Full wwPDB EM Validation Report (i)

Feb 4, 2024 – 02:20 PM EST

PDB ID	:	7UNV
EMDB ID	:	EMD-26634
Title	:	Pseudomonas aeruginosa 70S ribosome initiation complex bound to IF2-GDPCP (structure II-A)
Authors	:	Basu, R.S.; Sherman, M.B.; Gagnon, M.G.
Deposited on	:	2022-04-11
Resolution	:	2.70 Å(reported)
Based on initial models	:	3JCJ, 6SPG

This is a Full wwPDB EM Validation 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:

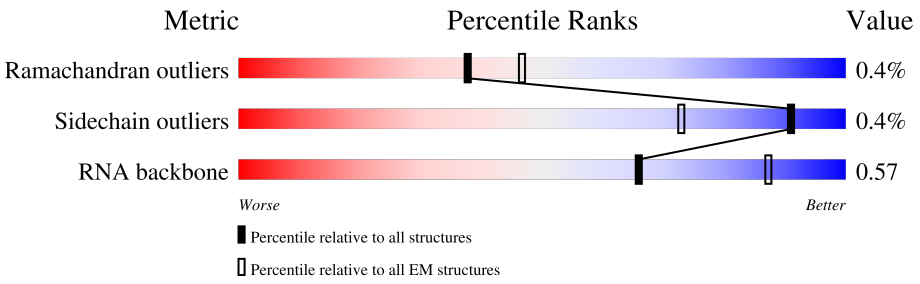
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	a	1536	81% 18% •
2	b	246	• 90% • 9%
3	c	228	• 91% 9%
4	d	206	99%
5	e	166	93% 7%
6	f	139	74% • 24%
7	g	156	5% 97% • •
8	h	130	98% ••

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Mol	Chain	Length	Quality of chain
9	i	130	95%
10	j	103	6%, 96%
11	k	129	92%, 8%
12	l	123	98%
13	m	118	96%
14	n	101	97%
15	o	89	98%
16	p	83	98%
17	q	88	91%, 9%
18	r	76	7%, 80%, 18%
19	s	91	90%, 9%
20	t	91	96%
21	u	71	87%, 13%
22	v	77	74%, 18%, 6%
23	w	24	25%, 75%
24	x	840	70%, 29%
25	A	2891	79%, 20%
26	B	120	84%, 12%
27	C	273	100%
28	D	211	99%
29	E	200	98%
30	F	179	96%
31	G	177	98%
32	H	148	49%, 51%
33	I	166	57%, 69%, 29%

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Mol	Chain	Length	Quality of chain
34	J	143	13% 93% 6%
35	L	142	100%
36	M	122	100%
37	N	144	100%
38	O	137	100%
39	P	129	93% 7%
40	Q	116	99%
41	R	116	97%
42	S	118	99%
43	T	103	98%
44	U	110	100%
45	V	99	95% 5%
46	W	104	98%
47	X	204	93% 7%
48	Y	85	88% 11%
49	Z	78	97%
50	1	63	97%
51	2	58	98%
52	3	71	17% 65% 34%
53	4	60	92% 8%
54	5	51	100%
55	6	44	100%
56	7	64	98%
57	8	38	100%

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 149599 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	1522	32675	14581	5999	10574	1521	0	0

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	b	224	1751	1104	320	317	10	0	0

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	c	208	1656	1047	313	291	5	0	0

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	205	1617	998	313	301	5	0	0

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	e	154	1134	711	210	207	6	0	0

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	f	106	857	534	159	158	6	0	0

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	152	1187	743	231	208	5	0	0

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	129	982	618	173	185	6	0	0

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	127	1010	625	203	181	1	0	0

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	99	787	493	147	146	1	0	0

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	119	879	545	171	161	2	0	0

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	122	959	588	198	169	4	0	0

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	114	892	544	182	162	4	0	0

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	n	100	800	494	167	136	3	0	0

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	o	88	703	434	139	129	1	0	0

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	p	81	636	397	125	113	1	0	0

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	q	80	645	404	124	115	2	0	0

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
18	r	62	480	307	85	88	0	0

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	s	83	663	422	129	109	3	0	0

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	t	87	671	414	138	117	2	0	0

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	u	62	506	316	103	86	1	0	0

- Molecule 22 is a RNA chain called P-site initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
22	v	76	1625	725	294	529	76	1	0	0

- Molecule 23 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
23	w	6	131	59	27	39	6	0	0

- Molecule 24 is a protein called Translation initiation factor IF-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	x	593	4275	2676	773	810	16	0	0

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
25	A	2884	61891	27621	11346	20041	2883	0	0

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
26	B	117	2495	1114	448	816	117	0	0

- Molecule 27 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	C	272	2072	1276	426	364	6	0	0

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	D	211	1588	981	304	297	6	0	0

- Molecule 29 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	E	200	1521	955	283	280	3	0	0

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	F	176	1406	899	249	254	4	0	0

- Molecule 31 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	G	175	1323	834	244	243	2	0	0

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	H	72	513	321	92	99	1	0	0

- Molecule 33 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	I	118	587	349	118	120	0	0

- Molecule 34 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	J	134	689	415	134	138	2	0	0

- Molecule 35 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	L	142	1130	718	206	202	4	0	0

- Molecule 36 is a protein called 50S ribosomal protein L14.

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

- Molecule 37 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
37	N	144	1066	654	215	194	3	0	0

- Molecule 38 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	O	137	1085	689	211	181	4	0	0

- Molecule 39 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
39	P	120	959	600	192	162	5	0	0

- Molecule 40 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Q	115	881	544	174	161	2	0	0

- Molecule 41 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	R	114	902	568	171	162	1	0	0

- Molecule 42 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
42	S	117	933	591	196	146	0	0

- Molecule 43 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	T	103	822	521	156	143	2	0	0

- Molecule 44 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	U	110	833	515	161	153	4	0	0

- Molecule 45 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	V	94	739	472	134	132	1	0	0

- Molecule 46 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	W	103	786	494	150	141	1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	X	190	1445	915	262	265	3	0	0

- Molecule 48 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
48	Y	76	575	364	111	100	0	0

- Molecule 49 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	Z	77	630	391	134	103	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	1	61	490	301	96	91	2	0	0

- Molecule 51 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
51	2	57	445	277	87	79	2	0	0

- Molecule 52 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
52	3	47	356	222	60	68	6	0	0

- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
53	4	55	440	264	93	82	1	0	0

- Molecule 54 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
54	5	51	426	272	78	75	1	0	0

- Molecule 55 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
55	6	44	365	222	87	54	2	0	0

- Molecule 56 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
56	7	63	506	314	108	81	3	0	0

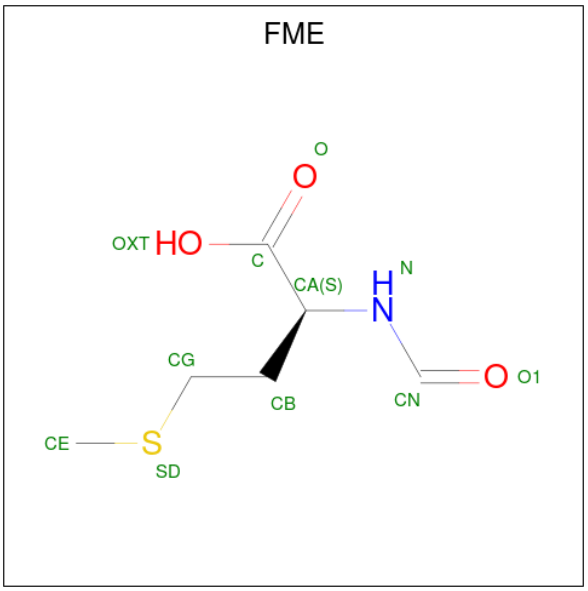
- Molecule 57 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
57	8	38	307	186	69	48	4	0	0

- Molecule 58 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

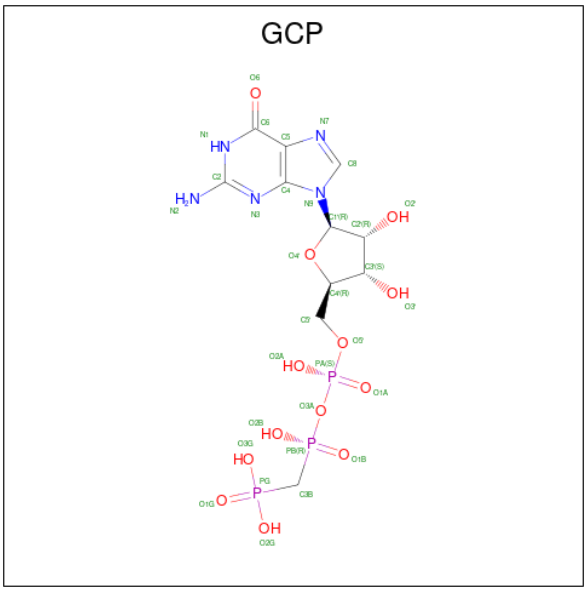
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	a	121	121	121	0
58	q	1	1	1	0
58	t	1	1	1	0
58	v	1	1	1	0
58	w	1	1	1	0
58	x	1	1	1	0
58	A	455	455	455	0
58	B	4	4	4	0
58	C	3	3	3	0
58	D	2	2	2	0
58	E	1	1	1	0
58	P	1	1	1	0
58	Y	1	1	1	0
58	4	1	1	1	0
58	7	1	1	1	0

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
59	v	1	10	6	1	2	1	0

- Molecule 60 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	x	1	32	11	5	13	3	0

- Molecule 61 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
61	3	1	1	1	0
			Total	Zn	
61	8	1	1	1	0

- Molecule 62 is water.

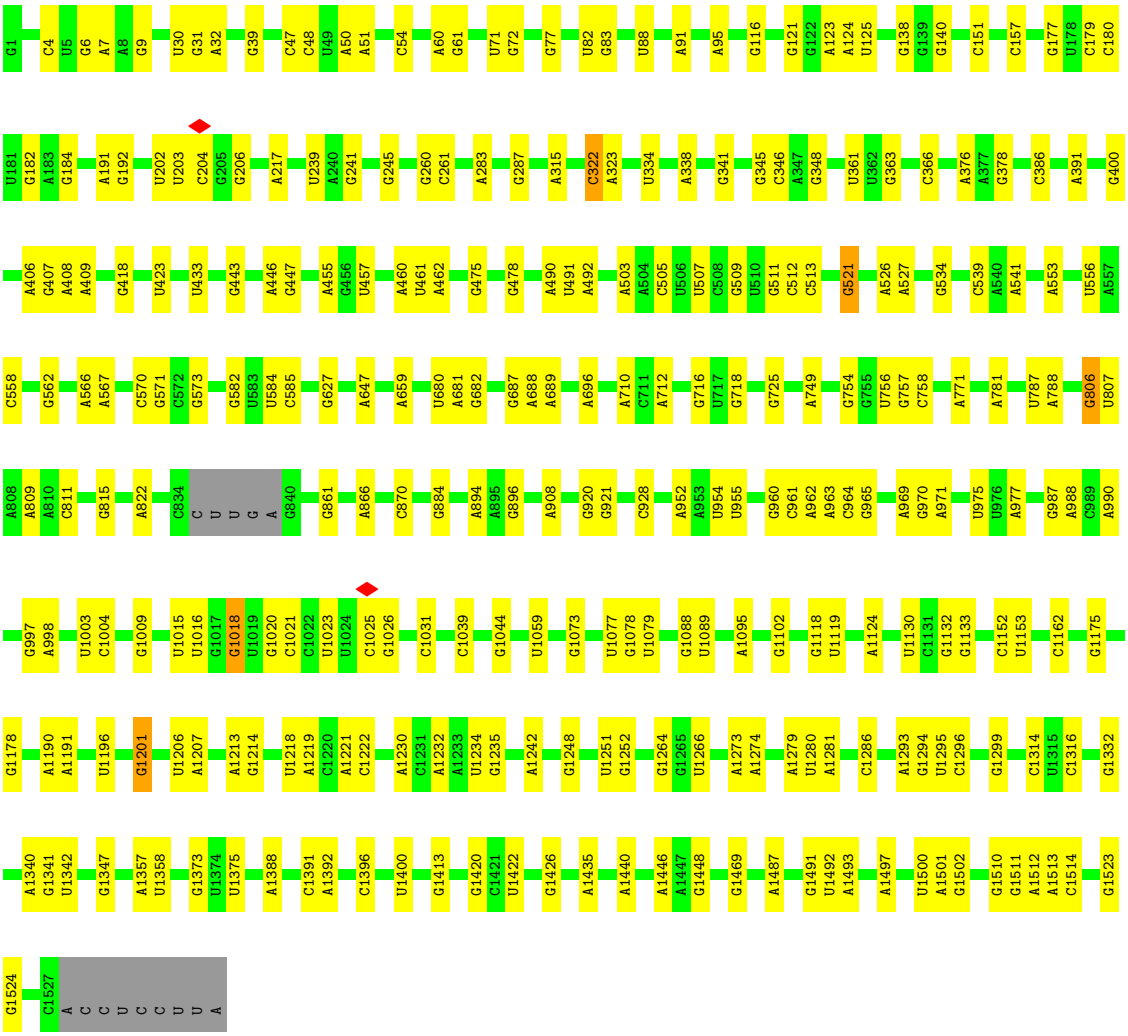
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
62	a	46	46	46	0
			Total	O	
62	k	1	1	1	0
			Total	O	
62	v	1	1	1	0
			Total	O	
62	w	1	1	1	0
			Total	O	
62	x	1	1	1	0
			Total	O	
62	A	238	238	238	0
			Total	O	
62	B	1	1	1	0
			Total	O	
62	C	2	2	2	0
			Total	O	
62	N	1	1	1	0
			Total	O	
62	4	2	2	2	0
			Total	O	
62	6	1	1	1	0

3 Residue-property plots (i)

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

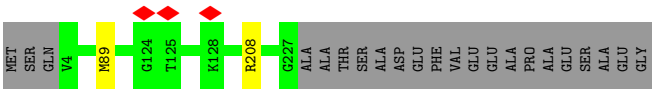
- Molecule 1: 16S Ribosomal RNA

Chain a: 81% 18%



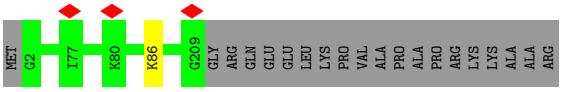
- Molecule 2: 30S ribosomal protein S2

Chain b: 90% 9%



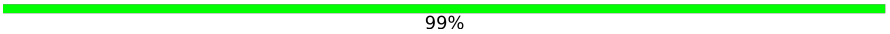
• Molecule 3: 30S ribosomal protein S3

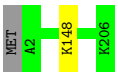
Chain c:



• Molecule 4: 30S ribosomal protein S4

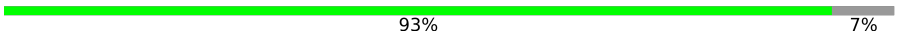
Chain d:

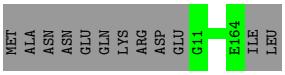




• Molecule 5: 30S ribosomal protein S5

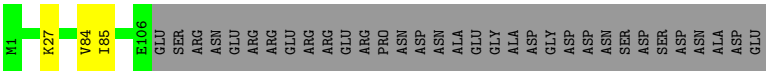
Chain e:





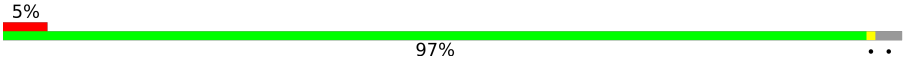
• Molecule 6: 30S ribosomal protein S6

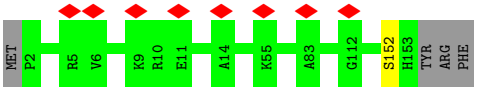
Chain f:



• Molecule 7: 30S ribosomal protein S7

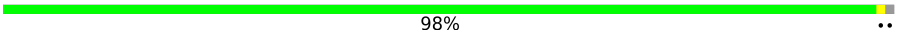
Chain g:

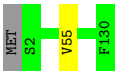




• Molecule 8: 30S ribosomal protein S8

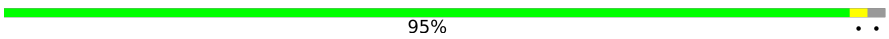
Chain h:

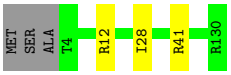




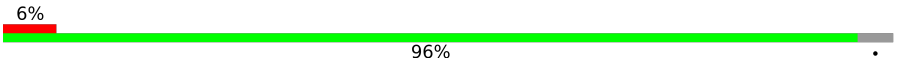
• Molecule 9: 30S ribosomal protein S9

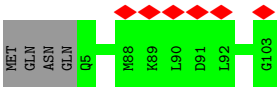
Chain i:





