wwPDB EM Validation Summary Report

Apr 22, 2025 – 04:21 pm BST

PDB ID	:	9GHA / pdb_00009gha
EMDB ID	:	EMD-51350
Title	:	Fusidic acid-locked Escherichia coli 70S ribosome with Staphylococcus aureus EF-G and a tRNA in pe/E chimeric state (CHI)
Authors	:	Gonzalez-Lopez, A.; Selmer, M.
Deposited on	:	2024-08-15
Resolution	:	2.24 Å(reported)
Based on initial models	:	9GHE, 8P2H, 7N2C

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:

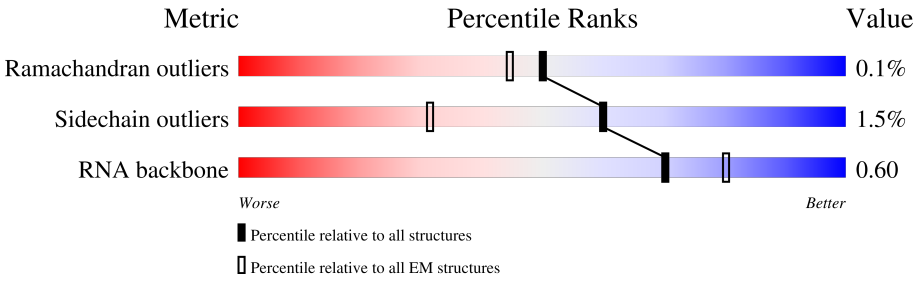
EMDB validation analysis	:	0.0.1.dev117
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.24 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	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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	0	55	87% · 9%
2	1	46	98% ·
3	2	65	95% · ·
4	3	38	97% ·
5	4	70	· 69% 31%
6	8	77	81% 19%
7	9	24	21% 79%
8	A	1554	· 82% 16% ·

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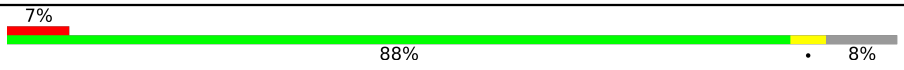
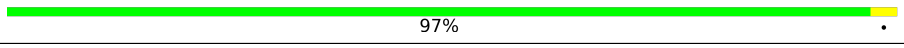
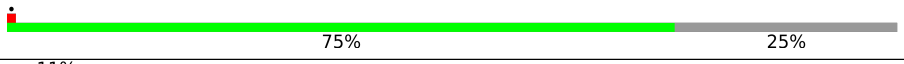
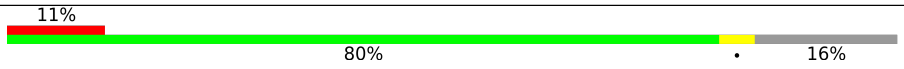
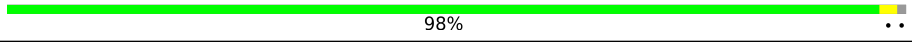
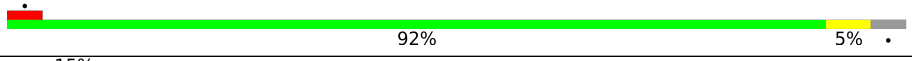
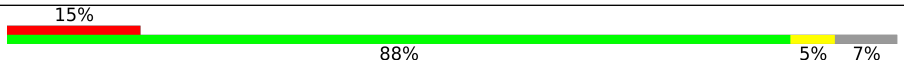
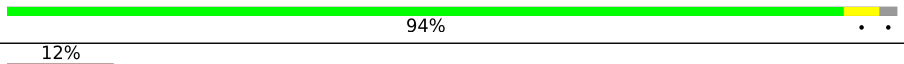
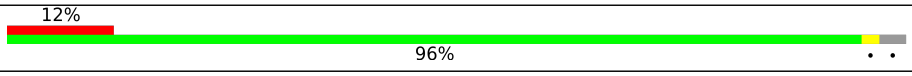
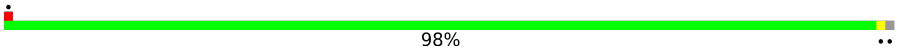
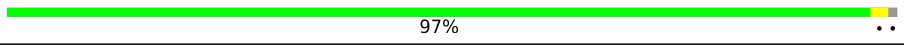
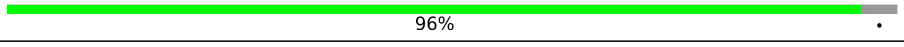
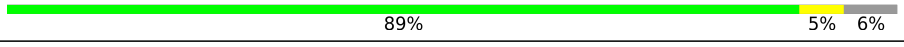
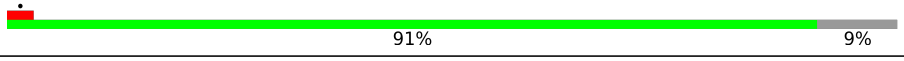
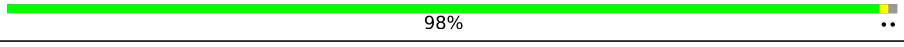
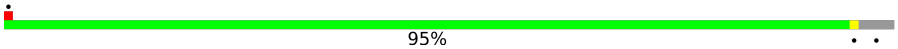
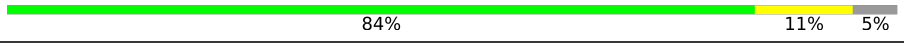
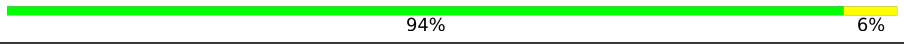
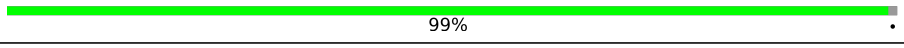
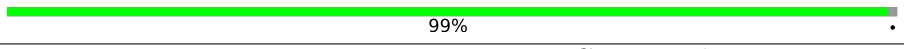
Mol	Chain	Length	Quality of chain
9	B	241	
10	C	233	
11	D	206	
12	E	167	
13	F	135	
14	G	179	
15	H	130	
16	I	130	
17	J	103	
18	K	129	
19	L	124	
20	M	118	
21	N	101	
22	O	89	
23	P	82	
24	Q	84	
25	R	75	
26	S	92	
27	T	87	
28	U	71	
29	W	693	
30	a	2930	
31	b	119	
32	c	273	
33	d	209	

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Mol	Chain	Length	Quality of chain
34	e	201	100%
35	f	179	94%
36	g	177	93%
37	h	149	28% 72%
38	i	142	98%
39	j	123	98%
40	k	144	99%
41	l	136	99%
42	m	127	93% 7%
43	n	117	97%
44	o	115	98%
45	p	118	98%
46	q	103	98%
47	r	110	99%
48	s	100	93% 7%
49	t	104	88% 11%
50	u	94	99%
51	v	85	88% 12%
52	w	78	97%
53	x	63	94% 5%
54	y	59	98%
55	z	57	95% 5%

2 Entry composition (i)

There are 60 unique types of molecules in this entry. The entry contains 145564 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	0	50	413	267	75	71	0	0

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	45	367	222	88	55	2	0	0

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	64	504	323	105	74	2	0	0

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	38	302	185	65	48	4	0	0

- Molecule 5 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	48	373	232	66	69	6	0	0

- Molecule 6 is a RNA chain called tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	8	77	1640	732	297	535	76	0	0

- Molecule 7 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	5	Total	C	N	O	P	0	0
			110	49	22	34	5		

- Molecule 8 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	1526	Total	C	N	O	P	0	0
			32757	14617	6009	10605	1526		

- Molecule 9 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	222	Total	C	N	O	S	0	0
			1737	1099	312	318	8		

- Molecule 10 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 11 is a protein called 30S ribosomal protein S4.

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

- Molecule 12 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	154	Total	C	N	O	S	0	0
			1135	706	215	208	6		

- Molecule 13 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	F	101	Total	C	N	O	S	0	0
			824	520	149	149	6		

- Molecule 14 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	150	Total	C	N	O	S	0	0
			1176	732	226	214	4		

- Molecule 15 is a protein called 30S ribosomal protein S8.

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

- Molecule 16 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	125	Total	C	N	O	S	0	0
			1001	622	200	176	3		

- Molecule 17 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	96	Total	C	N	O	S	0	0
			775	487	148	139	1		

- Molecule 18 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	modified residue	UNP P0A7R9

- Molecule 19 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 20 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 21 is a protein called 30S ribosomal protein S14.

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

- Molecule 22 is a protein called 30S ribosomal protein S15.

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

- Molecule 23 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 24 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 25 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	64	Total	C	N	O	S	0	0
			524	330	99	94	1		

- Molecule 26 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 27 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 28 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	U	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 29 is a protein called Elongation factor G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	666	Total	C	N	O	S	0	0
			5154	3232	865	1028	29		

- Molecule 30 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2782	Total	C	N	O	P	0	0
			59756	26665	11017	19292	2782		

- Molecule 31 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 32 is a protein called 50S ribosomal protein L2.

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

- Molecule 33 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	207	Total	C	N	O	S	0	0
			1552	972	286	291	3		

- Molecule 34 is a protein called 50S ribosomal protein L4.

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

- Molecule 35 is a protein called 50S ribosomal protein L5.

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

- Molecule 36 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	170	Total	C	N	O	S	0	0
			1273	803	232	236	2		

- Molecule 37 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 38 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	141	Total	C	N	O	S	0	0
			1121	709	211	198	3		

- Molecule 39 is a protein called 50S ribosomal protein L14.

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

- Molecule 40 is a protein called 50S ribosomal protein L15.

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

- Molecule 41 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	modified residue	UNP P0ADY7

- Molecule 42 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 43 is a protein called 50S ribosomal protein L18.

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

- Molecule 44 is a protein called 50S ribosomal protein L19.

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

- Molecule 45 is a protein called 50S ribosomal protein L20.

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

- Molecule 46 is a protein called 50S ribosomal protein L21.

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

- Molecule 47 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	109	Total	C	N	O	S	0	0
			845	526	162	154	3		

- Molecule 48 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

- Molecule 49 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
49	t	93	Total	C	N	O	0	0
			717	452	135	130		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	93	Total	C	N	O	S	0	0
			745	474	136	133	2		

- Molecule 51 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	75	Total	C	N	O	S	0	0
			569	353	113	102	1		

- Molecule 52 is a protein called 50S ribosomal protein L28.

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

- Molecule 53 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	60	Total	C	N	O	S	0	0
			491	303	96	91	1		

- Molecule 54 is a protein called 50S ribosomal protein L30.

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

- Molecule 55 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
57	A	14	Total	K	0
			14	14	
57	F	1	Total	K	0
			1	1	
57	a	74	Total	K	0
			74	74	
57	c	3	Total	K	0
			3	3	
57	e	1	Total	K	0
			1	1	
57	t	1	Total	K	0
			1	1	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	27	Total	Mg	0
			27	27	
58	W	1	Total	Mg	0
			1	1	
58	a	233	Total	Mg	0
			233	233	

Continued on next page...

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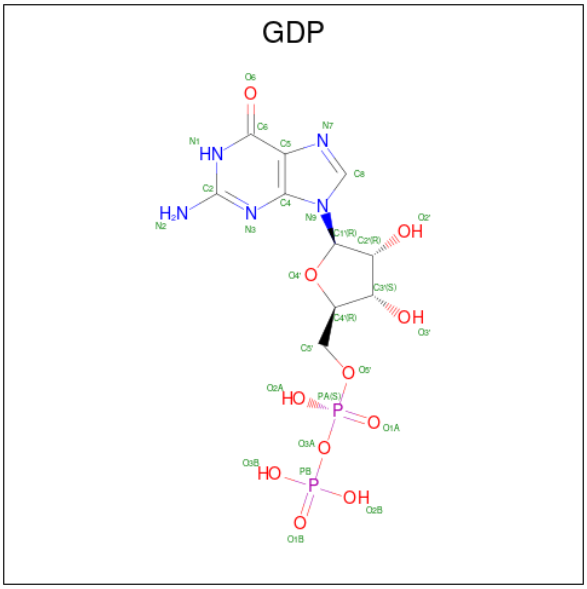
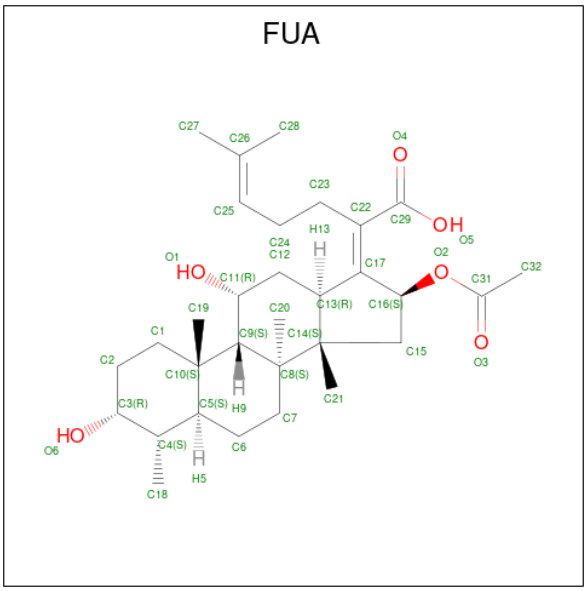
Mol	Chain	Residues	Atoms	AltConf
58	b	3	Total Mg 3 3	0
58	c	3	Total Mg 3 3	0
58	d	2	Total Mg 2 2	0
58	k	1	Total Mg 1 1	0
58	z	1	Total Mg 1 1	0

- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 60 is FUSIDIC ACID (CCD ID: FUA) (formula: $C_{31}H_{48}O_6$) (labeled as "Ligand of Interest" by depositor).



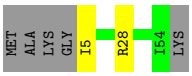
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
60	W	1	37	31	6	0

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.

