wwPDB EM Validation Summary Report (i)

Sep 16, 2026 – 03:45 AM EDT

PDB ID	:	7UNW / pdb_00007unw
EMDB ID	:	EMD-26635
Title	:	Pseudomonas aeruginosa 70S ribosome initiation complex bound to IF2-GDPCP (structure II-B)
Authors	:	Basu, R.S.; Sherman, M.B.; Gagnon, M.G.
Deposited on	:	2022-04-11
Resolution	:	2.60 Å(reported)
Based on initial models	:	3JCJ, 6SPG

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

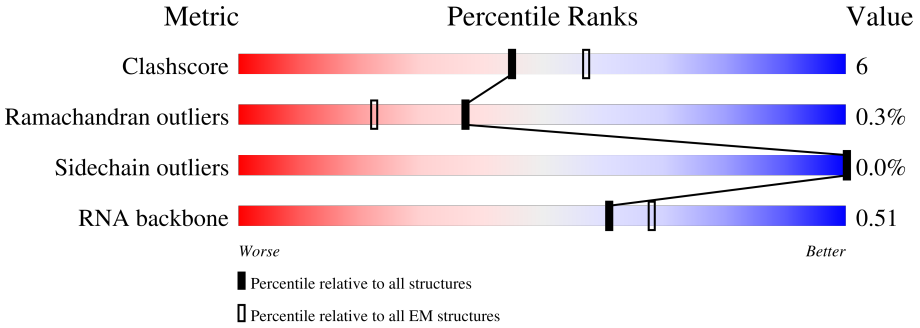
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

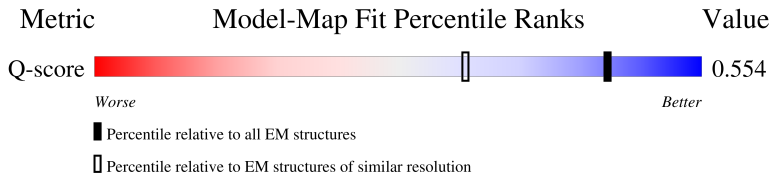
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8728 (2.10 - 3.10)

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	56% 37% 6% •
2	b	246	• 65% 26% • 9%
3	c	228	76% 15% 9%

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Mol	Chain	Length	Quality of chain
4	d	206	81% 19%
5	e	166	79% 14% 7%
6	f	139	42% 32% 24%
7	g	156	6% 68% 29%
8	h	130	76% 23%
9	i	130	69% 28%
10	j	103	7% 71% 25%
11	k	129	59% 33% 8%
12	l	123	82% 17%
13	m	118	59% 37%
14	n	101	73% 26%
15	o	89	83% 16%
16	p	83	83% 14%
17	q	88	67% 24% 9%
18	r	76	5% 76% 5% 18%
19	s	91	8% 65% 26% 9%
20	t	91	90% 5%
21	u	71	72% 15% 13%
22	v	77	45% 39% 13%
23	w	24	25% 75%
24	x	840	58% 12% 29%
25	A	2891	65% 29% 6%
26	B	120	70% 23%
27	C	273	89% 11%
28	D	211	85% 15%

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Mol	Chain	Length	Quality of chain
29	E	200	85% 15%
30	F	179	56% 41%
31	G	177	84% 15%
32	H	148	47% 51%
33	I	166	8% 61% 10% 29%
34	J	143	35% 90% 6%
35	L	142	89% 11%
36	M	122	80% 20%
37	N	144	96%
38	O	137	80% 20%
39	P	129	78% 16% 7%
40	Q	116	84% 16%
41	R	116	87% 11%
42	S	118	92% 7%
43	T	103	88% 11%
44	U	110	93% 7%
45	V	99	91% 5%
46	W	104	84% 15%
47	X	204	81% 12% 7%
48	Y	85	81% 8% 11%
49	Z	78	83% 15%
50	1	63	90% 6%
51	2	58	83% 16%
52	3	71	18% 46% 18% 34%
53	4	60	77% 15% 8%

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Mol	Chain	Length	Quality of chain
54	5	51	92% 8%
55	6	44	84% 16%
56	7	64	83% 16%
57	8	38	87% 13%

2 Entry composition (i)

There are 62 unique types of molecules in this entry. The entry contains 149945 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	1747	1102	320	315	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	1650	1044	310	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	793	496	150	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	4288	2685	769	818	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	1403	897	249	253	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	682	420	135	127	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	J	134	673	400	136	137	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	936	592	196	148	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

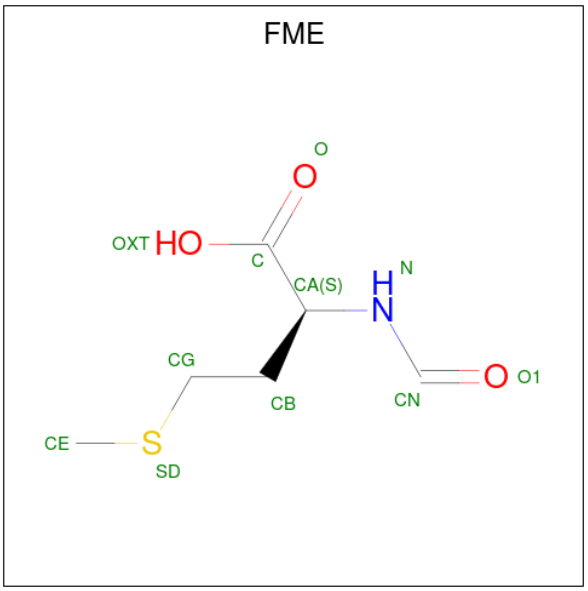
- Molecule 57 is a protein called 50S ribosomal protein L36.

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 (CCD ID: MG) (formula: Mg).

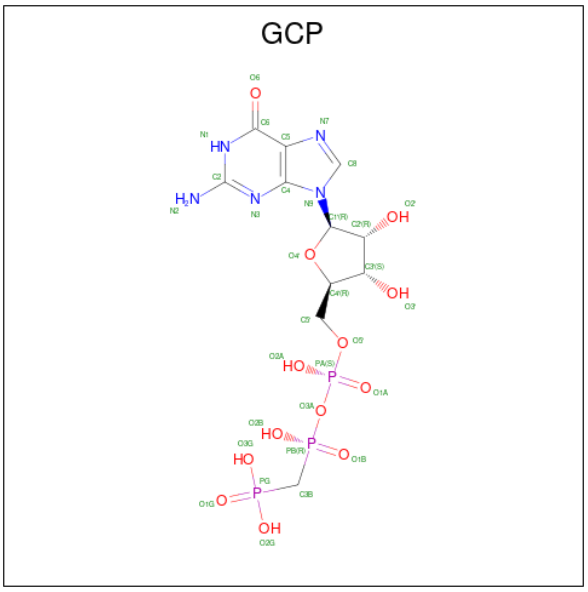
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
58	a	213	213	213	0
58	e	2	2	2	0
58	t	2	2	2	0
58	x	1	1	1	0
58	A	549	549	549	0
58	B	7	7	7	0
58	C	5	5	5	0
58	D	1	1	1	0
58	E	5	5	5	0
58	N	2	2	2	0
58	P	1	1	1	0
58	Y	1	1	1	0
58	4	3	3	3	0
58	6	2	2	2	0
58	7	2	2	2	0

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: 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 (CCD ID: GCP) (formula: $C_{11}H_{18}N_5O_{13}P_3$).



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

- Molecule 61 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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.

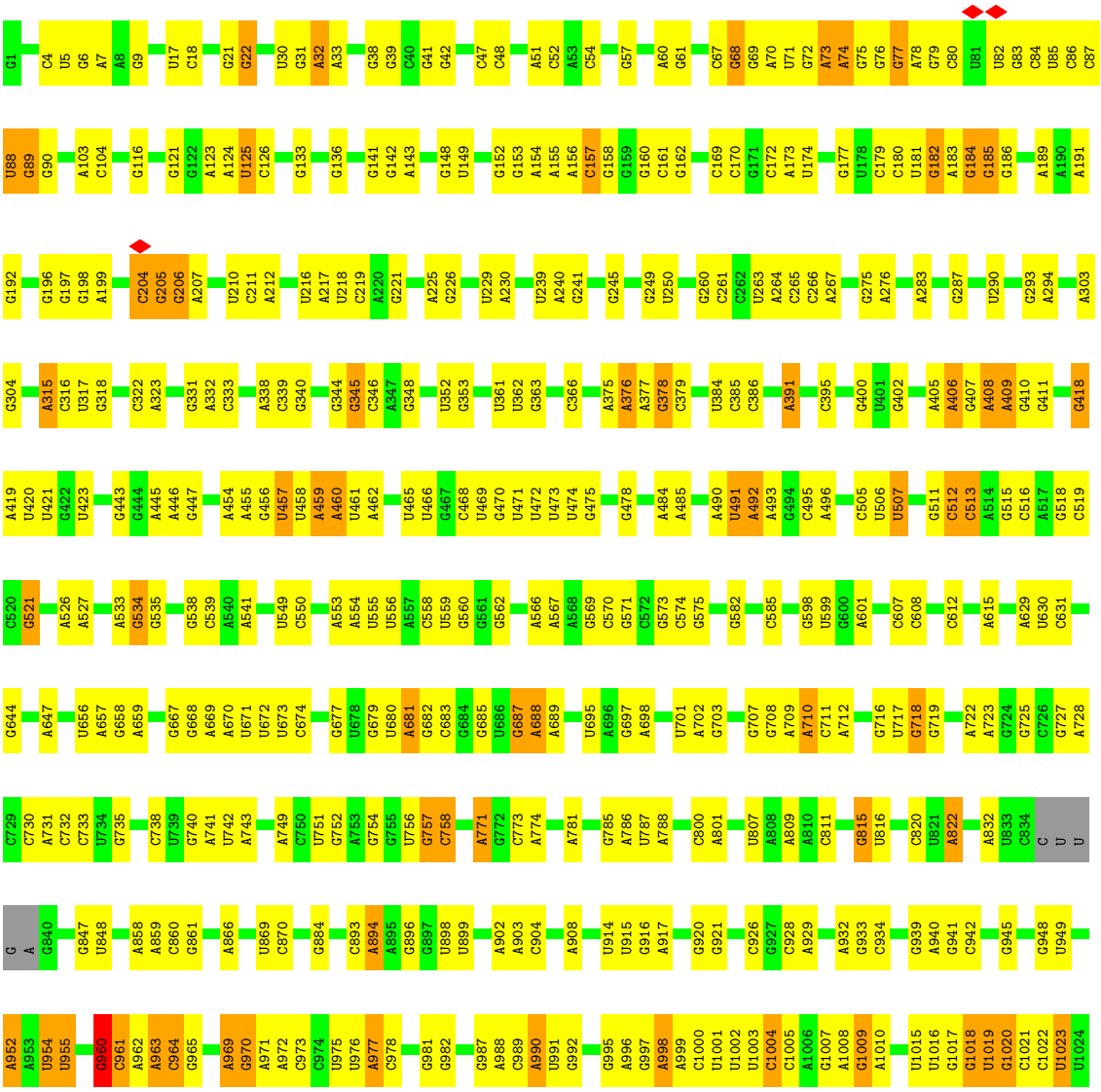
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
62	a	82	82	82	0
			Total	O	
62	w	1	1	1	0
			Total	O	
62	A	253	253	253	0
			Total	O	
62	B	6	6	6	0
			Total	O	
62	C	3	3	3	0
			Total	O	
62	D	1	1	1	0
			Total	O	
62	E	1	1	1	0
			Total	O	
62	V	1	1	1	0
			Total	O	
62	4	3	3	3	0
			Total	O	
62	6	1	1	1	0

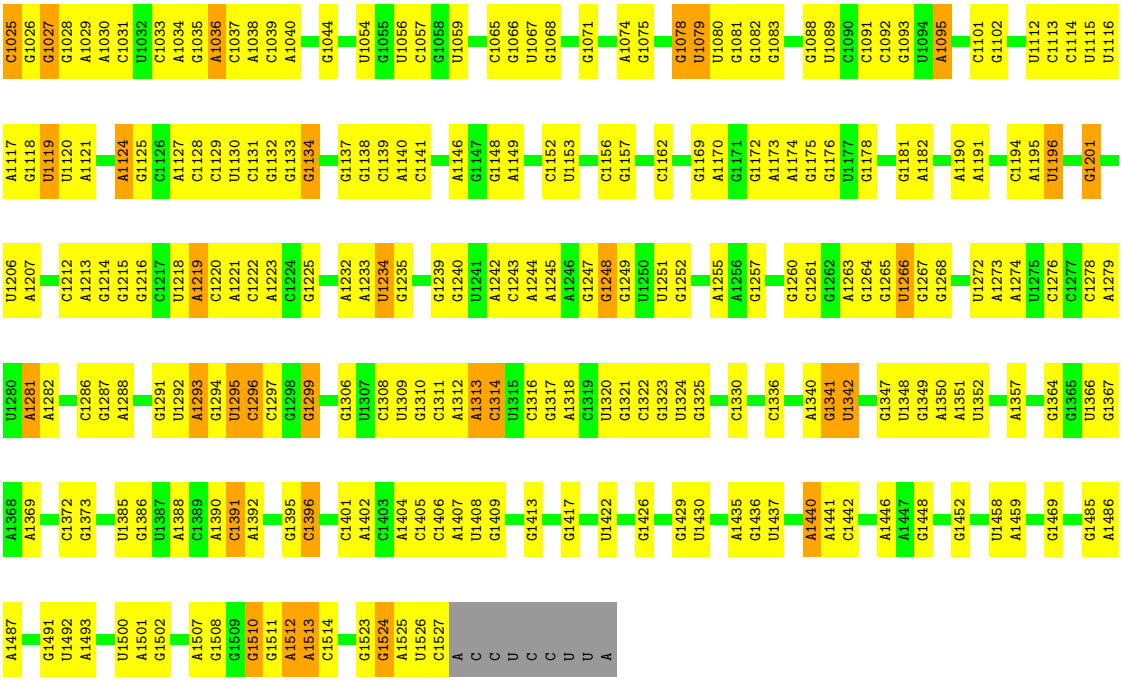
3 Residue-property plots (i)