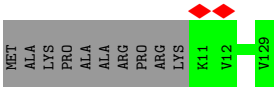
• Molecule 10: 30S ribosomal protein S10

Chain j: 

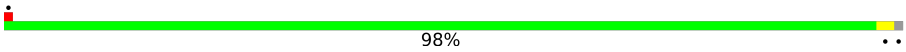


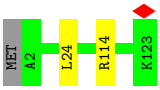
• Molecule 11: 30S ribosomal protein S11

Chain k:

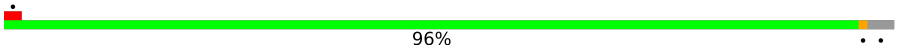


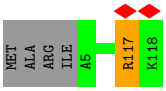
• Molecule 12: 30S ribosomal protein S12

Chain l: 

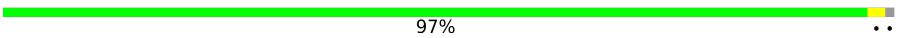


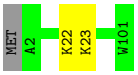
• Molecule 13: 30S ribosomal protein S13

Chain m: 

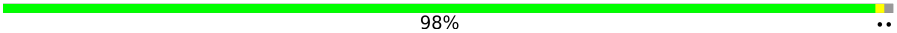


• Molecule 14: 30S ribosomal protein S14

Chain n: 



• Molecule 15: 30S ribosomal protein S15

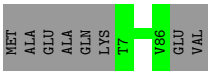
Chain o: 

• Molecule 16: 30S ribosomal protein S16

Chain p: 98%

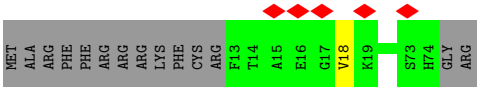
• Molecule 17: 30S ribosomal protein S17

Chain q: 91% 9%



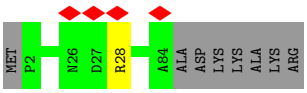
• Molecule 18: 30S ribosomal protein S18

Chain r: 7% 80% 18%



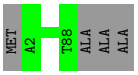
• Molecule 19: 30S ribosomal protein S19

Chain s: 90% 9%



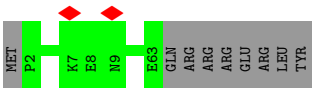
• Molecule 20: 30S ribosomal protein S20

Chain t: 96%



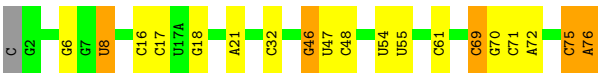
• Molecule 21: 30S ribosomal protein S21

Chain u: 87% 13%



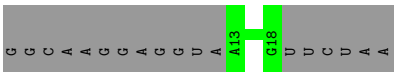
• Molecule 22: P-site initiator tRNA

Chain v: 74% 18% 6%



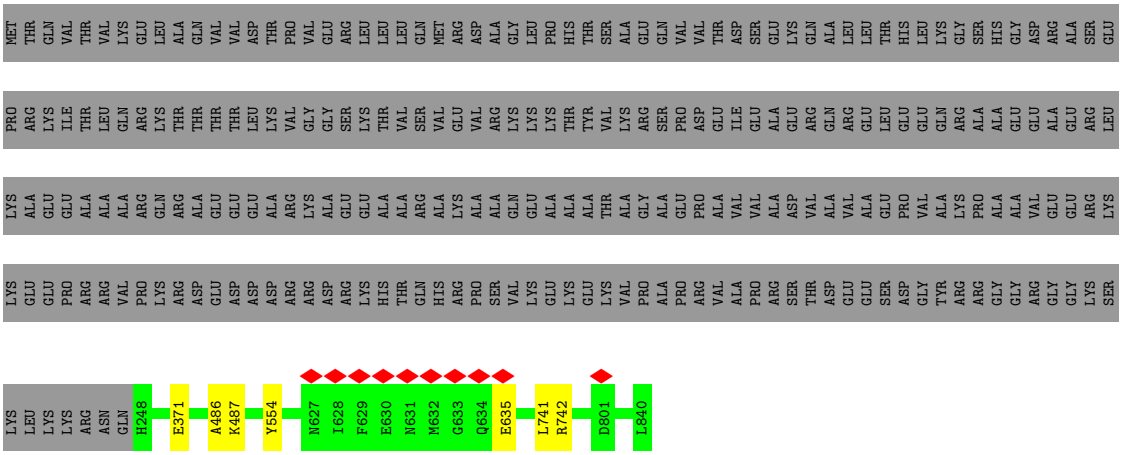
• Molecule 23: mRNA

Chain w: 25% 75%



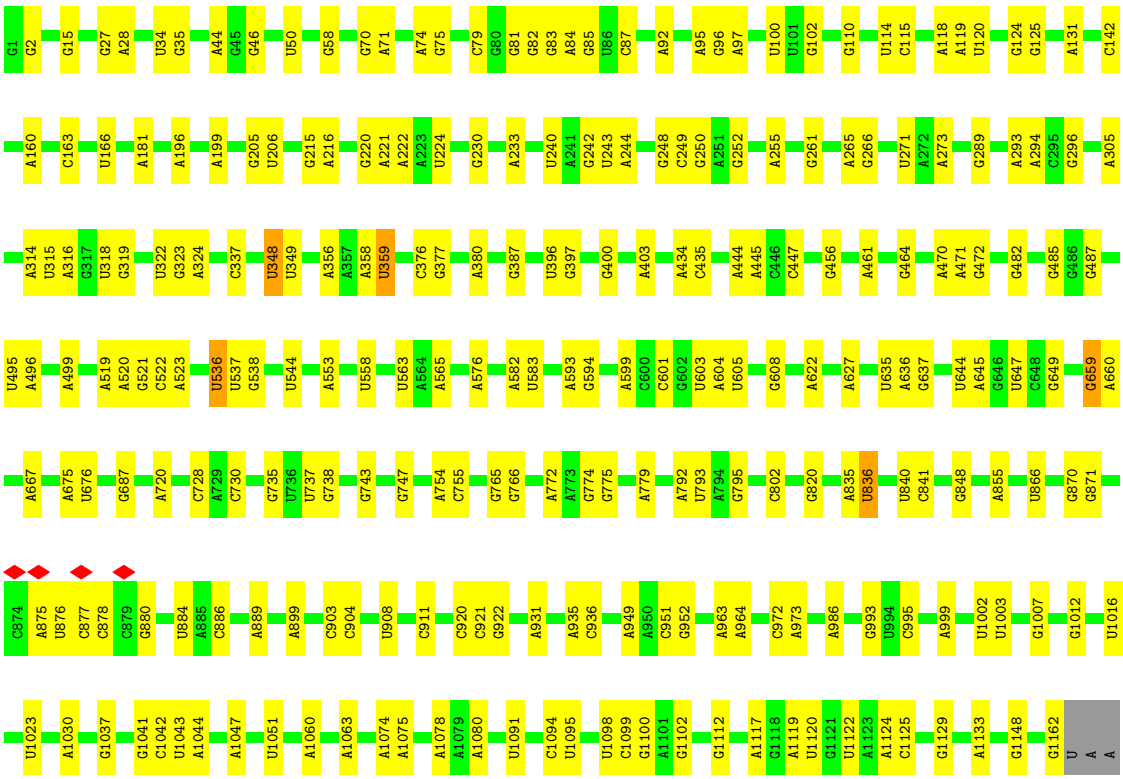
• Molecule 24: Translation initiation factor IF-2

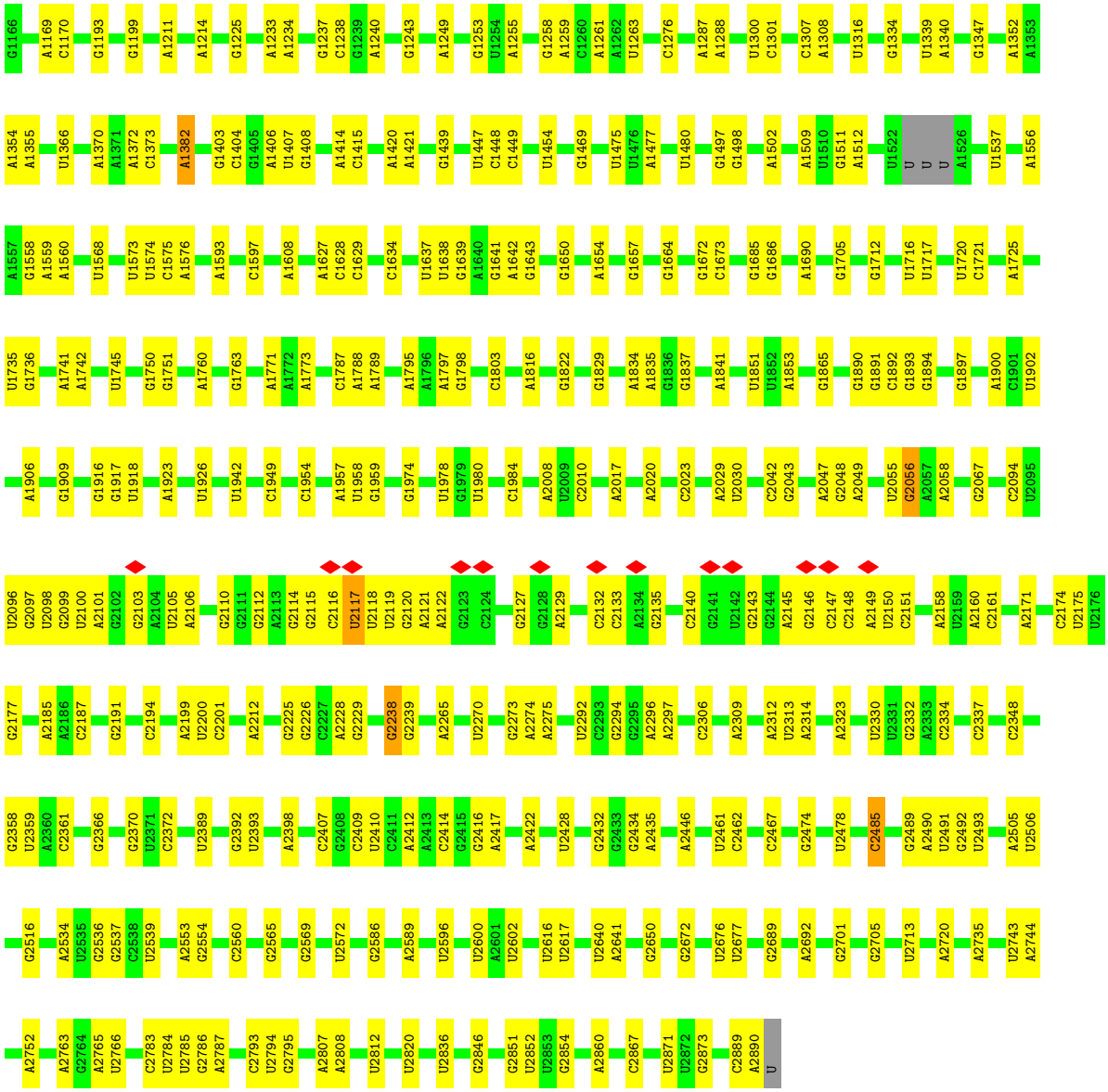
Chain x: 70% 29%



• Molecule 25: 23S Ribosomal RNA

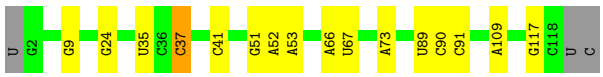
Chain A: 79% 20%





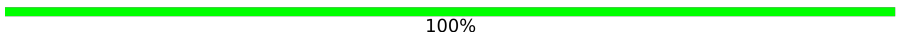
- Molecule 26: 5S Ribosomal RNA

Chain B:



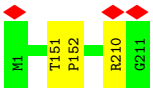
- Molecule 27: 50S ribosomal protein L2

Chain C:



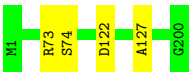
- Molecule 28: 50S ribosomal protein L3

Chain D: 99%



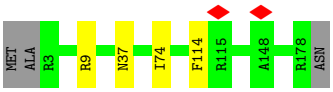
• Molecule 29: 50S ribosomal protein L4

Chain E: 98%



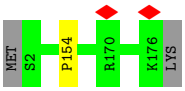
• Molecule 30: 50S ribosomal protein L5

Chain F: 96%



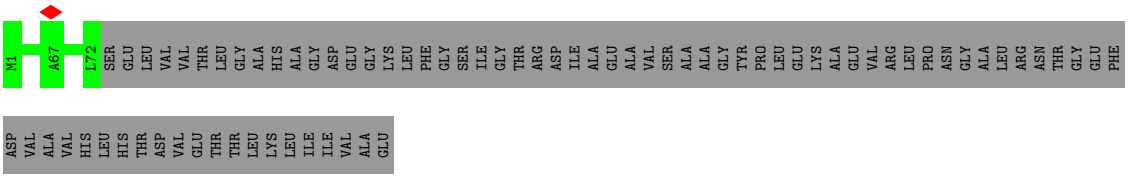
• Molecule 31: 50S ribosomal protein L6

Chain G: 98%



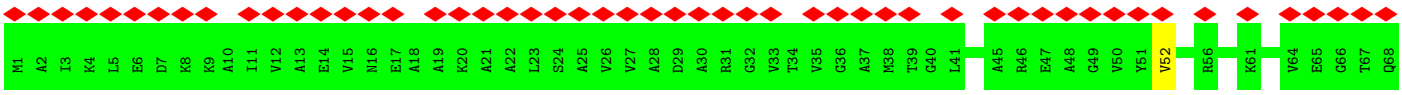
• Molecule 32: 50S ribosomal protein L9

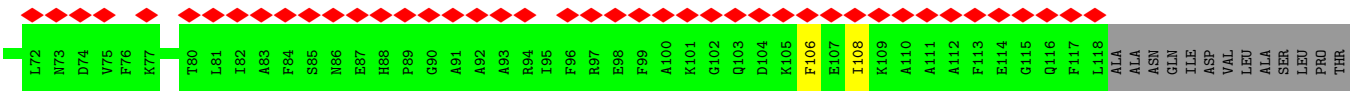
Chain H: 49% 51%

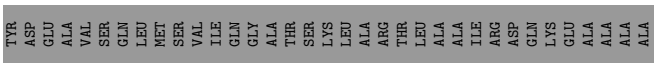


• Molecule 33: 50S ribosomal protein L10

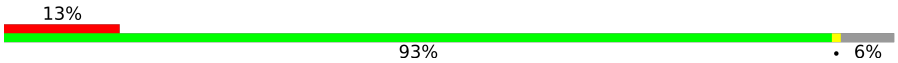
Chain I: 57% 69% 29%

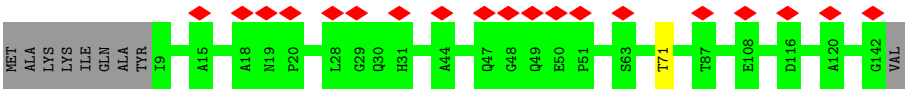




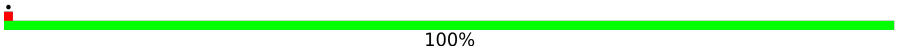


• Molecule 34: 50S ribosomal protein L11

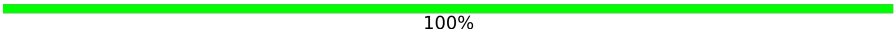
Chain J: 



• Molecule 35: 50S ribosomal protein L13

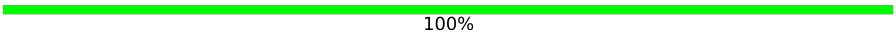
Chain L: 

• Molecule 36: 50S ribosomal protein L14

Chain M: 

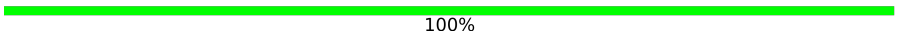
There are no outlier residues recorded for this chain.

• Molecule 37: 50S ribosomal protein L15

Chain N: 

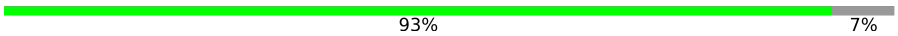
There are no outlier residues recorded for this chain.

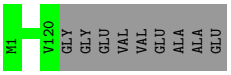
• Molecule 38: 50S ribosomal protein L16

Chain O: 

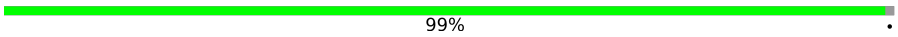
There are no outlier residues recorded for this chain.

