wwPDB EM Validation Summary Report

Nov 26, 2022 – 01:25 PM EST

PDB ID	:	7ST7
EMDB ID	:	EMD-25421
Title	:	Pre translocation intermediate stalled with viomycin and bound with EF-G in a GDP and Pi state (Structure III-vio)
Authors	:	Carbone, C.E.; Korostelev, A.A.
Deposited on	:	2021-11-12
Resolution	:	3.20 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:

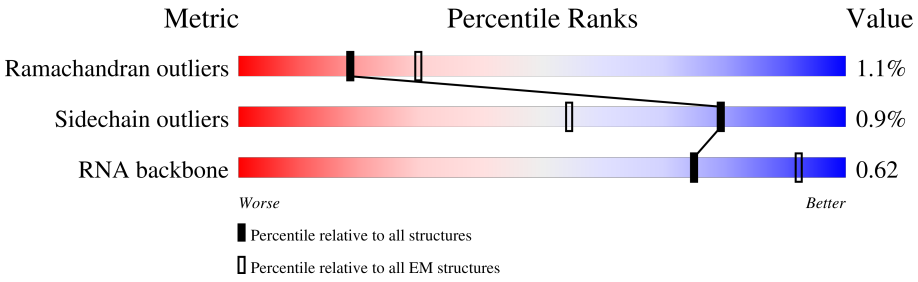
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	2903	85% 15%
2	2	120	90% 10%
3	b	271	97%
4	c	209	99%
5	d	201	99%
6	e	177	5% 98%
7	f	176	6% 98%
8	g	149	87% 99%

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Mol	Chain	Length	Quality of chain
9	a	223	30% 60% 40%
10	i	141	76% 96%
11	j	142	99%
12	k	122	97%
13	l	143	100%
14	m	136	99%
15	n	120	98%
16	o	116	99%
17	p	114	100%
18	q	117	99%
19	r	103	98%
20	s	110	100%
21	t	93	100%
22	u	102	98%
23	v	94	100%
24	w	75	100%
25	x	77	100%
26	y	63	6% 98%
27	z	58	97%
28	A	66	38% 97%
29	B	56	96%
30	C	50	24% 100%
31	D	46	98%
32	E	64	98%
33	F	38	100%

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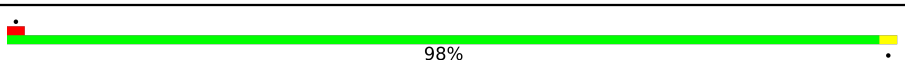
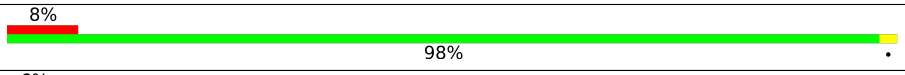
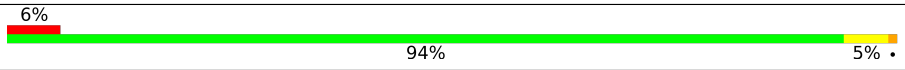
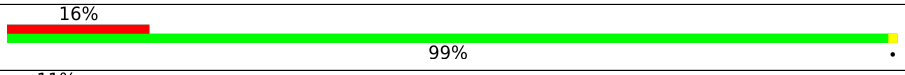
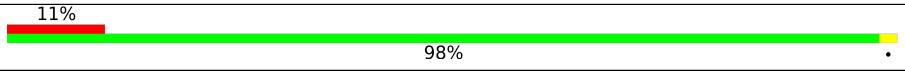
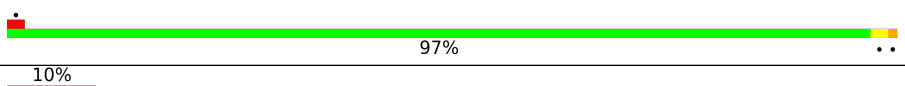
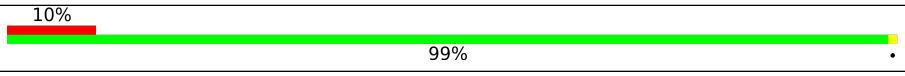
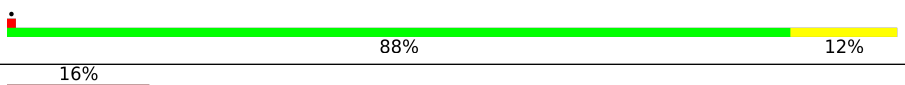
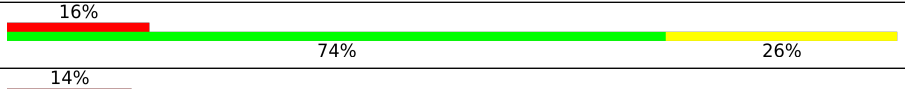
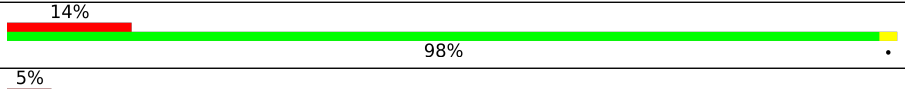
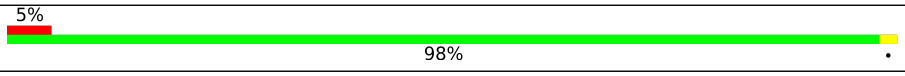
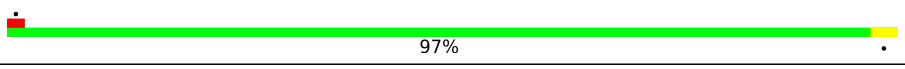
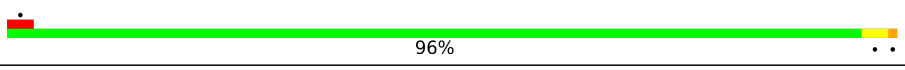
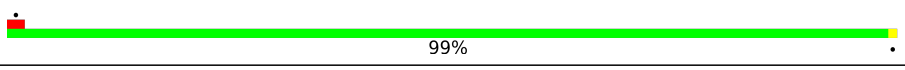
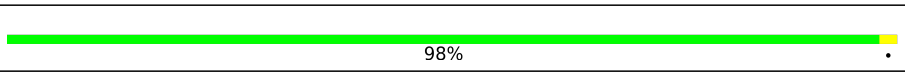
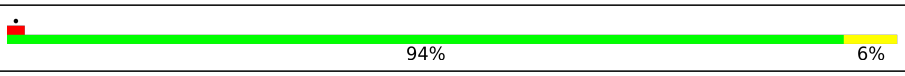
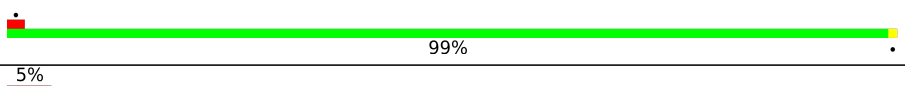
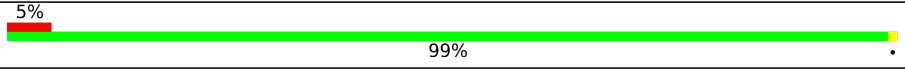
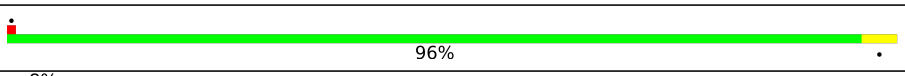
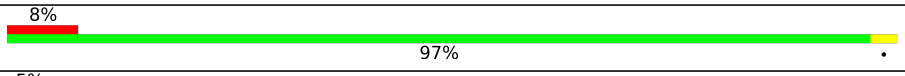
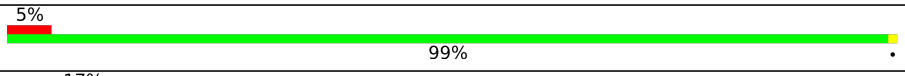
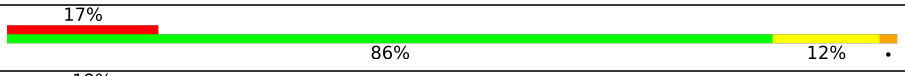
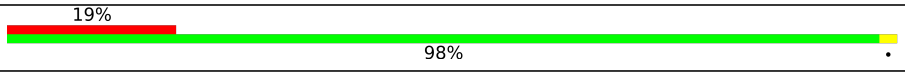
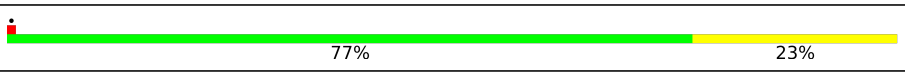
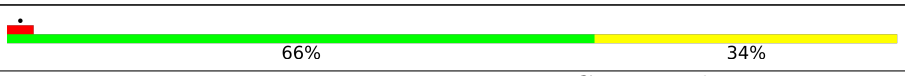
Mol	Chain	Length	Quality of chain
34	H	206	
35	L	151	
36	N	127	
37	O	98	
38	R	114	
39	S	100	
40	X	79	
41	3	1539	
42	4	19	
43	G	218	
44	I	205	
45	J	157	
46	K	100	
47	M	129	
48	P	116	
49	Q	123	
50	T	88	
51	U	82	
52	V	80	
53	W	65	
54	Y	85	
55	Z	65	
56	8	697	
57	6	77	
58	5	76	

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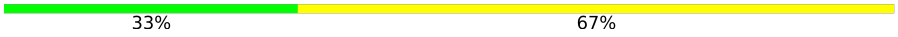
Mol	Chain	Length	Quality of chain
59	h	6	

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 153555 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called 5S rRNA.

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

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

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

- Molecule 5 is a protein called 50S ribosomal protein L4.

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

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

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

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L1.

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

- Molecule 10 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	i	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 11 is a protein called 50S ribosomal protein L13.

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

- Molecule 12 is a protein called 50S ribosomal protein L14.

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

- Molecule 13 is a protein called 50S ribosomal protein L15.

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

- Molecule 14 is a protein called 50S ribosomal protein L16.

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

- Molecule 15 is a protein called 50S ribosomal protein L17.

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

- Molecule 16 is a protein called 50S ribosomal protein L18.

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

- Molecule 17 is a protein called 50S ribosomal protein L19.

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

- Molecule 18 is a protein called 50S ribosomal protein L20.

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

- Molecule 19 is a protein called 50S ribosomal protein L21.

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

- Molecule 20 is a protein called 50S ribosomal protein L22.

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

- Molecule 21 is a protein called 50S ribosomal protein L23.

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

- Molecule 22 is a protein called 50S ribosomal protein L24.

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

- Molecule 23 is a protein called 50S ribosomal protein L25.

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

- Molecule 24 is a protein called 50S ribosomal protein L27.

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

- Molecule 25 is a protein called 50S ribosomal protein L28.

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

- Molecule 26 is a protein called 50S ribosomal protein L29.

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

- Molecule 27 is a protein called 50S ribosomal protein L30.

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

- Molecule 28 is a protein called 50S ribosomal protein L31.

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

- Molecule 29 is a protein called 50S ribosomal protein L32.

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

- Molecule 30 is a protein called 50S ribosomal protein L33.

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

- Molecule 31 is a protein called 50S ribosomal protein L34.

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

- Molecule 32 is a protein called 50S ribosomal protein L35.

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

- Molecule 33 is a protein called 50S ribosomal protein L36.

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

- Molecule 34 is a protein called 30S ribosomal protein S3.

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

- Molecule 35 is a protein called 30S ribosomal protein S7.

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

- Molecule 36 is a protein called 30S ribosomal protein S9.

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

- Molecule 37 is a protein called 30S ribosomal protein S10.

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

- Molecule 38 is a protein called 30S ribosomal protein S13.

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

- Molecule 39 is a protein called 30S ribosomal protein S14.

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

- Molecule 40 is a protein called 30S ribosomal protein S19.

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

- Molecule 41 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	3	1539	Total 33012	C 14725	N 6052	O 10697	P 1538	0	0

- Molecule 42 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	4	19	Total 413	C 186	N 85	O 124	P 18	0	0

- Molecule 43 is a protein called 30S ribosomal protein S2.

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

- Molecule 44 is a protein called 30S ribosomal protein S4.

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

- Molecule 45 is a protein called 30S ribosomal protein S5.

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

- Molecule 46 is a protein called 30S ribosomal protein S6.

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

- Molecule 47 is a protein called 30S ribosomal protein S8.

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

- Molecule 48 is a protein called 30S ribosomal protein S11.

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

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

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

- Molecule 50 is a protein called 30S ribosomal protein S15.

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

- Molecule 51 is a protein called 30S ribosomal protein S16.

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

- Molecule 52 is a protein called 30S ribosomal protein S17.

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

- Molecule 53 is a protein called 30S ribosomal protein S18.

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

- Molecule 54 is a protein called 30S ribosomal protein S20.

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

- Molecule 55 is a protein called 30S ribosomal protein S21.

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

- Molecule 56 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	8	697	Total	C	N	O	S	0	0
			5400	3403	929	1043	25		

- Molecule 57 is a RNA chain called tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

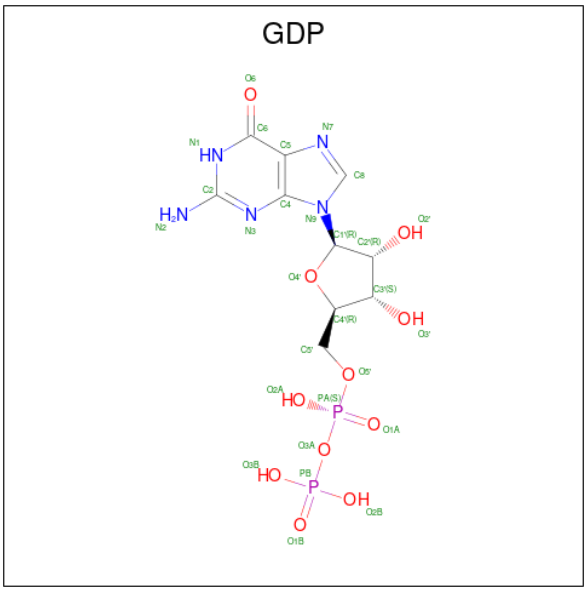
- Molecule 58 is a RNA chain called tRNA Pro.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	5	76	Total	C	N	O	P	0	0
			1625	723	290	536	76		

- Molecule 59 is a protein called Viomycin.

