wwPDB EM Validation Summary Report (i)

Jun 24, 2024 – 01:14 pm BST

PDB ID	:	8P2G
EMDB ID	:	EMD-17364
Title	:	Staphylococcus aureus 70S ribosome with elongation factor G locked with fusidic acid cyclopentane with a tRNA in pe/E chimeric state
Authors	:	Gonzalez-Lopez, A.; Selmer, M.
Deposited on	:	2023-05-16
Resolution	:	2.02 Å(reported)
Based on initial models	:	2XEX, 7SSD, 7NHM

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 (i) 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 (1)) were used in the production of this report:

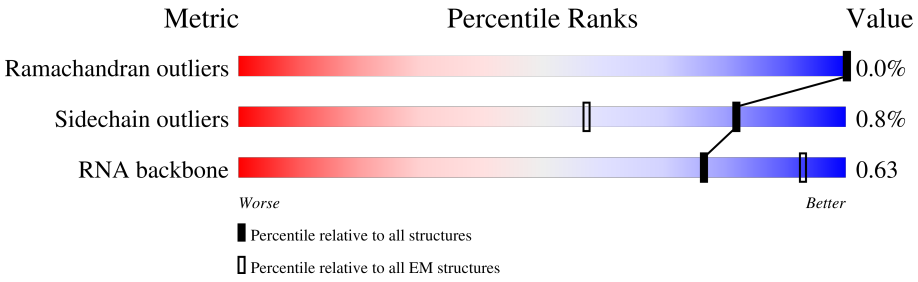
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.02 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	A	2923	86% 11%
2	B	115	86% 12%
3	D	77	86% 14%
4	E	693	17% 96%
5	G	277	99%
6	H	220	98%
7	I	207	98%
8	J	179	6% 98%

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Mol	Chain	Length	Quality of chain
9	K	178	98%
10	M	145	99%
11	N	122	100%
12	O	146	98%
13	P	144	92% 6%
14	Q	122	97%
15	R	119	100%
16	S	116	97%
17	T	118	97%
18	U	102	98%
19	V	117	93% 5%
20	W	91	98%
21	X	105	6% 97%
22	Y	217	43% 57%
23	Z	94	84% 16%
24	1	62	98%
25	2	69	94% 6%
26	3	59	95% 5%
27	4	84	37% 92% 8%
28	5	57	93% 7%
29	6	49	96%
30	7	45	93%
31	8	66	95%
32	9	37	100%
33	a	1555	86% 13%

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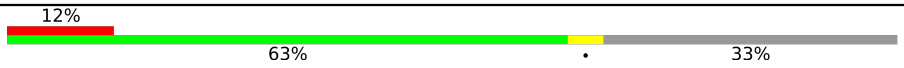
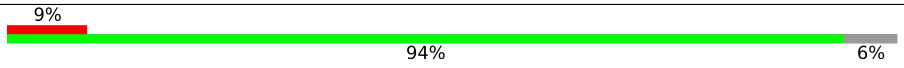
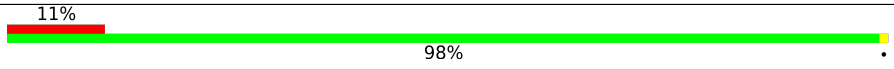
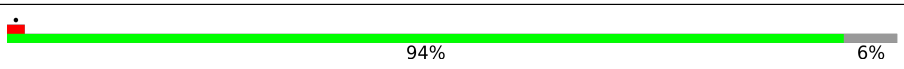
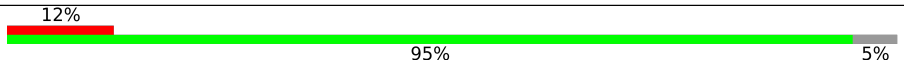
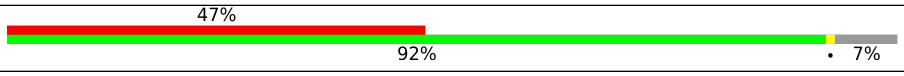
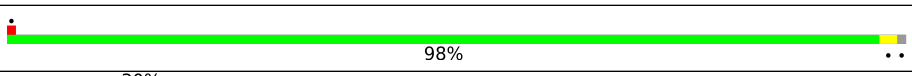
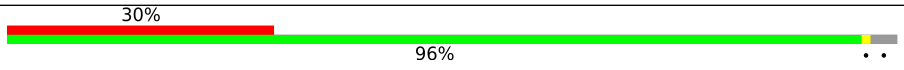
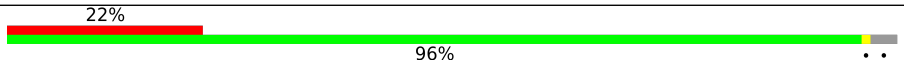
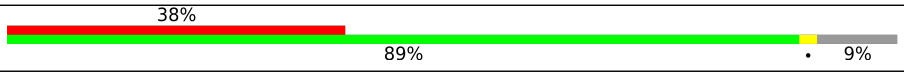
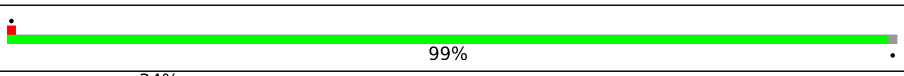
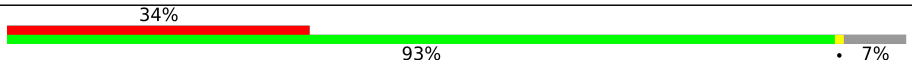
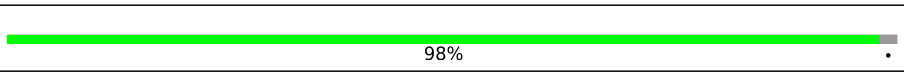
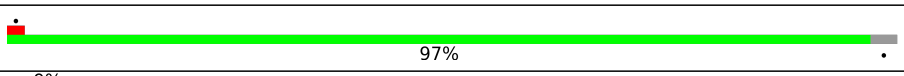
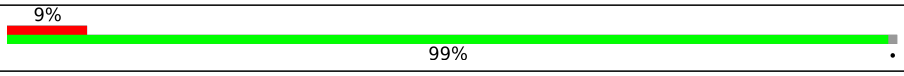
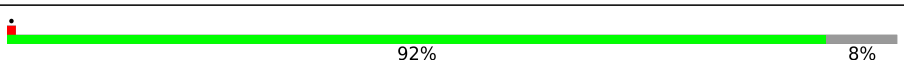
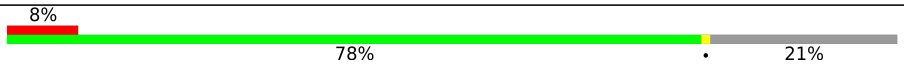
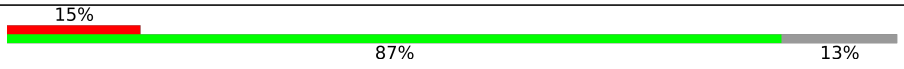
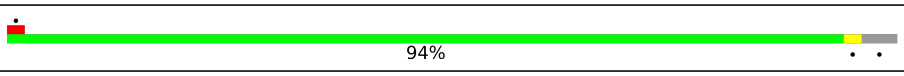
Mol	Chain	Length	Quality of chain
34	b	24	
35	c	255	
36	d	217	
37	e	200	
38	f	166	
39	g	98	
40	h	156	
41	i	132	
42	j	132	
43	k	102	
44	l	129	
45	m	137	
46	n	121	
47	o	61	
48	p	89	
49	q	91	
50	r	87	
51	s	80	
52	t	92	
53	u	83	

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 149701 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2844	61041	27258	11160	19776	2847	3	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	G	A	conflict	GB CP000253
A	1584	U	A	conflict	GB CP000253
A	2261	G	A	conflict	GB CP000253

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	113	2408	1076	431	788	113	0	0

- Molecule 3 is a RNA chain called tRNA.

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

- Molecule 4 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	669	5177	3248	868	1032	29	0	0

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	G	273	2085	1297	413	370	5	0	0

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	216	Total	C	N	O	S	0	0
			1637	1024	301	307	5		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	204	Total	C	N	O	S	0	0
			1564	981	286	295	2		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	176	Total	C	N	O	S	0	0
			1392	885	238	262	7		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	176	Total	C	N	O	S	0	0
			1372	852	251	266	3		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	144	Total	C	N	O	S	0	0
			1146	715	210	218	3		

- Molecule 11 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	N	122	Total	C	N	O	S	0	0
			920	572	174	170	4		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	O	145	Total	C	N	O	S	0	0
			1090	674	214	201	1		

- Molecule 13 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	P	136	Total	C	N	O	S	0	0
			1089	698	206	181	4		

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	R	119	Total	C	N	O	S	0	0
			922	574	174	173	1		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	S	114	Total	C	N	O	0	0
			922	580	185	157		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 21 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	X	102	Total	C	N	O	S	0	0
			787	497	144	144	2		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	94	Total	C	N	O	S	0	0
			738	471	131	134	2		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	Z	79	Total	C	N	O	0	0
			604	372	117	115		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1	61	Total	C	N	O	S	0	0
			481	298	104	78	1		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	2	65	Total	C	N	O	S	0	0
			535	329	100	105	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	3	56	Total	C	N	O	0	0
			436	271	82	83		

- Molecule 27 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	4	77	Total	C	N	O	S	0	0
			631	400	108	120	3		

- Molecule 28 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	5	53	Total	C	N	O	S	0	0
			422	256	86	75	5		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
5	?	-	ARG	deletion	UNP Q2FZF1

- Molecule 29 is a protein called Large ribosomal subunit protein bL33A.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	6	48	Total	C	N	O	S	0	0
			402	245	79	73	5		

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	43	Total	C	N	O	S	0	0
			367	225	89	52	1		

- Molecule 31 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	8	64	Total	C	N	O	S	0	0
			521	324	113	82	2		

- Molecule 32 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	9	37	Total	C	N	O	S	0	0
			296	186	60	45	5		

- Molecule 33 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	1534	Total	C	N	O	P	0	0
			32869	14681	5998	10656	1534		

- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	16	Total	C	N	O	P	0	0
			354	158	74	106	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	221	Total	C	N	O	S	0	0
			1781	1136	310	328	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	204	Total	C	N	O	S	0	0
			1612	1015	302	293	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	199	Total	C	N	O	S	0	0
			1617	1020	302	293	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	f	156	Total	C	N	O	S	0	0
			1160	730	213	215	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	g	93	Total	C	N	O	S	0	0
			773	489	136	146	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	h	145	Total	C	N	O	S	0	0
			1155	721	219	211	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	i	131	Total	C	N	O	S	0	0
			1032	652	183	193	4		

- Molecule 42 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	j	128	Total	C	N	O	S	0	0
			1016	629	203	183	1		

- Molecule 43 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	k	99	Total	C	N	O	S	0	0
			792	499	145	147	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	l	118	Total	C	N	O	S	0	0
			876	542	166	165	3		

- Molecule 45 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	m	135	Total	C	N	O	S	0	0
			1058	658	214	184	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	n	113	Total	C	N	O	S	0	0
			902	554	179	168	1		

- Molecule 47 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	o	60	Total	C	N	O	S	0	0
			501	317	100	79	5		

- Molecule 48 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	p	86	Total	C	N	O	S	0	0
			721	445	148	127	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	r	80	Total	C	N	O	S	0	0
			662	419	120	122	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	s	63	Total	C	N	O	S	0	0
			516	330	96	87	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	t	80	Total	C	N	O	S	0	0
			651	419	117	113	2		

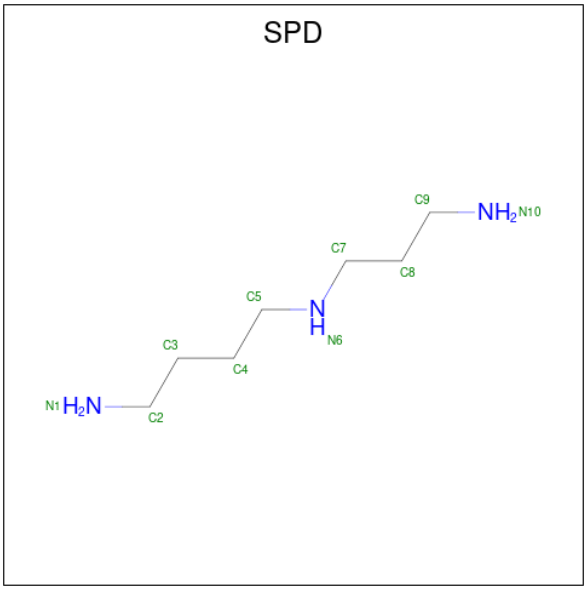
- Molecule 53 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

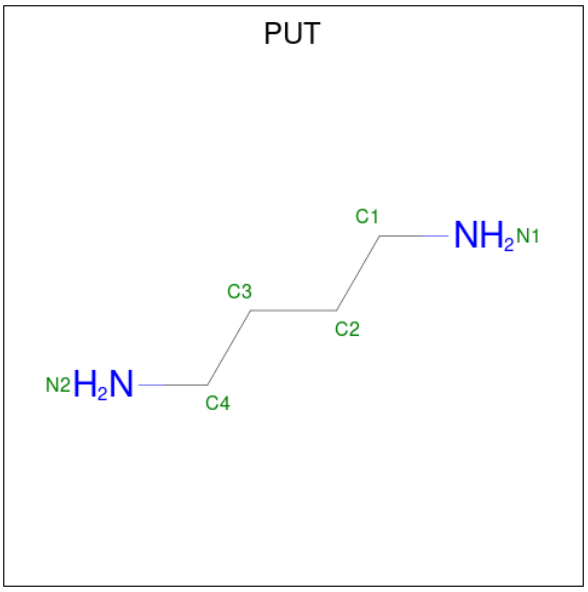
Mol	Chain	Residues	Atoms	AltConf
54	A	141	Total Mg 141 141	0
54	B	1	Total Mg 1 1	0
54	E	1	Total Mg 1 1	0
54	G	1	Total Mg 1 1	0
54	H	1	Total Mg 1 1	0
54	O	1	Total Mg 1 1	0
54	a	23	Total Mg 23 23	0

- Molecule 55 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).