• Molecule 39: 50S ribosomal protein L17

Chain P: 

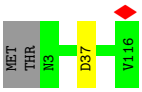


• Molecule 40: 50S ribosomal protein L18

Chain Q: 

• Molecule 41: 50S ribosomal protein L19

Chain R: 97%

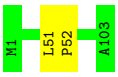


• Molecule 42: 50S ribosomal protein L20

Chain S: 99%

• Molecule 43: 50S ribosomal protein L21

Chain T: 98%



• Molecule 44: 50S ribosomal protein L22

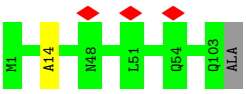
Chain U: 100%

• Molecule 45: 50S ribosomal protein L23

Chain V: 95% 5%

• Molecule 46: 50S ribosomal protein L24

Chain W: 98%

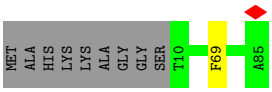


• Molecule 47: 50S ribosomal protein L25

Chain X: 93% 7%

• Molecule 48: 50S ribosomal protein L27

Chain Y: 88% 11%



• Molecule 49: 50S ribosomal protein L28

Chain Z: 97%

• Molecule 50: 50S ribosomal protein L29

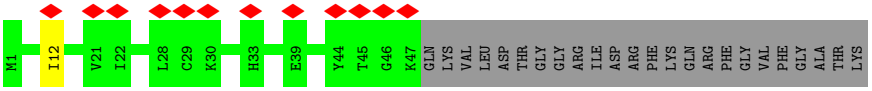
Chain 1: 97%

• Molecule 51: 50S ribosomal protein L30

Chain 2: 98%

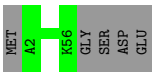
• Molecule 52: 50S ribosomal protein L31

Chain 3: 17% 65% 34%



• Molecule 53: 50S ribosomal protein L32

Chain 4: 92% 8%



• Molecule 54: 50S ribosomal protein L33

Chain 5: 100%

• Molecule 55: 50S ribosomal protein L34

Chain 6: 100%

There are no outlier residues recorded for this chain.

• Molecule 56: 50S ribosomal protein L35

Chain 7: 98%

• Molecule 57: 50S ribosomal protein L36

Chain 8: 100%

There are no outlier residues recorded for this chain.

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73337	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 ($e^-/Å^2$)	31	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.999	Depositor
Minimum map value	-0.674	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.065	Depositor
Recommended contour level	0.14	Depositor
Map size (Å)	435.2, 435.2, 435.2	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMU, 1MG, 6MZ, 4SU, 5MC, 2MA, 4OC, 2MG, FME, GCP, MA6, 7MG, ZN, OMC, MG, 5MU, OMG, PSU, UR3

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	a	0.29	0/36354	0.79	11/56707 (0.0%)
2	b	0.27	0/1779	0.58	0/2392
3	c	0.26	0/1685	0.54	0/2270
4	d	0.27	0/1636	0.56	0/2189
5	e	0.27	0/1148	0.57	0/1544
6	f	0.27	0/871	0.60	0/1172
7	g	0.25	0/1204	0.57	0/1609
8	h	0.26	0/993	0.52	0/1332
9	i	0.25	0/1022	0.60	0/1365
10	j	0.27	0/797	0.57	0/1076
11	k	0.26	0/895	0.53	0/1209
12	l	0.27	0/973	0.64	1/1303 (0.1%)
13	m	0.25	0/901	0.63	0/1209
14	n	0.25	0/812	0.62	0/1082
15	o	0.26	0/710	0.53	0/947
16	p	0.26	0/647	0.56	0/870
17	q	0.25	0/653	0.59	0/881
18	r	0.26	0/488	0.53	0/660
19	s	0.23	0/678	0.52	0/912
20	t	0.25	0/678	0.48	0/904
21	u	0.26	0/513	0.53	0/680
22	v	0.51	3/1725 (0.2%)	1.12	12/2689 (0.4%)
23	w	0.27	0/147	0.69	0/227
24	x	0.26	0/4325	0.54	1/5861 (0.0%)
25	A	0.39	0/68977	0.81	21/107590 (0.0%)
26	B	0.28	0/2789	0.79	2/4345 (0.0%)
27	C	0.28	0/2108	0.59	0/2831
28	D	0.29	0/1611	0.58	0/2167
29	E	0.27	0/1541	0.51	0/2075
30	F	0.26	0/1427	0.60	0/1917
31	G	0.26	0/1341	0.55	1/1805 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	H	0.24	0/516	0.50	0/696
33	I	0.23	0/586	0.45	0/813
34	J	0.25	0/688	0.45	0/953
35	L	0.27	0/1156	0.50	0/1559
36	M	0.27	0/947	0.58	0/1268
37	N	0.27	0/1078	0.59	0/1436
38	O	0.27	0/1105	0.56	0/1476
39	P	0.26	0/975	0.56	0/1304
40	Q	0.25	0/888	0.56	0/1183
41	R	0.30	0/911	0.53	0/1218
42	S	0.27	0/943	0.55	0/1253
43	T	0.27	0/835	0.54	0/1117
44	U	0.25	0/837	0.52	0/1114
45	V	0.26	0/749	0.50	0/1002
46	W	0.25	0/794	0.57	0/1062
47	X	0.26	0/1468	0.51	0/1987
48	Y	0.30	0/583	0.57	0/774
49	Z	0.29	0/641	0.58	0/854
50	1	0.22	0/491	0.45	0/654
51	2	0.25	0/449	0.52	0/602
52	3	0.23	0/364	0.48	0/494
53	4	0.25	0/446	0.55	0/594
54	5	0.26	0/433	0.52	0/576
55	6	0.26	0/368	0.66	0/482
56	7	0.24	0/511	0.57	0/668
57	8	0.25	0/308	0.62	0/404
All	All	0.33	3/160498 (0.0%)	0.75	49/239363 (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
28	D	0	1
43	T	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	76	A	N7-C5	-11.91	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	76	A	C5-C4	-8.39	1.32	1.38
22	v	76	A	C5-C6	-8.06	1.33	1.41

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	76	A	N1-C2-N3	-18.51	120.04	129.30
22	v	76	A	C2-N3-C4	18.36	119.78	110.60
22	v	76	A	O4'-C1'-N9	15.29	120.44	108.20
25	A	1094	C	OP1-P-O3'	-10.98	81.05	105.20
25	A	1094	C	OP2-P-O3'	-9.74	83.77	105.20
22	v	76	A	N3-C4-C5	-9.67	120.03	126.80
22	v	76	A	N7-C8-N9	-9.09	109.25	113.80
22	v	76	A	C5-N7-C8	7.99	107.89	103.90
25	A	536	U	C2-N1-C1'	7.89	127.16	117.70
12	l	24	LEU	CA-CB-CG	7.64	132.87	115.30
1	a	203	U	C2-N1-C1'	7.58	126.79	117.70
25	A	1300	U	C2-N1-C1'	7.49	126.69	117.70
22	v	76	A	N9-C4-C5	7.47	108.79	105.80
25	A	2117	U	C2-N1-C1'	7.36	126.53	117.70
25	A	536	U	N1-C2-O2	7.29	127.90	122.80
25	A	1095	U	OP1-P-OP2	7.29	130.53	119.60
22	v	75	C	OP1-P-O3'	7.28	121.21	105.20
31	G	154	PRO	C-N-CA	7.22	139.74	121.70
1	a	203	U	N1-C2-O2	6.93	127.65	122.80
22	v	76	A	C4-C5-C6	6.89	120.45	117.00
1	a	203	U	N3-C2-O2	-6.81	117.43	122.20
22	v	75	C	OP2-P-O3'	-6.70	90.47	105.20
25	A	2117	U	N1-C2-O2	6.67	127.47	122.80
25	A	536	U	N3-C2-O2	-6.65	117.55	122.20
25	A	359	U	N1-C2-O2	6.29	127.20	122.80
1	a	1018	G	C5-C6-O6	6.17	132.30	128.60
25	A	2117	U	N3-C2-O2	-6.15	117.89	122.20
25	A	359	U	C2-N1-C1'	6.11	125.03	117.70
25	A	359	U	N3-C2-O2	-6.09	117.94	122.20
22	v	69	C	C2-N1-C1'	5.54	124.89	118.80
1	a	1018	G	N1-C6-O6	-5.53	116.58	119.90
25	A	1300	U	N1-C2-O2	5.51	126.66	122.80
1	a	180	C	C6-N1-C2	-5.35	118.16	120.30
25	A	659	G	C4-N9-C1'	5.27	133.36	126.50
25	A	836	U	C2-N1-C1'	5.23	123.98	117.70
25	A	1301	C	C2-N1-C1'	5.21	124.53	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	46	G	N3-C2-N2	-5.19	116.27	119.90
24	x	741	LEU	CA-CB-CG	5.19	127.23	115.30
1	a	322	C	P-O3'-C3'	5.12	125.84	119.70
1	a	179	C	N1-C2-O2	5.11	121.96	118.90
25	A	1300	U	N3-C2-O2	-5.10	118.63	122.20
25	A	348	U	C2-N1-C1'	5.10	123.82	117.70
26	B	37	C	N1-C2-O2	5.08	121.95	118.90
26	B	37	C	C2-N1-C1'	5.08	124.39	118.80
25	A	1382	A	O4'-C1'-N9	5.07	112.26	108.20
25	A	536	U	C6-N1-C1'	-5.07	114.11	121.20
1	a	1286	C	N3-C2-O2	-5.03	118.38	121.90
1	a	180	C	N3-C2-O2	-5.01	118.39	121.90
1	a	806	G	P-O3'-C3'	5.01	125.71	119.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	D	151	THR	Peptide
43	T	51	LEU	Peptide

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	b	222/246 (90%)	205 (92%)	16 (7%)	1 (0%)	29 54
3	c	206/228 (90%)	194 (94%)	12 (6%)	0	100 100
4	d	203/206 (98%)	175 (86%)	28 (14%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	e	152/166 (92%)	139 (91%)	13 (9%)	0	100	100
6	f	104/139 (75%)	92 (88%)	10 (10%)	2 (2%)	8	20
7	g	150/156 (96%)	140 (93%)	9 (6%)	1 (1%)	22	46
8	h	127/130 (98%)	116 (91%)	10 (8%)	1 (1%)	19	43
9	i	125/130 (96%)	113 (90%)	11 (9%)	1 (1%)	19	43
10	j	97/103 (94%)	90 (93%)	7 (7%)	0	100	100
11	k	117/129 (91%)	112 (96%)	5 (4%)	0	100	100
12	l	120/123 (98%)	112 (93%)	8 (7%)	0	100	100
13	m	112/118 (95%)	99 (88%)	12 (11%)	1 (1%)	17	40
14	n	98/101 (97%)	87 (89%)	11 (11%)	0	100	100
15	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	p	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
17	q	78/88 (89%)	78 (100%)	0	0	100	100
18	r	60/76 (79%)	54 (90%)	5 (8%)	1 (2%)	9	23
19	s	81/91 (89%)	72 (89%)	9 (11%)	0	100	100
20	t	85/91 (93%)	84 (99%)	1 (1%)	0	100	100
21	u	60/71 (84%)	58 (97%)	2 (3%)	0	100	100
24	x	591/840 (70%)	544 (92%)	43 (7%)	4 (1%)	22	46
27	C	270/273 (99%)	255 (94%)	15 (6%)	0	100	100
28	D	209/211 (99%)	183 (88%)	24 (12%)	2 (1%)	15	37
29	E	198/200 (99%)	190 (96%)	6 (3%)	2 (1%)	15	37
30	F	174/179 (97%)	151 (87%)	20 (12%)	3 (2%)	9	23
31	G	173/177 (98%)	160 (92%)	13 (8%)	0	100	100
32	H	70/148 (47%)	65 (93%)	5 (7%)	0	100	100
33	I	116/166 (70%)	97 (84%)	16 (14%)	3 (3%)	5	13
34	J	132/143 (92%)	110 (83%)	21 (16%)	1 (1%)	19	43
35	L	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
36	M	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
37	N	142/144 (99%)	126 (89%)	16 (11%)	0	100	100
38	O	135/137 (98%)	132 (98%)	3 (2%)	0	100	100
39	P	118/129 (92%)	110 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	Q	113/116 (97%)	102 (90%)	11 (10%)	0	100	100
41	R	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
42	S	115/118 (98%)	111 (96%)	4 (4%)	0	100	100
43	T	101/103 (98%)	99 (98%)	1 (1%)	1 (1%)	15	37
44	U	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
45	V	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
46	W	101/104 (97%)	93 (92%)	7 (7%)	1 (1%)	15	37
47	X	188/204 (92%)	180 (96%)	8 (4%)	0	100	100
48	Y	74/85 (87%)	71 (96%)	2 (3%)	1 (1%)	11	28
49	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
50	1	59/63 (94%)	59 (100%)	0	0	100	100
51	2	55/58 (95%)	55 (100%)	0	0	100	100
52	3	45/71 (63%)	41 (91%)	3 (7%)	1 (2%)	6	17
53	4	53/60 (88%)	51 (96%)	2 (4%)	0	100	100
54	5	49/51 (96%)	47 (96%)	2 (4%)	0	100	100
55	6	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
56	7	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
57	8	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
All	All	6429/7157 (90%)	5976 (93%)	426 (7%)	27 (0%)	38	60

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	f	84	VAL
7	g	152	SER
8	h	55	VAL
13	m	117	ARG
24	x	635	GLU
28	D	152	PRO
29	E	122	ASP
30	F	74	ILE
43	T	52	PRO
52	3	12	ILE
6	f	85	ILE
24	x	486	ALA
30	F	37	ASN

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Mol	Chain	Res	Type
30	F	114	PHE
33	I	52	VAL
24	x	554	TYR
34	J	71	THR
46	W	14	ALA
48	Y	69	PHE
33	I	106	PHE
9	i	28	ILE
18	r	18	VAL
33	I	108	ILE
24	x	371	GLU
28	D	210	ARG
2	b	89	MET
29	E	127	ALA

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
2	b	184/202 (91%)	183 (100%)	1 (0%)	88 96
3	c	170/187 (91%)	169 (99%)	1 (1%)	86 95
4	d	171/174 (98%)	170 (99%)	1 (1%)	86 95
5	e	113/124 (91%)	113 (100%)	0	100 100
6	f	88/119 (74%)	87 (99%)	1 (1%)	73 90
7	g	118/122 (97%)	118 (100%)	0	100 100
8	h	108/109 (99%)	108 (100%)	0	100 100
9	i	104/106 (98%)	102 (98%)	2 (2%)	57 82
10	j	87/92 (95%)	87 (100%)	0	100 100
11	k	90/98 (92%)	90 (100%)	0	100 100
12	l	106/107 (99%)	105 (99%)	1 (1%)	78 92
13	m	95/99 (96%)	94 (99%)	1 (1%)	73 90
14	n	80/82 (98%)	78 (98%)	2 (2%)	47 76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	o	74/75 (99%)	73 (99%)	1 (1%)	67	86
16	p	64/65 (98%)	64 (100%)	0	100	100
17	q	73/79 (92%)	73 (100%)	0	100	100
18	r	48/64 (75%)	48 (100%)	0	100	100
19	s	72/78 (92%)	71 (99%)	1 (1%)	67	86
20	t	69/70 (99%)	69 (100%)	0	100	100
21	u	51/60 (85%)	51 (100%)	0	100	100
24	x	417/668 (62%)	415 (100%)	2 (0%)	88	96
27	C	212/213 (100%)	212 (100%)	0	100	100
28	D	162/162 (100%)	162 (100%)	0	100	100
29	E	157/158 (99%)	155 (99%)	2 (1%)	69	87
30	F	149/153 (97%)	148 (99%)	1 (1%)	84	94
31	G	138/141 (98%)	138 (100%)	0	100	100
32	H	44/107 (41%)	44 (100%)	0	100	100
33	I	2/122 (2%)	2 (100%)	0	100	100
34	J	13/110 (12%)	13 (100%)	0	100	100
35	L	119/119 (100%)	119 (100%)	0	100	100
36	M	102/102 (100%)	102 (100%)	0	100	100
37	N	106/106 (100%)	106 (100%)	0	100	100
38	O	110/110 (100%)	110 (100%)	0	100	100
39	P	99/104 (95%)	99 (100%)	0	100	100
40	Q	86/87 (99%)	86 (100%)	0	100	100
41	R	96/98 (98%)	95 (99%)	1 (1%)	76	91
42	S	86/88 (98%)	86 (100%)	0	100	100
43	T	86/86 (100%)	86 (100%)	0	100	100
44	U	87/87 (100%)	87 (100%)	0	100	100
45	V	79/82 (96%)	79 (100%)	0	100	100
46	W	84/88 (96%)	84 (100%)	0	100	100
47	X	154/164 (94%)	154 (100%)	0	100	100
48	Y	56/61 (92%)	56 (100%)	0	100	100
49	Z	66/67 (98%)	65 (98%)	1 (2%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
50	1	54/55 (98%)	54 (100%)	0	100	100
51	2	48/49 (98%)	48 (100%)	0	100	100
52	3	41/61 (67%)	41 (100%)	0	100	100
53	4	48/52 (92%)	48 (100%)	0	100	100
54	5	47/47 (100%)	47 (100%)	0	100	100
55	6	37/37 (100%)	37 (100%)	0	100	100
56	7	54/55 (98%)	54 (100%)	0	100	100
57	8	34/34 (100%)	34 (100%)	0	100	100
All	All	5038/5785 (87%)	5019 (100%)	19 (0%)	91	97

