG	Mainchain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/271 (99%)	233 (87%)	32 (12%)	4 (2%)	10	44
2	c	207/209 (99%)	182 (88%)	24 (12%)	1 (0%)	29	67
3	d	199/201 (99%)	175 (88%)	23 (12%)	1 (0%)	29	67
4	e	175/177 (99%)	153 (87%)	22 (13%)	0	100	100
5	f	174/176 (99%)	156 (90%)	18 (10%)	0	100	100
6	g	121/149 (81%)	102 (84%)	17 (14%)	2 (2%)	9	42
7	h	82/131 (63%)	63 (77%)	18 (22%)	1 (1%)	13	49
8	i	72/141 (51%)	58 (81%)	12 (17%)	2 (3%)	5	29
9	j	140/142 (99%)	124 (89%)	15 (11%)	1 (1%)	22	61
10	k	120/122 (98%)	98 (82%)	20 (17%)	2 (2%)	9	42
11	l	141/143 (99%)	116 (82%)	21 (15%)	4 (3%)	5	29
12	m	134/136 (98%)	123 (92%)	9 (7%)	2 (2%)	10	44
13	n	118/120 (98%)	101 (86%)	15 (13%)	2 (2%)	9	42
14	o	114/116 (98%)	102 (90%)	12 (10%)	0	100	100
15	p	112/114 (98%)	95 (85%)	16 (14%)	1 (1%)	17	56
16	q	115/117 (98%)	111 (96%)	4 (4%)	0	100	100
17	r	101/103 (98%)	84 (83%)	16 (16%)	1 (1%)	15	54
18	s	108/110 (98%)	97 (90%)	11 (10%)	0	100	100
19	t	91/93 (98%)	80 (88%)	11 (12%)	0	100	100
20	u	100/102 (98%)	74 (74%)	23 (23%)	3 (3%)	4	28
21	v	92/94 (98%)	77 (84%)	14 (15%)	1 (1%)	14	51
22	w	73/75 (97%)	63 (86%)	10 (14%)	0	100	100
23	x	75/77 (97%)	68 (91%)	7 (9%)	0	100	100
24	y	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
25	z	56/58 (97%)	53 (95%)	3 (5%)	0	100	100
26	A	64/66 (97%)	55 (86%)	8 (12%)	1 (2%)	9	43
27	B	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
28	C	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
29	D	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
30	E	62/64 (97%)	53 (86%)	6 (10%)	3 (5%)	2	17
31	F	36/38 (95%)	30 (83%)	6 (17%)	0	100	100
32	G	216/225 (96%)	178 (82%)	36 (17%)	2 (1%)	17	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	H	204/206 (99%)	183 (90%)	21 (10%)	0	100	100
34	I	203/205 (99%)	170 (84%)	32 (16%)	1 (0%)	29	67
35	J	155/157 (99%)	128 (83%)	24 (16%)	3 (2%)	8	39
36	K	98/100 (98%)	78 (80%)	19 (19%)	1 (1%)	15	54
37	L	149/151 (99%)	127 (85%)	21 (14%)	1 (1%)	22	61
38	M	127/129 (98%)	111 (87%)	16 (13%)	0	100	100
39	N	125/127 (98%)	98 (78%)	24 (19%)	3 (2%)	6	34
40	O	96/98 (98%)	81 (84%)	13 (14%)	2 (2%)	7	37
41	P	114/116 (98%)	87 (76%)	24 (21%)	3 (3%)	5	31
42	Q	121/123 (98%)	90 (74%)	29 (24%)	2 (2%)	9	42
43	R	112/114 (98%)	90 (80%)	19 (17%)	3 (3%)	5	30
44	S	98/100 (98%)	76 (78%)	22 (22%)	0	100	100
45	T	86/88 (98%)	71 (83%)	14 (16%)	1 (1%)	13	49
46	U	80/82 (98%)	66 (82%)	13 (16%)	1 (1%)	12	47
47	V	78/80 (98%)	61 (78%)	16 (20%)	1 (1%)	12	47
48	W	63/65 (97%)	48 (76%)	13 (21%)	2 (3%)	4	26
49	X	77/79 (98%)	68 (88%)	9 (12%)	0	100	100
50	Y	83/85 (98%)	76 (92%)	7 (8%)	0	100	100
51	Z	63/65 (97%)	39 (62%)	20 (32%)	4 (6%)	1	10
52	a	130/223 (58%)	104 (80%)	21 (16%)	5 (4%)	3	22
All	All	5836/6178 (94%)	4947 (85%)	822 (14%)	67 (1%)	18	51

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	83	VAL
6	g	9	VAL
17	r	54	VAL
30	E	30	HIS
30	E	31	ILE