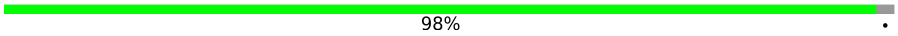
- Molecule 1: 50S ribosomal protein L33

Chain 0:



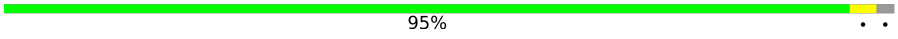
- Molecule 2: 50S ribosomal protein L34

Chain 1:



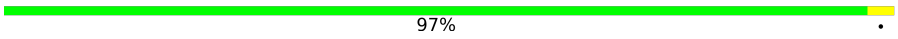
- Molecule 3: 50S ribosomal protein L35

Chain 2:



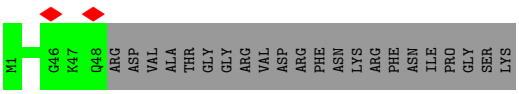
- Molecule 4: 50S ribosomal protein L36

Chain 3:



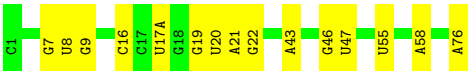
- Molecule 5: 50S ribosomal protein L31

Chain 4:



- Molecule 6: tRNA

Chain 8:

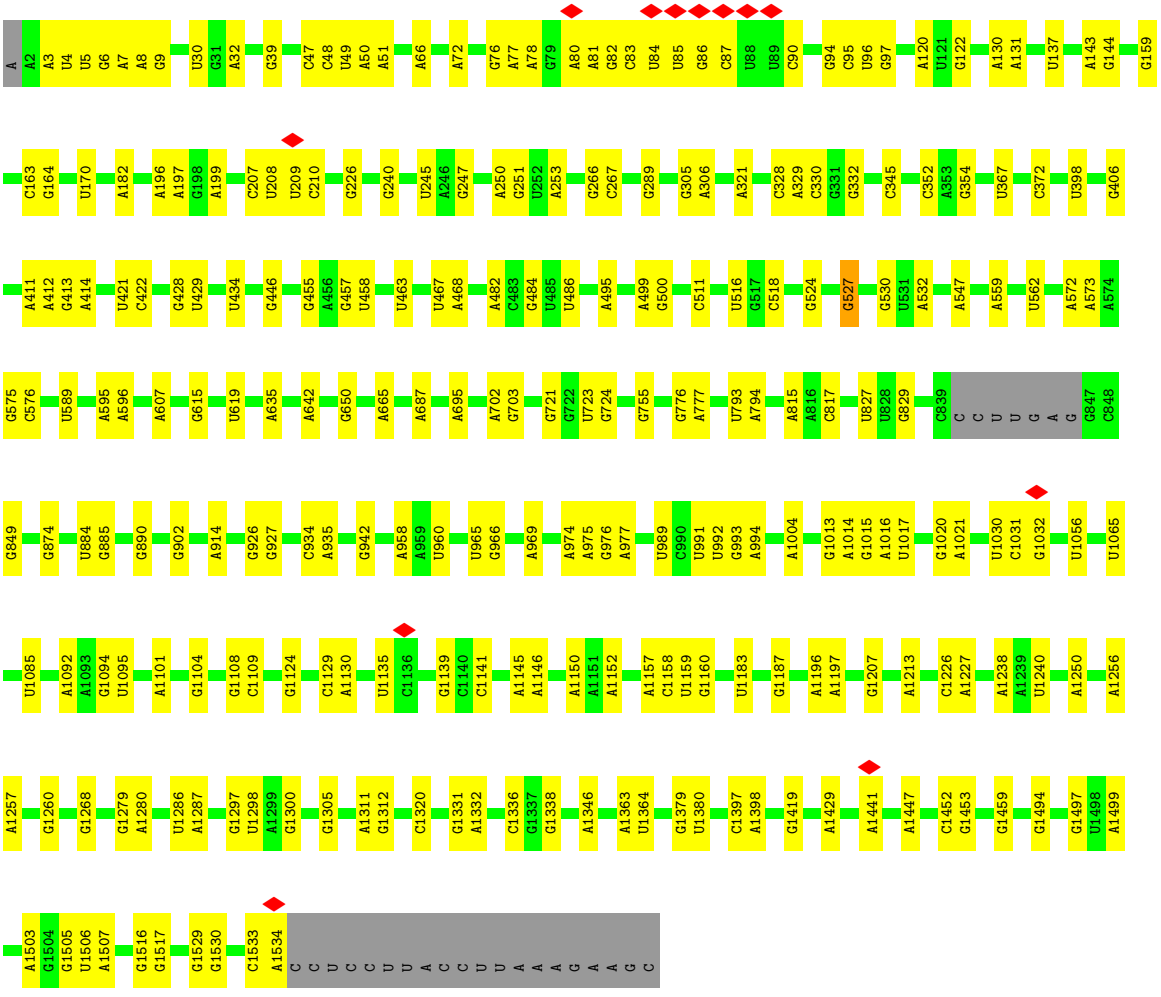


• Molecule 7: mRNA

Chain 9:

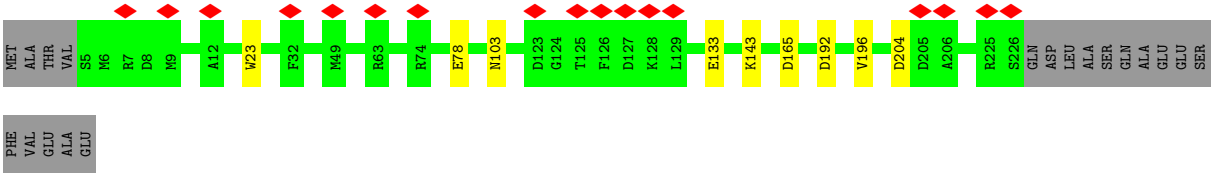
• Molecule 8: 16S rRNA

Chain A:



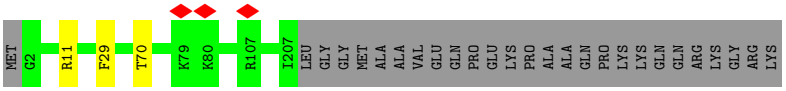
• Molecule 9: 30S ribosomal protein S2

Chain B:



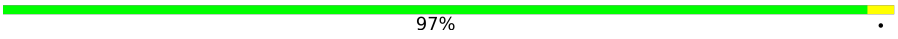
• Molecule 10: 30S ribosomal protein S3

Chain C:



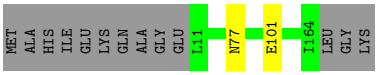
• Molecule 11: 30S ribosomal protein S4

Chain D:



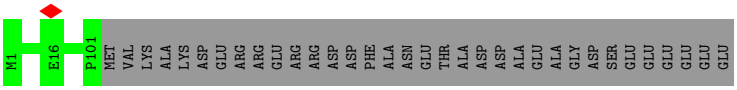
• Molecule 12: 30S ribosomal protein S5

Chain E:



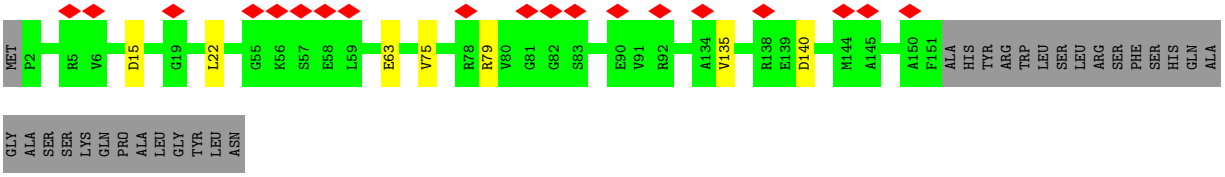
• Molecule 13: 30S ribosomal protein S6

Chain F:



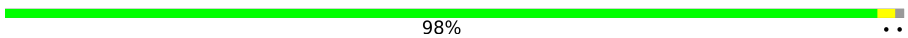
• Molecule 14: 30S ribosomal protein S7

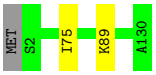
Chain G:



• Molecule 15: 30S ribosomal protein S8

Chain H:



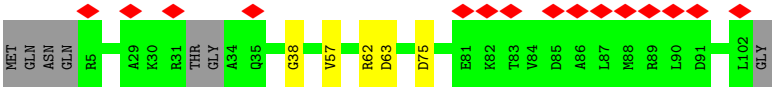


• Molecule 16: 30S ribosomal protein S9

Chain I:

• Molecule 17: 30S ribosomal protein S10

Chain J:

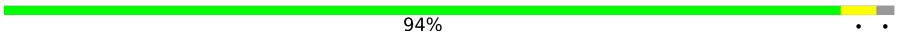


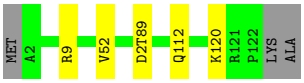
• Molecule 18: Small ribosomal subunit protein uS11

Chain K:

• Molecule 19: 30S ribosomal protein S12

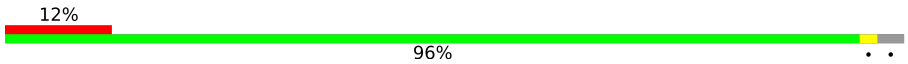
Chain L:

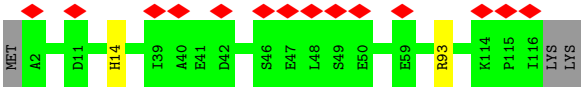




• Molecule 20: 30S ribosomal protein S13

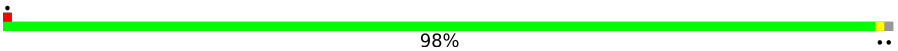
Chain M:

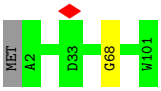




• Molecule 21: 30S ribosomal protein S14

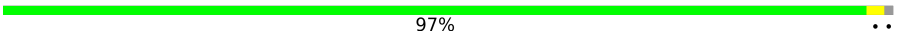
Chain N:





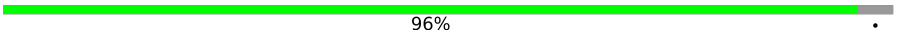
• Molecule 22: 30S ribosomal protein S15

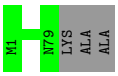
Chain O:



• Molecule 23: 30S ribosomal protein S16

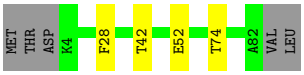
Chain P:





• Molecule 24: 30S ribosomal protein S17

Chain Q:

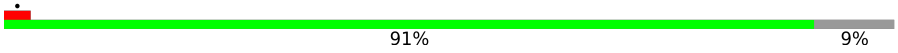


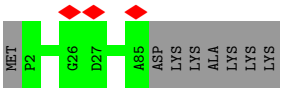
• Molecule 25: 30S ribosomal protein S18

Chain R:

• Molecule 26: 30S ribosomal protein S19

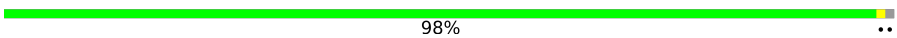
Chain S:

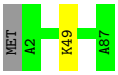




• Molecule 27: 30S ribosomal protein S20

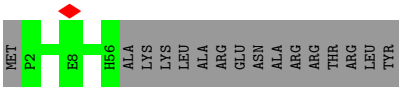
Chain T:





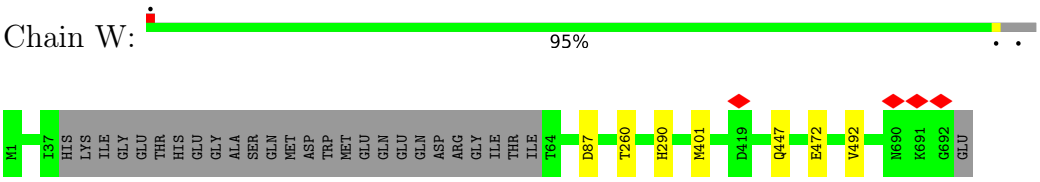
• Molecule 28: 30S ribosomal protein S21

Chain U:



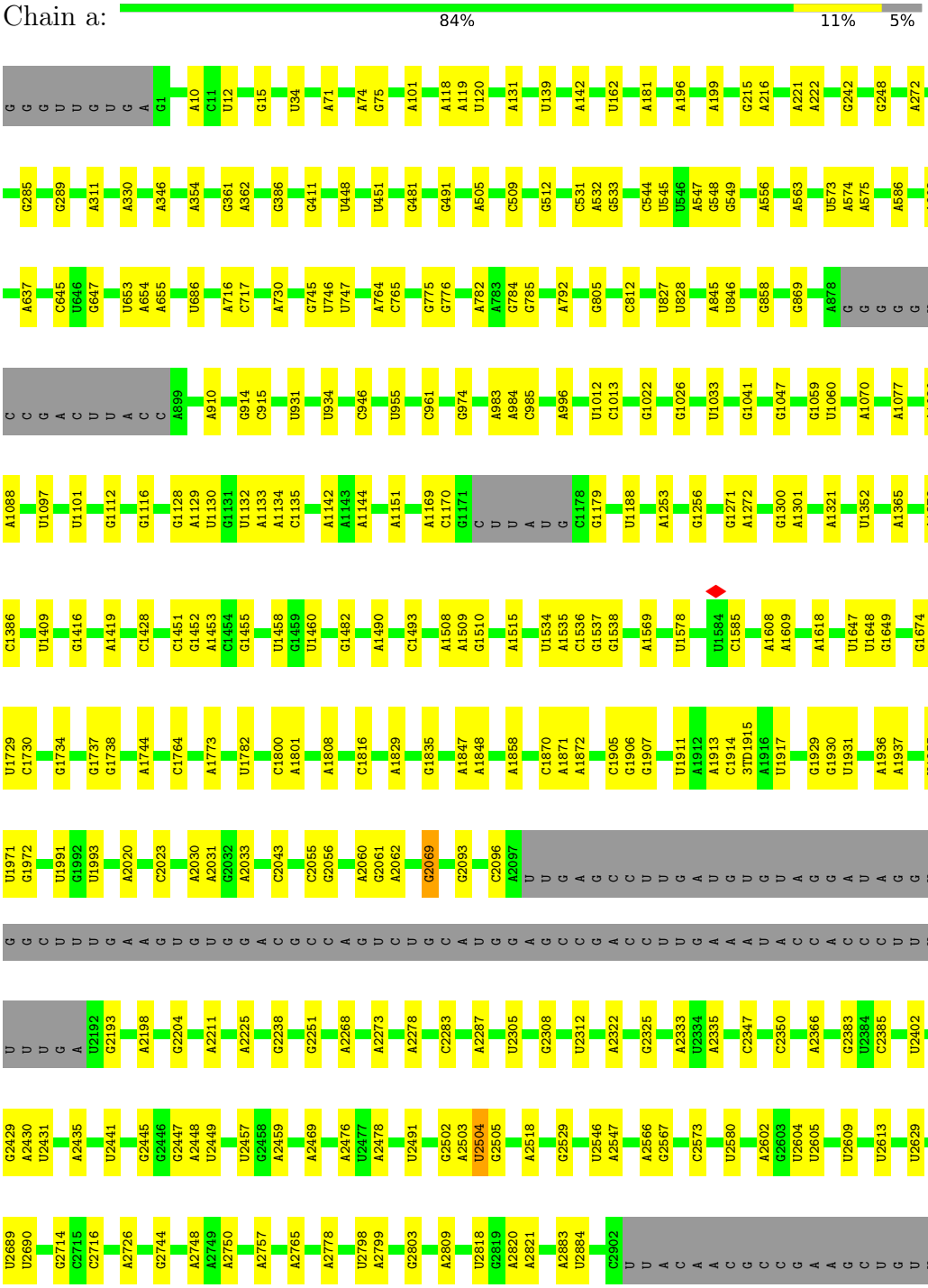
• Molecule 29: Elongation factor G

Chain W:



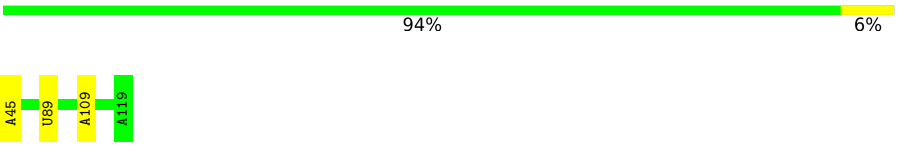
• Molecule 30: 23S rRNA

Chain a:



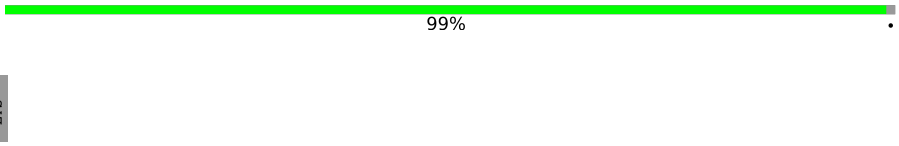
• Molecule 31: 5S rRNA

Chain b:



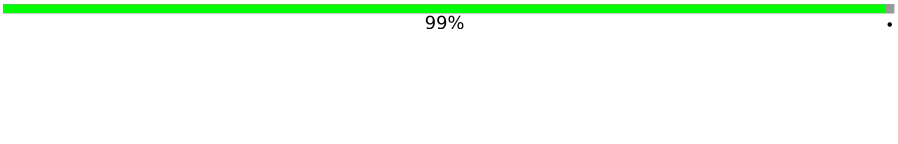
• Molecule 32: 50S ribosomal protein L2

Chain c:



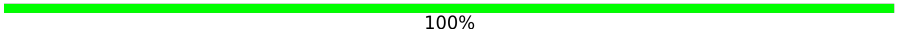
• Molecule 33: 50S ribosomal protein L3

Chain d:



• Molecule 34: 50S ribosomal protein L4

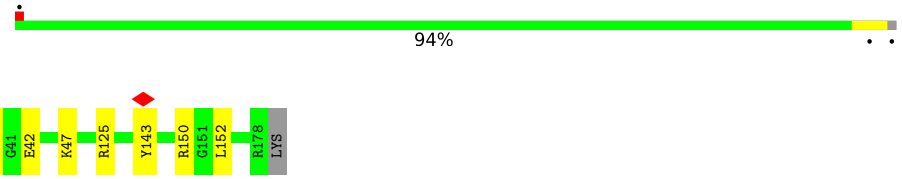
Chain e:



There are no outlier residues recorded for this chain.

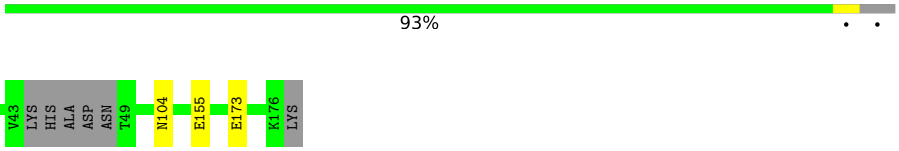
• Molecule 35: 50S ribosomal protein L5

Chain f:



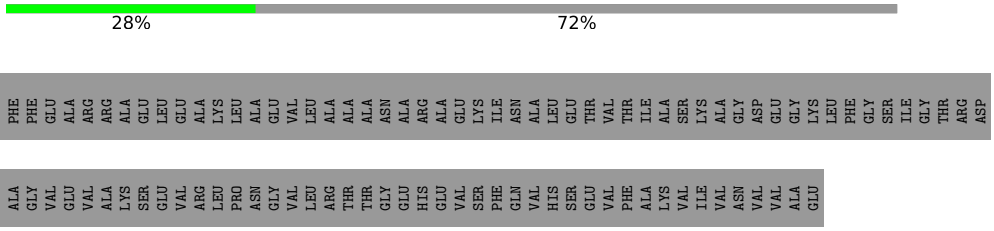
• Molecule 36: 50S ribosomal protein L6

Chain g:



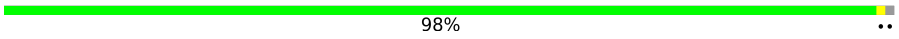
• Molecule 37: 50S ribosomal protein L9

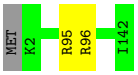
Chain h:



• Molecule 38: 50S ribosomal protein L13

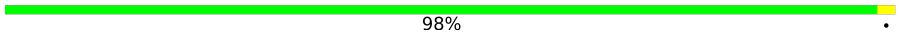
Chain i:





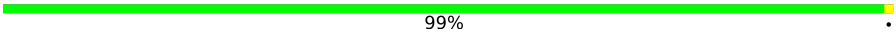
• Molecule 39: 50S ribosomal protein L14

Chain j:



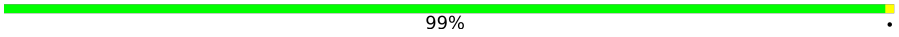
• Molecule 40: 50S ribosomal protein L15

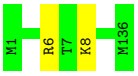
Chain k:



• Molecule 41: 50S ribosomal protein L16

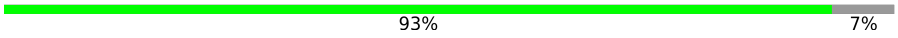
Chain l:





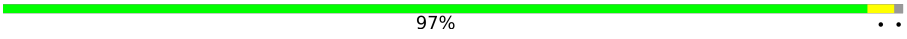
• Molecule 42: 50S ribosomal protein L17

Chain m:



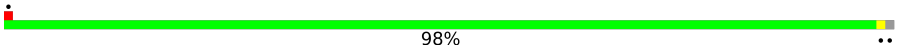
• Molecule 43: 50S ribosomal protein L18

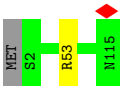
Chain n:



• Molecule 44: 50S ribosomal protein L19

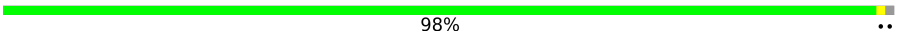
Chain o:





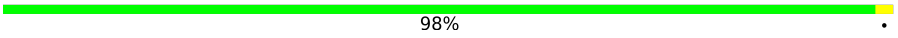
• Molecule 45: 50S ribosomal protein L20

Chain p:



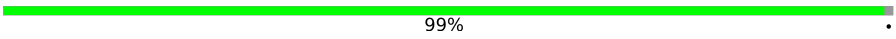
• Molecule 46: 50S ribosomal protein L21

Chain q:



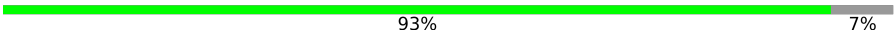
• Molecule 47: 50S ribosomal protein L22

Chain r:



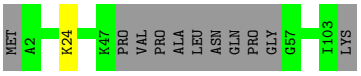
• Molecule 48: 50S ribosomal protein L23

Chain s:



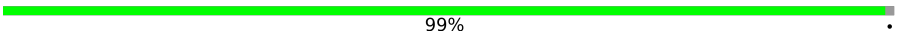
• Molecule 49: 50S ribosomal protein L24

Chain t:



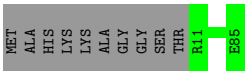
• Molecule 50: 50S ribosomal protein L25

Chain u:



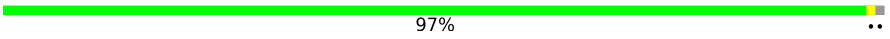
• Molecule 51: 50S ribosomal protein L27

Chain v:



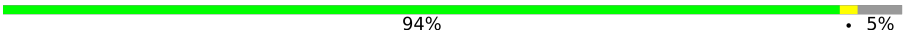
• Molecule 52: 50S ribosomal protein L28

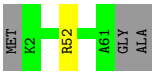
Chain w:



• Molecule 53: 50S ribosomal protein L29

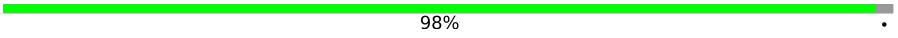
Chain x:





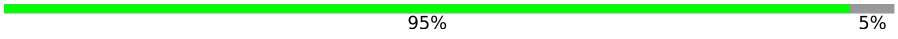
• Molecule 54: 50S ribosomal protein L30

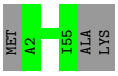
Chain y:



• Molecule 55: 50S ribosomal protein L32

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	88568	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.714	Depositor
Minimum map value	-0.317	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	388.8, 388.8, 388.8	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.648, 0.648, 0.648	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: PSU, MS6, ZN, MA6, 3TD, MEQ, MG, D2T, 4OC, H2U, 2MG, OMU, IAS, 6MZ, OMC, 5MU, 5MC, UR3, 4D4, GDP, FUA, G7M, 2MA, K, OMG, 1MG

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	0	0.31	0/420	0.52	0/560
2	1	0.29	0/370	0.61	0/487
3	2	0.32	0/513	0.55	0/676
4	3	0.30	0/303	0.57	0/397
5	4	0.31	0/380	0.53	0/508
6	8	0.46	0/1832	0.89	0/2855
7	9	0.55	0/123	0.86	0/190
8	A	0.44	0/36398	0.88	0/56774
9	B	0.29	0/1768	0.53	0/2381
10	C	0.28	0/1651	0.51	0/2225
11	D	0.29	0/1665	0.52	0/2227
12	E	0.29	0/1148	0.52	0/1545
13	F	0.28	0/843	0.49	0/1140
14	G	0.29	0/1190	0.53	0/1595
15	H	0.29	0/989	0.55	0/1326
16	I	0.29	0/1013	0.53	0/1350
17	J	0.28	0/784	0.59	0/1059
18	K	0.31	0/884	0.53	0/1191
19	L	0.29	0/945	0.58	0/1268
20	M	0.29	0/900	0.53	0/1204
21	N	0.30	0/817	0.51	0/1088
22	O	0.28	0/722	0.50	0/964
23	P	0.28	0/639	0.54	0/859
24	Q	0.28	0/650	0.53	0/871
25	R	0.29	0/532	0.52	0/715
26	S	0.32	0/685	0.52	0/922
27	T	0.28	0/676	0.50	0/895
28	U	0.31	0/467	0.58	0/620
29	W	0.29	0/5244	0.49	0/7091
30	a	0.42	0/66355	0.90	8/103511 (0.0%)
31	b	0.44	0/2850	0.90	0/4444

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	c	0.29	0/2121	0.56	0/2852
33	d	0.29	0/1562	0.54	0/2102
34	e	0.28	0/1571	0.51	0/2113
35	f	0.29	0/1434	0.52	0/1926
36	g	0.29	0/1291	0.54	0/1747
37	h	0.30	0/306	0.53	0/413
38	i	0.28	0/1144	0.54	0/1541
39	j	0.28	0/955	0.57	0/1279
40	k	0.31	0/1062	0.54	0/1413
41	l	0.29	0/1073	0.55	0/1433
42	m	0.28	0/958	0.55	0/1281
43	n	0.29	0/902	0.54	0/1209
44	o	0.29	0/929	0.55	0/1242
45	p	0.29	0/960	0.56	0/1278
46	q	0.29	0/829	0.54	0/1107
47	r	0.28	0/852	0.56	0/1142
48	s	0.27	0/744	0.51	0/994
49	t	0.30	0/721	0.54	0/956
50	u	0.29	0/758	0.54	0/1015
51	v	0.32	0/576	0.56	0/762
52	w	0.30	0/635	0.57	0/848
53	x	0.27	0/492	0.49	0/655
54	y	0.29	0/453	0.52	0/605
55	z	0.30	0/435	0.56	0/581
All	All	0.39	0/156519	0.81	8/233432 (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
3	2	0	1
4	3	0	1
10	C	0	1
11	D	0	1
14	G	0	1
16	I	0	2
17	J	0	2
18	K	0	1
19	L	0	1
36	g	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
38	i	0	1
45	p	0	1
52	w	0	1
53	x	0	1
All	All	0	16

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	512	G	O4'-C1'-N9	7.53	114.23	108.20
30	a	2447	G	C3'-C2'-C1'	-5.94	96.75	101.50
30	a	2546	U	O3'-P-O5'	-5.94	92.71	104.00
30	a	512	G	C1'-O4'-C4'	-5.93	105.16	109.90
30	a	1936	A	C1'-O4'-C4'	-5.50	105.50	109.90