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	208	ARG
3	c	86	LYS
4	d	148	LYS
6	f	27	LYS
9	i	12	ARG
9	i	41	ARG
12	l	114	ARG
13	m	117	ARG
14	n	22	LYS
14	n	23	LYS
15	o	88	ARG
19	s	28	ARG
24	x	487	LYS
24	x	742	ARG
29	E	73	ARG
29	E	74	SER
30	F	9	ARG
41	R	37	ASP
49	Z	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
3	c	139	GLN
4	d	41	HIS

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Mol	Chain	Res	Type
4	d	152	GLN
5	e	20	ASN
6	f	58	HIS
6	f	63	ASN
7	g	28	ASN
8	h	4	GLN
10	j	58	ASN
11	k	24	HIS
11	k	28	ASN
11	k	85	ASN
11	k	118	HIS
12	l	46	ASN
12	l	59	ASN
12	l	73	ASN
14	n	45	GLN
15	o	37	ASN
20	t	13	GLN
24	x	298	GLN
24	x	399	HIS
24	x	457	ASN
24	x	668	GLN
27	C	22	GLN
27	C	61	HIS
27	C	261	ASN
28	D	126	ASN
30	F	37	ASN
30	F	127	ASN
35	L	23	GLN
36	M	56	GLN
39	P	16	HIS
40	Q	39	GLN
41	R	3	ASN
41	R	39	GLN
45	V	28	GLN
45	V	90	GLN
47	X	25	ASN
48	Y	29	GLN
48	Y	40	GLN
50	1	31	GLN
55	6	29	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1517/1536 (98%)	268 (17%)	0
22	v	75/77 (97%)	16 (21%)	0
23	w	5/24 (20%)	0	0
25	A	2878/2891 (99%)	548 (19%)	47 (1%)
26	B	116/120 (96%)	14 (12%)	2 (1%)
All	All	4591/4648 (98%)	846 (18%)	49 (1%)

All (846) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	C
1	a	6	G
1	a	7	A
1	a	9	G
1	a	30	U
1	a	31	G
1	a	32	A
1	a	39	G
1	a	47	C
1	a	48	C
1	a	50	A
1	a	51	A
1	a	54	C
1	a	60	A
1	a	61	G
1	a	71	U
1	a	72	G
1	a	77	G
1	a	82	U
1	a	83	G
1	a	88	U
1	a	91	A
1	a	95	A
1	a	116	G
1	a	121	G
1	a	123	A
1	a	124	A
1	a	125	U
1	a	138	G
1	a	140	G
1	a	151	C
1	a	157	C
1	a	177	G

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Mol	Chain	Res	Type
1	a	182	G
1	a	184	G
1	a	191	A
1	a	192	G
1	a	202	U
1	a	204	C
1	a	206	G
1	a	217	A
1	a	239	U
1	a	241	G
1	a	245	G
1	a	260	G
1	a	261	C
1	a	283	A
1	a	287	G
1	a	315	A
1	a	322	C
1	a	323	A
1	a	334	U
1	a	338	A
1	a	341	G
1	a	345	G
1	a	346	C
1	a	348	G
1	a	361	U
1	a	363	G
1	a	366	C
1	a	376	A
1	a	378	G
1	a	386	C
1	a	391	A
1	a	400	G
1	a	406	A
1	a	407	G
1	a	408	A
1	a	409	A
1	a	418	G
1	a	423	U
1	a	433	U
1	a	443	G
1	a	446	A
1	a	447	G

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Mol	Chain	Res	Type
1	a	455	A
1	a	457	U
1	a	460	A
1	a	461	U
1	a	462	A
1	a	475	G
1	a	478	G
1	a	490	A
1	a	491	U
1	a	492	A
1	a	503	A
1	a	505	C
1	a	507	U
1	a	509	G
1	a	511	G
1	a	512	C
1	a	513	C
1	a	521	7MG
1	a	526	A
1	a	527	A
1	a	534	G
1	a	539	C
1	a	541	A
1	a	553	A
1	a	556	U
1	a	558	C
1	a	562	G
1	a	566	A
1	a	567	A
1	a	570	C
1	a	571	G
1	a	573	G
1	a	582	G
1	a	584	U
1	a	585	C
1	a	627	G
1	a	647	A
1	a	659	A
1	a	680	U
1	a	681	A
1	a	682	G
1	a	687	G

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Mol	Chain	Res	Type
1	a	688	A
1	a	689	A
1	a	696	A
1	a	710	A
1	a	712	A
1	a	716	G
1	a	718	G
1	a	725	G
1	a	749	A
1	a	754	G
1	a	756	U
1	a	757	G
1	a	758	C
1	a	771	A
1	a	781	A
1	a	787	U
1	a	788	A
1	a	806	G
1	a	807	U
1	a	809	A
1	a	811	C
1	a	815	G
1	a	822	A
1	a	861	G
1	a	866	A
1	a	870	C
1	a	884	G
1	a	894	A
1	a	896	G
1	a	908	A
1	a	920	G
1	a	921	G
1	a	928	C
1	a	952	A
1	a	954	U
1	a	955	U
1	a	962	A
1	a	963	A
1	a	964	C
1	a	965	G
1	a	969	A
1	a	970	G

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Mol	Chain	Res	Type
1	a	971	A
1	a	975	U
1	a	977	A
1	a	987	G
1	a	988	A
1	a	990	A
1	a	997	G
1	a	998	A
1	a	1003	U
1	a	1004	C
1	a	1009	G
1	a	1015	U
1	a	1016	U
1	a	1018	G
1	a	1020	G
1	a	1021	C
1	a	1023	U
1	a	1025	C
1	a	1026	G
1	a	1031	C
1	a	1039	C
1	a	1044	G
1	a	1059	U
1	a	1073	G
1	a	1077	U
1	a	1078	G
1	a	1079	U
1	a	1088	G
1	a	1089	U
1	a	1095	A
1	a	1102	G
1	a	1118	G
1	a	1119	U
1	a	1124	A
1	a	1130	U
1	a	1132	G
1	a	1133	G
1	a	1152	C
1	a	1153	U
1	a	1162	C
1	a	1175	G
1	a	1178	G

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Mol	Chain	Res	Type
1	a	1190	A
1	a	1191	A
1	a	1196	U
1	a	1201	2MG
1	a	1206	U
1	a	1207	A
1	a	1213	A
1	a	1214	G
1	a	1218	U
1	a	1219	A
1	a	1221	A
1	a	1222	C
1	a	1230	A
1	a	1232	A
1	a	1234	U
1	a	1235	G
1	a	1242	A
1	a	1248	G
1	a	1251	U
1	a	1252	G
1	a	1264	G
1	a	1266	U
1	a	1273	A
1	a	1274	A
1	a	1279	A
1	a	1280	U
1	a	1281	A
1	a	1293	A
1	a	1294	G
1	a	1295	U
1	a	1296	C
1	a	1299	G
1	a	1314	C
1	a	1316	C
1	a	1332	G
1	a	1340	A
1	a	1341	G
1	a	1342	U
1	a	1347	G
1	a	1357	A
1	a	1358	U
1	a	1373	G

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Mol	Chain	Res	Type
1	a	1375	U
1	a	1388	A
1	a	1391	C
1	a	1392	A
1	a	1400	U
1	a	1413	G
1	a	1420	G
1	a	1422	U
1	a	1426	G
1	a	1435	A
1	a	1440	A
1	a	1446	A
1	a	1448	G
1	a	1469	G
1	a	1487	A
1	a	1491	G
1	a	1493	A
1	a	1497	A
1	a	1500	U
1	a	1501	A
1	a	1502	G
1	a	1511	G
1	a	1514	C
1	a	1523	G
1	a	1524	G
22	v	6	G
22	v	8	4SU
22	v	16	C
22	v	17	C
22	v	18	G
22	v	21	A
22	v	46	G
22	v	47	U
22	v	48	C
22	v	61	C
22	v	69	C
22	v	70	G
22	v	71	C
22	v	72	A
22	v	75	C
22	v	76	A
25	A	2	G

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Mol	Chain	Res	Type
25	A	15	G
25	A	28	A
25	A	34	U
25	A	35	G
25	A	44	A
25	A	46	G
25	A	50	U
25	A	58	G
25	A	70	G
25	A	71	A
25	A	74	A
25	A	75	G
25	A	79	C
25	A	82	G
25	A	83	G
25	A	84	A
25	A	85	G
25	A	92	A
25	A	95	A
25	A	96	G
25	A	97	A
25	A	100	U
25	A	102	G
25	A	110	G
25	A	114	U
25	A	115	C
25	A	118	A
25	A	119	A
25	A	120	U
25	A	124	G
25	A	125	G
25	A	131	A
25	A	142	C
25	A	160	A
25	A	163	C
25	A	166	U
25	A	181	A
25	A	196	A
25	A	199	A
25	A	205	G
25	A	206	U
25	A	215	G

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Mol	Chain	Res	Type
25	A	216	A
25	A	220	G
25	A	221	A
25	A	222	A
25	A	224	U
25	A	230	G
25	A	233	A
25	A	240	U
25	A	242	G
25	A	243	U
25	A	244	A
25	A	248	G
25	A	249	C
25	A	250	G
25	A	252	G
25	A	255	A
25	A	261	G
25	A	265	A
25	A	266	G
25	A	271	U
25	A	273	A
25	A	289	G
25	A	293	A
25	A	294	A
25	A	296	G
25	A	305	A
25	A	315	U
25	A	316	A
25	A	318	U
25	A	319	G
25	A	322	U
25	A	323	G
25	A	324	A
25	A	337	C
25	A	348	U
25	A	349	U
25	A	356	A
25	A	358	A
25	A	359	U
25	A	376	C
25	A	377	G
25	A	380	A

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Mol	Chain	Res	Type
25	A	387	G
25	A	396	U
25	A	397	G
25	A	400	G
25	A	403	A
25	A	435	C
25	A	445	A
25	A	447	C
25	A	456	G
25	A	461	A
25	A	464	G
25	A	471	A
25	A	472	G
25	A	482	G
25	A	485	G
25	A	487	G
25	A	495	U
25	A	496	A
25	A	499	A
25	A	519	A
25	A	520	A
25	A	521	G
25	A	522	C
25	A	523	A
25	A	536	U
25	A	537	U
25	A	538	G
25	A	544	U
25	A	553	A
25	A	558	U
25	A	563	U
25	A	565	A
25	A	576	A
25	A	582	A
25	A	583	U
25	A	593	A
25	A	594	G
25	A	599	A
25	A	601	C
25	A	603	U
25	A	604	A
25	A	605	U

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Mol	Chain	Res	Type
25	A	608	G
25	A	622	A
25	A	627	A
25	A	635	U
25	A	636	A
25	A	637	G
25	A	644	U
25	A	645	A
25	A	647	U
25	A	649	G
25	A	659	G
25	A	660	A
25	A	667	A
25	A	675	A
25	A	676	U
25	A	687	G
25	A	720	A
25	A	728	C
25	A	730	C
25	A	737	U
25	A	738	G
25	A	743	G
25	A	747	G
25	A	754	A
25	A	755	C
25	A	765	G
25	A	766	G
25	A	772	A
25	A	774	G
25	A	775	G
25	A	779	A
25	A	793	U
25	A	795	G
25	A	802	C
25	A	820	G
25	A	835	A
25	A	836	U
25	A	841	C
25	A	848	G
25	A	855	A
25	A	866	U
25	A	870	G

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Mol	Chain	Res	Type
25	A	871	G
25	A	875	A
25	A	876	U
25	A	877	C
25	A	878	C
25	A	880	G
25	A	884	U
25	A	886	C
25	A	889	A
25	A	899	A
25	A	903	C
25	A	904	C
25	A	908	U
25	A	911	C
25	A	921	C
25	A	922	G
25	A	931	A
25	A	935	A
25	A	936	C
25	A	949	A
25	A	951	C
25	A	952	G
25	A	964	A
25	A	972	C
25	A	973	A
25	A	986	A
25	A	993	G
25	A	995	C
25	A	999	A
25	A	1002	U
25	A	1003	U
25	A	1007	G
25	A	1012	G
25	A	1016	U
25	A	1017	A
25	A	1023	U
25	A	1030	A
25	A	1037	G
25	A	1041	G
25	A	1043	U
25	A	1044	A
25	A	1047	A

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Mol	Chain	Res	Type
25	A	1051	U
25	A	1060	A
25	A	1063	A
25	A	1074	A
25	A	1075	A
25	A	1078	A
25	A	1080	A
25	A	1091	U
25	A	1099	C
25	A	1100	G
25	A	1102	G
25	A	1112	G
25	A	1117	A
25	A	1119	A
25	A	1120	U
25	A	1122	U
25	A	1124	A
25	A	1125	C
25	A	1129	G
25	A	1133	A
25	A	1148	G
25	A	1162	G
25	A	1169	A
25	A	1170	C
25	A	1193	G
25	A	1199	G
25	A	1211	A
25	A	1214	A
25	A	1225	G
25	A	1234	A
25	A	1237	G
25	A	1238	C
25	A	1240	A
25	A	1243	G
25	A	1249	A
25	A	1253	G
25	A	1255	A
25	A	1258	G
25	A	1259	A
25	A	1261	A
25	A	1263	U
25	A	1276	C

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Mol	Chain	Res	Type
25	A	1287	A
25	A	1288	A
25	A	1307	C
25	A	1308	A
25	A	1316	U
25	A	1334	G
25	A	1339	U
25	A	1347	G
25	A	1352	A
25	A	1354	A
25	A	1355	A
25	A	1366	U
25	A	1370	A
25	A	1372	A
25	A	1373	C
25	A	1382	A
25	A	1403	G
25	A	1404	C
25	A	1406	A
25	A	1407	U
25	A	1408	G
25	A	1414	A
25	A	1415	C
25	A	1420	A
25	A	1421	A
25	A	1439	G
25	A	1447	U
25	A	1448	C
25	A	1449	C
25	A	1454	U
25	A	1469	G
25	A	1475	U
25	A	1477	A
25	A	1480	U
25	A	1497	G
25	A	1498	G
25	A	1502	A
25	A	1509	A
25	A	1511	G
25	A	1512	A
25	A	1537	U
25	A	1556	A

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Mol	Chain	Res	Type
25	A	1558	G
25	A	1559	A
25	A	1560	A
25	A	1568	U
25	A	1573	U
25	A	1574	U
25	A	1575	C
25	A	1576	A
25	A	1593	A
25	A	1597	C
25	A	1628	C
25	A	1629	C
25	A	1634	C
25	A	1637	U
25	A	1638	U
25	A	1639	G
25	A	1641	G
25	A	1643	G
25	A	1650	G
25	A	1654	A
25	A	1657	G
25	A	1664	G
25	A	1673	C
25	A	1685	G
25	A	1686	G
25	A	1690	A
25	A	1705	G
25	A	1712	G
25	A	1716	U
25	A	1717	U
25	A	1720	U
25	A	1721	C
25	A	1725	A
25	A	1735	U
25	A	1736	G
25	A	1742	A
25	A	1745	U
25	A	1750	G
25	A	1751	G
25	A	1760	A
25	A	1763	G
25	A	1771	A

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Mol	Chain	Res	Type
25	A	1773	A
25	A	1787	C
25	A	1788	A
25	A	1789	A
25	A	1795	A
25	A	1797	A
25	A	1798	G
25	A	1803	C
25	A	1816	A
25	A	1829	G
25	A	1835	A
25	A	1837	G
25	A	1841	A
25	A	1851	U
25	A	1853	A
25	A	1865	G
25	A	1890	G
25	A	1892	C
25	A	1893	G
25	A	1894	G
25	A	1897	G
25	A	1900	A
25	A	1906	A
25	A	1909	G
25	A	1916	G
25	A	1917	G
25	A	1918	U
25	A	1923	A
25	A	1942	U
25	A	1954	C
25	A	1957	A
25	A	1958	U
25	A	1959	G
25	A	1974	G
25	A	1978	U
25	A	1980	U
25	A	1984	C
25	A	2008	A
25	A	2010	C
25	A	2020	A
25	A	2023	C
25	A	2030	U

