wwPDB EM Validation Summary Report

Nov 4, 2023 – 12:41 PM EDT

PDB ID	:	7S1G
EMDB ID	:	EMD-24800
Title	:	wild-type Escherichia coli stalled ribosome with antibiotic linezolid
Authors	:	Young, I.D.; Stojkovic, V.; Tsai, K.; Lee, D.J.; Fraser, J.S.; Galonic Fujimori, D.
Deposited on	:	2021-09-02
Resolution	:	2.48 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:

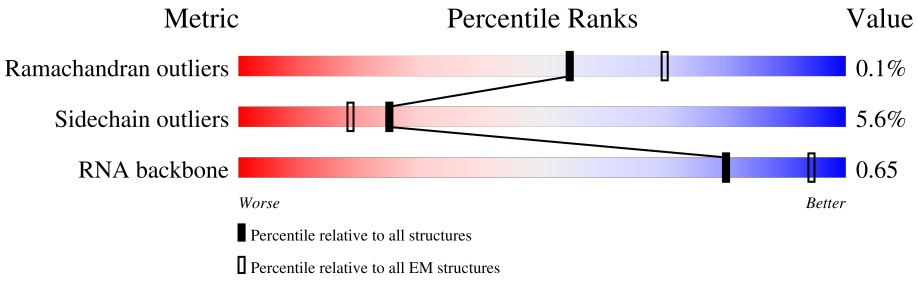
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.48 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 <=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	92	5% 80% 5% 14%
2	2	87	5% 91% 7%
3	3	71	30% 90% 8%
4	4	15	40% 60%
5	A	76	75% 25%
6	C	1540	89% 11%
7	D	240	15% 82% 9% 9%
8	E	233	85% 12%

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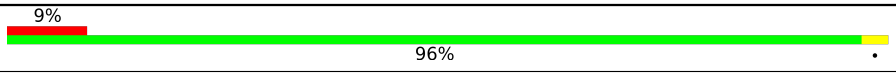
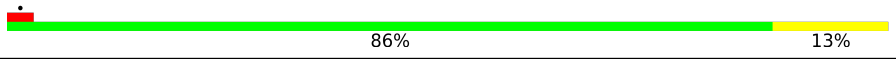
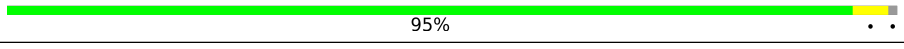
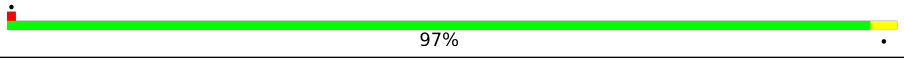
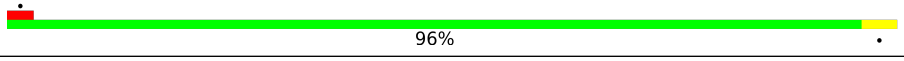
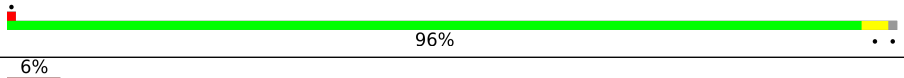
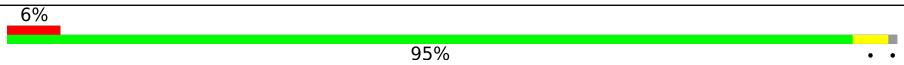
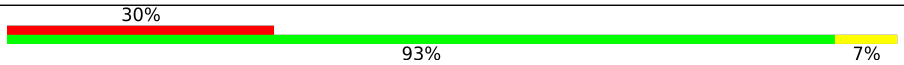
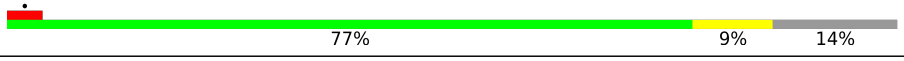
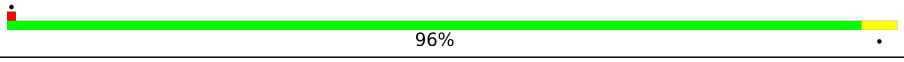
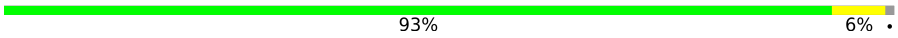
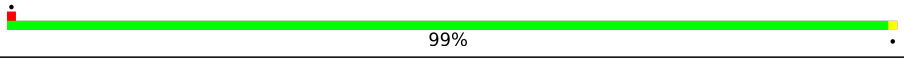
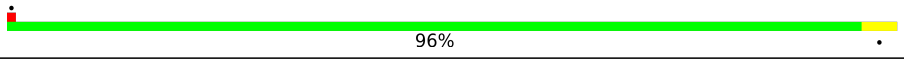
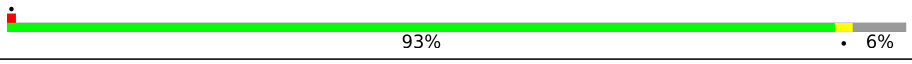
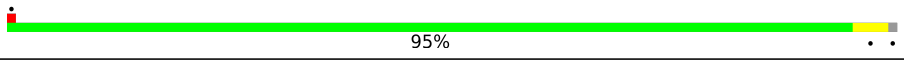
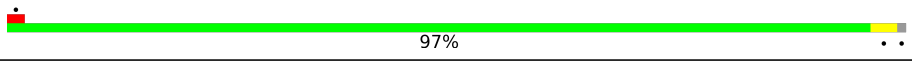
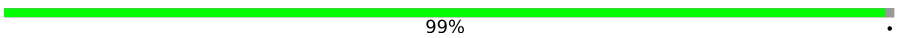
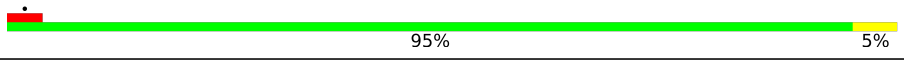
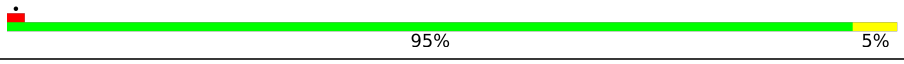
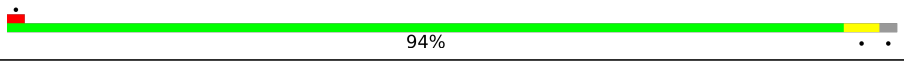
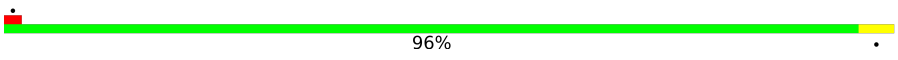
Mol	Chain	Length	Quality of chain
9	F	206	
10	G	167	
11	H	135	
12	I	2904	
13	J	120	
14	K	273	
15	L	209	
16	M	201	
17	N	179	
18	O	177	
19	P	149	
20	Q	70	
21	R	142	
22	S	123	
23	T	144	
24	U	136	
25	V	127	
26	W	117	
27	X	115	
28	Y	118	
29	Z	103	
30	a	110	
31	b	100	
32	c	104	
33	d	94	

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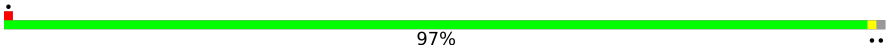
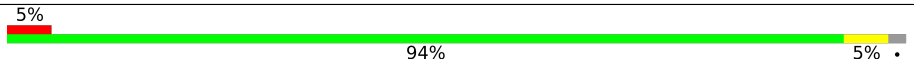
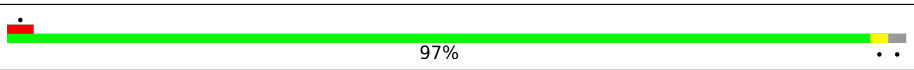
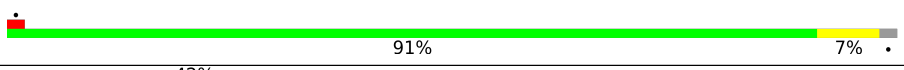
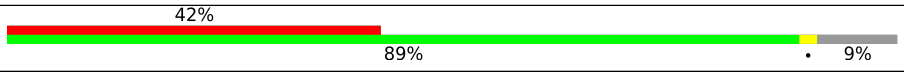
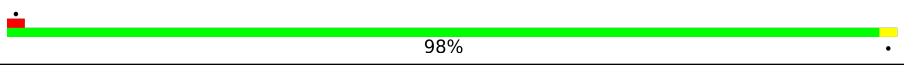
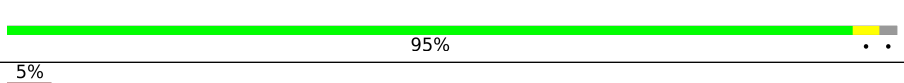
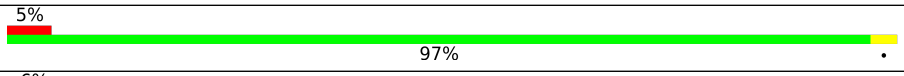
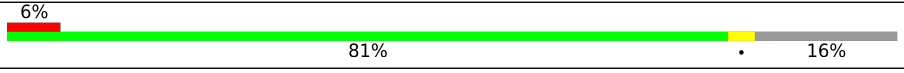
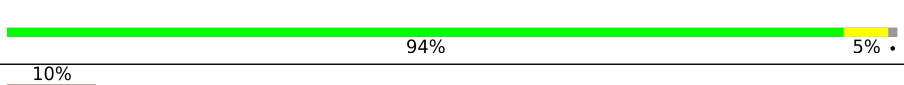
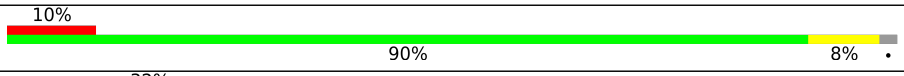
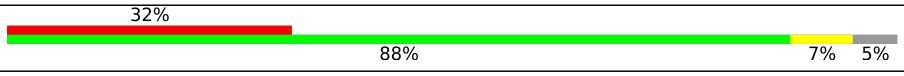
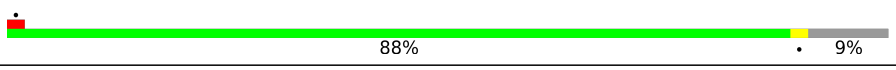
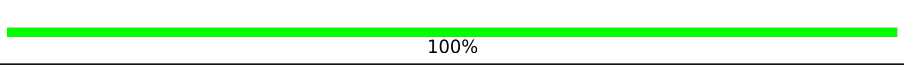
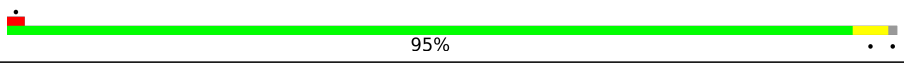
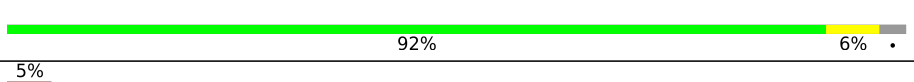
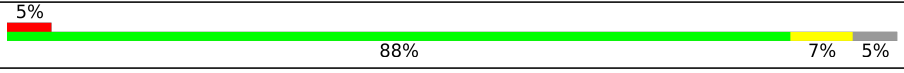
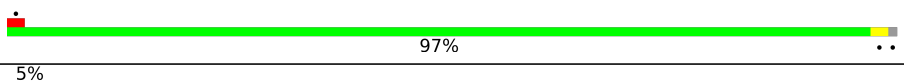
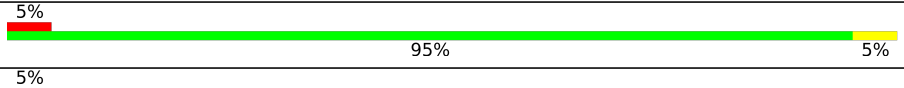
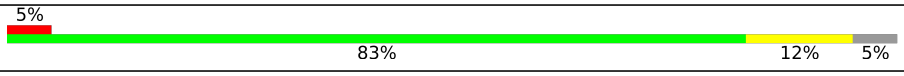
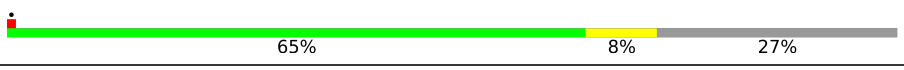
Mol	Chain	Length	Quality of chain
34	e	85	
35	f	78	
36	g	63	
37	h	59	
38	i	57	
39	j	55	
40	k	46	
41	l	65	
42	m	38	
43	n	179	
44	o	130	
45	p	130	
46	q	103	
47	r	129	
48	s	5	
49	t	124	
50	u	118	
51	v	101	
52	w	89	
53	x	82	
54	y	84	
55	z	75	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 240851 atoms, of which 96713 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 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	1	79	Total	C	H	N	O	S	0	0
			1303	408	666	120	107	2		

- Molecule 2 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	2	85	Total	C	H	N	O	S	0	0
			1380	411	715	137	114	3		

- Molecule 3 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	3	70	Total	C	H	N	O	S	0	0
			1219	366	629	125	98	1		

- Molecule 4 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	4	6	Total	C	H	N	O	P	0	0
			190	56	65	20	43	6		

- Molecule 5 is a RNA chain called tRNA(PHE).