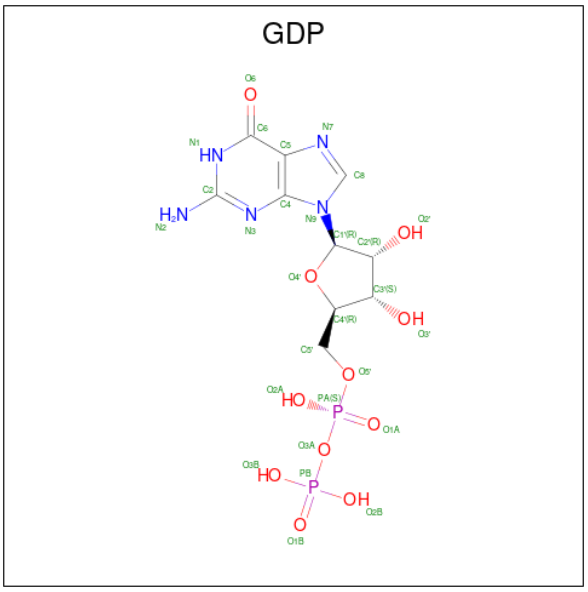
Mol	Chain	Residues	Atoms	AltConf
55	A	1	Total C N 10 7 3	0
55	A	1	Total C N 10 7 3	0
55	A	1	Total C N 10 7 3	0

- Molecule 56 is 1,4-DIAMINOBUTANE (three-letter code: PUT) (formula: $C_4H_{12}N_2$).



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

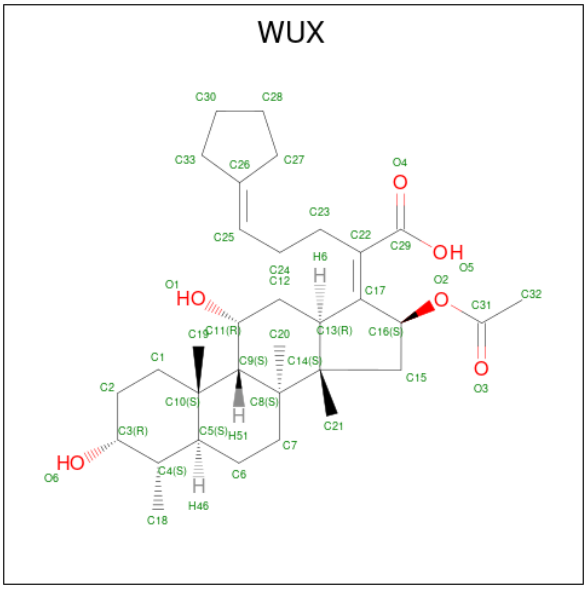
- Molecule 57 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 58 is 2-[(3 {R},4 {S},5 {S},8 {S},9 {S},10 {S},11 {R},13 {S},14 {S},16 {S})-16-acetyloxy-4,8,10,14-tetramethyl-3,11-bis(oxidanyl)-1,2,3,4,5,6,7,9,11,12,13,15,16,17-tetrad

ecahydrocyclopenta[a]phenanthren-17-yl]-5-cyclopentyl-pentanoic acid (three-letter code: WUX) (formula: $C_{33}H_{54}O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
58	E	1	Total C O 39 33 6	0

- Molecule 59 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
59	5	1	Total Zn 1 1	0
59	9	1	Total Zn 1 1	0
59	o	1	Total Zn 1 1	0

- Molecule 60 is water.

Mol	Chain	Residues	Atoms	AltConf
60	A	2684	Total O 2684 2684	0
60	B	7	Total O 7 7	0
60	D	1	Total O 1 1	0
60	E	8	Total O 8 8	0

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Mol	Chain	Residues	Atoms	AltConf
60	G	78	Total O 78 78	0
60	H	49	Total O 49 49	0
60	I	42	Total O 42 42	0
60	M	14	Total O 14 14	0
60	N	14	Total O 14 14	0
60	O	41	Total O 41 41	0
60	P	12	Total O 12 12	0
60	Q	13	Total O 13 13	0
60	S	12	Total O 12 12	0
60	T	30	Total O 30 30	0
60	U	16	Total O 16 16	0
60	V	26	Total O 26 26	0
60	W	7	Total O 7 7	0
60	X	1	Total O 1 1	0
60	Z	14	Total O 14 14	0
60	1	4	Total O 4 4	0
60	3	2	Total O 2 2	0
60	5	11	Total O 11 11	0
60	7	20	Total O 20 20	0
60	8	34	Total O 34 34	0
60	9	2	Total O 2 2	0

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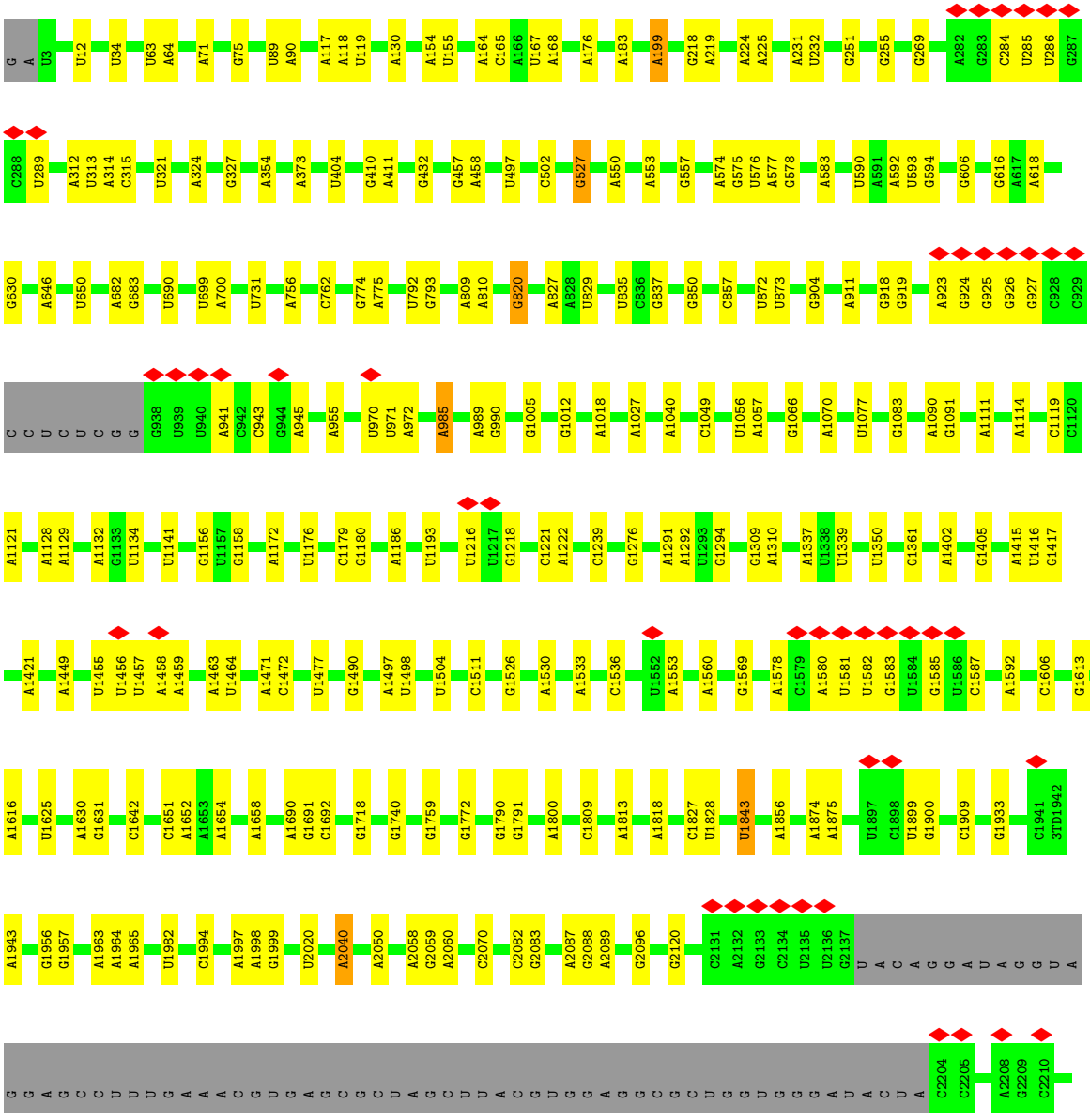
Mol	Chain	Residues	Atoms		AltConf
60	a	27	Total 27	O 27	0

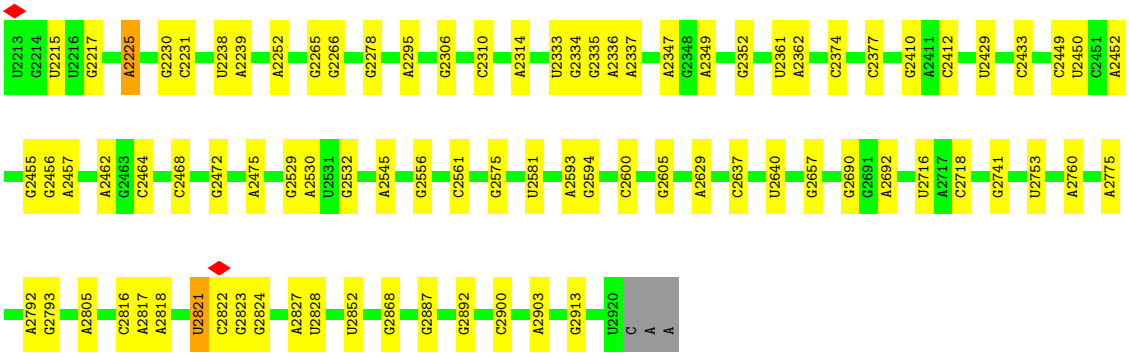
3 Residue-property plots (i)

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: 23S ribosomal RNA

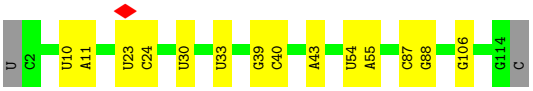
Chain A:





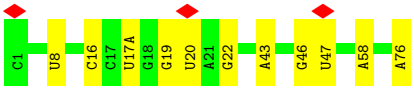
• Molecule 2: 5S ribosomal RNA

Chain B:



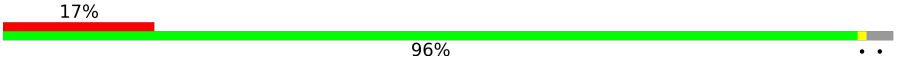
• Molecule 3: tRNA

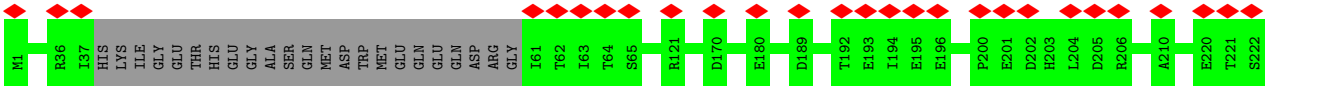
Chain D:

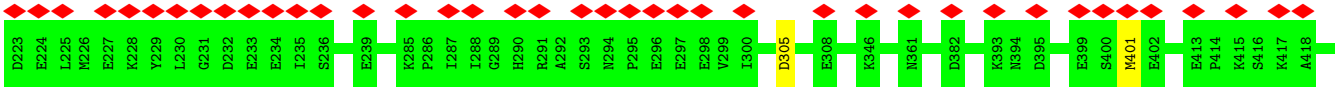


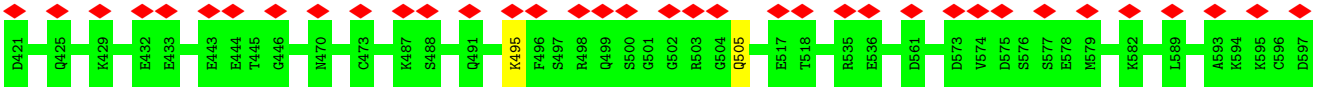
• Molecule 4: Elongation factor G

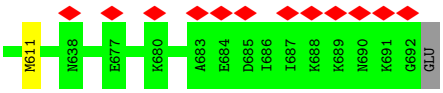
Chain E:





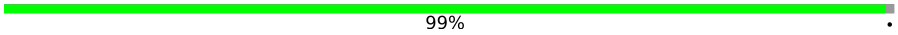


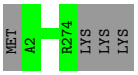




• Molecule 5: 50S ribosomal protein L2

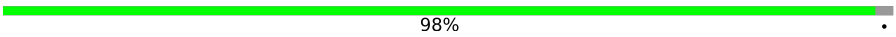
Chain G:

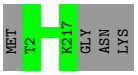




• Molecule 6: 50S ribosomal protein L3

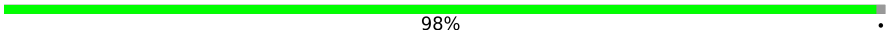
Chain H:

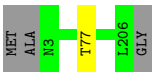




• Molecule 7: 50S ribosomal protein L4

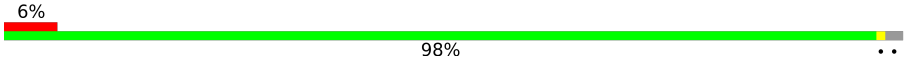
Chain I:

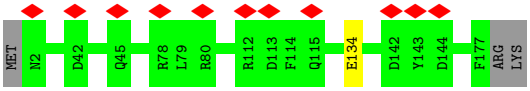




• Molecule 8: 50S ribosomal protein L5

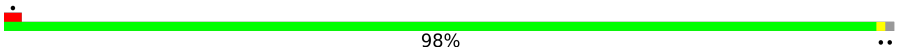
Chain J:

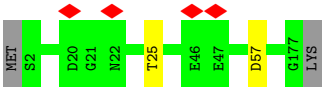




• Molecule 9: 50S ribosomal protein L6

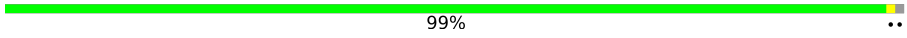
Chain K:

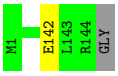




• Molecule 10: 50S ribosomal protein L13

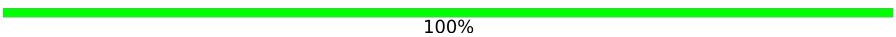
Chain M:





• Molecule 11: 50S ribosomal protein L14

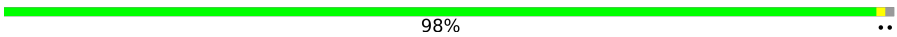
Chain N:

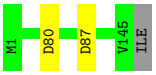


There are no outlier residues recorded for this chain.