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	b	216/216 (100%)	208 (96%)	8 (4%)	34	68
2	c	164/164 (100%)	162 (99%)	2 (1%)	71	88
3	d	165/165 (100%)	162 (98%)	3 (2%)	59	82
4	e	148/148 (100%)	146 (99%)	2 (1%)	67	86
5	f	137/137 (100%)	134 (98%)	3 (2%)	52	79
6	g	98/114 (86%)	96 (98%)	2 (2%)	55	80
7	h	66/100 (66%)	64 (97%)	2 (3%)	41	73
8	i	60/109 (55%)	58 (97%)	2 (3%)	38	71
9	j	116/116 (100%)	115 (99%)	1 (1%)	78	91
10	k	103/103 (100%)	101 (98%)	2 (2%)	57	81
11	l	102/102 (100%)	98 (96%)	4 (4%)	32	67
12	m	109/109 (100%)	104 (95%)	5 (5%)	27	63
13	n	100/100 (100%)	100 (100%)	0	100	100
14	o	86/86 (100%)	85 (99%)	1 (1%)	71	88
15	p	99/99 (100%)	97 (98%)	2 (2%)	55	80
16	q	89/89 (100%)	85 (96%)	4 (4%)	27	63
17	r	84/84 (100%)	81 (96%)	3 (4%)	35	69
18	s	93/93 (100%)	92 (99%)	1 (1%)	73	88
19	t	80/80 (100%)	78 (98%)	2 (2%)	47	77
20	u	83/83 (100%)	81 (98%)	2 (2%)	49	77
21	v	78/78 (100%)	78 (100%)	0	100	100
22	w	57/57 (100%)	57 (100%)	0	100	100
23	x	67/67 (100%)	67 (100%)	0	100	100
24	y	55/55 (100%)	53 (96%)	2 (4%)	35	69
25	z	48/48 (100%)	45 (94%)	3 (6%)	18	52
26	A	59/59 (100%)	59 (100%)	0	100	100
27	B	47/47 (100%)	47 (100%)	0	100	100
28	C	45/45 (100%)	45 (100%)	0	100	100
29	D	38/38 (100%)	38 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	E	51/51 (100%)	51 (100%)	0	100	100
31	F	34/34 (100%)	33 (97%)	1 (3%)	42	74
32	G	180/186 (97%)	179 (99%)	1 (1%)	86	94
33	H	170/170 (100%)	165 (97%)	5 (3%)	42	74
34	I	172/172 (100%)	167 (97%)	5 (3%)	42	74
35	J	119/119 (100%)	118 (99%)	1 (1%)	81	93
36	K	87/87 (100%)	84 (97%)	3 (3%)	37	70
37	L	124/124 (100%)	121 (98%)	3 (2%)	49	77
38	M	104/104 (100%)	104 (100%)	0	100	100
39	N	105/105 (100%)	101 (96%)	4 (4%)	33	67
40	O	86/86 (100%)	86 (100%)	0	100	100
41	P	89/89 (100%)	85 (96%)	4 (4%)	27	63
42	Q	103/103 (100%)	102 (99%)	1 (1%)	76	90
43	R	92/92 (100%)	90 (98%)	2 (2%)	52	79
44	S	83/83 (100%)	83 (100%)	0	100	100
45	T	76/76 (100%)	74 (97%)	2 (3%)	46	76
46	U	65/65 (100%)	65 (100%)	0	100	100
47	V	74/74 (100%)	74 (100%)	0	100	100
48	W	56/56 (100%)	53 (95%)	3 (5%)	22	58
49	X	70/70 (100%)	69 (99%)	1 (1%)	67	86
50	Y	65/65 (100%)	65 (100%)	0	100	100
51	Z	55/55 (100%)	52 (94%)	3 (6%)	21	57
52	a	110/174 (63%)	107 (97%)	3 (3%)	44	75
All	All	4862/5031 (97%)	4764 (98%)	98 (2%)	57	80

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	G	224	ARG
36	K	75	GLU
33	H	84	GLU
34	I	170	LEU
39	N	57	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
35	J	82	HIS
46	U	29	ASN
46	U	26	ASN
47	V	8	GLN
14	o	29	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	3	1538/1539 (99%)	171 (11%)	7 (0%)
54	1	2902/2903 (99%)	354 (12%)	17 (0%)
55	2	119/120 (99%)	9 (7%)	1 (0%)
56	5	76/77 (98%)	11 (14%)	0
56	6	76/77 (98%)	19 (25%)	0
57	4	17/18 (94%)	5 (29%)	0
58	7	76/77 (98%)	11 (14%)	4 (5%)
All	All	4804/4811 (99%)	580 (12%)	29 (0%)

5 of 580 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	3	4	U
53	3	6	G
53	3	7	A
53	3	9	G
53	3	22	G

5 of 29 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	1	858	G
58	7	40	C
54	1	1475	G
55	2	88	C
54	1	1130	U

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
59	FME	5	101	56	8,9,10	0.49	0	7,9,11	1.08	1 (14%)

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
59	FME	5	101	56	-	1/7/9/11	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	5	101	FME	O-C-CA	-2.25	118.87	124.78

There are no chirality outliers.