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	2	13	ARG	Sidechain
4	3	36	ARG	Sidechain
10	C	11	ARG	Sidechain
11	D	184	ARG	Sidechain
14	G	79	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	
1	0	48/55 (87%)	48 (100%)	0	0	100	100
2	1	43/46 (94%)	43 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	46/70 (66%)	45 (98%)	1 (2%)	0	100	100
9	B	220/241 (91%)	214 (97%)	5 (2%)	1 (0%)	25	24
10	C	204/233 (88%)	197 (97%)	7 (3%)	0	100	100
11	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
12	E	152/167 (91%)	148 (97%)	4 (3%)	0	100	100
13	F	99/135 (73%)	95 (96%)	4 (4%)	0	100	100
14	G	148/179 (83%)	145 (98%)	3 (2%)	0	100	100
15	H	127/130 (98%)	124 (98%)	2 (2%)	1 (1%)	16	13
16	I	123/130 (95%)	118 (96%)	5 (4%)	0	100	100
17	J	92/103 (89%)	88 (96%)	3 (3%)	1 (1%)	12	8
18	K	113/129 (88%)	107 (95%)	6 (5%)	0	100	100
19	L	118/124 (95%)	111 (94%)	7 (6%)	0	100	100
20	M	113/118 (96%)	110 (97%)	3 (3%)	0	100	100
21	N	98/101 (97%)	95 (97%)	2 (2%)	1 (1%)	13	9
22	O	86/89 (97%)	85 (99%)	1 (1%)	0	100	100
23	P	77/82 (94%)	74 (96%)	3 (4%)	0	100	100
24	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
25	R	62/75 (83%)	62 (100%)	0	0	100	100
26	S	82/92 (89%)	81 (99%)	1 (1%)	0	100	100
27	T	84/87 (97%)	84 (100%)	0	0	100	100
28	U	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
29	W	662/693 (96%)	647 (98%)	15 (2%)	0	100	100
32	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
33	d	204/209 (98%)	198 (97%)	6 (3%)	0	100	100
34	e	199/201 (99%)	194 (98%)	5 (2%)	0	100	100
35	f	175/179 (98%)	170 (97%)	4 (2%)	1 (1%)	22	20
36	g	166/177 (94%)	164 (99%)	2 (1%)	0	100	100
37	h	39/149 (26%)	37 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
38	i	139/142 (98%)	138 (99%)	1 (1%)	0	100 100
39	j	121/123 (98%)	117 (97%)	4 (3%)	0	100 100
40	k	142/144 (99%)	136 (96%)	5 (4%)	1 (1%)	19 17
41	l	132/136 (97%)	129 (98%)	3 (2%)	0	100 100
42	m	116/127 (91%)	112 (97%)	4 (3%)	0	100 100
43	n	114/117 (97%)	110 (96%)	4 (4%)	0	100 100
44	o	112/115 (97%)	110 (98%)	2 (2%)	0	100 100
45	p	115/118 (98%)	114 (99%)	1 (1%)	0	100 100
46	q	101/103 (98%)	100 (99%)	0	1 (1%)	13 9
47	r	107/110 (97%)	105 (98%)	2 (2%)	0	100 100
48	s	91/100 (91%)	88 (97%)	3 (3%)	0	100 100
49	t	89/104 (86%)	88 (99%)	1 (1%)	0	100 100
50	u	91/94 (97%)	88 (97%)	3 (3%)	0	100 100
51	v	73/85 (86%)	71 (97%)	2 (3%)	0	100 100
52	w	75/78 (96%)	75 (100%)	0	0	100 100
53	x	58/63 (92%)	58 (100%)	0	0	100 100
54	y	56/59 (95%)	55 (98%)	1 (2%)	0	100 100
55	z	52/57 (91%)	51 (98%)	1 (2%)	0	100 100
All	All	6064/6606 (92%)	5915 (98%)	142 (2%)	7 (0%)	50 55

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	J	57	VAL
35	f	42	GLU
9	B	165	ASP
40	k	29	LYS
15	H	75	ILE

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	0	46/49 (94%)	44 (96%)	2 (4%)	25 26
2	1	37/38 (97%)	37 (100%)	0	100 100
3	2	51/52 (98%)	50 (98%)	1 (2%)	50 57
4	3	34/34 (100%)	34 (100%)	0	100 100
5	4	44/62 (71%)	44 (100%)	0	100 100
9	B	184/199 (92%)	176 (96%)	8 (4%)	25 26
10	C	170/190 (90%)	168 (99%)	2 (1%)	67 75
11	D	172/173 (99%)	167 (97%)	5 (3%)	37 43
12	E	117/126 (93%)	115 (98%)	2 (2%)	56 64
13	F	88/116 (76%)	88 (100%)	0	100 100
14	G	124/147 (84%)	118 (95%)	6 (5%)	21 21
15	H	104/105 (99%)	103 (99%)	1 (1%)	73 79
16	I	103/107 (96%)	99 (96%)	4 (4%)	27 30
17	J	85/90 (94%)	83 (98%)	2 (2%)	44 50
18	K	89/98 (91%)	89 (100%)	0	100 100
19	L	101/103 (98%)	98 (97%)	3 (3%)	36 42
20	M	93/96 (97%)	91 (98%)	2 (2%)	47 54
21	N	83/84 (99%)	83 (100%)	0	100 100
22	O	76/77 (99%)	74 (97%)	2 (3%)	41 47
23	P	64/65 (98%)	64 (100%)	0	100 100
24	Q	73/78 (94%)	69 (94%)	4 (6%)	18 16
25	R	55/65 (85%)	55 (100%)	0	100 100
26	S	72/79 (91%)	72 (100%)	0	100 100
27	T	65/66 (98%)	64 (98%)	1 (2%)	60 69
28	U	48/61 (79%)	48 (100%)	0	100 100
29	W	556/579 (96%)	549 (99%)	7 (1%)	65 73
32	c	216/218 (99%)	215 (100%)	1 (0%)	86 90
33	d	162/163 (99%)	162 (100%)	0	100 100
34	e	165/165 (100%)	165 (100%)	0	100 100
35	f	148/150 (99%)	141 (95%)	7 (5%)	22 23
36	g	132/138 (96%)	128 (97%)	4 (3%)	36 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
37	h	32/114 (28%)	32 (100%)	0	100 100
38	i	115/116 (99%)	114 (99%)	1 (1%)	75 82
39	j	104/104 (100%)	102 (98%)	2 (2%)	52 60
40	k	103/103 (100%)	103 (100%)	0	100 100
41	l	107/107 (100%)	105 (98%)	2 (2%)	52 60
42	m	98/103 (95%)	98 (100%)	0	100 100
43	n	86/87 (99%)	83 (96%)	3 (4%)	31 35
44	o	99/100 (99%)	98 (99%)	1 (1%)	73 79
45	p	89/90 (99%)	89 (100%)	0	100 100
46	q	84/84 (100%)	83 (99%)	1 (1%)	67 75
47	r	92/93 (99%)	92 (100%)	0	100 100
48	s	80/84 (95%)	80 (100%)	0	100 100
49	t	76/85 (89%)	75 (99%)	1 (1%)	65 73
50	u	77/78 (99%)	77 (100%)	0	100 100
51	v	56/63 (89%)	56 (100%)	0	100 100
52	w	67/68 (98%)	67 (100%)	0	100 100
53	x	54/55 (98%)	54 (100%)	0	100 100
54	y	48/49 (98%)	48 (100%)	0	100 100
55	z	46/48 (96%)	46 (100%)	0	100 100
All	All	5070/5404 (94%)	4995 (98%)	75 (2%)	60 69

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
35	f	143	TYR
43	n	90	VAL
35	f	152	LEU
39	j	49	ARG
14	G	135	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 34 such sidechains are listed below:

Mol	Chain	Res	Type
46	q	12	HIS

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Mol	Chain	Res	Type
46	q	43	ASN
50	u	49	ASN
17	J	58	ASN
14	G	148	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
30	a	2774/2930 (94%)	298 (10%)	0
31	b	118/119 (99%)	7 (5%)	0
6	8	76/77 (98%)	15 (19%)	3 (3%)
7	9	4/24 (16%)	0	0
8	A	1521/1554 (97%)	233 (15%)	47 (3%)
All	All	4493/4704 (95%)	553 (12%)	50 (1%)

5 of 553 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	8	7	G
6	8	8	U
6	8	9	G
6	8	16	C
6	8	17(A)	U

5 of 50 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	1031	C
8	A	1157	A
8	A	1505	G
8	A	1092	A
8	A	1124	G

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

39 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	$\#\|Z\| > 2$
8	4OC	A	1402	8	20,23,24	0.39	0	26,32,35	0.42	0
8	2MG	A	1207	8	18,26,27	1.04	2 (11%)	16,38,41	0.73	0
30	PSU	a	2604	30	18,21,22	0.91	1 (5%)	22,30,33	0.75	1 (4%)
8	2MG	A	1516	8	18,26,27	1.02	2 (11%)	16,38,41	0.82	0
30	6MZ	a	2030	30	18,25,26	0.70	0	16,36,39	0.75	1 (6%)
30	OMC	a	2498	30,58	19,22,23	0.28	0	26,31,34	0.53	0
30	PSU	a	2504	57,30	18,21,22	0.85	1 (5%)	22,30,33	0.76	0
19	D2T	L	89	19	7,9,10	0.94	0	6,11,13	1.85	4 (66%)
30	PSU	a	955	30	18,21,22	0.88	1 (5%)	22,30,33	0.65	0
30	2MA	a	2503	57,30,58	19,25,26	0.99	1 (5%)	21,37,40	1.78	5 (23%)
8	G7M	A	527	8	20,26,27	1.13	2 (10%)	17,39,42	0.30	0
30	PSU	a	1911	30	18,21,22	0.92	1 (5%)	22,30,33	0.66	0
30	OMU	a	2552	30	19,22,23	0.21	0	26,31,34	0.40	0
8	5MC	A	1407	8	18,22,23	0.32	0	26,32,35	0.54	0
41	4D4	l	81	41	9,11,12	0.55	0	8,13,15	0.70	0
30	PSU	a	2457	30	18,21,22	0.88	1 (5%)	22,30,33	0.62	0
18	IAS	K	119	18	6,7,8	0.91	0	6,8,10	0.99	0
30	OMG	a	2251	57,30	18,26,27	1.00	2 (11%)	19,38,41	0.69	0
30	6MZ	a	1618	30	18,25,26	0.66	0	16,36,39	0.74	1 (6%)
30	5MU	a	1939	57,30	19,22,23	0.30	0	28,32,35	0.37	0
33	MEQ	d	150	33	8,9,10	0.43	0	5,10,12	0.54	0
30	2MG	a	2445	30	18,26,27	1.01	2 (11%)	16,38,41	0.75	0
8	5MC	A	967	8	18,22,23	0.33	0	26,32,35	0.49	0
30	2MG	a	1835	30	18,26,27	1.02	2 (11%)	16,38,41	0.70	0
8	UR3	A	1498	8	19,22,23	0.28	0	26,32,35	0.64	0
30	PSU	a	746	30,58	18,21,22	0.95	1 (5%)	22,30,33	0.60	0
30	PSU	a	2580	57,30	18,21,22	0.90	1 (5%)	22,30,33	0.85	1 (4%)
30	5MU	a	747	30	19,22,23	0.26	0	28,32,35	0.42	0
8	MA6	A	1519	8	18,26,27	0.73	0	19,38,41	0.58	0
30	PSU	a	1917	30	18,21,22	0.89	1 (5%)	22,30,33	0.52	0
30	H2U	a	2449	30	18,21,22	0.60	0	21,30,33	0.88	2 (9%)
30	PSU	a	2605	30	18,21,22	0.90	1 (5%)	22,30,33	0.75	0
30	5MC	a	1962	30	18,22,23	0.34	0	26,32,35	0.50	0
30	G7M	a	2069	30	20,26,27	1.11	3 (15%)	17,39,42	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
30	3TD	a	1915	30	18,22,23	0.98	1 (5%)	22,32,35	0.62	0
8	PSU	A	516	8	18,21,22	0.91	1 (5%)	22,30,33	0.59	0
8	2MG	A	966	8	18,26,27	1.02	2 (11%)	16,38,41	0.70	0
30	1MG	a	745	30	18,26,27	0.97	1 (5%)	19,39,42	0.52	0
8	MA6	A	1518	8	18,26,27	0.75	0	19,38,41	0.45	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
8	4OC	A	1402	8	-	0/9/29/30	0/2/2/2
8	2MG	A	1207	8	-	0/5/27/28	0/3/3/3
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
8	2MG	A	1516	8	-	0/5/27/28	0/3/3/3
30	6MZ	a	2030	30	-	2/5/27/28	0/3/3/3
30	OMC	a	2498	30,58	-	0/9/27/28	0/2/2/2
30	PSU	a	2504	57,30	-	2/7/25/26	0/2/2/2
19	D2T	L	89	19	-	4/7/12/14	-
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
30	2MA	a	2503	57,30,58	-	1/3/25/26	0/3/3/3
8	G7M	A	527	8	-	2/3/25/26	0/3/3/3
30	PSU	a	1911	30	-	2/7/25/26	0/2/2/2
30	OMU	a	2552	30	-	0/9/27/28	0/2/2/2
8	5MC	A	1407	8	-	0/7/25/26	0/2/2/2
41	4D4	l	81	41	-	1/11/12/14	-
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
18	IAS	K	119	18	-	2/7/7/8	-
30	OMG	a	2251	57,30	-	1/5/27/28	0/3/3/3
30	6MZ	a	1618	30	-	0/5/27/28	0/3/3/3
30	5MU	a	1939	57,30	-	0/7/25/26	0/2/2/2
33	MEQ	d	150	33	-	2/8/9/11	-
30	2MG	a	2445	30	-	1/5/27/28	0/3/3/3
8	5MC	A	967	8	-	0/7/25/26	0/2/2/2
30	2MG	a	1835	30	-	0/5/27/28	0/3/3/3
8	UR3	A	1498	8	-	0/7/25/26	0/2/2/2
30	PSU	a	746	30,58	-	2/7/25/26	0/2/2/2
30	PSU	a	2580	57,30	-	0/7/25/26	0/2/2/2
30	5MU	a	747	30	-	1/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MA6	A	1519	8	-	0/7/29/30	0/3/3/3
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	2/7/25/26	0/2/2/2
30	G7M	a	2069	30	-	2/3/25/26	0/3/3/3
30	3TD	a	1915	30	-	0/7/25/26	0/2/2/2
8	PSU	A	516	8	-	0/7/25/26	0/2/2/2
8	2MG	A	966	8	-	2/5/27/28	0/3/3/3
30	1MG	a	745	30	-	0/3/25/26	0/3/3/3
8	MA6	A	1518	8	-	0/7/29/30	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	746	PSU	C6-C5	3.77	1.39	1.35
30	a	1915	3TD	C6-C5	3.71	1.39	1.35
30	a	1911	PSU	C6-C5	3.65	1.39	1.35
8	A	516	PSU	C6-C5	3.58	1.39	1.35
30	a	2580	PSU	C6-C5	3.58	1.39	1.35

