



wwPDB EM Validation Summary Report ⓘ

Oct 19, 2021 – 04:21 pm BST

PDB ID : 7PJS
EMDB ID : EMD-13458
Title : Structure of the 70S ribosome with tRNAs in the classical pre-translocation state and apramycin (C)
Authors : Petrychenko, V.; Peng, B.Z.; Schwarzer, A.C.; Peske, F.; Rodnina, M.V.; Fischer, N.
Deposited on : 2021-08-24
Resolution : 2.35 Å (reported)
Based on initial models : 4AQY, 5LZD, 6YSS

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.0.dev97
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.2

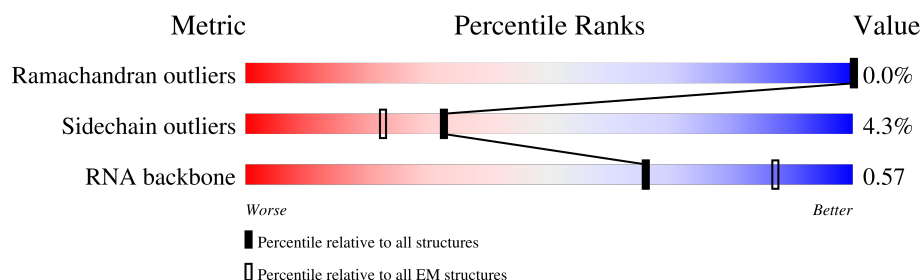
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.




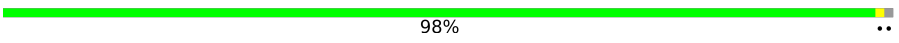
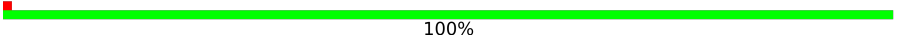
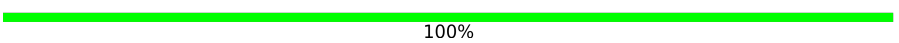
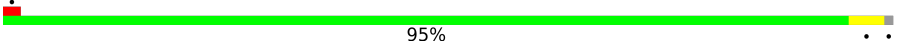
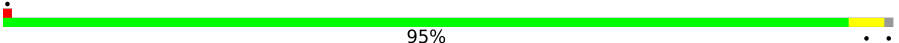


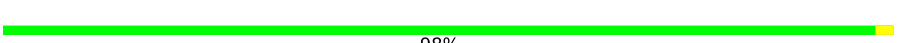
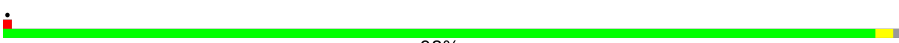
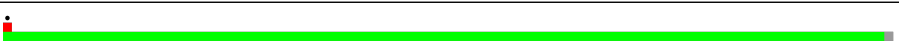



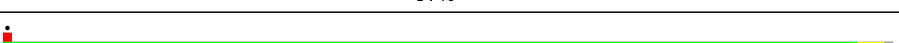
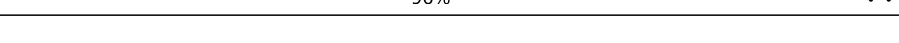
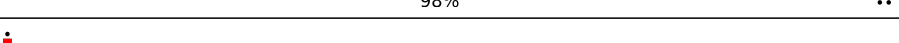
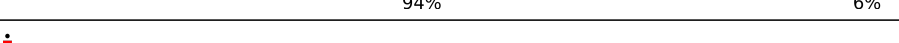
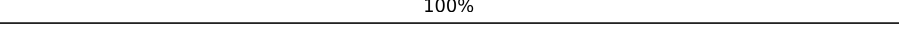
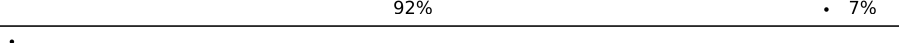
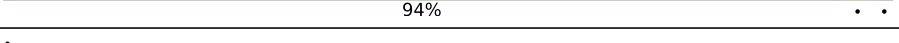
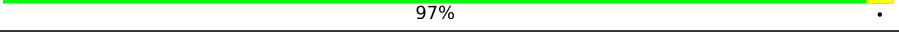

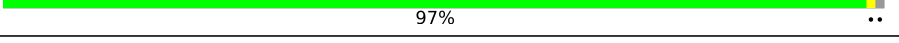
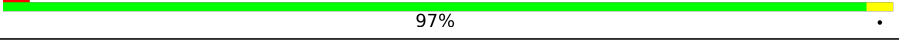
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	0	57	
2	1	55	
3	2	46	
4	3	65	
5	4	38	
6	5	165	
7	6	70	
8	A	2903	




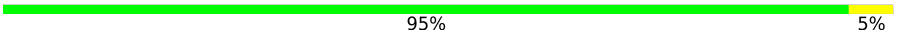
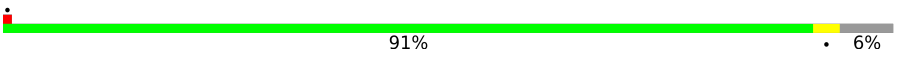


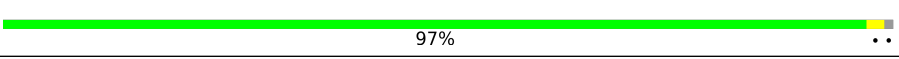
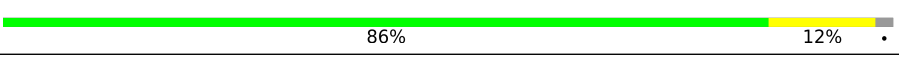

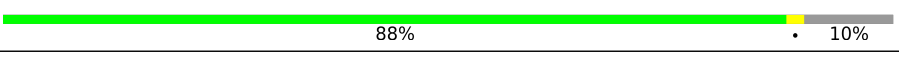
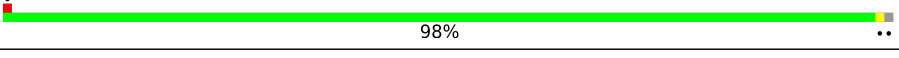

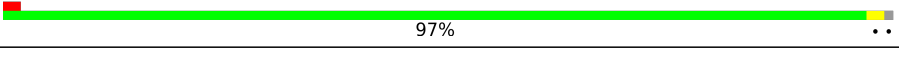
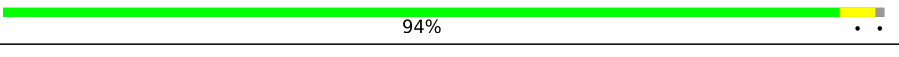
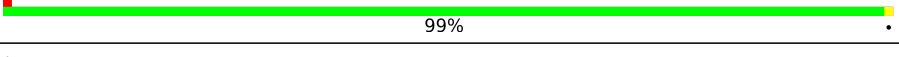
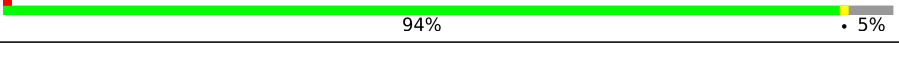


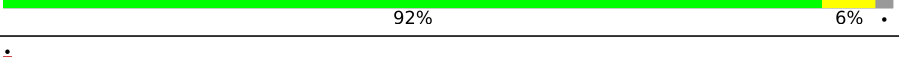



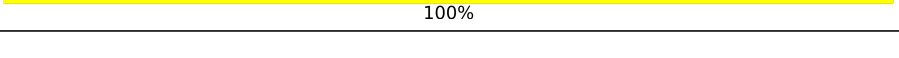
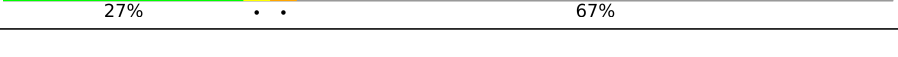
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Mol	Chain	Length	Quality of chain
9	B	120	 78%22%
10	C	273	 98%..
11	D	209	 100%
12	E	201	 100%
13	F	179	 95%..
14	G	177	 95%..
15	H	149	 48%90%10%
16	I	142	 96%99%.
17	J	142	 98%.
18	K	123	 98%..
19	L	144	 99%.
20	M	136	 97%.
21	N	127	 93%6%
22	O	117	 97%..
23	P	115	 96%..
24	Q	118	 98%..
25	R	103	 94%6%
26	S	110	 100%
27	T	100	 92%7%
28	U	104	 94%..
29	V	94	 97%.
30	W	85	 88%12%
31	X	78	 97%..
32	Y	63	 97%.
33	Z	59	 95%..

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Mol	Chain	Length	Quality of chain
34	a	1542	
35	b	240	
36	c	233	
37	d	206	
38	e	167	
39	f	135	
40	g	179	
41	h	130	
42	i	130	
43	j	103	
44	k	129	
45	l	124	
46	m	118	
47	n	102	
48	o	89	
49	p	82	
50	q	84	
51	r	75	
52	s	92	
53	t	87	
54	u	71	
55	v	77	
56	w	76	
57	y	2	
58	z	33	

2 Entry composition

There are 63 unique types of molecules in this entry. The entry contains 147741 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 L32.

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

- Molecule 2 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	1	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 3 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 4 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	5	131	Total	C	N	O	0	0
			647	385	131	131		

- Molecule 7 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

- Molecule 8 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	2903	Total	C	N	O	P	0	0
			62338	27816	11471	20148	2903		

- Molecule 9 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	120	Total	C	N	O	P	0	0
			2570	1144	468	838	120		

- Molecule 10 is a protein called 50S ribosomal protein L2.

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

- Molecule 11 is a protein called 50S ribosomal protein L3.

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

- Molecule 12 is a protein called 50S ribosomal protein L4.

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

- Molecule 13 is a protein called 50S ribosomal protein L5.

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

- Molecule 14 is a protein called 50S ribosomal protein L6.

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

- Molecule 15 is a protein called 50S ribosomal protein L9.

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

- Molecule 16 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	141	Total	C	N	O	S	0	0
			693	411	141	141			

- Molecule 17 is a protein called 50S ribosomal protein L13.

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

- Molecule 18 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 19 is a protein called 50S ribosomal protein L15.

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

- Molecule 20 is a protein called 50S ribosomal protein L16.

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

- Molecule 21 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 22 is a protein called 50S ribosomal protein L18.

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

- Molecule 23 is a protein called 50S ribosomal protein L19.

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

- Molecule 24 is a protein called 50S ribosomal protein L20.

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

- Molecule 25 is a protein called 50S ribosomal protein L21.

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

- Molecule 26 is a protein called 50S ribosomal protein L22.

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

- Molecule 27 is a protein called 50S ribosomal protein L23.

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

- Molecule 28 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	U	102	Total	C	N	O	0	0
			779	492	146	141		

- Molecule 29 is a protein called 50S ribosomal protein L25.

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

- Molecule 30 is a protein called 50S ribosomal protein L27.

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

- Molecule 31 is a protein called 50S ribosomal protein L28.

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

- Molecule 32 is a protein called 50S ribosomal protein L29.

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

- Molecule 33 is a protein called 50S ribosomal protein L30.

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

- Molecule 34 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	a	1540	Total	C	N	O	P	0	0
			33050	14748	6057	10705	1540		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	b	218	Total	C	N	O	S	0	0
			1704	1081	305	311	7		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	0	0
			1141	709	218	208	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	f	100	Total	C	N	O	S	0	0
			817	515	148	148	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	g	151	Total	C	N	O	S	0	0
			1181	735	227	215	4		

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

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

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

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	k	116	Total	C	N	O	S	0	0
			869	535	173	158	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
46	m	114	Total	C	N	O	S	0	0
			883	546	178	156	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			799	498	165	133	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP C3SR07

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	q	80	Total	C	N	O	S	0	0
			648	411	121	113	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
51	r	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	82	Total	C	N	O	S	0	0
			658	421	125	110	2		

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

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

- Molecule 54 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			506	313	105	87	1		

- Molecule 55 is a RNA chain called P-site tRNA(fMet).

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1642	733	297	534	77	1		

- Molecule 56 is a RNA chain called P-site fMet-Phe-tRNA(Phe).

Mol	Chain	Residues	Atoms						AltConf	Trace
56	w	76	Total	C	N	O	P	S	0	0
			1631	731	291	531	76	2		

- Molecule 57 is a protein called Dipeptide (FME-PHE).