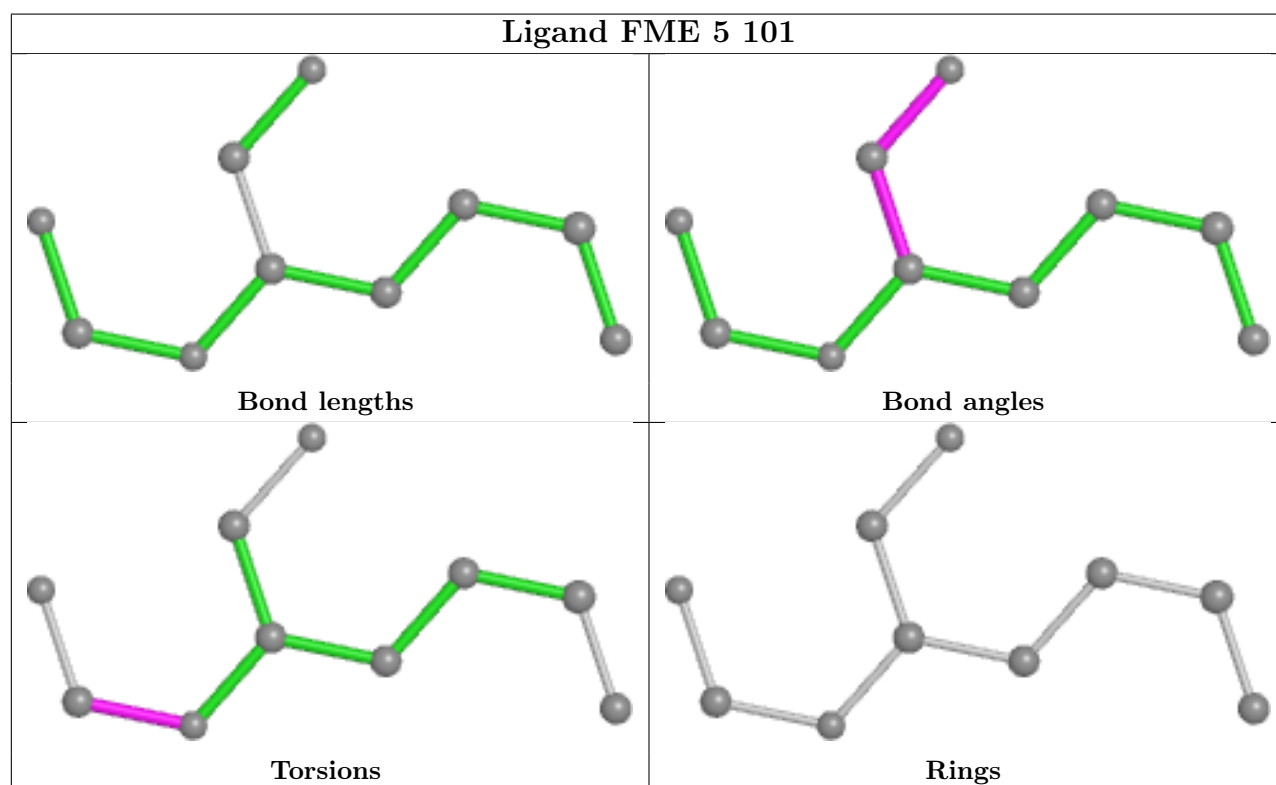
All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	5	101	FME	O1-CN-N-CA

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

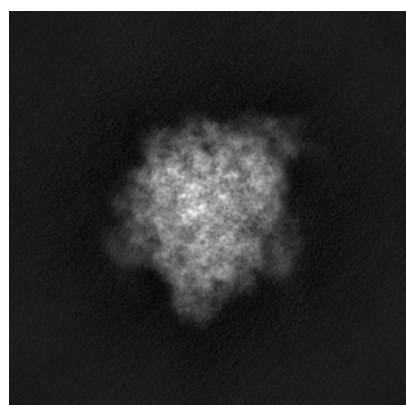
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22672. These allow visual inspection of the internal detail of the map and identification of artifacts.

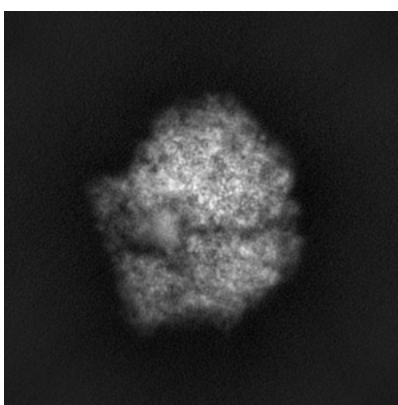
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

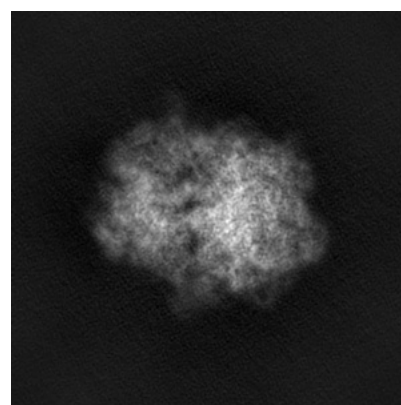
6.1.1 Primary map



X



Y

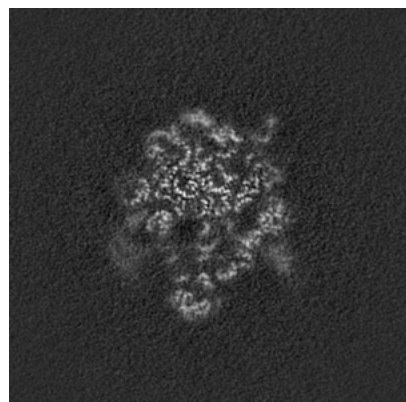


Z

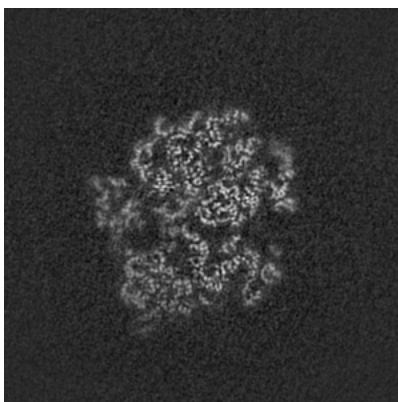
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