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	a	2503	2MA	C5-C6-N1	-5.42	117.45	121.01
30	a	2503	2MA	C5-C6-N6	4.25	126.81	120.35
30	a	2580	PSU	C3'-C2'-C1'	2.75	104.84	101.64
19	L	89	D2T	OD1-CG-CB	-2.58	117.03	122.44
30	a	2503	2MA	CM2-C2-N1	2.37	120.85	117.15

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	L	89	D2T	CA-CB-CG-OD1
19	L	89	D2T	CA-CB-CG-OD2
30	a	746	PSU	C2'-C1'-C5-C4
30	a	1911	PSU	O4'-C1'-C5-C4
30	a	1911	PSU	O4'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 369 ligands modelled in this entry, 367 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
60	FUA	W	703	-	39,40,40	1.48	2 (5%)	49,64,64	0.91	2 (4%)
59	GDP	W	701	58	24,30,30	0.95	2 (8%)	30,47,47	0.63	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
60	FUA	W	703	-	-	7/15/92/92	0/4/4/4
59	GDP	W	701	58	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	W	703	FUA	C29-C22	-8.49	1.35	1.47
59	W	701	GDP	C5-C6	-2.61	1.42	1.47
60	W	703	FUA	O5-C29	-2.32	1.23	1.30
59	W	701	GDP	C8-N7	-2.09	1.31	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	W	703	FUA	C14-C8-C9	-2.20	105.10	109.40
60	W	703	FUA	C16-O2-C31	2.16	120.34	117.06

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

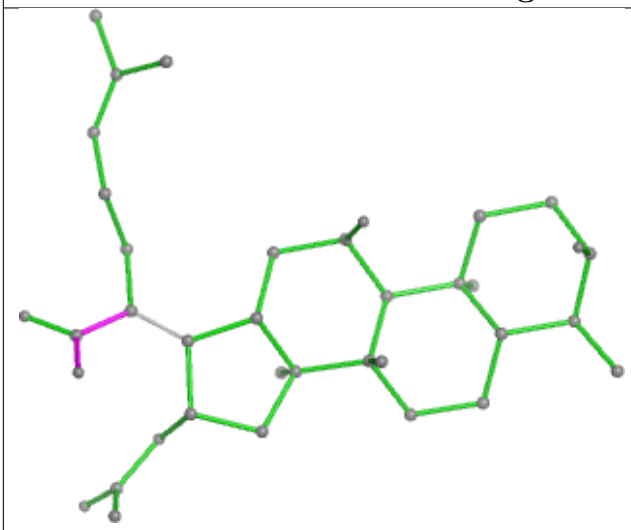
Mol	Chain	Res	Type	Atoms
60	W	703	FUA	C13-C17-C22-C29
60	W	703	FUA	C32-C31-O2-C16
60	W	703	FUA	O3-C31-O2-C16
60	W	703	FUA	C29-C22-C23-C24
60	W	703	FUA	C17-C22-C29-O4

There are no ring outliers.

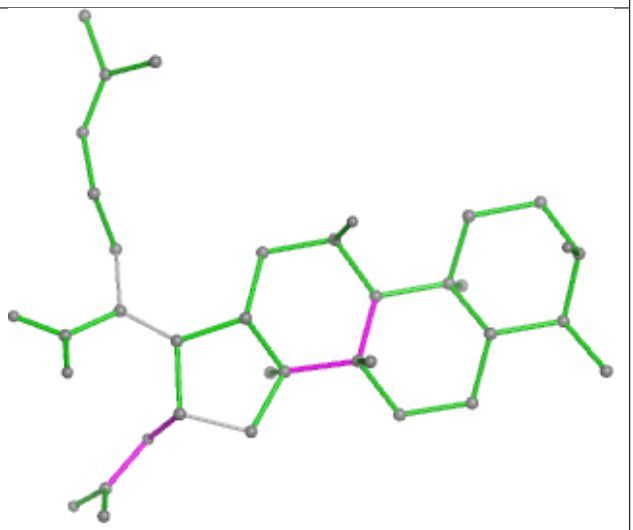
No monomer is involved in short contacts.

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.

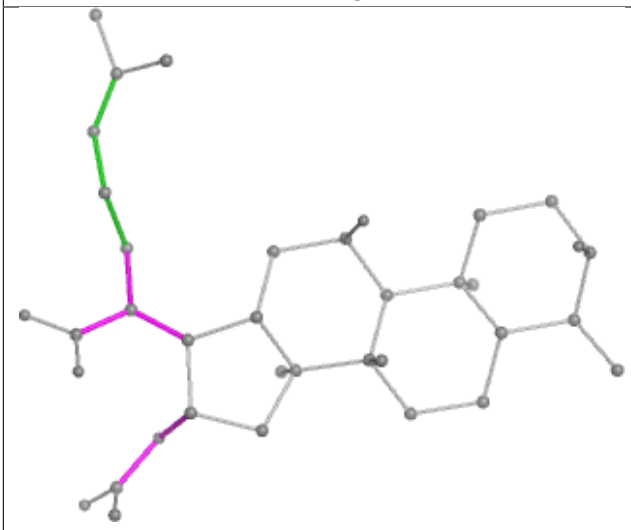
Ligand FUA W 703



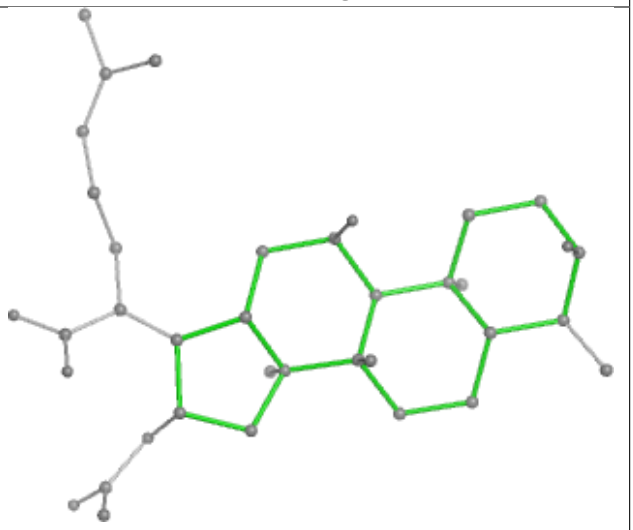
Bond lengths



Bond angles

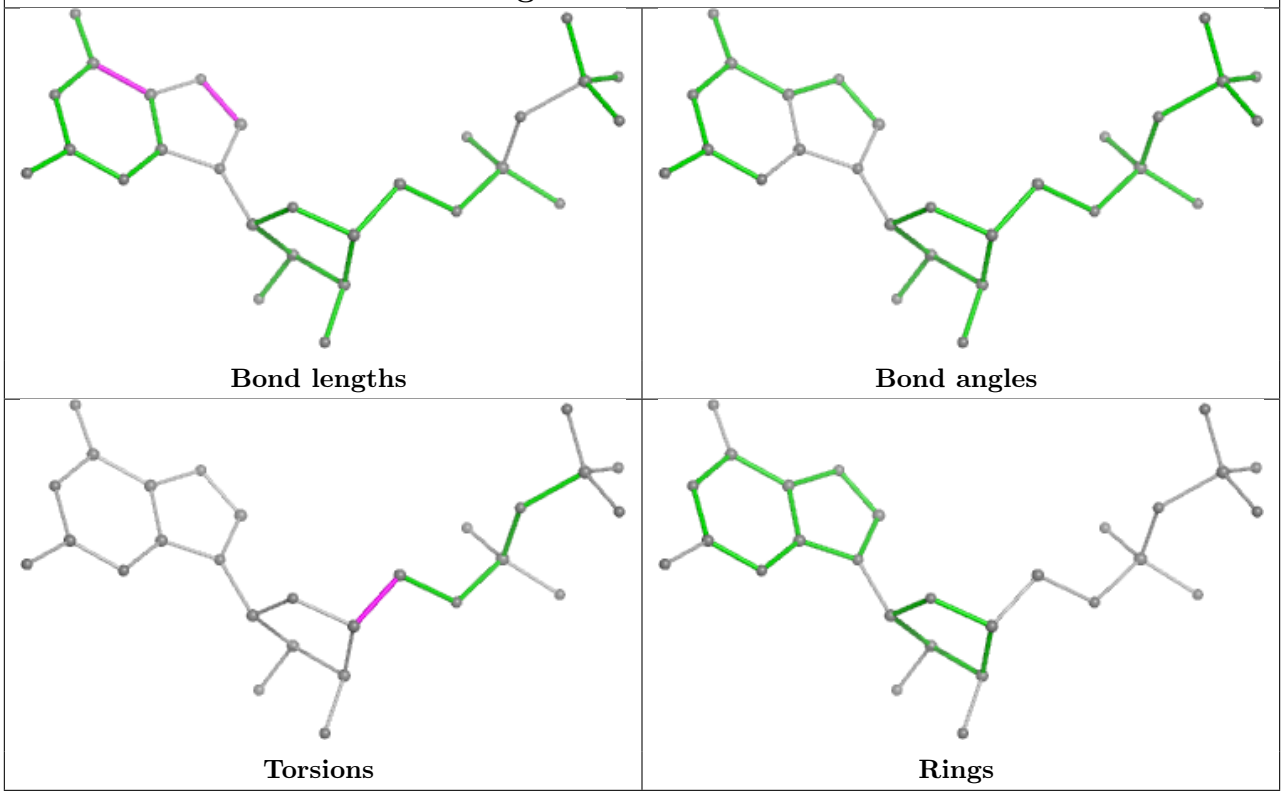


Torsions



Rings

Ligand GDP W 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.

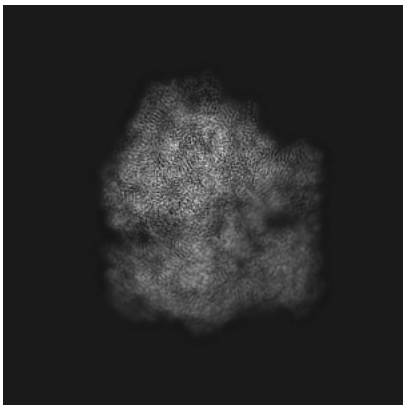
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51350. These allow visual inspection of the internal detail of the map and identification of artifacts.

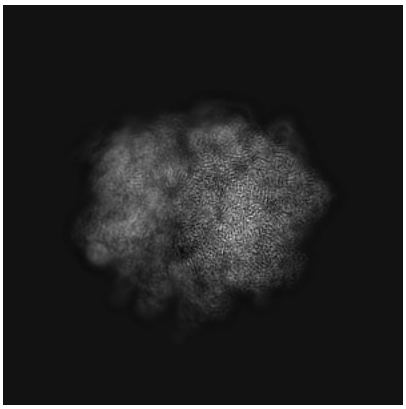
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

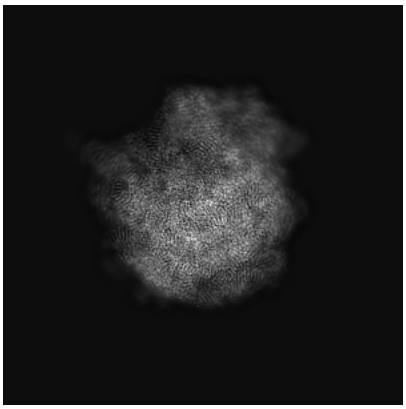
6.1.1 Primary map



X

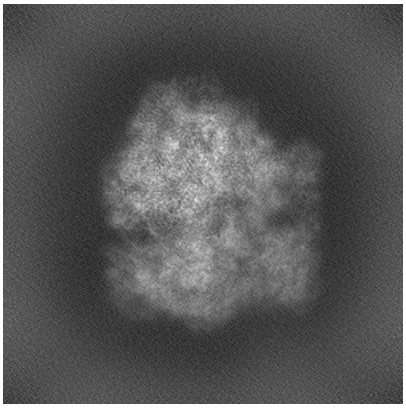


Y

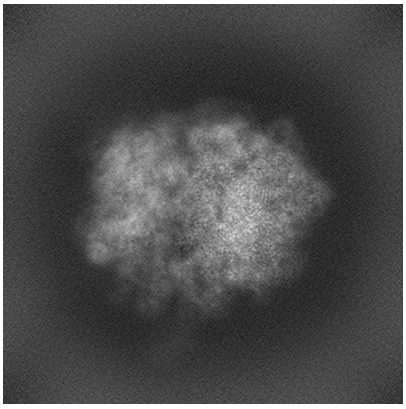


Z

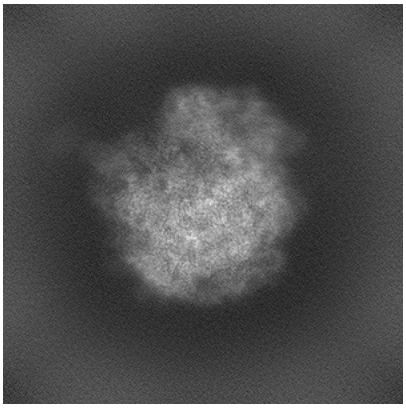
6.1.2 Raw map



X



Y

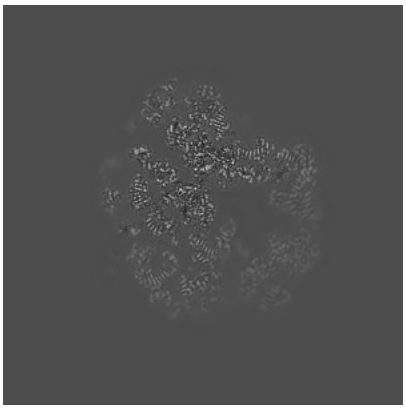


Z

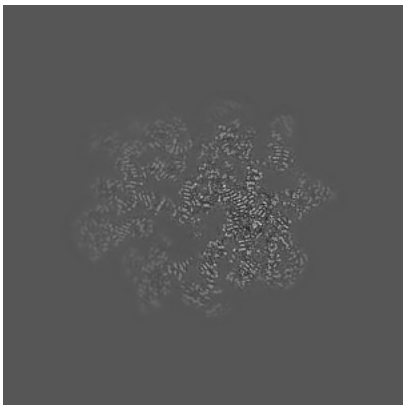
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