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

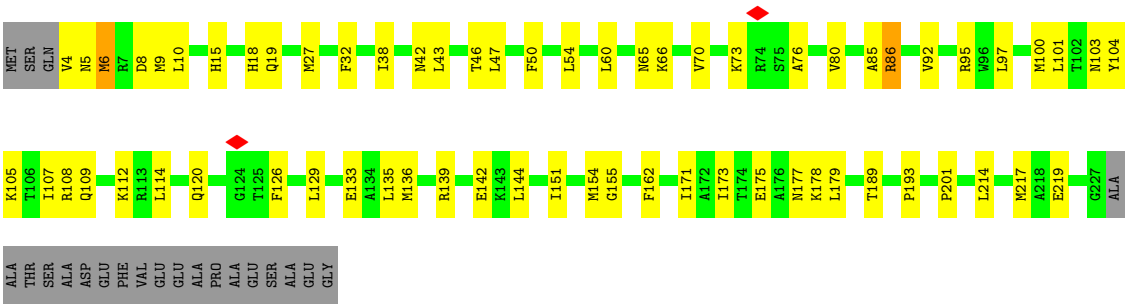
Chain a: 56% 37% 6%





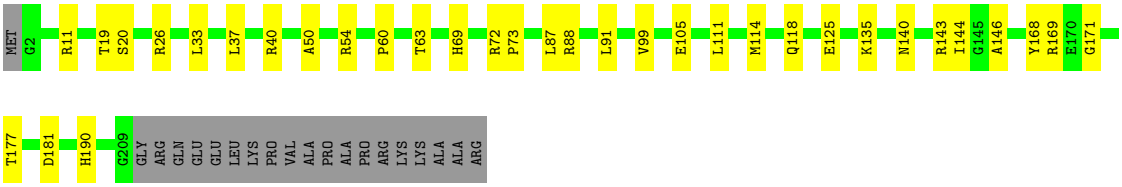
- Molecule 2: 30S ribosomal protein S2

Chain b:



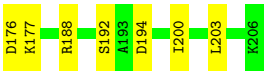
- Molecule 3: 30S ribosomal protein S3

Chain c:



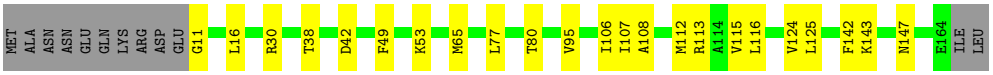
- Molecule 4: 30S ribosomal protein S4

Chain d:



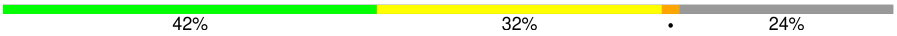
• Molecule 5: 30S ribosomal protein S5

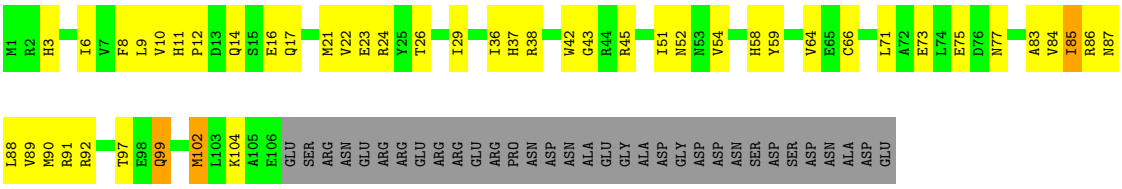
Chain e:



• Molecule 6: 30S ribosomal protein S6

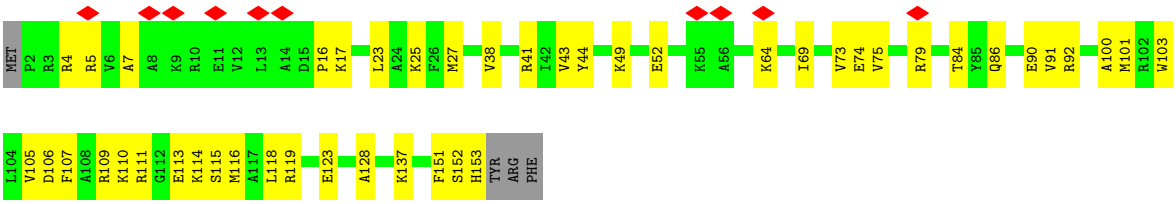
Chain f:





• Molecule 7: 30S ribosomal protein S7

Chain g:

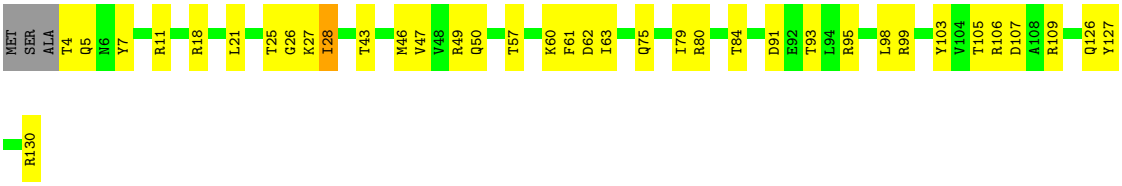


• Molecule 8: 30S ribosomal protein S8

Chain h:

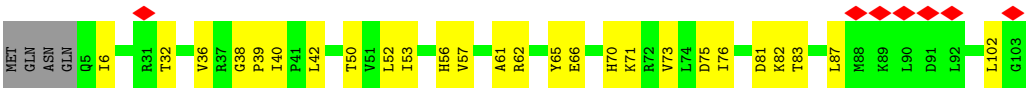
• Molecule 9: 30S ribosomal protein S9

Chain i:



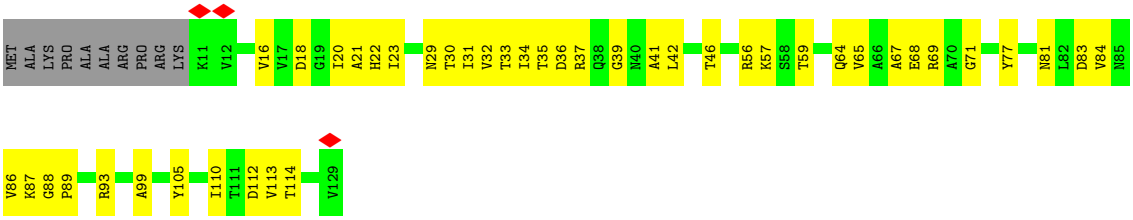
• Molecule 10: 30S ribosomal protein S10

Chain j:



- Molecule 11: 30S ribosomal protein S11

Chain k:

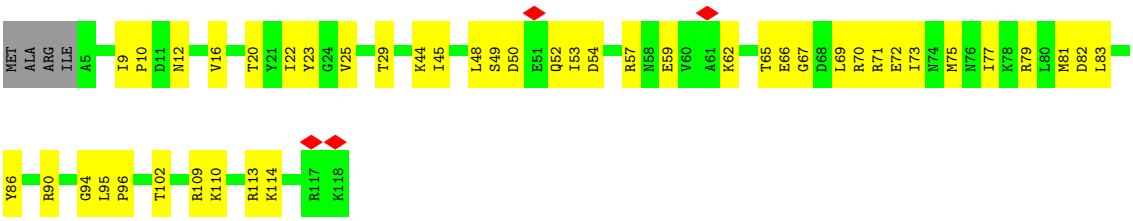


- Molecule 12: 30S ribosomal protein S12

Chain l:

- Molecule 13: 30S ribosomal protein S13

Chain m:

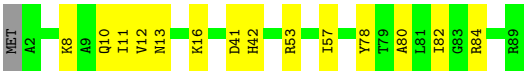


- Molecule 14: 30S ribosomal protein S14

Chain n:

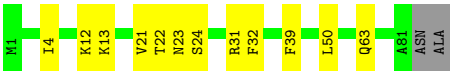
- Molecule 15: 30S ribosomal protein S15

Chain o:



- Molecule 16: 30S ribosomal protein S16

Chain p:

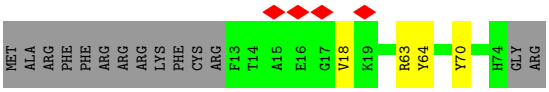


- Molecule 17: 30S ribosomal protein S17

Chain q:

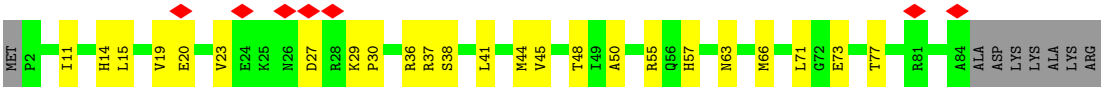
- Molecule 18: 30S ribosomal protein S18

Chain r:



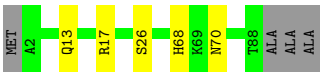
- Molecule 19: 30S ribosomal protein S19

Chain s:



- Molecule 20: 30S ribosomal protein S20

Chain t:

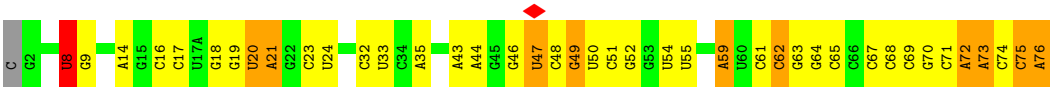


- Molecule 21: 30S ribosomal protein S21

Chain u:

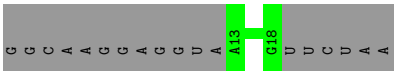
- Molecule 22: P-site initiator tRNA

Chain v:



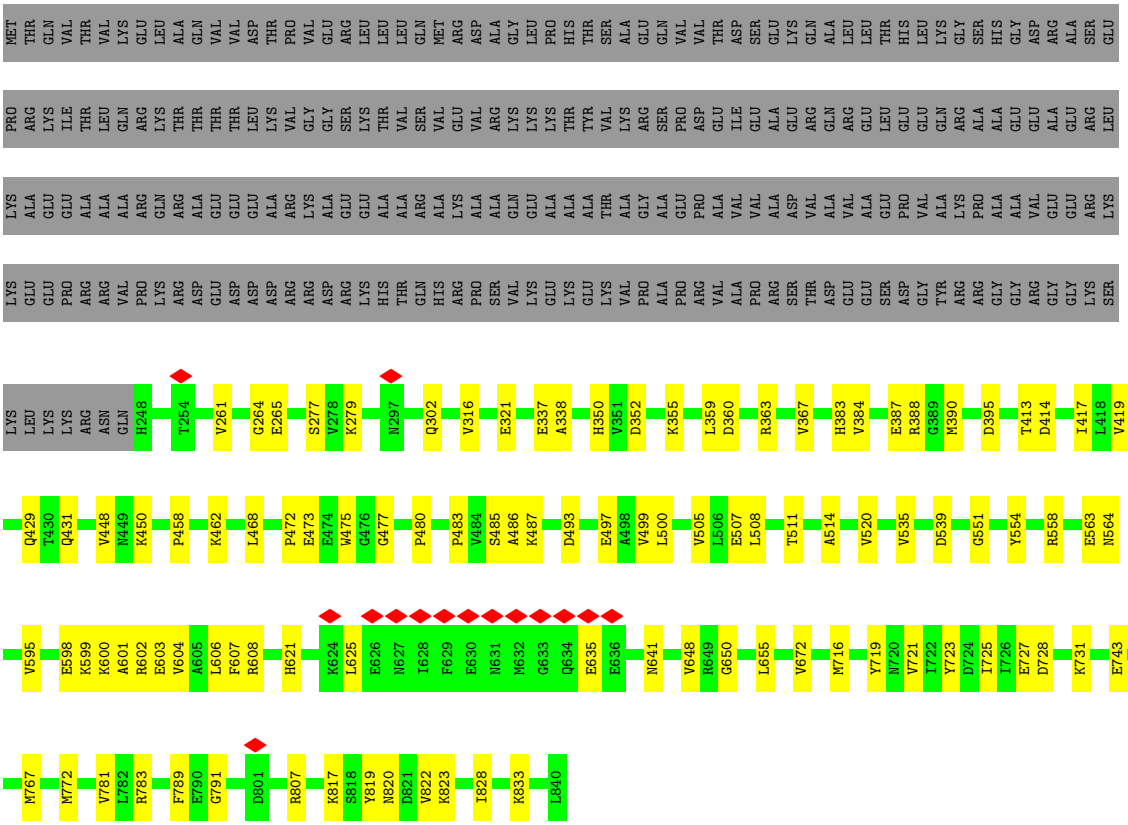
• Molecule 23: mRNA

Chain w:



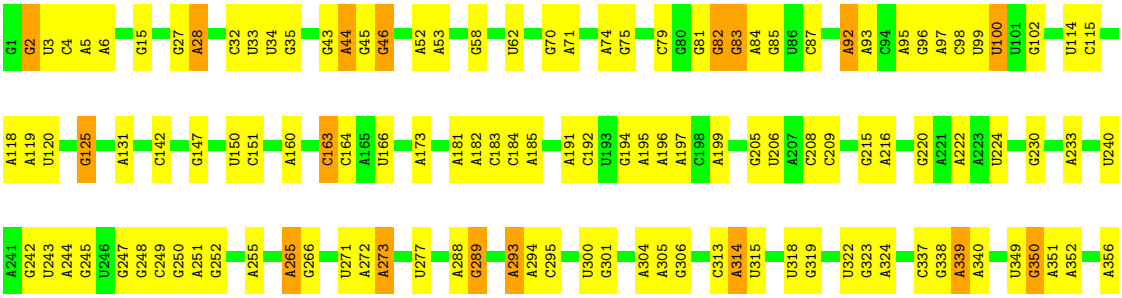
• Molecule 24: Translation initiation factor IF-2

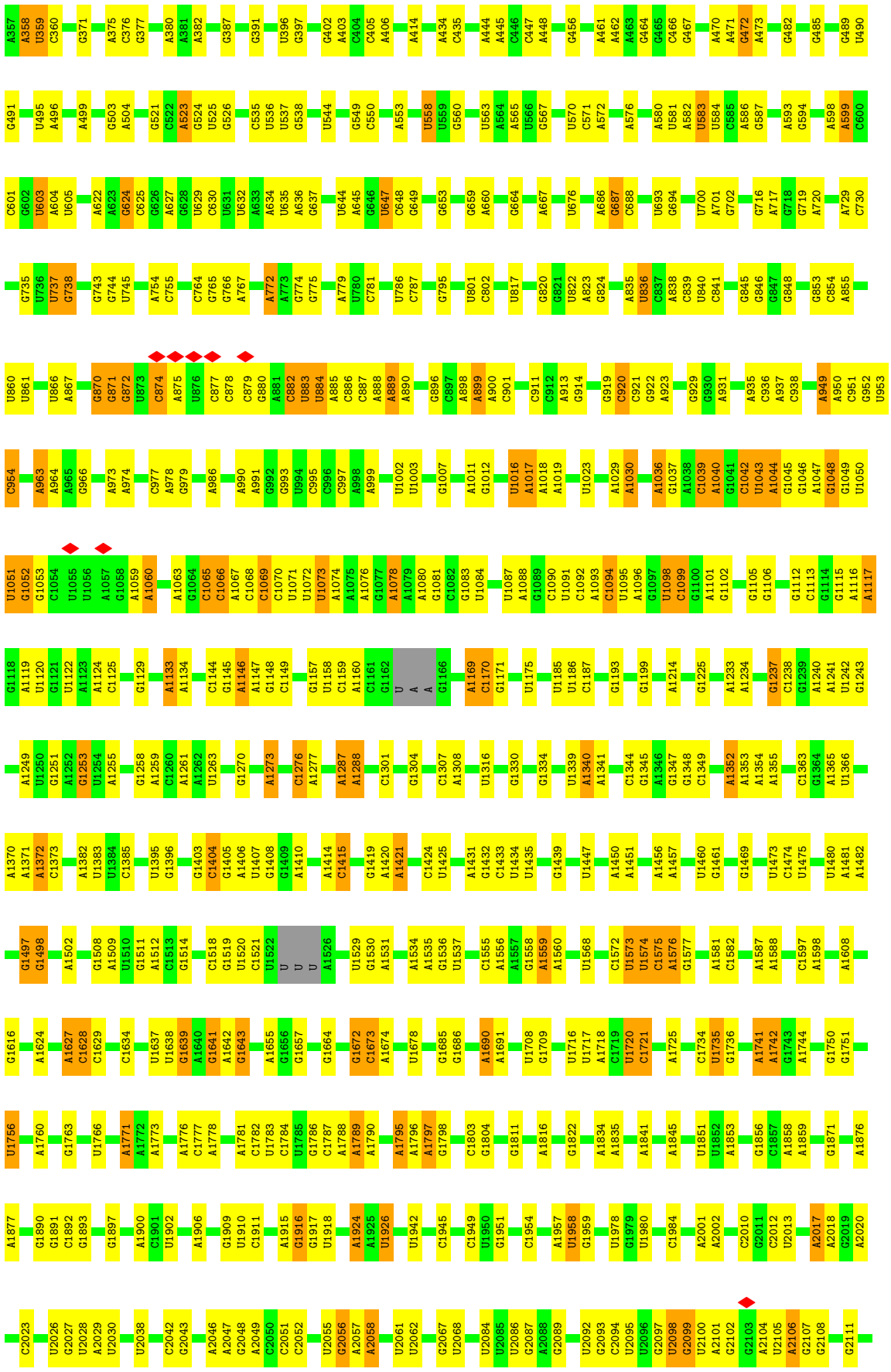
Chain x:



• Molecule 25: 23S Ribosomal RNA

Chain A:




A357 A358 U359 C360 G371 A375 C376 G377 A380 A381 A382 G387 G391 U396 G397 G402 A403 C404 C405 A406 A414 A434 C435 A444 A445 C446 C447 A448 G456 A461 A462 A463 G464 G465 C466 G467 A470 A471 G472 A473 G482 G485 G489 U490
G491 U495 A496 A499 G503 A504 G521 C522 A523 G524 U525 G526 C535 U536 U537 G538 U544 G549 C550 A553 U558 U559 G560 U563 A564 A565 U566 G567 U570 C571 A572 A576 A580 U581 A582 U583 U584 C585 A586 G587 A593 G594 A598 A599 C600
C601 G602 U603 A604 U605 A622 A623 G624 C625 G626 A627 G628 U629 C630 U631 U632 A633 A634 U635 A636 G637 U644 A645 G646 U647 C648 G649 G653 G659 A660 G664 A667 U676 A686 G687 C688 U693 G694 U700 A701 G702 G716 A717 G718 G719 A720 A729 C730
G735 U736 U737 G738 G743 G744 U745 A754 C755 C764 G765 G766 A767 A772 A773 G774 G775 A779 U780 C781 U786 C787 G795 U801 C802 U817 G820 G821 U822 A823 G824 A835 U836 C837 A838 C839 U840 C841 G845 G846 G847 G848 G853 C854 A855
U860 U861 U866 A867 G870 G871 G872 U873 C874 A875 U876 C877 C878 C879 G880 A881 C882 U883 U884 A885 C886 C887 A888 A889 A890 G896 C897 A898 A899 A900 C901 C911 C912 A913 G914 G919 C920 C921 G922 A923 G929 G930 A931 A935 C936 A937 C938 A949 A950 C951 G952 U953
C954 A963 A964 A965 G966 A973 A974 C977 A978 G979 A986 A990 A991 G992 G993 U994 C995 C996 C997 A998 A999 U1002 U1003 G1007 A1011 G1012 U1016 A1017 A1018 A1019 U1023 A1029 A1030 A1036 G1037 A1038 C1039 A1040 G1041 C1042 U1043 A1044 G1045 G1046 A1047 G1048 G1049 U1050
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G1118 A1119 U1120 G1121 U1122 A1123 A1124 C1125 G1129 A1133 A1134 C1144 G1145 A1146 A1147 G1148 C1149 G1157 U1158 C1159 A1160 C1161 G1162 U A A A G1166 A1169 C1170 G1171 U1175 U1185 U1186 C1187 G1193 G1199 A1214 G1225 A1233 A1234 G1237 C1238 G1239 A1240 A1241 U1242 G1243
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A1370 A1371 A1372 C1373 A1382 U1383 U1384 C1385 U1395 G1396 G1403 C1404 G1405 A1406 U1407 G1408 G1409 A1410 A1414 C1415 G1419 A1420 A1421 C1424 U1425 A1431 G1432 C1433 U1434 U1435 G1439 U1447 A1450 A1451 A1456 A1457 U1460 G1461 G1469 U1473 C1474 U1475 U1480 A1481 A1482
G1497 G1498 A1502 G1508 A1509 U1510 G1511 A1512 C1513 G1514 C1518 G1519 U1520 C1521 U1522 U U U U A1526 U1529 G1530 A1531 A1534 A1535 G1536 U1537 C1555 A1556 A1557 G1558 A1559 A1560 U1568 C1572 U1573 U1574 C1575 A1576 G1577 A1581 C1582 A1587 A1588 C1597 A1598 A1608
G1616 A1624 A1627 C1628 C1629 C1634 U1637 U1638 G1639 A1640 G1641 A1642 G1643 A1655 G1656 G1657 G1664 G1672 C1673 A1674 U1678 G1685 G1686 A1690 A1691 U1708 G1709 U1716 U1717 A1718 C1719 U1720 C1721 A1725 C1734 U1735 G1736 A1741 A1742 G1743 A1744 G1750 G1751
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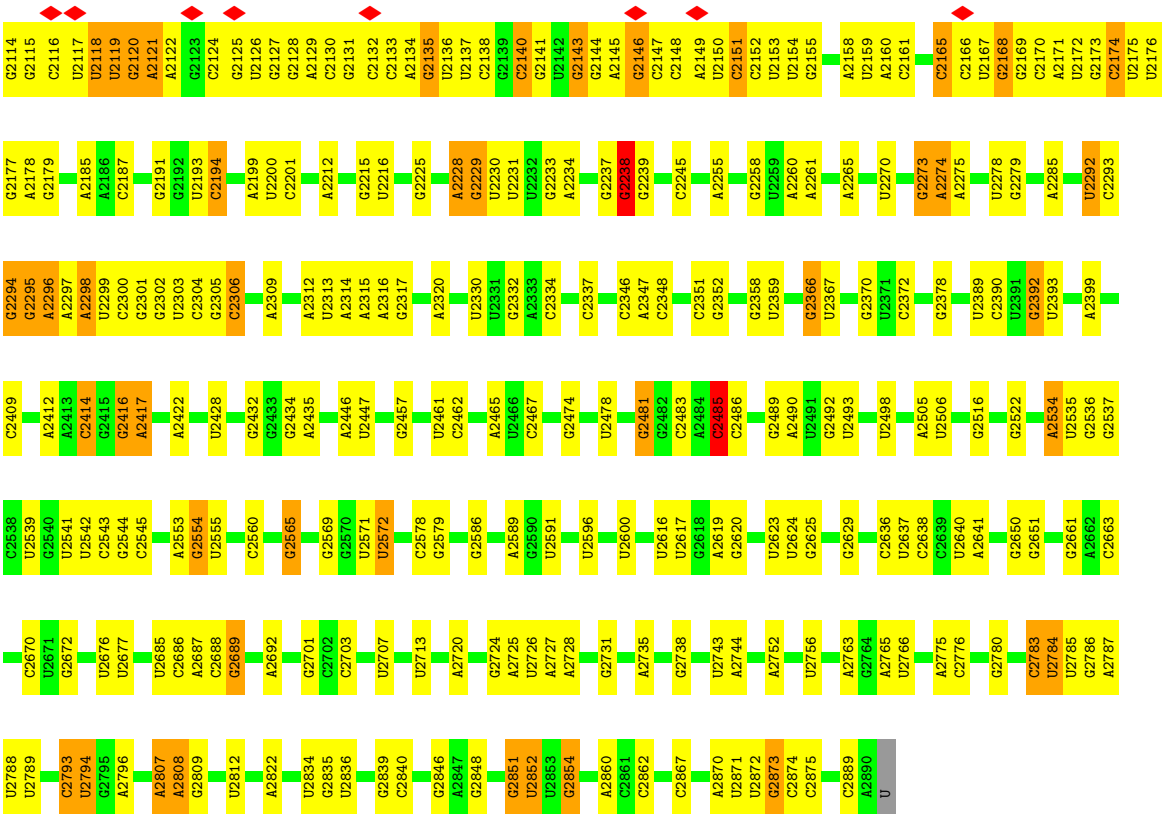
C2023 U2026 G2027 U2028 A2029 U2030 U2038 C2042 G2043 A2046 A2047 G2048 A2049 C2050 C2051 C2052 U2055 G2056 A2057 A2058 U2061 U2062 G2067 U2068 U2084 U2085 U2086 G2087 A2088 G2089 U2092 G2093 C2094 U2095 U2096 G2097 U2098 G2099 U2100 A2101 G2102 G2103 A2104 U2105 A2106 G2107 G2108 G2111



- Molecule 26: 5S Ribosomal RNA

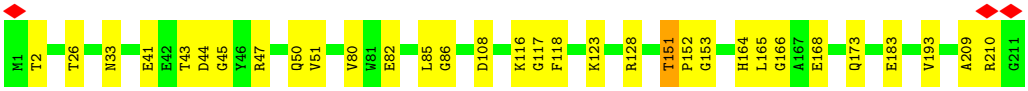
Chain B:

- Molecule 27: 50S ribosomal protein L2

Chain C:

- Molecule 28: 50S ribosomal protein L3

Chain D:

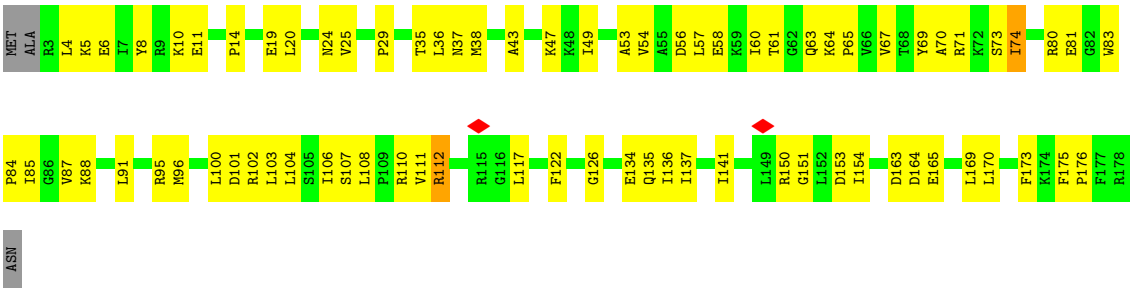


- Molecule 29: 50S ribosomal protein L4

Chain E:

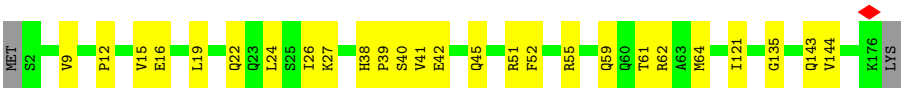
• Molecule 30: 50S ribosomal protein L5

Chain F:



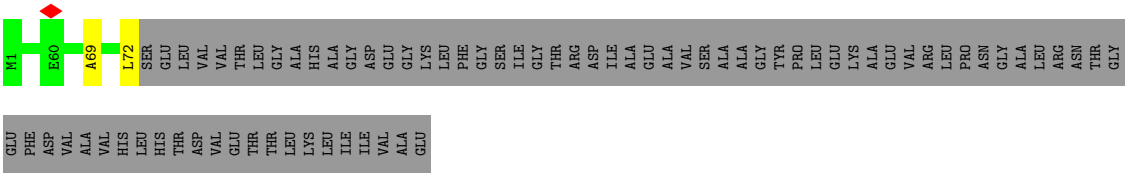
• Molecule 31: 50S ribosomal protein L6

Chain G:



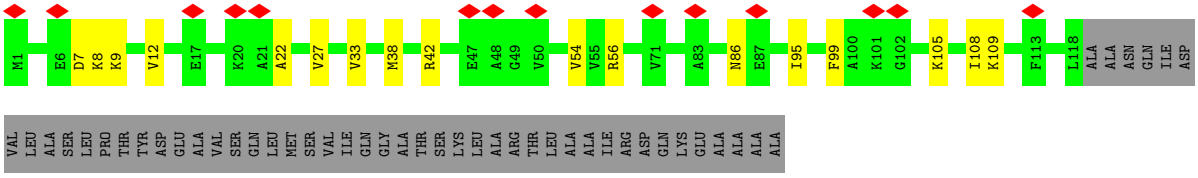
• Molecule 32: 50S ribosomal protein L9

Chain H:



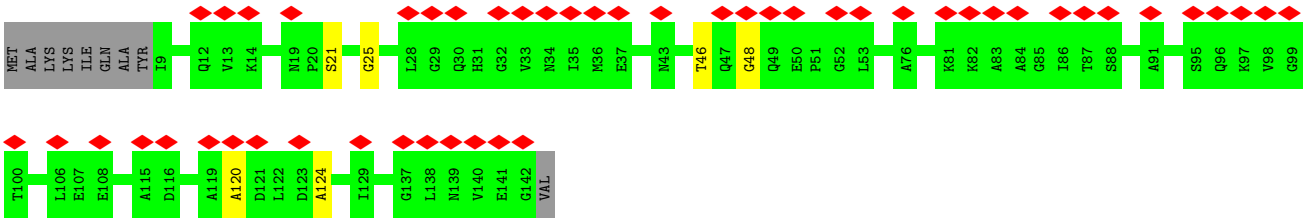
• Molecule 33: 50S ribosomal protein L10

Chain I:



• Molecule 34: 50S ribosomal protein L11

Chain J:

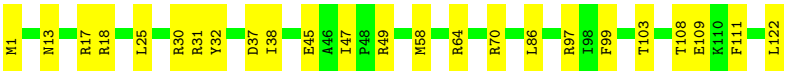


• Molecule 35: 50S ribosomal protein L13

Chain L:

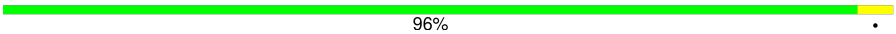
• Molecule 36: 50S ribosomal protein L14

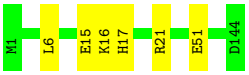
Chain M:



• Molecule 37: 50S ribosomal protein L15

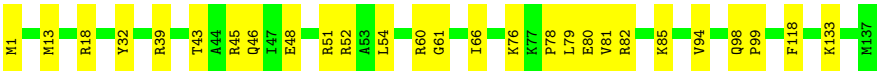
Chain N:





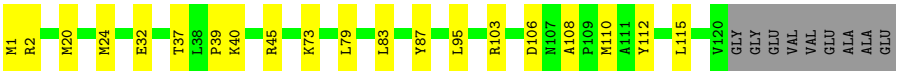
• Molecule 38: 50S ribosomal protein L16

Chain O:



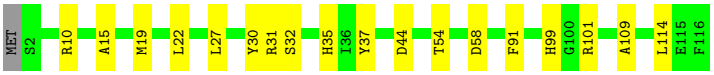
• Molecule 39: 50S ribosomal protein L17

Chain P:



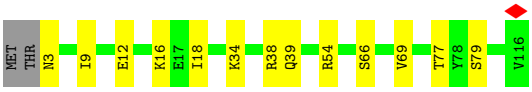
• Molecule 40: 50S ribosomal protein L18

Chain Q:



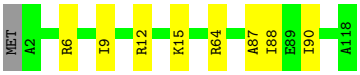
- Molecule 41: 50S ribosomal protein L19

Chain R:



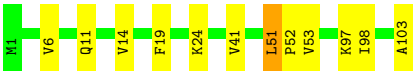
- Molecule 42: 50S ribosomal protein L20

Chain S:



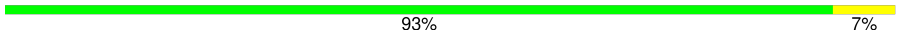
- Molecule 43: 50S ribosomal protein L21

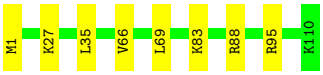
Chain T:



- Molecule 44: 50S ribosomal protein L22

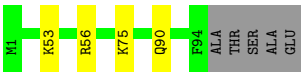
Chain U:





- Molecule 45: 50S ribosomal protein L23

Chain V:



- Molecule 46: 50S ribosomal protein L24

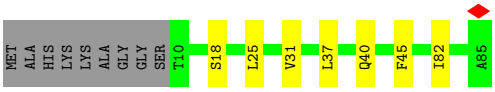
Chain W:

- Molecule 47: 50S ribosomal protein L25

Chain X:

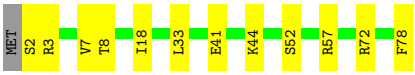
- Molecule 48: 50S ribosomal protein L27

Chain Y:



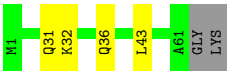
- Molecule 49: 50S ribosomal protein L28

Chain Z:



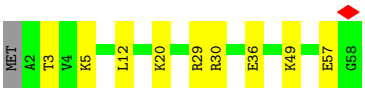
- Molecule 50: 50S ribosomal protein L29

Chain 1:



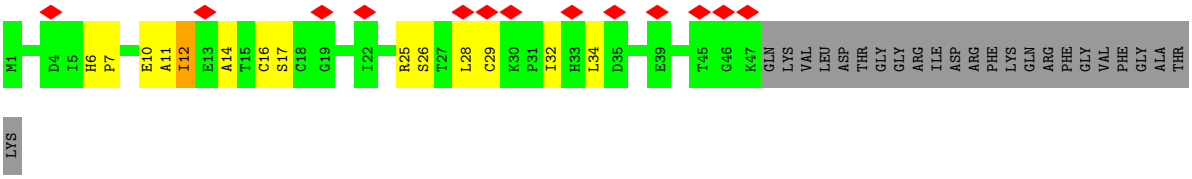
- Molecule 51: 50S ribosomal protein L30

Chain 2:



- Molecule 52: 50S ribosomal protein L31

Chain 3:

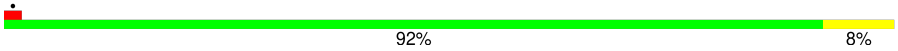


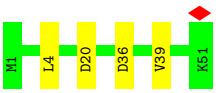
- Molecule 53: 50S ribosomal protein L32

Chain 4:

- Molecule 54: 50S ribosomal protein L33

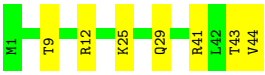
Chain 5:





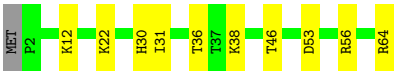
- Molecule 55: 50S ribosomal protein L34

Chain 6:



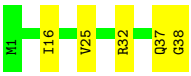
- Molecule 56: 50S ribosomal protein L35

Chain 7:



- Molecule 57: 50S ribosomal protein L36

Chain 8:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	98715	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	1.936	Depositor
Minimum map value	-0.654	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.13	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: PSU, MG, 1MG, UR3, OMC, 5MU, 6MZ, GCP, 5MC, FME, OMU, ZN, 4OC, 7MG, MA6, 4SU, OMG, 2MA, 2MG

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	0.20	0/36354	0.30	0/56707
2	b	0.16	0/1775	0.42	0/2387
3	c	0.15	0/1679	0.32	0/2263
4	d	0.20	0/1636	0.35	0/2189
5	e	0.20	0/1148	0.37	0/1544
6	f	0.18	0/871	0.49	0/1172
7	g	0.14	0/1204	0.32	0/1609
8	h	0.18	0/993	0.34	0/1332
9	i	0.14	0/1022	0.36	0/1365
10	j	0.14	0/803	0.32	0/1083
11	k	0.16	0/895	0.32	0/1209
12	l	0.21	0/973	0.38	0/1303
13	m	0.14	0/901	0.39	0/1209
14	n	0.15	0/812	0.34	0/1082
15	o	0.17	0/710	0.28	0/947
16	p	0.18	0/647	0.36	0/870
17	q	0.17	0/653	0.36	0/881
18	r	0.17	0/488	0.31	0/660
19	s	0.11	0/678	0.31	0/912
20	t	0.18	0/678	0.28	0/904
21	u	0.15	0/513	0.33	0/680
22	v	0.24	0/1725	0.42	3/2689 (0.1%)
23	w	0.19	0/147	0.18	0/227
24	x	0.17	0/4339	0.38	0/5878
25	A	0.31	0/68977	0.36	2/107590 (0.0%)
26	B	0.21	0/2789	0.29	0/4345
27	C	0.26	0/2108	0.37	0/2831
28	D	0.29	0/1611	0.47	1/2167 (0.0%)
29	E	0.23	0/1541	0.32	0/2075
30	F	0.16	0/1424	0.45	1/1913 (0.1%)
31	G	0.19	0/1341	0.32	0/1805

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	H	0.13	0/516	0.31	0/696
33	I	0.10	0/683	0.31	0/937
34	J	0.09	0/672	0.26	0/929
35	L	0.25	0/1156	0.34	0/1559
36	M	0.32	0/947	0.44	0/1268
37	N	0.24	0/1078	0.41	0/1436
38	O	0.27	0/1105	0.35	0/1476
39	P	0.29	0/975	0.41	0/1304
40	Q	0.19	0/888	0.34	0/1183
41	R	0.30	0/911	0.34	0/1218
42	S	0.27	0/946	0.33	0/1257
43	T	0.25	0/835	0.33	0/1117
44	U	0.24	0/837	0.29	0/1114
45	V	0.22	0/749	0.33	0/1002
46	W	0.21	0/794	0.40	0/1062
47	X	0.21	0/1468	0.33	0/1987
48	Y	0.25	0/583	0.37	0/774
49	Z	0.24	0/641	0.33	0/854
50	1	0.19	0/491	0.29	0/654
51	2	0.31	0/449	0.39	0/602
52	3	0.11	0/364	0.36	0/494
53	4	0.24	0/446	0.34	0/594
54	5	0.17	0/433	0.30	0/576
55	6	0.28	0/368	0.37	0/482
56	7	0.25	0/511	0.31	0/668
57	8	0.25	0/308	0.40	0/404
All	All	0.26	0/160589	0.34	7/239475 (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
42	S	0	1
43	T	0	1
All	All	0	3