• Molecule 12: 50S ribosomal protein L15

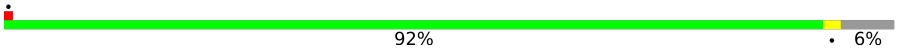
Chain O:

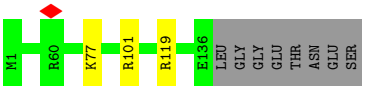




• Molecule 13: 50S ribosomal protein L16

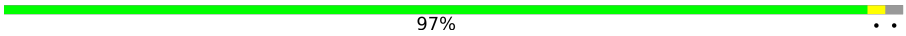
Chain P:

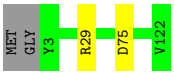




• Molecule 14: 50S ribosomal protein L17

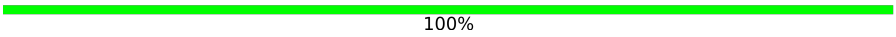
Chain Q:





• Molecule 15: 50S ribosomal protein L18

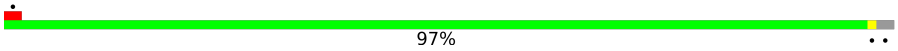
Chain R:

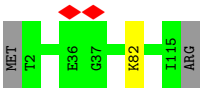


There are no outlier residues recorded for this chain.

• Molecule 16: 50S ribosomal protein L19

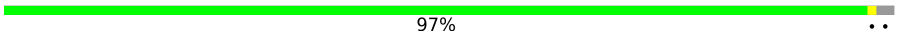
Chain S:





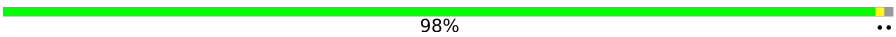
• Molecule 17: 50S ribosomal protein L20

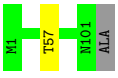
Chain T:



• Molecule 18: 50S ribosomal protein L21

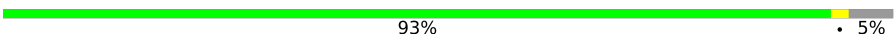
Chain U:

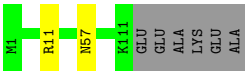




• Molecule 19: 50S ribosomal protein L22

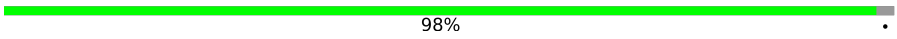
Chain V:





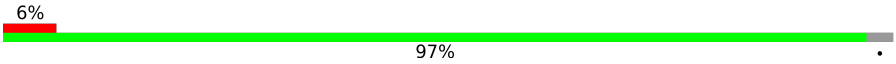
• Molecule 20: 50S ribosomal protein L23

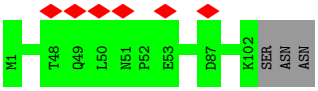
Chain W:



• Molecule 21: 50S ribosomal protein L24

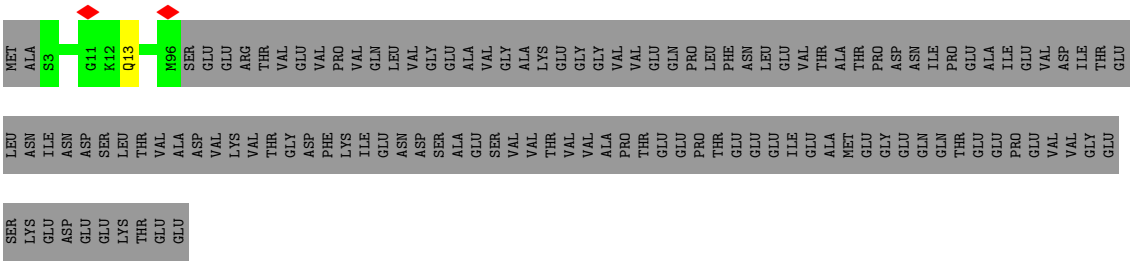
Chain X:





• Molecule 22: 50S ribosomal protein L25

Chain Y:

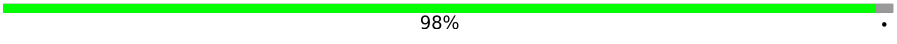


• Molecule 23: 50S ribosomal protein L27

Chain Z:

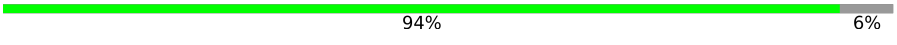
• Molecule 24: 50S ribosomal protein L28

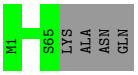
Chain 1:



• Molecule 25: 50S ribosomal protein L29

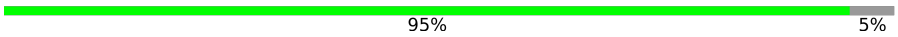
Chain 2:

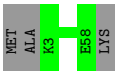




• Molecule 26: 50S ribosomal protein L30

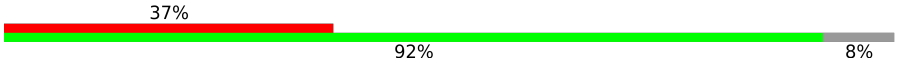
Chain 3:

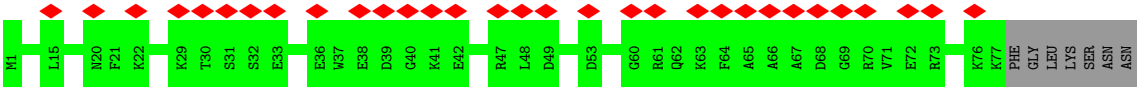




• Molecule 27: 50S ribosomal protein L31 type B

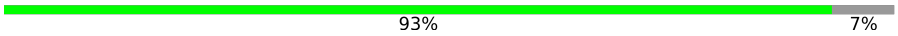
Chain 4:

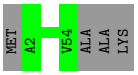




• Molecule 28: Large ribosomal subunit protein bL32

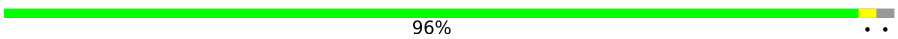
Chain 5:





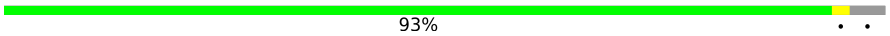
• Molecule 29: Large ribosomal subunit protein bL33A

Chain 6:



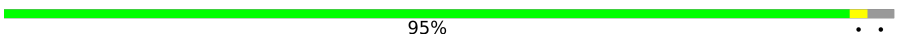
• Molecule 30: 50S ribosomal protein L34

Chain 7:



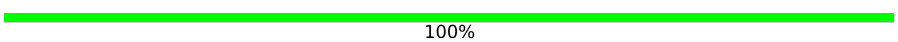
• Molecule 31: 50S ribosomal protein L35

Chain 8:



• Molecule 32: 50S ribosomal protein L36

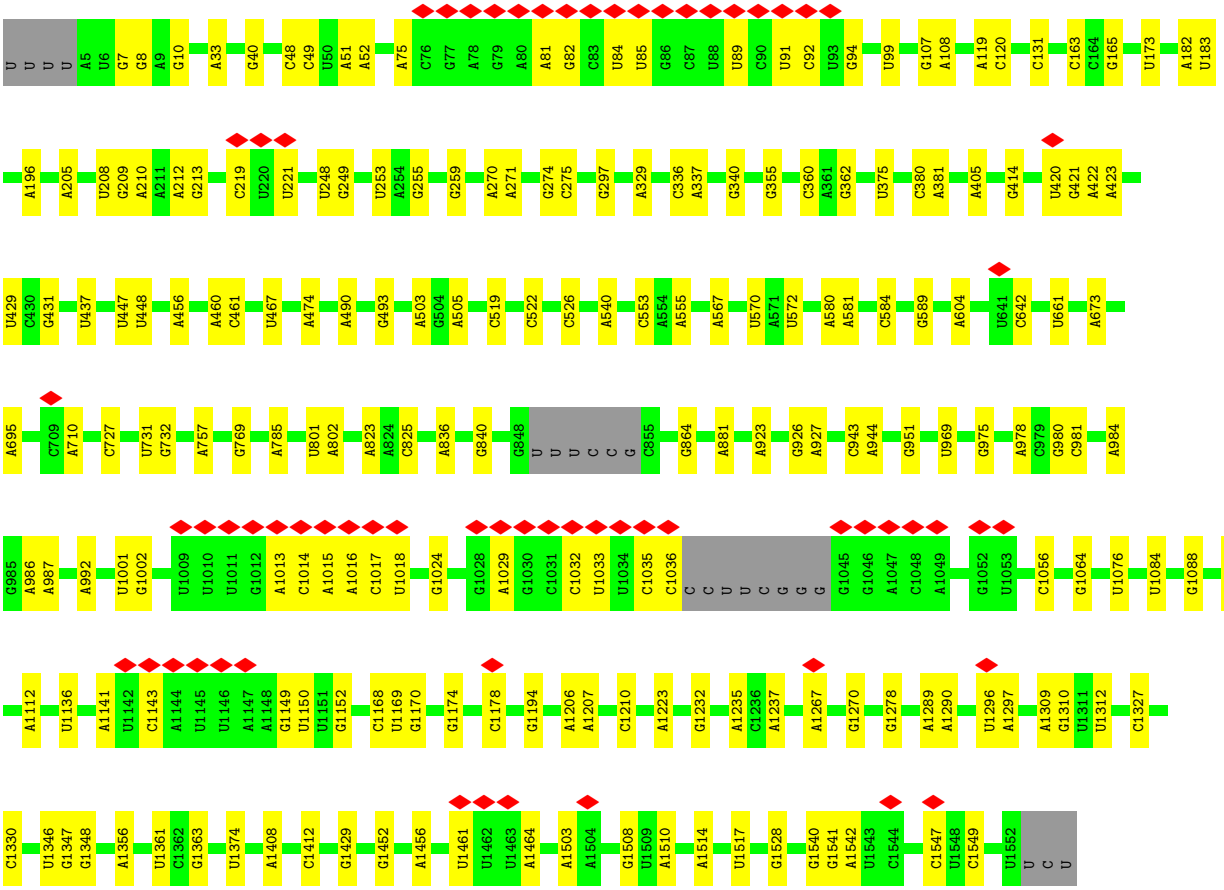
Chain 9:



There are no outlier residues recorded for this chain.

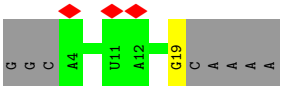
• Molecule 33: 16S ribosomal RNA

Chain a:



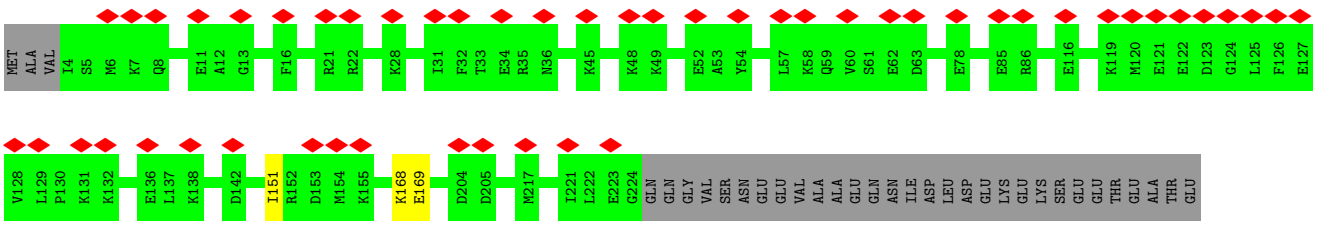
• Molecule 34: mRNA

Chain b:



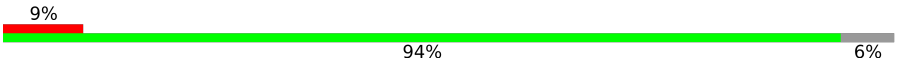
• Molecule 35: 30S ribosomal protein S2

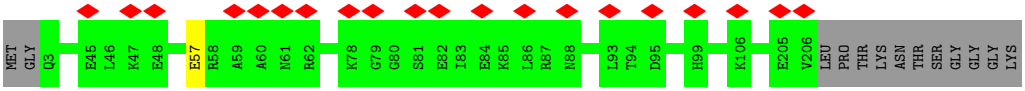
Chain c:



• Molecule 36: 30S ribosomal protein S3

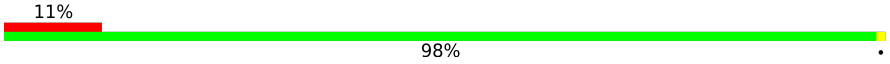
Chain d:

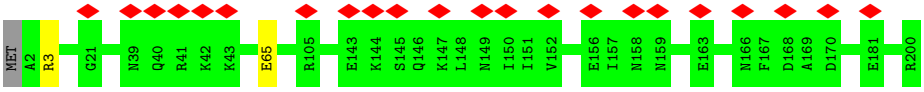




• Molecule 37: 30S ribosomal protein S4

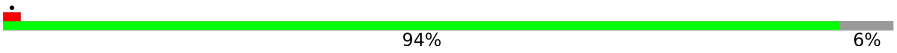
Chain e:

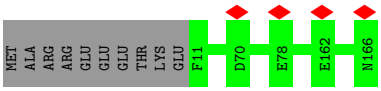




• Molecule 38: 30S ribosomal protein S5

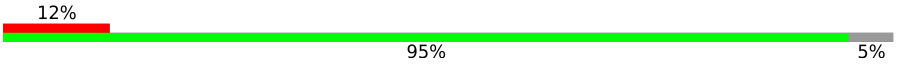
Chain f:

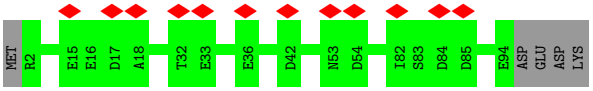




• Molecule 39: 30S ribosomal protein S6

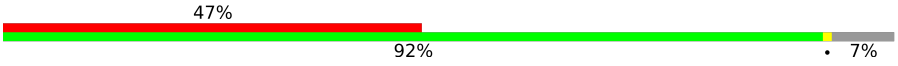
Chain g:

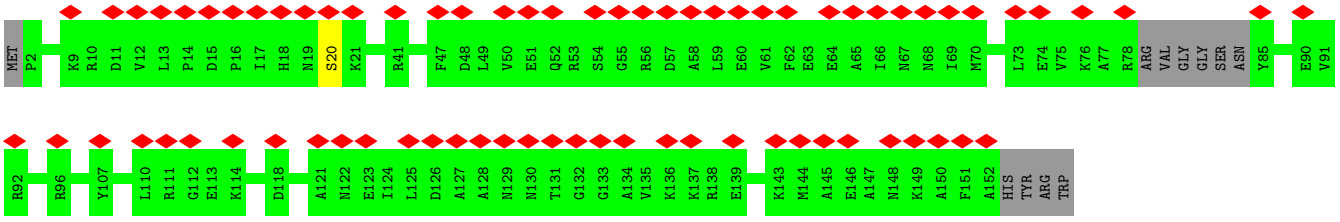




• Molecule 40: 30S ribosomal protein S7

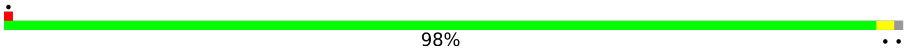
Chain h:

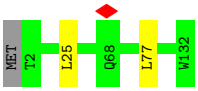




• Molecule 41: 30S ribosomal protein S8

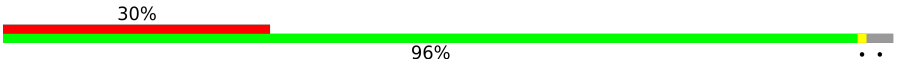
Chain i:

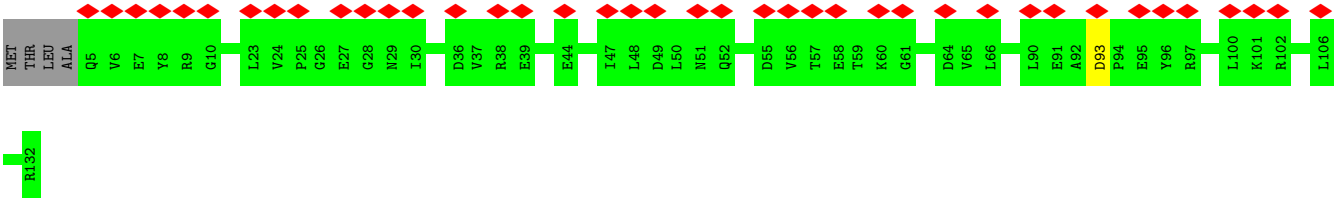




• Molecule 42: 30S ribosomal protein S9

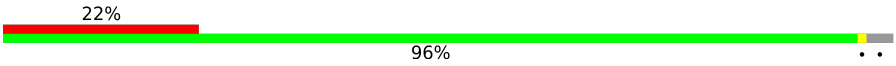
Chain j:

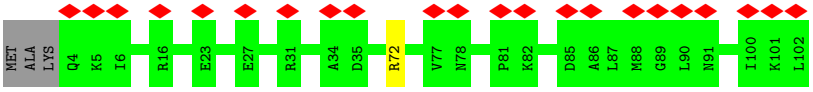




• Molecule 43: Small ribosomal subunit protein uS10

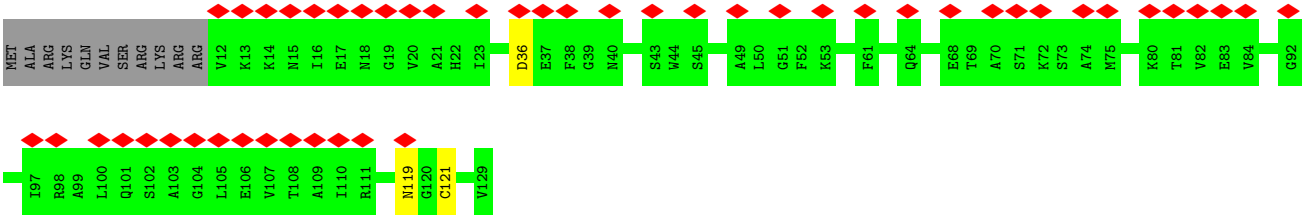
Chain k:





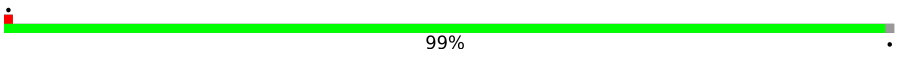
• Molecule 44: 30S ribosomal protein S11

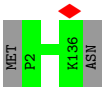
Chain l:



• Molecule 45: 30S ribosomal protein S12

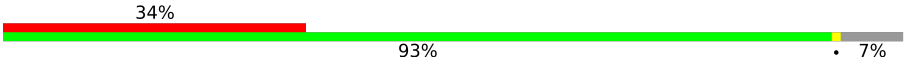
Chain m:

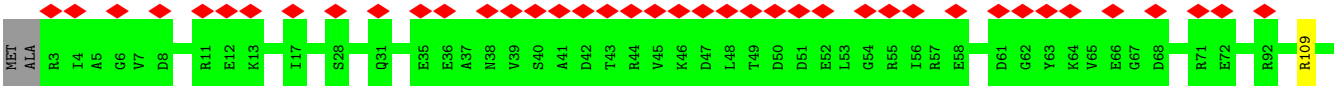


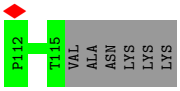


• Molecule 46: 30S ribosomal protein S13

Chain n:

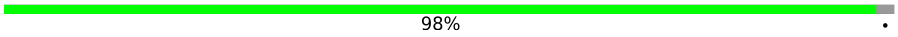






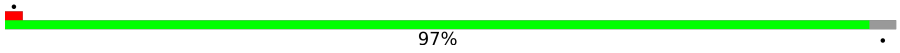
• Molecule 47: 30S ribosomal protein S14 type Z

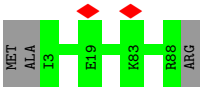
Chain o:



• Molecule 48: 30S ribosomal protein S15

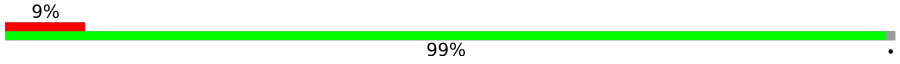
Chain p:

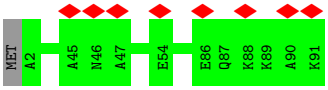




• Molecule 49: 30S ribosomal protein S16

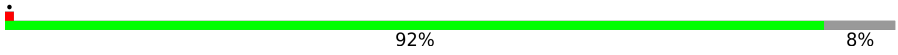
Chain q:

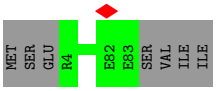




• Molecule 50: 30S ribosomal protein S17

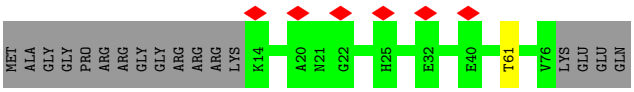
Chain r:





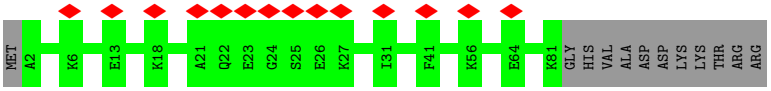
• Molecule 51: 30S ribosomal protein S18

Chain s:



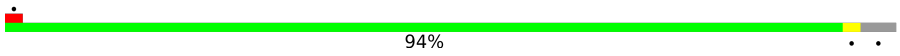
• Molecule 52: 30S ribosomal protein S19

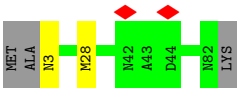
Chain t:



• Molecule 53: 30S ribosomal protein S20

Chain u:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	303005	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	27.77	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	165000	Depositor
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	5.371	Depositor
Minimum map value	-2.346	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	509.59998, 509.59998, 509.59998	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.728, 0.728, 0.728	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, 2MG, UR3, WUX, H2U, GDP, 4OC, ZN, MA6, SPD, 3TD, G7M, 2MA, 5MU, PUT, MG, 5MC

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	A	0.50	0/68163	0.86	21/106299 (0.0%)
2	B	0.36	0/2692	0.78	0/4193
3	D	0.28	0/1832	0.76	0/2855
4	E	0.25	0/5267	0.48	0/7123
5	G	0.28	0/2120	0.59	0/2847
6	H	0.30	0/1661	0.55	0/2227
7	I	0.28	0/1587	0.55	0/2143
8	J	0.25	0/1410	0.48	0/1893
9	K	0.26	0/1390	0.53	0/1870
10	M	0.28	0/1168	0.52	0/1573
11	N	0.28	0/927	0.61	0/1243
12	O	0.30	0/1104	0.57	0/1471
13	P	0.30	0/1113	0.59	0/1493
14	Q	0.28	0/956	0.61	0/1277
15	R	0.27	0/931	0.53	0/1244
16	S	0.26	0/934	0.62	0/1249
17	T	0.31	0/955	0.59	0/1265
18	U	0.29	0/803	0.55	0/1073
19	V	0.30	0/861	0.61	0/1159
20	W	0.29	0/733	0.57	0/978
21	X	0.27	0/796	0.48	0/1063
22	Y	0.28	0/746	0.51	0/1000
23	Z	0.29	0/610	0.61	0/811
24	1	0.27	0/487	0.60	0/649
25	2	0.26	0/536	0.54	0/713
26	3	0.25	0/438	0.56	0/590
27	4	0.26	0/647	0.46	0/868
28	5	0.29	0/429	0.63	0/571
29	6	0.28	0/407	0.58	0/545
30	7	0.29	0/371	0.71	0/484
31	8	0.28	0/526	0.65	0/690

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	9	0.28	0/299	0.55	0/393
33	a	0.32	0/36619	0.77	1/57097 (0.0%)
34	b	0.24	0/399	0.71	0/622
35	c	0.25	0/1808	0.46	0/2426
36	d	0.24	0/1634	0.52	0/2195
37	e	0.25	0/1647	0.51	0/2211
38	f	0.26	0/1174	0.53	0/1583
39	g	0.25	0/784	0.52	0/1052
40	h	0.23	0/1170	0.50	0/1572
41	i	0.25	0/1044	0.54	0/1401
42	j	0.24	0/1032	0.55	0/1386
43	k	0.24	0/804	0.52	0/1083
44	l	0.24	0/891	0.52	0/1203
45	m	0.26	0/1075	0.57	0/1439
46	n	0.23	0/909	0.57	0/1218
47	o	0.27	0/511	0.55	0/678
48	p	0.24	0/730	0.55	0/975
49	q	0.25	0/723	0.52	0/971
50	r	0.25	0/670	0.51	0/895
51	s	0.26	0/525	0.55	0/704
52	t	0.25	0/668	0.47	0/896
53	u	0.24	0/606	0.46	0/810
All	All	0.39	0/158322	0.76	22/236269 (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
17	T	0	1

There are no bond length outliers.

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	557	G	O4'-C1'-N9	6.07	113.05	108.20
1	A	2040	A	O5'-P-OP1	-5.98	100.32	105.70
33	a	1033	U	C2-N1-C1'	5.93	124.82	117.70
1	A	199	A	O4'-C1'-N9	5.48	112.58	108.20
1	A	1843	U	N3-C2-O2	-5.43	118.40	122.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	T	50	ARG	Sidechain

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	
4	E	665/693 (96%)	650 (98%)	15 (2%)	0	100	100
5	G	271/277 (98%)	265 (98%)	6 (2%)	0	100	100
6	H	214/220 (97%)	204 (95%)	10 (5%)	0	100	100
7	I	202/207 (98%)	200 (99%)	2 (1%)	0	100	100
8	J	174/179 (97%)	171 (98%)	3 (2%)	0	100	100
9	K	174/178 (98%)	168 (97%)	6 (3%)	0	100	100
10	M	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
11	N	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
12	O	143/146 (98%)	136 (95%)	7 (5%)	0	100	100
13	P	134/144 (93%)	131 (98%)	3 (2%)	0	100	100
14	Q	118/122 (97%)	116 (98%)	2 (2%)	0	100	100
15	R	117/119 (98%)	114 (97%)	3 (3%)	0	100	100
16	S	112/116 (97%)	110 (98%)	2 (2%)	0	100	100
17	T	114/118 (97%)	113 (99%)	1 (1%)	0	100	100
18	U	99/102 (97%)	97 (98%)	2 (2%)	0	100	100
19	V	109/117 (93%)	108 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	W	87/91 (96%)	86 (99%)	1 (1%)	0	100	100
21	X	100/105 (95%)	96 (96%)	4 (4%)	0	100	100
22	Y	92/217 (42%)	91 (99%)	1 (1%)	0	100	100
23	Z	77/94 (82%)	75 (97%)	2 (3%)	0	100	100
24	1	59/62 (95%)	59 (100%)	0	0	100	100
25	2	63/69 (91%)	63 (100%)	0	0	100	100
26	3	54/59 (92%)	52 (96%)	2 (4%)	0	100	100
27	4	75/84 (89%)	73 (97%)	2 (3%)	0	100	100
28	5	51/57 (90%)	49 (96%)	2 (4%)	0	100	100
29	6	46/49 (94%)	44 (96%)	2 (4%)	0	100	100
30	7	41/45 (91%)	41 (100%)	0	0	100	100
31	8	62/66 (94%)	61 (98%)	1 (2%)	0	100	100
32	9	35/37 (95%)	35 (100%)	0	0	100	100
35	c	219/255 (86%)	208 (95%)	11 (5%)	0	100	100
36	d	202/217 (93%)	196 (97%)	6 (3%)	0	100	100
37	e	197/200 (98%)	192 (98%)	5 (2%)	0	100	100
38	f	154/166 (93%)	148 (96%)	6 (4%)	0	100	100
39	g	91/98 (93%)	87 (96%)	4 (4%)	0	100	100
40	h	141/156 (90%)	138 (98%)	3 (2%)	0	100	100
41	i	129/132 (98%)	123 (95%)	6 (5%)	0	100	100
42	j	126/132 (96%)	123 (98%)	3 (2%)	0	100	100
43	k	97/102 (95%)	94 (97%)	3 (3%)	0	100	100
44	l	116/129 (90%)	109 (94%)	6 (5%)	1 (1%)	17	10
45	m	133/137 (97%)	130 (98%)	3 (2%)	0	100	100
46	n	111/121 (92%)	105 (95%)	6 (5%)	0	100	100
47	o	58/61 (95%)	57 (98%)	1 (2%)	0	100	100
48	p	84/89 (94%)	81 (96%)	3 (4%)	0	100	100
49	q	88/91 (97%)	86 (98%)	2 (2%)	0	100	100
50	r	78/87 (90%)	76 (97%)	2 (3%)	0	100	100
51	s	61/80 (76%)	61 (100%)	0	0	100	100
52	t	78/92 (85%)	76 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
53	u	78/83 (94%)	77 (99%)	1 (1%)	0	100	100
All	All	5991/6468 (93%)	5831 (97%)	159 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
44	l	121	CYS