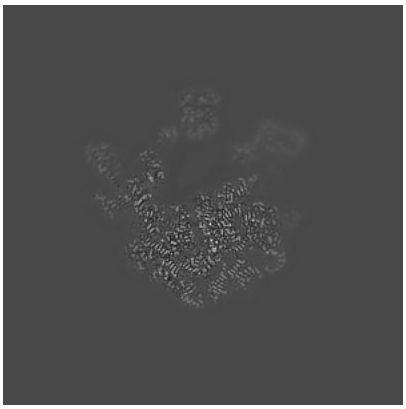
6.2.1 Primary map



X Index: 300

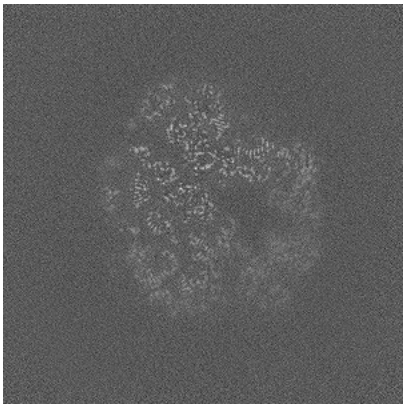


Y Index: 300

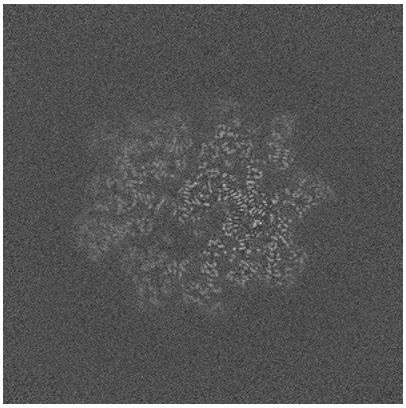


Z Index: 300

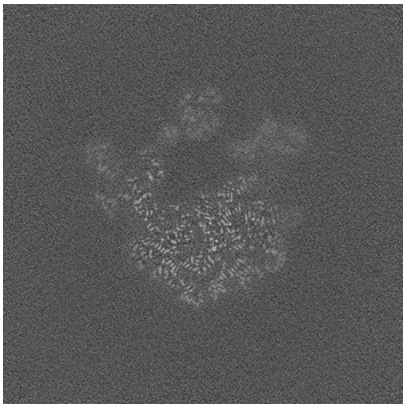
6.2.2 Raw map



X Index: 300



Y Index: 300

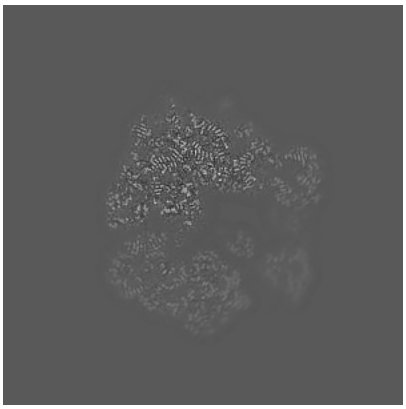


Z Index: 300

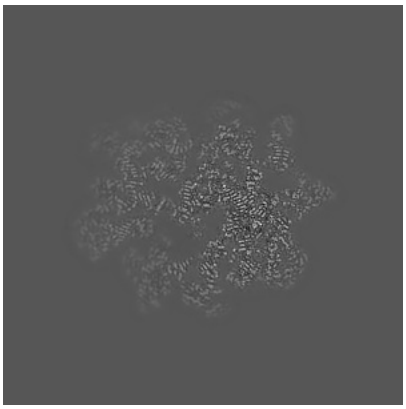
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

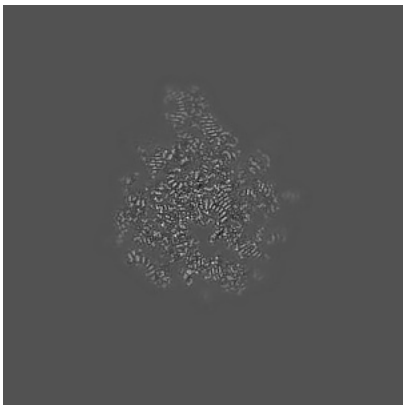
6.3.1 Primary map



X Index: 268

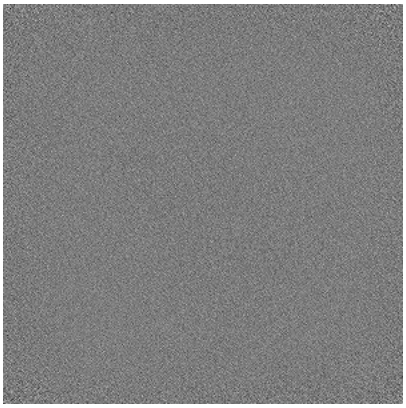


Y Index: 300

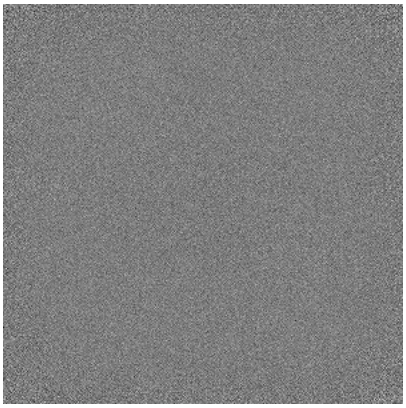


Z Index: 372

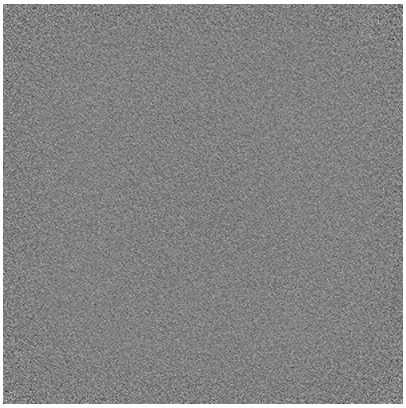
6.3.2 Raw map



X Index: 0



Y Index: 0

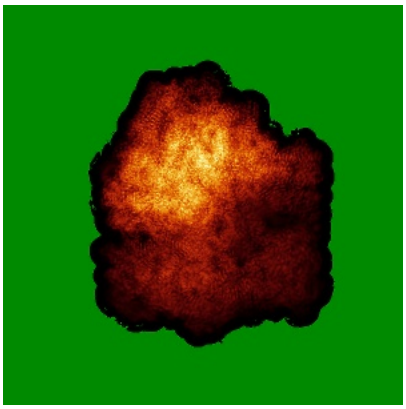


Z Index: 0

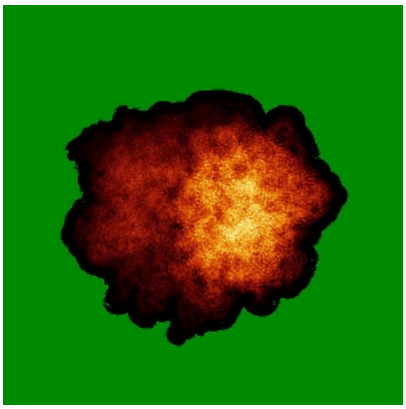
The images above show the largest variance slices of the map in three orthogonal directions.

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

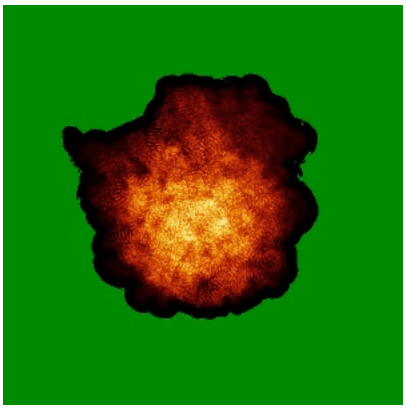
6.4.1 Primary map



X

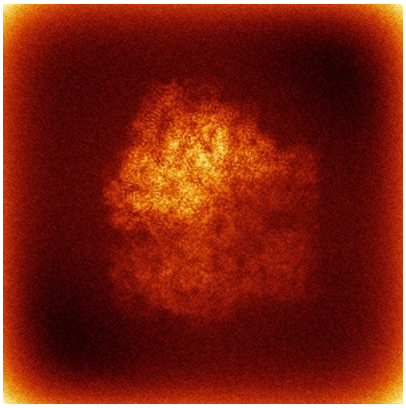


Y

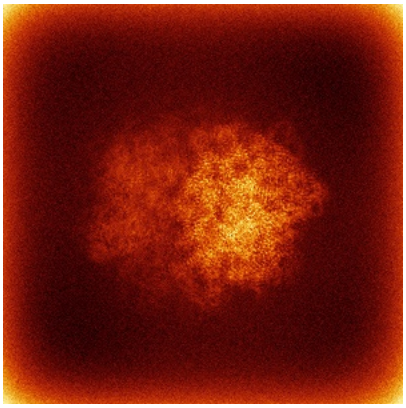


Z

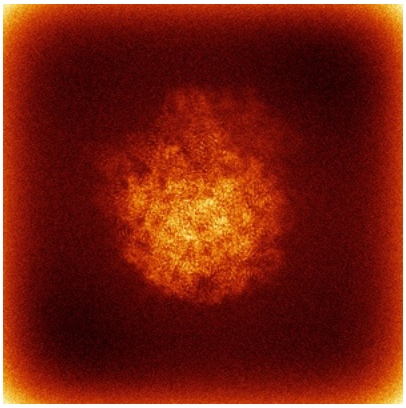
6.4.2 Raw map



X



Y

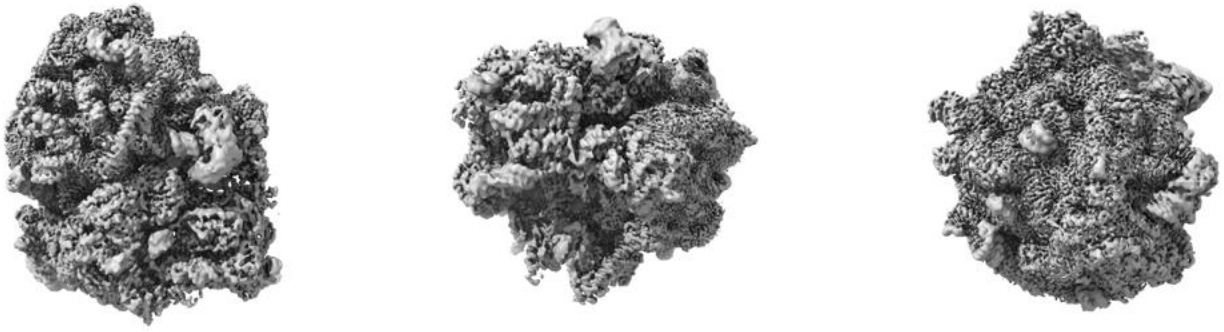


Z

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)

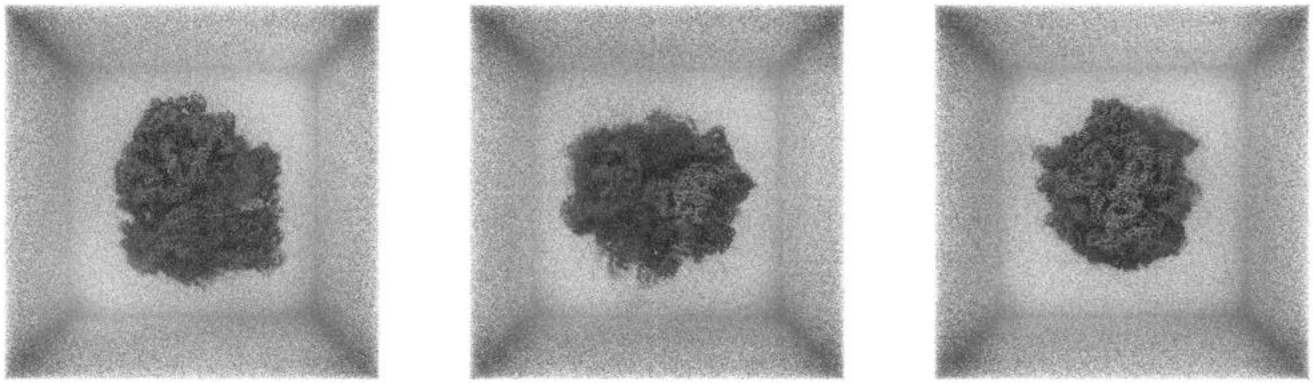
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