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	v	75	C	OP2-P-O3'	-12.10	71.71	108.00
22	v	75	C	OP1-P-O3'	9.20	135.60	108.00
25	A	1094	C	OP1-P-O3'	-8.82	81.53	108.00
30	F	106	ILE	N-CA-C	-8.38	105.75	113.71
25	A	1094	C	OP2-P-O3'	-8.16	83.53	108.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	D	151	THR	Peptide
42	S	87	ALA	Peptide
43	T	51	LEU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	32675	0	16461	415	0
2	b	1747	0	1781	44	0
3	c	1650	0	1695	21	0
4	d	1617	0	1650	25	0
5	e	1134	0	1181	16	0
6	f	857	0	836	34	0
7	g	1187	0	1244	32	0
8	h	982	0	1036	23	0
9	i	1010	0	1052	27	0
10	j	793	0	833	19	0
11	k	879	0	896	30	0
12	l	959	0	1009	14	0
13	m	892	0	933	34	0
14	n	800	0	837	24	0
15	o	703	0	727	7	0
16	p	636	0	646	7	0
17	q	645	0	689	12	0
18	r	480	0	488	2	0
19	s	663	0	697	20	0
20	t	671	0	722	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	u	506	0	537	7	0
22	v	1625	0	828	20	0
23	w	131	0	66	0	0
24	x	4288	0	4238	66	0
25	A	61891	0	31144	454	0
26	B	2495	0	1263	12	0
27	C	2072	0	2152	22	0
28	D	1588	0	1603	20	0
29	E	1521	0	1581	20	0
30	F	1403	0	1466	54	0
31	G	1323	0	1386	19	0
32	H	513	0	514	1	0
33	I	682	0	535	12	0
34	J	673	0	357	4	0
35	L	1130	0	1160	12	0
36	M	938	0	1012	16	0
37	N	1066	0	1112	5	0
38	O	1085	0	1157	20	0
39	P	959	0	1005	17	0
40	Q	881	0	920	13	0
41	R	902	0	960	8	0
42	S	936	0	1025	6	0
43	T	822	0	858	6	0
44	U	833	0	897	6	0
45	V	739	0	788	3	0
46	W	786	0	836	10	0
47	X	1445	0	1486	14	0
48	Y	575	0	598	6	0
49	Z	630	0	653	9	0
50	1	490	0	520	2	0
51	2	445	0	472	8	0
52	3	356	0	342	9	0
53	4	440	0	437	8	0
54	5	426	0	457	2	0
55	6	365	0	409	5	0
56	7	506	0	569	7	0
57	8	307	0	342	3	0
58	4	3	0	0	0	0
58	6	2	0	0	0	0
58	7	2	0	0	0	0
58	A	549	0	0	0	0
58	B	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	C	5	0	0	0	0
58	D	1	0	0	0	0
58	E	5	0	0	0	0
58	N	2	0	0	0	0
58	P	1	0	0	0	0
58	Y	1	0	0	0	0
58	a	213	0	0	0	0
58	e	2	0	0	0	0
58	t	2	0	0	0	0
58	x	1	0	0	0	0
59	v	10	0	10	0	0
60	x	32	0	14	2	0
61	3	1	0	0	0	0
61	8	1	0	0	0	0
62	4	3	0	0	0	0
62	6	1	0	0	0	0
62	A	253	0	0	2	0
62	B	6	0	0	0	0
62	C	3	0	0	0	0
62	D	1	0	0	0	0
62	E	1	0	0	0	0
62	V	1	0	0	0	0
62	a	82	0	0	0	0
62	w	1	0	0	0	0
All	All	149945	0	101122	1555	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

The worst 5 of 1555 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:A:2106:A:H61	25:A:2155:G:N2	1.46	1.13
25:A:2106:A:N6	25:A:2155:G:H21	1.54	1.05
1:a:1020:G:H1	1:a:1029:A:N6	1.56	1.03
1:a:1020:G:H1	1:a:1029:A:H61	1.01	0.97
25:A:1083:G:H21	25:A:1088:A:H62	1.17	0.90

There are no symmetry-related clashes.

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%)	204 (92%)	16 (7%)	2 (1%)	14 30
3	c	206/228 (90%)	191 (93%)	15 (7%)	0	100 100
4	d	203/206 (98%)	174 (86%)	29 (14%)	0	100 100
5	e	152/166 (92%)	142 (93%)	10 (7%)	0	100 100
6	f	104/139 (75%)	92 (88%)	9 (9%)	3 (3%)	3 6
7	g	150/156 (96%)	145 (97%)	4 (3%)	1 (1%)	18 38
8	h	127/130 (98%)	118 (93%)	9 (7%)	0	100 100
9	i	125/130 (96%)	108 (86%)	16 (13%)	1 (1%)	16 34
10	j	97/103 (94%)	91 (94%)	6 (6%)	0	100 100
11	k	117/129 (91%)	111 (95%)	6 (5%)	0	100 100
12	l	120/123 (98%)	112 (93%)	8 (7%)	0	100 100
13	m	112/118 (95%)	96 (86%)	16 (14%)	0	100 100
14	n	98/101 (97%)	90 (92%)	8 (8%)	0	100 100
15	o	86/89 (97%)	84 (98%)	2 (2%)	0	100 100
16	p	79/83 (95%)	75 (95%)	4 (5%)	0	100 100
17	q	78/88 (89%)	77 (99%)	1 (1%)	0	100 100
18	r	60/76 (79%)	53 (88%)	6 (10%)	1 (2%)	7 15
19	s	81/91 (89%)	76 (94%)	5 (6%)	0	100 100
20	t	85/91 (93%)	84 (99%)	1 (1%)	0	100 100
21	u	60/71 (84%)	56 (93%)	4 (7%)	0	100 100
24	x	591/840 (70%)	543 (92%)	45 (8%)	3 (0%)	24 46
27	C	270/273 (99%)	252 (93%)	18 (7%)	0	100 100
28	D	209/211 (99%)	187 (90%)	20 (10%)	2 (1%)	12 28
29	E	198/200 (99%)	189 (96%)	8 (4%)	1 (0%)	24 46
30	F	174/179 (97%)	147 (84%)	24 (14%)	3 (2%)	7 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	G	173/177 (98%)	162 (94%)	11 (6%)	0	100	100
32	H	70/148 (47%)	65 (93%)	5 (7%)	0	100	100
33	I	116/166 (70%)	93 (80%)	22 (19%)	1 (1%)	14	30
34	J	132/143 (92%)	114 (86%)	18 (14%)	0	100	100
35	L	140/142 (99%)	135 (96%)	5 (4%)	0	100	100
36	M	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
37	N	142/144 (99%)	125 (88%)	17 (12%)	0	100	100
38	O	135/137 (98%)	130 (96%)	5 (4%)	0	100	100
39	P	118/129 (92%)	113 (96%)	5 (4%)	0	100	100
40	Q	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
41	R	112/116 (97%)	106 (95%)	6 (5%)	0	100	100
42	S	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
43	T	101/103 (98%)	99 (98%)	1 (1%)	1 (1%)	12	28
44	U	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
45	V	92/99 (93%)	89 (97%)	3 (3%)	0	100	100
46	W	101/104 (97%)	92 (91%)	8 (8%)	1 (1%)	12	28
47	X	188/204 (92%)	180 (96%)	8 (4%)	0	100	100
48	Y	74/85 (87%)	72 (97%)	2 (3%)	0	100	100
49	Z	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
50	1	59/63 (94%)	58 (98%)	1 (2%)	0	100	100
51	2	55/58 (95%)	55 (100%)	0	0	100	100
52	3	45/71 (63%)	39 (87%)	5 (11%)	1 (2%)	5	10
53	4	53/60 (88%)	52 (98%)	1 (2%)	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%)	5968 (93%)	440 (7%)	21 (0%)	37	58

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	f	85	ILE

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Mol	Chain	Res	Type
6	f	102	MET
24	x	486	ALA
24	x	635	GLU
28	D	152	PRO

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	183/202 (91%)	183 (100%)	0	100	100
3	c	169/187 (90%)	169 (100%)	0	100	100
4	d	171/174 (98%)	171 (100%)	0	100	100
5	e	113/124 (91%)	113 (100%)	0	100	100
6	f	88/119 (74%)	88 (100%)	0	100	100
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%)	104 (100%)	0	100	100
10	j	88/92 (96%)	88 (100%)	0	100	100
11	k	90/98 (92%)	90 (100%)	0	100	100
12	l	106/107 (99%)	106 (100%)	0	100	100
13	m	95/99 (96%)	95 (100%)	0	100	100
14	n	80/82 (98%)	80 (100%)	0	100	100
15	o	74/75 (99%)	74 (100%)	0	100	100
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%)	72 (100%)	0	100	100
20	t	69/70 (99%)	69 (100%)	0	100	100
21	u	51/60 (85%)	51 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	x	419/668 (63%)	419 (100%)	0	100	100
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%)	157 (100%)	0	100	100
30	F	149/153 (97%)	149 (100%)	0	100	100
31	G	138/141 (98%)	138 (100%)	0	100	100
32	H	44/107 (41%)	44 (100%)	0	100	100
33	I	29/122 (24%)	29 (100%)	0	100	100
34	J	4/110 (4%)	4 (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%)	68	86
42	S	87/88 (99%)	87 (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%)	66 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
57	8	34/34 (100%)	34 (100%)	0	100	100
All	All	5058/5785 (87%)	5057 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	R	66	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
44	U	23	GLN
45	V	87	GLN
51	2	33	HIS
12	l	112	GLN
12	l	77	HIS

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1520/1536 (98%)	267 (17%)	0
22	v	75/77 (97%)	21 (28%)	0
23	w	5/24 (20%)	0	0
25	A	2881/2891 (99%)	545 (18%)	47 (1%)
26	B	116/120 (96%)	18 (15%)	2 (1%)
All	All	4597/4648 (98%)	851 (18%)	49 (1%)

5 of 851 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	C
1	a	5	U
1	a	6	G
1	a	7	A
1	a	9	G

5 of 49 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	1574	U
25	A	2029	A
25	A	1627	A
25	A	1741	A
25	A	2228	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	$\#\|Z\| > 2$
1	4OC	a	1396	58,1	20,23,24	0.74	0	25,32,35	0.92	1 (4%)
22	PSU	v	55	22	18,21,22	1.35	2 (11%)	21,30,33	1.99	3 (14%)
1	MA6	a	1513	1	23,26,27	1.45	5 (21%)	33,38,41	2.41	14 (42%)
25	1MG	A	735	25	23,26,27	1.11	3 (13%)	33,39,42	1.70	5 (15%)
22	4SU	v	8	22	18,21,22	1.96	4 (22%)	25,30,33	1.86	5 (20%)
25	7MG	A	2056	25	23,26,27	1.37	4 (17%)	27,39,42	2.67	7 (25%)
25	2MA	A	2490	58,25	22,25,26	1.44	6 (27%)	32,37,40	2.33	9 (28%)
25	2MG	A	1822	25	23,26,27	1.28	3 (13%)	33,38,41	2.21	6 (18%)
25	5MC	A	1949	25	19,22,23	1.45	3 (15%)	26,32,35	1.11	2 (7%)
1	7MG	a	521	1	23,26,27	1.32	3 (13%)	27,39,42	2.63	7 (25%)
25	6MZ	A	2017	25	22,25,26	1.81	6 (27%)	29,36,39	3.53	10 (34%)
1	2MG	a	1201	1	23,26,27	1.28	4 (17%)	33,38,41	2.20	7 (21%)
25	2MG	A	2432	58,25	23,26,27	1.32	5 (21%)	33,38,41	2.24	7 (21%)
25	OMC	A	2485	58,25	19,22,23	0.82	0	25,31,34	1.02	1 (4%)
25	6MZ	A	1608	25	22,25,26	1.82	6 (27%)	29,36,39	3.45	10 (34%)
1	5MC	a	961	1	19,22,23	1.42	3 (15%)	26,32,35	1.13	2 (7%)
25	OMG	A	2238	25	23,26,27	1.26	3 (13%)	32,38,41	1.95	5 (15%)
22	5MU	v	54	22	19,22,23	1.41	6 (31%)	27,32,35	2.05	5 (18%)
25	OMU	A	2539	25	19,22,23	1.32	3 (15%)	25,31,34	1.88	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	MA6	a	1512	1	23,26,27	1.46	4 (17%)	33,38,41	2.43	13 (39%)
1	2MG	a	1510	1	23,26,27	1.25	3 (13%)	33,38,41	2.21	6 (18%)
1	UR3	a	1492	1	19,22,23	0.92	1 (5%)	26,32,35	1.77	3 (11%)
22	5MC	v	32	22	19,22,23	1.43	3 (15%)	26,32,35	1.28	3 (11%)
1	2MG	a	960	1	23,26,27	1.27	3 (13%)	33,38,41	2.17	6 (18%)
25	UR3	A	1902	25	19,22,23	0.99	1 (5%)	26,32,35	1.73	3 (11%)
25	5MU	A	1926	58,25	19,22,23	1.40	4 (21%)	27,32,35	2.20	6 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	4OC	a	1396	58,1	-	0/9/29/30	0/2/2/2
22	PSU	v	55	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1513	1	-	4/11/29/30	0/3/3/3
25	1MG	A	735	25	-	0/7/25/26	0/3/3/3
22	4SU	v	8	22	-	1/7/25/26	0/2/2/2
25	7MG	A	2056	25	-	2/7/37/38	0/3/3/3
25	2MA	A	2490	58,25	-	1/7/25/26	0/3/3/3
25	2MG	A	1822	25	-	0/9/27/28	0/3/3/3
25	5MC	A	1949	25	-	0/7/25/26	0/2/2/2
1	7MG	a	521	1	-	1/7/37/38	0/3/3/3
25	6MZ	A	2017	25	-	2/9/27/28	0/3/3/3
1	2MG	a	1201	1	-	3/9/27/28	0/3/3/3
25	2MG	A	2432	58,25	-	1/9/27/28	0/3/3/3
25	OMC	A	2485	58,25	-	1/9/27/28	0/2/2/2
25	6MZ	A	1608	25	-	0/9/27/28	0/3/3/3
1	5MC	a	961	1	-	0/7/25/26	0/2/2/2
25	OMG	A	2238	25	-	2/9/27/28	0/3/3/3
22	5MU	v	54	22	-	0/7/25/26	0/2/2/2
25	OMU	A	2539	25	-	0/9/27/28	0/2/2/2
1	MA6	a	1512	1	-	2/11/29/30	0/3/3/3
1	2MG	a	1510	1	-	0/9/27/28	0/3/3/3
1	UR3	a	1492	1	-	0/7/25/26	0/2/2/2
22	5MC	v	32	22	-	0/7/25/26	0/2/2/2
1	2MG	a	960	1	-	0/9/27/28	0/3/3/3
25	UR3	A	1902	25	-	0/7/25/26	0/2/2/2
25	5MU	A	1926	58,25	-	0/7/25/26	0/2/2/2

The worst 5 of 88 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1608	6MZ	C6-N6	5.22	1.40	1.34
25	A	2017	6MZ	C6-N6	5.09	1.40	1.34
25	A	1949	5MC	C5-C4	5.08	1.48	1.44
22	v	8	4SU	C4-S4	-5.03	1.59	1.68
1	a	961	5MC	C5-C4	4.84	1.47	1.44

The worst 5 of 150 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2017	6MZ	C9-N6-C6	-15.30	108.66	122.85
25	A	1608	6MZ	C9-N6-C6	-14.63	109.29	122.85
1	a	521	7MG	N9-C4-N3	8.98	138.62	125.46
25	A	2056	7MG	N9-C4-N3	8.91	138.52	125.46
25	A	2490	2MA	C5-C4-N3	-8.22	118.52	127.18

There are no chirality outliers.