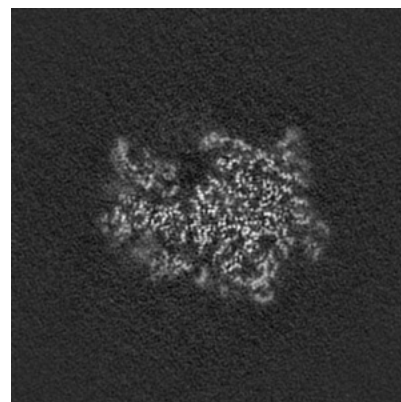
6.2.1 Primary map



X Index: 200



Y Index: 200

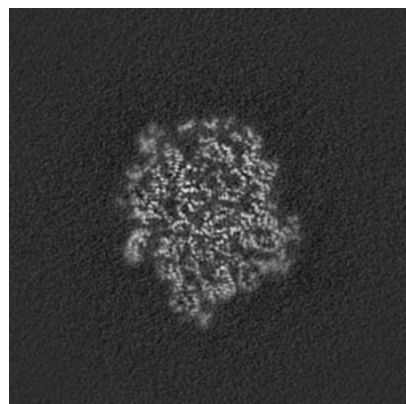


Z Index: 200

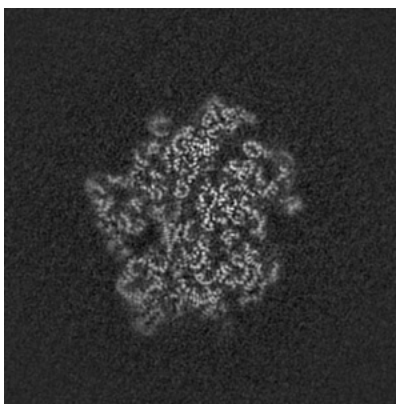
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

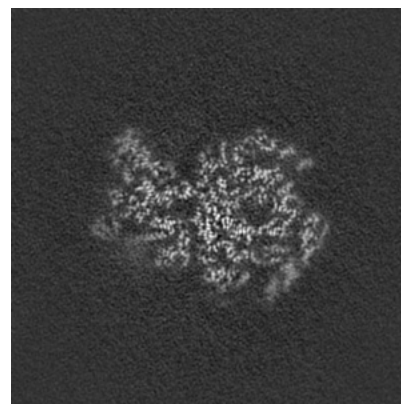
6.3.1 Primary map



X Index: 223



Y Index: 193

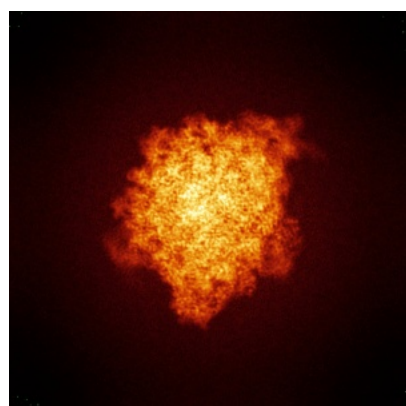


Z Index: 215

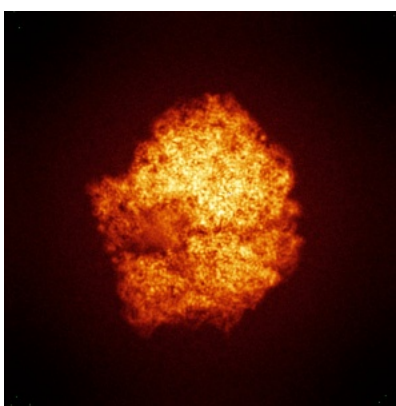
The images above show the largest variance slices of the map in three orthogonal directions.

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

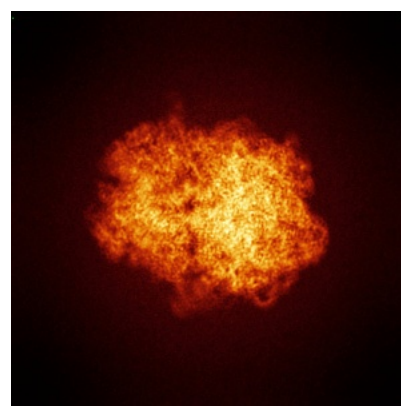
6.4.1 Primary map



X



Y



Z

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 3.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