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Mol	Chain	Res	Type
25	A	2042	C
25	A	2043	G
25	A	2047	A
25	A	2048	G
25	A	2049	A
25	A	2055	U
25	A	2056	7MG
25	A	2058	A
25	A	2067	G
25	A	2094	C
25	A	2096	U
25	A	2097	G
25	A	2098	U
25	A	2099	G
25	A	2100	U
25	A	2101	A
25	A	2103	G
25	A	2105	U
25	A	2106	A
25	A	2110	G
25	A	2112	G
25	A	2114	G
25	A	2115	G
25	A	2116	C
25	A	2117	U
25	A	2118	U
25	A	2119	U
25	A	2120	G
25	A	2121	A
25	A	2122	A
25	A	2127	G
25	A	2129	A
25	A	2132	C
25	A	2133	C
25	A	2135	G
25	A	2140	C
25	A	2143	G
25	A	2145	A
25	A	2146	G
25	A	2147	C
25	A	2148	C
25	A	2150	U

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Mol	Chain	Res	Type
25	A	2151	C
25	A	2158	A
25	A	2160	A
25	A	2161	C
25	A	2171	A
25	A	2174	C
25	A	2175	U
25	A	2177	G
25	A	2185	A
25	A	2187	C
25	A	2191	G
25	A	2194	C
25	A	2199	A
25	A	2200	U
25	A	2201	C
25	A	2212	A
25	A	2225	G
25	A	2226	G
25	A	2229	G
25	A	2238	OMG
25	A	2239	G
25	A	2265	A
25	A	2270	U
25	A	2274	A
25	A	2275	A
25	A	2292	U
25	A	2294	G
25	A	2296	A
25	A	2297	A
25	A	2306	C
25	A	2309	A
25	A	2312	A
25	A	2313	U
25	A	2314	A
25	A	2323	A
25	A	2330	U
25	A	2332	G
25	A	2334	C
25	A	2337	C
25	A	2348	C
25	A	2358	G
25	A	2359	U

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Mol	Chain	Res	Type
25	A	2361	C
25	A	2366	G
25	A	2370	G
25	A	2372	C
25	A	2389	U
25	A	2393	U
25	A	2398	A
25	A	2407	C
25	A	2409	C
25	A	2410	U
25	A	2412	A
25	A	2414	C
25	A	2416	G
25	A	2417	A
25	A	2422	A
25	A	2428	U
25	A	2434	G
25	A	2435	A
25	A	2446	A
25	A	2462	C
25	A	2467	C
25	A	2474	G
25	A	2478	U
25	A	2485	OMC
25	A	2489	G
25	A	2491	U
25	A	2492	G
25	A	2493	U
25	A	2505	A
25	A	2506	U
25	A	2516	G
25	A	2534	A
25	A	2537	G
25	A	2553	A
25	A	2554	G
25	A	2560	C
25	A	2565	G
25	A	2569	G
25	A	2572	U
25	A	2586	G
25	A	2589	A
25	A	2596	U

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Mol	Chain	Res	Type
25	A	2600	U
25	A	2602	U
25	A	2616	U
25	A	2617	U
25	A	2640	U
25	A	2641	A
25	A	2650	G
25	A	2672	G
25	A	2676	U
25	A	2677	U
25	A	2689	G
25	A	2692	A
25	A	2701	G
25	A	2705	G
25	A	2713	U
25	A	2720	A
25	A	2735	A
25	A	2744	A
25	A	2752	A
25	A	2763	A
25	A	2765	A
25	A	2766	U
25	A	2783	C
25	A	2784	U
25	A	2785	U
25	A	2786	G
25	A	2787	A
25	A	2794	U
25	A	2795	G
25	A	2807	A
25	A	2808	A
25	A	2812	U
25	A	2820	U
25	A	2836	U
25	A	2846	G
25	A	2852	U
25	A	2854	G
25	A	2860	A
25	A	2867	C
25	A	2871	U
25	A	2873	G
25	A	2889	C

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Mol	Chain	Res	Type
25	A	2890	A
26	B	9	G
26	B	24	G
26	B	35	U
26	B	37	C
26	B	41	C
26	B	52	A
26	B	53	A
26	B	67	U
26	B	73	A
26	B	89	U
26	B	90	C
26	B	91	C
26	B	109	A
26	B	117	G

All (49) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	27	G
25	A	81	G
25	A	83	G
25	A	87	C
25	A	114	U
25	A	243	U
25	A	265	A
25	A	314	A
25	A	434	A
25	A	444	A
25	A	470	A
25	A	687	G
25	A	774	G
25	A	792	A
25	A	840	U
25	A	920	C
25	A	963	A
25	A	1016	U
25	A	1042	C
25	A	1098	U
25	A	1099	C
25	A	1169	A
25	A	1233	A

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Mol	Chain	Res	Type
25	A	1340	A
25	A	1407	U
25	A	1448	C
25	A	1497	G
25	A	1574	U
25	A	1627	A
25	A	1642	A
25	A	1672	G
25	A	1741	A
25	A	1834	A
25	A	1891	G
25	A	1917	G
25	A	2029	A
25	A	2149	A
25	A	2228	A
25	A	2273	G
25	A	2274	A
25	A	2392	G
25	A	2461	U
25	A	2536	G
25	A	2743	U
25	A	2783	C
25	A	2793	C
25	A	2851	G
26	B	51	G
26	B	66	A

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

26 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	$\#\|Z\| > 2$
25	2MA	A	2490	58,25	17,25,26	0.95	1 (5%)	17,37,40	1.01	2 (11%)
1	UR3	a	1492	1	19,22,23	0.97	1 (5%)	26,32,35	1.47	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
25	UR3	A	1902	25	19,22,23	1.02	1 (5%)	26,32,35	1.46	2 (7%)
1	4OC	a	1396	1	20,23,24	0.73	0	26,32,35	0.98	2 (7%)
25	6MZ	A	2017	25	18,25,26	1.13	2 (11%)	16,36,39	4.51	4 (25%)
22	4SU	v	8	22	18,21,22	1.85	4 (22%)	26,30,33	1.84	5 (19%)
22	5MU	v	54	22	19,22,23	1.42	5 (26%)	28,32,35	2.07	5 (17%)
25	2MG	A	1822	25	18,26,27	0.92	1 (5%)	16,38,41	1.10	2 (12%)
25	1MG	A	735	25	18,26,27	0.68	0	19,39,42	1.04	2 (10%)
1	2MG	a	1201	1	18,26,27	0.93	1 (5%)	16,38,41	1.11	2 (12%)
25	5MC	A	1949	25	18,22,23	0.91	2 (11%)	26,32,35	1.09	2 (7%)
25	6MZ	A	1608	25	18,25,26	1.17	2 (11%)	16,36,39	4.29	4 (25%)
1	5MC	a	961	1	18,22,23	0.94	2 (11%)	26,32,35	1.11	2 (7%)
1	2MG	a	960	1	18,26,27	0.88	1 (5%)	16,38,41	1.22	2 (12%)
25	OMU	A	2539	25	19,22,23	1.24	3 (15%)	26,31,34	1.75	5 (19%)
1	MA6	a	1513	1	19,26,27	0.90	1 (5%)	18,38,41	1.89	6 (33%)
1	7MG	a	521	1	22,26,27	1.31	3 (13%)	29,39,42	2.56	7 (24%)
25	OMC	A	2485	58,25	19,22,23	0.83	0	26,31,34	0.89	1 (3%)
1	2MG	a	1510	1	18,26,27	0.91	1 (5%)	16,38,41	1.19	2 (12%)
25	7MG	A	2056	58,25	22,26,27	1.32	3 (13%)	29,39,42	2.53	7 (24%)
1	MA6	a	1512	1	19,26,27	0.92	1 (5%)	18,38,41	1.85	6 (33%)
25	2MG	A	2432	58,25	18,26,27	0.95	1 (5%)	16,38,41	1.17	2 (12%)
25	5MU	A	1926	25	19,22,23	1.40	5 (26%)	28,32,35	2.14	6 (21%)
25	OMG	A	2238	25	18,26,27	0.96	1 (5%)	19,38,41	1.03	2 (10%)
22	5MC	v	32	22	18,22,23	0.96	2 (11%)	26,32,35	1.28	3 (11%)
22	PSU	v	55	22	18,21,22	1.35	2 (11%)	22,30,33	1.89	3 (13%)

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
25	2MA	A	2490	58,25	-	2/3/25/26	0/3/3/3
1	UR3	a	1492	1	-	0/7/25/26	0/2/2/2
25	UR3	A	1902	25	-	0/7/25/26	0/2/2/2
1	4OC	a	1396	1	-	2/9/29/30	0/2/2/2
25	6MZ	A	2017	25	-	2/5/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	4SU	v	8	22	-	1/7/25/26	0/2/2/2
22	5MU	v	54	22	-	0/7/25/26	0/2/2/2
25	2MG	A	1822	25	-	0/5/27/28	0/3/3/3
25	1MG	A	735	25	-	0/3/25/26	0/3/3/3
1	2MG	a	1201	1	-	3/5/27/28	0/3/3/3
25	5MC	A	1949	25	-	0/7/25/26	0/2/2/2
25	6MZ	A	1608	25	-	0/5/27/28	0/3/3/3
1	5MC	a	961	1	-	0/7/25/26	0/2/2/2
1	2MG	a	960	1	-	0/5/27/28	0/3/3/3
25	OMU	A	2539	25	-	0/9/27/28	0/2/2/2
1	MA6	a	1513	1	-	3/7/29/30	0/3/3/3
1	7MG	a	521	1	-	2/7/37/38	0/3/3/3
25	OMC	A	2485	58,25	-	1/9/27/28	0/2/2/2
1	2MG	a	1510	1	-	0/5/27/28	0/3/3/3
25	7MG	A	2056	58,25	-	2/7/37/38	0/3/3/3
1	MA6	a	1512	1	-	1/7/29/30	0/3/3/3
25	2MG	A	2432	58,25	-	0/5/27/28	0/3/3/3
25	5MU	A	1926	25	-	0/7/25/26	0/2/2/2
25	OMG	A	2238	25	-	2/5/27/28	0/3/3/3
22	5MC	v	32	22	-	1/7/25/26	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	8	4SU	C4-S4	-4.48	1.59	1.68
22	v	8	4SU	C4-N3	-3.62	1.33	1.37
25	A	2056	7MG	C4-N9	-3.37	1.33	1.37
25	A	1608	6MZ	C6-N6	3.31	1.40	1.35
25	A	2017	6MZ	C6-N6	3.23	1.40	1.35
22	v	55	PSU	C6-C5	3.21	1.39	1.35
22	v	8	4SU	C5-C4	-3.02	1.38	1.42
1	a	521	7MG	C4-N9	-2.96	1.34	1.37
25	A	1926	5MU	C4-N3	-2.92	1.33	1.38
1	a	521	7MG	C5-C4	2.88	1.47	1.38
25	A	2238	OMG	C6-N1	-2.80	1.33	1.37
25	A	2432	2MG	C6-N1	-2.79	1.33	1.37
25	A	1822	2MG	C6-N1	-2.75	1.33	1.37
25	A	2539	OMU	C4-N3	-2.74	1.33	1.38
25	A	2056	7MG	C5-C4	2.73	1.47	1.38
25	A	2056	7MG	C6-N1	-2.71	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	v	54	5MU	C6-C5	2.68	1.39	1.34
22	v	55	PSU	C4-N3	-2.64	1.33	1.38
22	v	54	5MU	C4-N3	-2.62	1.34	1.38
1	a	1201	2MG	C6-N1	-2.61	1.34	1.37
1	a	961	5MC	C6-C5	2.61	1.38	1.34
22	v	8	4SU	C2-N3	-2.59	1.33	1.38
25	A	1926	5MU	C6-C5	2.56	1.38	1.34
22	v	32	5MC	C6-C5	2.56	1.38	1.34
1	a	1510	2MG	C6-N1	-2.54	1.34	1.37
1	a	521	7MG	C6-N1	-2.53	1.34	1.38
25	A	1949	5MC	C6-C5	2.53	1.38	1.34
25	A	2539	OMU	C2-N3	-2.52	1.33	1.38
25	A	1926	5MU	C6-N1	-2.51	1.33	1.38
1	a	960	2MG	C6-N1	-2.47	1.34	1.37
25	A	1949	5MC	C6-N1	-2.44	1.33	1.38
22	v	32	5MC	C6-N1	-2.43	1.33	1.38
22	v	54	5MU	C2-N1	2.43	1.42	1.38
25	A	1926	5MU	C2-N3	-2.38	1.33	1.38
1	a	961	5MC	C6-N1	-2.38	1.34	1.38
1	a	1512	MA6	C5-C4	2.33	1.47	1.40
1	a	1513	MA6	C5-C4	2.31	1.47	1.40
22	v	54	5MU	C4-C5	2.31	1.48	1.44
22	v	54	5MU	C6-N1	-2.27	1.34	1.38
25	A	1608	6MZ	C5-C4	2.23	1.46	1.40
25	A	2539	OMU	C5-C4	-2.19	1.38	1.43
25	A	1902	UR3	C2-N1	2.19	1.41	1.38
25	A	2017	6MZ	C5-C4	2.17	1.46	1.40
25	A	1926	5MU	C4-C5	2.07	1.48	1.44
1	a	1492	UR3	C2-N1	2.01	1.41	1.38
25	A	2490	2MA	C2-N3	2.01	1.35	1.31

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2017	6MZ	C9-N6-C6	-16.16	108.95	122.87
25	A	1608	6MZ	C9-N6-C6	-15.46	109.56	122.87
1	a	521	7MG	N9-C4-N3	9.12	139.12	125.47
25	A	2056	7MG	N9-C4-N3	8.84	138.70	125.47
25	A	2017	6MZ	C2-N1-C6	6.20	121.91	116.59
1	a	1492	UR3	C4-N3-C2	-6.00	118.91	124.56
22	v	55	PSU	N1-C2-N3	5.96	121.89	115.13
25	A	1608	6MZ	C2-N1-C6	5.81	121.58	116.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	1902	UR3	C4-N3-C2	-5.59	119.30	124.56
25	A	2056	7MG	N9-C8-N7	-5.58	95.40	103.38
1	a	521	7MG	C5-C4-N3	-5.55	117.55	128.13
25	A	1926	5MU	C4-N3-C2	-5.45	120.29	127.35
22	v	8	4SU	C5-C4-N3	5.39	119.69	114.69
25	A	2056	7MG	C5-C4-N3	-5.27	118.08	128.13
25	A	1926	5MU	N3-C2-N1	5.20	121.80	114.89
1	a	521	7MG	N9-C8-N7	-5.20	95.94	103.38
22	v	54	5MU	C4-N3-C2	-5.15	120.69	127.35
22	v	54	5MU	N3-C2-N1	4.92	121.42	114.89
22	v	8	4SU	C4-N3-C2	-4.64	122.83	127.34
25	A	2539	OMU	C4-N3-C2	-4.62	120.48	126.58
25	A	1926	5MU	C5-C4-N3	4.59	119.23	115.31
22	v	54	5MU	C5-C4-N3	4.44	119.10	115.31
1	a	521	7MG	C2-N3-C4	4.28	119.93	112.30
25	A	2539	OMU	N3-C2-N1	4.22	120.49	114.89
25	A	1926	5MU	C5-C6-N1	-4.16	119.06	123.34
25	A	2056	7MG	C2-N3-C4	4.15	119.69	112.30
1	a	1512	MA6	N1-C6-N6	4.14	121.42	117.06
22	v	55	PSU	C4-N3-C2	-3.94	120.67	126.34
22	v	54	5MU	O4-C4-C5	-3.91	120.37	124.90
25	A	1926	5MU	O4-C4-C5	-3.84	120.45	124.90
25	A	2539	OMU	C5-C4-N3	3.80	120.53	114.84
1	a	1513	MA6	C10-N6-C6	-3.59	108.64	119.51
22	v	54	5MU	C5-C6-N1	-3.50	119.74	123.34
1	a	1512	MA6	C10-N6-C6	-3.46	109.03	119.51
22	v	55	PSU	O2-C2-N1	-3.39	119.06	122.79
22	v	32	5MC	C5-C6-N1	-3.38	119.86	123.34
1	a	1513	MA6	N3-C2-N1	-3.37	123.41	128.68
1	a	961	5MC	C5-C6-N1	-3.35	119.90	123.34
25	A	1949	5MC	C5-C6-N1	-3.34	119.90	123.34
25	A	2017	6MZ	N3-C2-N1	-3.31	123.50	128.68
22	v	8	4SU	C5-C4-S4	-3.29	120.23	124.47
1	a	1513	MA6	C9-N6-C6	-3.25	109.67	119.51
25	A	1608	6MZ	N3-C2-N1	-3.22	123.64	128.68
1	a	1512	MA6	N3-C2-N1	-3.18	123.71	128.68
25	A	2539	OMU	O4-C4-C5	-3.11	119.68	125.16
22	v	8	4SU	N3-C2-N1	3.04	118.93	114.89
25	A	2017	6MZ	C4-C5-N7	-3.04	106.23	109.40
1	a	1513	MA6	N1-C6-N6	3.01	120.22	117.06
1	a	1513	MA6	C4-C5-N7	-2.96	106.32	109.40
22	v	32	5MC	C5-C4-N3	-2.86	118.59	121.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	32	5MC	O2-C2-N3	-2.83	117.73	122.33
25	A	1926	5MU	O2-C2-N1	-2.78	119.09	122.79
1	a	1512	MA6	C9-N6-C6	-2.75	111.20	119.51
1	a	521	7MG	C5-C6-N1	2.66	115.68	110.99
1	a	1513	MA6	C10-N6-C9	-2.65	107.57	116.12
1	a	1512	MA6	C4-C5-N7	-2.64	106.65	109.40
25	A	2056	7MG	C5-C6-N1	2.62	115.61	110.99
25	A	1608	6MZ	C4-C5-N7	-2.62	106.67	109.40
25	A	2432	2MG	C5-C6-N1	2.51	118.39	113.95
25	A	1902	UR3	C1'-N1-C2	2.48	121.18	116.99
25	A	1949	5MC	C5-C4-N3	-2.47	119.00	121.67
1	a	961	5MC	C5-C4-N3	-2.46	119.02	121.67
25	A	2490	2MA	C5-C6-N1	2.46	118.27	114.02
1	a	1510	2MG	C5-C6-N1	2.44	118.25	113.95
22	v	8	4SU	C1'-N1-C2	2.42	121.95	117.57
25	A	2056	7MG	C5-C4-N9	-2.41	103.21	106.35
1	a	1510	2MG	C8-N7-C5	2.41	107.58	102.99
25	A	735	1MG	C8-N7-C5	2.40	107.55	102.99
1	a	1396	4OC	C6-C5-C4	2.39	119.89	116.96
25	A	2490	2MA	C8-N7-C5	2.36	107.50	102.99
1	a	960	2MG	C5-C6-N1	2.34	118.08	113.95
1	a	960	2MG	C8-N7-C5	2.33	107.42	102.99
1	a	521	7MG	C5-C4-N9	-2.32	103.33	106.35
25	A	1822	2MG	C5-C6-N1	2.32	118.04	113.95
25	A	1822	2MG	C8-N7-C5	2.31	107.40	102.99
25	A	735	1MG	C5-C6-N1	2.31	117.37	113.90
25	A	2432	2MG	C8-N7-C5	2.30	107.38	102.99
1	a	1201	2MG	C5-C6-N1	2.30	118.02	113.95
25	A	2485	OMC	O2-C2-N3	-2.28	118.63	122.33
25	A	2238	OMG	C5-C6-N1	2.24	117.90	113.95
1	a	1201	2MG	C8-N7-C5	2.22	107.23	102.99
25	A	2238	OMG	C8-N7-C5	2.22	107.21	102.99
1	a	1396	4OC	O2-C2-N3	-2.21	118.73	122.33
1	a	1512	MA6	C10-N6-C9	-2.20	109.02	116.12
25	A	2539	OMU	O2-C2-N1	-2.10	120.00	122.79
1	a	521	7MG	O6-C6-C5	-2.07	122.46	127.54
25	A	2056	7MG	O6-C6-C5	-2.04	122.54	127.54