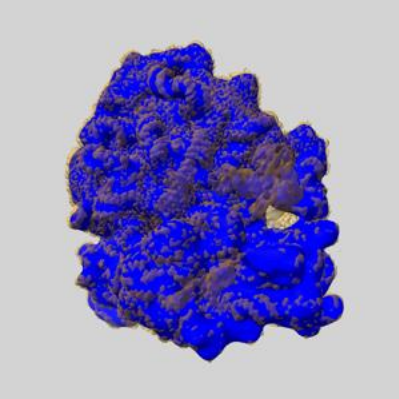
6.6 Mask visualisation

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

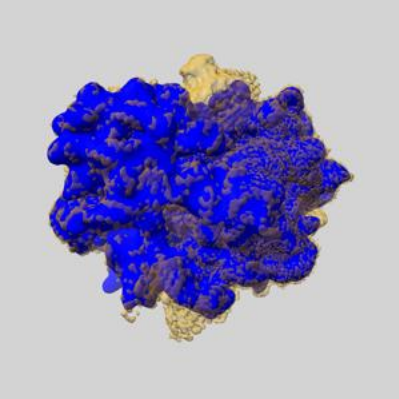
A mask typically either:

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

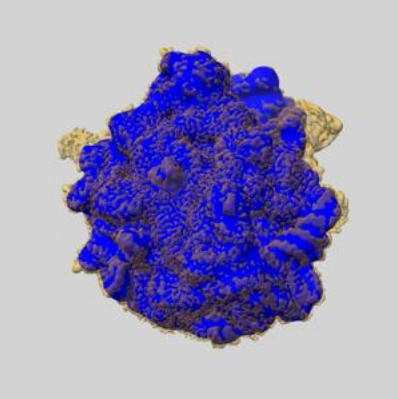
6.6.1 emd_51350_msk_1.map



X



Y

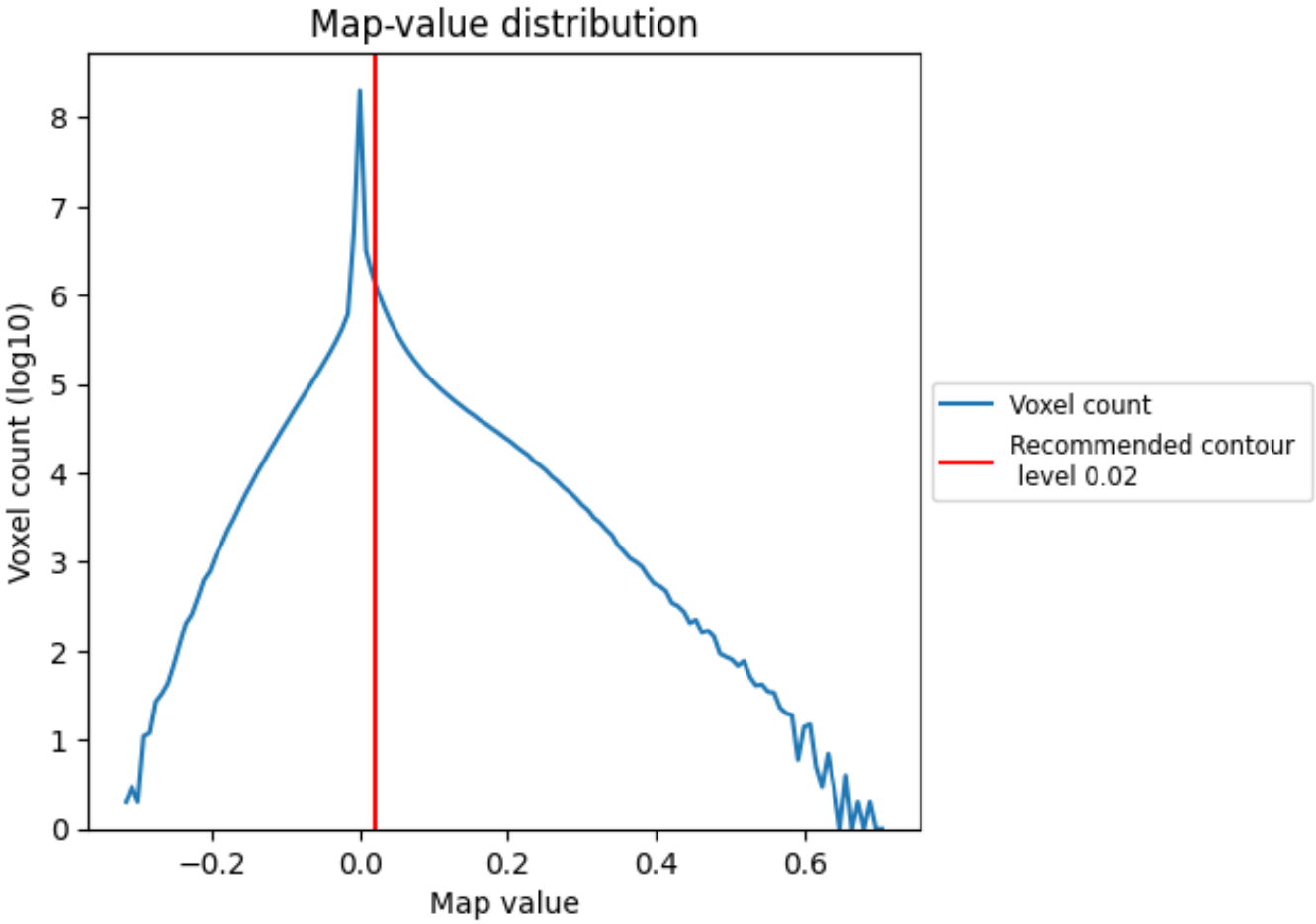


Z

7 Map analysis

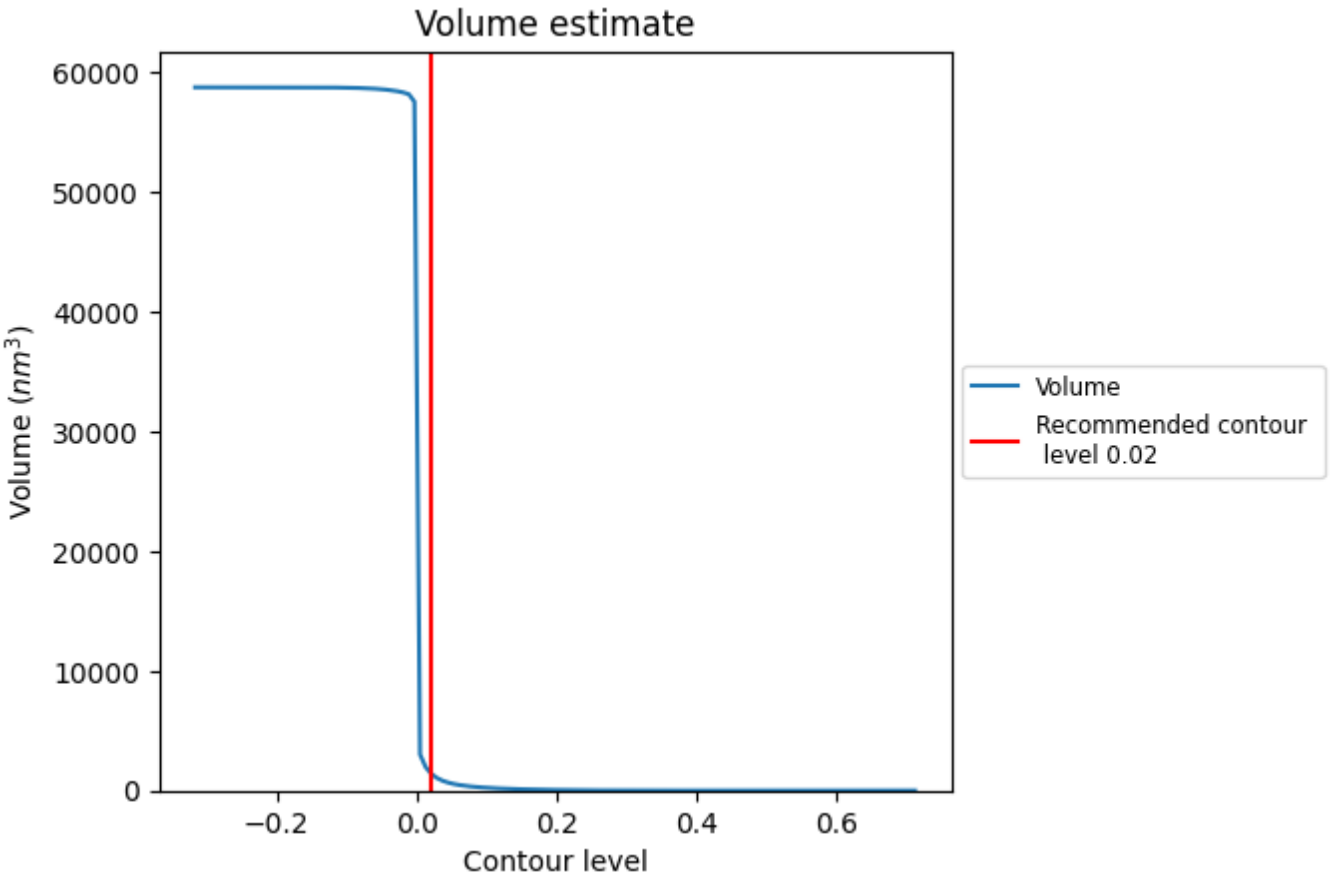
This section contains the results of statistical analysis of the map.

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.

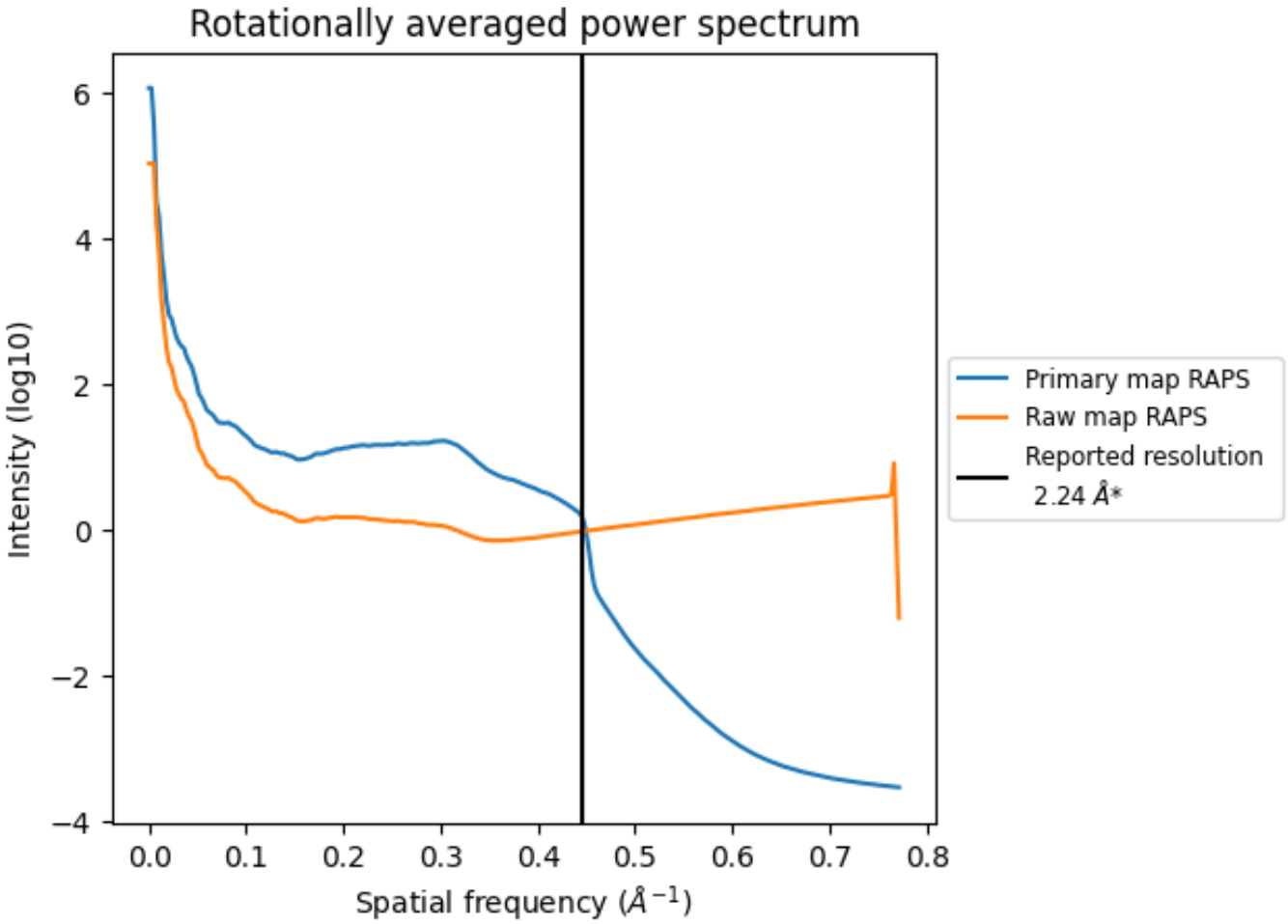
7.2 Volume estimate (i)



The volume at the recommended contour level is 1500 nm^3; this corresponds to an approximate mass of 1355 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)