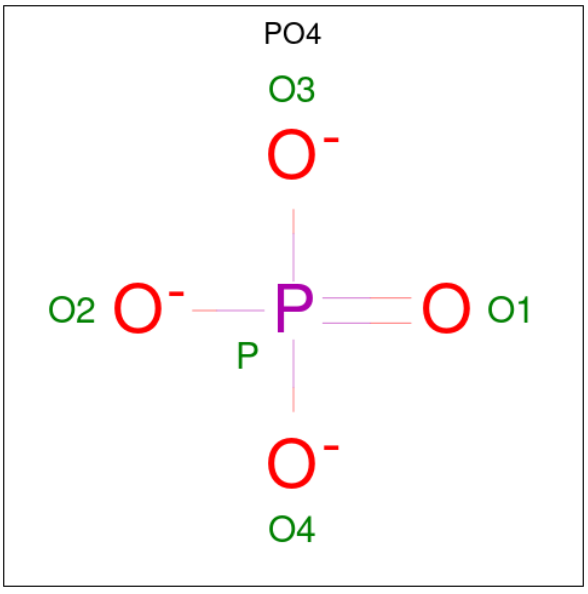
Mol	Chain	Residues	Atoms				AltConf	Trace
59	h	6	Total	C	N	O	0	0
			48	25	13	10		

- Molecule 60 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
60	8	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 61 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P) (labeled as "Ligand of Interest" by depositor).



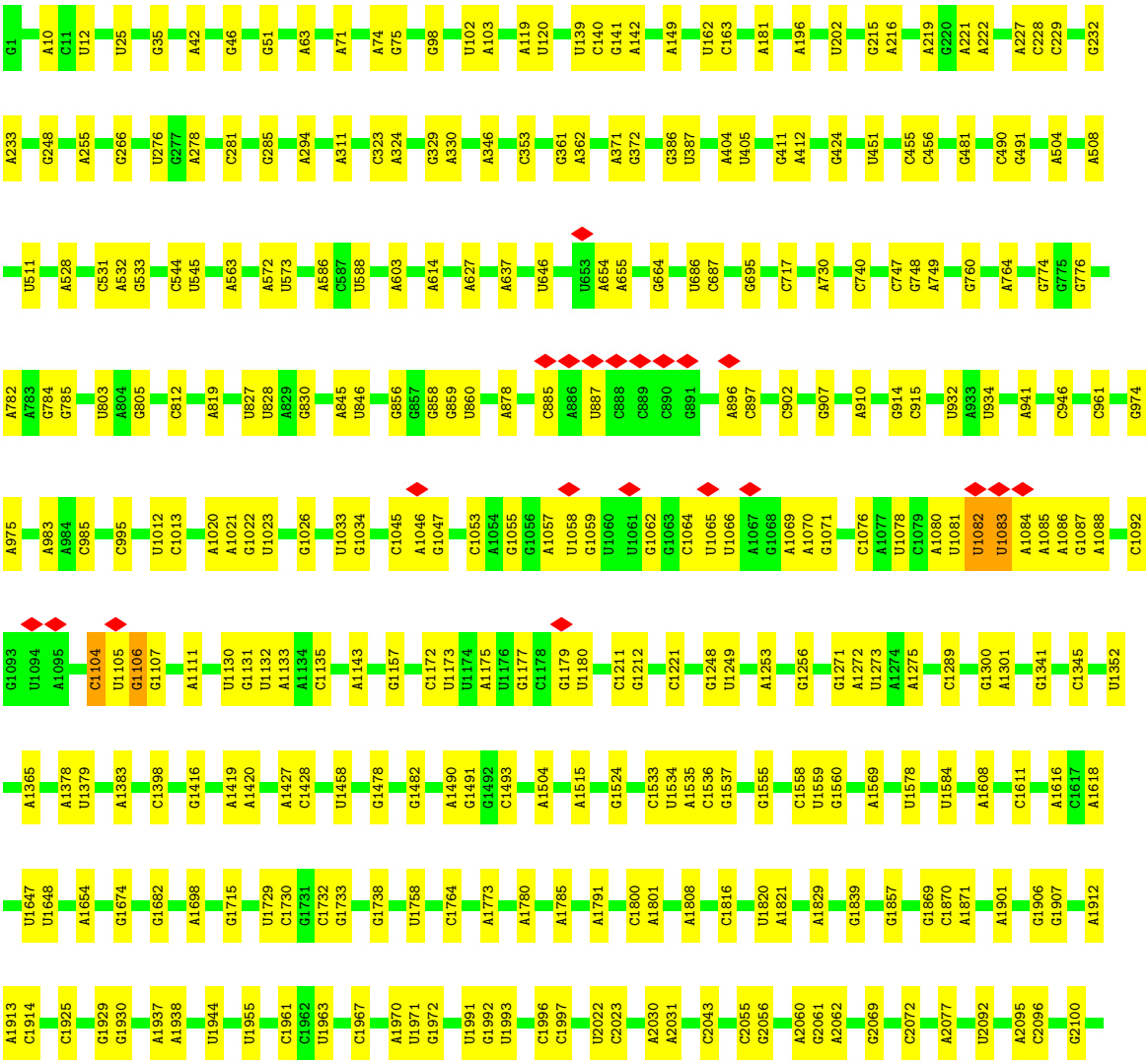
Mol	Chain	Residues	Atoms			AltConf
61	8	1	Total	O	P	0
			5	4	1	

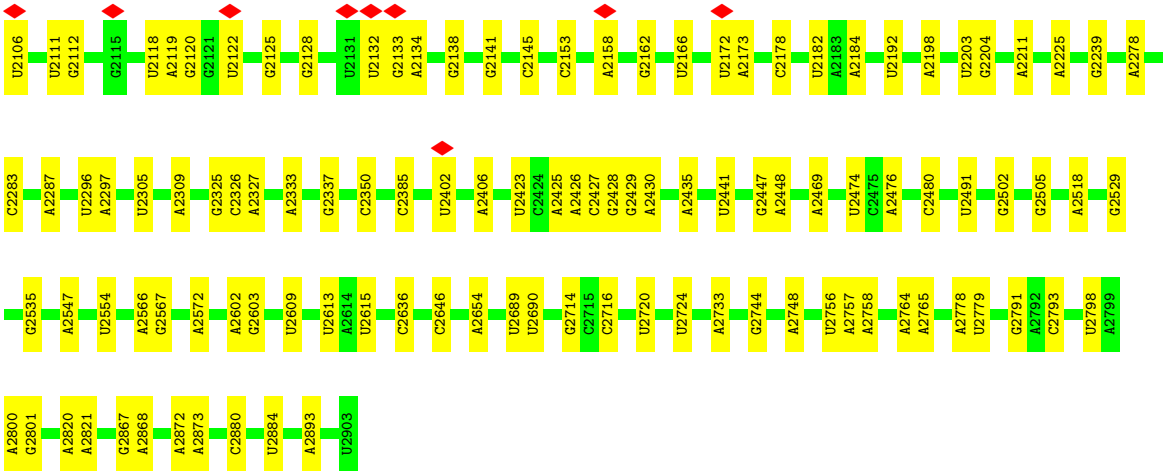
3 Residue-property plots (i)

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: 23S rRNA

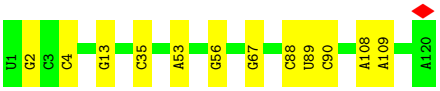
Chain 1:





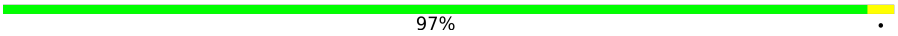
• Molecule 2: 5S rRNA

Chain 2:



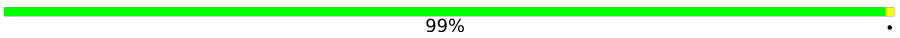
• Molecule 3: 50S ribosomal protein L2

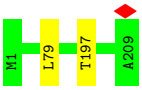
Chain b:



• Molecule 4: 50S ribosomal protein L3

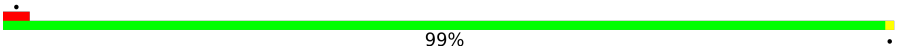
Chain c:

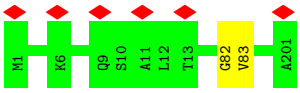




• Molecule 5: 50S ribosomal protein L4

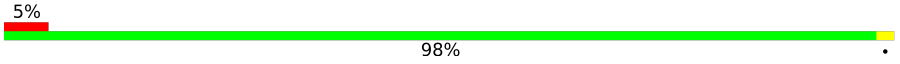
Chain d:

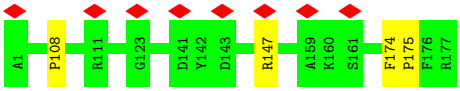




• Molecule 6: 50S ribosomal protein L5

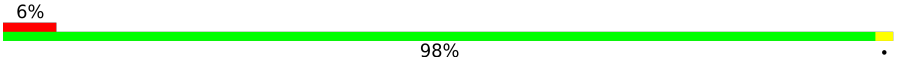
Chain e:

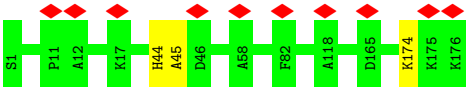




• Molecule 7: 50S ribosomal protein L6

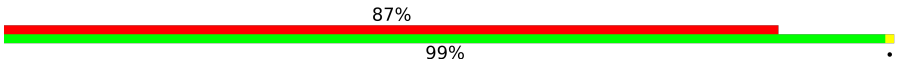
Chain f:

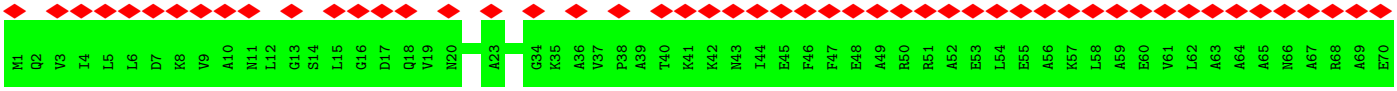


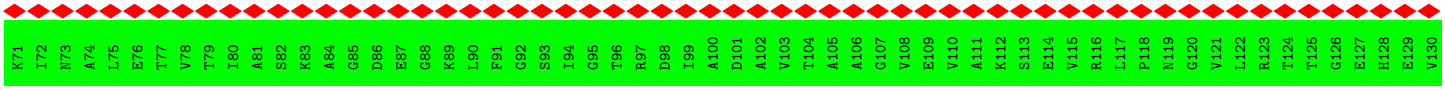


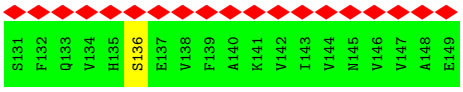
• Molecule 8: 50S ribosomal protein L9

Chain g:



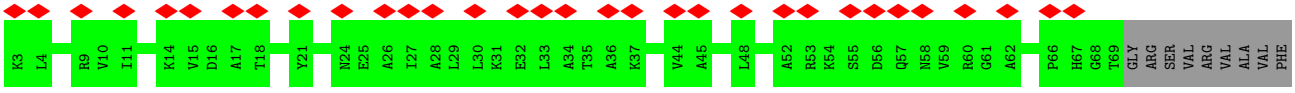


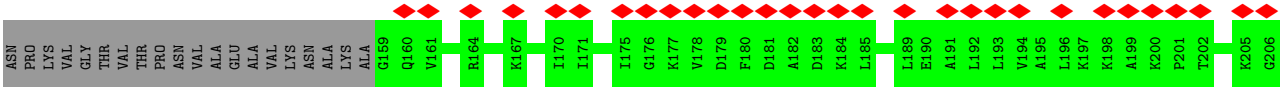


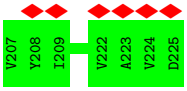


• Molecule 9: 50S ribosomal protein L1

Chain a:

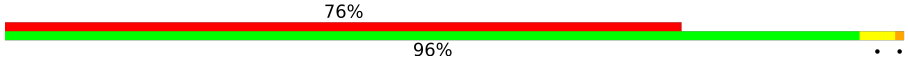


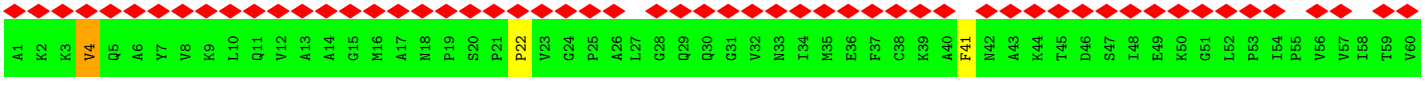


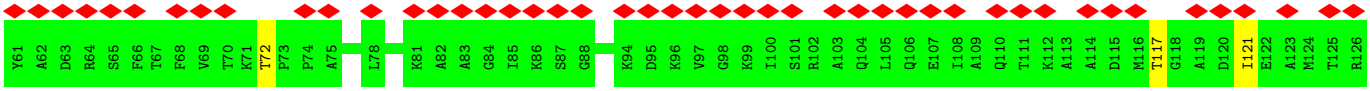


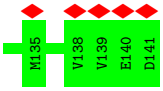
• Molecule 10: 50S ribosomal protein L11

Chain i:



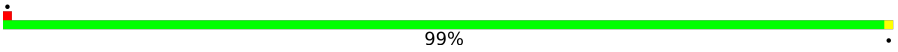






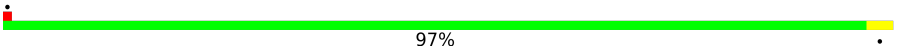
• Molecule 11: 50S ribosomal protein L13

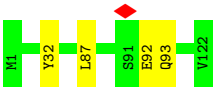
Chain j:



• Molecule 12: 50S ribosomal protein L14

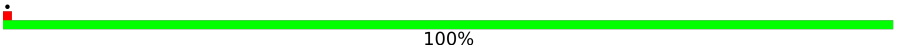
Chain k:

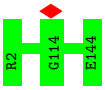




• Molecule 13: 50S ribosomal protein L15

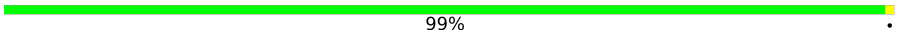
Chain l:





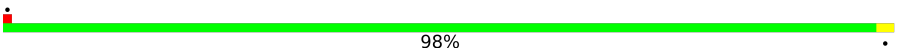
• Molecule 14: 50S ribosomal protein L16

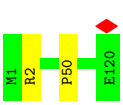
Chain m:



• Molecule 15: 50S ribosomal protein L17

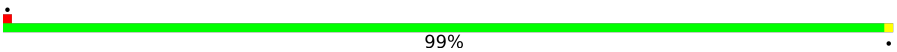
Chain n:

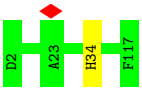




• Molecule 16: 50S ribosomal protein L18

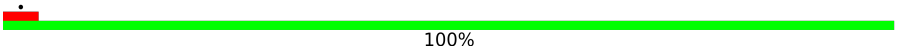
Chain o:

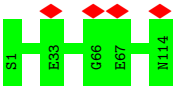




• Molecule 17: 50S ribosomal protein L19

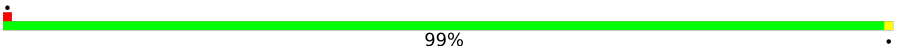
Chain p:

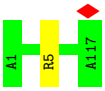




• Molecule 18: 50S ribosomal protein L20

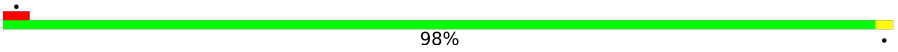
Chain q:

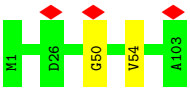




• Molecule 19: 50S ribosomal protein L21

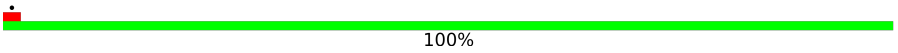
Chain r:

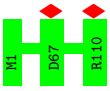




• Molecule 20: 50S ribosomal protein L22

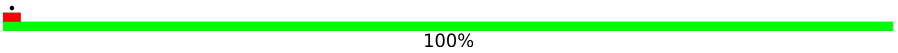
Chain s:





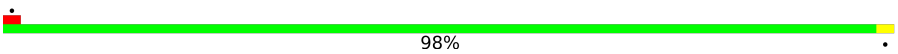
• Molecule 21: 50S ribosomal protein L23

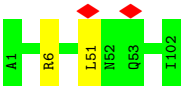
Chain t:



• Molecule 22: 50S ribosomal protein L24

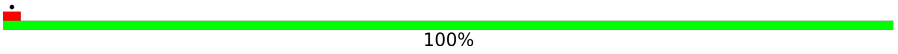
Chain u:

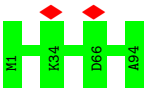




• Molecule 23: 50S ribosomal protein L25

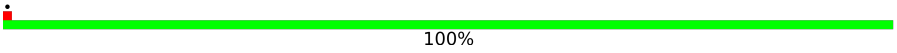
Chain v:





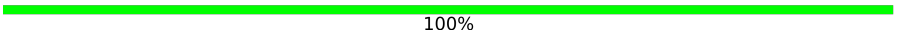
• Molecule 24: 50S ribosomal protein L27

Chain w:



• Molecule 25: 50S ribosomal protein L28

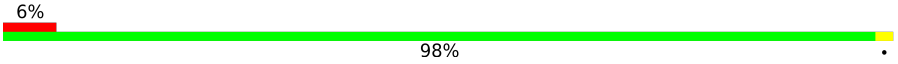
Chain x:

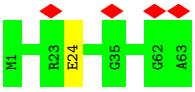


There are no outlier residues recorded for this chain.

• Molecule 26: 50S ribosomal protein L29

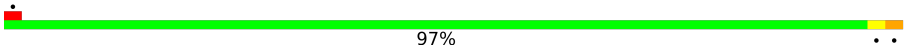
Chain y:

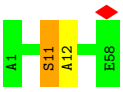




• Molecule 27: 50S ribosomal protein L30

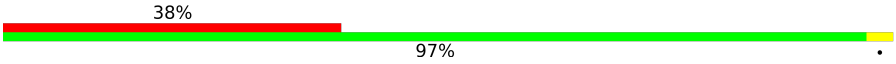
Chain z:

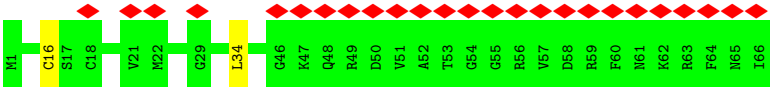




• Molecule 28: 50S ribosomal protein L31

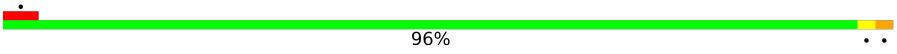
Chain A:

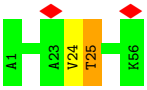




• Molecule 29: 50S ribosomal protein L32

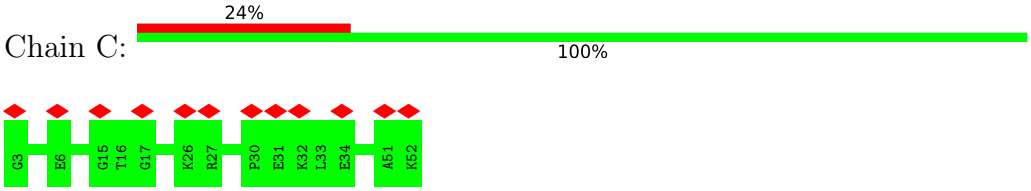
Chain B:





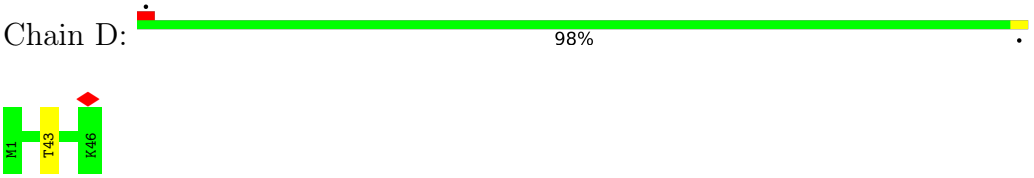
• Molecule 30: 50S ribosomal protein L33

Chain C:



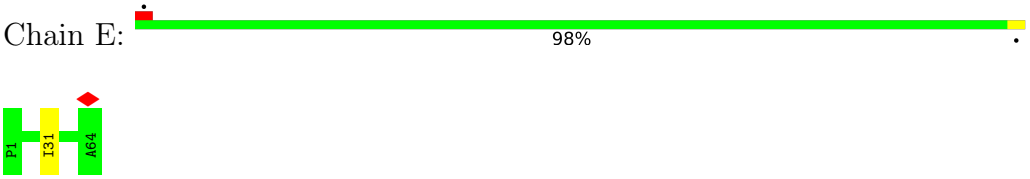
• Molecule 31: 50S ribosomal protein L34

Chain D:



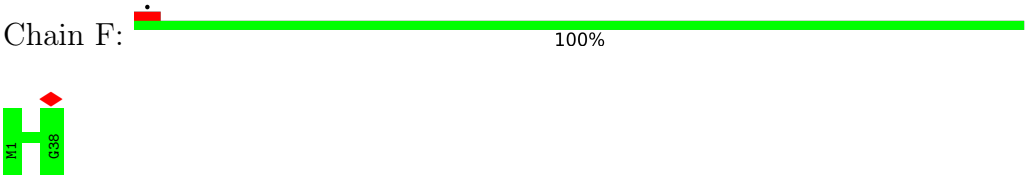
• Molecule 32: 50S ribosomal protein L35

Chain E:



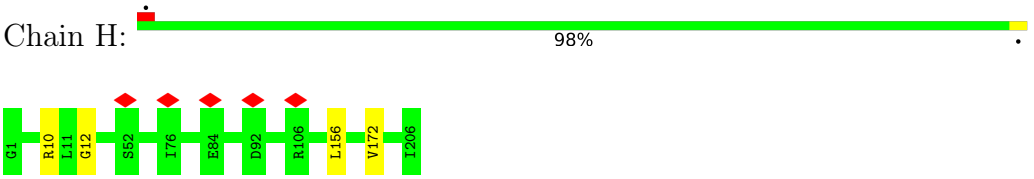
• Molecule 33: 50S ribosomal protein L36

Chain F:



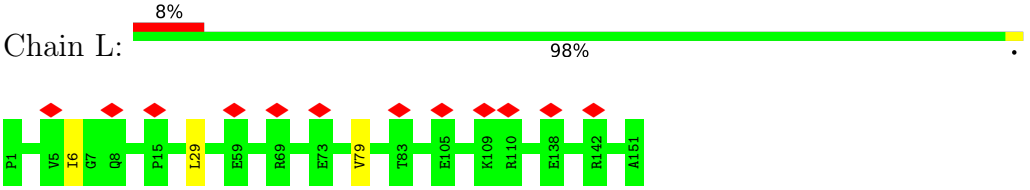
• Molecule 34: 30S ribosomal protein S3

Chain H:



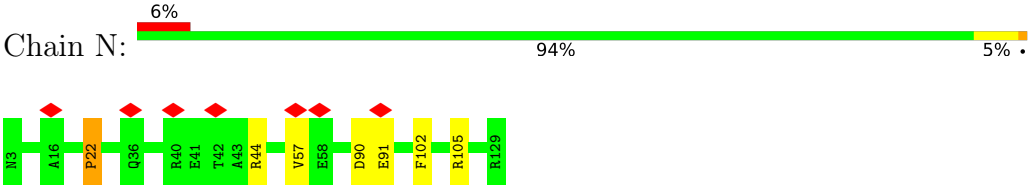
• Molecule 35: 30S ribosomal protein S7

Chain L:



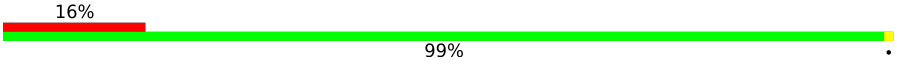
• Molecule 36: 30S ribosomal protein S9

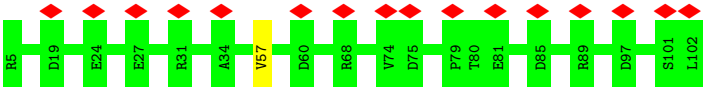
Chain N:



• Molecule 37: 30S ribosomal protein S10

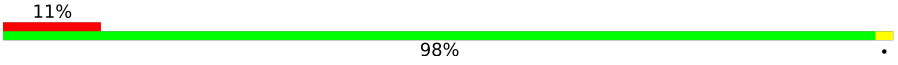
Chain O:

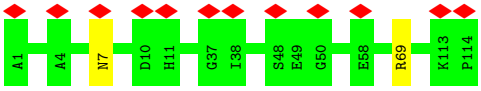




• Molecule 38: 30S ribosomal protein S13

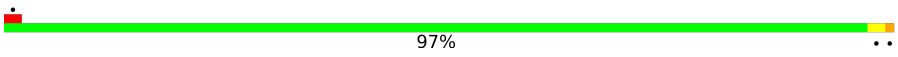
Chain R:

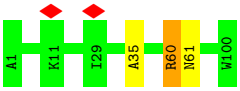




• Molecule 39: 30S ribosomal protein S14

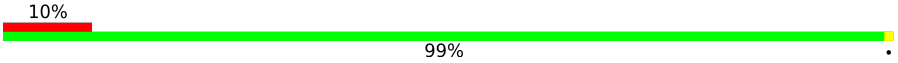
Chain S:

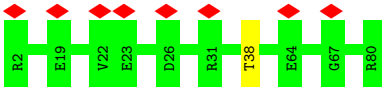




• Molecule 40: 30S ribosomal protein S19

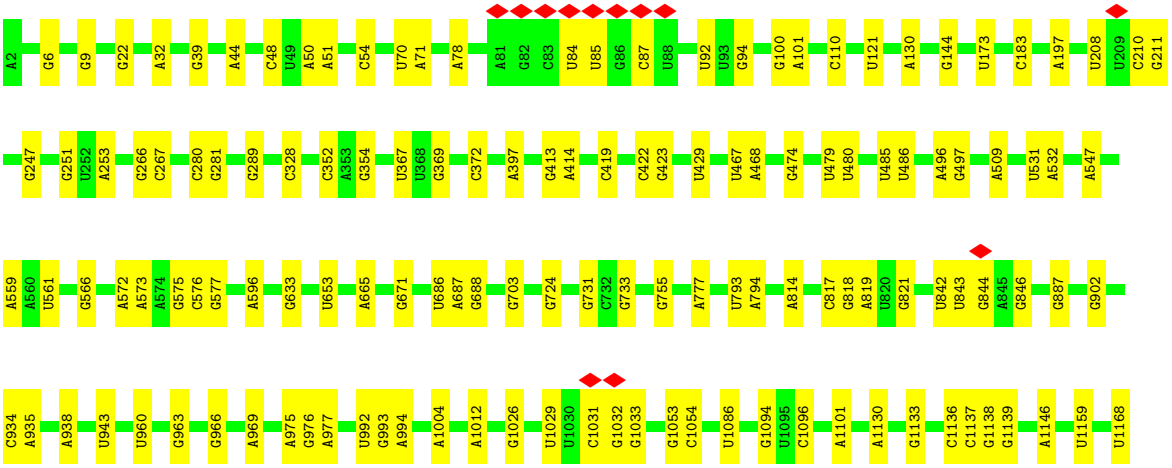
Chain X:

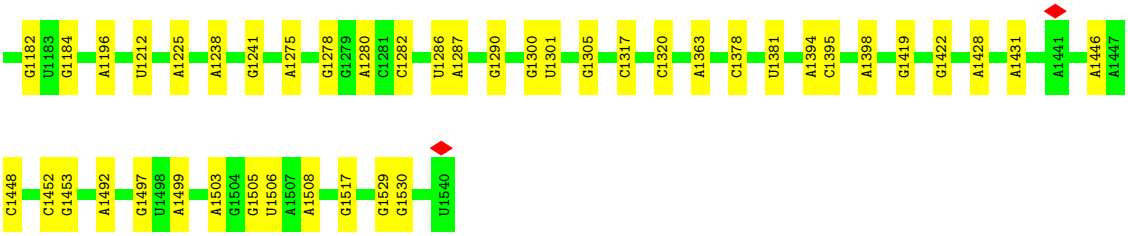




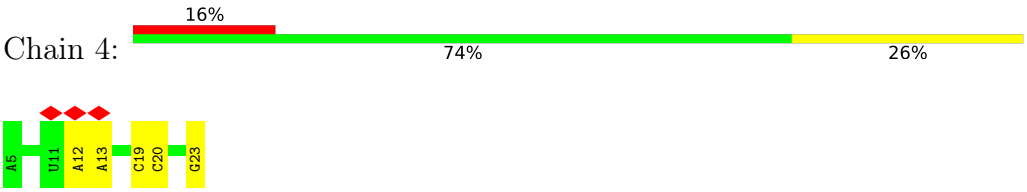
• Molecule 41: 16S rRNA

Chain 3:

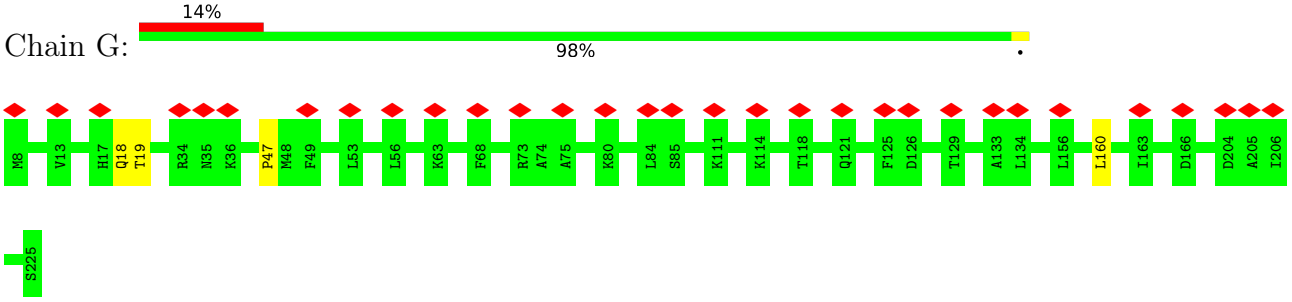




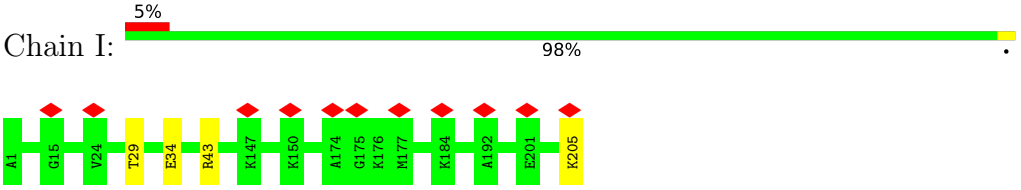
• Molecule 42: mRNA



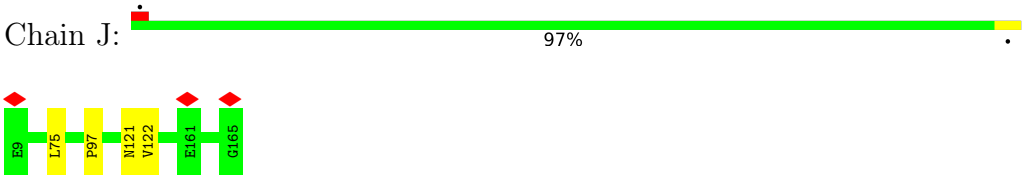
• Molecule 43: 30S ribosomal protein S2



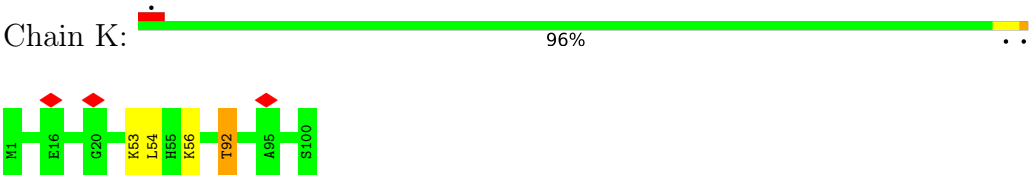
• Molecule 44: 30S ribosomal protein S4



• Molecule 45: 30S ribosomal protein S5

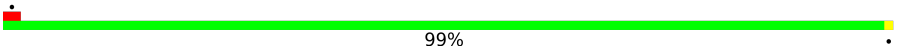


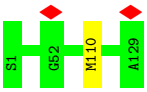
• Molecule 46: 30S ribosomal protein S6



• Molecule 47: 30S ribosomal protein S8

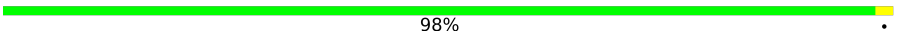
Chain M:

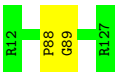




• Molecule 48: 30S ribosomal protein S11

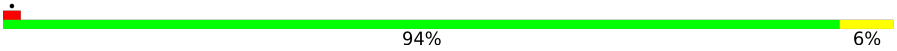
Chain P:

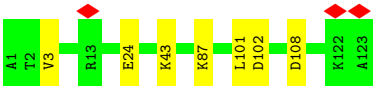




• Molecule 49: 30S ribosomal protein S12

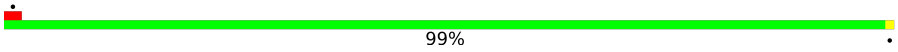
Chain Q:

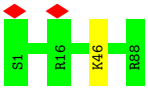




• Molecule 50: 30S ribosomal protein S15

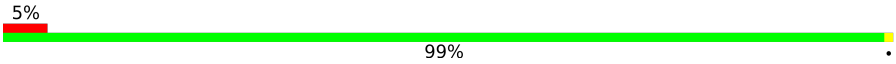
Chain T:

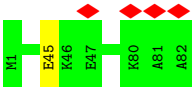




• Molecule 51: 30S ribosomal protein S16

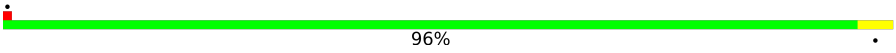
Chain U:





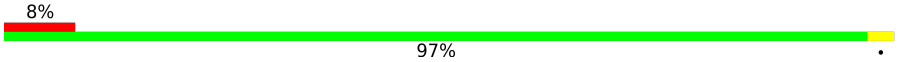
• Molecule 52: 30S ribosomal protein S17

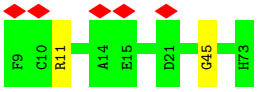
Chain V:



• Molecule 53: 30S ribosomal protein S18

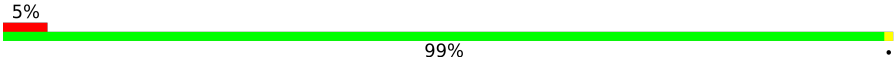
Chain W:

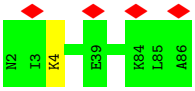




• Molecule 54: 30S ribosomal protein S20

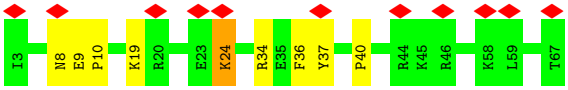
Chain Y:





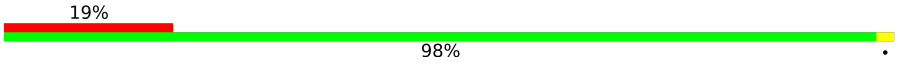
• Molecule 55: 30S ribosomal protein S21

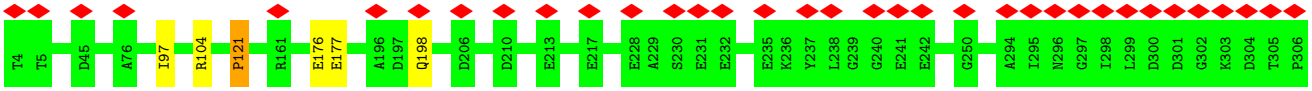
Chain Z:

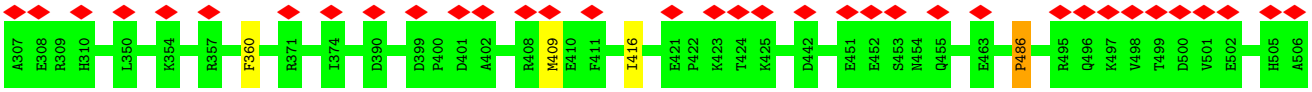


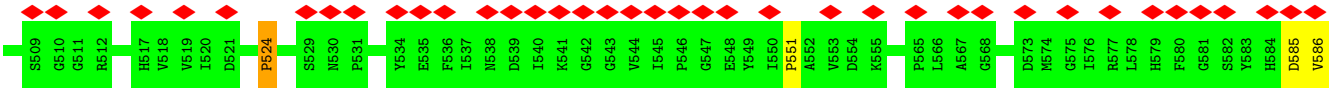
• Molecule 56: Elongation factor G

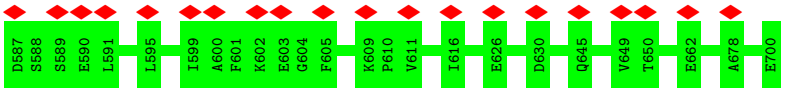
Chain 8:





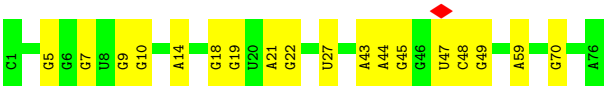






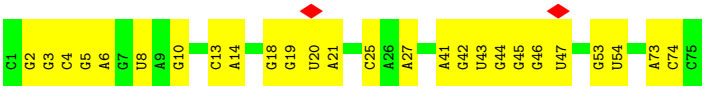
• Molecule 57: tRNA fMet

Chain 6:



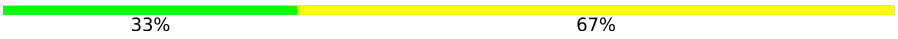
• Molecule 58: tRNA Pro

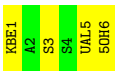
Chain 5:



• Molecule 59: Viomycin

Chain h:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	20167	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	30.5	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	20.132	Depositor
Minimum map value	-8.010	Depositor
Average map value	0.009	Depositor
Map value standard deviation	1.134	Depositor
Recommended contour level	2.65	Depositor
Map size (Å)	389.76, 389.76, 389.76	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.87, 0.87, 0.87	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: DPP, GDP, UAL, KBE, PO4, 5OH

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	0.38	5/69796 (0.0%)	0.66	7/108888 (0.0%)
2	2	0.37	0/2872	0.66	0/4479
3	b	0.33	0/2122	0.67	1/2852 (0.0%)
4	c	0.32	0/1586	0.62	0/2134
5	d	0.31	0/1571	0.58	1/2113 (0.0%)
6	e	0.35	0/1435	0.64	0/1926
7	f	0.31	0/1343	0.61	0/1816
8	g	0.35	0/1122	0.64	0/1515
9	a	0.33	0/1034	0.69	0/1387
10	i	0.38	0/1046	0.74	1/1410 (0.1%)
11	j	0.31	0/1152	0.57	0/1551
12	k	0.36	0/948	0.71	1/1268 (0.1%)
13	l	0.31	0/1054	0.67	0/1403
14	m	0.34	0/1093	0.61	0/1460
15	n	0.31	0/974	0.61	0/1301
16	o	0.29	0/902	0.61	0/1209
17	p	0.33	0/929	0.62	0/1242
18	q	0.31	0/960	0.50	0/1278
19	r	0.34	0/829	0.69	1/1107 (0.1%)
20	s	0.29	0/864	0.57	0/1156
21	t	0.33	0/745	0.57	0/994
22	u	0.33	0/788	0.66	1/1051 (0.1%)
23	v	0.31	0/766	0.57	0/1025
24	w	0.30	0/582	0.54	0/769
25	x	0.31	0/635	0.60	0/848
26	y	0.28	0/510	0.54	0/677
27	z	0.35	0/453	0.73	2/605 (0.3%)
28	A	0.34	0/532	0.63	1/709 (0.1%)
29	B	0.35	0/450	0.66	0/599
30	C	0.29	0/417	0.55	0/554
31	D	0.32	0/380	0.64	0/498
32	E	0.32	0/513	0.63	0/676

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
33	F	0.30	0/303	0.59	0/397
34	H	0.31	0/1652	0.58	0/2225
35	L	0.34	0/1196	0.61	0/1602
36	N	0.36	0/1034	0.73	1/1375 (0.1%)
37	O	0.31	0/797	0.64	0/1077
38	R	0.29	0/893	0.60	0/1193
39	S	0.29	0/817	0.61	0/1088
40	X	0.32	0/653	0.63	0/877
41	3	0.40	0/36963	0.66	2/57662 (0.0%)
42	4	0.54	0/465	0.62	0/725
43	G	0.35	0/1736	0.67	2/2338 (0.1%)
44	I	0.32	0/1665	0.67	0/2227
45	J	0.33	0/1170	0.68	0/1573
46	K	0.37	0/836	0.74	0/1128
47	M	0.31	0/989	0.58	0/1326
48	P	0.32	0/886	0.67	0/1195
49	Q	0.36	0/969	0.77	1/1300 (0.1%)
50	T	0.28	0/722	0.56	0/964
51	U	0.31	0/659	0.64	0/884
52	V	0.33	0/658	0.60	0/881
53	W	0.31	0/545	0.65	1/731 (0.1%)
54	Y	0.28	0/671	0.52	0/888
55	Z	0.42	0/551	0.89	2/728 (0.3%)
56	8	0.34	0/5502	0.67	3/7446 (0.0%)
57	6	0.36	0/1832	0.66	0/2855
58	5	0.43	0/1815	0.76	1/2829 (0.0%)
59	h	2.45	1/11 (9.1%)	0.82	0/13
All	All	0.37	6/166393 (0.0%)	0.66	29/248027 (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
1	1	0	3
46	K	0	1
All	All	0	4

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1082	U	O3'-P	8.82	1.71	1.61
1	1	1104	C	O3'-P	7.67	1.70	1.61
1	1	1104	C	C3'-O3'	6.99	1.51	1.42
1	1	1082	U	N1-C2	-6.58	1.32	1.38
1	1	1086	A	C5-C6	-6.17	1.35	1.41