Mol	Chain	Residues	Atoms					AltConf	Trace
57	y	2	Total	C	N	O	S	0	0
			21	15	2	3	1		

- Molecule 58 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	11	Total	C	N	O	P	0	0
			230	103	35	81	11		

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	0	1	Total	Mg	0
			1	1	
59	A	258	Total	Mg	0
			258	258	
59	B	4	Total	Mg	0
			4	4	
59	C	2	Total	Mg	0
			2	2	
59	D	1	Total	Mg	0
			1	1	
59	N	1	Total	Mg	0
			1	1	
59	O	1	Total	Mg	0
			1	1	
59	P	1	Total	Mg	0
			1	1	
59	a	92	Total	Mg	0
			92	92	

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Mol	Chain	Residues	Atoms		AltConf
59	m	1	Total	Mg	0
			1	1	
59	n	1	Total	Mg	0
			1	1	

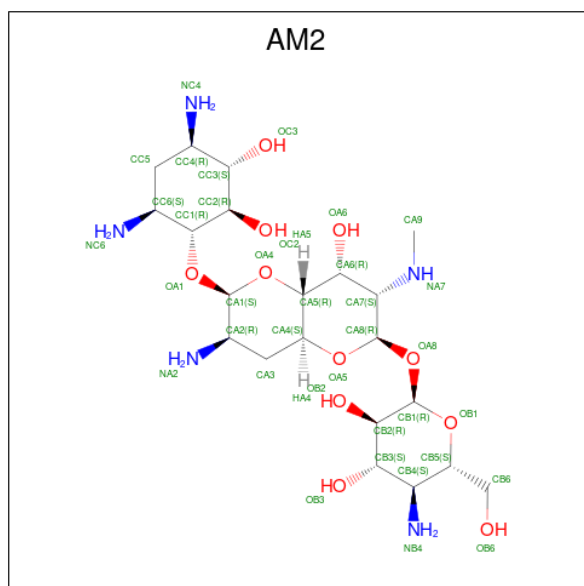
- Molecule 60 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	4	1	Total	Zn	0
			1	1	
60	6	1	Total	Zn	0
			1	1	

- Molecule 61 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
61	A	1	Total	Na	0
			1	1	
61	B	1	Total	Na	0
			1	1	

- Molecule 62 is APRAMYCIN (three-letter code: AM2) (formula: C₂₁H₄₁N₅O₁₁).



Mol	Chain	Residues	Atoms				AltConf
62	a	1	Total	C	N	O	0
			148	84	20	44	

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Mol	Chain	Residues	Atoms				AltConf
62	a	1	Total 148	C 84	N 20	O 44	0
62	a	1	Total 148	C 84	N 20	O 44	0
62	a	1	Total 148	C 84	N 20	O 44	0

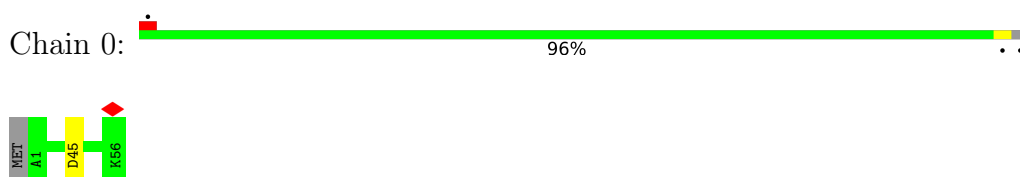
- Molecule 63 is water.

Mol	Chain	Residues	Atoms		AltConf
63	A	5	Total 5	O 5	0
63	a	15	Total 15	O 15	0
63	z	2	Total 2	O 2	0

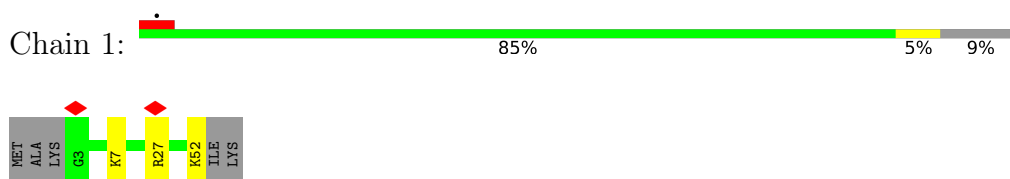
3 Residue-property plots [i](#)

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.

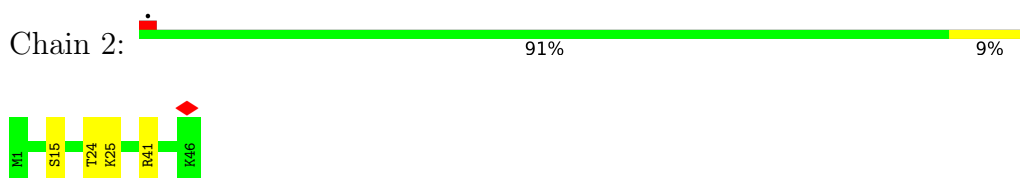
- Molecule 1: 50S ribosomal protein L32



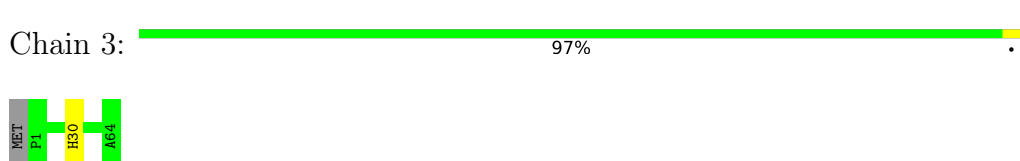
- Molecule 2: 50S ribosomal protein L33



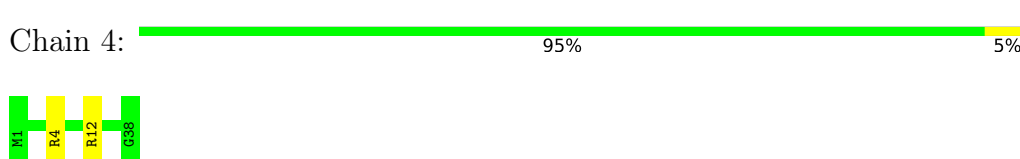
- Molecule 3: 50S ribosomal protein L34



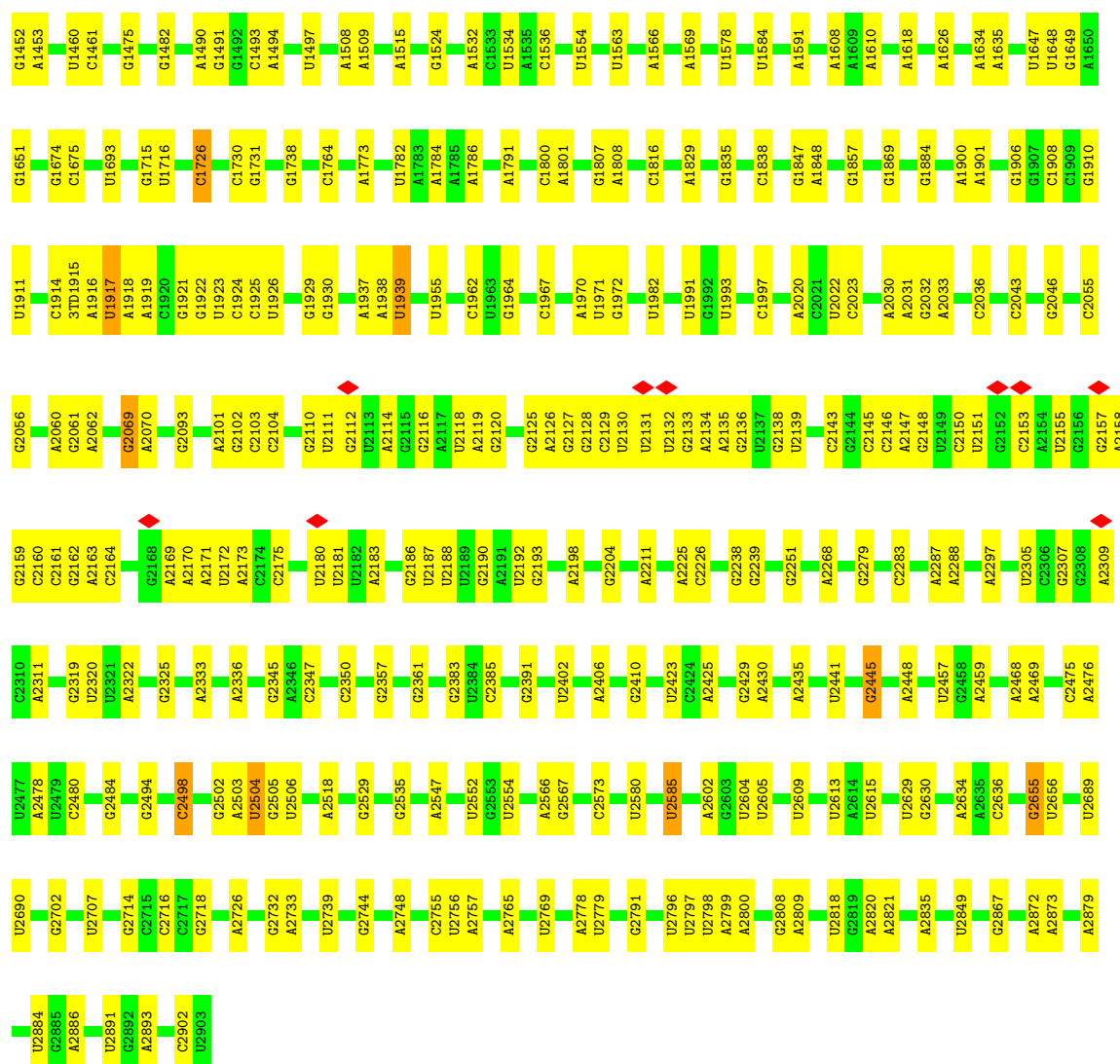
- Molecule 4: 50S ribosomal protein L35



- Molecule 5: 50S ribosomal protein L36

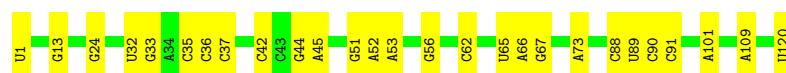


- Molecule 6: 50S ribosomal protein L10



• Molecule 9: 5S ribosomal RNA

Chain B: 78% 22%



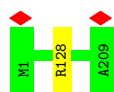
• Molecule 10: 50S ribosomal protein L2

Chain C: 98% ..



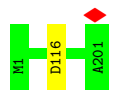
• Molecule 11: 50S ribosomal protein L3

Chain D: 100%



- Molecule 12: 50S ribosomal protein L4

Chain E: 100%



- Molecule 13: 50S ribosomal protein L5

Chain F: 95%



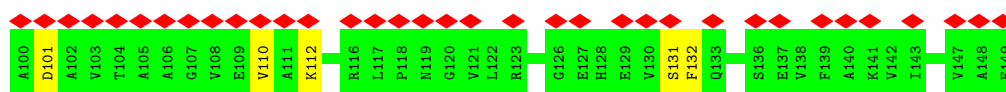
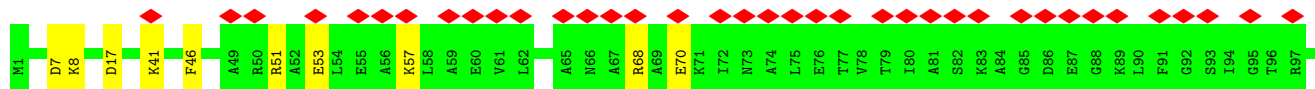
- Molecule 14: 50S ribosomal protein L6

Chain G: 95%



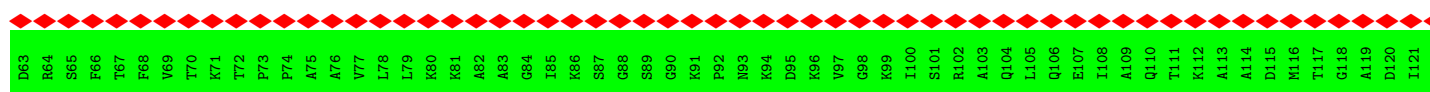
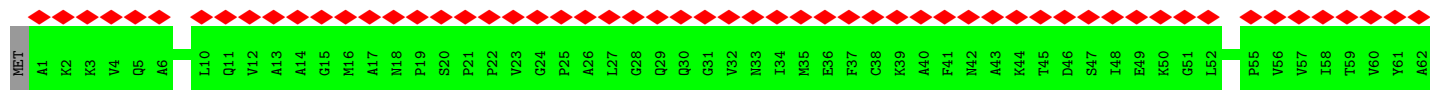
- Molecule 15: 50S ribosomal protein L9

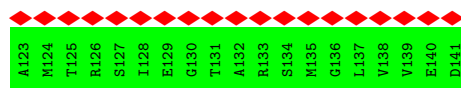
Chain H: 48%



- Molecule 16: 50S ribosomal protein L11

Chain I: 96%





- Molecule 17: 50S ribosomal protein L13

Chain J: 98%



- Molecule 18: 50S ribosomal protein L14

Chain K: 98%



- Molecule 19: 50S ribosomal protein L15

Chain L: 99%



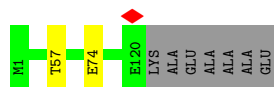
- Molecule 20: 50S ribosomal protein L16

Chain M: 97%



- Molecule 21: 50S ribosomal protein L17

Chain N: 93%



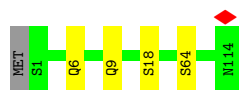
- Molecule 22: 50S ribosomal protein L18

Chain O: 97%



- Molecule 23: 50S ribosomal protein L19

Chain P:  96% ..