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1201	2MG	O4'-C4'-C5'-O5'
1	a	1201	2MG	C3'-C4'-C5'-O5'
25	A	2017	6MZ	O4'-C4'-C5'-O5'
25	A	2238	OMG	O4'-C4'-C5'-O5'
1	a	521	7MG	C3'-C4'-C5'-O5'
1	a	1396	4OC	O4'-C4'-C5'-O5'
1	a	1513	MA6	O4'-C4'-C5'-O5'
25	A	2056	7MG	O4'-C4'-C5'-O5'
25	A	2056	7MG	C3'-C4'-C5'-O5'
25	A	2238	OMG	C3'-C4'-C5'-O5'
1	a	521	7MG	O4'-C4'-C5'-O5'
25	A	2017	6MZ	C3'-C4'-C5'-O5'
1	a	1396	4OC	C3'-C4'-C5'-O5'
1	a	1513	MA6	C3'-C4'-C5'-O5'
25	A	2485	OMC	O4'-C4'-C5'-O5'
1	a	1512	MA6	C5-C6-N6-C9
1	a	1513	MA6	C5-C6-N6-C9
1	a	1201	2MG	C4'-C5'-O5'-P
22	v	8	4SU	O4'-C4'-C5'-O5'
25	A	2490	2MA	C4'-C5'-O5'-P
25	A	2490	2MA	O4'-C4'-C5'-O5'
22	v	32	5MC	C2'-C1'-N1-C2

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 599 ligands modelled in this entry, 597 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	$\#\|Z\| > 2$
59	FME	v	102	22	8,9,10	0.43	0	7,9,11	1.31	0
60	GCP	x	902	58	27,34,34	1.42	5 (18%)	34,54,54	1.91	8 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	FME	v	102	22	-	1/7/9/11	-
60	GCP	x	902	58	-	1/15/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	x	902	GCP	C5-C6	3.99	1.48	1.41
60	x	902	GCP	PG-O3G	2.67	1.61	1.54
60	x	902	GCP	PG-O2G	2.58	1.60	1.54
60	x	902	GCP	C5-C4	2.35	1.47	1.40
60	x	902	GCP	PB-O3A	2.02	1.60	1.58

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	x	902	GCP	C2-N3-C4	4.78	120.82	115.36
60	x	902	GCP	C4-C5-C6	-4.03	116.95	120.80
60	x	902	GCP	C2-N1-C6	4.03	122.33	115.93
60	x	902	GCP	C5-C6-N1	-3.87	118.13	123.43
60	x	902	GCP	N3-C2-N1	-3.29	122.83	127.22
60	x	902	GCP	PB-O3A-PA	-3.09	122.76	132.56
60	x	902	GCP	C4-C5-N7	-2.66	106.62	109.40
60	x	902	GCP	C3'-C2'-C1'	2.29	104.42	100.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

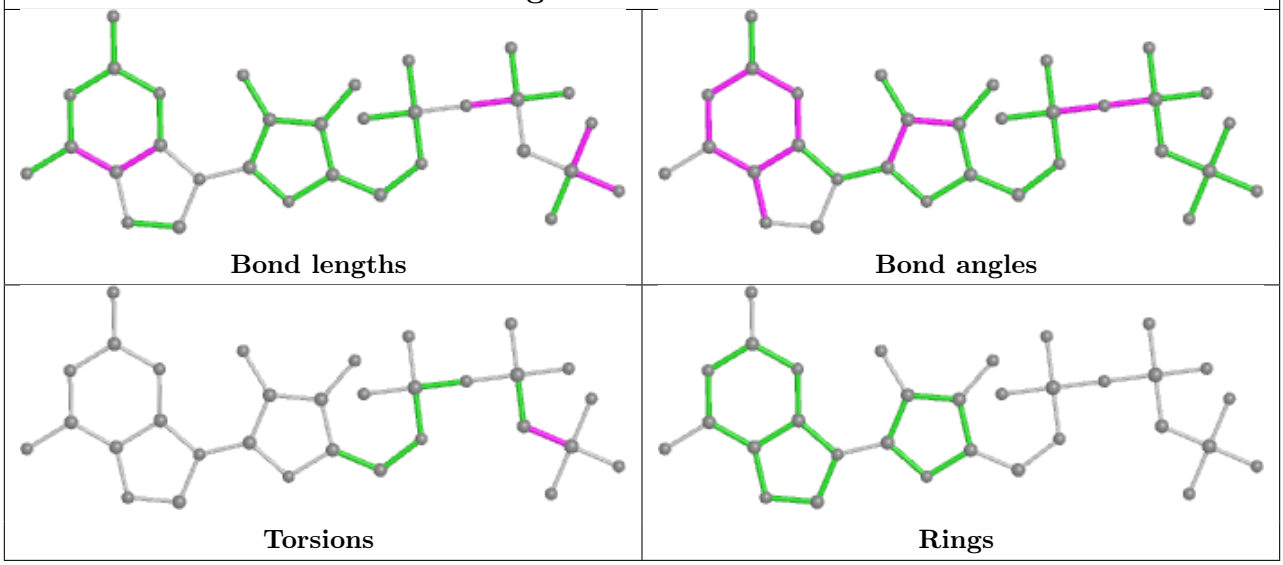
Mol	Chain	Res	Type	Atoms
59	v	102	FME	CB-CG-SD-CE
60	x	902	GCP	PB-C3B-PG-O1G

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 GCP x 902



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.

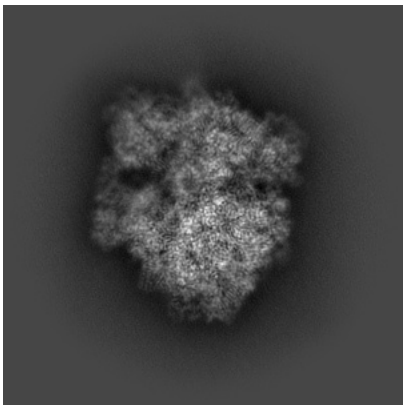
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26634. These allow visual inspection of the internal detail of the map and identification of artifacts.

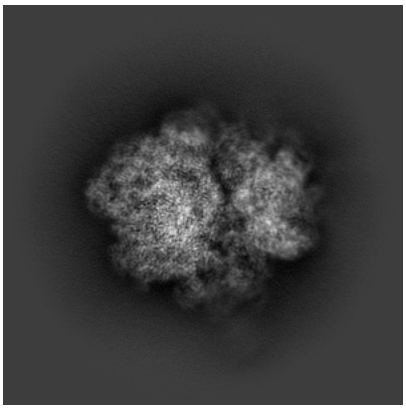
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

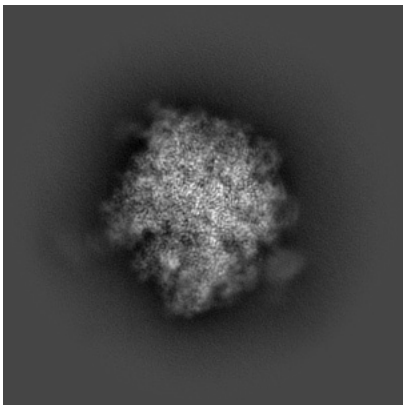
6.1.1 Primary map



X

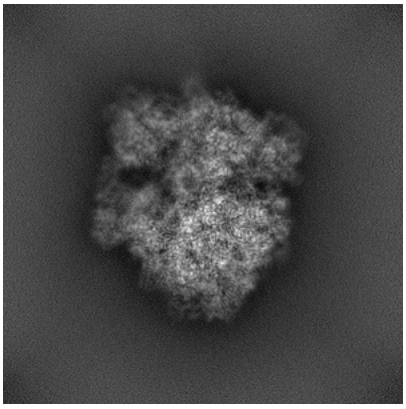


Y

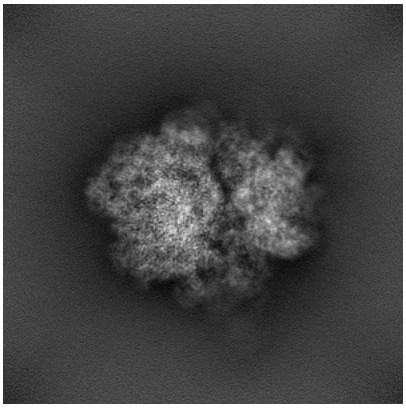


Z

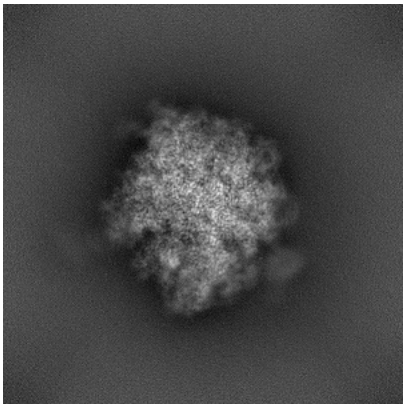
6.1.2 Raw map



X



Y

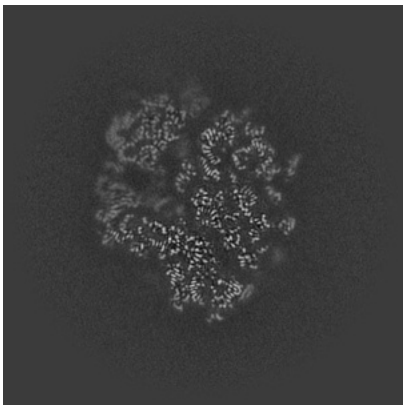


Z

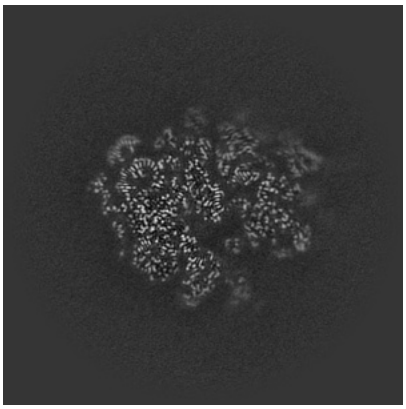
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

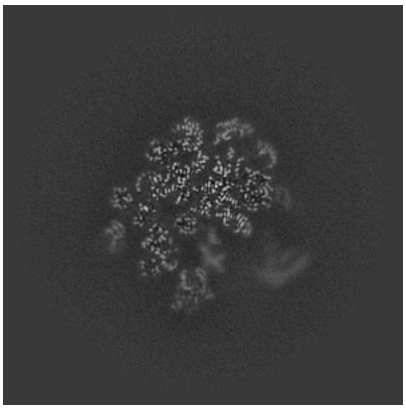
6.2.1 Primary map



X Index: 256

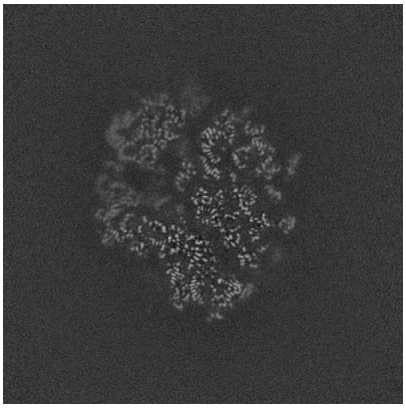


Y Index: 256

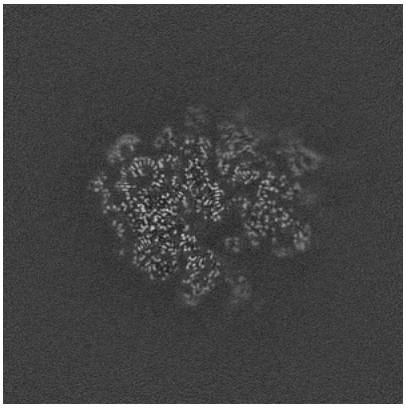


Z Index: 256

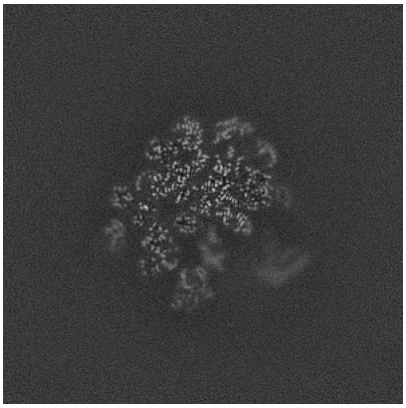
6.2.2 Raw map



X Index: 256



Y Index: 256

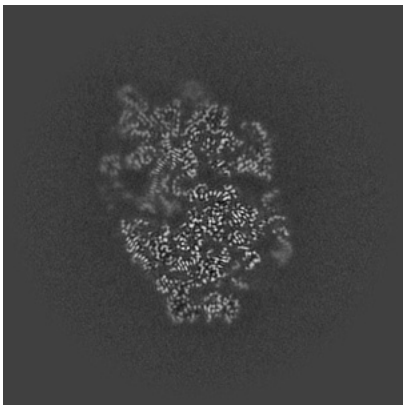


Z Index: 256

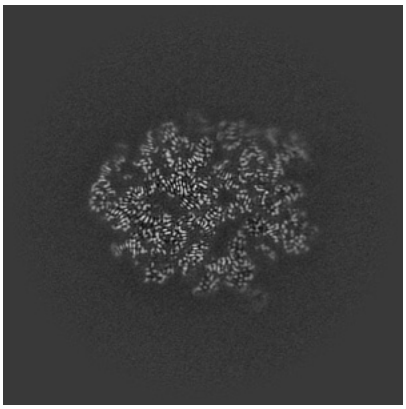
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