5 of 20 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1513	MA6	C5-C6-N6-C9
25	A	2238	OMG	O4'-C4'-C5'-O5'
25	A	2056	7MG	O4'-C4'-C5'-O5'
1	a	1201	2MG	O4'-C4'-C5'-O5'
1	a	1201	2MG	C3'-C4'-C5'-O5'

There are no ring outliers.

11 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1396	4OC	1	0
1	a	1513	MA6	3	0
22	v	8	4SU	2	0
25	A	2017	6MZ	1	0
25	A	2485	OMC	1	0
1	a	961	5MC	1	0
25	A	2238	OMG	1	0
1	a	1512	MA6	2	0
1	a	1510	2MG	1	0
1	a	960	2MG	1	0
25	A	1926	5MU	2	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 800 ligands modelled in this entry, 798 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
60	GCP	x	902	58	32,34,34	1.40	5 (15%)	49,54,54	1.76	8 (16%)
59	FME	v	101	22	8,9,10	0.43	0	8,9,11	1.20	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
60	GCP	x	902	58	-	0/19/38/38	0/3/3/3
59	FME	v	101	22	-	2/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
60	x	902	GCP	C5-C4	2.90	1.46	1.38
60	x	902	GCP	PG-O2G	2.79	1.61	1.55
60	x	902	GCP	C6-N1	-2.72	1.33	1.38
60	x	902	GCP	PG-O3G	2.70	1.61	1.55
60	x	902	GCP	C5-N7	-2.22	1.34	1.39

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	x	902	GCP	C5-C4-N3	-5.99	118.85	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
60	x	902	GCP	C2-N3-C4	4.96	120.84	112.30
60	x	902	GCP	N9-C4-N3	4.49	134.94	125.95
60	x	902	GCP	C6-C5-N7	3.31	136.32	130.29
60	x	902	GCP	PB-O3A-PA	-2.92	122.83	132.37

There are no chirality outliers.

All (2) torsion outliers are listed below:

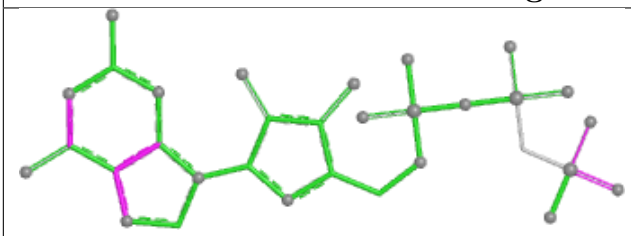
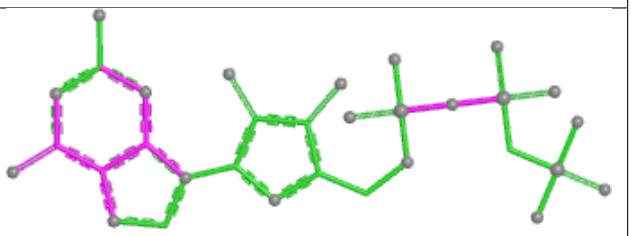
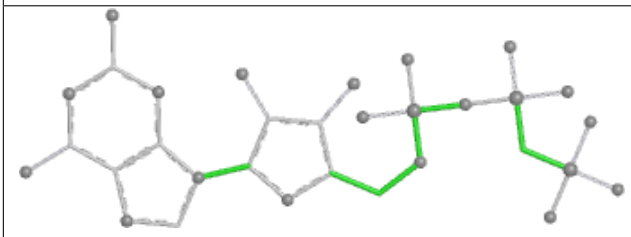
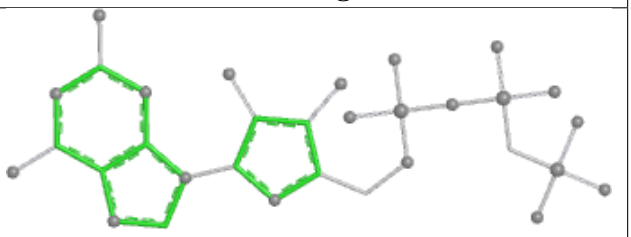
Mol	Chain	Res	Type	Atoms
59	v	101	FME	N-CA-CB-CG
59	v	101	FME	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	x	902	GCP	2	0

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	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

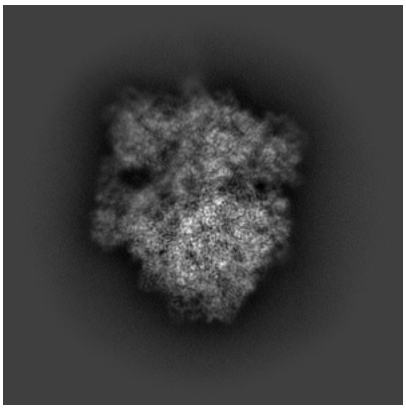
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-26635. 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



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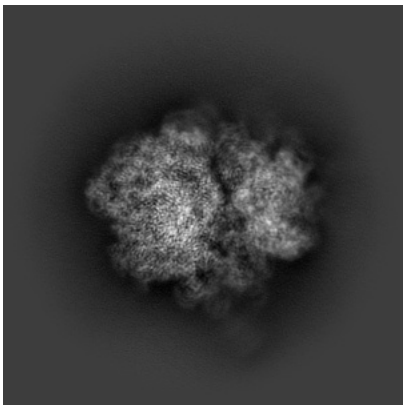

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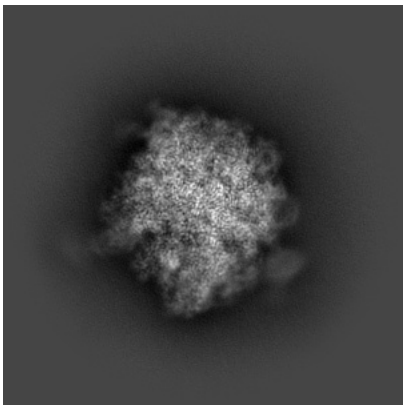
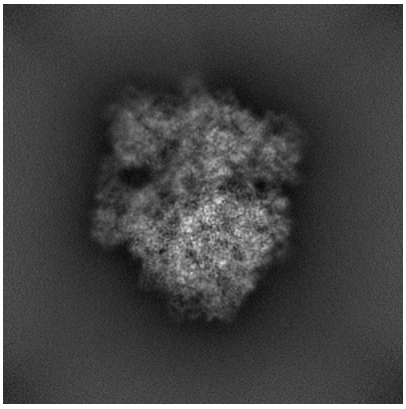


Z

6.1.2 Raw map



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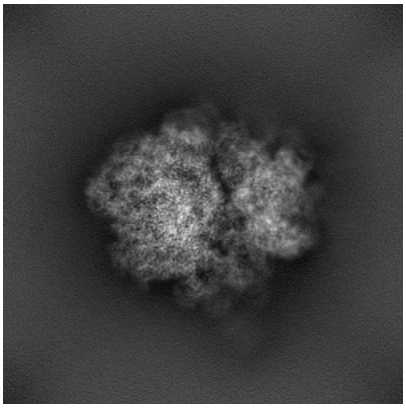

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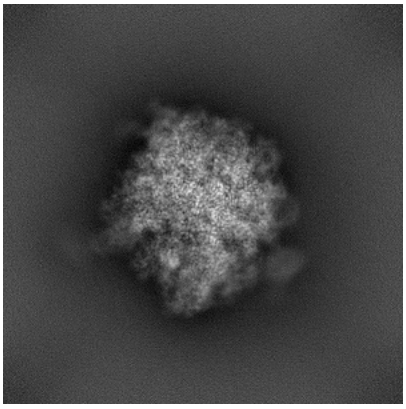
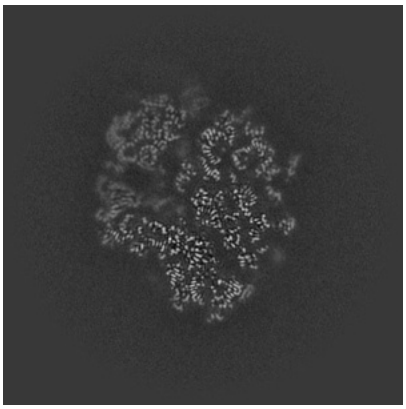


Z

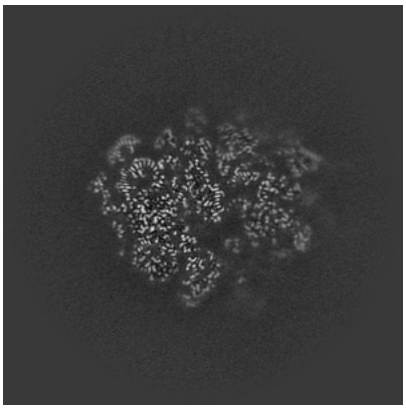
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 256



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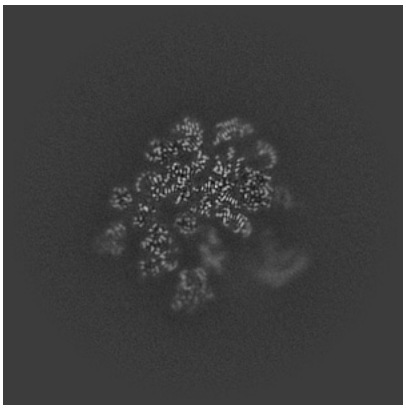
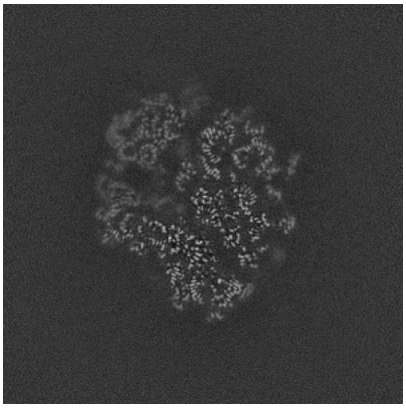
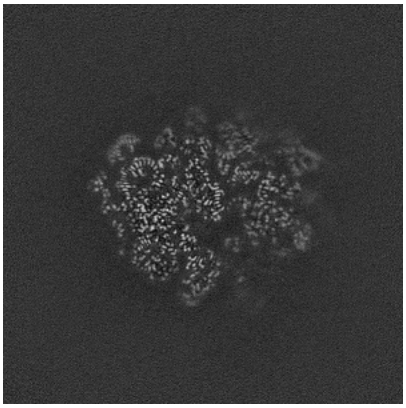


Z Index: 256

6.2.2 Raw map



X Index: 256



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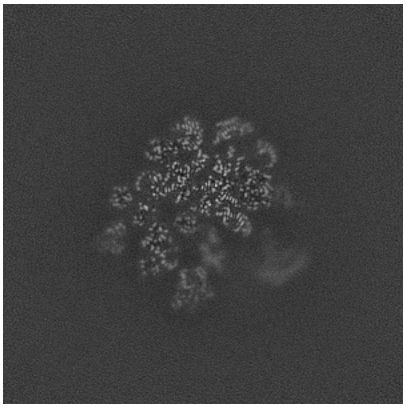
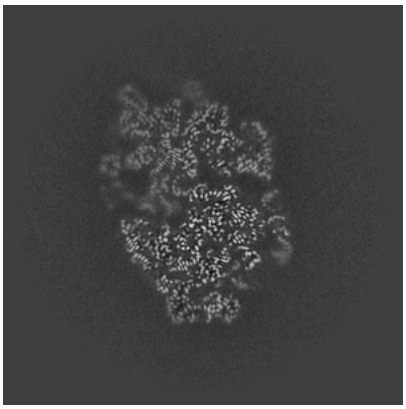


Z Index: 256

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

6.3 Largest variance slices (i)

6.3.1 Primary map



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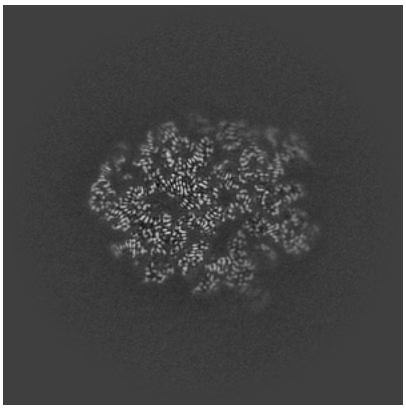
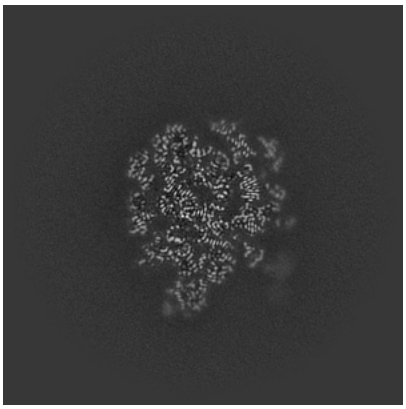
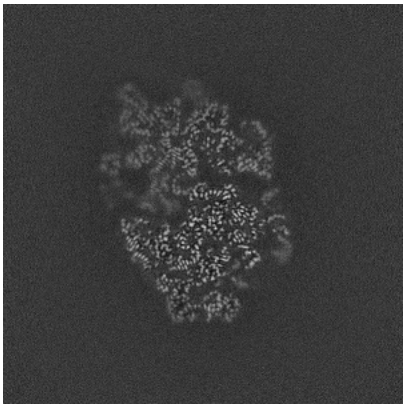