- Molecule 24: 50S ribosomal protein L20

Chain Q:  98% ..



- Molecule 25: 50S ribosomal protein L21

Chain R:  94% 6%



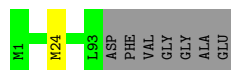
- Molecule 26: 50S ribosomal protein L22

Chain S:  100%



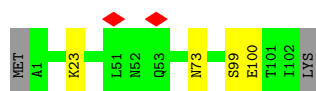
- Molecule 27: 50S ribosomal protein L23

Chain T:  92% 7%



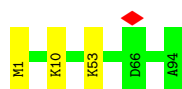
- Molecule 28: 50S ribosomal protein L24

Chain U:  94% ..

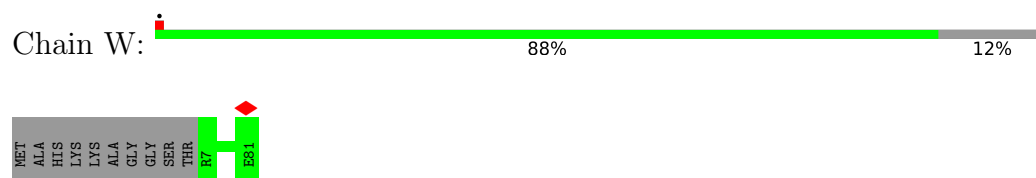


- Molecule 29: 50S ribosomal protein L25

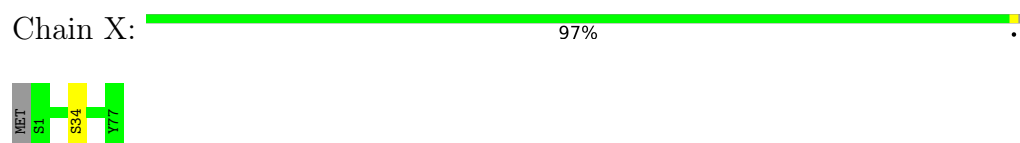
Chain V:  97% .



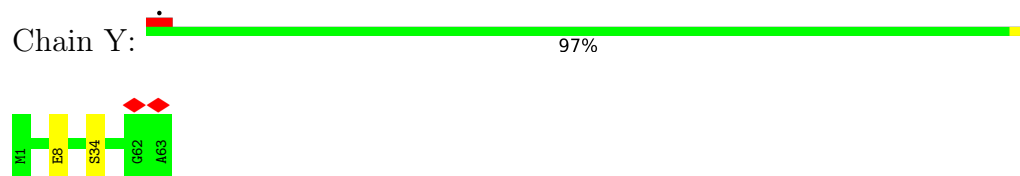
- Molecule 30: 50S ribosomal protein L27



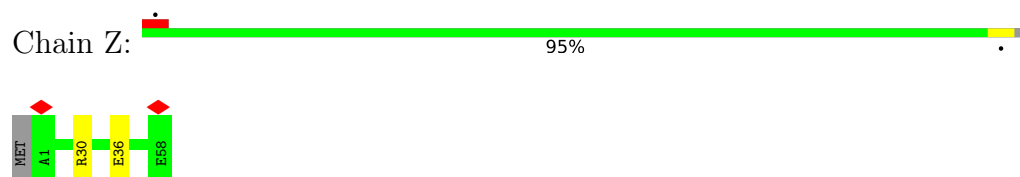
- Molecule 31: 50S ribosomal protein L28



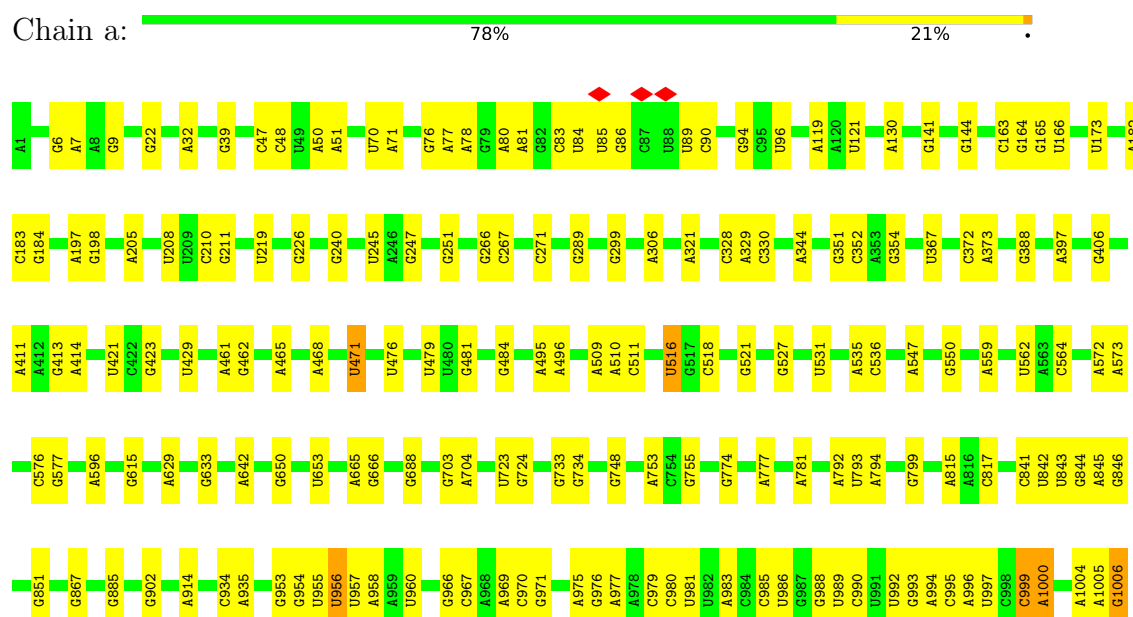
- Molecule 32: 50S ribosomal protein L29



- Molecule 33: 50S ribosomal protein L30

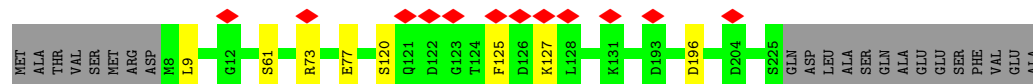
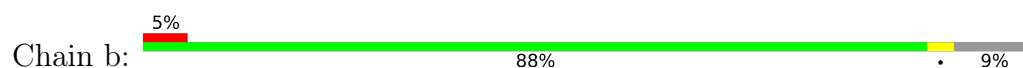


- Molecule 34: 16S ribosomal RNA

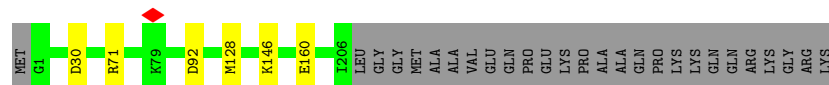
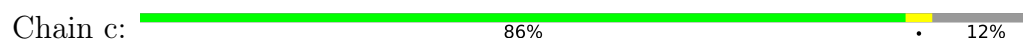




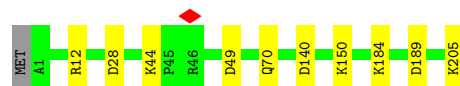
• Molecule 35: 30S ribosomal protein S2



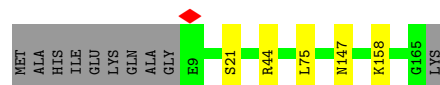
• Molecule 36: 30S ribosomal protein S3



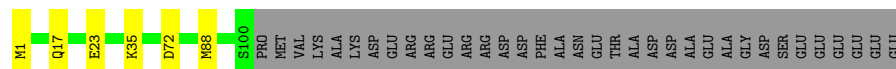
• Molecule 37: 30S ribosomal protein S4



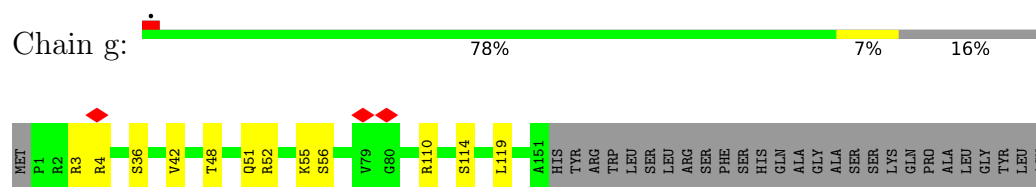
• Molecule 38: 30S ribosomal protein S5



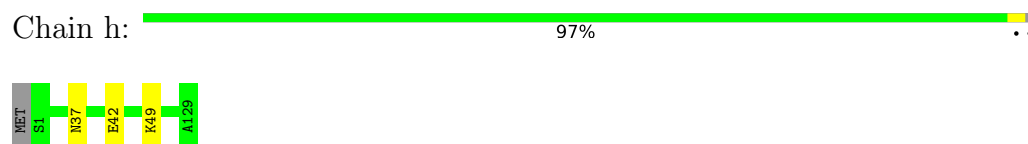
• Molecule 39: 30S ribosomal protein S6



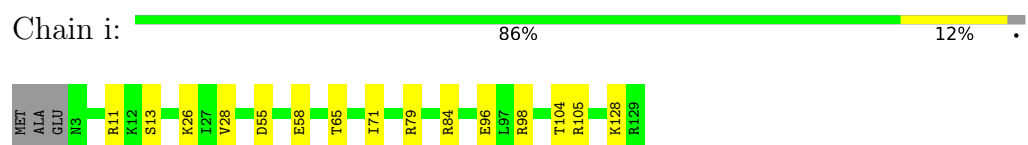
- Molecule 40: 30S ribosomal protein S7



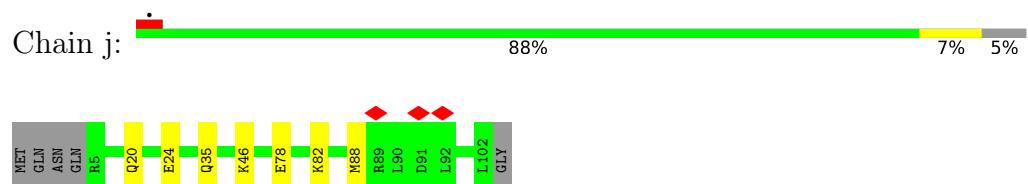
- Molecule 41: 30S ribosomal protein S8



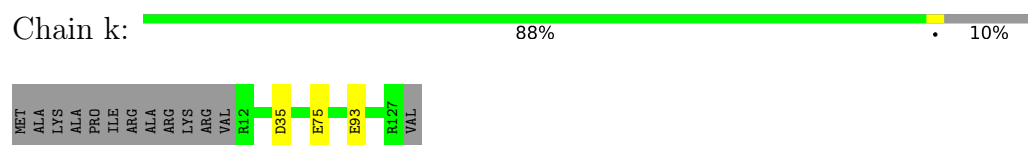
- Molecule 42: 30S ribosomal protein S9



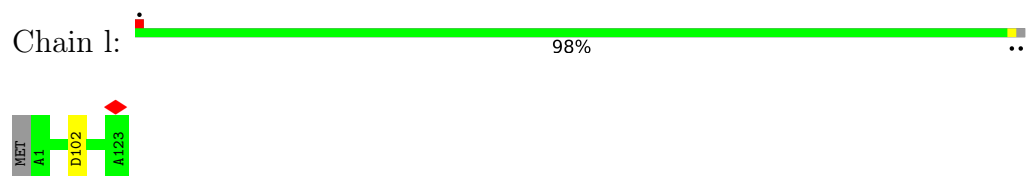
- Molecule 43: 30S ribosomal protein S10



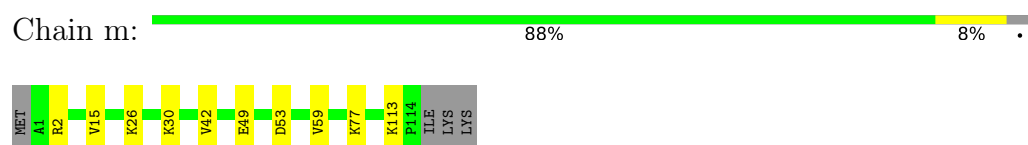
- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



- Molecule 47: 30S ribosomal protein S14

Chain n:  97% ..



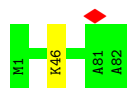
- Molecule 48: 30S ribosomal protein S15

Chain o:  94% ..



- Molecule 49: 30S ribosomal protein S16

Chain p:  99% .




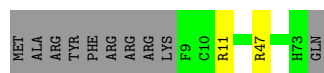
- Molecule 50: 30S ribosomal protein S17

Chain q:  94% . 5%




- Molecule 51: 30S ribosomal protein S18

Chain r:  84% . 13%




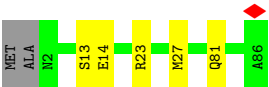
- Molecule 52: 30S ribosomal protein S19

Chain s:  84% 5% 11%

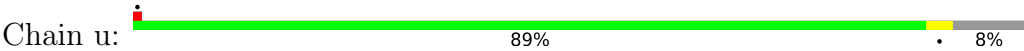


- Molecule 53: 30S ribosomal protein S20

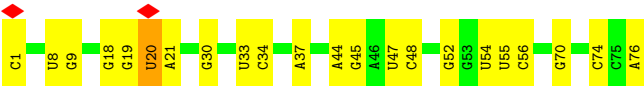
Chain t:  92% 6% .