Mol	Chain	Residues	Atoms						AltConf	Trace
5	A	76	Total	C	H	N	O	P	0	0
			2444	724	820	292	532	76		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	C	1540	Total	C	H	N	O	P	0	0
			49665	14735	16628	6057	10705	1540		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	D	218	Total	C	H	N	O	S	0	0
			3438	1081	1734	305	311	7		

- Molecule 8 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	E	206	Total	C	H	N	O	S	0	0
			3321	1028	1697	305	288	3		

- Molecule 9 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	F	205	Total	C	H	N	O	S	0	0
			3352	1026	1709	315	298	4		

- Molecule 10 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	G	150	Total	C	H	N	O	S	0	0
			2254	687	1149	211	201	6		

- Molecule 11 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	H	100	Total	C	H	N	O	S	0	0
			1625	515	808	148	148	6		

- Molecule 12 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	2898	Total	C	H	N	O	P	0	0
			93550	27768	31321	11448	20115	2898		

- Molecule 13 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	J	118	Total	C	H	N	O	P	0	0
			3809	1126	1280	464	821	118		

- Molecule 14 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	K	271	Total	C	H	N	O	S	2	0
			4263	1294	2170	427	365	7		

- Molecule 15 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	L	209	Total	C	H	N	O	S	0	0
			3184	979	1619	288	294	4		

- Molecule 16 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	M	201	Total	C	H	N	O	S	0	0
			3172	974	1620	283	290	5		

- Molecule 17 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	N	177	Total	C	H	N	O	S	0	0
			2855	899	1445	249	256	6		

- Molecule 18 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	O	176	Total	C	H	N	O	S	0	0
			2696	832	1373	243	246	2		

- Molecule 19 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	P	149	Total	C	H	N	O	S	0	0
			2259	699	1148	197	214	1		

- Molecule 20 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	Q	60	Total	C	H	N	O	S	0	0
			963	299	483	90	85	6		

- Molecule 21 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	R	142	Total	C	H	N	O	S	0	0
			2292	714	1163	212	199	4		

- Molecule 22 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	S	122	Total	C	H	N	O	S	0	0
			1951	587	1013	180	165	6		

- Molecule 23 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	T	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 24 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	U	136	Total	C	H	N	O	S	0	0
			2231	686	1156	205	178	6		

- Molecule 25 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	V	120	Total	C	H	N	O	S	0	0
			1961	593	1001	196	166	5		

- Molecule 26 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	W	116	Total	C	H	N	O	0	0
			1817	552	925	178	162		

- Molecule 27 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	X	114	Total	C	H	N	O	S	0	0
			1880	574	963	179	163	1		

- Molecule 28 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Y	117	Total	C	H	N	O	0	0
			1968	604	1021	192	151		

- Molecule 29 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	Z	103	Total	C	H	N	O	S	0	0
			1657	516	841	153	145	2		

- Molecule 30 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	a	110	Total	C	H	N	O	S	0	0
			1780	532	923	166	156	3		

- Molecule 31 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	b	93	Total	C	H	N	O	S	0	0
			1546	466	808	139	131	2		

- Molecule 32 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	102	Total	C	H	N	O	0	0
			1611	492	832	146	141		

- Molecule 33 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	d	94	Total	C	H	N	O	S	0	0
			1534	479	781	137	134	3		

- Molecule 34 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
34	e	75	Total	C	H	N	O	S	0	0
			1168	356	593	116	102	1		

- Molecule 35 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
35	f	77	Total	C	H	N	O	S	0	0
			1278	388	653	129	106	2		

- Molecule 36 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms						AltConf	Trace
36	g	62	Total	C	H	N	O	S	0	0
			1033	308	532	98	94	1		

- Molecule 37 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
37	h	58	Total	C	H	N	O	S	0	0
			938	281	489	87	79	2		

- Molecule 38 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms						AltConf	Trace
38	i	56	Total	C	H	N	O	S	0	0
			904	269	460	94	80	1		

- Molecule 39 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	50	Total	C	H	N	O	0	0
			851	263	442	75	71		

- Molecule 40 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms						AltConf	Trace
40	k	46	Total	C	H	N	O	S	0	0
			795	228	418	90	57	2		

- Molecule 41 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
41	l	64	Total	C	H	N	O	S	0	0
			1077	323	573	105	74	2		

- Molecule 42 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms						AltConf	Trace
42	m	38	Total	C	H	N	O	S	0	0
			645	185	343	65	48	4		

- Molecule 43 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms						AltConf	Trace
43	n	151	Total	C	H	N	O	S	0	0
			2419	735	1238	227	215	4		

- Molecule 44 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms						AltConf	Trace
44	o	129	Total	C	H	N	O	S	0	0
			2011	616	1032	173	184	6		

- Molecule 45 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms						AltConf	Trace
45	p	127	Total	C	H	N	O	S	0	0
			2093	634	1071	206	179	3		

- Molecule 46 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms						AltConf	Trace
46	q	98	Total	C	H	N	O	S	0	0
			1615	493	829	150	142	1		

- Molecule 47 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms						AltConf	Trace
47	r	117	Total	C	H	N	O	S	0	0
			1765	540	888	174	160	3		

- Molecule 48 is a protein called nascent peptide chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
48	s	5	Total	C	H	N	O	S	0	0
			91	32	47	6	5	1		

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms						AltConf	Trace
49	t	123	Total	C	H	N	O	S	0	0
			1972	590	1017	196	165	4		

- Molecule 50 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms						AltConf	Trace
50	u	115	Total	C	H	N	O	S	0	0
			1845	552	954	179	157	3		

- Molecule 51 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms						AltConf	Trace
51	v	96	Total	C	H	N	O	S	0	0
			1600	483	826	160	128	3		

- Molecule 52 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms						AltConf	Trace
52	w	88	Total	C	H	N	O	S	0	0
			1441	437	731	143	129	1		

- Molecule 53 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms						AltConf	Trace
53	x	82	Total	C	H	N	O	S	0	0
			1315	406	666	128	114	1		

- Molecule 54 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms						AltConf	Trace
54	y	80	Total	C	H	N	O	S	0	0
			1341	411	693	121	113	3		

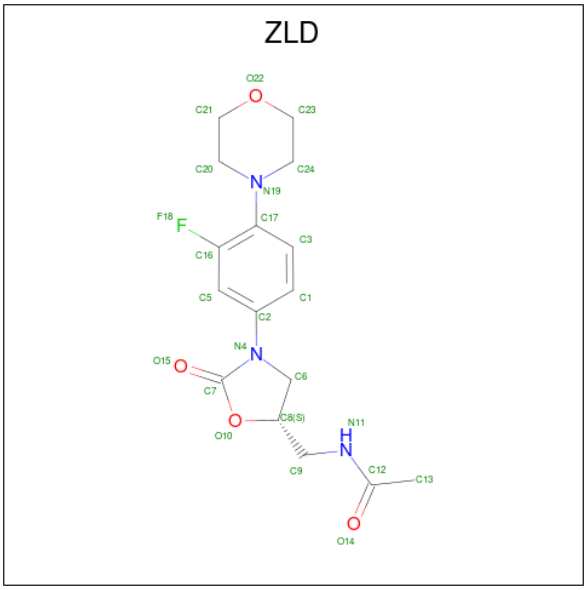
- Molecule 55 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	55	Total	C	H	N	O	0	0
			934	288	479	86	81		

- Molecule 56 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	C	83	Total Mg 83 83	0
56	I	110	Total Mg 110 110	0
56	K	1	Total Mg 1 1	0
56	L	1	Total Mg 1 1	0
56	V	1	Total Mg 1 1	0

- Molecule 57 is N-{[(5S)-3-(3-fluoro-4-morpholin-4-ylphenyl)-2-oxo-1,3-oxazolidin-5-yl]methyl}acetamide (three-letter code: ZLD) (formula: $C_{16}H_{20}FN_3O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
57	I	1	Total 44	C 16	F 1	H 20	N 3	O 4	0

- Molecule 58 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
58	Q	1	Total Zn 1 1	0
58	m	1	Total Zn 1 1	0

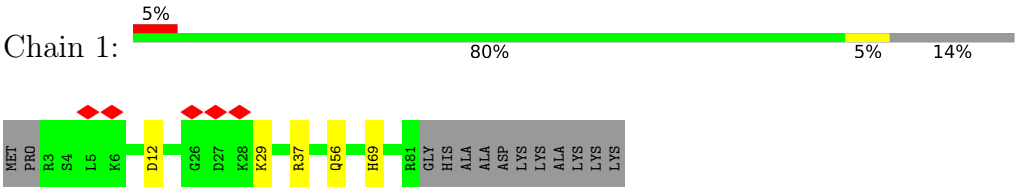
- Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	C	3	Total H O 9 6 3	0
59	I	37	Total H O 111 74 37	0
59	c	1	Total H O 3 2 1	0
59	k	1	Total H O 3 2 1	0

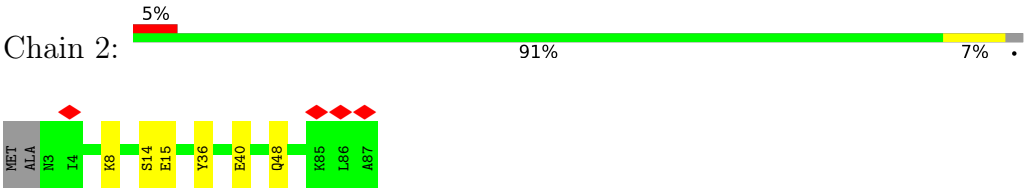
3 Residue-property plots (i)

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

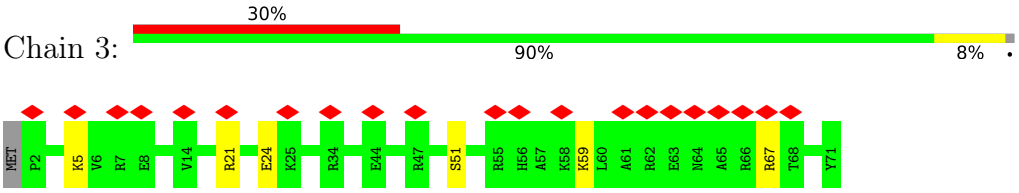
• Molecule 1: 30S ribosomal protein S19



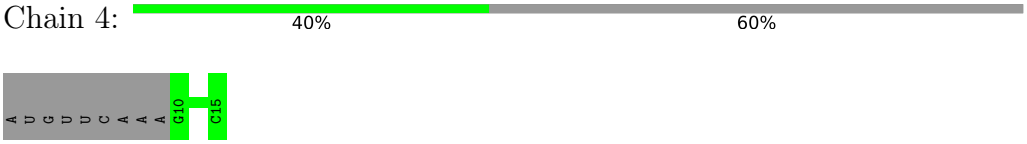
• Molecule 2: 30S ribosomal protein S20



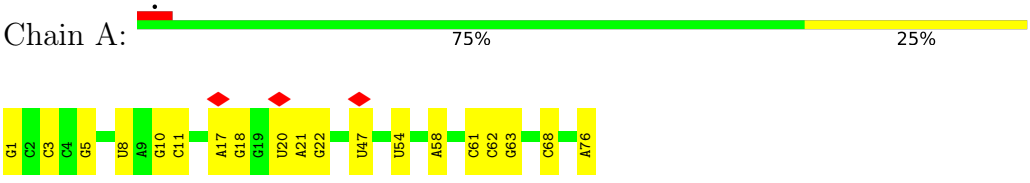
• Molecule 3: 30S ribosomal protein S21



• Molecule 4: mRNA

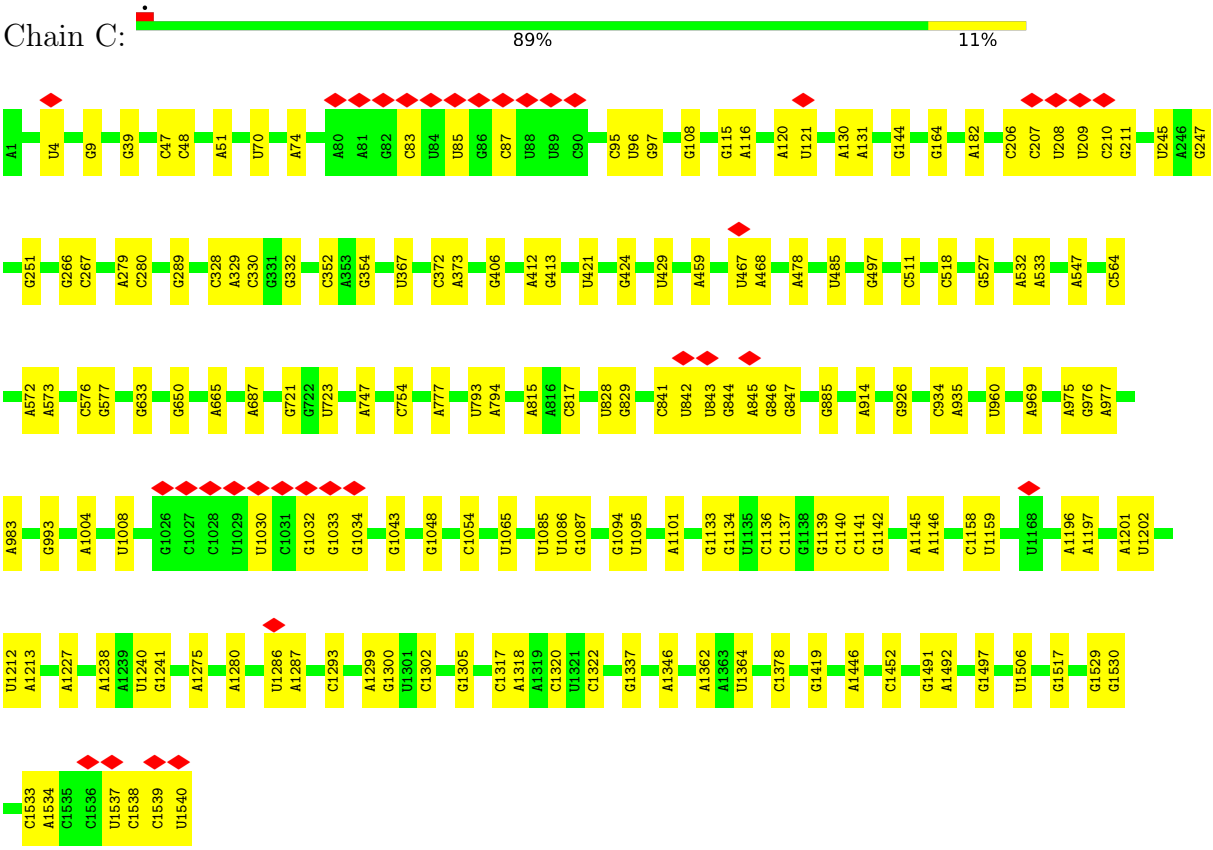


• Molecule 5: tRNA(PHE)