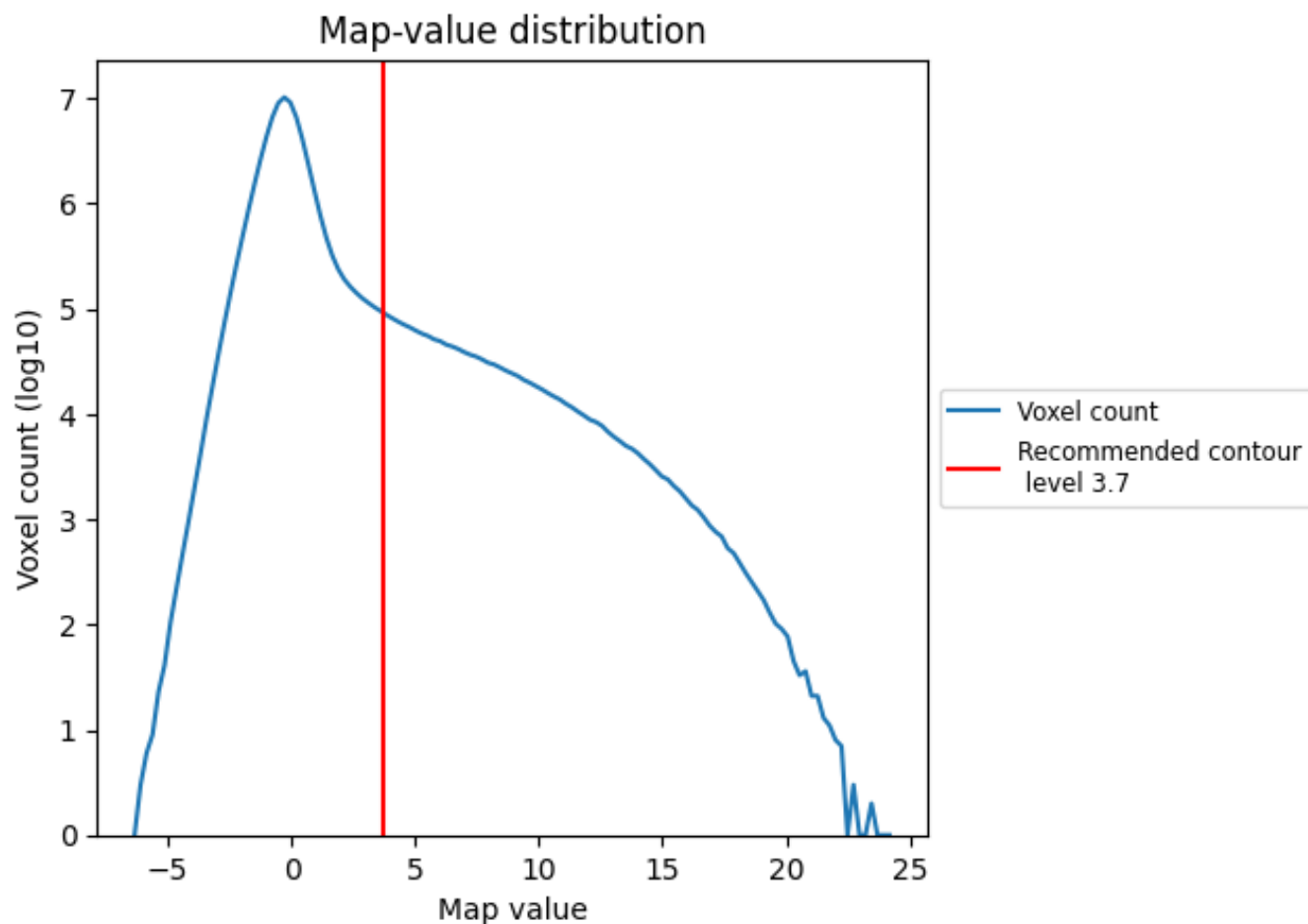
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

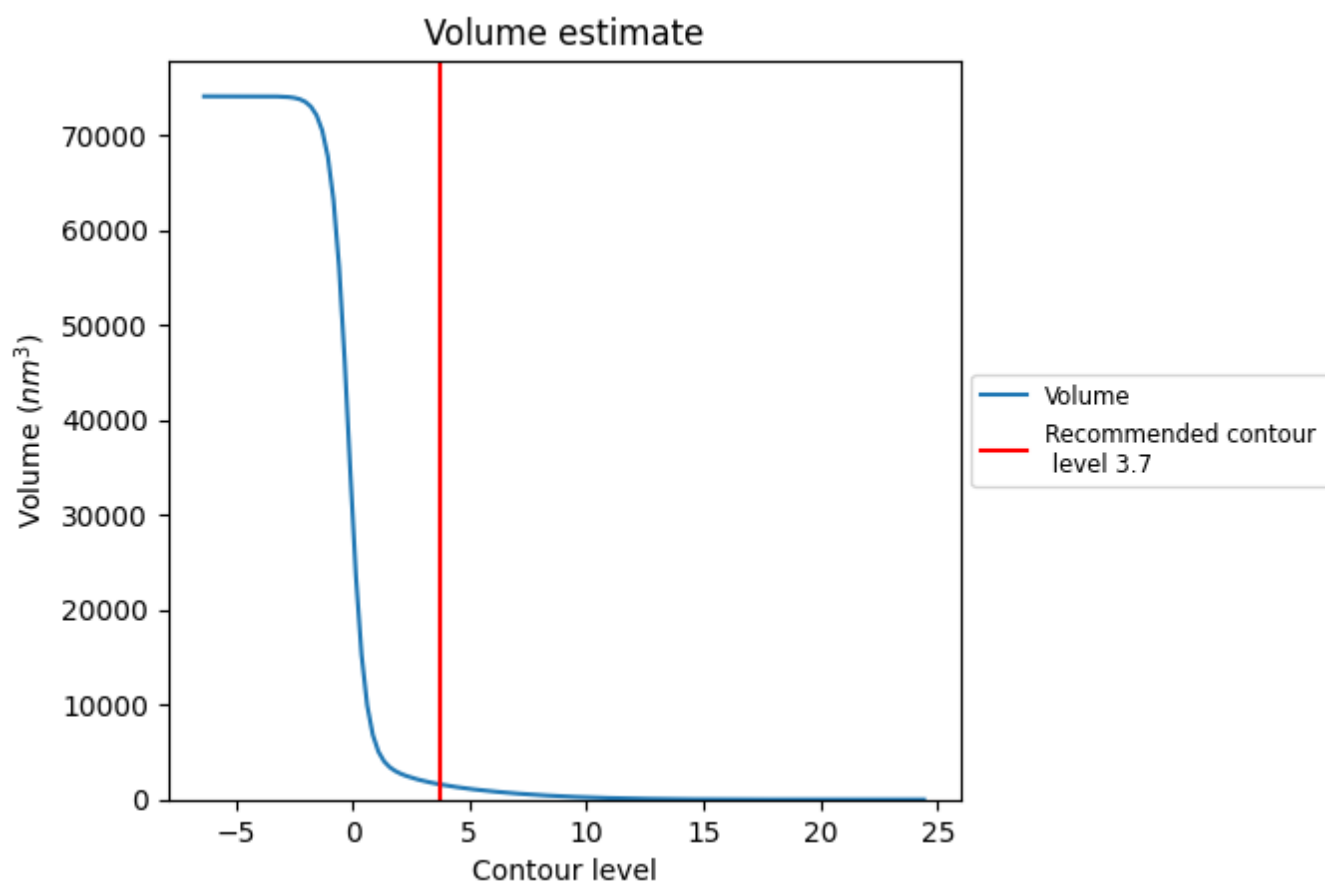
This section contains the results of statistical analysis of the map.