• Molecule 54: 30S ribosomal protein S21



• Molecule 55: P-site tRNA(fMet)



• Molecule 56: P-site fMet-Phe-tRNA(Phe)



• Molecule 57: Dipeptide (FME-PHE)



• Molecule 58: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	537761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1200	Depositor
Magnification	59000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	21.985	Depositor
Minimum map value	-5.122	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.0	Depositor
Map size (Å)	334.08, 334.08, 334.08	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.6525, 0.6525, 0.6525	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: UR3, G7M, 6MZ, MA6, AM2, 4SU, OMU, MG, H2U, OMC, PSU, 3TD, FME, OMG, 2MG, 5MU, 1MG, 4OC, ZN, MIA, 2MA, NA, 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	0	0.31	0/450	0.65	1/599 (0.2%)
2	1	0.31	0/416	0.53	0/554
3	2	0.29	0/380	0.66	0/498
4	3	0.30	0/513	0.53	0/676
5	4	0.32	0/303	0.61	0/397
6	5	0.24	0/646	0.43	0/898
7	6	0.31	0/531	0.71	0/709
8	A	0.59	1/69266 (0.0%)	0.80	23/108055 (0.0%)
9	B	0.54	1/2873 (0.0%)	0.78	0/4478
10	C	0.34	0/2121	0.58	0/2852
11	D	0.33	0/1586	0.54	0/2134
12	E	0.31	0/1571	0.50	0/2113
13	F	0.31	0/1434	0.58	0/1926
14	G	0.29	0/1343	0.53	0/1816
15	H	0.32	0/1122	0.68	0/1515
16	I	0.25	0/692	0.45	0/960
17	J	0.33	0/1152	0.52	0/1551
18	K	0.33	0/947	0.60	0/1268
19	L	0.32	0/1054	0.60	0/1403
20	M	0.33	0/1093	0.58	0/1460
21	N	0.30	0/973	0.56	0/1301
22	O	0.31	0/902	0.60	0/1209
23	P	0.32	0/929	0.56	0/1242
24	Q	0.33	0/960	0.53	0/1278
25	R	0.34	0/829	0.59	0/1107
26	S	0.29	0/864	0.53	0/1156
27	T	0.31	0/744	0.55	0/994
28	U	0.31	0/787	0.52	0/1051
29	V	0.32	0/766	0.53	0/1025
30	W	0.32	0/582	0.54	0/769
31	X	0.33	0/635	0.59	0/848

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	0.30	0/510	0.58	0/677
33	Z	0.28	0/453	0.58	0/605
34	a	0.53	0/36725	0.83	25/57285 (0.0%)
35	b	0.29	0/1735	0.57	1/2338 (0.0%)
36	c	0.31	0/1651	0.55	0/2225
37	d	0.29	0/1665	0.55	0/2227
38	e	0.31	0/1154	0.55	0/1554
39	f	0.31	0/835	0.59	0/1128
40	g	0.28	0/1195	0.58	0/1602
41	h	0.30	0/989	0.50	0/1326
42	i	0.31	0/1034	0.64	0/1375
43	j	0.34	0/796	0.69	0/1077
44	k	0.31	0/885	0.63	0/1195
45	l	0.34	0/969	0.63	1/1300 (0.1%)
46	m	0.30	0/892	0.62	0/1193
47	n	0.28	0/811	0.55	0/1081
48	o	0.27	0/722	0.55	0/964
49	p	0.31	0/659	0.58	0/884
50	q	0.32	0/657	0.58	0/881
51	r	0.33	0/544	0.56	0/731
52	s	0.31	0/675	0.59	0/908
53	t	0.27	0/671	0.48	0/888
54	u	0.33	0/512	0.60	0/683
55	v	0.51	1/1745 (0.1%)	0.80	0/2716
56	w	0.36	0/1650	0.82	1/2569 (0.0%)
57	y	0.43	0/11	0.26	0/13
58	z	0.49	0/255	1.18	3/394 (0.8%)
All	All	0.51	3/158864 (0.0%)	0.76	55/237661 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	1	U	OP3-P	-10.68	1.48	1.61
55	v	1	C	OP3-P	-10.66	1.48	1.61
8	A	1	G	OP3-P	-10.60	1.48	1.61

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	z	-1	C	OP2-P-O3'	-10.72	81.61	105.20
58	z	-1	C	OP1-P-O3'	-10.70	81.67	105.20
34	a	999	C	C2-N1-C1'	9.50	129.25	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	999	C	C6-N1-C1'	-7.77	111.47	120.80
8	A	2506	U	C2-N1-C1'	7.61	126.83	117.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	54/57 (95%)	54 (100%)	0	0	100	100
2	1	48/55 (87%)	48 (100%)	0	0	100	100
3	2	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
4	3	62/65 (95%)	59 (95%)	3 (5%)	0	100	100
5	4	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
6	5	129/165 (78%)	116 (90%)	13 (10%)	0	100	100
7	6	64/70 (91%)	57 (89%)	7 (11%)	0	100	100
10	C	269/273 (98%)	256 (95%)	13 (5%)	0	100	100
11	D	207/209 (99%)	197 (95%)	10 (5%)	0	100	100
12	E	199/201 (99%)	197 (99%)	2 (1%)	0	100	100
13	F	175/179 (98%)	161 (92%)	14 (8%)	0	100	100
14	G	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
15	H	147/149 (99%)	128 (87%)	19 (13%)	0	100	100
16	I	139/142 (98%)	130 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	J	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
18	K	120/123 (98%)	116 (97%)	4 (3%)	0	100	100
19	L	141/144 (98%)	133 (94%)	8 (6%)	0	100	100
20	M	134/136 (98%)	129 (96%)	5 (4%)	0	100	100
21	N	118/127 (93%)	113 (96%)	5 (4%)	0	100	100
22	O	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
23	P	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
24	Q	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
25	R	101/103 (98%)	95 (94%)	5 (5%)	1 (1%)	15	15
26	S	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
27	T	91/100 (91%)	91 (100%)	0	0	100	100
28	U	100/104 (96%)	92 (92%)	8 (8%)	0	100	100
29	V	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
30	W	73/85 (86%)	69 (94%)	4 (6%)	0	100	100
31	X	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
32	Y	61/63 (97%)	61 (100%)	0	0	100	100
33	Z	56/59 (95%)	56 (100%)	0	0	100	100
35	b	216/240 (90%)	203 (94%)	13 (6%)	0	100	100
36	c	204/233 (88%)	195 (96%)	9 (4%)	0	100	100
37	d	203/206 (98%)	190 (94%)	13 (6%)	0	100	100
38	e	155/167 (93%)	152 (98%)	3 (2%)	0	100	100
39	f	98/135 (73%)	94 (96%)	4 (4%)	0	100	100
40	g	149/179 (83%)	145 (97%)	4 (3%)	0	100	100
41	h	127/130 (98%)	125 (98%)	2 (2%)	0	100	100
42	i	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
43	j	96/103 (93%)	85 (88%)	11 (12%)	0	100	100
44	k	114/129 (88%)	106 (93%)	8 (7%)	0	100	100
45	l	121/124 (98%)	116 (96%)	5 (4%)	0	100	100
46	m	112/118 (95%)	108 (96%)	4 (4%)	0	100	100
47	n	99/102 (97%)	98 (99%)	1 (1%)	0	100	100
48	o	86/89 (97%)	80 (93%)	6 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
49	p	80/82 (98%)	76 (95%)	4 (5%)	0	100	100
50	q	78/84 (93%)	76 (97%)	2 (3%)	0	100	100
51	r	63/75 (84%)	61 (97%)	2 (3%)	0	100	100
52	s	80/92 (87%)	79 (99%)	1 (1%)	0	100	100
53	t	83/87 (95%)	81 (98%)	2 (2%)	0	100	100
54	u	63/71 (89%)	61 (97%)	2 (3%)	0	100	100
All	All	5850/6220 (94%)	5602 (96%)	247 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
25	R	51	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	47/48 (98%)	47 (100%)	0	100	100
2	1	45/49 (92%)	42 (93%)	3 (7%)	16	17
3	2	38/38 (100%)	34 (90%)	4 (10%)	7	6
4	3	51/52 (98%)	50 (98%)	1 (2%)	55	66
5	4	34/34 (100%)	32 (94%)	2 (6%)	19	22
7	6	59/62 (95%)	49 (83%)	10 (17%)	2	1
10	C	216/218 (99%)	213 (99%)	3 (1%)	67	78
11	D	164/164 (100%)	163 (99%)	1 (1%)	86	93
12	E	165/165 (100%)	164 (99%)	1 (1%)	86	93
13	F	148/150 (99%)	141 (95%)	7 (5%)	26	31
14	G	137/138 (99%)	130 (95%)	7 (5%)	24	27
15	H	114/114 (100%)	99 (87%)	15 (13%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	J	116/116 (100%)	113 (97%)	3 (3%)	46	56
18	K	103/104 (99%)	101 (98%)	2 (2%)	57	68
19	L	102/103 (99%)	102 (100%)	0	100	100
20	M	109/109 (100%)	105 (96%)	4 (4%)	34	42
21	N	100/103 (97%)	98 (98%)	2 (2%)	55	66
22	O	86/87 (99%)	83 (96%)	3 (4%)	36	44
23	P	99/100 (99%)	95 (96%)	4 (4%)	31	39
24	Q	89/90 (99%)	88 (99%)	1 (1%)	73	84
25	R	84/84 (100%)	79 (94%)	5 (6%)	19	21
26	S	93/93 (100%)	93 (100%)	0	100	100
27	T	80/84 (95%)	79 (99%)	1 (1%)	69	80
28	U	83/85 (98%)	79 (95%)	4 (5%)	25	30
29	V	78/78 (100%)	75 (96%)	3 (4%)	33	41
30	W	57/63 (90%)	57 (100%)	0	100	100
31	X	67/68 (98%)	66 (98%)	1 (2%)	65	76
32	Y	55/55 (100%)	53 (96%)	2 (4%)	35	43
33	Z	48/49 (98%)	46 (96%)	2 (4%)	30	36
35	b	180/198 (91%)	173 (96%)	7 (4%)	32	40
36	c	170/190 (90%)	164 (96%)	6 (4%)	36	44
37	d	172/173 (99%)	162 (94%)	10 (6%)	20	22
38	e	114/126 (90%)	109 (96%)	5 (4%)	28	34
39	f	87/116 (75%)	81 (93%)	6 (7%)	15	15
40	g	124/147 (84%)	112 (90%)	12 (10%)	8	7
41	h	104/105 (99%)	101 (97%)	3 (3%)	42	52
42	i	105/107 (98%)	90 (86%)	15 (14%)	3	3
43	j	86/90 (96%)	79 (92%)	7 (8%)	11	11
44	k	89/99 (90%)	86 (97%)	3 (3%)	37	46
45	l	103/104 (99%)	103 (100%)	0	100	100
46	m	92/96 (96%)	82 (89%)	10 (11%)	6	6
47	n	79/84 (94%)	77 (98%)	2 (2%)	47	58
48	o	76/77 (99%)	72 (95%)	4 (5%)	22	26

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	p	65/65 (100%)	64 (98%)	1 (2%)	65	76
50	q	74/78 (95%)	73 (99%)	1 (1%)	67	78
51	r	56/65 (86%)	54 (96%)	2 (4%)	35	43
52	s	72/79 (91%)	67 (93%)	5 (7%)	15	15
53	t	65/66 (98%)	60 (92%)	5 (8%)	13	12
54	u	46/61 (75%)	44 (96%)	2 (4%)	29	35
57	y	1/1 (100%)	0	1 (100%)	0	0
All	All	4627/4830 (96%)	4429 (96%)	198 (4%)	33	35

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	e	44	ARG
42	i	28	VAL
39	f	1	MET
40	g	51	GLN
42	i	96	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
36	c	99	GLN
39	f	3	HIS
47	n	49	GLN
32	Y	36	GLN
32	Y	15	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
34	a	1536/1542 (99%)	312 (20%)	0
55	v	76/77 (98%)	18 (23%)	0
56	w	74/76 (97%)	18 (24%)	0
58	z	10/33 (30%)	1 (10%)	0
8	A	2898/2903 (99%)	517 (17%)	37 (1%)
9	B	119/120 (99%)	23 (19%)	4 (3%)
All	All	4713/4751 (99%)	889 (18%)	41 (0%)

5 of 889 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	A	10	A
8	A	15	G
8	A	23	G
8	A	34	U
8	A	35	G