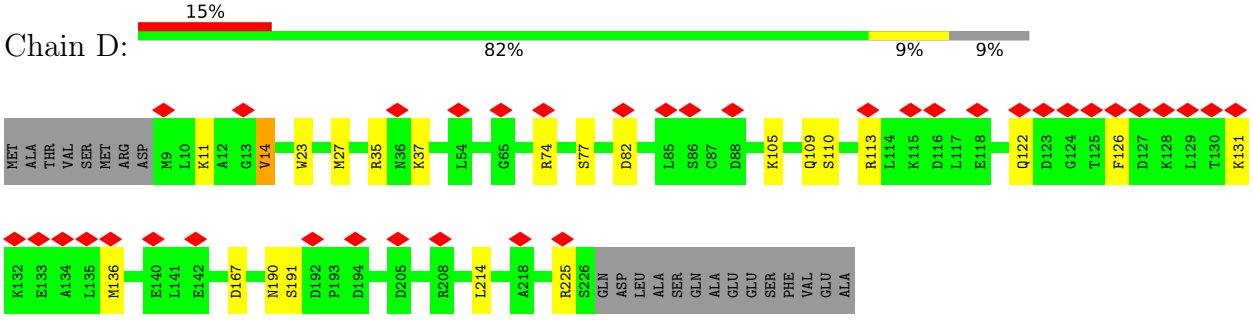
• Molecule 6: 16S rRNA

Chain C:



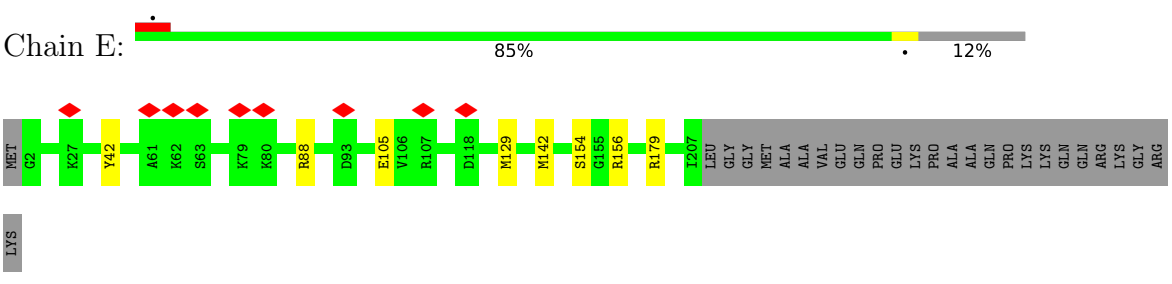
• Molecule 7: 30S ribosomal protein S2

Chain D:



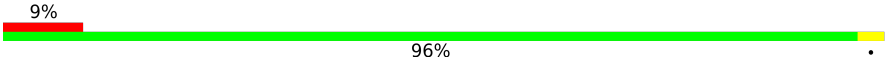
• Molecule 8: 30S ribosomal protein S3

Chain E:



• Molecule 9: 30S ribosomal protein S4

Chain F:



• Molecule 10: 30S ribosomal protein S5

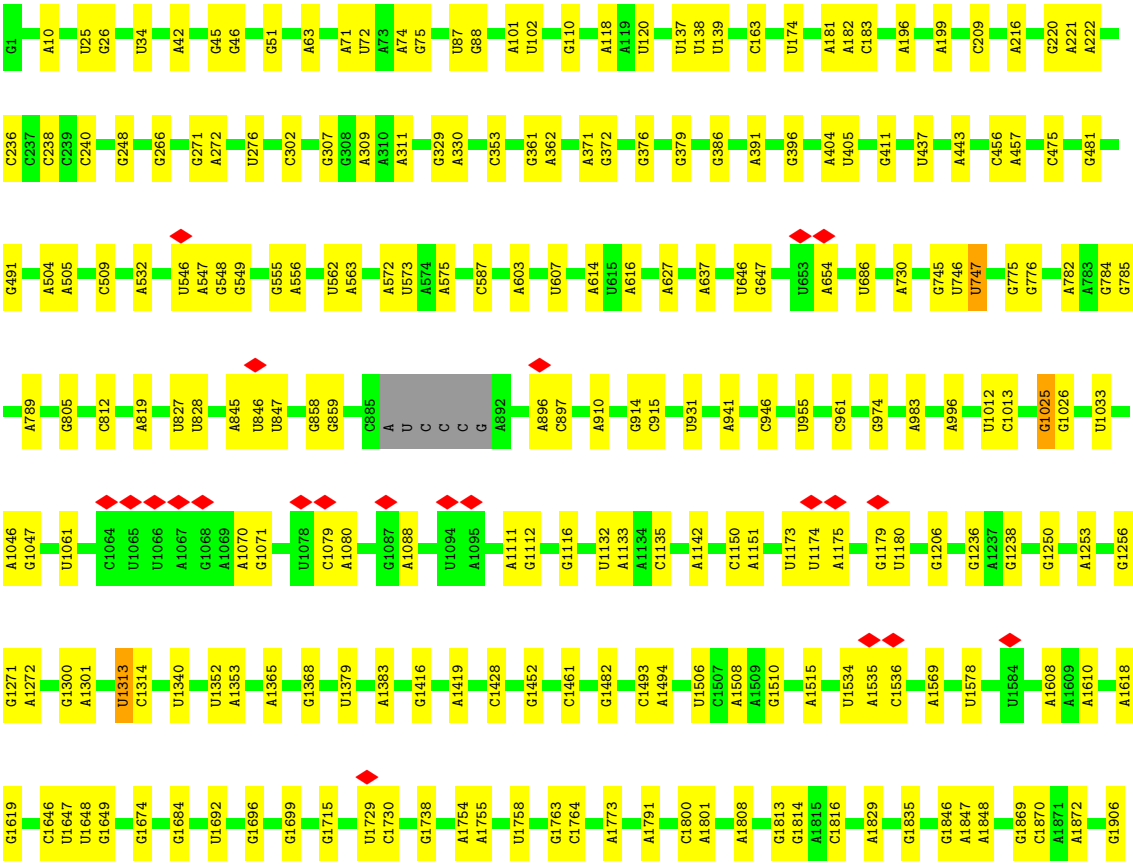
Chain G:

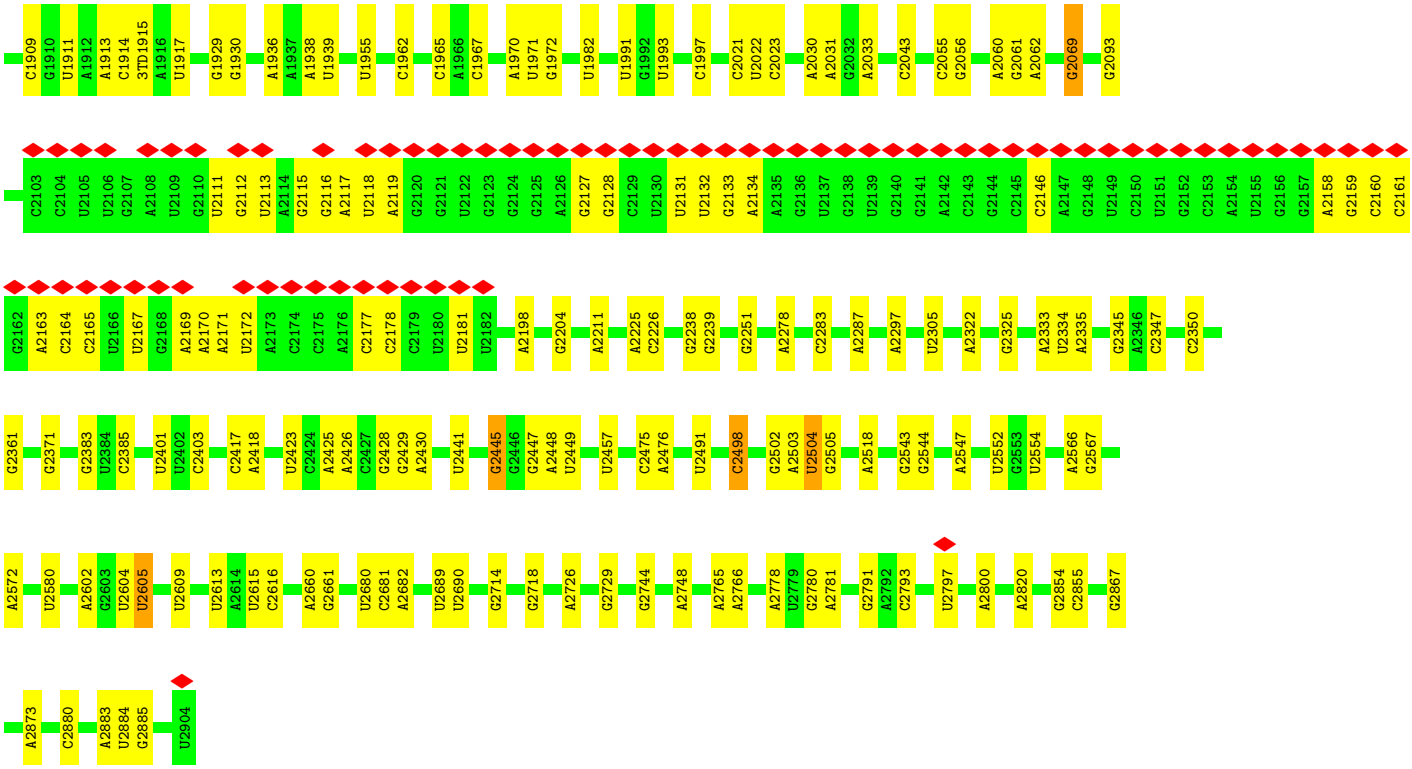
• Molecule 11: 30S ribosomal protein S6

Chain H:

• Molecule 12: 23S rRNA

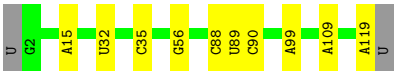
Chain I:





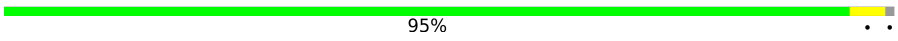
• Molecule 13: 5S rRNA

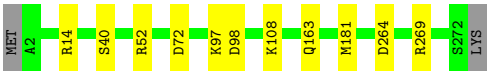
Chain J:



• Molecule 14: 50S ribosomal protein L2

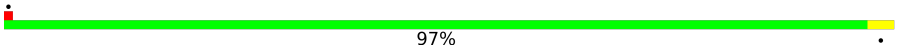
Chain K:

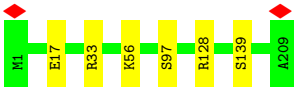




• Molecule 15: 50S ribosomal protein L3

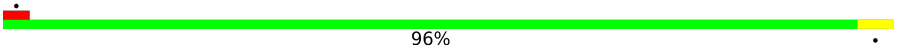
Chain L:

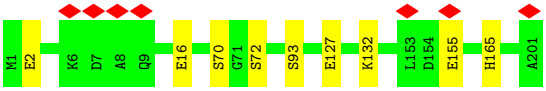




• Molecule 16: 50S ribosomal protein L4

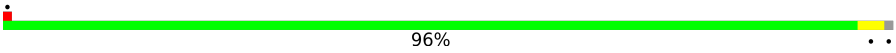
Chain M:

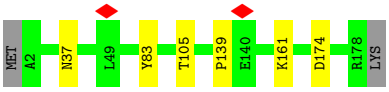




• Molecule 17: 50S ribosomal protein L5

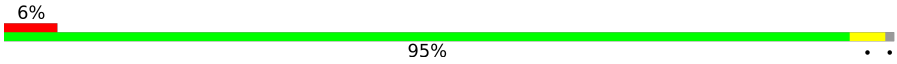
Chain N:

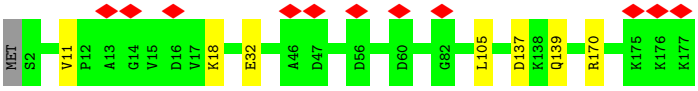




• Molecule 18: 50S ribosomal protein L6

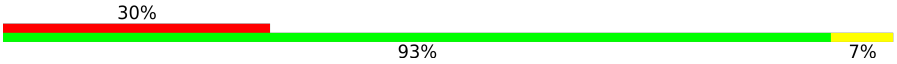
Chain O:

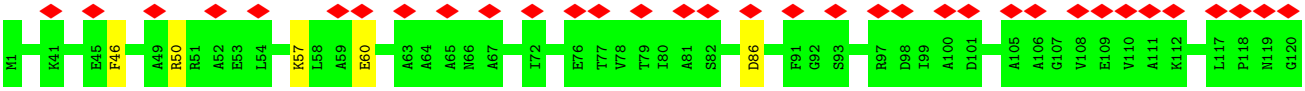


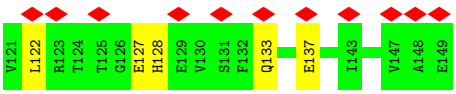


• Molecule 19: 50S ribosomal protein L9

Chain P:

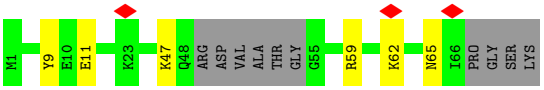






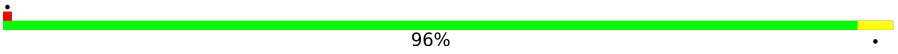
• Molecule 20: 50S ribosomal protein L31

Chain Q:



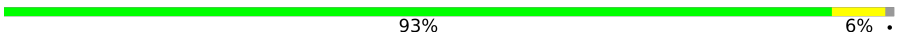
• Molecule 21: 50S ribosomal protein L13

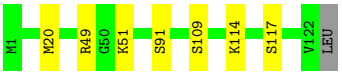
Chain R:



• Molecule 22: 50S ribosomal protein L14

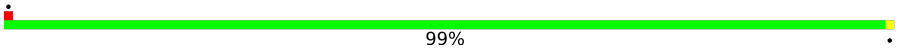
Chain S:

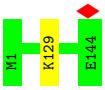




• Molecule 23: 50S ribosomal protein L15

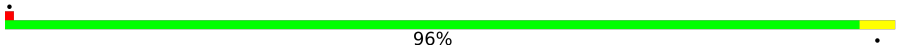
Chain T:

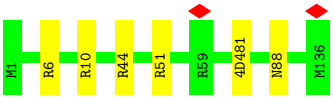




• Molecule 24: 50S ribosomal protein L16

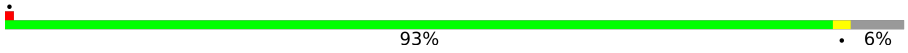
Chain U:

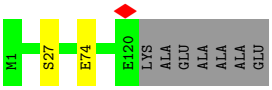




• Molecule 25: 50S ribosomal protein L17

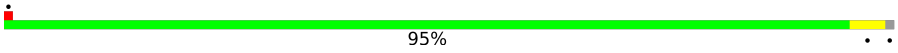
Chain V:

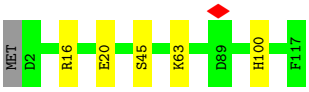




• Molecule 26: 50S ribosomal protein L18

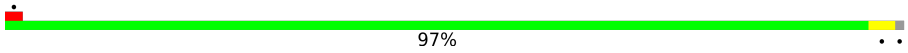
Chain W:

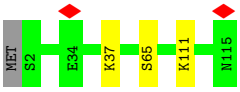




• Molecule 27: 50S ribosomal protein L19

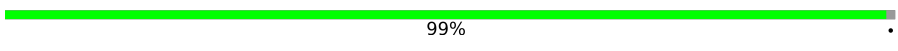
Chain X:





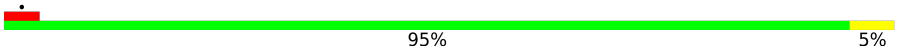
• Molecule 28: 50S ribosomal protein L20

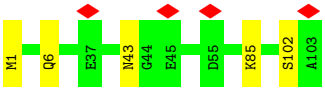
Chain Y:



• Molecule 29: 50S ribosomal protein L21

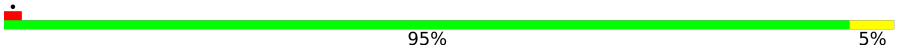
Chain Z:





• Molecule 30: 50S ribosomal protein L22

Chain a:

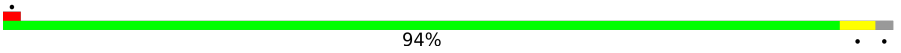


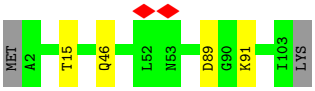
• Molecule 31: 50S ribosomal protein L23

Chain b:

• Molecule 32: 50S ribosomal protein L24

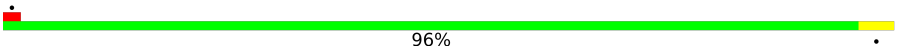
Chain c:

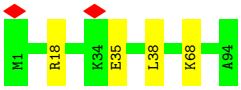




• Molecule 33: 50S ribosomal protein L25

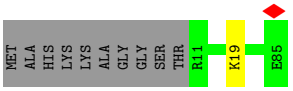
Chain d:





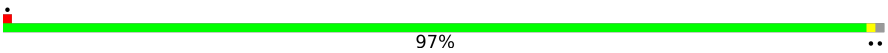
• Molecule 34: 50S ribosomal protein L27

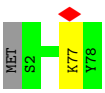
Chain e:



• Molecule 35: 50S ribosomal protein L28

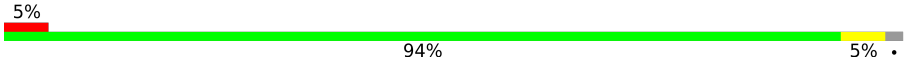
Chain f:

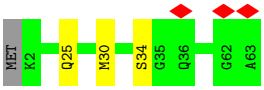




• Molecule 36: 50S ribosomal protein L29

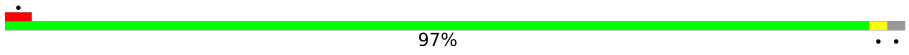
Chain g:

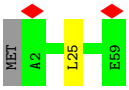




• Molecule 37: 50S ribosomal protein L30

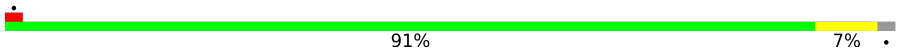
Chain h:

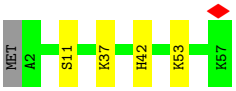




• Molecule 38: 50S ribosomal protein L32

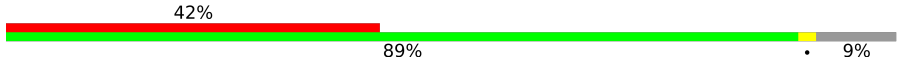
Chain i:

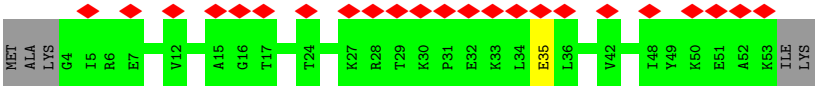




• Molecule 39: 50S ribosomal protein L33

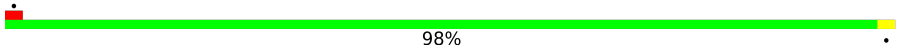
Chain j:





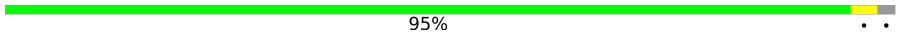
• Molecule 40: 50S ribosomal protein L34

Chain k:



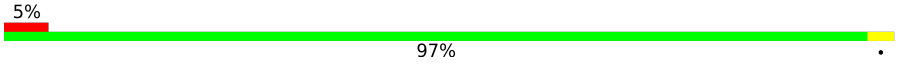
• Molecule 41: 50S ribosomal protein L35

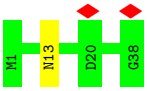
Chain l:



• Molecule 42: 50S ribosomal protein L36

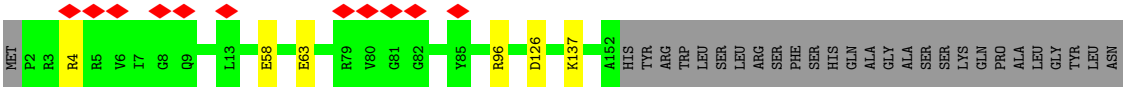
Chain m:





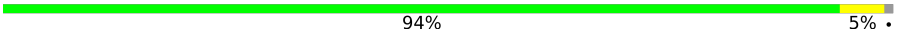
• Molecule 43: 30S ribosomal protein S7

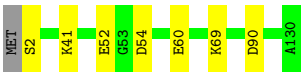
Chain n:



• Molecule 44: 30S ribosomal protein S8

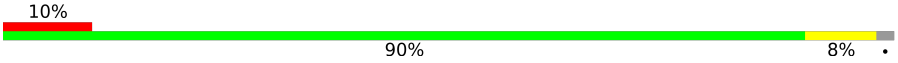
Chain o:

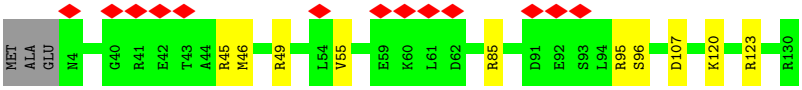




• Molecule 45: 30S ribosomal protein S9

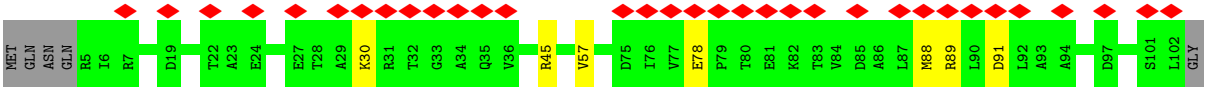
Chain p:





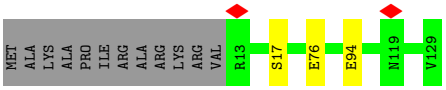
• Molecule 46: 30S ribosomal protein S10

Chain q:



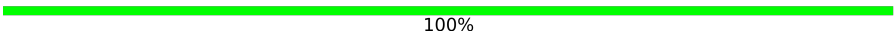
• Molecule 47: 30S ribosomal protein S11

Chain r:



• Molecule 48: nascent peptide chain

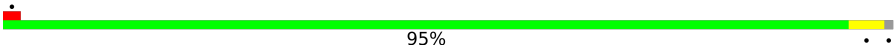
Chain s:



There are no outlier residues recorded for this chain.

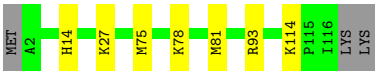
• Molecule 49: 30S ribosomal protein S12

Chain t:



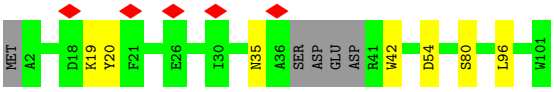
• Molecule 50: 30S ribosomal protein S13

Chain u:



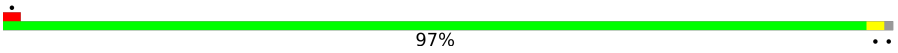
• Molecule 51: 30S ribosomal protein S14

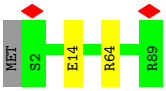
Chain v:



• Molecule 52: 30S ribosomal protein S15

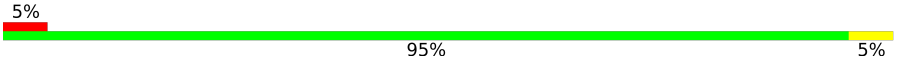
Chain w:

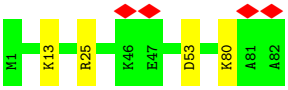




• Molecule 53: 30S ribosomal protein S16

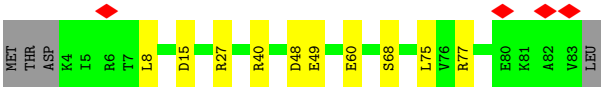
Chain x:





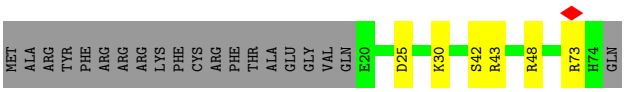
• Molecule 54: 30S ribosomal protein S17

Chain y:



• Molecule 55: 30S ribosomal protein S18

Chain z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	176779	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 ($e^-/Å^2$)	67.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	21.751	Depositor
Minimum map value	-8.832	Depositor
Average map value	-0.004	Depositor
Map value standard deviation	0.721	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8125, 0.8125, 0.8125	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 4D4, ZN, 1MG, ZLD, 5MC, 6MZ, H2U, OMC, PSU, MG, 2MA, 2MG, G7M, 3TD, OMG, 5MU