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	1	1082	U	OP2-P-O3'	11.81	131.18	105.20
1	1	1082	U	C2'-C3'-O3'	11.21	134.17	109.50
1	1	1083	U	O5'-P-OP2	-10.09	96.62	105.70
1	1	1082	U	C5'-C4'-C3'	-7.92	103.33	116.00
58	5	43	U	OP2-P-O3'	7.47	121.62	105.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	202	U	Sidechain
1	1	25	U	Sidechain
1	1	511	U	Sidechain
46	K	53	LYS	Peptide

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
3	b	269/271 (99%)	231 (86%)	33 (12%)	5 (2%)	8 39

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	c	207/209 (99%)	181 (87%)	25 (12%)	1 (0%)	29	67
5	d	199/201 (99%)	188 (94%)	10 (5%)	1 (0%)	29	67
6	e	175/177 (99%)	155 (89%)	18 (10%)	2 (1%)	14	51
7	f	174/176 (99%)	152 (87%)	19 (11%)	3 (2%)	9	42
8	g	147/149 (99%)	133 (90%)	13 (9%)	1 (1%)	22	61
9	a	130/223 (58%)	112 (86%)	18 (14%)	0	100	100
10	i	139/141 (99%)	117 (84%)	20 (14%)	2 (1%)	11	46
11	j	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	22	61
12	k	120/122 (98%)	99 (82%)	19 (16%)	2 (2%)	9	42
13	l	141/143 (99%)	121 (86%)	20 (14%)	0	100	100
14	m	134/136 (98%)	126 (94%)	8 (6%)	0	100	100
15	n	118/120 (98%)	101 (86%)	17 (14%)	0	100	100
16	o	114/116 (98%)	103 (90%)	10 (9%)	1 (1%)	17	56
17	p	112/114 (98%)	102 (91%)	10 (9%)	0	100	100
18	q	115/117 (98%)	110 (96%)	4 (4%)	1 (1%)	17	56
19	r	101/103 (98%)	85 (84%)	15 (15%)	1 (1%)	15	54
20	s	108/110 (98%)	99 (92%)	9 (8%)	0	100	100
21	t	91/93 (98%)	78 (86%)	13 (14%)	0	100	100
22	u	100/102 (98%)	81 (81%)	18 (18%)	1 (1%)	15	54
23	v	92/94 (98%)	86 (94%)	6 (6%)	0	100	100
24	w	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
25	x	75/77 (97%)	72 (96%)	3 (4%)	0	100	100
26	y	61/63 (97%)	57 (93%)	3 (5%)	1 (2%)	9	43
27	z	56/58 (97%)	51 (91%)	4 (7%)	1 (2%)	8	41
28	A	64/66 (97%)	57 (89%)	7 (11%)	0	100	100
29	B	54/56 (96%)	48 (89%)	5 (9%)	1 (2%)	8	39
30	C	48/50 (96%)	46 (96%)	2 (4%)	0	100	100
31	D	44/46 (96%)	41 (93%)	3 (7%)	0	100	100
32	E	62/64 (97%)	56 (90%)	5 (8%)	1 (2%)	9	43
33	F	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
34	H	204/206 (99%)	184 (90%)	19 (9%)	1 (0%)	29	67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
35	L	149/151 (99%)	129 (87%)	18 (12%)	2 (1%)	12 47
36	N	125/127 (98%)	94 (75%)	26 (21%)	5 (4%)	3 21
37	O	96/98 (98%)	78 (81%)	17 (18%)	1 (1%)	15 54
38	R	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	17 56
39	S	98/100 (98%)	80 (82%)	15 (15%)	3 (3%)	4 26
40	X	77/79 (98%)	69 (90%)	8 (10%)	0	100 100
43	G	216/218 (99%)	187 (87%)	28 (13%)	1 (0%)	29 67
44	I	203/205 (99%)	177 (87%)	24 (12%)	2 (1%)	15 54
45	J	155/157 (99%)	131 (84%)	20 (13%)	4 (3%)	5 31
46	K	98/100 (98%)	82 (84%)	13 (13%)	3 (3%)	4 26
47	M	127/129 (98%)	119 (94%)	8 (6%)	0	100 100
48	P	114/116 (98%)	90 (79%)	22 (19%)	2 (2%)	8 41
49	Q	121/123 (98%)	98 (81%)	17 (14%)	6 (5%)	2 16
50	T	86/88 (98%)	77 (90%)	8 (9%)	1 (1%)	13 49
51	U	80/82 (98%)	69 (86%)	10 (12%)	1 (1%)	12 47
52	V	78/80 (98%)	67 (86%)	10 (13%)	1 (1%)	12 47
53	W	63/65 (97%)	57 (90%)	6 (10%)	0	100 100
54	Y	83/85 (98%)	80 (96%)	3 (4%)	0	100 100
55	Z	63/65 (97%)	43 (68%)	15 (24%)	5 (8%)	1 6
56	8	695/697 (100%)	622 (90%)	65 (9%)	8 (1%)	13 49
59	h	2/6 (33%)	1 (50%)	1 (50%)	0	100 100
All	All	6544/6743 (97%)	5750 (88%)	721 (11%)	73 (1%)	18 51

5 of 73 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	d	83	VAL
6	e	175	PRO
7	f	45	ALA
8	g	136	SER
12	k	92	GLU

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
3	b	216/216 (100%)	213 (99%)	3 (1%)	67 86
4	c	164/164 (100%)	163 (99%)	1 (1%)	86 94
5	d	165/165 (100%)	165 (100%)	0	100 100
6	e	148/148 (100%)	146 (99%)	2 (1%)	67 86
7	f	137/137 (100%)	137 (100%)	0	100 100
8	g	114/114 (100%)	114 (100%)	0	100 100
9	a	110/174 (63%)	110 (100%)	0	100 100
10	i	109/109 (100%)	105 (96%)	4 (4%)	34 68
11	j	116/116 (100%)	115 (99%)	1 (1%)	78 91
12	k	103/103 (100%)	102 (99%)	1 (1%)	76 90
13	l	102/102 (100%)	102 (100%)	0	100 100
14	m	109/109 (100%)	108 (99%)	1 (1%)	78 91
15	n	100/100 (100%)	98 (98%)	2 (2%)	55 80
16	o	86/86 (100%)	86 (100%)	0	100 100
17	p	99/99 (100%)	99 (100%)	0	100 100
18	q	89/89 (100%)	89 (100%)	0	100 100
19	r	84/84 (100%)	84 (100%)	0	100 100
20	s	93/93 (100%)	93 (100%)	0	100 100
21	t	80/80 (100%)	80 (100%)	0	100 100
22	u	83/83 (100%)	83 (100%)	0	100 100
23	v	78/78 (100%)	78 (100%)	0	100 100
24	w	57/57 (100%)	57 (100%)	0	100 100
25	x	67/67 (100%)	67 (100%)	0	100 100
26	y	55/55 (100%)	55 (100%)	0	100 100
27	z	48/48 (100%)	48 (100%)	0	100 100
28	A	59/59 (100%)	58 (98%)	1 (2%)	60 83

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
29	B	47/47 (100%)	45 (96%)	2 (4%)	29 64
30	C	45/45 (100%)	45 (100%)	0	100 100
31	D	38/38 (100%)	37 (97%)	1 (3%)	46 76
32	E	51/51 (100%)	51 (100%)	0	100 100
33	F	34/34 (100%)	34 (100%)	0	100 100
34	H	170/170 (100%)	167 (98%)	3 (2%)	59 82
35	L	124/124 (100%)	123 (99%)	1 (1%)	81 93
36	N	105/105 (100%)	103 (98%)	2 (2%)	57 81
37	O	86/86 (100%)	86 (100%)	0	100 100
38	R	92/92 (100%)	91 (99%)	1 (1%)	73 88
39	S	83/83 (100%)	82 (99%)	1 (1%)	71 88
40	X	70/70 (100%)	69 (99%)	1 (1%)	67 86
43	G	180/180 (100%)	178 (99%)	2 (1%)	73 88
44	I	172/172 (100%)	170 (99%)	2 (1%)	71 88
45	J	119/119 (100%)	119 (100%)	0	100 100
46	K	87/87 (100%)	86 (99%)	1 (1%)	73 88
47	M	104/104 (100%)	103 (99%)	1 (1%)	76 90
48	P	89/89 (100%)	89 (100%)	0	100 100
49	Q	103/103 (100%)	103 (100%)	0	100 100
50	T	76/76 (100%)	76 (100%)	0	100 100
51	U	65/65 (100%)	65 (100%)	0	100 100
52	V	74/74 (100%)	72 (97%)	2 (3%)	44 75
53	W	56/56 (100%)	55 (98%)	1 (2%)	59 82
54	Y	65/65 (100%)	64 (98%)	1 (2%)	65 85
55	Z	55/55 (100%)	52 (94%)	3 (6%)	21 57
56	8	574/574 (100%)	568 (99%)	6 (1%)	76 90
59	h	2/2 (100%)	2 (100%)	0	100 100
All	All	5437/5501 (99%)	5390 (99%)	47 (1%)	79 91

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
43	G	47	PRO

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Mol	Chain	Res	Type
52	V	40	THR
43	G	160	LEU
46	K	92	THR
54	Y	4	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 74 such sidechains are listed below:

Mol	Chain	Res	Type
46	K	94	HIS
56	8	85	ASN
48	P	37	GLN
53	W	51	GLN
13	l	99	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2902/2903 (99%)	413 (14%)	11 (0%)
2	2	119/120 (99%)	12 (10%)	1 (0%)
41	3	1538/1539 (99%)	175 (11%)	3 (0%)
42	4	18/19 (94%)	5 (27%)	0
57	6	76/77 (98%)	18 (23%)	0
58	5	75/76 (98%)	22 (29%)	4 (5%)
All	All	4728/4734 (99%)	645 (13%)	19 (0%)

5 of 645 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	10	A
1	1	12	U
1	1	35	G
1	1	42	A
1	1	46	G

5 of 19 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	3	1012	A
58	5	41	A
58	5	45	G

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Mol	Chain	Res	Type
58	5	3	G
1	1	2326	C

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

4 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	$\#\|Z\| > 2$
59	5OH	h	6	59	8,12,13	0.78	0	3,16,18	1.51	1 (33%)
59	DPP	h	2	59	3,5,6	0.55	0	1,5,7	0.08	0
59	UAL	h	5	59	7,8,9	2.30	3 (42%)	5,9,11	2.92	2 (40%)
59	KBE	h	1	59	8,8,9	0.60	0	7,8,10	1.20	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	5OH	h	6	59	-	0/2/18/20	0/1/1/1
59	DPP	h	2	59	-	0/2/4/6	-
59	UAL	h	5	59	-	0/3/7/9	-
59	KBE	h	1	59	-	0/7/7/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	h	5	UAL	C1-N1	-4.87	1.32	1.40
59	h	5	UAL	C-CA	-2.91	1.40	1.45
59	h	5	UAL	CA-N	2.00	1.40	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
59	h	5	UAL	CA-CB-N1	-5.31	115.59	125.60
59	h	5	UAL	O-C-CA	-3.22	121.29	125.39
59	h	6	5OH	CR-CB-CA	-2.37	110.06	112.61
59	h	1	KBE	CB-CA-C	-2.07	109.21	112.25

There are no chirality outliers.

There are no torsion outliers.

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)

2 ligands 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	$\#\|Z\| > 2$
61	PO4	8	802	-	4,4,4	1.11	0	6,6,6	0.68	0
60	GDP	8	801	-	24,30,30	0.93	1 (4%)	30,47,47	1.44	5 (16%)

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
60	GDP	8	801	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	8	801	GDP	C6-N1	-2.40	1.34	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	8	801	GDP	PA-O3A-PB	-4.36	117.86	132.83
60	8	801	GDP	C3'-C2'-C1'	2.57	104.84	100.98
60	8	801	GDP	C5-C6-N1	2.30	118.02	113.95
60	8	801	GDP	C8-N7-C5	2.22	107.22	102.99
60	8	801	GDP	O6-C6-C5	-2.07	120.33	124.37

There are no chirality outliers.

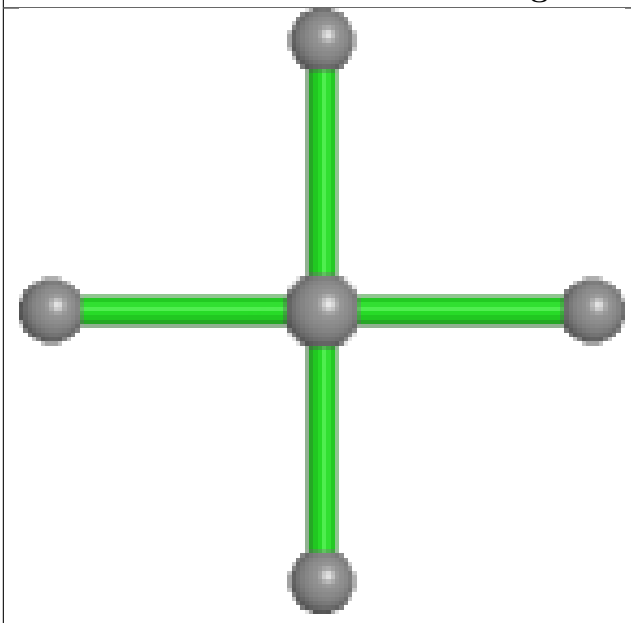
There are no torsion outliers.

There are no ring outliers.

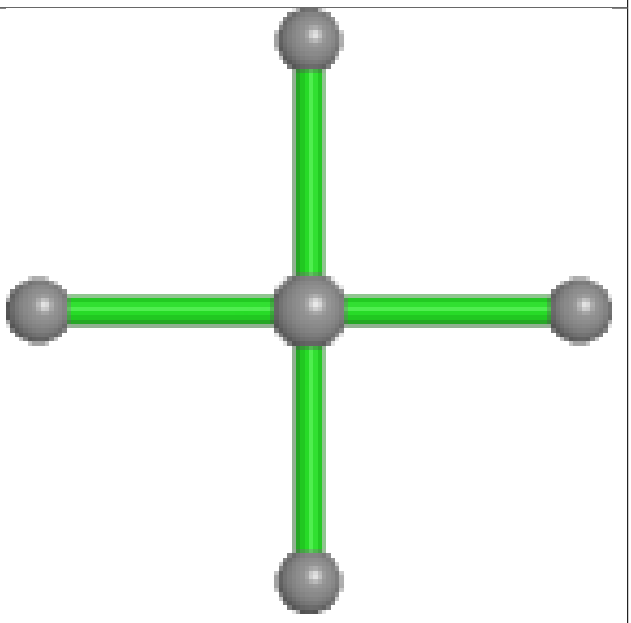
No monomer is involved in short contacts.