5 of 41 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	A	2158	A
8	A	2796	U
8	A	2192	U
8	A	2468	A
9	B	36	C

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

46 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	5MU	A	1939	8	15,22,23	2.90	3 (20%)	16,32,35	2.92	2 (12%)
55	4SU	v	8	55	14,21,22	3.35	5 (35%)	15,30,33	1.25	2 (13%)
34	MA6	a	1519	34	19,26,27	1.00	1 (5%)	18,38,41	2.76	2 (11%)
34	G7M	a	527	34	20,26,27	3.43	7 (35%)	20,39,42	2.29	4 (20%)
57	FME	y	101	57	8,9,10	0.88	0	7,9,11	1.81	2 (28%)
55	PSU	v	55	55	17,21,22	0.99	1 (5%)	20,30,33	3.20	7 (35%)
8	PSU	A	2504	8	17,21,22	1.06	2 (11%)	20,30,33	3.13	6 (30%)
8	PSU	A	955	8	17,21,22	1.10	3 (17%)	20,30,33	3.02	6 (30%)
8	PSU	A	1917	8	17,21,22	1.04	2 (11%)	20,30,33	3.09	6 (30%)
8	PSU	A	2604	8	17,21,22	1.06	2 (11%)	20,30,33	3.02	6 (30%)
8	6MZ	A	1618	8	18,25,26	2.14	3 (16%)	16,36,39	1.85	3 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	PSU	A	2457	8	17,21,22	1.11	3 (17%)	20,30,33	2.96	6 (30%)
55	5MU	v	54	55	15,22,23	2.86	3 (20%)	16,32,35	2.83	2 (12%)
8	G7M	A	2069	8	20,26,27	3.41	8 (40%)	20,39,42	2.72	7 (35%)
34	2MG	a	1516	34	19,26,27	4.79	8 (42%)	21,38,41	2.36	8 (38%)
8	5MC	A	1962	8	15,22,23	3.18	5 (33%)	19,32,35	1.19	2 (10%)
8	PSU	A	1911	8	17,21,22	1.07	3 (17%)	20,30,33	3.04	6 (30%)
34	2MG	a	966	34	19,26,27	4.75	8 (42%)	21,38,41	2.12	8 (38%)
56	G7M	w	46	56	20,26,27	3.50	8 (40%)	20,39,42	2.52	5 (25%)
8	6MZ	A	2030	8	18,25,26	2.05	3 (16%)	16,36,39	2.30	3 (18%)
34	5MC	a	967	34	15,22,23	3.16	5 (33%)	19,32,35	1.24	3 (15%)
56	PSU	w	55	56	17,21,22	1.15	3 (17%)	20,30,33	3.07	7 (35%)
56	PSU	w	32	56	17,21,22	1.00	1 (5%)	20,30,33	3.15	7 (35%)
8	OMG	A	2251	8,55,59	18,26,27	3.49	7 (38%)	20,38,41	1.81	4 (20%)
8	5MC	A	747	8	15,22,23	3.12	5 (33%)	19,32,35	1.33	3 (15%)
56	5MU	w	54	56	15,22,23	2.85	3 (20%)	16,32,35	2.76	2 (12%)
8	OMC	A	2498	8,59	15,22,23	3.44	5 (33%)	17,31,34	1.27	1 (5%)
8	3TD	A	1915	8	17,22,23	3.68	6 (35%)	19,32,35	1.80	4 (21%)
55	H2U	v	20	55	18,21,22	3.08	5 (27%)	21,30,33	1.98	5 (23%)
8	PSU	A	2605	8	17,21,22	1.07	2 (11%)	20,30,33	3.04	5 (25%)
56	PSU	w	39	56	17,21,22	0.99	2 (11%)	20,30,33	3.06	6 (30%)
8	2MA	A	2503	8,59	17,25,26	3.75	5 (29%)	19,37,40	1.86	4 (21%)
34	PSU	a	516	34,59	17,21,22	0.97	1 (5%)	20,30,33	3.10	6 (30%)
8	2MG	A	1835	8	19,26,27	4.77	7 (36%)	21,38,41	2.14	8 (38%)
8	PSU	A	2580	8	17,21,22	1.16	3 (17%)	20,30,33	3.15	8 (40%)
8	OMU	A	2552	8,59	14,22,23	3.26	5 (35%)	14,31,34	0.73	0
34	4OC	a	1402	34	16,23,24	3.19	6 (37%)	17,32,35	1.30	1 (5%)
34	5MC	a	1407	34	15,22,23	3.14	5 (33%)	19,32,35	1.23	2 (10%)
8	PSU	A	746	8,59	17,21,22	1.09	2 (11%)	20,30,33	3.19	7 (35%)
34	MA6	a	1518	34	19,26,27	1.00	1 (5%)	18,38,41	2.71	2 (11%)
8	2MG	A	2445	8	19,26,27	4.72	8 (42%)	21,38,41	2.22	8 (38%)
34	2MG	a	1207	34	19,26,27	4.82	8 (42%)	21,38,41	2.15	8 (38%)
34	UR3	a	1498	34	14,22,23	2.79	4 (28%)	15,32,35	0.69	0
56	4SU	w	8	56	14,21,22	3.34	5 (35%)	15,30,33	1.25	2 (13%)
8	1MG	A	745	8	18,26,27	3.54	5 (27%)	19,39,42	2.26	2 (10%)
56	MIA	w	37	56	24,31,32	2.51	4 (16%)	26,44,47	3.11	9 (34%)

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	5MU	A	1939	8	-	4/5/25/26	0/2/2/2
55	4SU	v	8	55	-	0/5/25/26	0/2/2/2
34	MA6	a	1519	34	-	1/7/29/30	0/3/3/3
34	G7M	a	527	34	-	1/3/25/26	0/3/3/3
57	FME	y	101	57	-	5/7/9/11	-
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
8	PSU	A	2504	8	-	2/7/25/26	0/2/2/2
8	PSU	A	955	8	-	0/7/25/26	0/2/2/2
8	PSU	A	1917	8	-	2/7/25/26	0/2/2/2
8	PSU	A	2604	8	-	0/7/25/26	0/2/2/2
8	6MZ	A	1618	8	-	0/5/27/28	0/3/3/3
8	PSU	A	2457	8	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	0/5/25/26	0/2/2/2
8	G7M	A	2069	8	-	1/3/25/26	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
8	5MC	A	1962	8	-	2/5/25/26	0/2/2/2
8	PSU	A	1911	8	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	0/5/27/28	0/3/3/3
56	G7M	w	46	56	-	0/3/25/26	0/3/3/3
8	6MZ	A	2030	8	-	2/5/27/28	0/3/3/3
34	5MC	a	967	34	-	0/5/25/26	0/2/2/2
56	PSU	w	55	56	-	0/7/25/26	0/2/2/2
56	PSU	w	32	56	-	2/7/25/26	0/2/2/2
8	OMG	A	2251	8,55,59	-	1/5/27/28	0/3/3/3
8	5MC	A	747	8	-	0/5/25/26	0/2/2/2
56	5MU	w	54	56	-	0/5/25/26	0/2/2/2
8	OMC	A	2498	8,59	-	2/7/27/28	0/2/2/2
8	3TD	A	1915	8	-	2/7/25/26	0/2/2/2
55	H2U	v	20	55	-	3/7/38/39	0/2/2/2
8	PSU	A	2605	8	-	0/7/25/26	0/2/2/2
56	PSU	w	39	56	-	3/7/25/26	0/2/2/2
8	2MA	A	2503	8,59	-	2/3/25/26	0/3/3/3
34	PSU	a	516	34,59	-	0/7/25/26	0/2/2/2
8	2MG	A	1835	8	-	2/5/27/28	0/3/3/3
8	PSU	A	2580	8	-	0/7/25/26	0/2/2/2
8	OMU	A	2552	8,59	-	1/7/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
34	5MC	a	1407	34	-	0/5/25/26	0/2/2/2
8	PSU	A	746	8,59	-	3/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	0/7/29/30	0/3/3/3
8	2MG	A	2445	8	-	2/5/27/28	0/3/3/3
34	2MG	a	1207	34	-	0/5/27/28	0/3/3/3
34	UR3	a	1498	34	-	0/5/25/26	0/2/2/2
56	4SU	w	8	56	-	0/5/25/26	0/2/2/2
8	1MG	A	745	8	-	0/3/25/26	0/3/3/3
56	MIA	w	37	56	-	2/11/33/34	0/3/3/3

The worst 5 of 191 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	a	1207	2MG	C2-N2	15.71	1.47	1.34
34	a	1516	2MG	C2-N2	15.65	1.47	1.34
8	A	1835	2MG	C2-N2	15.52	1.47	1.34
34	a	966	2MG	C2-N2	15.37	1.47	1.34
8	A	2445	2MG	C2-N2	15.30	1.47	1.34

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	516	PSU	N1-C2-N3	-10.66	119.96	128.43
55	v	55	PSU	N1-C2-N3	-10.56	120.03	128.43
56	w	32	PSU	N1-C2-N3	-10.44	120.13	128.43
8	A	746	PSU	N1-C2-N3	-10.40	120.16	128.43
56	w	39	PSU	N1-C2-N3	-10.33	120.22	128.43

There are no chirality outliers.

5 of 49 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	v	20	H2U	O4'-C4'-C5'-O5'
55	v	55	PSU	O4'-C1'-C5-C4
55	v	55	PSU	O4'-C1'-C5-C6
8	A	746	PSU	O4'-C1'-C5-C4
8	A	746	PSU	O4'-C1'-C5-C6

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 371 ligands modelled in this entry, 367 are monoatomic - leaving 4 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
62	AM2	a	1685	-	40,40,40	1.67	7 (17%)	53,60,60	1.08	5 (9%)
62	AM2	a	1684	-	40,40,40	1.62	8 (20%)	53,60,60	1.10	3 (5%)
62	AM2	a	1689	-	40,40,40	1.64	8 (20%)	53,60,60	1.09	4 (7%)
62	AM2	a	1682	-	40,40,40	1.61	9 (22%)	53,60,60	1.05	3 (5%)

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
62	AM2	a	1685	-	-	4/12/84/84	0/4/4/4
62	AM2	a	1684	-	-	4/12/84/84	0/4/4/4
62	AM2	a	1689	-	-	3/12/84/84	0/4/4/4
62	AM2	a	1682	-	-	1/12/84/84	0/4/4/4

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	a	1685	AM2	OA4-CA1	4.60	1.53	1.41
62	a	1689	AM2	OA4-CA1	4.58	1.53	1.41
62	a	1684	AM2	OA4-CA1	4.49	1.53	1.41

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
62	a	1682	AM2	OA4-CA1	4.32	1.52	1.41
62	a	1685	AM2	OA4-CA5	3.77	1.49	1.44

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
62	a	1684	AM2	CA9-NA7-CA7	-3.48	109.32	114.38
62	a	1682	AM2	CA9-NA7-CA7	-3.46	109.35	114.38
62	a	1684	AM2	CA1-OA1-CC1	-3.28	109.83	117.96
62	a	1689	AM2	CA9-NA7-CA7	-3.19	109.74	114.38
62	a	1689	AM2	CA1-OA1-CC1	-3.08	110.35	117.96

There are no chirality outliers.