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	
4	E	559/579 (96%)	554 (99%)	5 (1%)	78	82
5	G	220/224 (98%)	220 (100%)	0	100	100
6	H	174/177 (98%)	174 (100%)	0	100	100
7	I	168/169 (99%)	167 (99%)	1 (1%)	86	89
8	J	155/158 (98%)	154 (99%)	1 (1%)	86	89
9	K	153/155 (99%)	151 (99%)	2 (1%)	69	72
10	M	123/123 (100%)	122 (99%)	1 (1%)	81	85
11	N	100/100 (100%)	100 (100%)	0	100	100
12	O	111/112 (99%)	109 (98%)	2 (2%)	59	61
13	P	113/119 (95%)	110 (97%)	3 (3%)	44	44
14	Q	101/102 (99%)	99 (98%)	2 (2%)	55	57
15	R	95/95 (100%)	95 (100%)	0	100	100
16	S	100/102 (98%)	99 (99%)	1 (1%)	76	80
17	T	96/98 (98%)	96 (100%)	0	100	100
18	U	86/86 (100%)	85 (99%)	1 (1%)	71	75
19	V	90/94 (96%)	88 (98%)	2 (2%)	52	53
20	W	80/82 (98%)	80 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	X	87/90 (97%)	87 (100%)	0	100	100
22	Y	83/190 (44%)	82 (99%)	1 (1%)	71	75
23	Z	62/75 (83%)	62 (100%)	0	100	100
24	1	51/52 (98%)	51 (100%)	0	100	100
25	2	59/62 (95%)	59 (100%)	0	100	100
26	3	51/53 (96%)	51 (100%)	0	100	100
27	4	69/75 (92%)	69 (100%)	0	100	100
28	5	48/50 (96%)	48 (100%)	0	100	100
29	6	46/47 (98%)	45 (98%)	1 (2%)	52	53
30	7	39/40 (98%)	38 (97%)	1 (3%)	46	46
31	8	55/57 (96%)	54 (98%)	1 (2%)	59	61
32	9	35/35 (100%)	35 (100%)	0	100	100
35	c	192/221 (87%)	189 (98%)	3 (2%)	62	66
36	d	166/175 (95%)	165 (99%)	1 (1%)	86	89
37	e	174/175 (99%)	172 (99%)	2 (1%)	73	77
38	f	122/131 (93%)	122 (100%)	0	100	100
39	g	81/86 (94%)	81 (100%)	0	100	100
40	h	123/132 (93%)	122 (99%)	1 (1%)	81	85
41	i	112/113 (99%)	110 (98%)	2 (2%)	59	61
42	j	106/109 (97%)	105 (99%)	1 (1%)	78	82
43	k	89/91 (98%)	88 (99%)	1 (1%)	73	77
44	l	94/104 (90%)	92 (98%)	2 (2%)	53	55
45	m	117/119 (98%)	117 (100%)	0	100	100
46	n	98/104 (94%)	97 (99%)	1 (1%)	76	80
47	o	52/53 (98%)	52 (100%)	0	100	100
48	p	79/81 (98%)	79 (100%)	0	100	100
49	q	76/77 (99%)	76 (100%)	0	100	100
50	r	75/82 (92%)	75 (100%)	0	100	100
51	s	56/68 (82%)	55 (98%)	1 (2%)	59	61
52	t	70/80 (88%)	70 (100%)	0	100	100
53	u	67/69 (97%)	65 (97%)	2 (3%)	41	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5158/5471 (94%)	5116 (99%)	42 (1%)	82 85

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
36	d	57	GLU
43	k	72	ARG
37	e	3	ARG
41	i	25	LEU
44	l	119	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
4	E	447	GLN
21	X	49	GLN
22	Y	10	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2837/2923 (97%)	316 (11%)	21 (0%)
2	B	112/115 (97%)	14 (12%)	0
3	D	76/77 (98%)	11 (14%)	0
33	a	1528/1555 (98%)	201 (13%)	0
34	b	15/24 (62%)	1 (6%)	0
All	All	4568/4694 (97%)	543 (11%)	21 (0%)

5 of 543 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	34	U
1	A	63	U
1	A	64	A
1	A	71	A
1	A	75	G

5 of 21 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	2238	U
1	A	2457	A
1	A	2827	A
1	A	2817	A
1	A	2449	C

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

15 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	$\#\|Z\| > 2$
1	2MA	A	2530	1,54	17,25,26	0.85	1 (5%)	17,37,40	0.61	0
33	2MG	a	975	33	18,26,27	0.96	2 (11%)	16,38,41	0.78	0
1	3TD	A	1942[A]	1	19,22,23	0.58	0	21,32,35	0.56	0
33	4OC	a	1412	33	20,23,24	0.30	0	26,32,35	1.09	2 (7%)
33	MA6	a	1529	33	18,26,27	0.76	0	19,38,41	0.68	0
1	3TD	A	1942[B]	1	19,22,23	0.57	0	21,32,35	0.57	0
33	MA6	a	1530	33	18,26,27	0.76	0	19,38,41	0.69	0
1	OMG	A	2278	1,54	18,26,27	0.99	2 (11%)	19,38,41	0.62	0
33	UR3	a	1509	33	19,22,23	0.29	0	26,32,35	0.36	0
33	5MC	a	976	33	18,22,23	0.31	0	26,32,35	0.43	0
1	2MG	A	2472	1	18,26,27	0.98	2 (11%)	16,38,41	0.66	0
1	5MU	A	1966	1	19,22,23	0.33	0	28,32,35	0.40	0
1	H2U	A	2476	1	18,21,22	0.36	0	21,30,33	0.44	0
33	G7M	a	535	33	20,26,27	0.58	0	17,39,42	0.42	0
1	5MU	A	792	1	19,22,23	0.32	0	28,32,35	0.37	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	2MA	A	2530	1,54	-	2/3/25/26	0/3/3/3
33	2MG	a	975	33	-	0/5/27/28	0/3/3/3
1	3TD	A	1942[A]	1	-	0/7/25/26	0/2/2/2
33	4OC	a	1412	33	-	0/9/29/30	0/2/2/2
33	MA6	a	1529	33	-	0/7/29/30	0/3/3/3
1	3TD	A	1942[B]	1	-	2/7/25/26	0/2/2/2
33	MA6	a	1530	33	-	3/7/29/30	0/3/3/3
1	OMG	A	2278	1,54	-	0/5/27/28	0/3/3/3
33	UR3	a	1509	33	-	0/7/25/26	0/2/2/2
33	5MC	a	976	33	-	0/7/25/26	0/2/2/2
1	2MG	A	2472	1	-	0/5/27/28	0/3/3/3
1	5MU	A	1966	1	-	0/7/25/26	0/2/2/2
1	H2U	A	2476	1	-	0/7/38/39	0/2/2/2
33	G7M	a	535	33	-	1/3/25/26	0/3/3/3
1	5MU	A	792	1	-	0/7/25/26	0/2/2/2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2278	OMG	C5-C6	-2.52	1.42	1.47
33	a	975	2MG	C5-C6	-2.31	1.42	1.47
1	A	2472	2MG	C8-N7	-2.18	1.31	1.35
1	A	2530	2MA	C8-N7	-2.15	1.31	1.35
33	a	975	2MG	C5-C4	-2.06	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a	1412	4OC	O3'-C3'-C2'	3.60	121.39	111.17
33	a	1412	4OC	O3'-C3'-C4'	3.14	120.12	111.05

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1942[B]	3TD	C3'-C4'-C5'-O5'
1	A	1942[B]	3TD	O4'-C4'-C5'-O5'
33	a	1530	MA6	O4'-C4'-C5'-O5'
33	a	1530	MA6	C3'-C4'-C5'-O5'
1	A	2530	2MA	O4'-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 178 ligands modelled in this entry, 172 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
55	SPD	A	3109	-	9,9,9	0.10	0	8,8,8	0.15	0
58	WUX	E	703	-	42,43,43	0.45	1 (2%)	47,68,68	0.55	0
56	PUT	A	3110	-	5,5,5	0.09	0	4,4,4	0.12	0
57	GDP	E	701	54	24,30,30	0.89	2 (8%)	30,47,47	0.84	1 (3%)
55	SPD	A	3107	-	9,9,9	0.12	0	8,8,8	0.21	0
55	SPD	A	3108	-	9,9,9	0.12	0	8,8,8	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	SPD	A	3109	-	-	1/7/7/7	-
58	WUX	E	703	-	-	4/15/99/99	0/5/5/5
56	PUT	A	3110	-	-	1/3/3/3	-
57	GDP	E	701	54	-	2/12/32/32	0/3/3/3
55	SPD	A	3107	-	-	2/7/7/7	-
55	SPD	A	3108	-	-	4/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	E	701	GDP	C5-C6	-2.25	1.42	1.47
58	E	703	WUX	C29-C22	2.03	1.50	1.47
57	E	701	GDP	C8-N7	-2.03	1.31	1.35

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	E	701	GDP	PA-O3A-PB	3.34	144.29	132.83

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

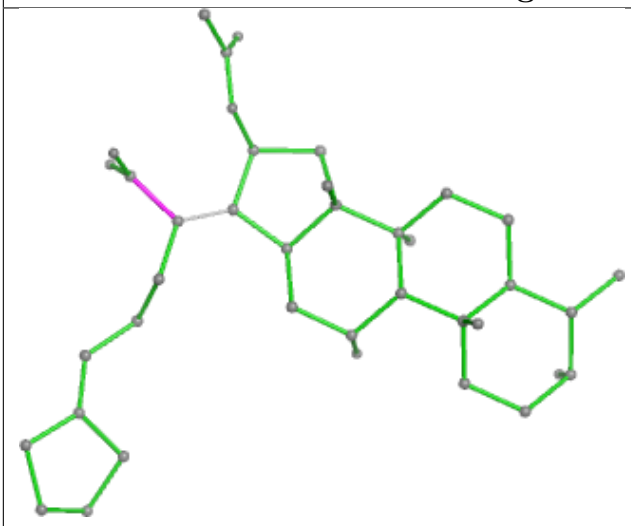
Mol	Chain	Res	Type	Atoms
58	E	703	WUX	C23-C22-C29-O4
58	E	703	WUX	C23-C22-C29-O5
55	A	3108	SPD	N6-C7-C8-C9
58	E	703	WUX	C22-C23-C24-C25
55	A	3107	SPD	C4-C5-N6-C7

There are no ring outliers.

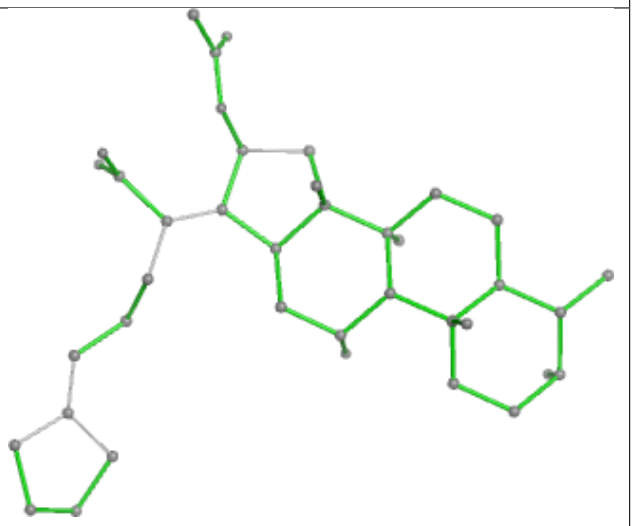
No monomer is involved in short contacts.

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.

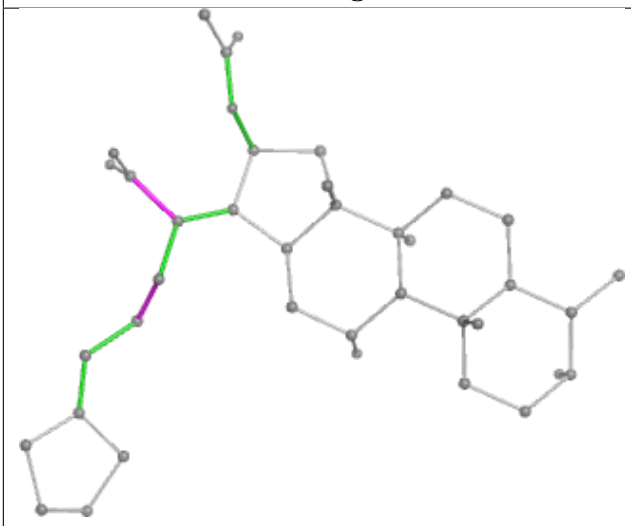
Ligand WUX E 703



Bond lengths



Bond angles



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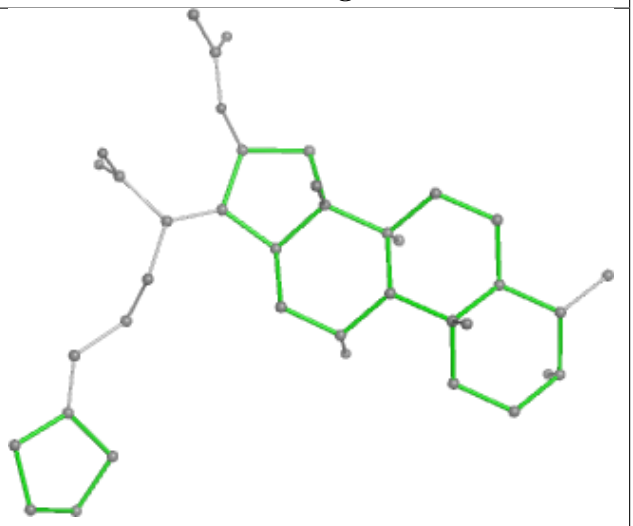
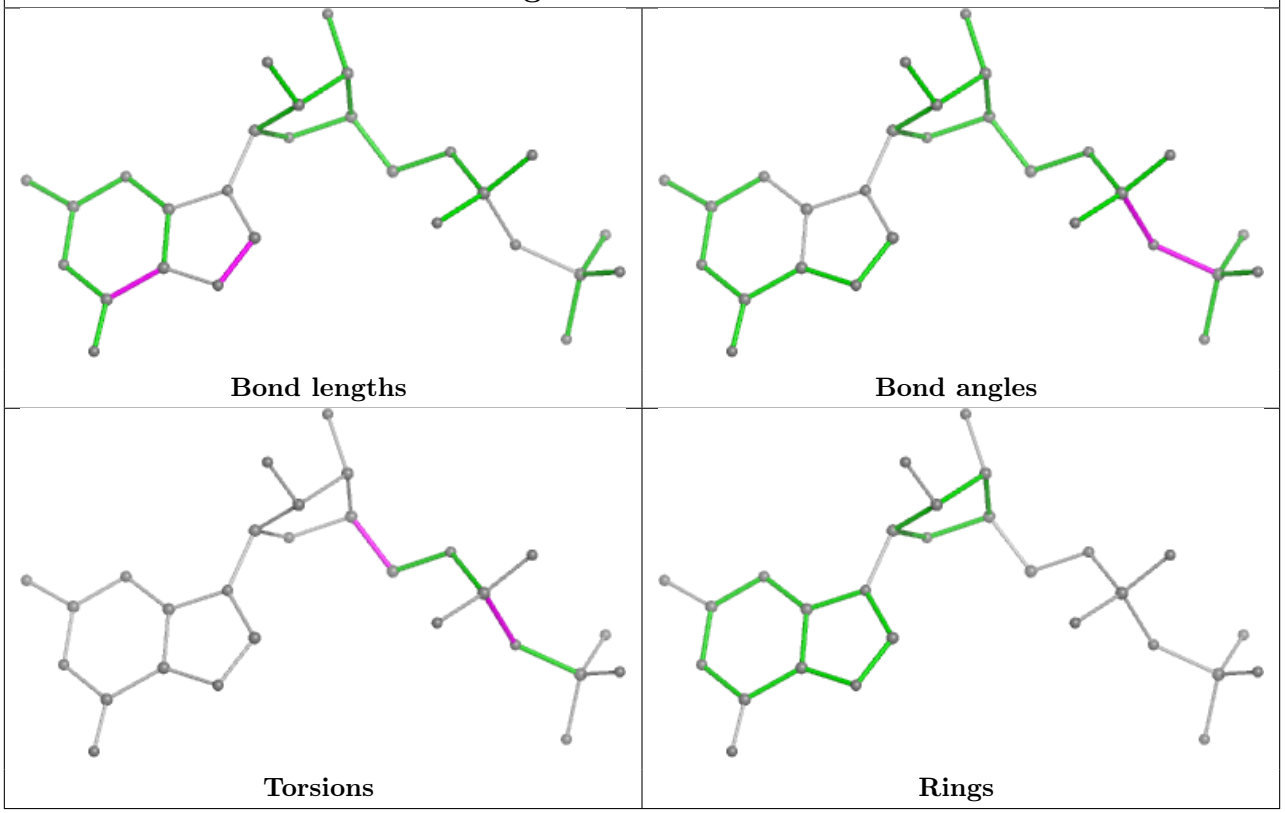


Rings

Ligand GDP E 701



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.