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.

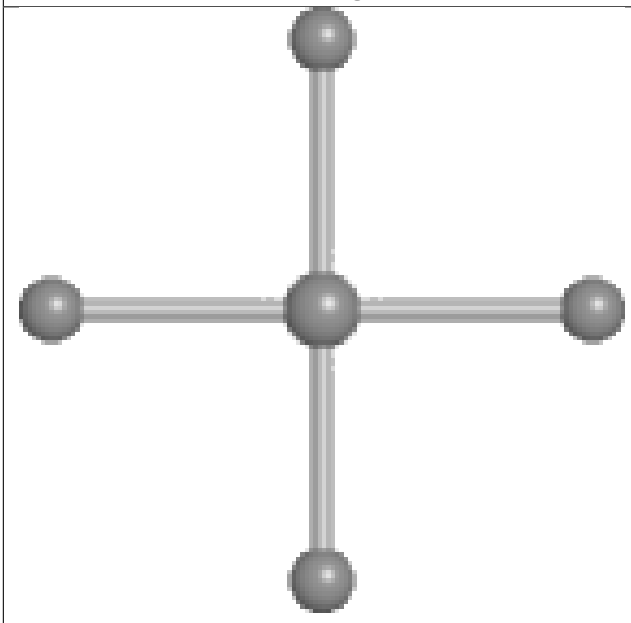
Ligand PO4 8 802



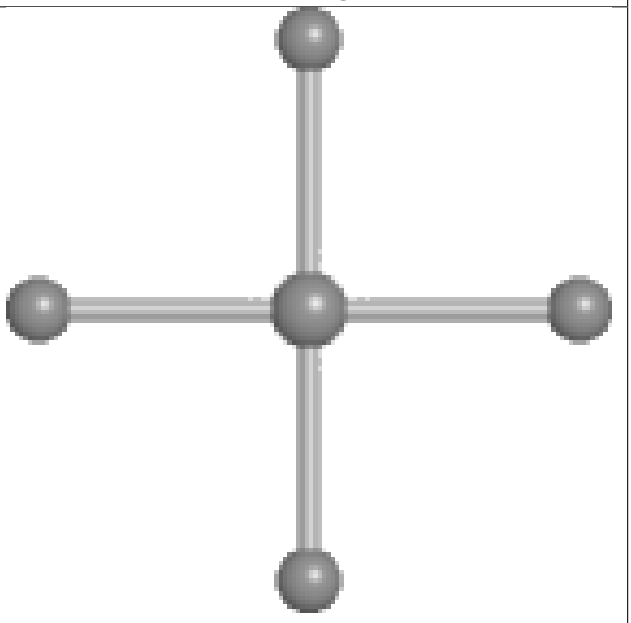
Bond lengths



Bond angles

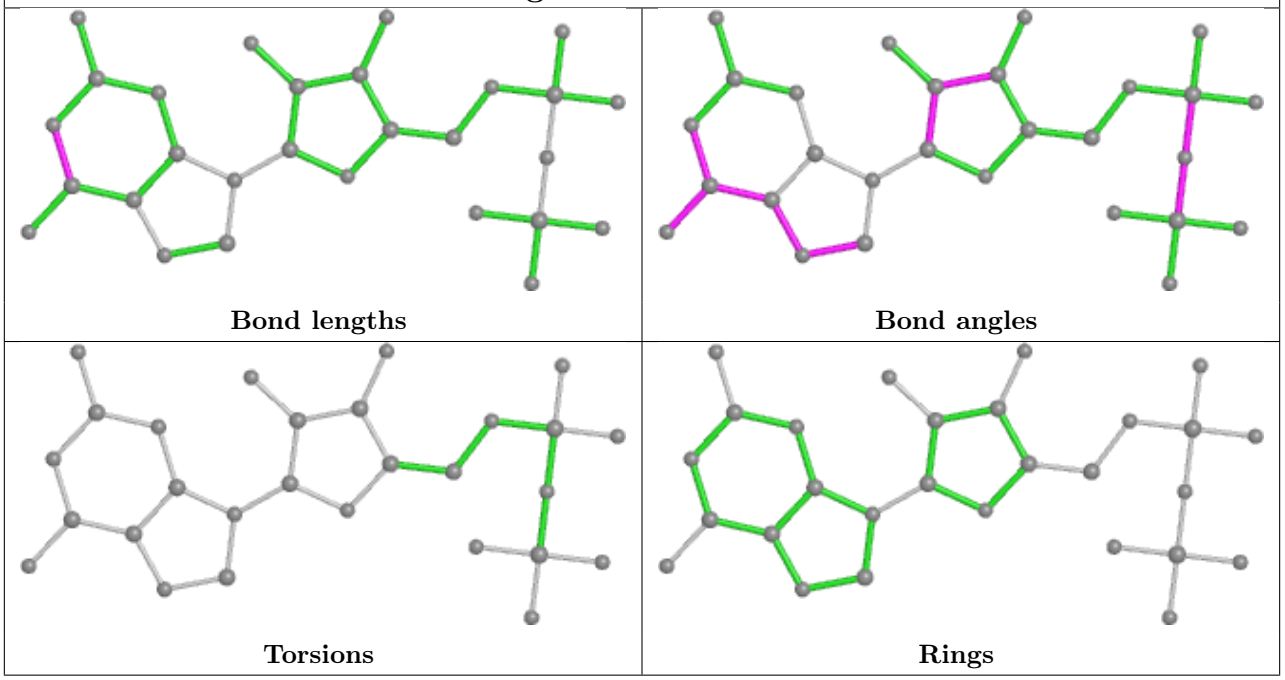


Torsions



Rings

Ligand GDP 8 801



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.

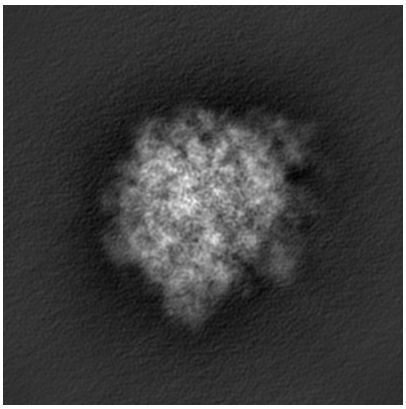
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-25421. These allow visual inspection of the internal detail of the map and identification of artifacts.

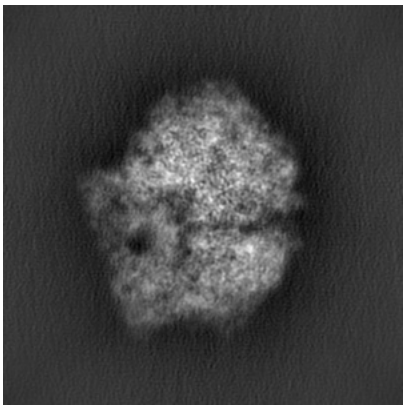
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

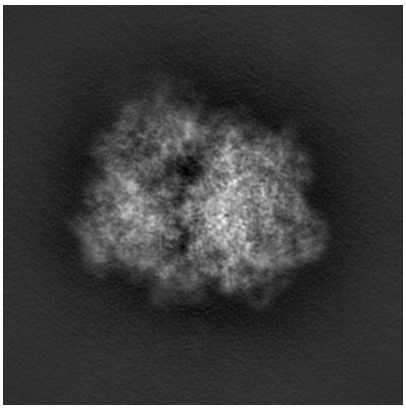
6.1.1 Primary map



X

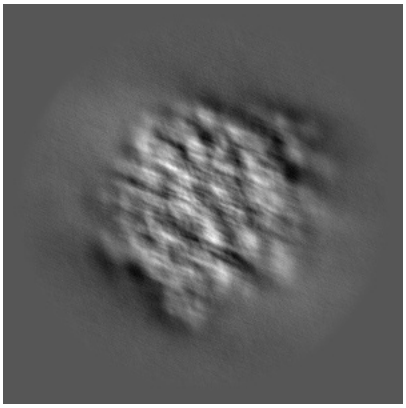


Y

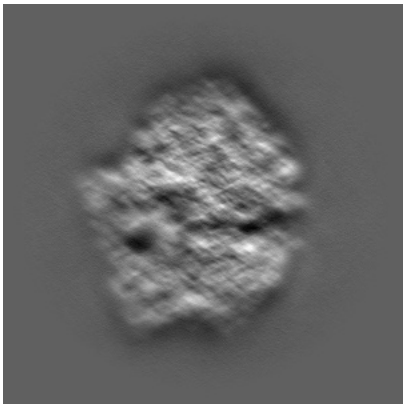


Z

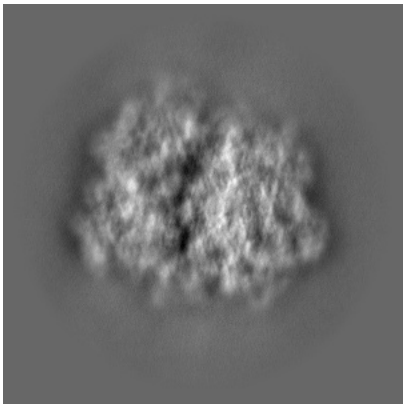
6.1.2 Raw map



X



Y

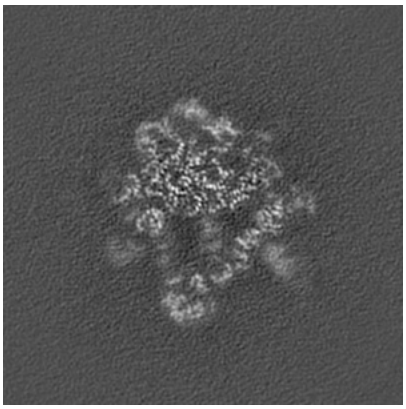


Z

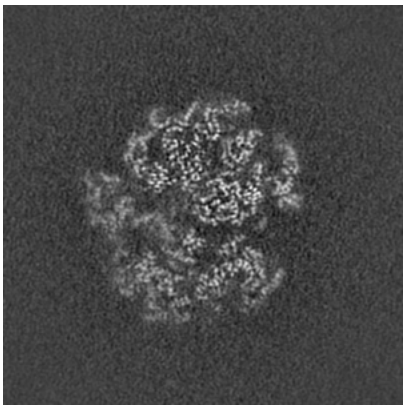
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

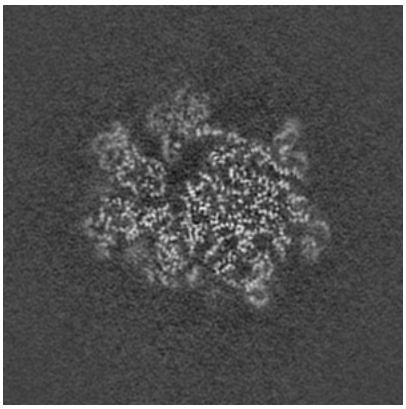
6.2.1 Primary map



X Index: 224

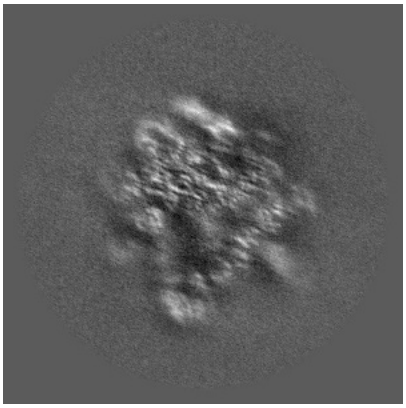


Y Index: 224

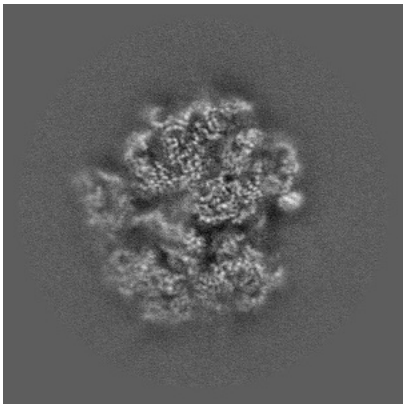


Z Index: 224

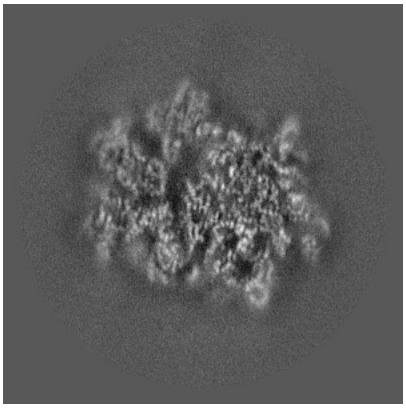
6.2.2 Raw map



X Index: 224



Y Index: 224

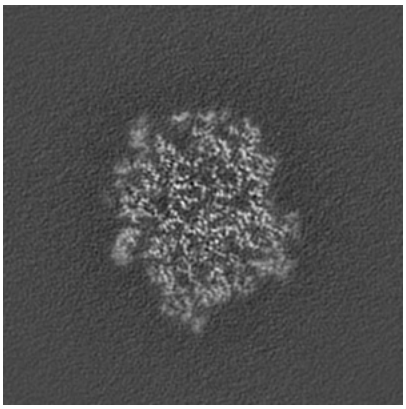


Z Index: 224

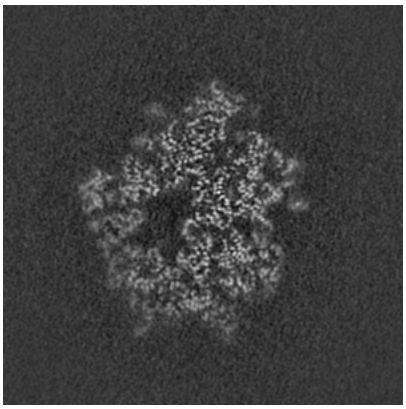
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