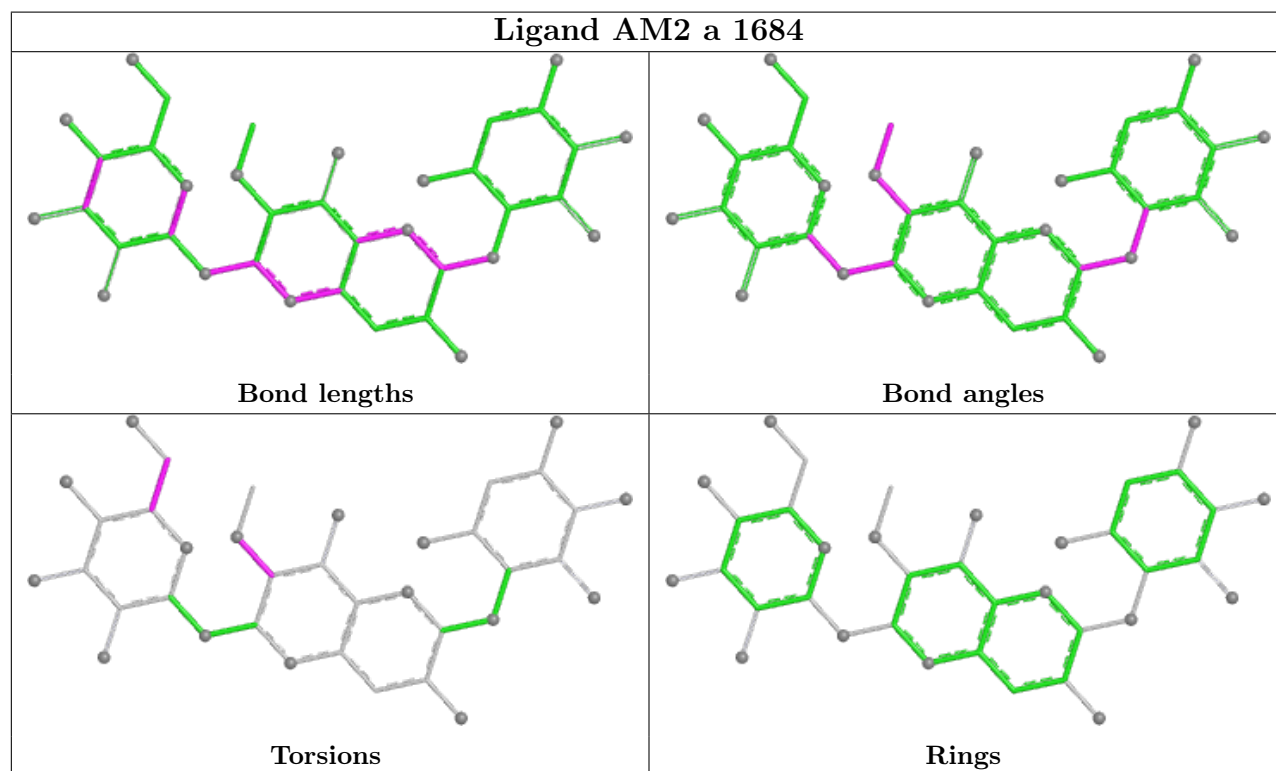
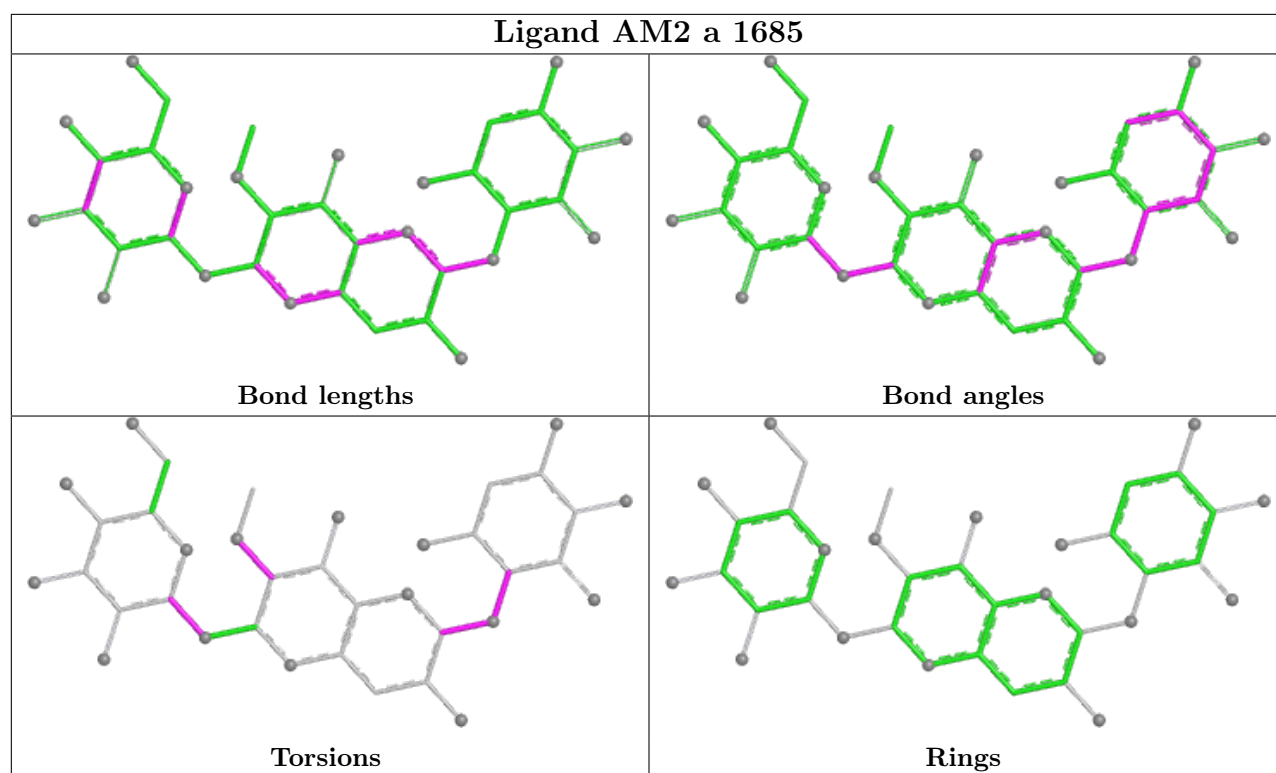
5 of 12 torsion outliers are listed below:

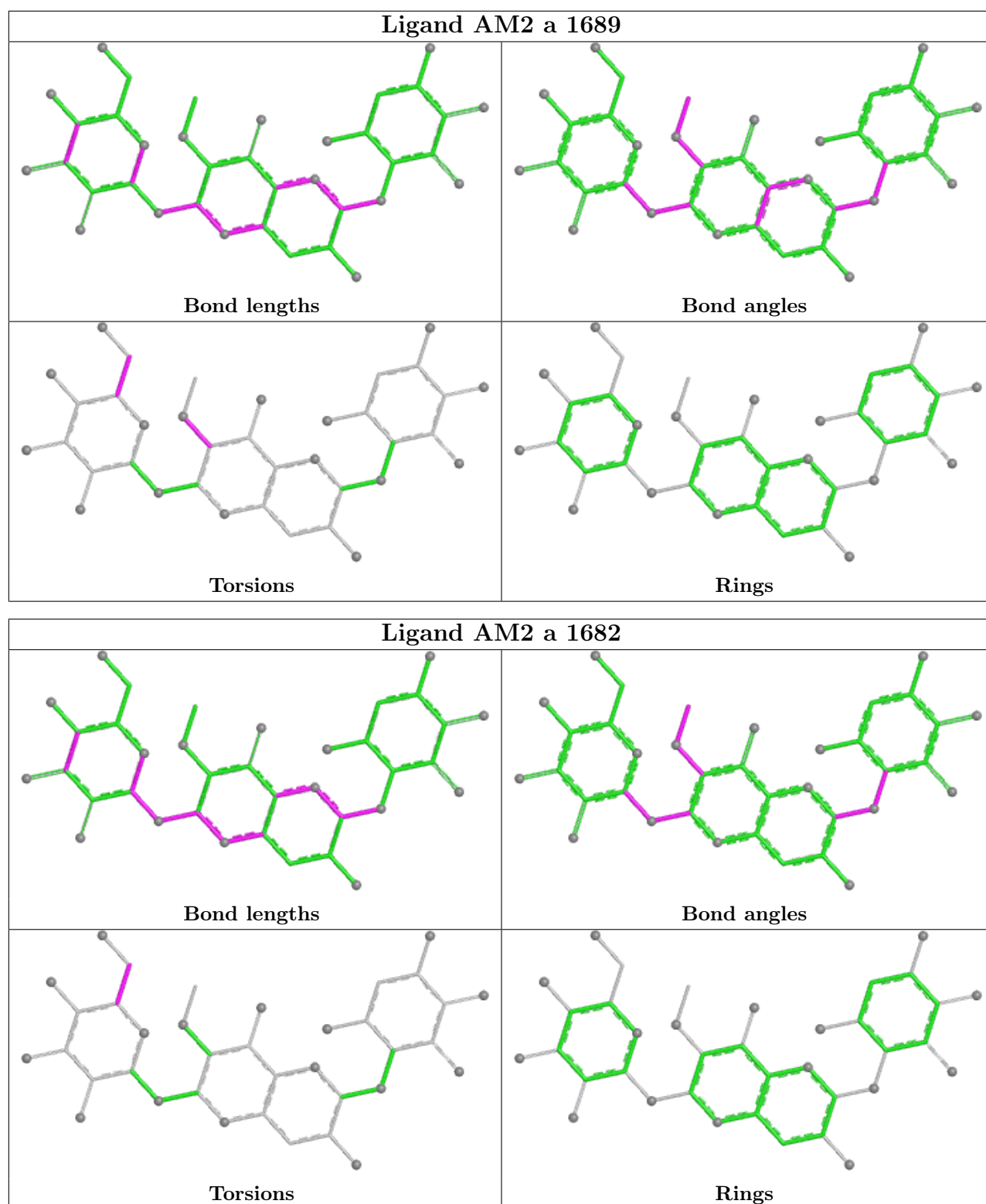
Mol	Chain	Res	Type	Atoms
62	a	1684	AM2	CA6-CA7-NA7-CA9
62	a	1684	AM2	CA8-CA7-NA7-CA9
62	a	1685	AM2	CA8-CA7-NA7-CA9
62	a	1684	AM2	OB1-CB5-CB6-OB6
62	a	1684	AM2	CB4-CB5-CB6-OB6

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

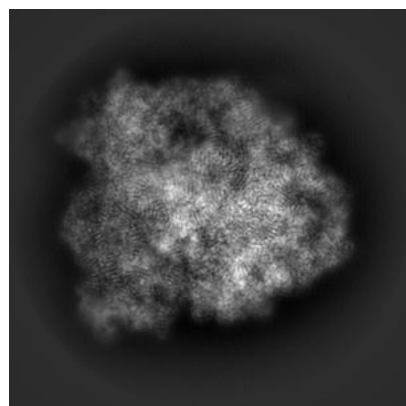
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13458. These allow visual inspection of the internal detail of the map and identification of artifacts.

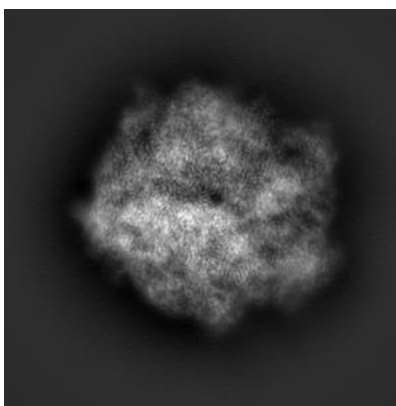
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

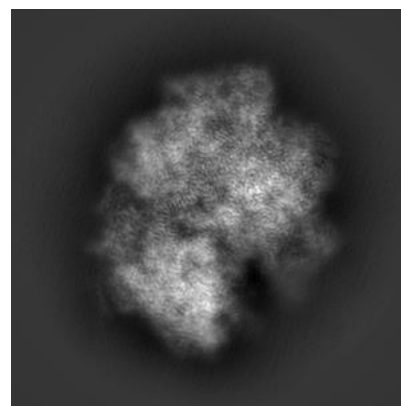
6.1.1 Primary map



X

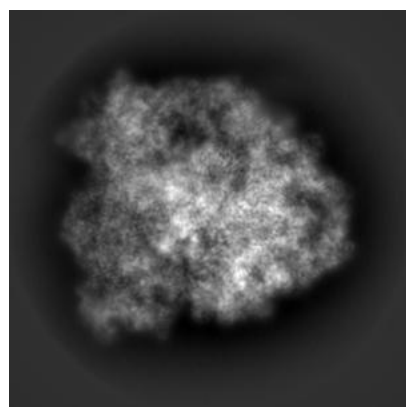


Y

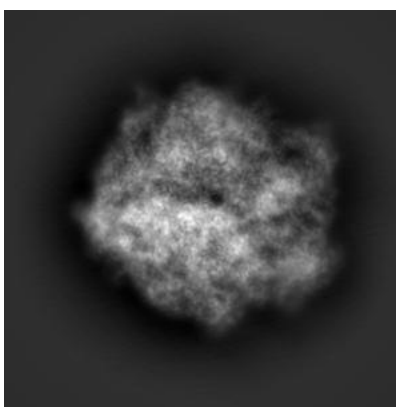


Z

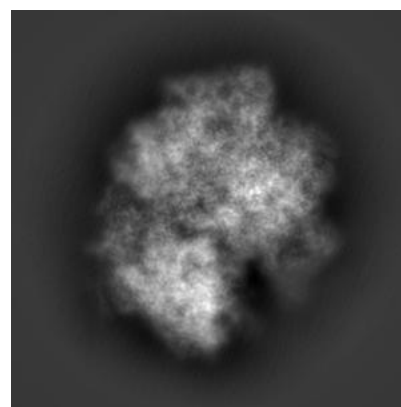
6.1.2 Raw map



X



Y

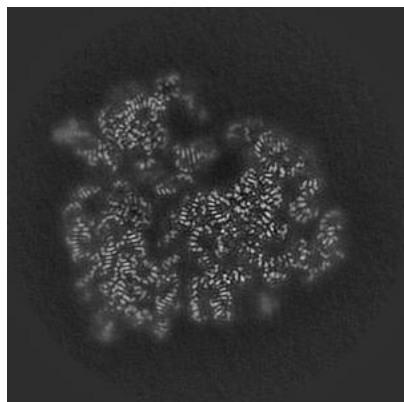


Z

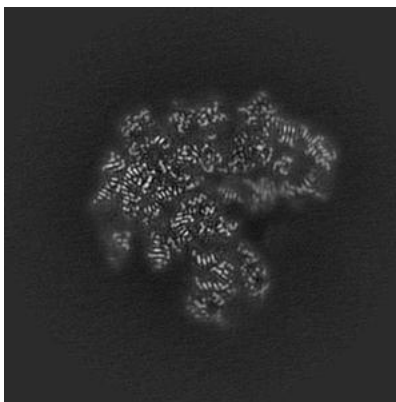
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