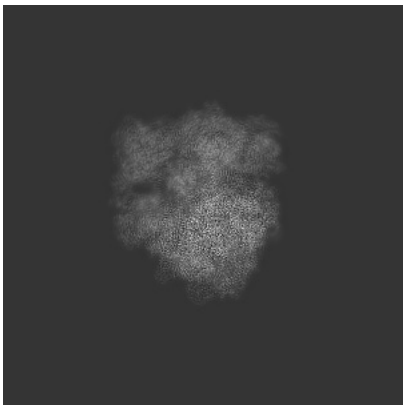
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-17364. These allow visual inspection of the internal detail of the map and identification of artifacts.

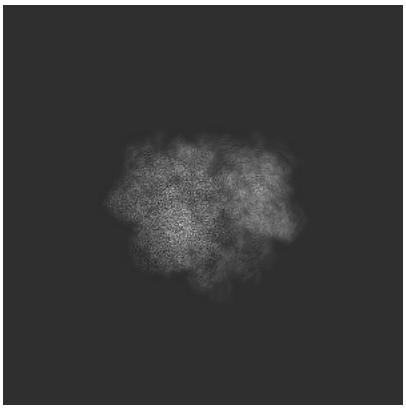
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

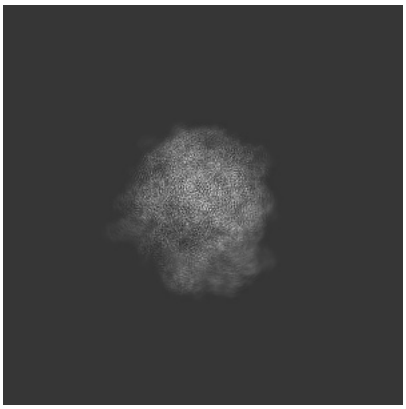
6.1.1 Primary map



X

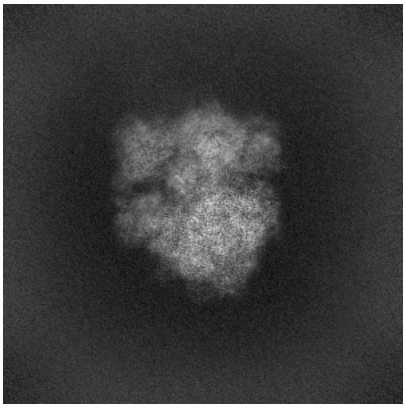


Y

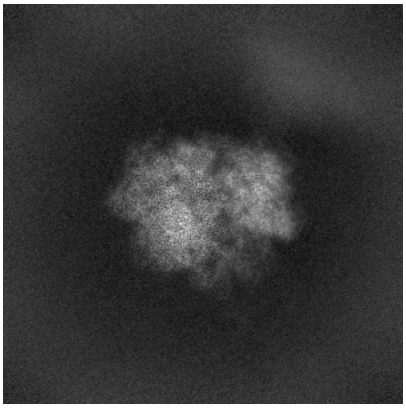


Z

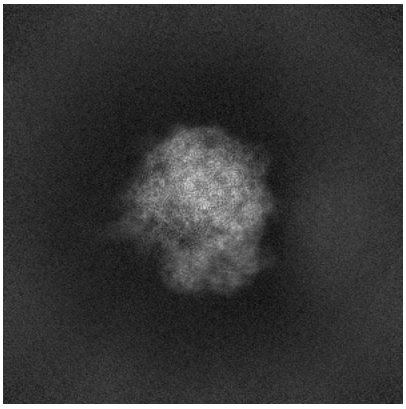
6.1.2 Raw map



X



Y

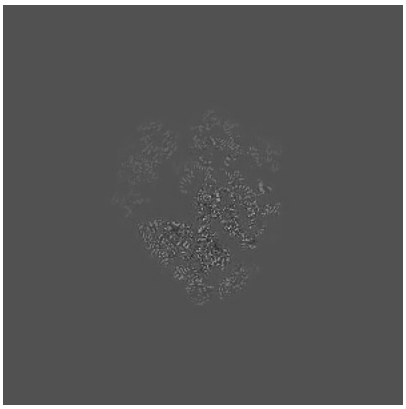


Z

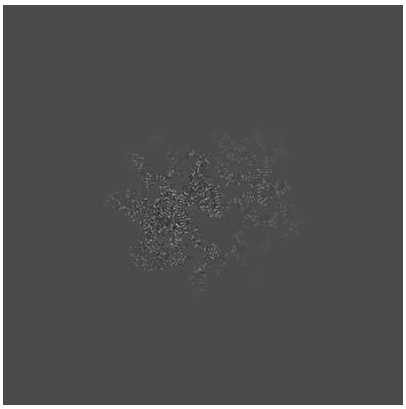
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



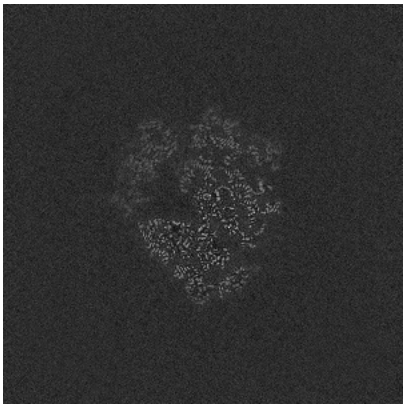
X Index: 350



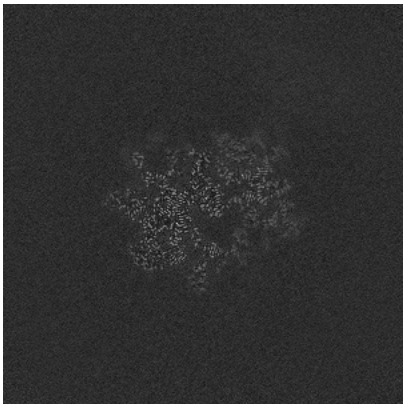
Y Index: 350

Z Index: 350

6.2.2 Raw map



X Index: 350



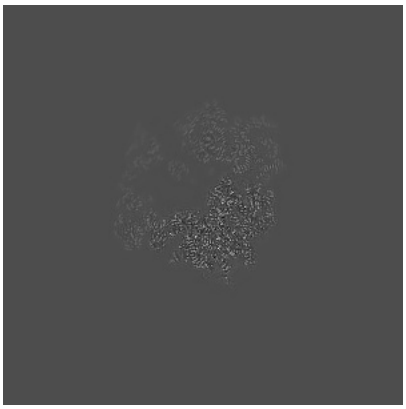
Y Index: 350

Z Index: 350

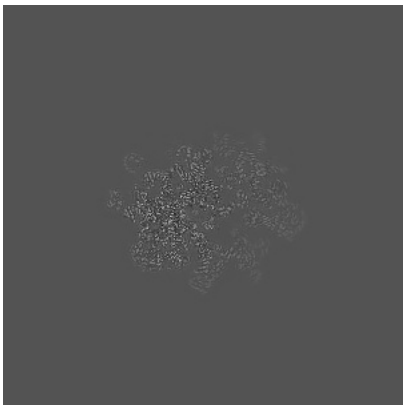
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

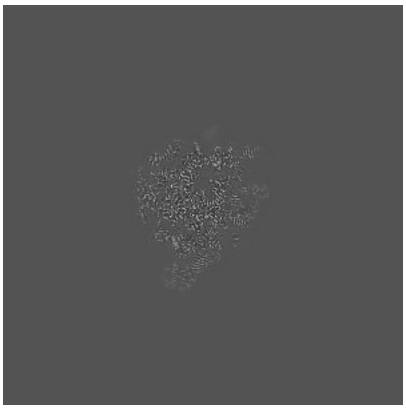
6.3.1 Primary map



X Index: 318

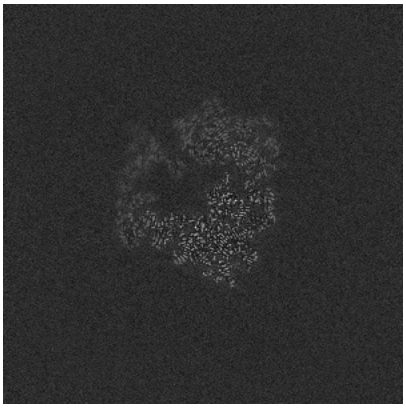


Y Index: 358

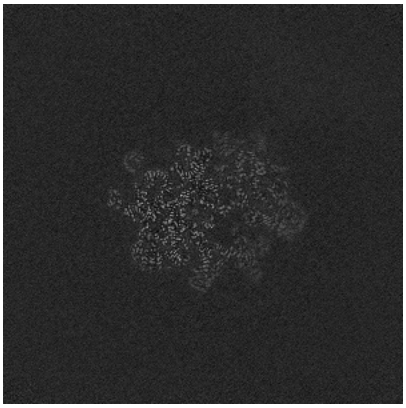


Z Index: 293

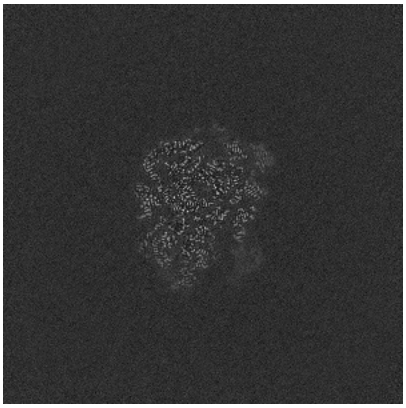
6.3.2 Raw map



X Index: 323



Y Index: 358

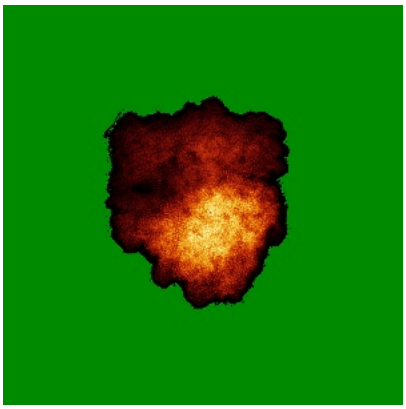


Z Index: 309

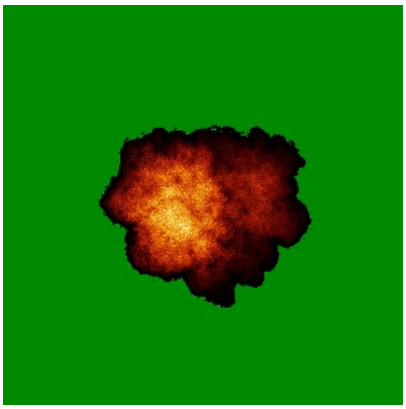
The images above show the largest variance slices of the map in three orthogonal directions.

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

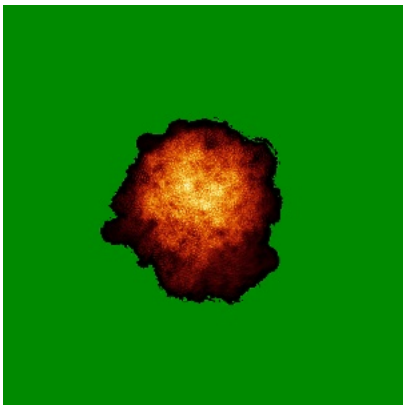
6.4.1 Primary map



X

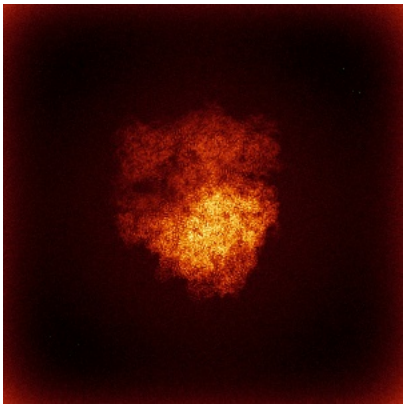


Y

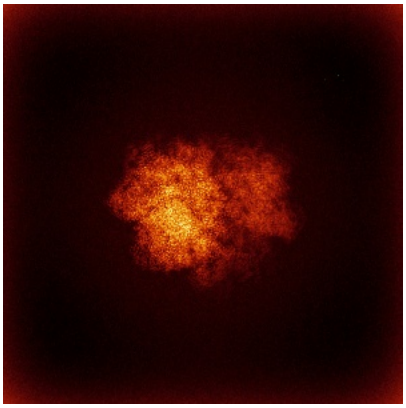


Z

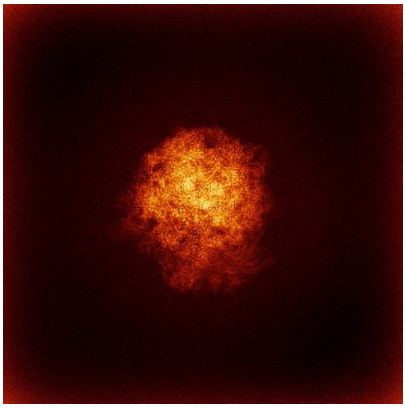
6.4.2 Raw map



X



Y

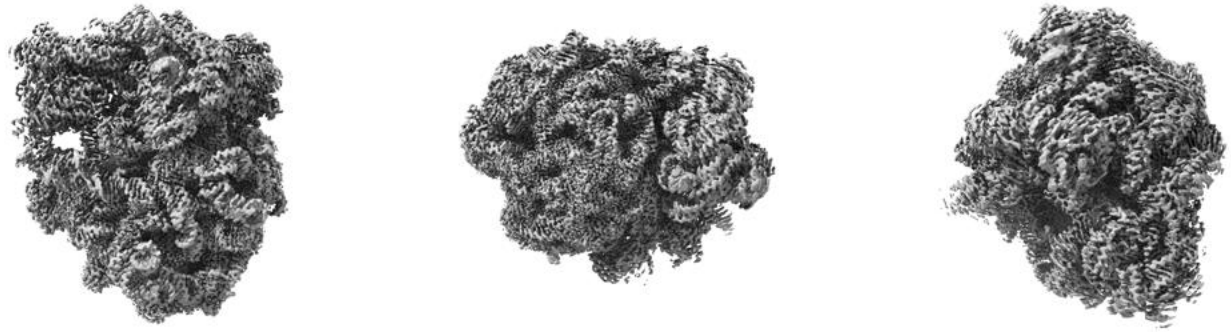


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

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.