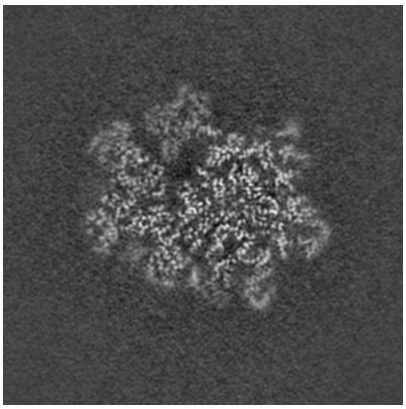
6.3.1 Primary map



X Index: 251

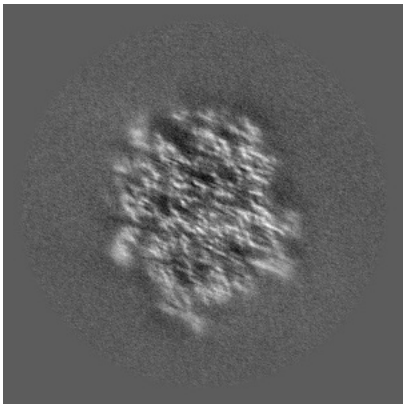


Y Index: 209

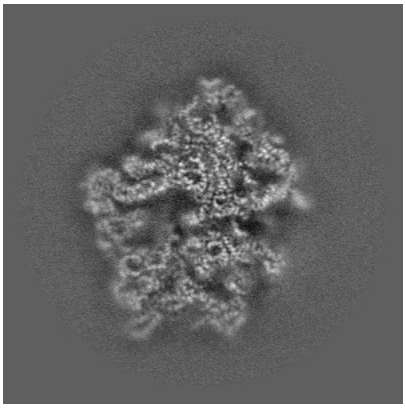


Z Index: 227

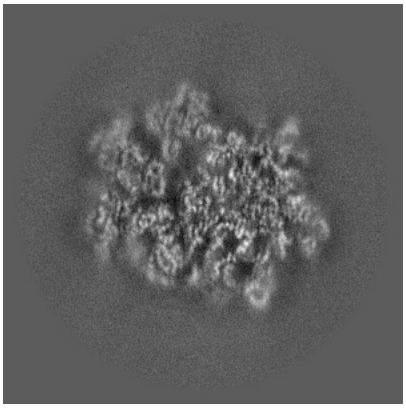
6.3.2 Raw map



X Index: 251



Y Index: 200



Z Index: 226

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 2.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map

X Y Z

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

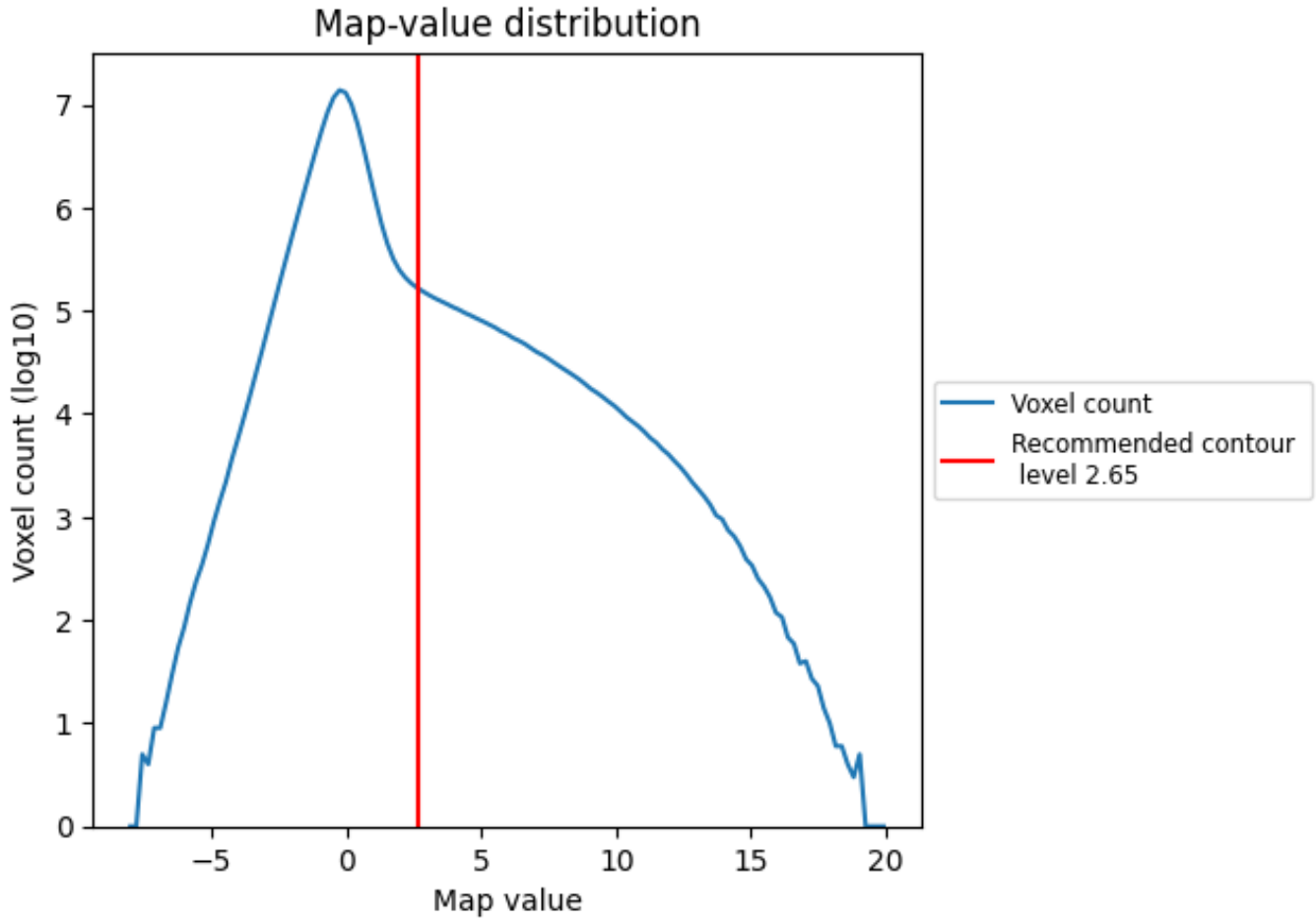
6.5 Mask visualisation (i)

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

7 Map analysis

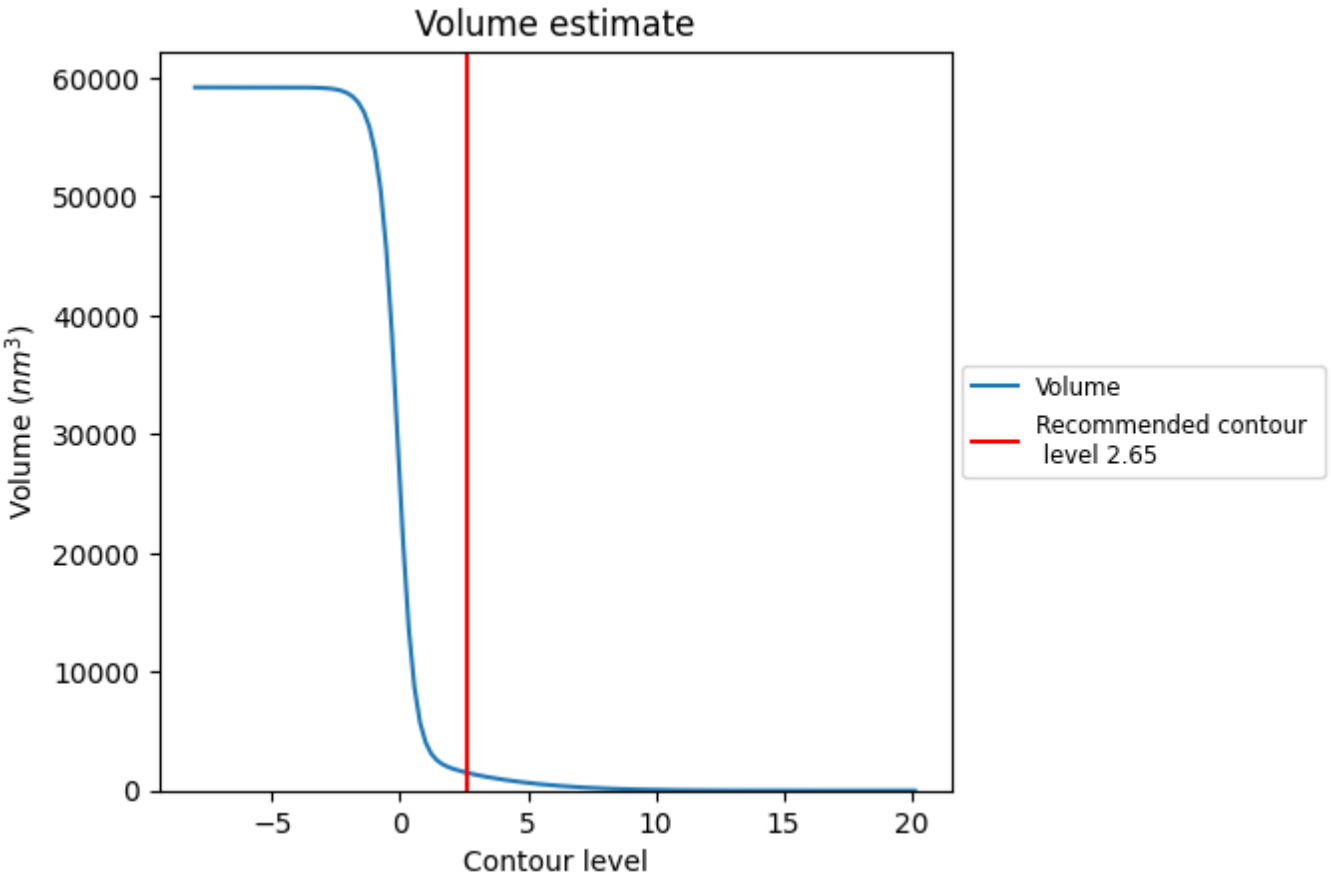
This section contains the results of statistical analysis of the map.

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.

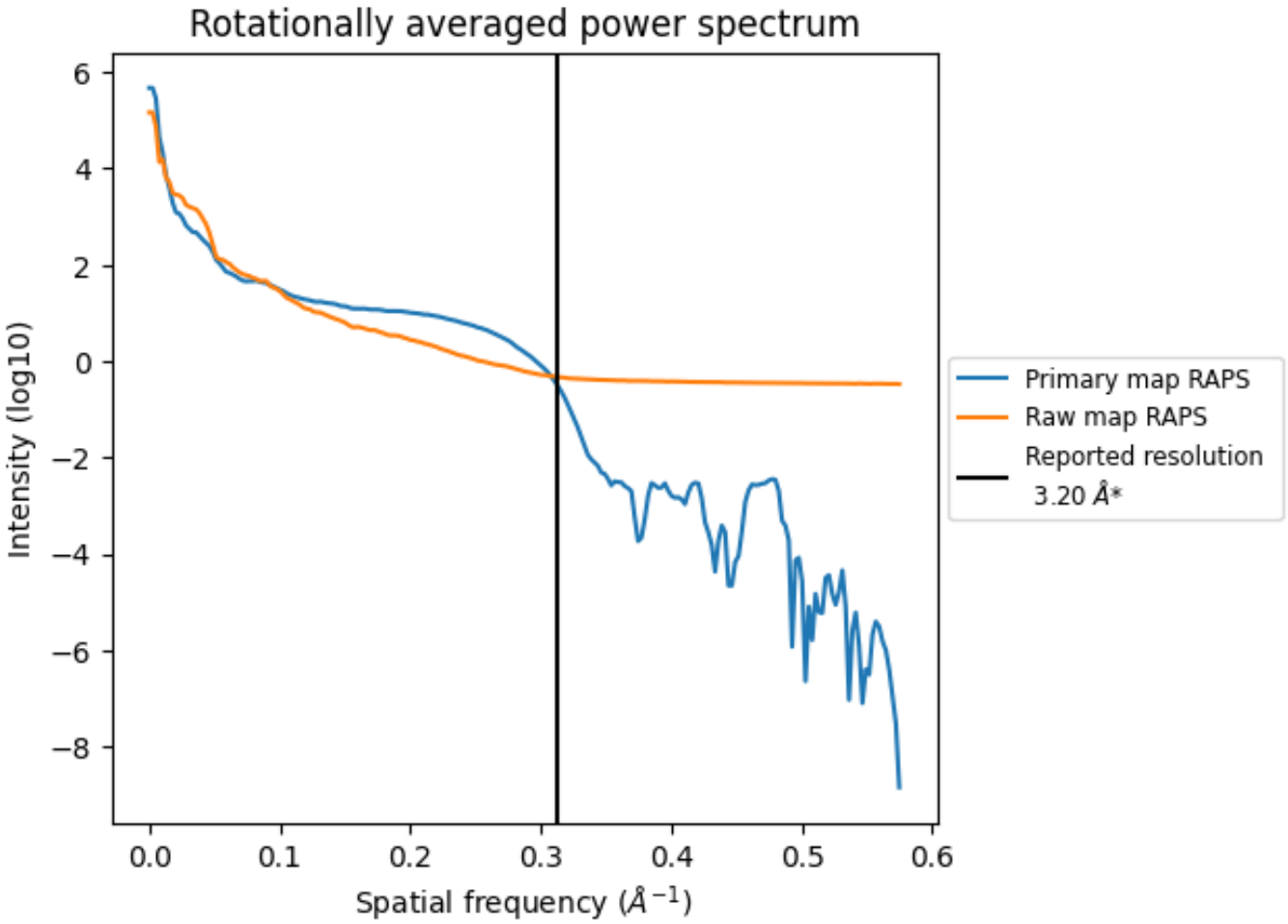
7.2 Volume estimate (i)



The volume at the recommended contour level is 1485 nm^3; this corresponds to an approximate mass of 1341 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)