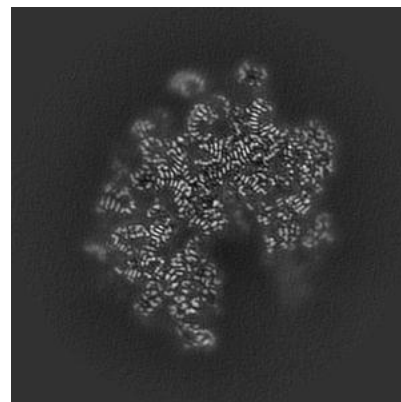
6.2.1 Primary map



X Index: 256

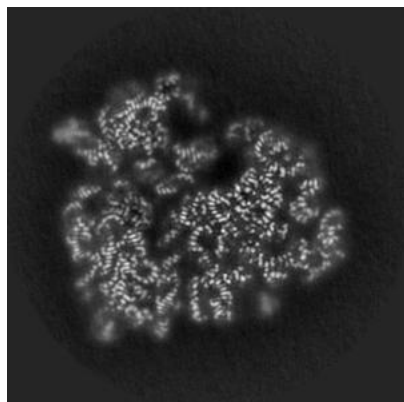


Y Index: 256

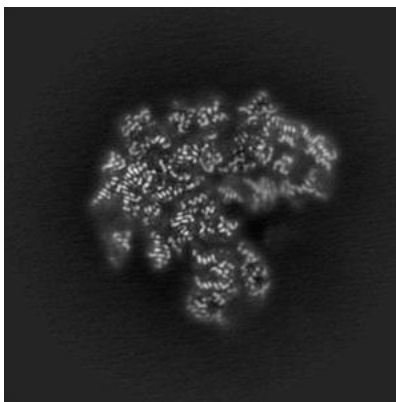


Z Index: 256

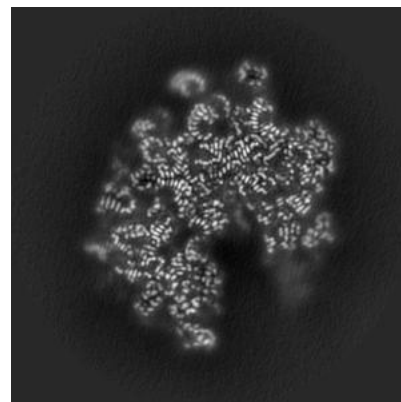
6.2.2 Raw map



X Index: 144



Y Index: 144

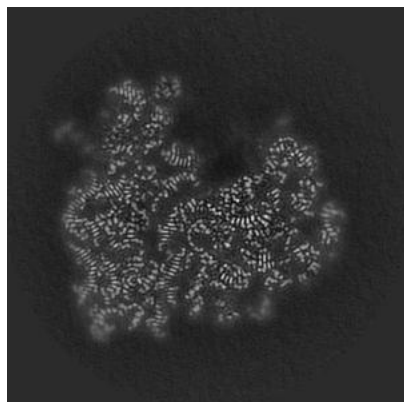


Z Index: 144

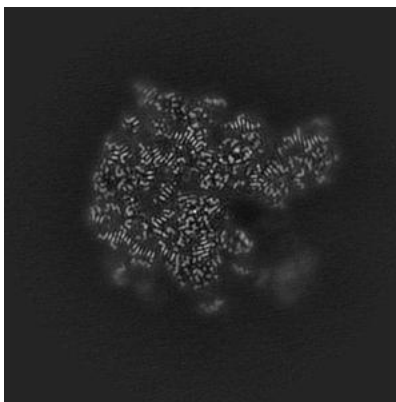
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

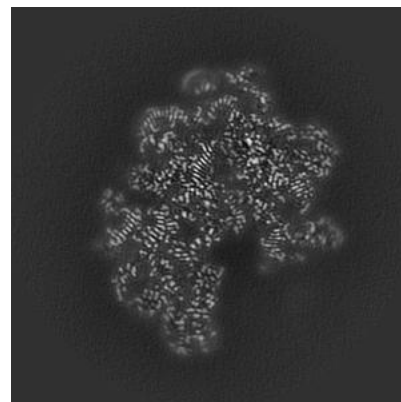
6.3.1 Primary map



X Index: 246

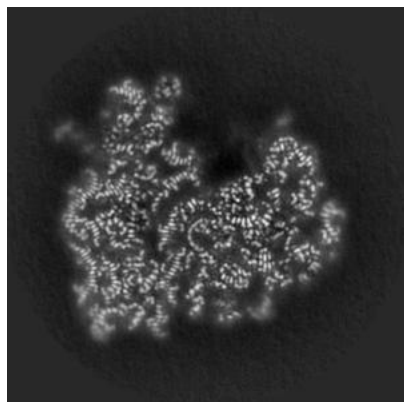


Y Index: 285

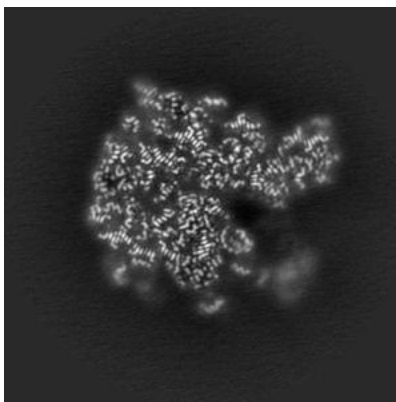


Z Index: 242

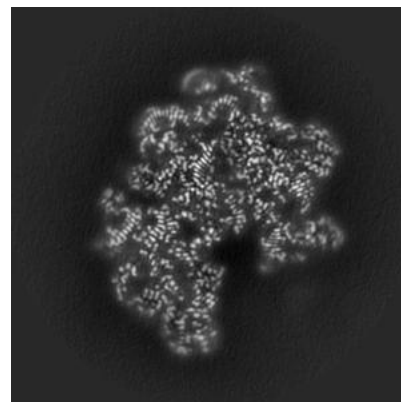
6.3.2 Raw map



X Index: 138



Y Index: 160



Z Index: 136

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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

6.4.2 Raw map



X



Y



Z

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

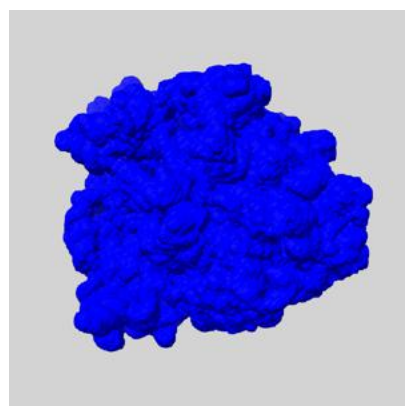
6.5 Mask visualisation [i](#)

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

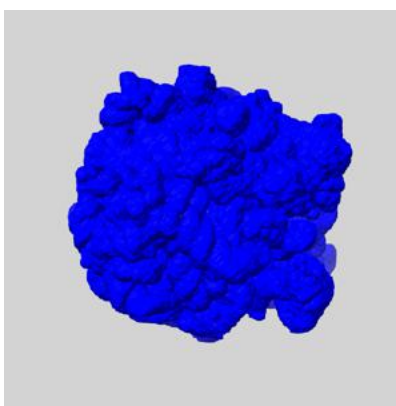
A mask typically either:

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

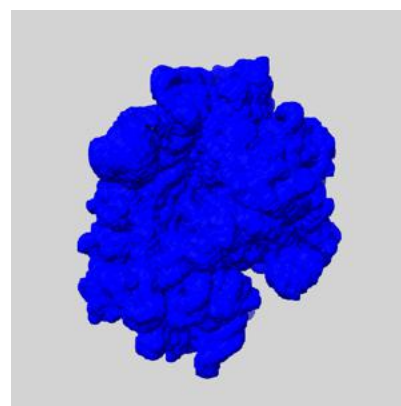
6.5.1 emd_13458_msk_1.map [i](#)