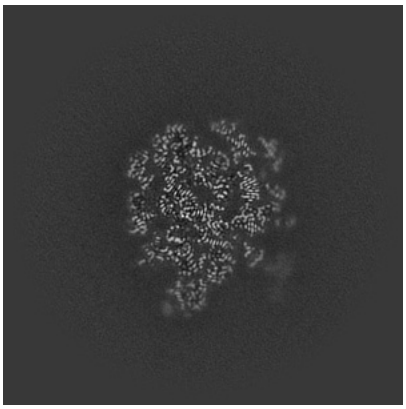
6.3.1 Primary map



X Index: 270

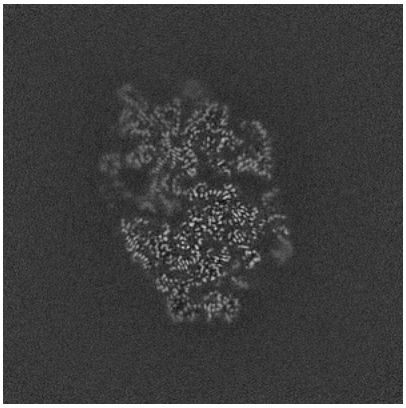


Y Index: 270

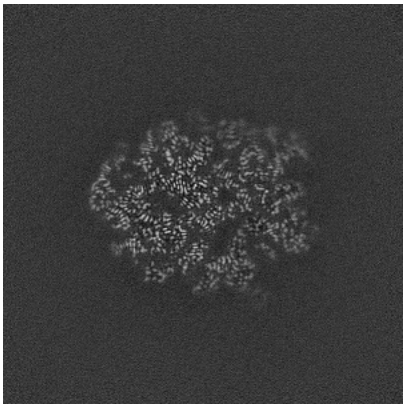


Z Index: 211

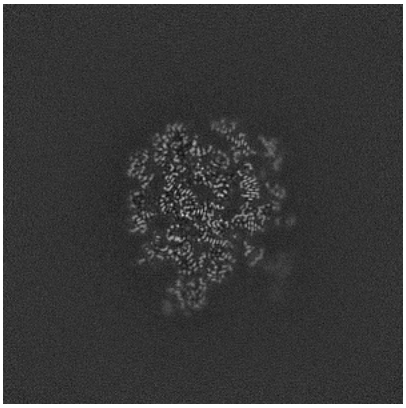
6.3.2 Raw map



X Index: 270



Y Index: 270

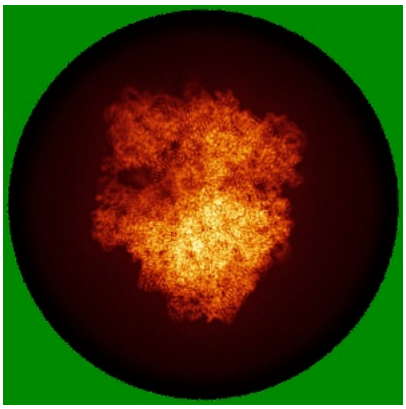


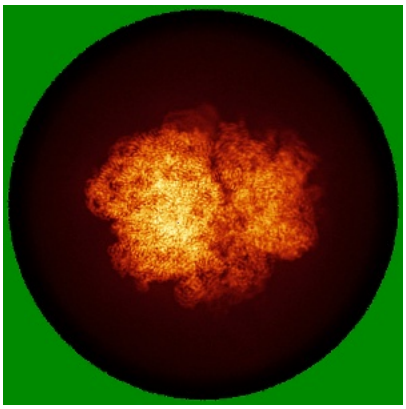
Z Index: 211

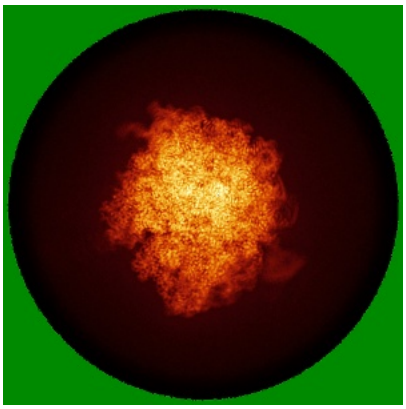
The images above show the largest variance slices of the map in three orthogonal directions.

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

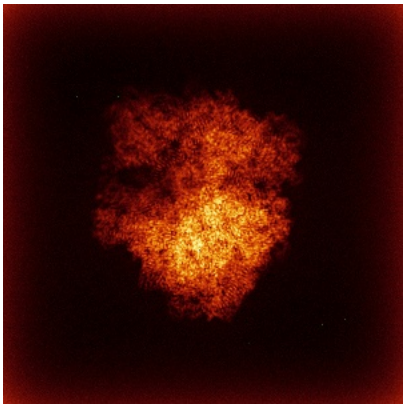
6.4.1 Primary map

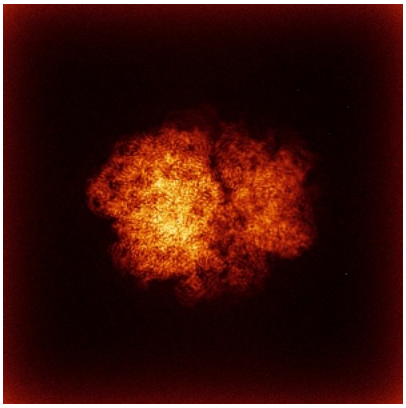

X

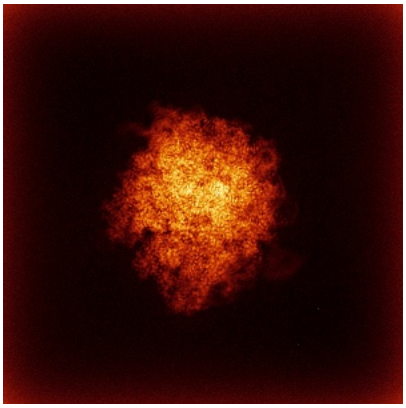

Y


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 0.14. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

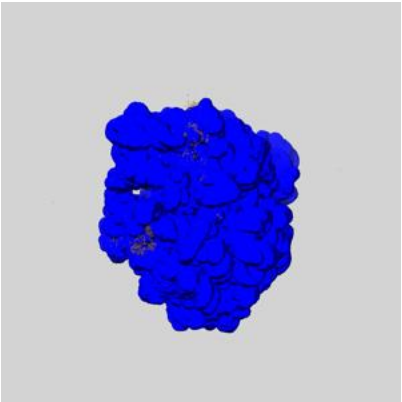
6.6 Mask visualisation (i)

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

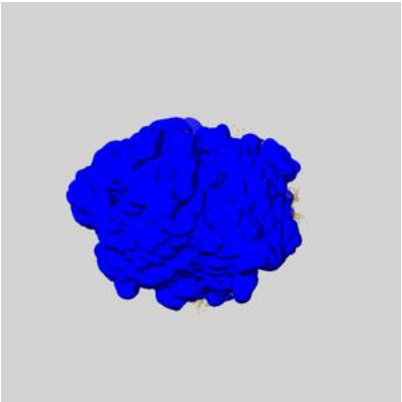
A mask typically either:

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

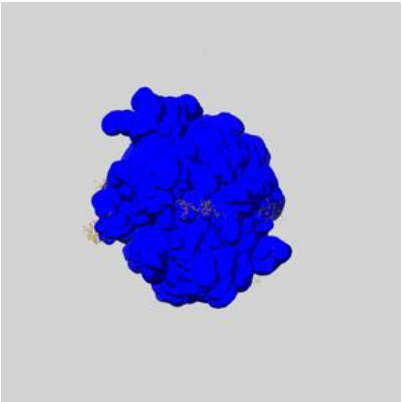
6.6.1 emd_26634_msk_1.map (i)



X



Y

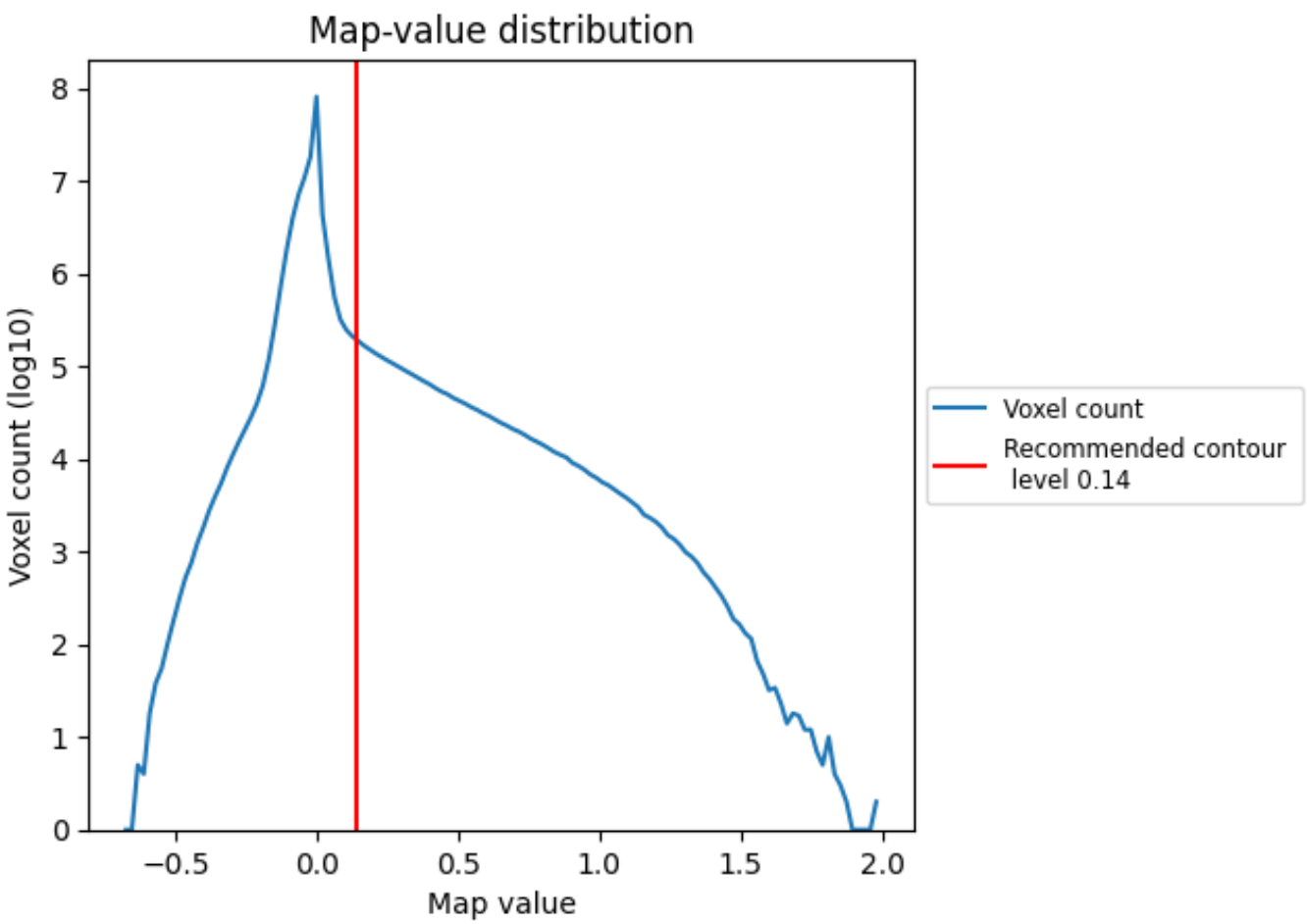


Z

7 Map analysis (i)

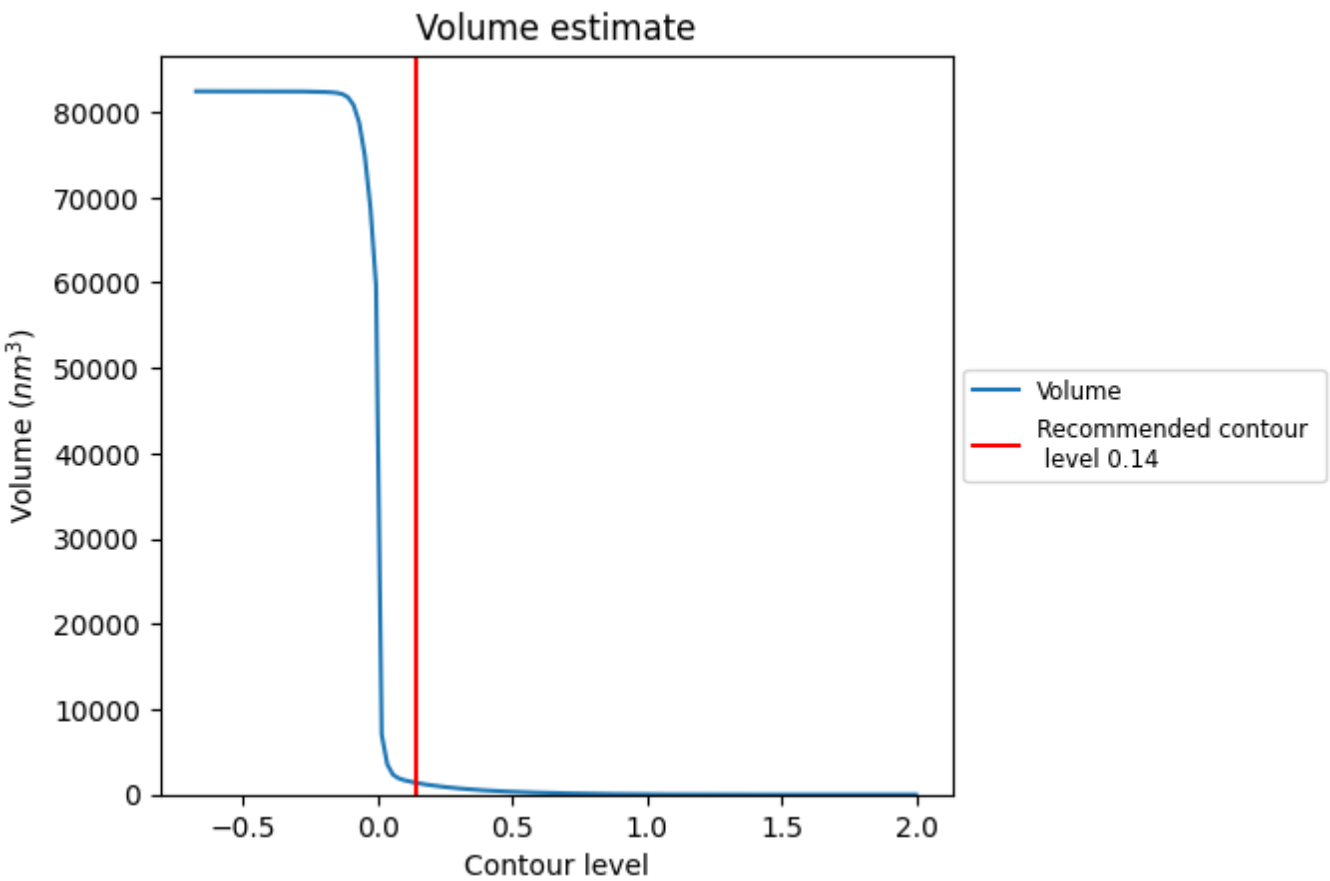
This section contains the results of statistical analysis of the map.

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.