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	0.24	0/652	0.53	0/877
2	2	0.24	0/671	0.50	0/888
3	3	0.26	0/598	0.63	0/792
4	4	0.16	0/138	0.66	0/212
5	A	0.17	0/1815	0.70	1/2828 (0.0%)
6	C	0.18	0/36991	0.66	2/57705 (0.0%)
7	D	0.24	0/1735	0.49	0/2338
8	E	0.24	0/1651	0.54	0/2225
9	F	0.24	0/1665	0.54	0/2227
10	G	0.24	0/1118	0.55	0/1504
11	H	0.25	0/835	0.53	0/1128
12	I	0.20	0/69121	0.66	6/107828 (0.0%)
13	J	0.16	0/2828	0.65	0/4410
14	K	0.25	0/2139	0.58	0/2876
15	L	0.26	0/1586	0.52	0/2134
16	M	0.25	0/1571	0.53	0/2113
17	N	0.25	0/1434	0.54	0/1926
18	O	0.26	0/1343	0.51	0/1816
19	P	0.26	0/1122	0.53	0/1515
20	Q	0.26	0/488	0.56	0/649
21	R	0.25	0/1152	0.51	0/1551
22	S	0.26	0/947	0.58	0/1268
23	T	0.25	0/1062	0.57	0/1413
24	U	0.25	0/1081	0.55	0/1443
25	V	0.24	0/973	0.57	0/1301
26	W	0.25	0/902	0.57	0/1209
27	X	0.24	0/929	0.55	0/1242
28	Y	0.25	0/960	0.54	0/1278
29	Z	0.26	0/829	0.54	0/1107
30	a	0.24	0/864	0.52	0/1156
31	b	0.24	0/744	0.51	0/994

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.25	0/787	0.52	0/1051
33	d	0.27	0/766	0.54	0/1025
34	e	0.25	0/582	0.55	0/769
35	f	0.23	0/635	0.59	0/848
36	g	0.26	0/502	0.53	0/667
37	h	0.23	0/453	0.55	0/605
38	i	0.24	0/450	0.60	0/599
39	j	0.25	0/416	0.50	0/554
40	k	0.24	0/380	0.66	0/498
41	l	0.23	0/513	0.52	0/676
42	m	0.25	0/303	0.59	0/397
43	n	0.24	0/1195	0.53	0/1602
44	o	0.25	0/989	0.51	0/1326
45	p	0.24	0/1034	0.61	0/1375
46	q	0.23	0/796	0.58	0/1077
47	r	0.25	0/893	0.56	0/1205
48	s	0.37	0/45	0.38	0/57
49	t	0.24	0/969	0.58	0/1300
50	u	0.24	0/900	0.59	0/1204
51	v	0.24	0/785	0.59	0/1043
52	w	0.24	0/718	0.56	0/959
53	x	0.25	0/659	0.56	0/884
54	y	0.24	0/657	0.54	0/881
55	z	0.25	0/462	0.54	0/621
All	All	0.21	0/155833	0.63	9/233176 (0.0%)

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	2418	A	OP1-P-OP2	-6.93	109.20	119.60
5	A	1	G	OP1-P-OP2	-6.79	109.42	119.60
12	I	2401	U	OP1-P-OP2	-6.72	109.52	119.60
12	I	1025	G	OP1-P-OP2	-6.68	109.58	119.60
12	I	2616	C	OP1-P-OP2	-6.48	109.88	119.60

There are no chirality outliers.

There are no planarity outliers.

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	1	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
2	2	83/87 (95%)	82 (99%)	1 (1%)	0	100	100
3	3	68/71 (96%)	68 (100%)	0	0	100	100
7	D	216/240 (90%)	208 (96%)	7 (3%)	1 (0%)	29	46
8	E	204/233 (88%)	203 (100%)	1 (0%)	0	100	100
9	F	203/206 (98%)	195 (96%)	7 (3%)	1 (0%)	29	46
10	G	148/167 (89%)	140 (95%)	8 (5%)	0	100	100
11	H	98/135 (73%)	97 (99%)	1 (1%)	0	100	100
14	K	271/273 (99%)	262 (97%)	9 (3%)	0	100	100
15	L	207/209 (99%)	200 (97%)	7 (3%)	0	100	100
16	M	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
17	N	175/179 (98%)	171 (98%)	4 (2%)	0	100	100
18	O	174/177 (98%)	174 (100%)	0	0	100	100
19	P	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
20	Q	56/70 (80%)	56 (100%)	0	0	100	100
21	R	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
22	S	120/123 (98%)	118 (98%)	2 (2%)	0	100	100
23	T	142/144 (99%)	140 (99%)	2 (1%)	0	100	100
24	U	133/136 (98%)	131 (98%)	2 (2%)	0	100	100
25	V	118/127 (93%)	118 (100%)	0	0	100	100
26	W	114/117 (97%)	110 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	X	112/115 (97%)	111 (99%)	1 (1%)	0	100	100
28	Y	115/118 (98%)	115 (100%)	0	0	100	100
29	Z	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
30	a	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
31	b	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
32	c	100/104 (96%)	98 (98%)	2 (2%)	0	100	100
33	d	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
34	e	73/85 (86%)	73 (100%)	0	0	100	100
35	f	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
36	g	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
37	h	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
38	i	54/57 (95%)	54 (100%)	0	0	100	100
39	j	48/55 (87%)	45 (94%)	3 (6%)	0	100	100
40	k	44/46 (96%)	44 (100%)	0	0	100	100
41	l	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
42	m	36/38 (95%)	36 (100%)	0	0	100	100
43	n	149/179 (83%)	148 (99%)	1 (1%)	0	100	100
44	o	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
45	p	125/130 (96%)	118 (94%)	6 (5%)	1 (1%)	19	33
46	q	96/103 (93%)	89 (93%)	6 (6%)	1 (1%)	15	26
47	r	115/129 (89%)	111 (96%)	4 (4%)	0	100	100
48	s	3/5 (60%)	3 (100%)	0	0	100	100
49	t	121/124 (98%)	114 (94%)	7 (6%)	0	100	100
50	u	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
51	v	92/101 (91%)	90 (98%)	2 (2%)	0	100	100
52	w	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
53	x	80/82 (98%)	77 (96%)	3 (4%)	0	100	100
54	y	78/84 (93%)	74 (95%)	4 (5%)	0	100	100
55	z	53/75 (71%)	53 (100%)	0	0	100	100
All	All	5558/5917 (94%)	5423 (98%)	131 (2%)	4 (0%)	54	71

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	F	28	ILE
45	p	55	VAL
46	q	57	VAL
7	D	14	VAL

5.3.2 Protein sidechains (i)

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	1	70/79 (89%)	65 (93%)	5 (7%)	14 26
2	2	65/66 (98%)	59 (91%)	6 (9%)	9 16
3	3	60/61 (98%)	54 (90%)	6 (10%)	7 13
7	D	180/198 (91%)	158 (88%)	22 (12%)	5 8
8	E	170/190 (90%)	162 (95%)	8 (5%)	26 46
9	F	172/173 (99%)	166 (96%)	6 (4%)	36 59
10	G	113/126 (90%)	109 (96%)	4 (4%)	36 59
11	H	87/116 (75%)	81 (93%)	6 (7%)	15 28
14	K	218/218 (100%)	207 (95%)	11 (5%)	24 43
15	L	164/164 (100%)	158 (96%)	6 (4%)	34 57
16	M	165/165 (100%)	156 (94%)	9 (6%)	21 39
17	N	148/150 (99%)	142 (96%)	6 (4%)	30 53
18	O	137/138 (99%)	130 (95%)	7 (5%)	24 42
19	P	114/114 (100%)	104 (91%)	10 (9%)	10 18
20	Q	55/62 (89%)	49 (89%)	6 (11%)	6 11
21	R	116/116 (100%)	110 (95%)	6 (5%)	23 41
22	S	103/104 (99%)	96 (93%)	7 (7%)	16 28
23	T	103/103 (100%)	102 (99%)	1 (1%)	76 89
24	U	108/108 (100%)	103 (95%)	5 (5%)	27 47
25	V	100/103 (97%)	98 (98%)	2 (2%)	55 77
26	W	86/87 (99%)	81 (94%)	5 (6%)	20 36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	X	99/100 (99%)	96 (97%)	3 (3%)	41 65
28	Y	89/90 (99%)	89 (100%)	0	100 100
29	Z	84/84 (100%)	79 (94%)	5 (6%)	19 34
30	a	93/93 (100%)	88 (95%)	5 (5%)	22 40
31	b	80/84 (95%)	75 (94%)	5 (6%)	18 32
32	c	83/85 (98%)	79 (95%)	4 (5%)	25 45
33	d	78/78 (100%)	74 (95%)	4 (5%)	24 42
34	e	57/63 (90%)	56 (98%)	1 (2%)	59 80
35	f	67/68 (98%)	66 (98%)	1 (2%)	65 83
36	g	54/55 (98%)	51 (94%)	3 (6%)	21 38
37	h	48/49 (98%)	47 (98%)	1 (2%)	53 76
38	i	47/48 (98%)	43 (92%)	4 (8%)	10 19
39	j	45/49 (92%)	44 (98%)	1 (2%)	52 75
40	k	38/38 (100%)	37 (97%)	1 (3%)	46 70
41	l	51/52 (98%)	49 (96%)	2 (4%)	32 55
42	m	34/34 (100%)	33 (97%)	1 (3%)	42 66
43	n	124/147 (84%)	118 (95%)	6 (5%)	25 45
44	o	104/105 (99%)	97 (93%)	7 (7%)	16 29
45	p	105/107 (98%)	96 (91%)	9 (9%)	10 18
46	q	86/90 (96%)	80 (93%)	6 (7%)	15 27
47	r	90/99 (91%)	87 (97%)	3 (3%)	38 61
48	s	4/4 (100%)	4 (100%)	0	100 100
49	t	103/104 (99%)	98 (95%)	5 (5%)	25 44
50	u	93/96 (97%)	86 (92%)	7 (8%)	13 24
51	v	79/84 (94%)	72 (91%)	7 (9%)	9 17
52	w	75/77 (97%)	73 (97%)	2 (3%)	44 69
53	x	65/65 (100%)	61 (94%)	4 (6%)	18 33
54	y	74/78 (95%)	64 (86%)	10 (14%)	4 6
55	z	48/65 (74%)	42 (88%)	6 (12%)	4 8
All	All	4631/4832 (96%)	4374 (94%)	257 (6%)	25 39

5 of 257 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
51	v	42	TRP
53	x	25	ARG
18	O	32	GLU
17	N	174	ASP
54	y	27	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
21	R	132	HIS
29	Z	82	HIS
53	x	63	GLN
43	n	86	GLN
20	Q	30	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	I	2892/2904 (99%)	355 (12%)	30 (1%)
13	J	117/120 (97%)	10 (8%)	0
4	4	5/15 (33%)	0	0
5	A	75/76 (98%)	17 (22%)	3 (4%)
6	C	1539/1540 (99%)	169 (10%)	7 (0%)
All	All	4628/4655 (99%)	551 (11%)	40 (0%)

5 of 551 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	3	C
5	A	5	G
5	A	8	U
5	A	11	C
5	A	17	A

5 of 40 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	I	1847	A
12	I	2447	G
12	I	1913	A
12	I	2159	G

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Mol	Chain	Res	Type
12	I	2660	A

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	5MC	I	1962	12	18,22,23	0.85	1 (5%)	26,32,35	1.11	3 (11%)
12	3TD	I	1915	12	18,22,23	0.95	1 (5%)	22,32,35	1.74	2 (9%)
12	G7M	I	2069	12	20,26,27	0.96	1 (5%)	17,39,42	0.49	0
12	PSU	I	1917	12	18,21,22	0.92	0	22,30,33	1.83	3 (13%)
12	PSU	I	2504	12,56	18,21,22	0.95	1 (5%)	22,30,33	1.83	4 (18%)
12	2MA	I	2503	12,56	17,25,26	0.83	1 (5%)	17,37,40	0.94	1 (5%)
12	6MZ	I	1618	12	18,25,26	1.02	2 (11%)	16,36,39	2.00	4 (25%)
12	PSU	I	955	12	18,21,22	0.94	0	22,30,33	1.82	3 (13%)
12	5MU	I	1939	12	19,22,23	1.01	2 (10%)	28,32,35	2.08	6 (21%)
12	PSU	I	2605	12	18,21,22	0.95	0	22,30,33	1.85	4 (18%)
12	5MU	I	747	12	19,22,23	1.01	2 (10%)	28,32,35	2.10	6 (21%)
12	1MG	I	745	12	18,26,27	1.20	2 (11%)	19,39,42	1.32	3 (15%)
12	PSU	I	1911	12	18,21,22	0.91	0	22,30,33	1.84	3 (13%)
12	OMC	I	2498	12,56	19,22,23	0.89	1 (5%)	26,31,34	0.95	1 (3%)
12	2MG	I	2445	12	18,26,27	1.24	2 (11%)	16,38,41	1.28	2 (12%)
24	4D4	U	81	24	9,11,12	2.15	2 (22%)	8,13,15	2.15	4 (50%)
12	PSU	I	2604	12	18,21,22	0.92	1 (5%)	22,30,33	1.85	4 (18%)
12	PSU	I	2580	12	18,21,22	0.97	1 (5%)	22,30,33	1.87	5 (22%)
12	PSU	I	746	12,56	18,21,22	0.99	1 (5%)	22,30,33	1.75	4 (18%)
12	OMG	I	2251	5,12	18,26,27	1.20	2 (11%)	19,38,41	1.39	4 (21%)
12	H2U	I	2449	12	18,21,22	0.45	0	21,30,33	0.88	1 (4%)
12	2MG	I	1835	12	18,26,27	1.23	2 (11%)	16,38,41	1.28	2 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
12	PSU	I	2457	12	18,21,22	0.94	1 (5%)	22,30,33	1.85	4 (18%)
12	OMU	I	2552	12	19,22,23	0.94	1 (5%)	26,31,34	1.84	6 (23%)
12	6MZ	I	2030	12	18,25,26	1.04	2 (11%)	16,36,39	2.07	4 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	5MC	I	1962	12	-	0/7/25/26	0/2/2/2
12	3TD	I	1915	12	-	2/7/25/26	0/2/2/2
12	G7M	I	2069	12	-	1/3/25/26	0/3/3/3
12	PSU	I	1917	12	-	0/7/25/26	0/2/2/2
12	PSU	I	2504	12,56	-	2/7/25/26	0/2/2/2
12	2MA	I	2503	12,56	-	2/3/25/26	0/3/3/3
12	6MZ	I	1618	12	-	2/5/27/28	0/3/3/3
12	PSU	I	955	12	-	0/7/25/26	0/2/2/2
12	5MU	I	1939	12	-	0/7/25/26	0/2/2/2
12	PSU	I	2605	12	-	2/7/25/26	0/2/2/2
12	5MU	I	747	12	-	0/7/25/26	0/2/2/2
12	1MG	I	745	12	-	0/3/25/26	0/3/3/3
12	PSU	I	1911	12	-	0/7/25/26	0/2/2/2
12	OMC	I	2498	12,56	-	1/9/27/28	0/2/2/2
12	2MG	I	2445	12	-	2/5/27/28	0/3/3/3
24	4D4	U	81	24	-	1/11/12/14	-
12	PSU	I	2604	12	-	0/7/25/26	0/2/2/2
12	PSU	I	2580	12	-	0/7/25/26	0/2/2/2
12	PSU	I	746	12,56	-	1/7/25/26	0/2/2/2
12	OMG	I	2251	5,12	-	0/5/27/28	0/3/3/3
12	H2U	I	2449	12	-	0/7/38/39	0/2/2/2
12	2MG	I	1835	12	-	0/5/27/28	0/3/3/3
12	PSU	I	2457	12	-	0/7/25/26	0/2/2/2
12	OMU	I	2552	12	-	0/9/27/28	0/2/2/2
12	6MZ	I	2030	12	-	2/5/27/28	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	81	4D4	CZ-NE	5.24	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	U	81	4D4	CZ-NH2	3.11	1.44	1.32
12	I	2069	G7M	C8-N9	2.97	1.38	1.33
12	I	1835	2MG	C5-C6	-2.87	1.41	1.47
12	I	2251	OMG	C5-C6	-2.80	1.41	1.47