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.

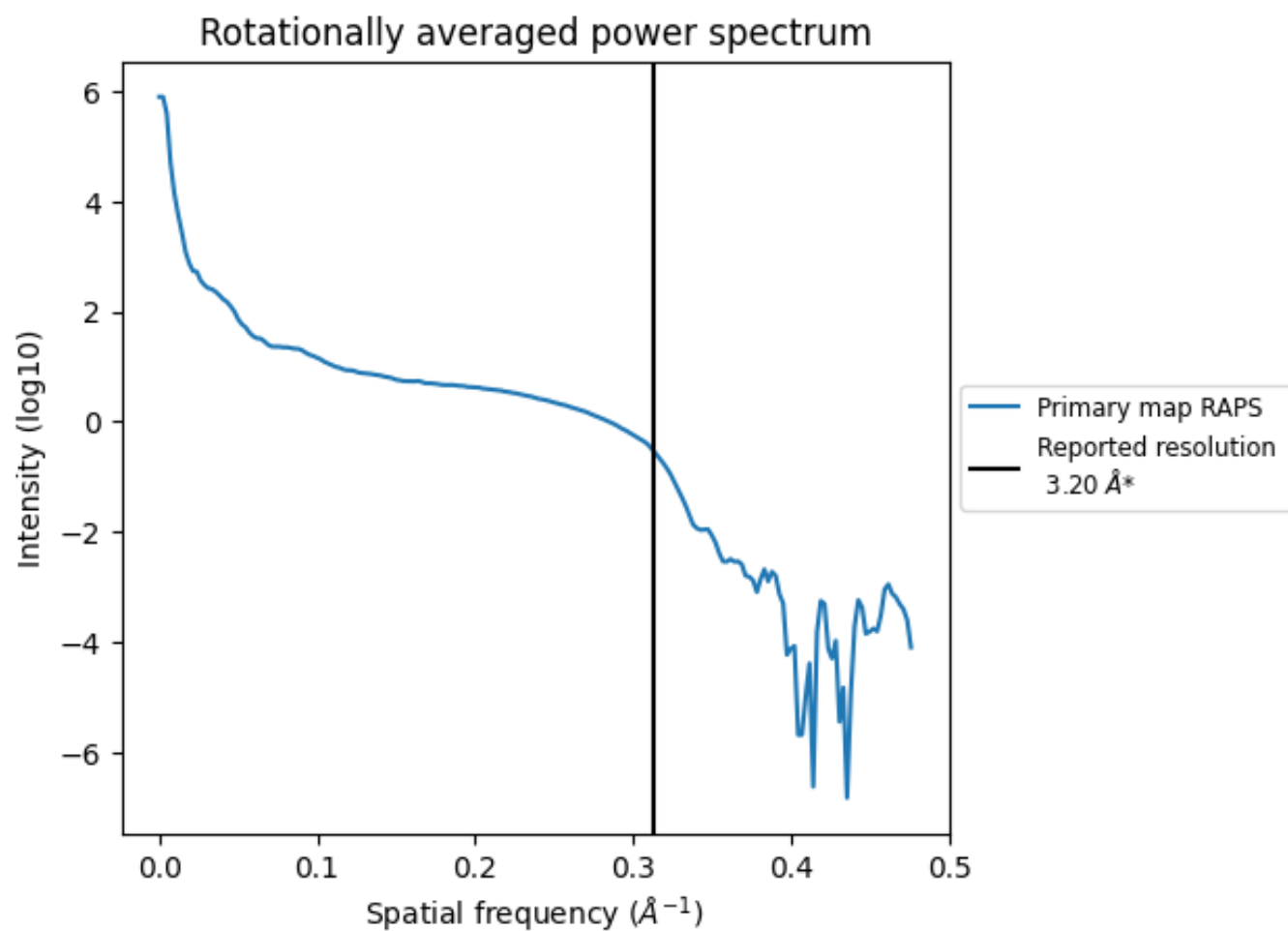
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1619 nm³; this corresponds to an approximate mass of 1462 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 0.312 Å⁻¹

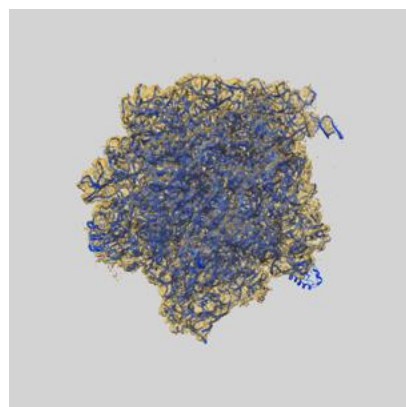
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

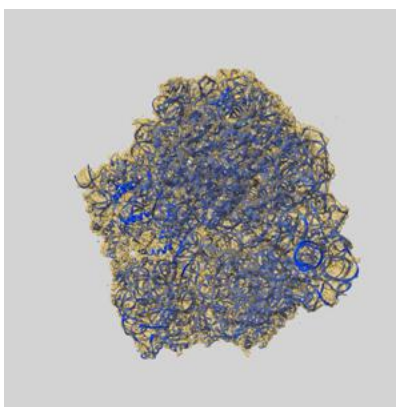
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22672 and PDB model 7K53. Per-residue inclusion information can be found in section [3](#) on page [16](#).