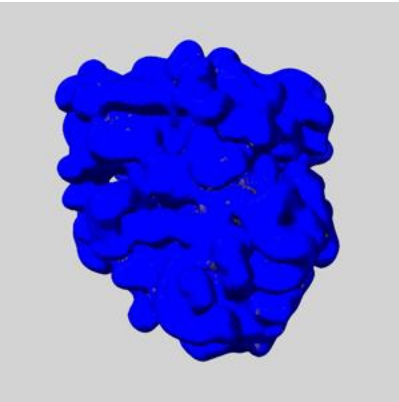
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

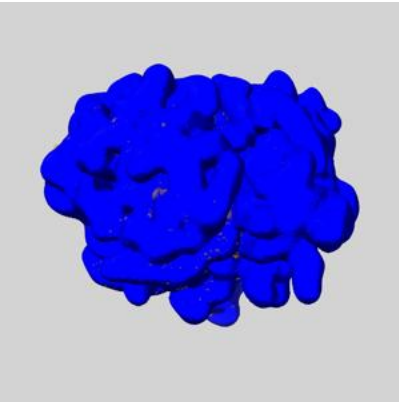
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

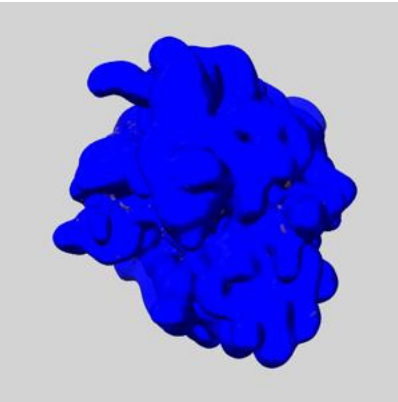
6.6.1 emd_17364_msk_1.map (i)



X



Y

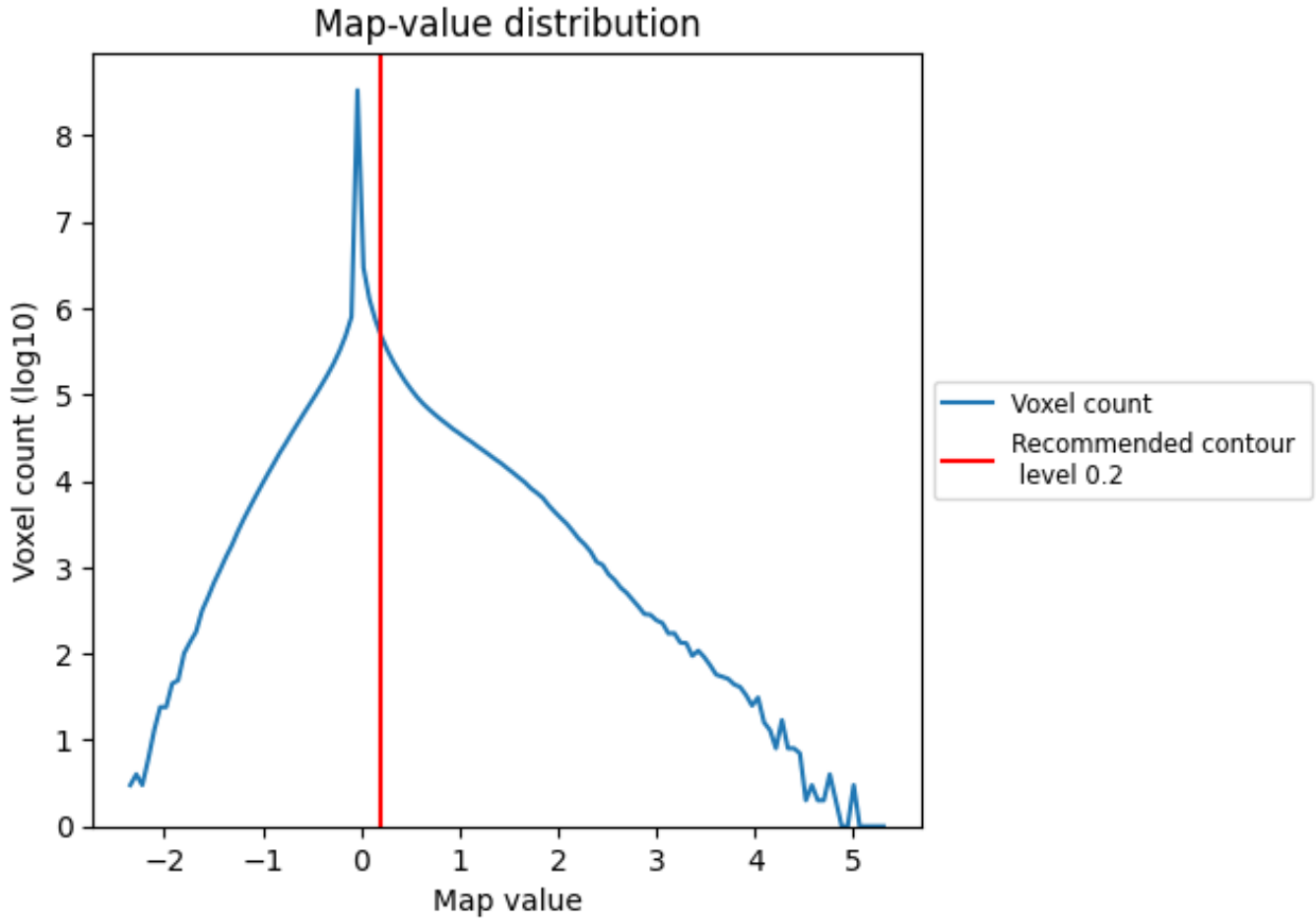


Z

7 Map analysis

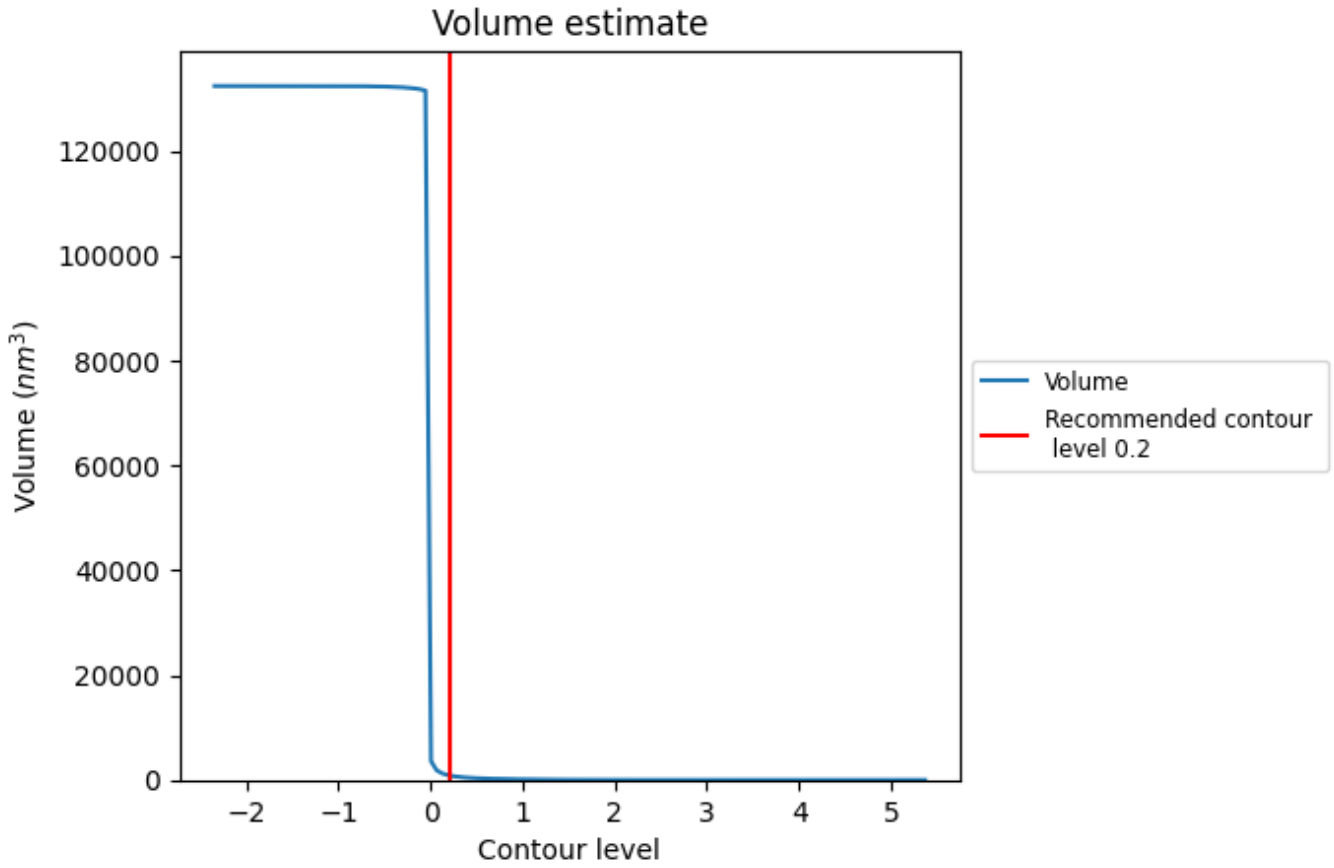
This section contains the results of statistical analysis of the map.

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.

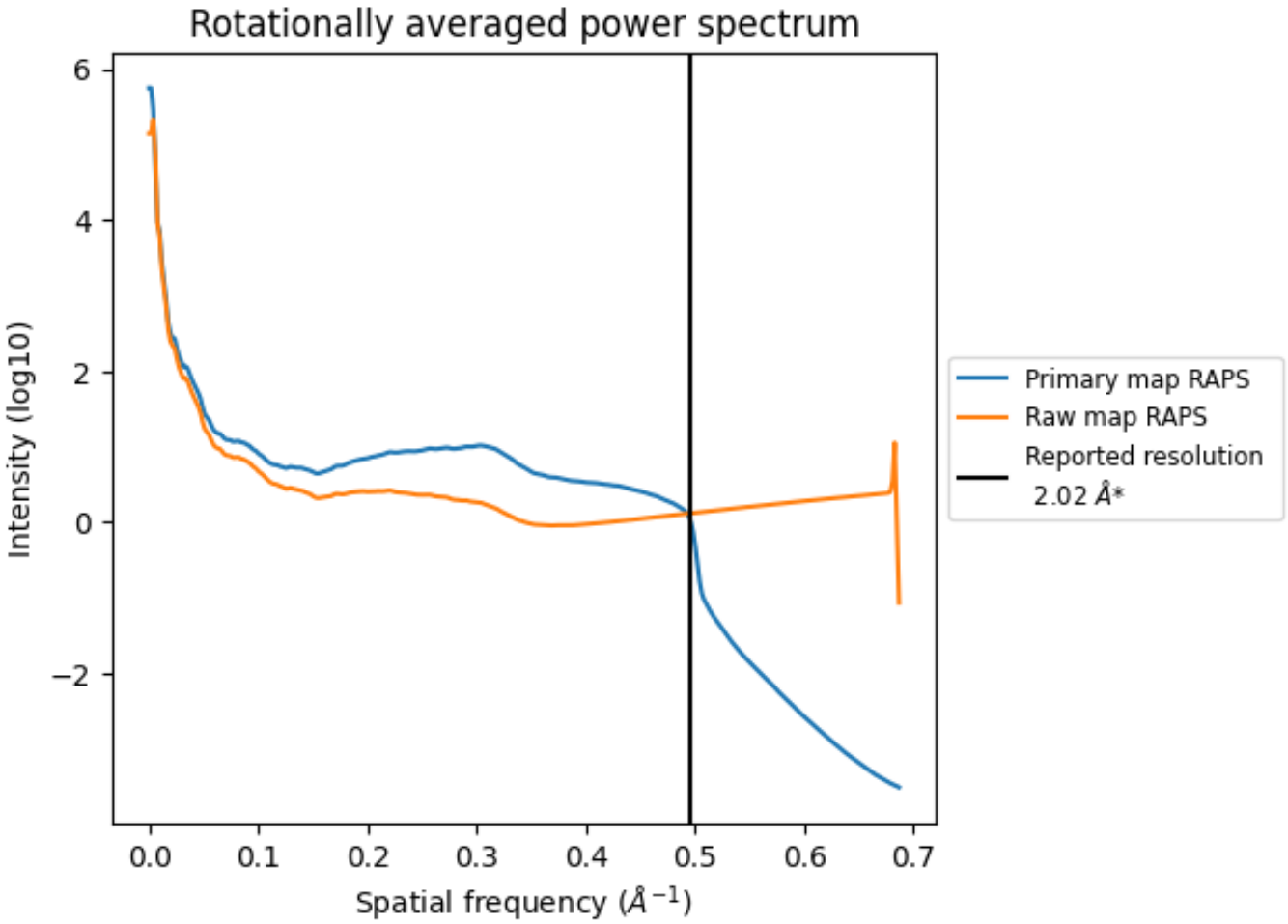
7.2 Volume estimate



The volume at the recommended contour level is 878 nm^3; this corresponds to an approximate mass of 793 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)