X



Y

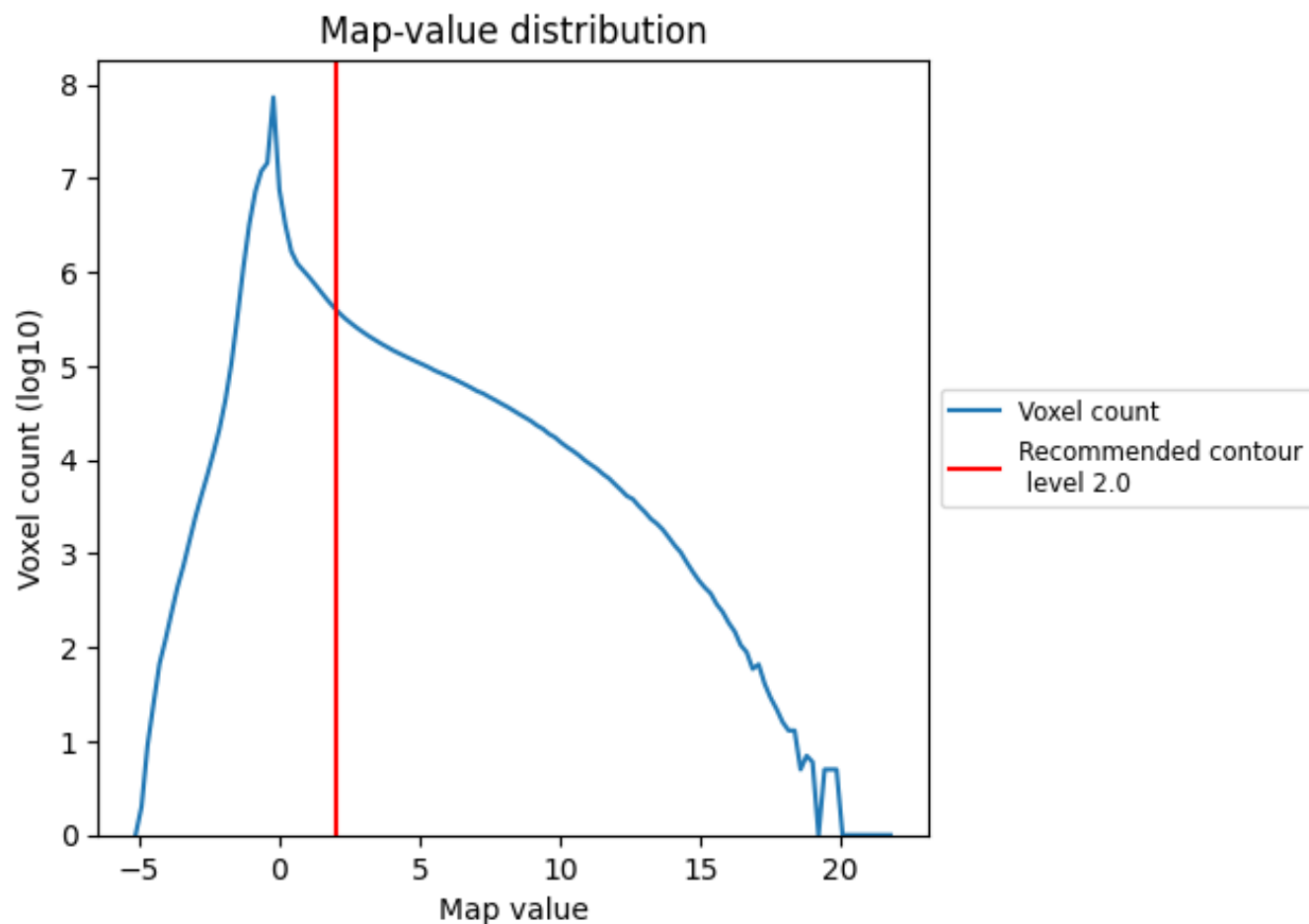


Z

7 Map analysis [i](#)

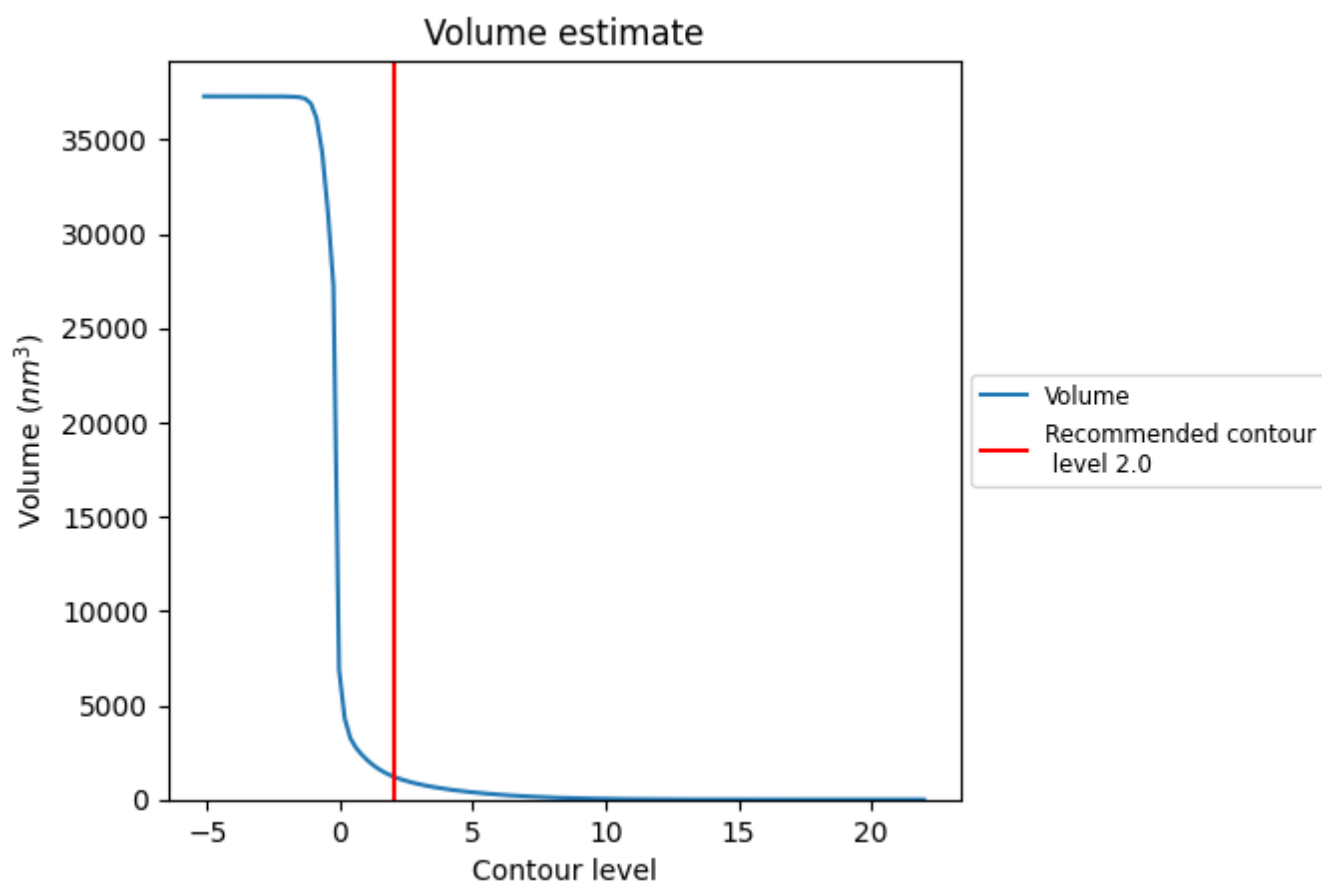
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1226 nm³; this corresponds to an approximate mass of 1108 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.

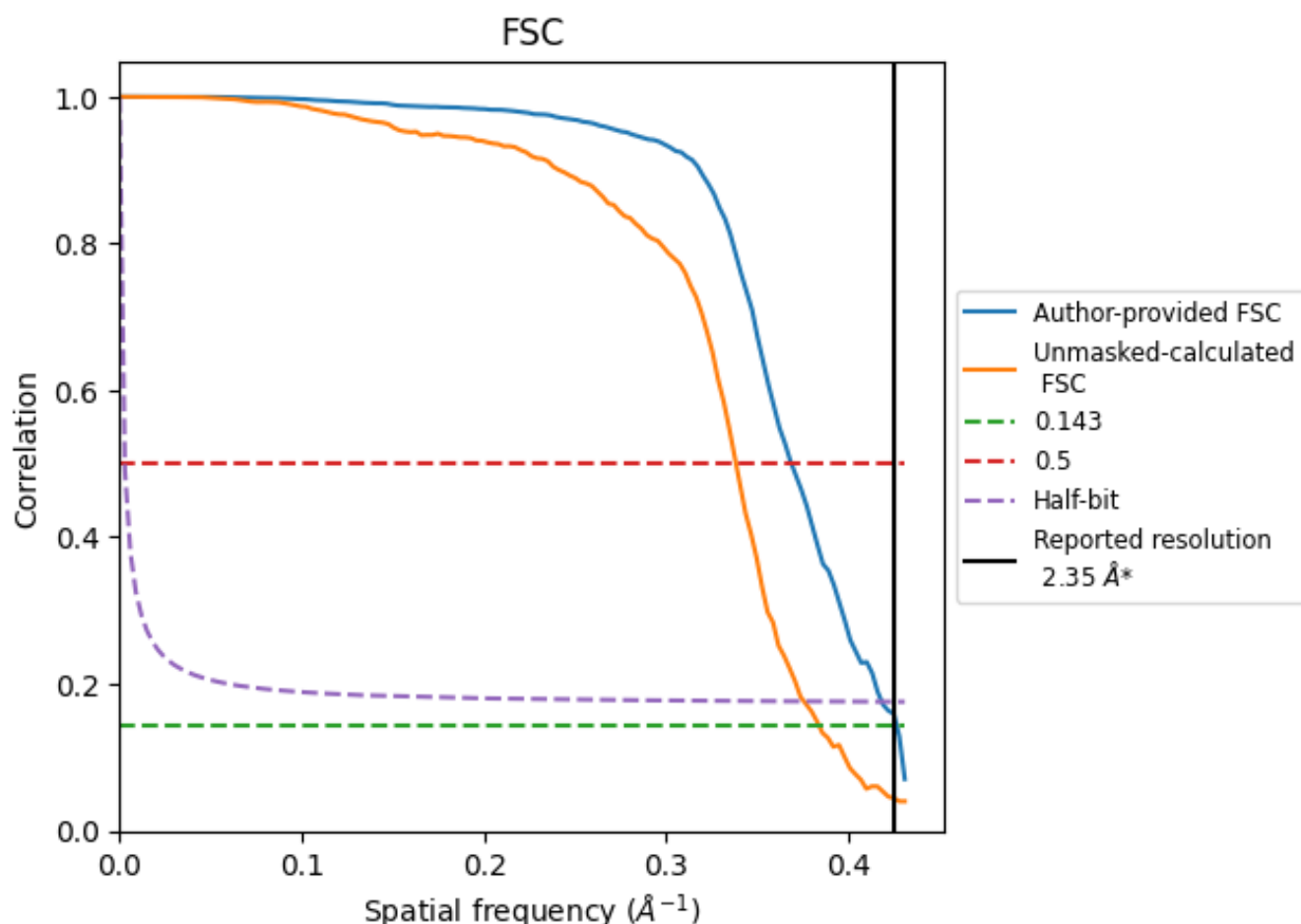
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.426 Å⁻¹

8.2 Resolution estimates [i](#)

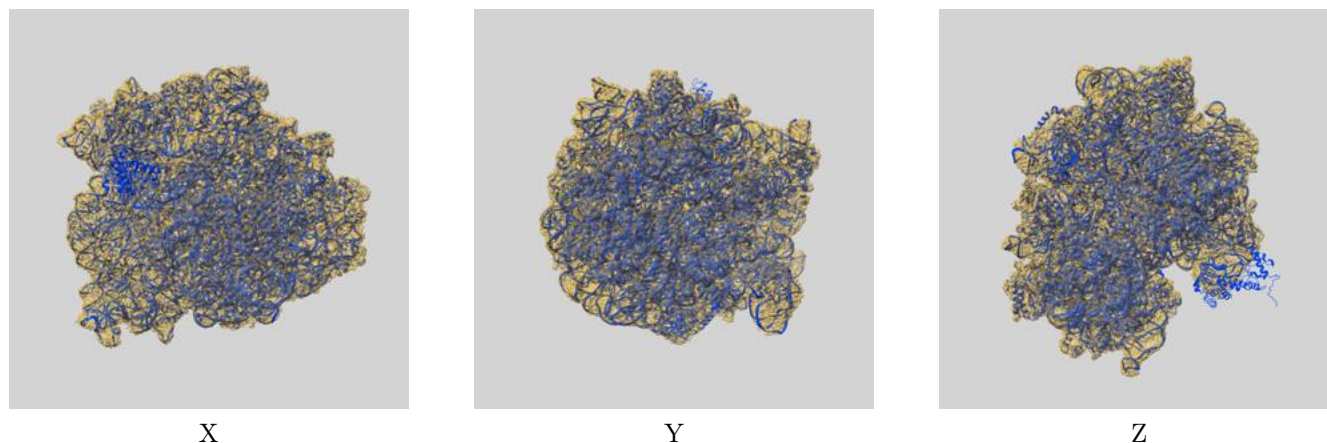
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.35	-	-
Author-provided FSC curve	2.34	2.71	2.39
Unmasked-calculated*	2.60	2.96	2.66

*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 2.60 differs from the reported value 2.35 by more than 10 %

9 Map-model fit [i](#)

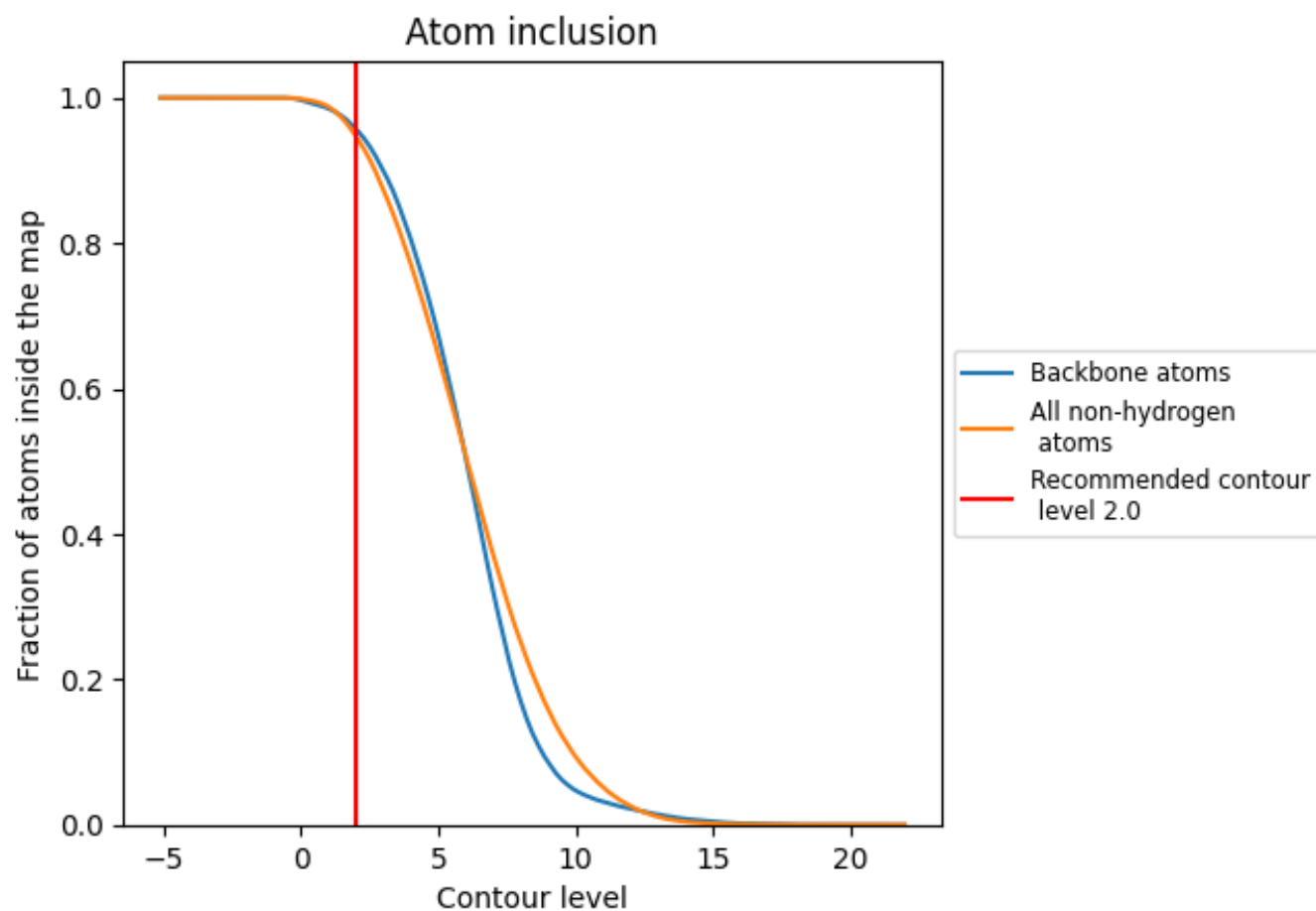
This section contains information regarding the fit between EMDB map EMD-13458 and PDB model 7PJS. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 2.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.