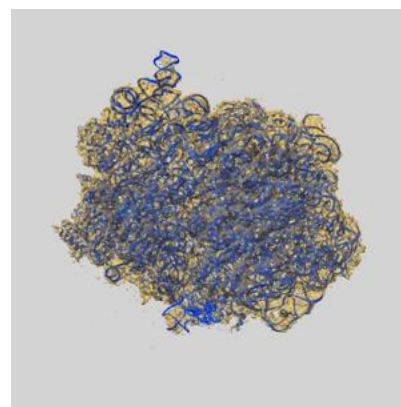
9.1 Map-model overlay [i](#)



X



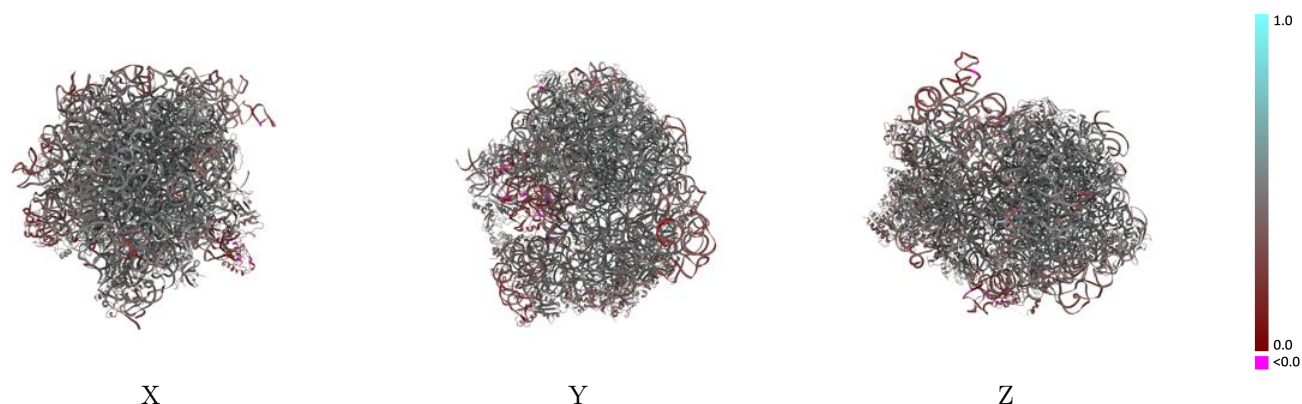
Y



Z

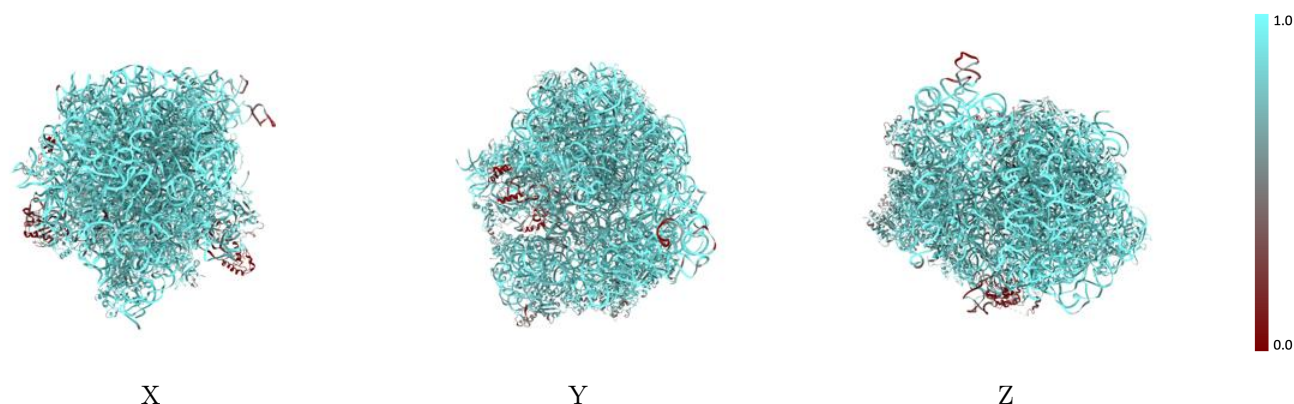
The images above show the 3D surface view of the map at the recommended contour level 3.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