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	I	1915	3TD	N1-C2-N3	5.94	120.83	116.14
12	I	747	5MU	C4-N3-C2	-5.57	120.14	127.35
12	I	1939	5MU	C4-N3-C2	-5.47	120.27	127.35
12	I	1618	6MZ	C2-N1-C6	5.28	121.12	116.59
12	I	2030	6MZ	C2-N1-C6	5.28	121.12	116.59

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	I	1618	6MZ	O4'-C4'-C5'-O5'
12	I	1618	6MZ	C3'-C4'-C5'-O5'
12	I	1915	3TD	C3'-C4'-C5'-O5'
12	I	1915	3TD	O4'-C4'-C5'-O5'
12	I	2445	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 199 ligands modelled in this entry, 198 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	$\#\|Z\| > 2$
57	ZLD	I	3111	56	26,26,26	1.39	3 (11%)	36,36,36	1.95	10 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	ZLD	I	3111	56	-	0/13/33/33	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	I	3111	ZLD	C7-N4	4.15	1.40	1.36
57	I	3111	ZLD	O10-C8	-3.39	1.41	1.46
57	I	3111	ZLD	C9-C8	3.10	1.55	1.51

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	I	3111	ZLD	C6-N4-C7	-4.96	108.40	111.28
57	I	3111	ZLD	C8-O10-C7	4.86	113.98	110.15
57	I	3111	ZLD	O10-C7-N4	-3.28	107.57	109.83
57	I	3111	ZLD	C8-C6-N4	3.03	104.86	101.81
57	I	3111	ZLD	C6-C8-C9	2.89	116.28	113.08

There are no chirality outliers.

There are no torsion outliers.

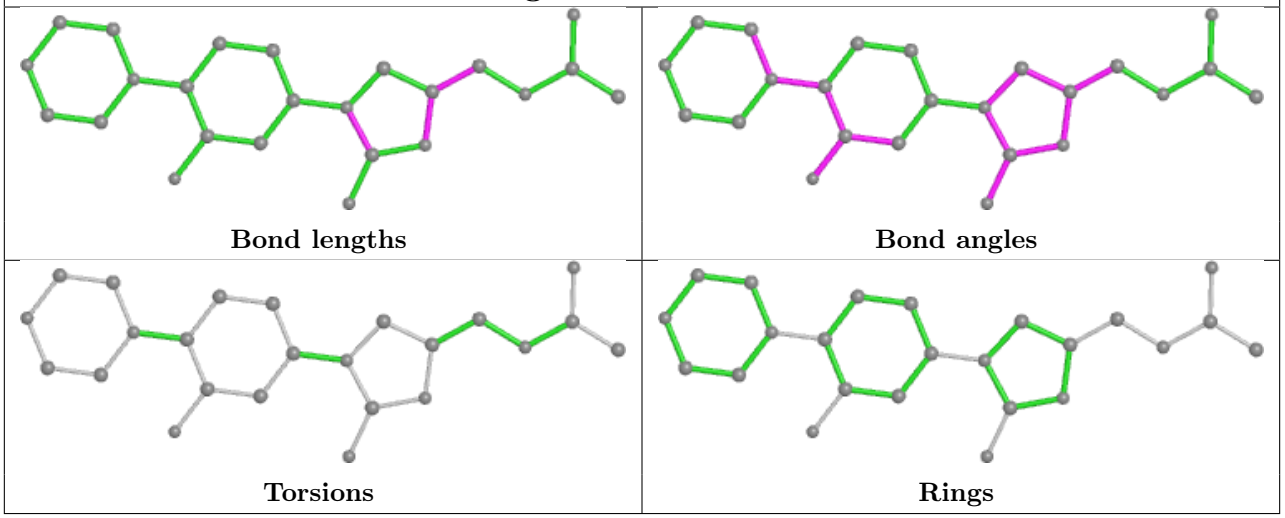
There are no ring outliers.

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 then 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.

Ligand ZLD I 3111



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.

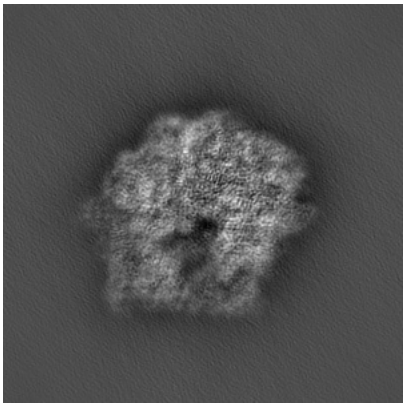
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24800. These allow visual inspection of the internal detail of the map and identification of artifacts.

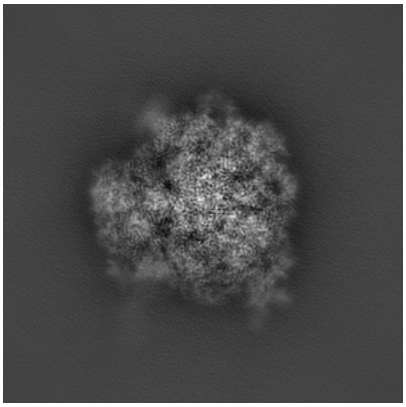
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

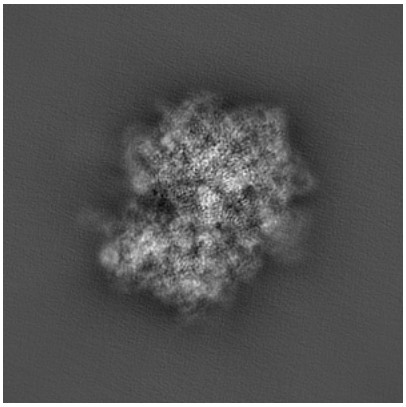
6.1.1 Primary map



X



Y

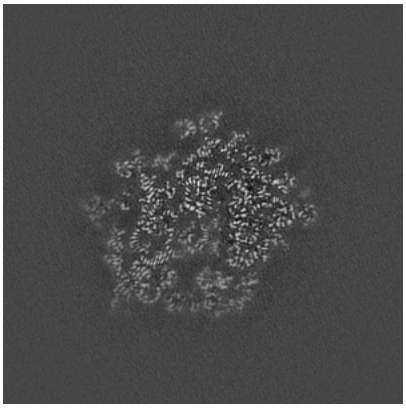


Z

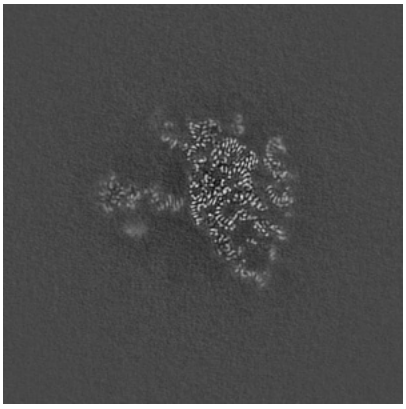
The images above show the map projected in three orthogonal directions.

6.2 Central slices

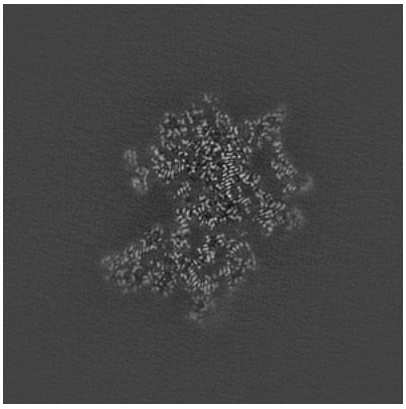
6.2.1 Primary map



X Index: 256



Y Index: 256

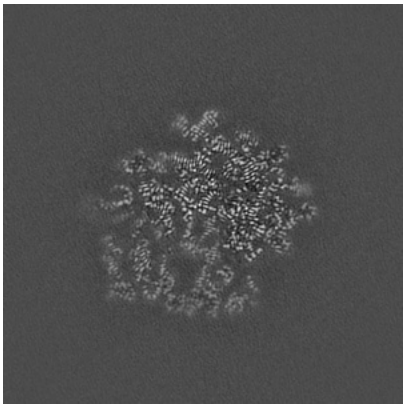


Z Index: 256

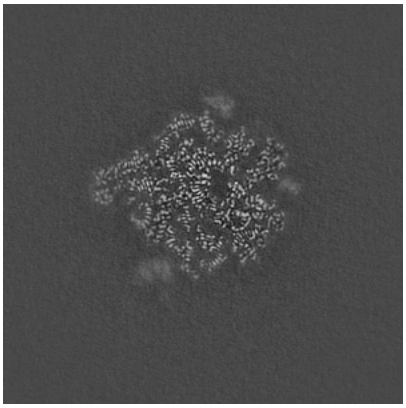
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

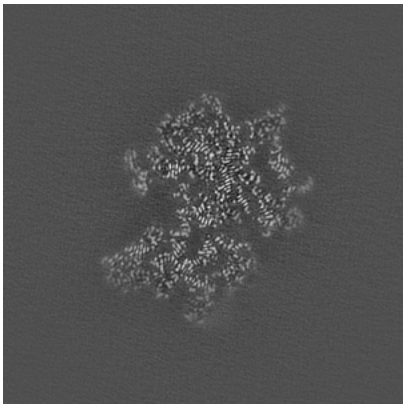
6.3.1 Primary map



X Index: 263



Y Index: 293

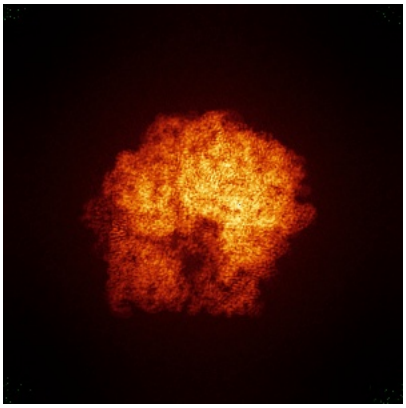


Z Index: 254

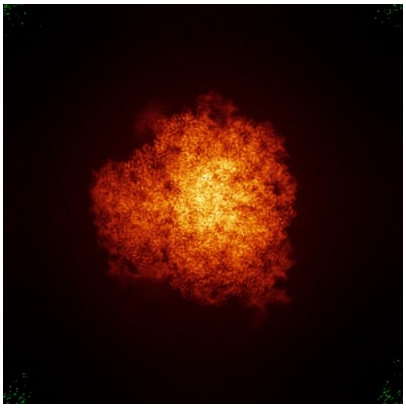
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