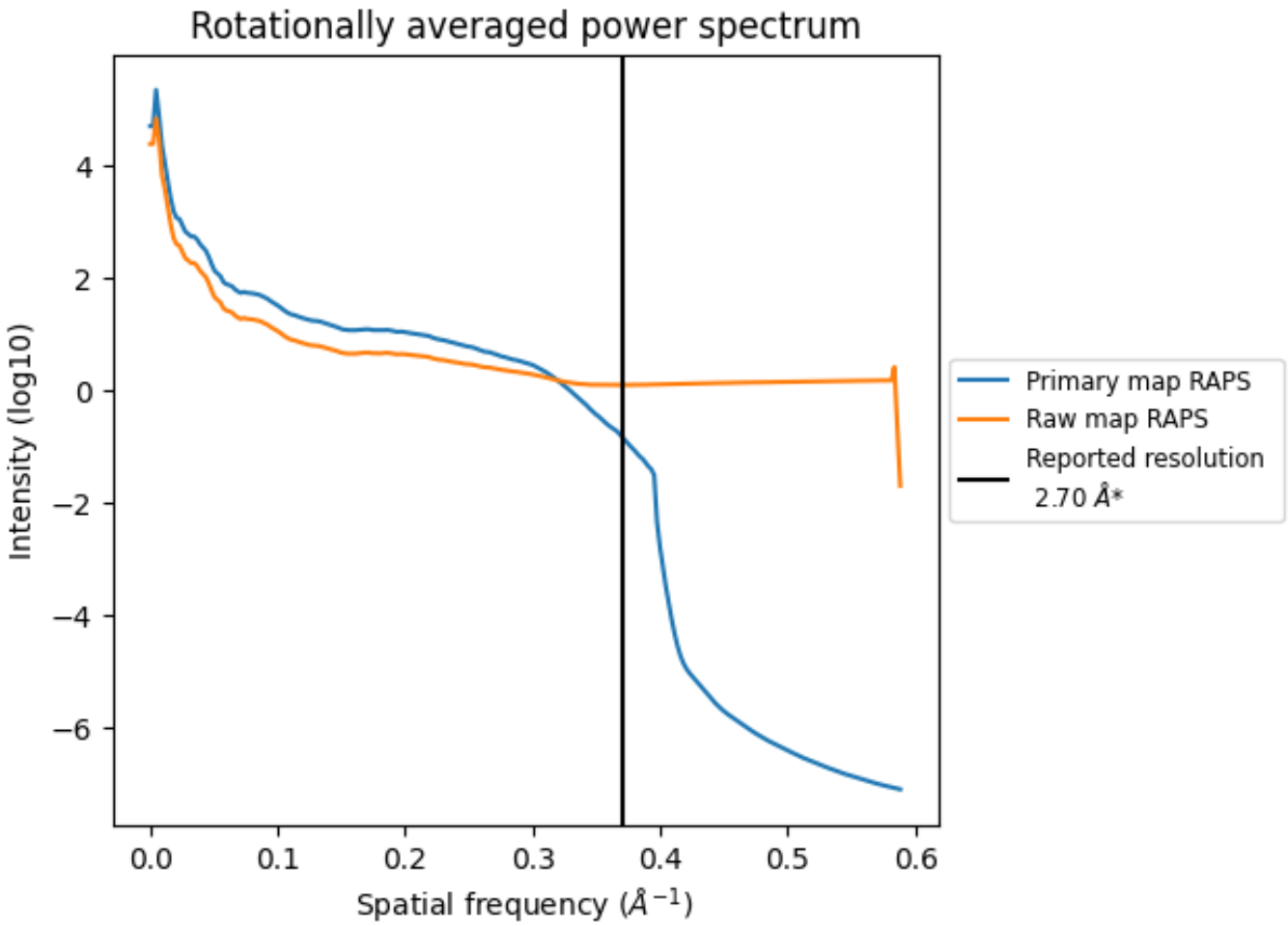
7.2 Volume estimate (i)



The volume at the recommended contour level is 1392 nm^3; this corresponds to an approximate mass of 1258 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)

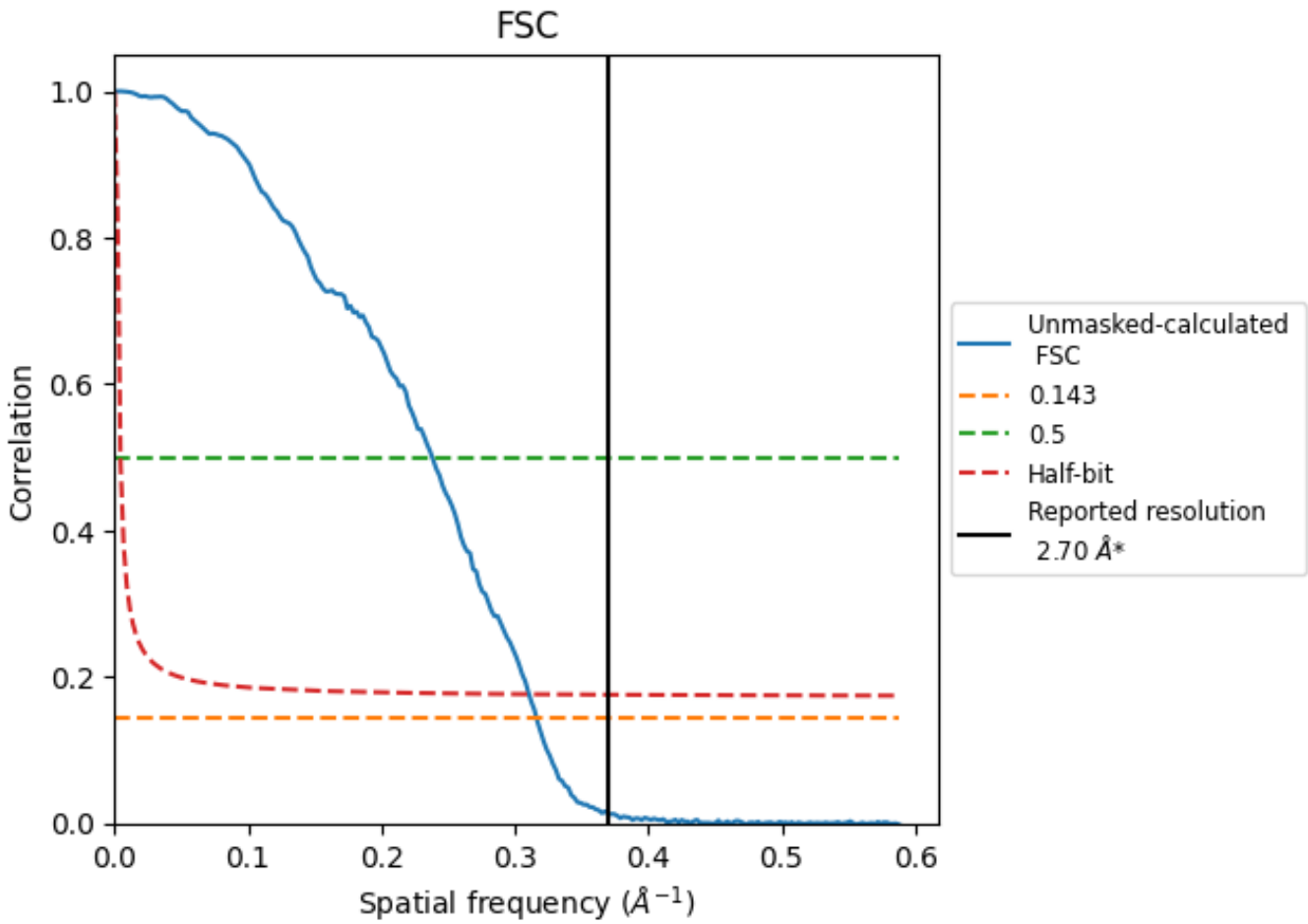


*Reported resolution corresponds to spatial frequency of 0.370 Å^{-1}

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 0.370 Å^{-1}

8.2 Resolution estimates (i)

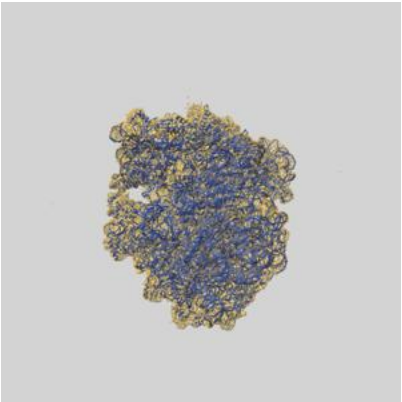
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.16	4.20	3.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.16 differs from the reported value 2.7 by more than 10 %

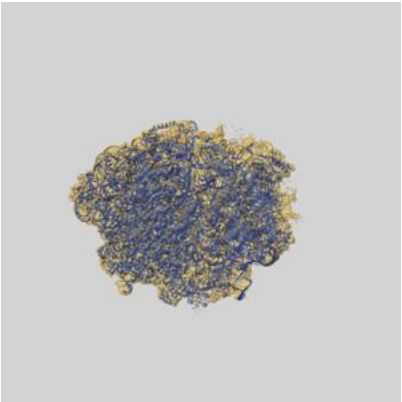
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26634 and PDB model 7UNV. Per-residue inclusion information can be found in section 3 on page 16.

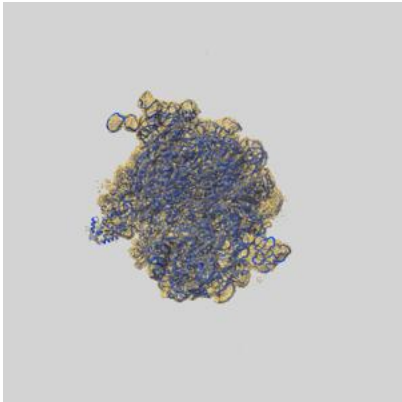
9.1 Map-model overlay (i)



X



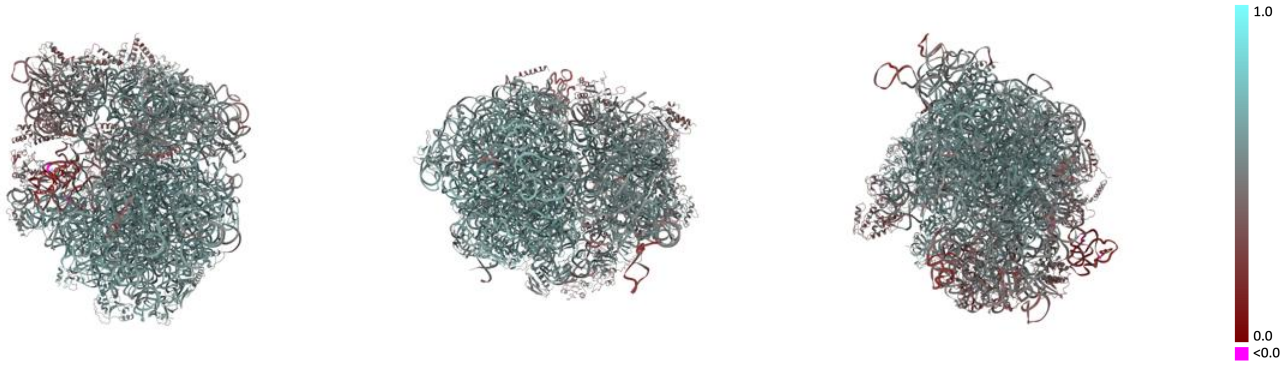
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.14 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

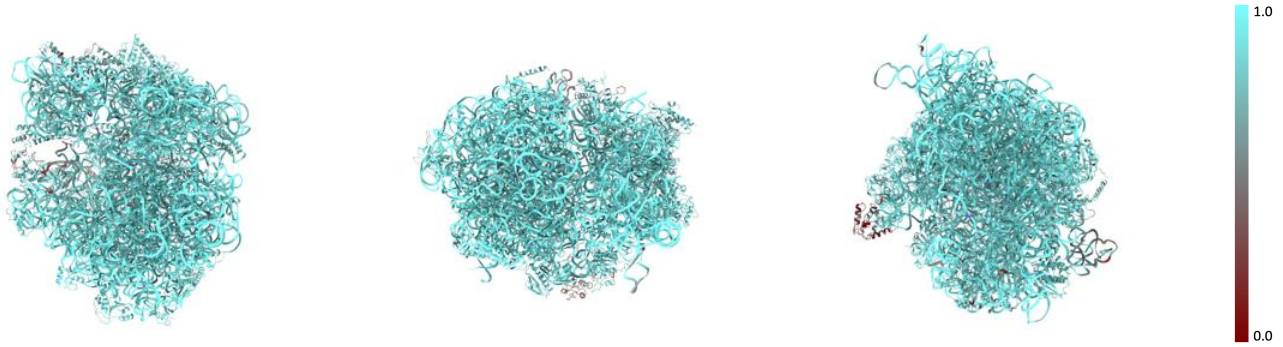
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

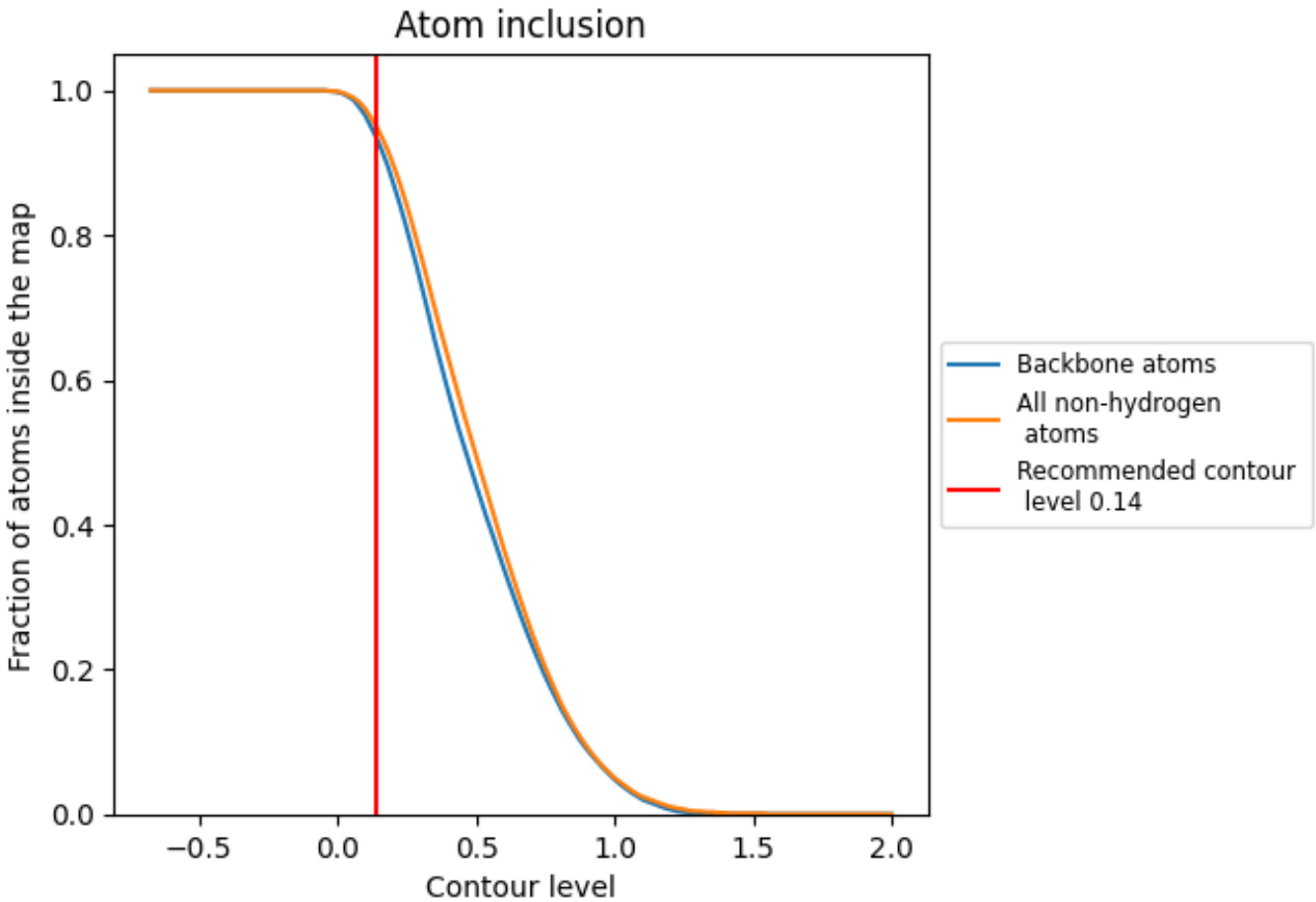
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.14).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 95% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.14) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9500	0.5540
1	0.9250	0.5560
2	0.9610	0.5990
3	0.5810	0.3460
4	0.9410	0.5940
5	0.9010	0.5720
6	0.9710	0.6220
7	0.9780	0.6260
8	0.9420	0.6070
A	0.9820	0.5920
B	0.9920	0.5470
C	0.9640	0.6130
D	0.9480	0.5980
E	0.9510	0.5880
F	0.8220	0.4250
G	0.8970	0.5390
H	0.8080	0.4670
I	0.2610	0.3650
J	0.7740	0.3840
L	0.9640	0.6020
M	0.9470	0.6060
N	0.9600	0.5970
O	0.9520	0.6130
P	0.9710	0.6060
Q	0.9210	0.5310
R	0.9420	0.5960
S	0.9730	0.6120
T	0.9470	0.5850
U	0.9470	0.5970
V	0.9440	0.5810
W	0.8820	0.5380
X	0.9250	0.5570
Y	0.9590	0.6120
Z	0.9550	0.5980
a	0.9850	0.5300

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Chain	Atom inclusion	Q-score
b	0.8080	0.4340
c	0.8580	0.4940
d	0.8960	0.5280
e	0.9170	0.5460
f	0.8440	0.4070
g	0.7830	0.3990
h	0.9120	0.5380
i	0.8530	0.4210
j	0.7850	0.4350
k	0.8450	0.4570
l	0.9300	0.5780
m	0.8130	0.3890
n	0.8630	0.4420
o	0.9210	0.5200
p	0.9450	0.5580
q	0.9250	0.5380
r	0.8010	0.4440
s	0.7800	0.3840
t	0.9240	0.5330
u	0.7860	0.4480
v	0.9410	0.4170
w	0.9770	0.5630
x	0.8900	0.5250