Y Index: 270

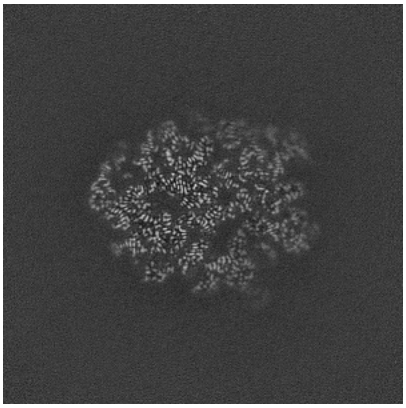


Z Index: 211

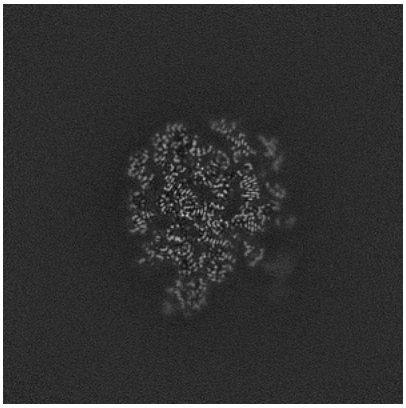
6.3.2 Raw map



X Index: 270



Y Index: 270

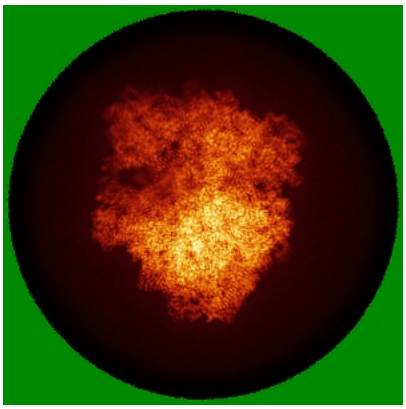


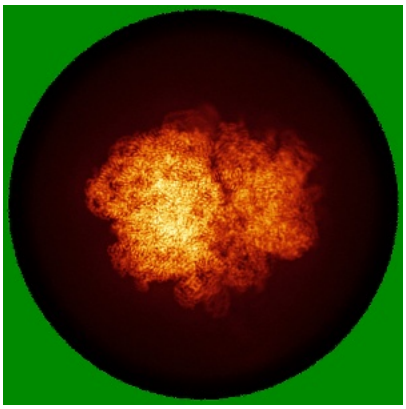
Z Index: 211

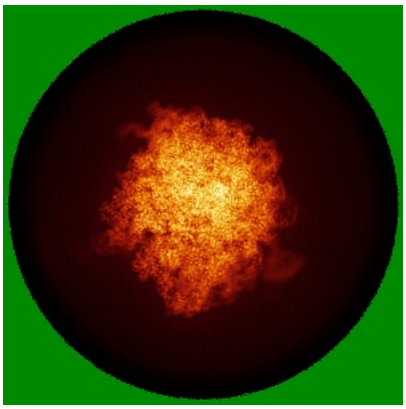
The images above show the largest variance slices of the map in three orthogonal directions.

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

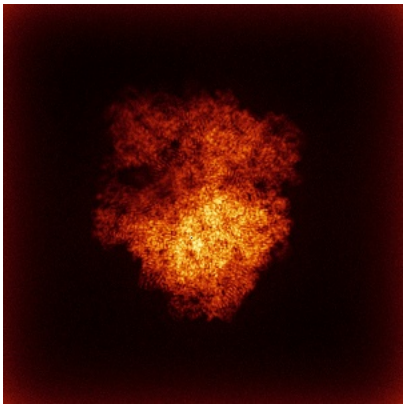
6.4.1 Primary map

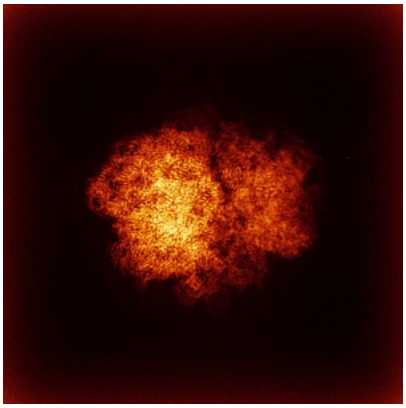

X

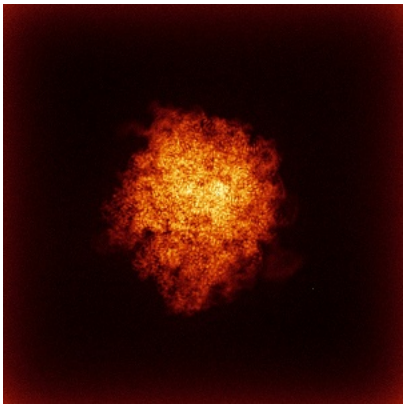

Y


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 0.13. 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.

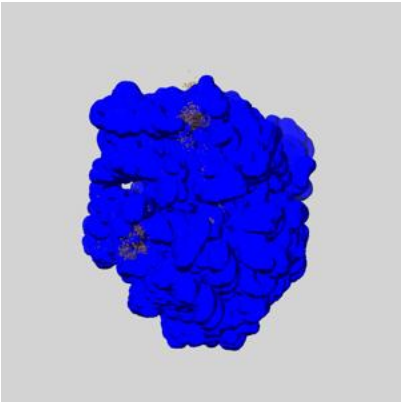
6.6 Mask visualisation (i)

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

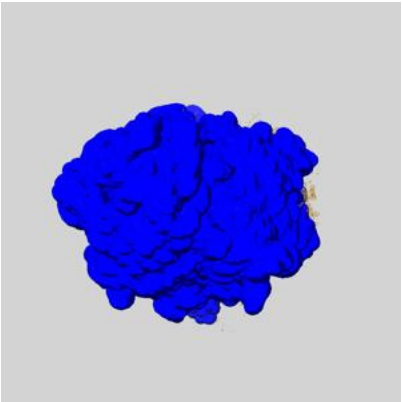
A mask typically either:

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

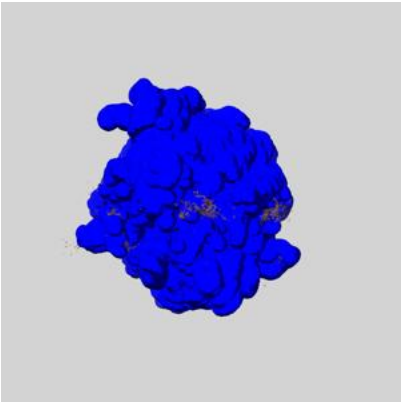
6.6.1 emd_26635_msk_1.map (i)



X



Y

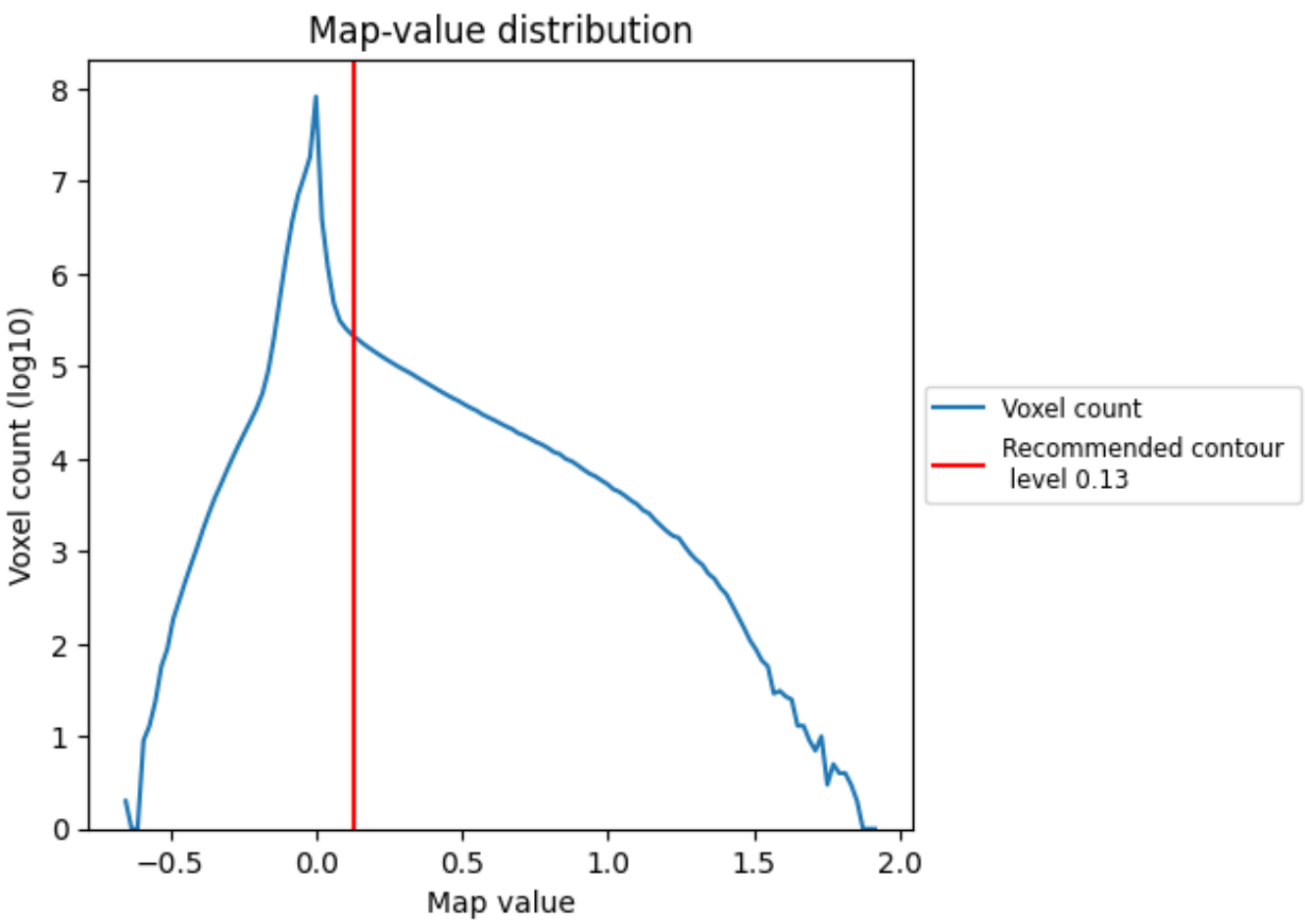


Z

7 Map analysis (i)

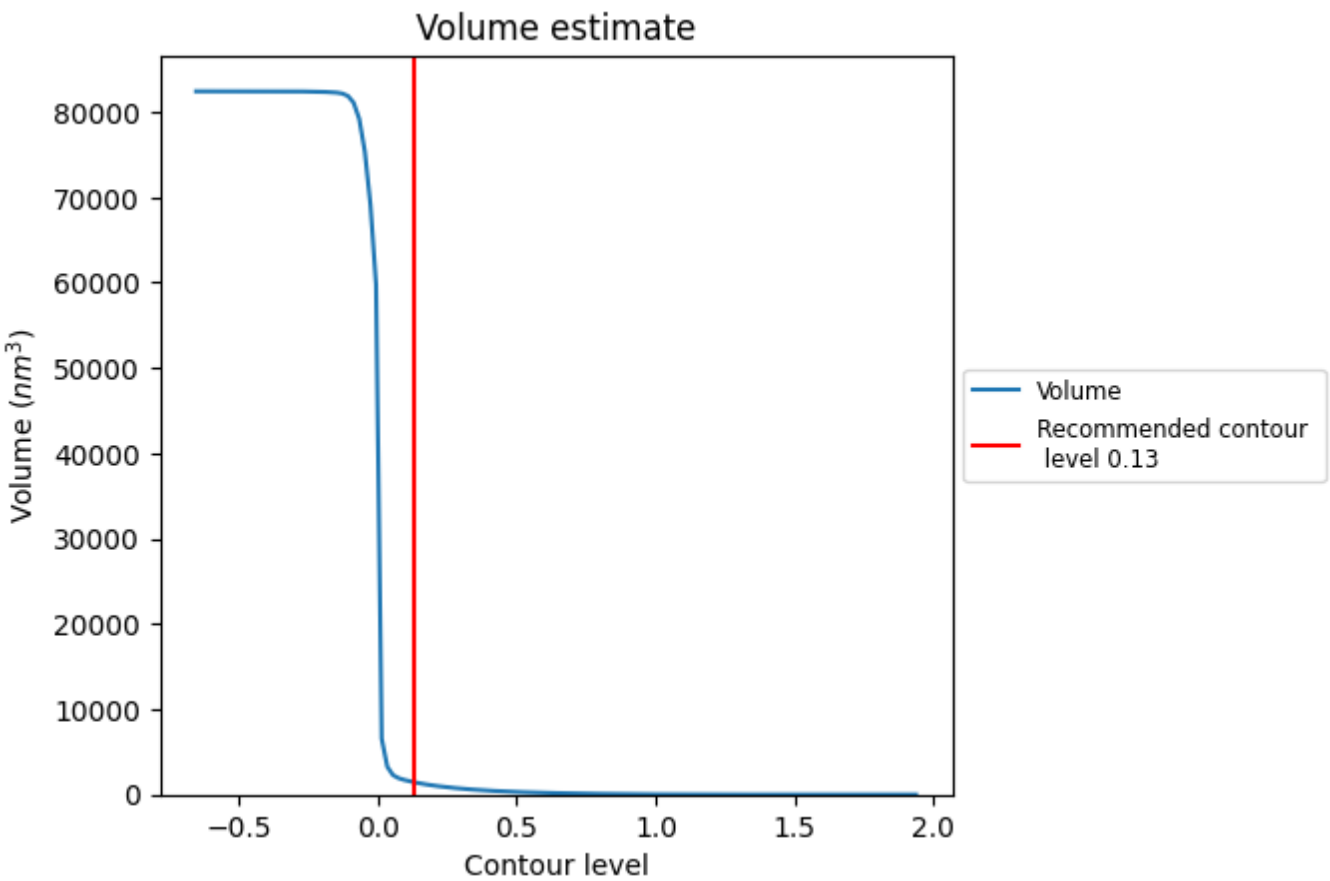
This section contains the results of statistical analysis of the map.