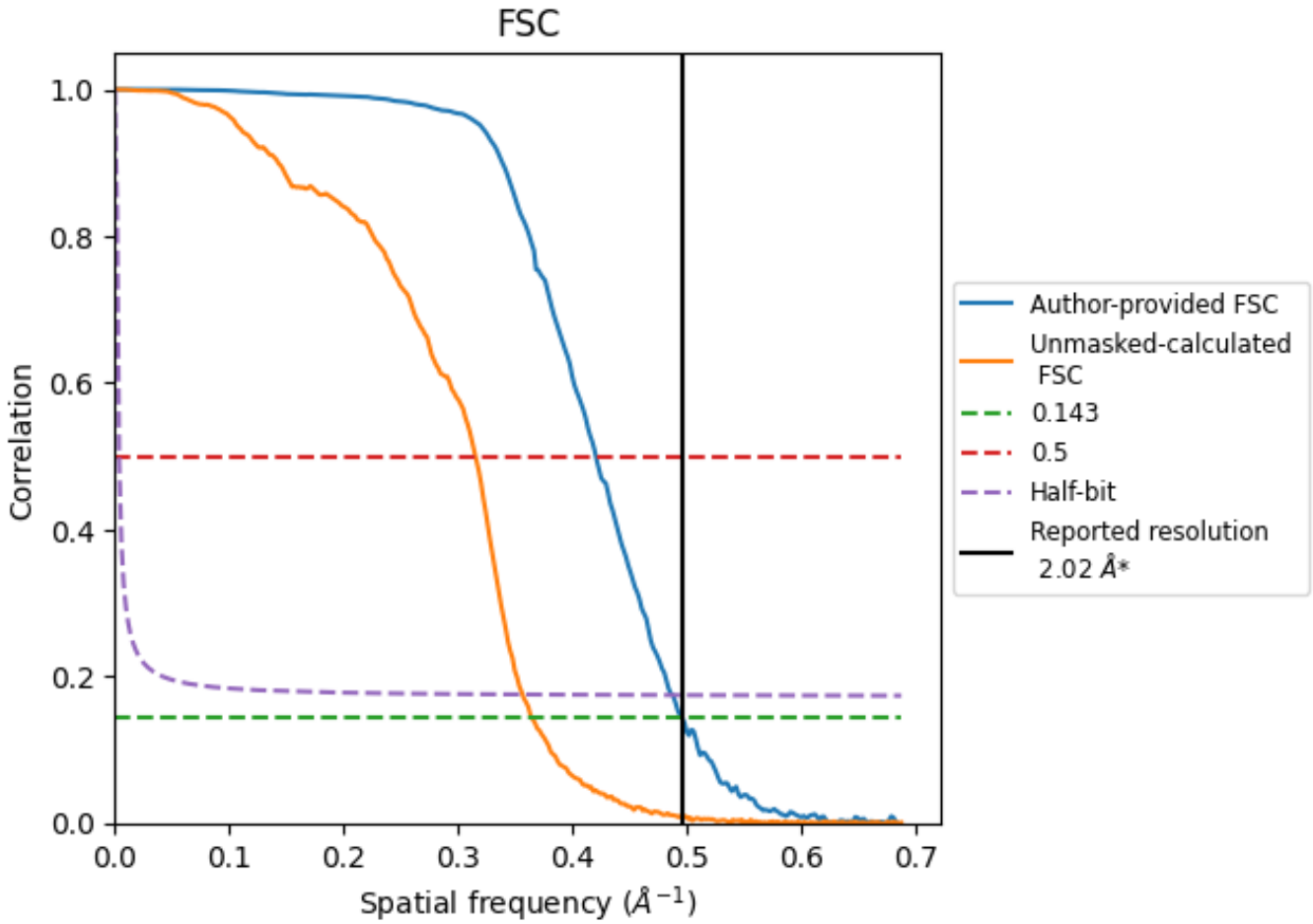


*Reported resolution corresponds to spatial frequency of 0.495 Å^{-1}

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 0.495 Å^{-1}

8.2 Resolution estimates (i)

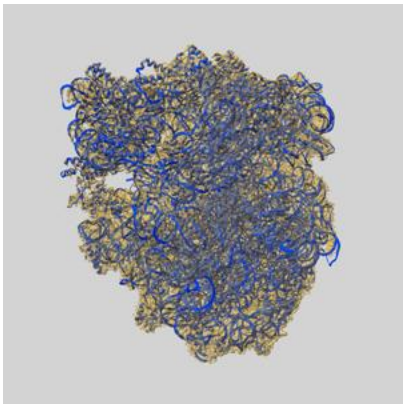
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.02	-	-
Author-provided FSC curve	2.02	2.38	2.05
Unmasked-calculated*	2.74	3.18	2.81

*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 2.74 differs from the reported value 2.02 by more than 10 %

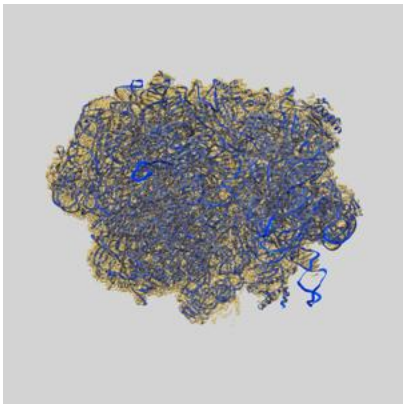
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-17364 and PDB model 8P2G. Per-residue inclusion information can be found in section 3 on page 18.

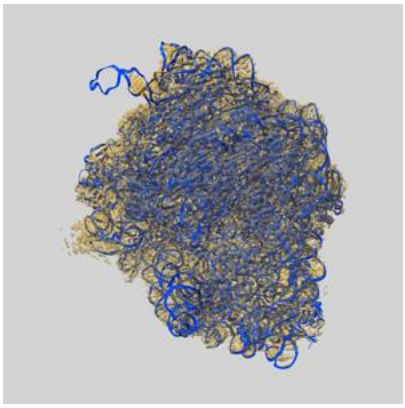
9.1 Map-model overlay



X



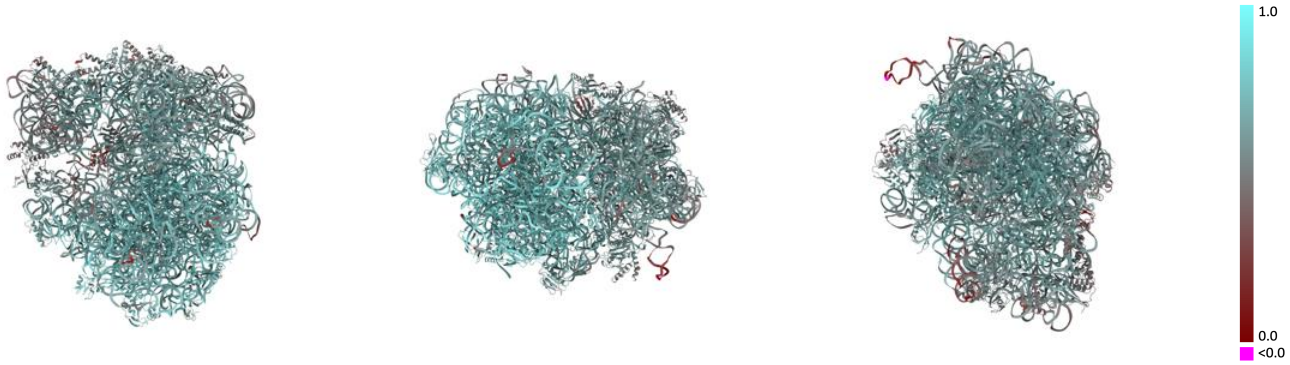
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.2 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.

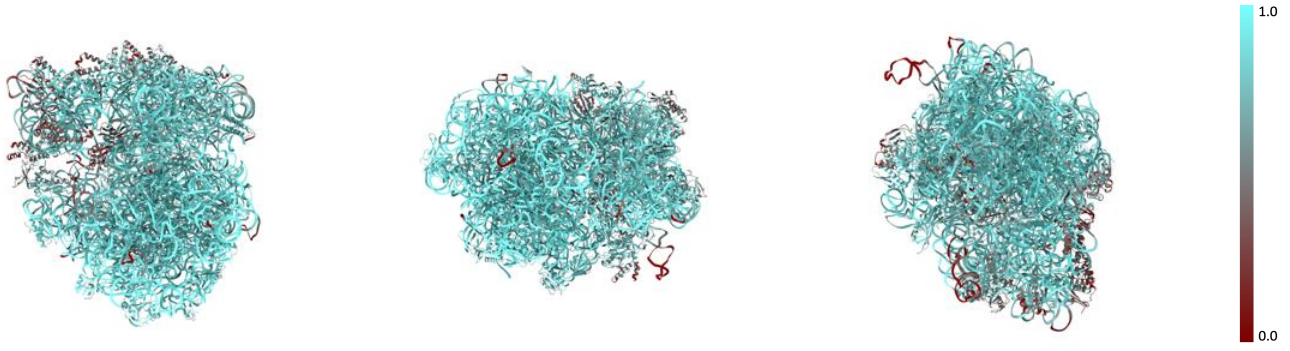
9.2 Q-score mapped to coordinate model



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.

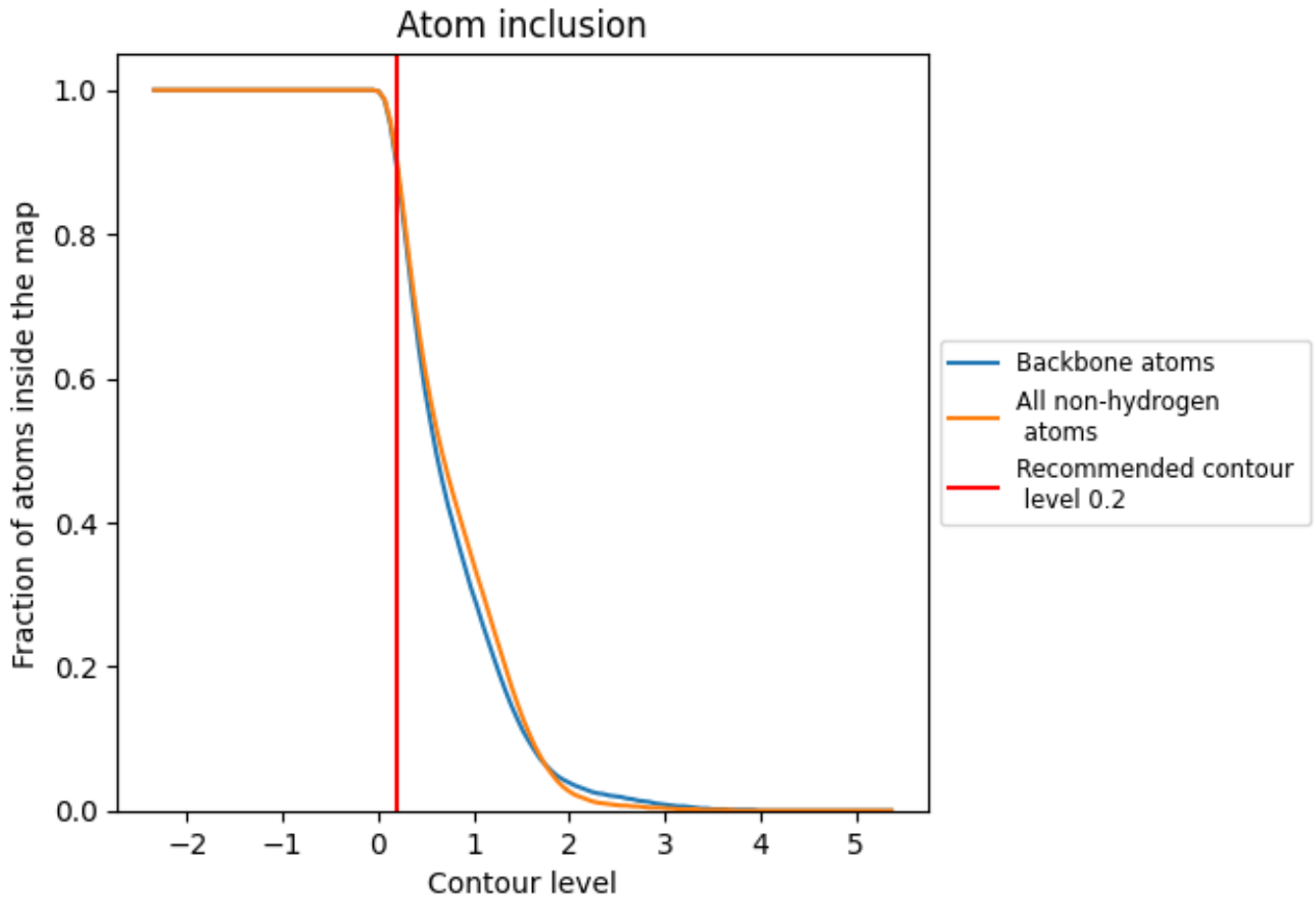
9.3 Atom inclusion mapped to coordinate model



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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 89% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8970	0.6800
1	0.9550	0.7240
2	0.9130	0.7070
3	0.9770	0.7720
4	0.5200	0.5110
5	0.9680	0.7770
6	0.9380	0.7110
7	0.9910	0.8040
8	0.9980	0.8050
9	0.9590	0.7600
A	0.9670	0.7400
B	0.9710	0.6700
D	0.8320	0.5880
E	0.6810	0.5720
G	0.9780	0.7860
H	0.9740	0.7830
I	0.9540	0.7550
J	0.7220	0.5760
K	0.8620	0.6300
M	0.9720	0.7750
N	0.9860	0.7870
O	0.9610	0.7570
P	0.9640	0.7580
Q	0.9730	0.7840
R	0.9070	0.6560
S	0.9550	0.7590
T	0.9860	0.7960
U	0.9680	0.7670
V	0.9700	0.7830
W	0.9510	0.7350
X	0.8600	0.6510
Y	0.8770	0.6440
Z	0.9690	0.7710
a	0.8870	0.6160
b	0.6130	0.5370

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c	0.6010	0.5320
d	0.7450	0.5800
e	0.7350	0.5560
f	0.8970	0.6530
g	0.6940	0.5650
h	0.4300	0.4790
i	0.8380	0.6030
j	0.6240	0.5520
k	0.6570	0.5470
l	0.4800	0.4110
m	0.9110	0.6650
n	0.5180	0.5010
o	0.8790	0.6510
p	0.8310	0.6050
q	0.7800	0.5860
r	0.8030	0.5910
s	0.7650	0.5650
t	0.6380	0.5480
u	0.8730	0.6380