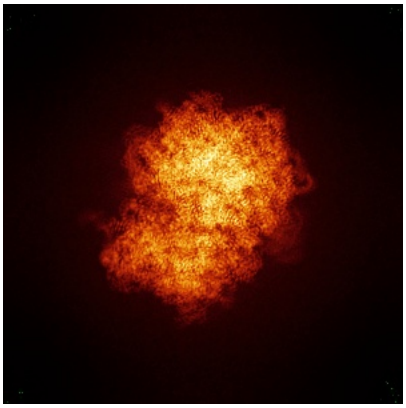
6.4.1 Primary map



X



Y

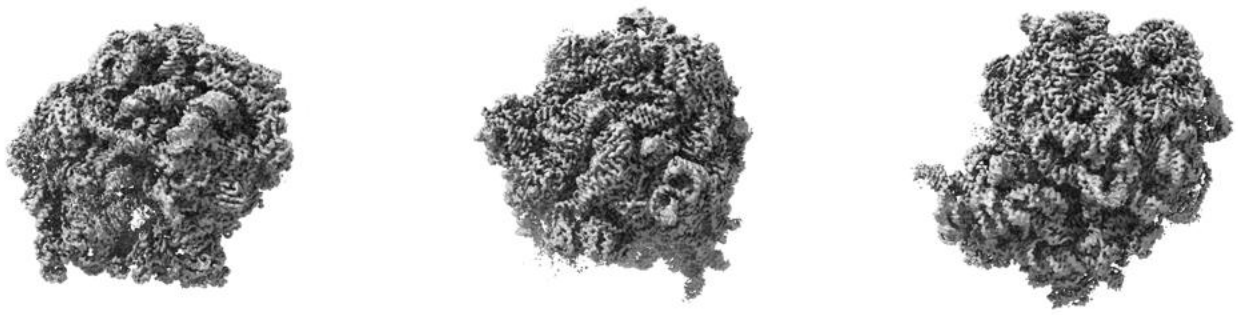


Z

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



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

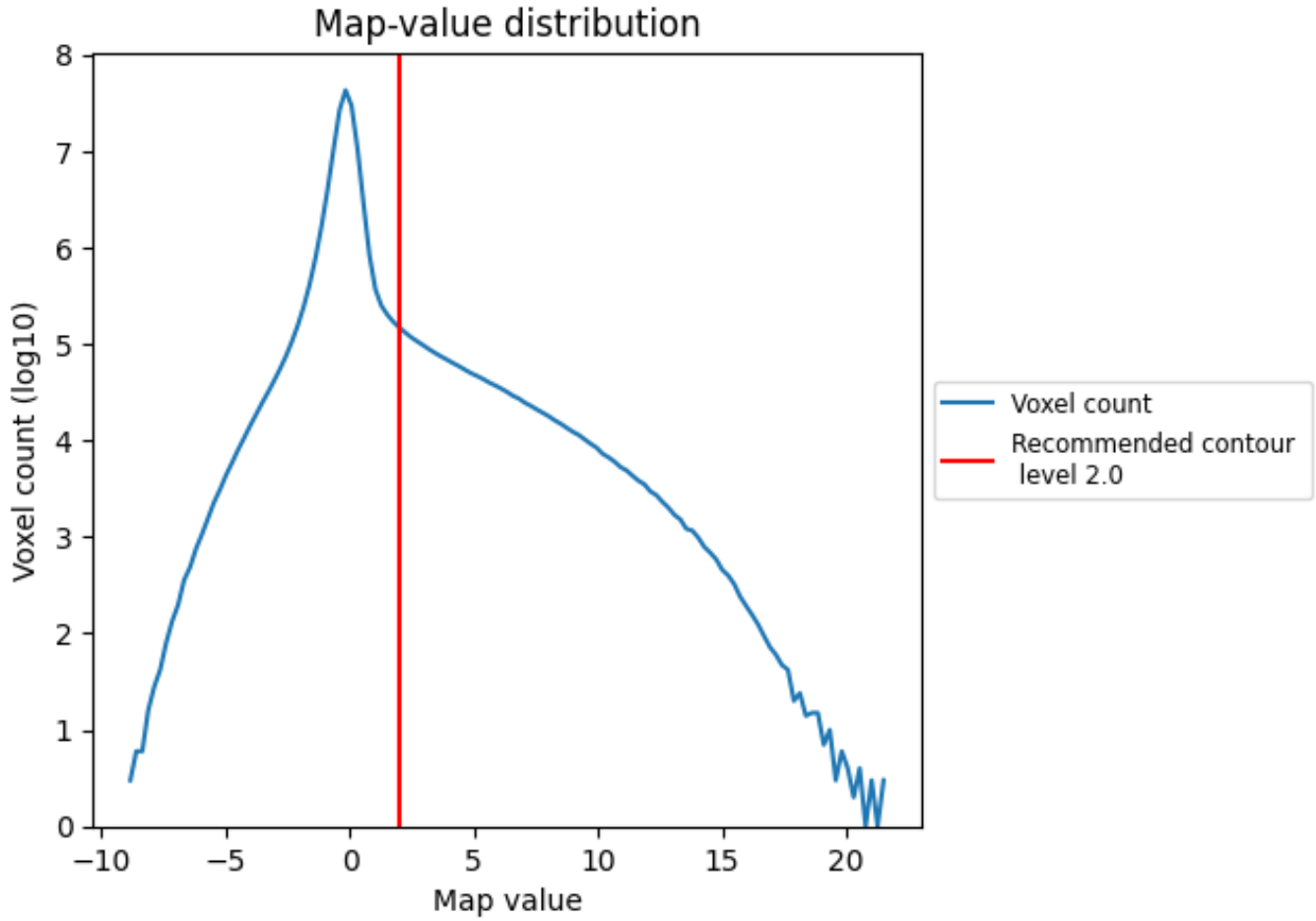
6.6 Mask visualisation (i)

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

7 Map analysis

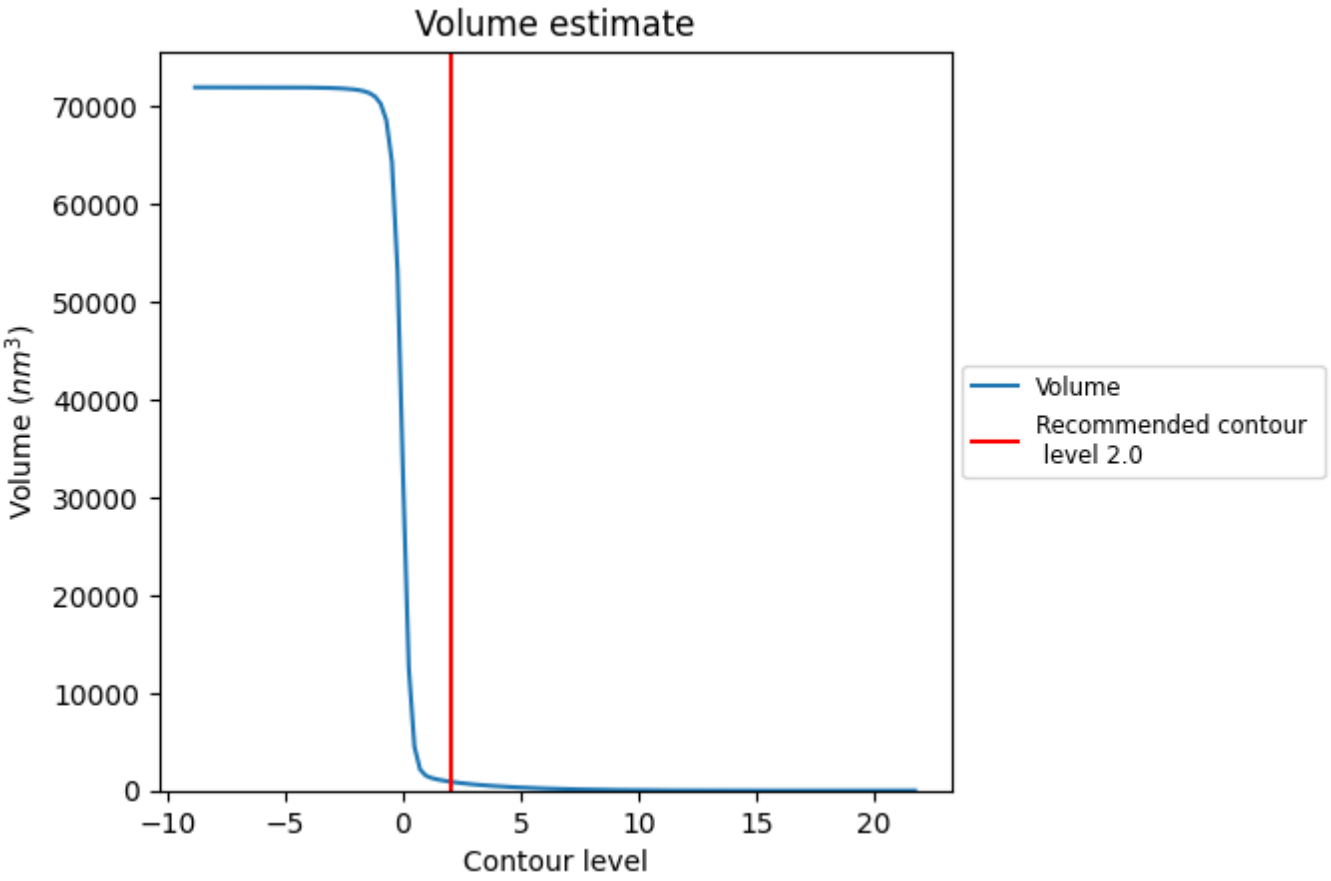
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

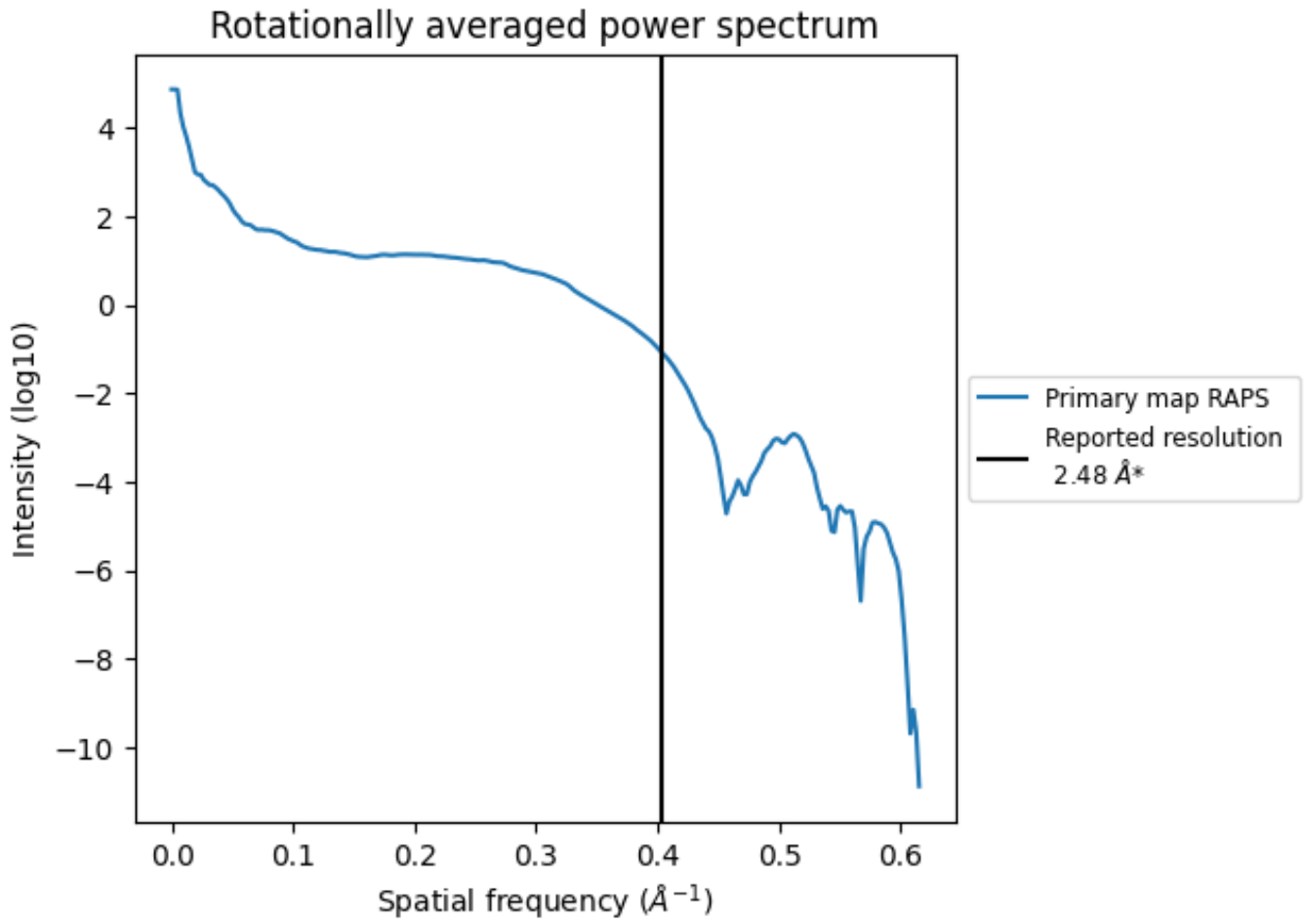
7.2 Volume estimate (i)



The volume at the recommended contour level is 910 nm^3; this corresponds to an approximate mass of 822 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 (i)