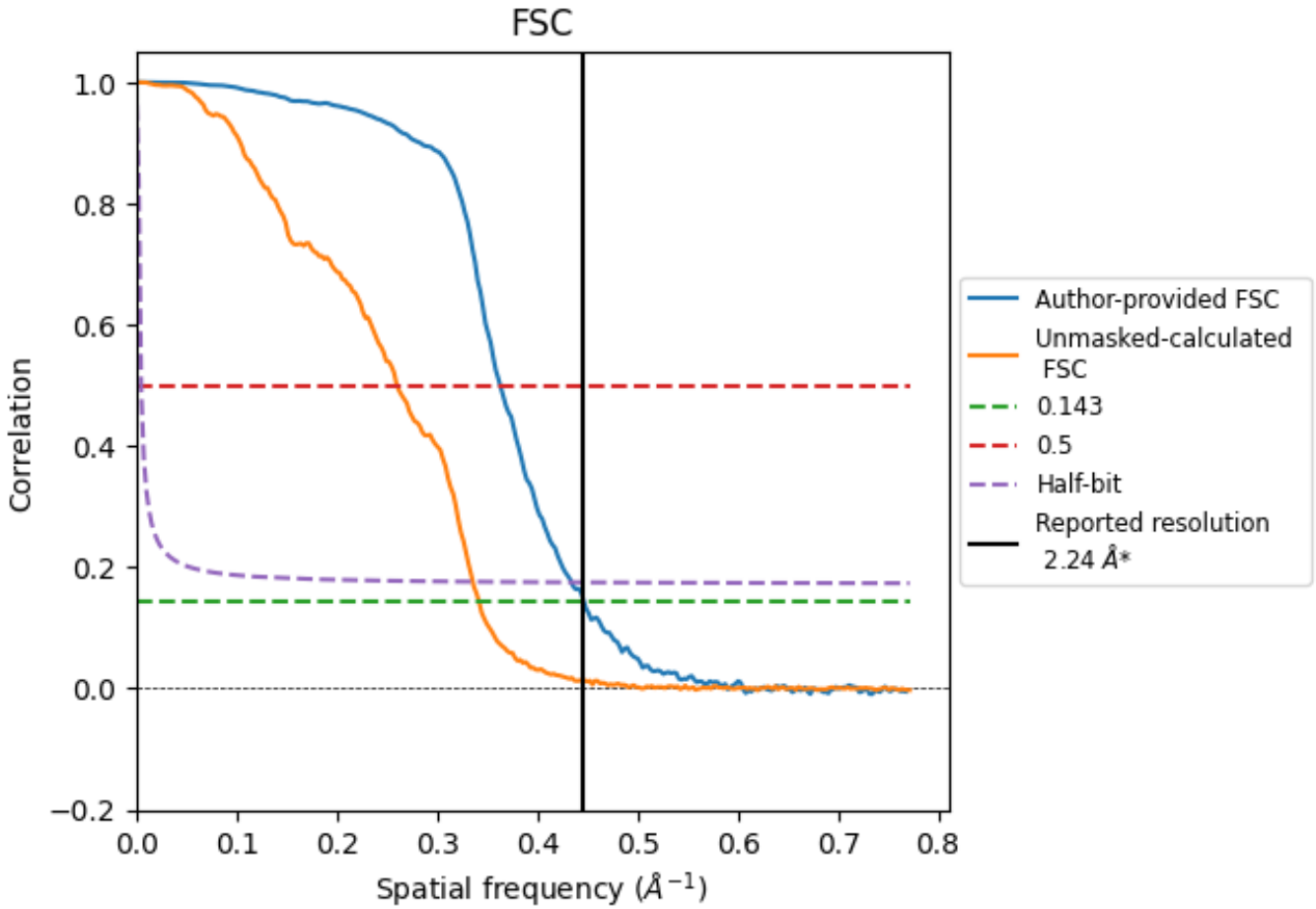


*Reported resolution corresponds to spatial frequency of 0.446 Å^{-1}

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 0.446 $Å^{-1}$

8.2 Resolution estimates (i)

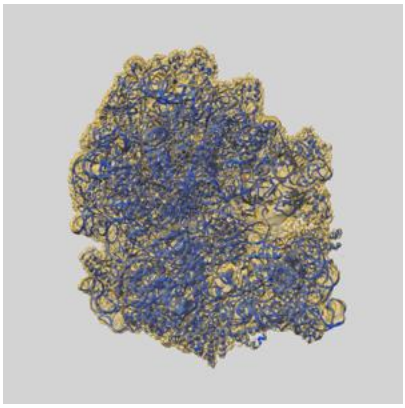
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.24	-	-
Author-provided FSC curve	2.24	2.75	2.30
Unmasked-calculated*	2.92	3.84	2.98

*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 2.92 differs from the reported value 2.24 by more than 10 %

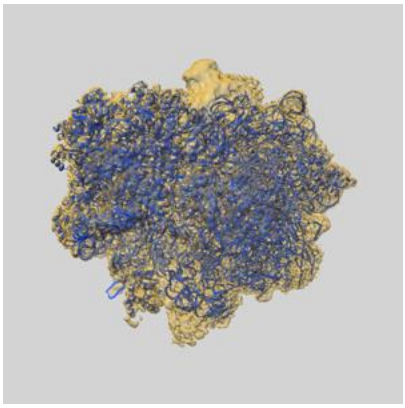
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51350 and PDB model 9GHA. Per-residue inclusion information can be found in section 3 on page 16.

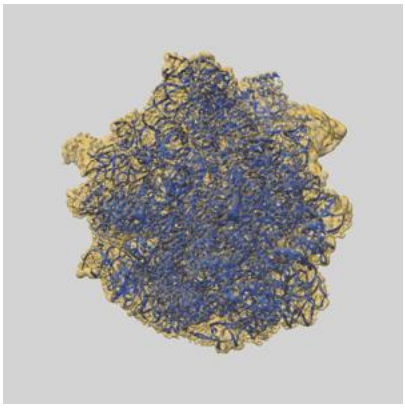
9.1 Map-model overlay



X



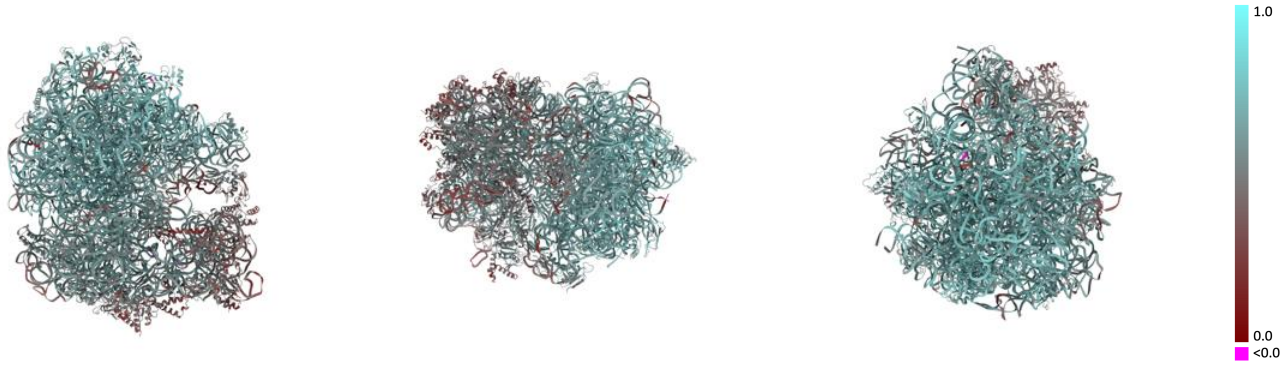
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 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.

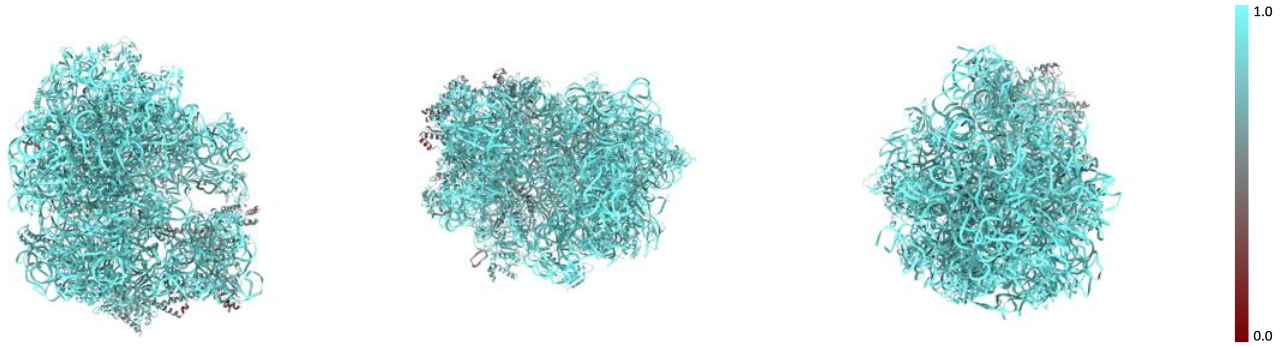
9.2 Q-score mapped to coordinate model



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.

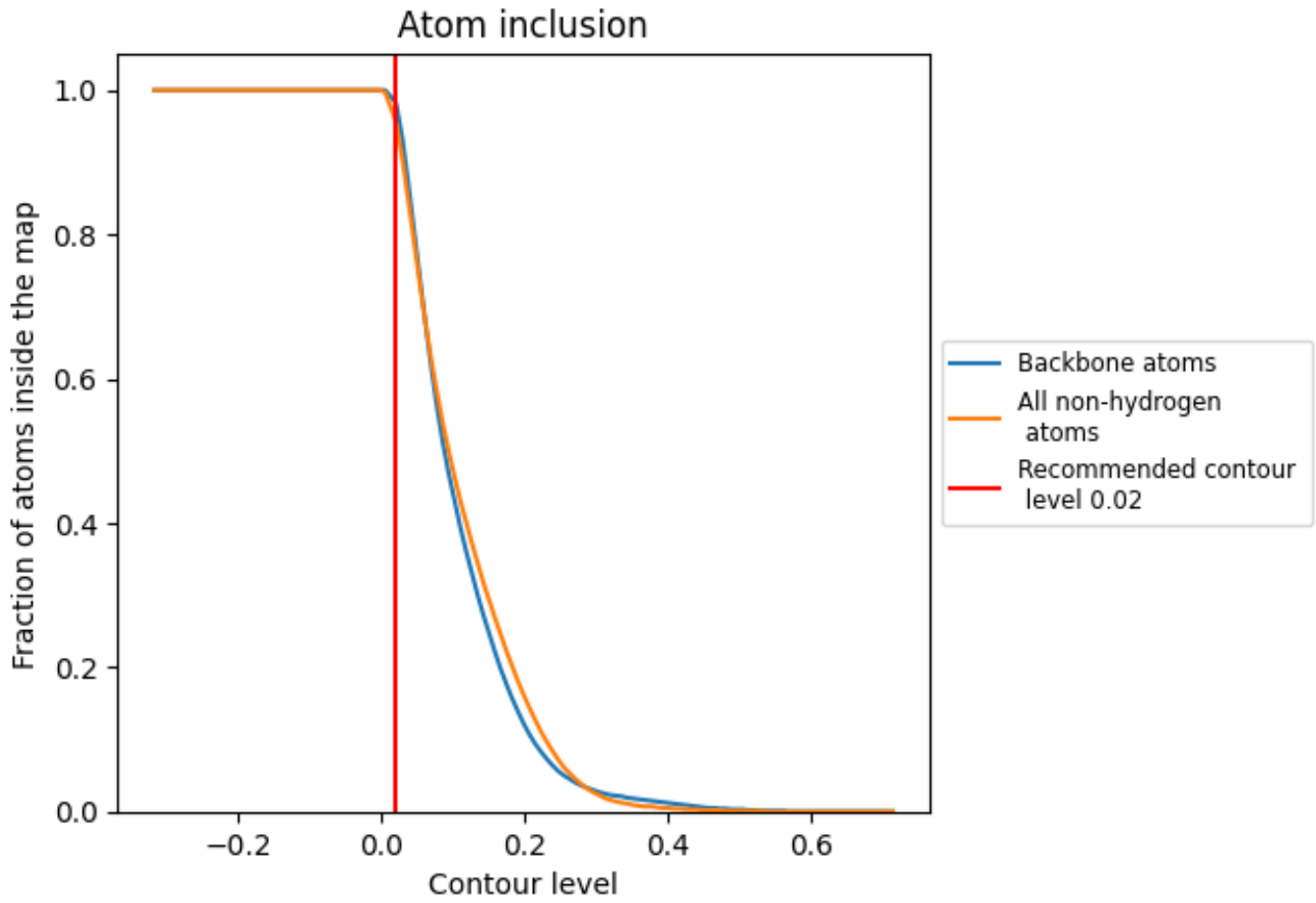
9.3 Atom inclusion mapped to coordinate model



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 (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 96% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.6150
0	0.9460	0.6380
1	0.9970	0.7540
2	0.9940	0.7340
3	0.9930	0.6730
4	0.7980	0.3930
8	0.9290	0.4840
9	0.8730	0.5040
A	0.9740	0.5540
B	0.6740	0.3880
C	0.8280	0.4780
D	0.8720	0.4780
E	0.9200	0.5390
F	0.8780	0.4970
G	0.6590	0.3370
H	0.9170	0.5450
I	0.8110	0.4350
J	0.7150	0.4190
K	0.9040	0.5440
L	0.9340	0.5650
M	0.7040	0.4140
N	0.8820	0.4880
O	0.9250	0.5580
P	0.9490	0.5510
Q	0.9330	0.5690
R	0.9180	0.5330
S	0.8220	0.4580
T	0.9360	0.5530
U	0.8500	0.5020
W	0.8390	0.4790
a	0.9930	0.6860
b	0.9950	0.6280
c	0.9890	0.7120
d	0.9730	0.7060
e	0.9590	0.6740

Continued on next page...

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Chain	Atom inclusion	Q-score
f	0.8550	0.4730
g	0.9410	0.5910
h	0.9430	0.5840
i	0.9790	0.7090
j	0.9780	0.6920
k	0.9800	0.7030
l	0.9760	0.6830
m	0.9970	0.7360
n	0.9570	0.6110
o	0.9550	0.6700
p	0.9920	0.7360
q	0.9510	0.6680
r	0.9810	0.7100
s	0.9520	0.6460
t	0.9660	0.6480
u	0.9340	0.6210
v	0.9730	0.6990
w	0.9770	0.6920
x	0.9400	0.6260
y	0.9660	0.6950
z	0.9830	0.7150