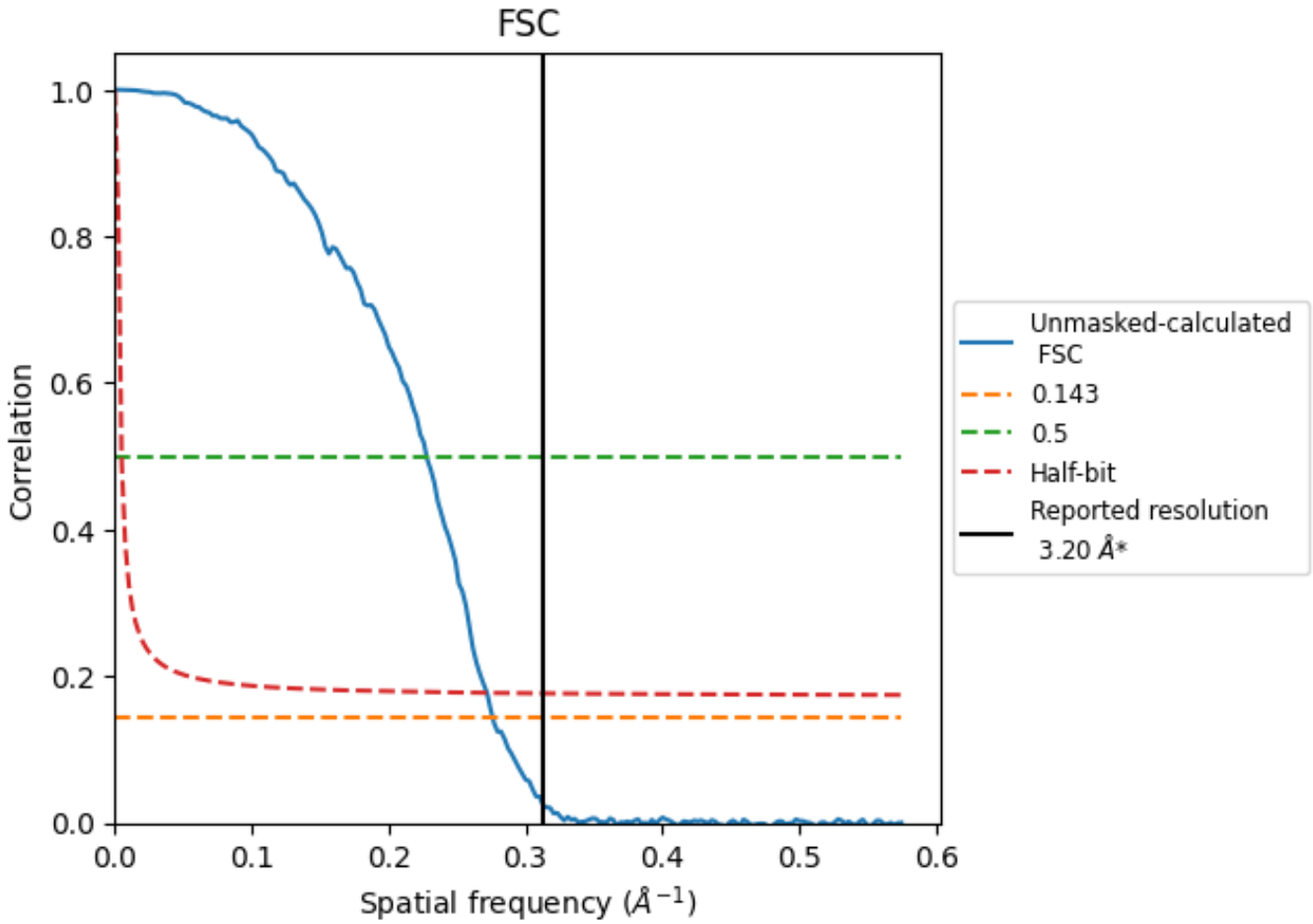


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

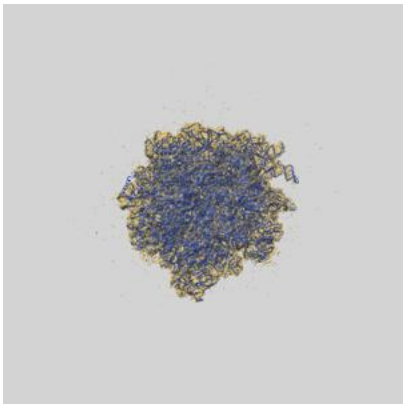
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.62	4.39	3.68

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.62 differs from the reported value 3.2 by more than 10 %

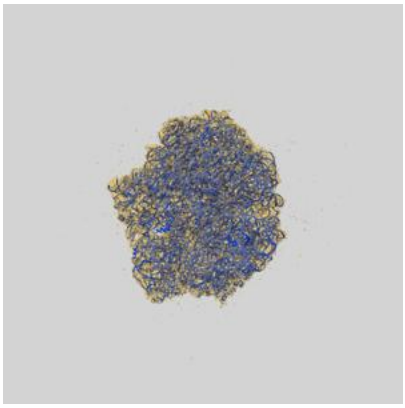
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-25421 and PDB model 7ST7. Per-residue inclusion information can be found in section 3 on page 16.

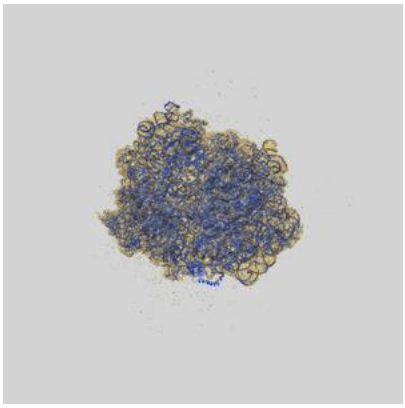
9.1 Map-model overlay



X



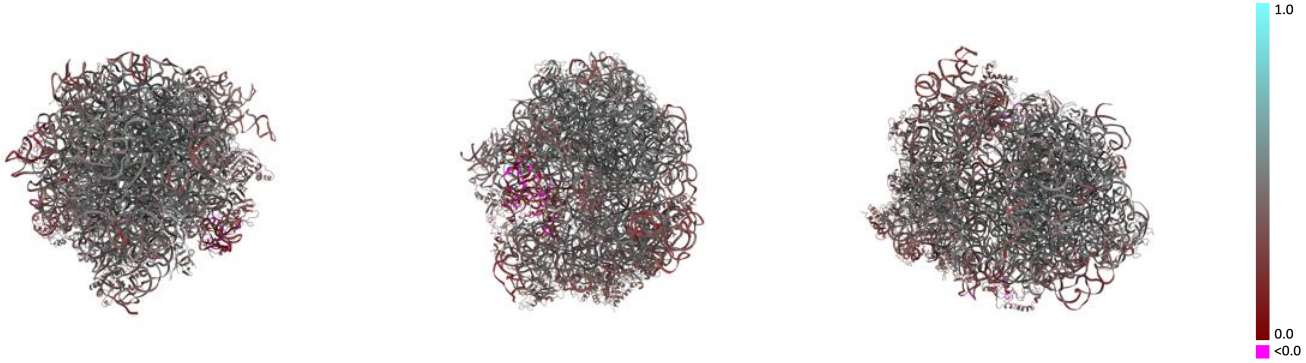
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.65 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.

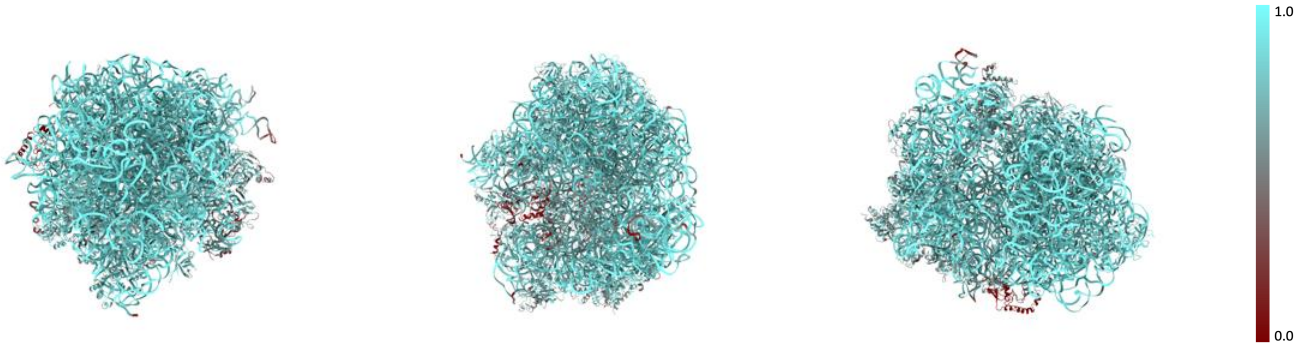
9.2 Q-score mapped to coordinate model (i)



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.

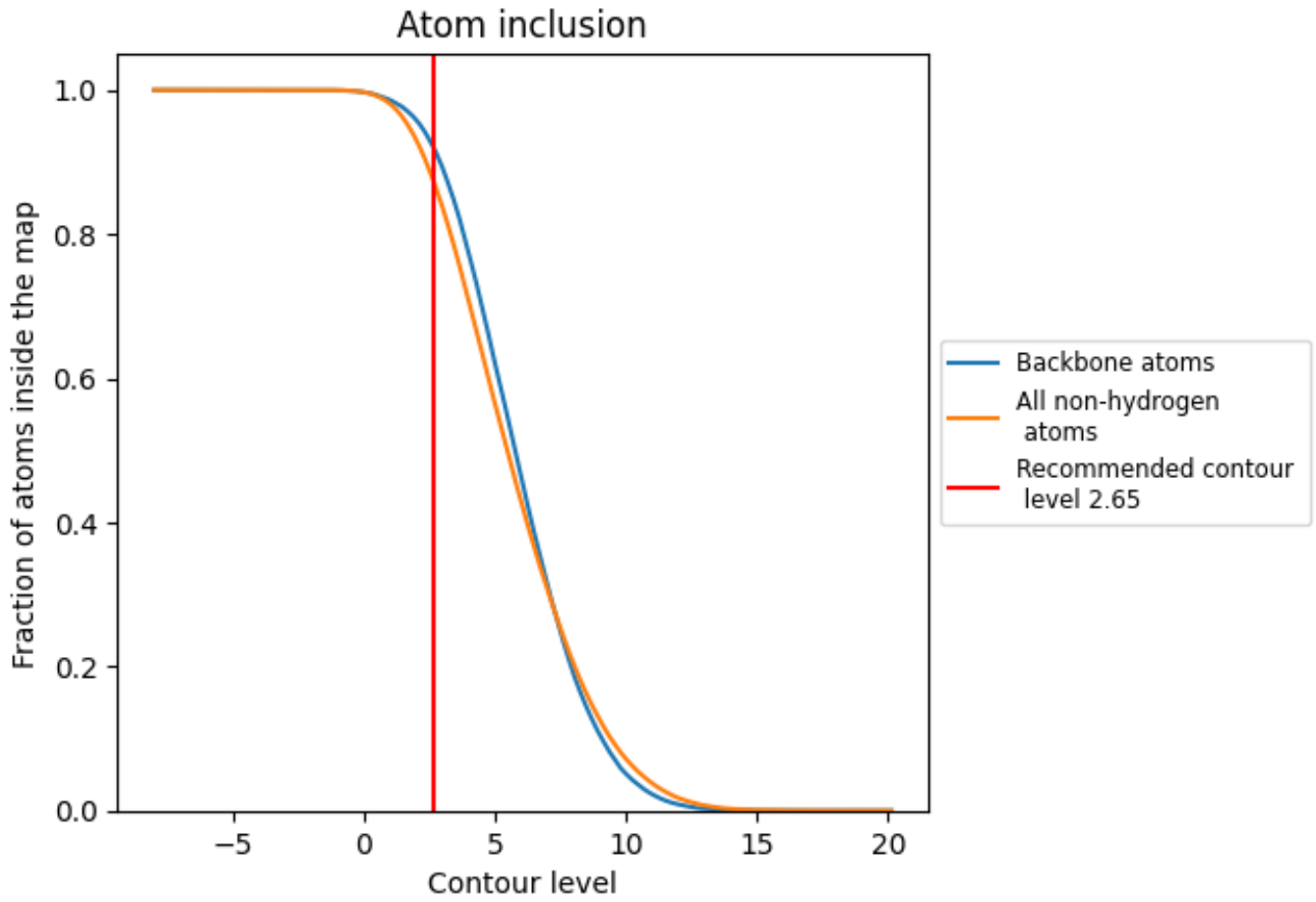
9.3 Atom inclusion mapped to coordinate model (i)



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 (2.65).

9.4 Atom inclusion (i)



At the recommended contour level, 92% of all backbone atoms, 87% 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 (2.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8737	0.4170
1	0.9467	0.4330
2	0.9502	0.3950
3	0.9318	0.4040
4	0.7119	0.3500
5	0.8203	0.2800
6	0.8866	0.3560
8	0.6142	0.3610
A	0.5488	0.2820
B	0.8505	0.4670
C	0.6020	0.4440
D	0.8901	0.4930
E	0.8839	0.4980
F	0.7877	0.4840
G	0.6360	0.3710
H	0.7460	0.4200
I	0.7597	0.3730
J	0.8167	0.4460
K	0.7792	0.3680
L	0.6795	0.3660
M	0.8167	0.4440
N	0.7569	0.3710
O	0.6785	0.3770
P	0.8381	0.4440
Q	0.8056	0.4730
R	0.7312	0.3740
S	0.7920	0.3860
T	0.8391	0.4310
U	0.7799	0.4250
V	0.8404	0.4260
W	0.8000	0.4220
X	0.7508	0.3750
Y	0.7769	0.3740
Z	0.6448	0.3370
a	0.4426	0.2350

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Chain	Atom inclusion	Q-score
b	0.8726	0.4980
c	0.8628	0.4830
d	0.8138	0.4510
e	0.7584	0.3800
f	0.7602	0.3920
g	0.1296	0.3110
h	0.8333	0.4660
i	0.2446	0.2020
j	0.8709	0.4710
k	0.8326	0.4900
l	0.8474	0.4590
m	0.8445	0.4790
n	0.8960	0.4760
o	0.8389	0.4110
p	0.8142	0.4730
q	0.8822	0.4760
r	0.8432	0.4640
s	0.8409	0.4770
t	0.8077	0.4470
u	0.8255	0.4340
v	0.8238	0.4420
w	0.8748	0.4880
x	0.8453	0.4780
y	0.8028	0.4010
z	0.8444	0.4650