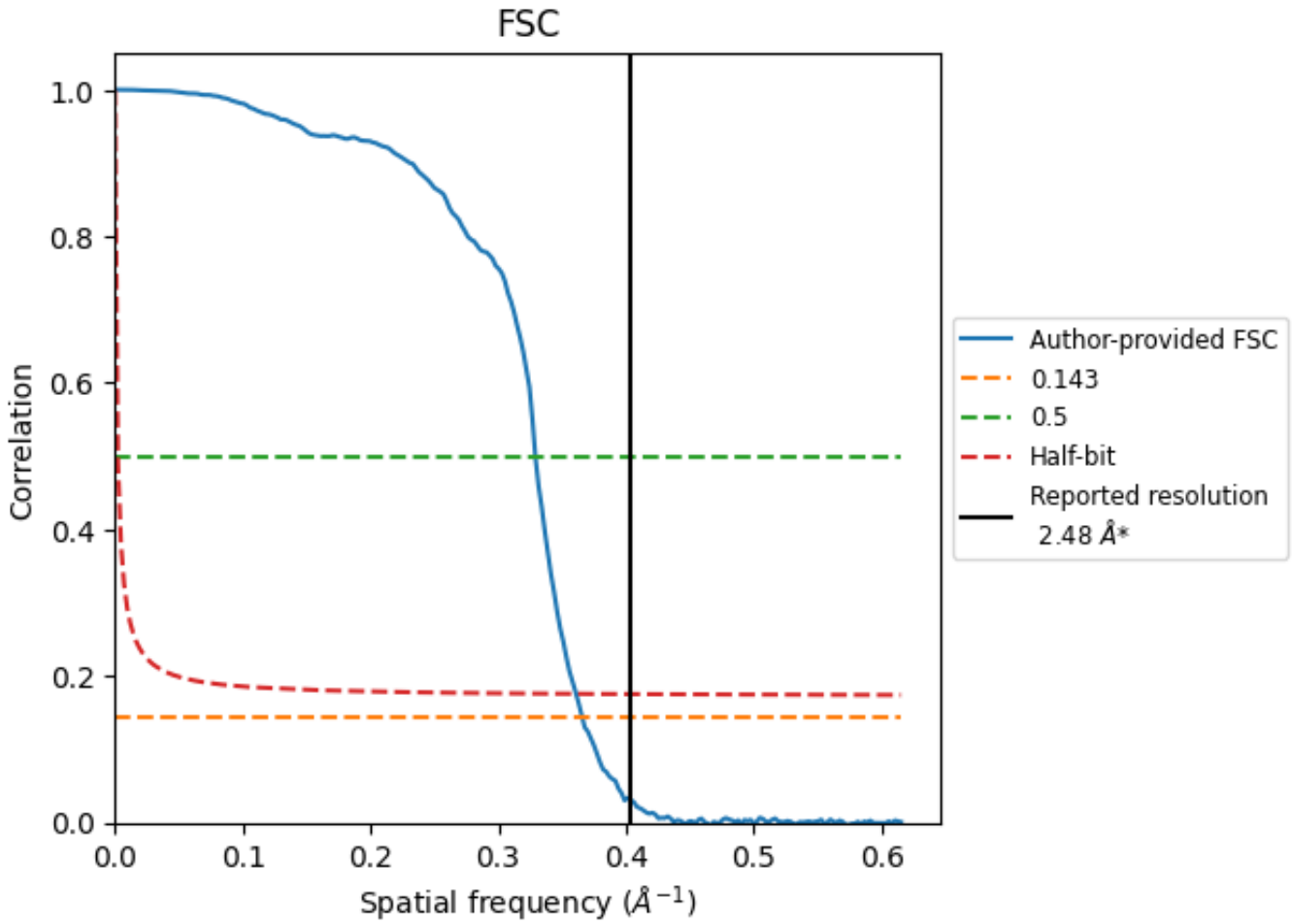


*Reported resolution corresponds to spatial frequency of 0.403 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.403 Å^{-1}

8.2 Resolution estimates (i)

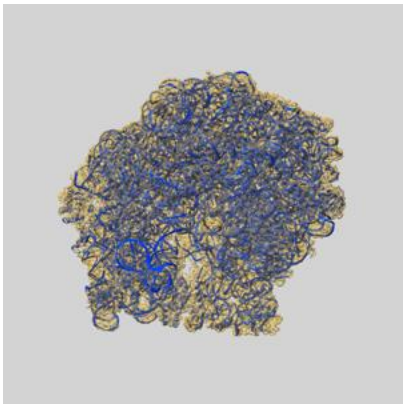
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.48	-	-
Author-provided FSC curve	2.73	3.04	2.77
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.73 differs from the reported value 2.48 by more than 10 %

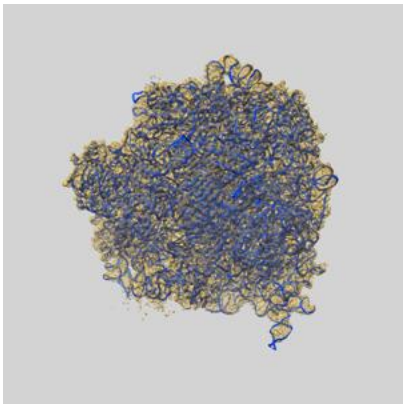
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24800 and PDB model 7S1G. Per-residue inclusion information can be found in section 3 on page 15.

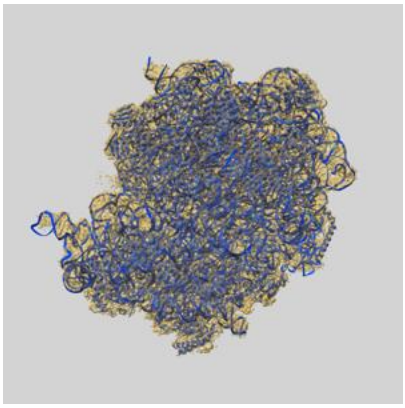
9.1 Map-model overlay



X



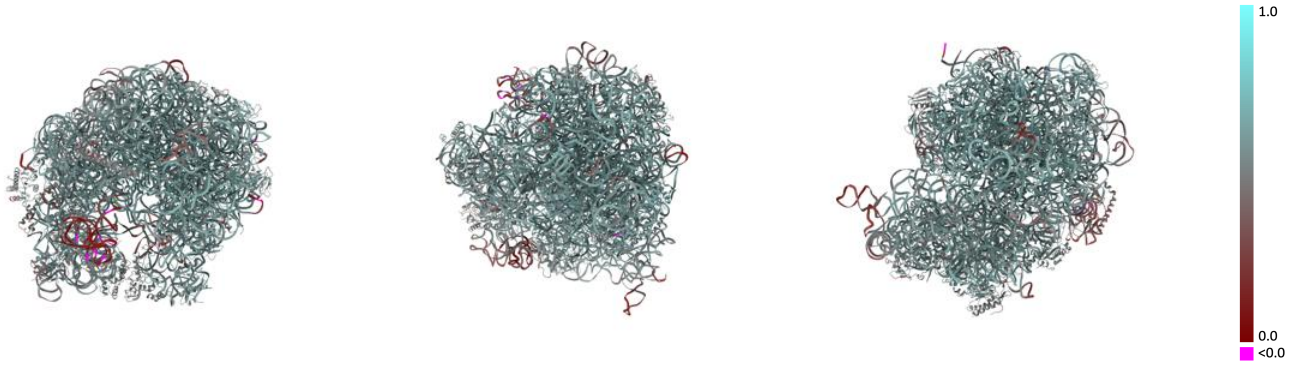
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.0 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.

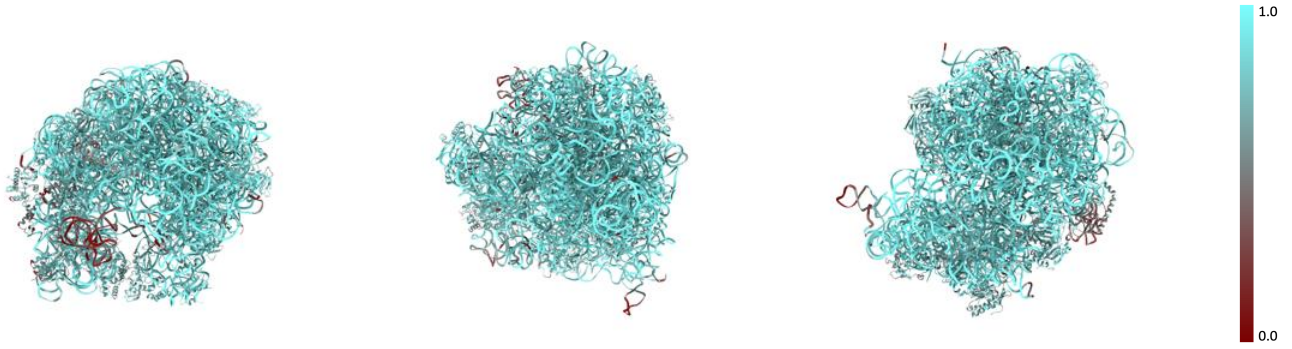
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

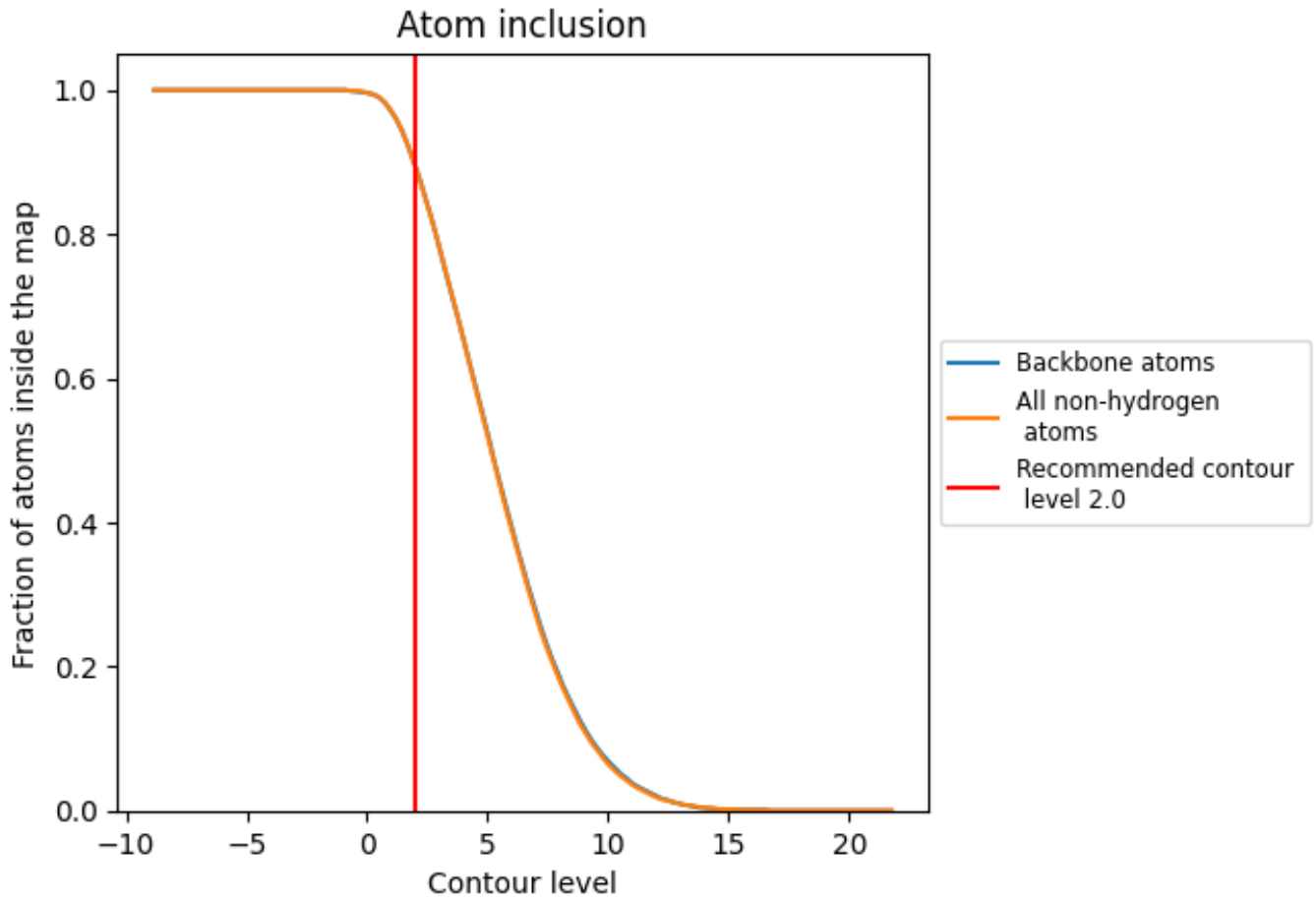
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (2.0).

9.4 Atom inclusion (i)



At the recommended contour level, 89% 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 (2.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8940	0.5740
1	0.7660	0.5210
2	0.8000	0.5390
3	0.5210	0.4780
4	0.9120	0.5840
A	0.8940	0.5460
C	0.9330	0.5760
D	0.6360	0.4970
E	0.7590	0.5500
F	0.7280	0.5250
G	0.8560	0.5900
H	0.8200	0.5320
I	0.9390	0.5800
J	0.9610	0.5790
K	0.9280	0.6210
L	0.9010	0.6120
M	0.8180	0.5750
N	0.7590	0.5210
O	0.7740	0.5140
P	0.5310	0.4460
Q	0.7160	0.4830
R	0.8980	0.6080
S	0.8850	0.6120
T	0.8740	0.6010
U	0.8720	0.6020
V	0.9250	0.6190
W	0.8100	0.5530
X	0.8830	0.6070
Y	0.9240	0.6160
Z	0.8480	0.5920
a	0.8730	0.6120
b	0.8170	0.5750
c	0.8100	0.5600
d	0.8240	0.5820
e	0.9030	0.6180

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	0.8970	0.6060
g	0.7930	0.5340
h	0.8560	0.5890
i	0.8780	0.5990
j	0.3970	0.4840
k	0.9180	0.6260
l	0.9250	0.6310
m	0.8870	0.6070
n	0.7290	0.5160
o	0.8510	0.5980
p	0.7390	0.5130
q	0.5560	0.4860
r	0.8340	0.5610
s	0.8640	0.6450
t	0.8500	0.5880
u	0.8020	0.5470
v	0.7630	0.5410
w	0.8600	0.5800
x	0.8100	0.5430
y	0.7860	0.5510
z	0.8780	0.5760