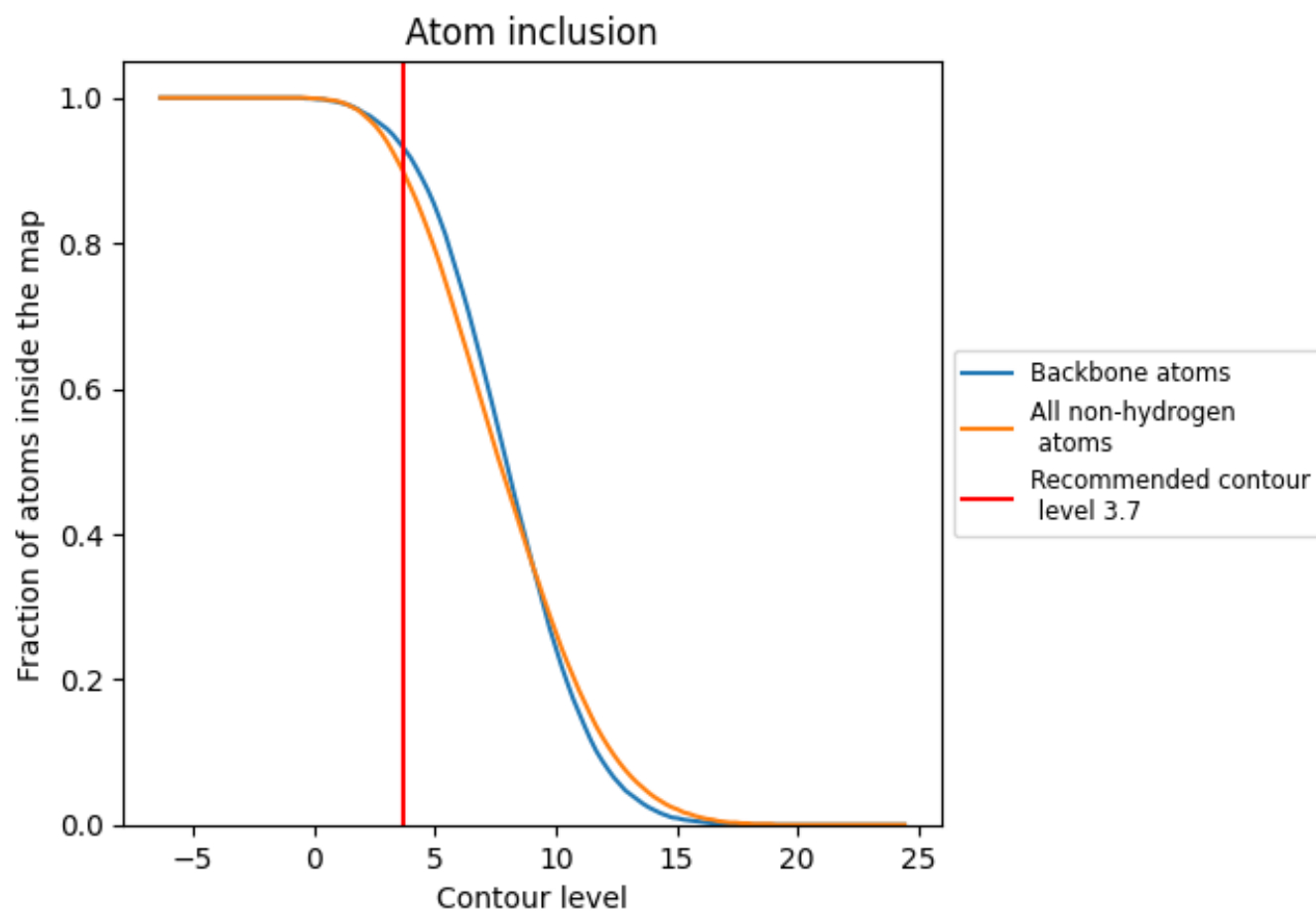
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.7).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (3.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.4370
1	 0.9600	 0.4520
2	 0.9740	 0.4390
3	 0.9480	 0.4300
4	 0.7140	 0.3000
5	 0.9440	 0.4200
6	 0.5080	 0.2160
7	 0.7810	 0.3180
A	 0.7250	 0.3910
B	 0.9370	 0.4880
C	 0.7240	 0.4590
D	 0.9300	 0.5040
E	 0.9160	 0.5050
F	 0.8800	 0.4920
G	 0.6700	 0.3990
H	 0.7830	 0.4460
I	 0.7530	 0.4100
J	 0.8710	 0.4550
K	 0.8390	 0.4160
L	 0.7800	 0.4080
M	 0.8600	 0.4660
N	 0.7650	 0.4110
O	 0.6140	 0.3920
P	 0.8660	 0.4460
Q	 0.8510	 0.4510
R	 0.8120	 0.4150
S	 0.8110	 0.4260
T	 0.8930	 0.4440
U	 0.7880	 0.4340
V	 0.8860	 0.4400
W	 0.8600	 0.4410
X	 0.7940	 0.4030
Y	 0.8110	 0.4130
Z	 0.7240	 0.3640
a	 0.1600	 0.2510



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9200	 0.5070
c	 0.9010	 0.4820
d	 0.8150	 0.4560
e	 0.8310	 0.4230
f	 0.7900	 0.4130
g	 0.2680	 0.3300
h	 0.0530	 0.1940
i	 0.2140	 0.2370
j	 0.8980	 0.4750
k	 0.8890	 0.4850
l	 0.8870	 0.4790
m	 0.9000	 0.4870
n	 0.9100	 0.4730
o	 0.8580	 0.4360
p	 0.8910	 0.4780
q	 0.9170	 0.4910
r	 0.8580	 0.4690
s	 0.8720	 0.4750
t	 0.8660	 0.4570
u	 0.8360	 0.4280
v	 0.8280	 0.4530
w	 0.8840	 0.4760
x	 0.9030	 0.4890
y	 0.7870	 0.4060
z	 0.8760	 0.4760