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.

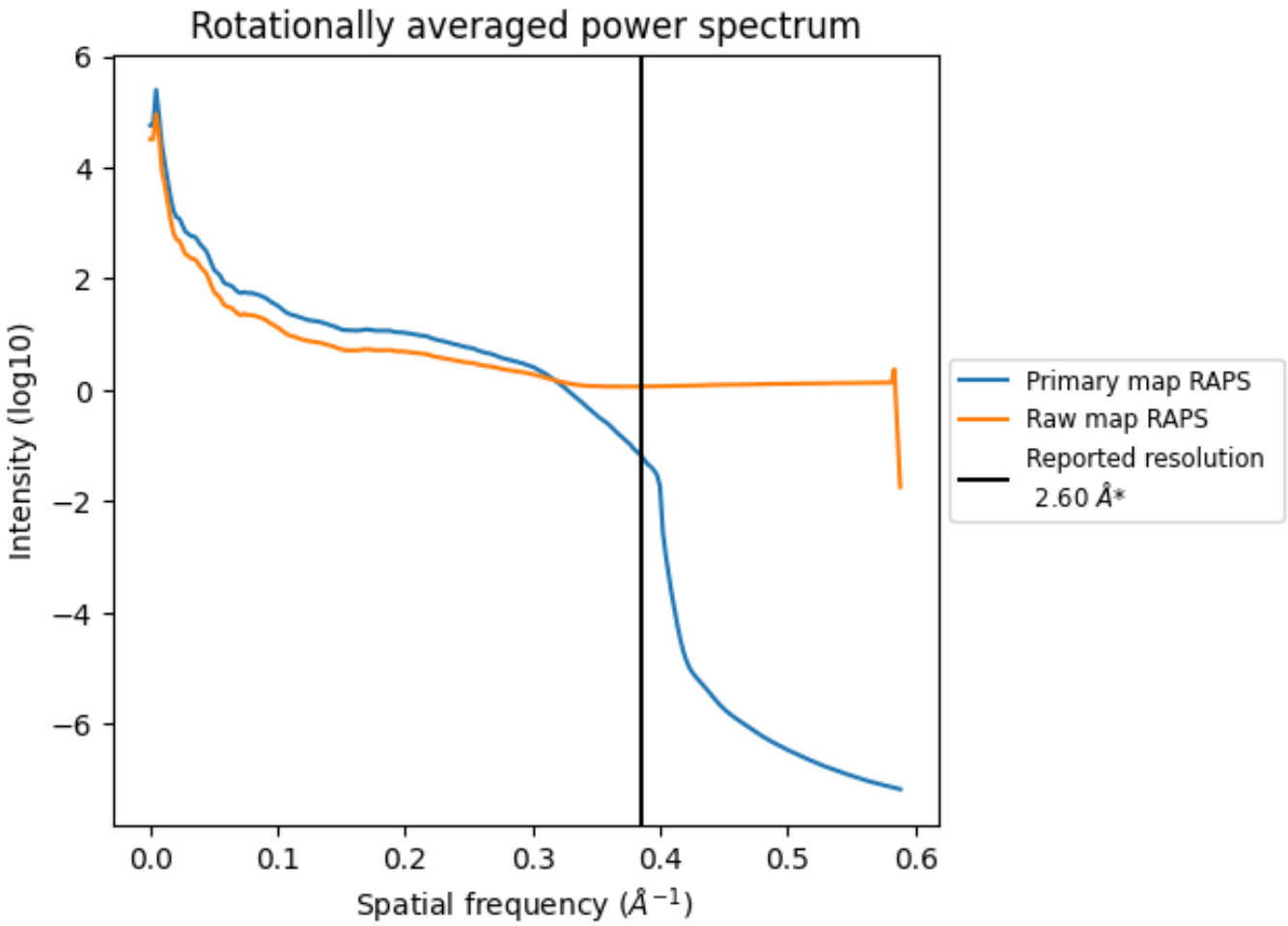
7.2 Volume estimate (i)



The volume at the recommended contour level is 1450 nm^3; this corresponds to an approximate mass of 1310 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)

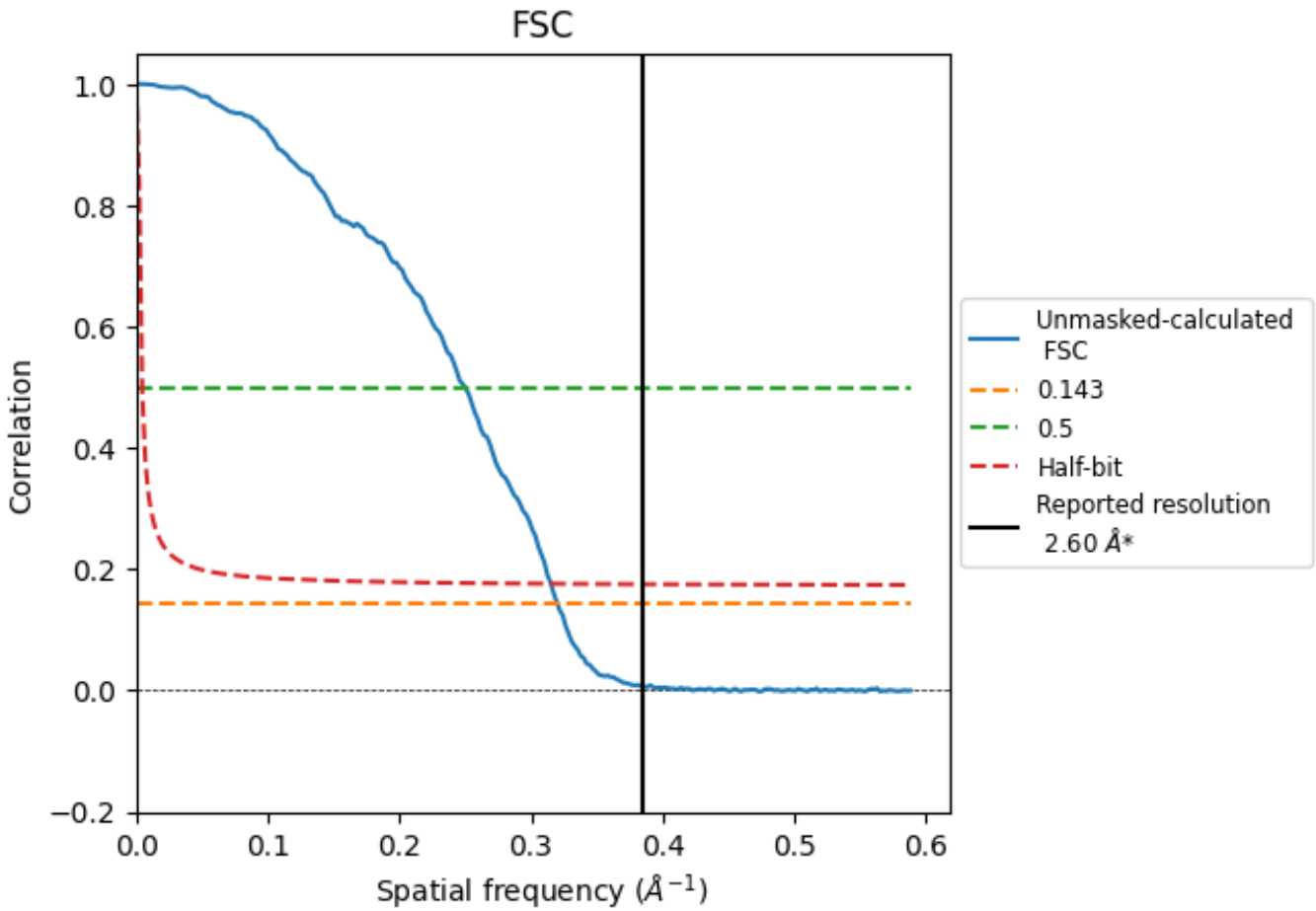


*Reported resolution corresponds to spatial frequency of 0.385 Å^{-1}

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 0.385 Å^{-1}

8.2 Resolution estimates (i)

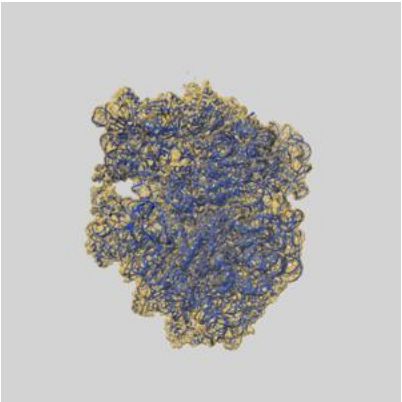
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.12	4.00	3.17

*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 3.12 differs from the reported value 2.6 by more than 10 %

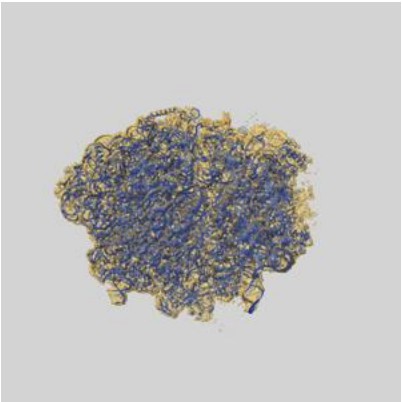
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-26635 and PDB model 7UNW. Per-residue inclusion information can be found in section 3 on page 17.

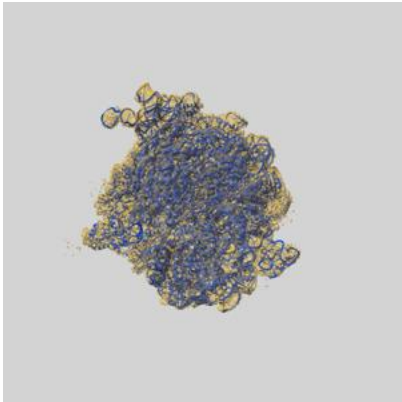
9.1 Map-model overlay (i)



X



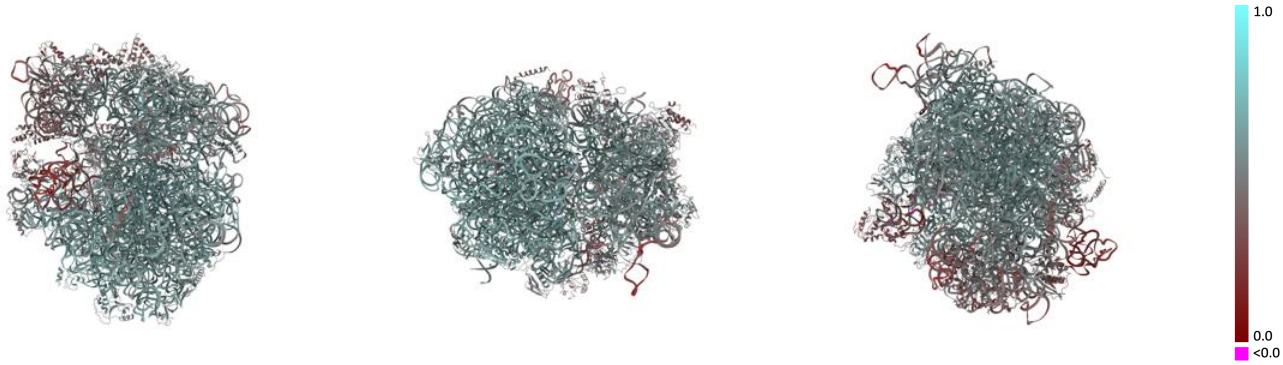
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.13 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.

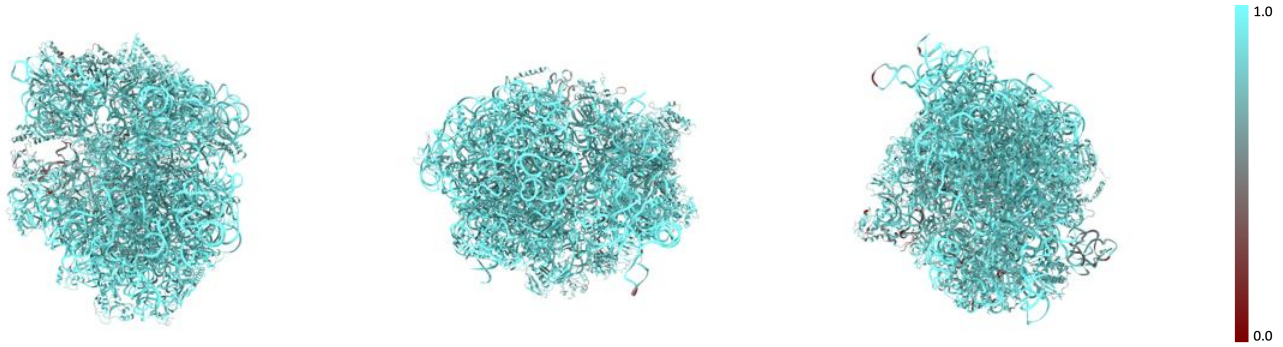
9.2 Q-score mapped to coordinate model (i)



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.

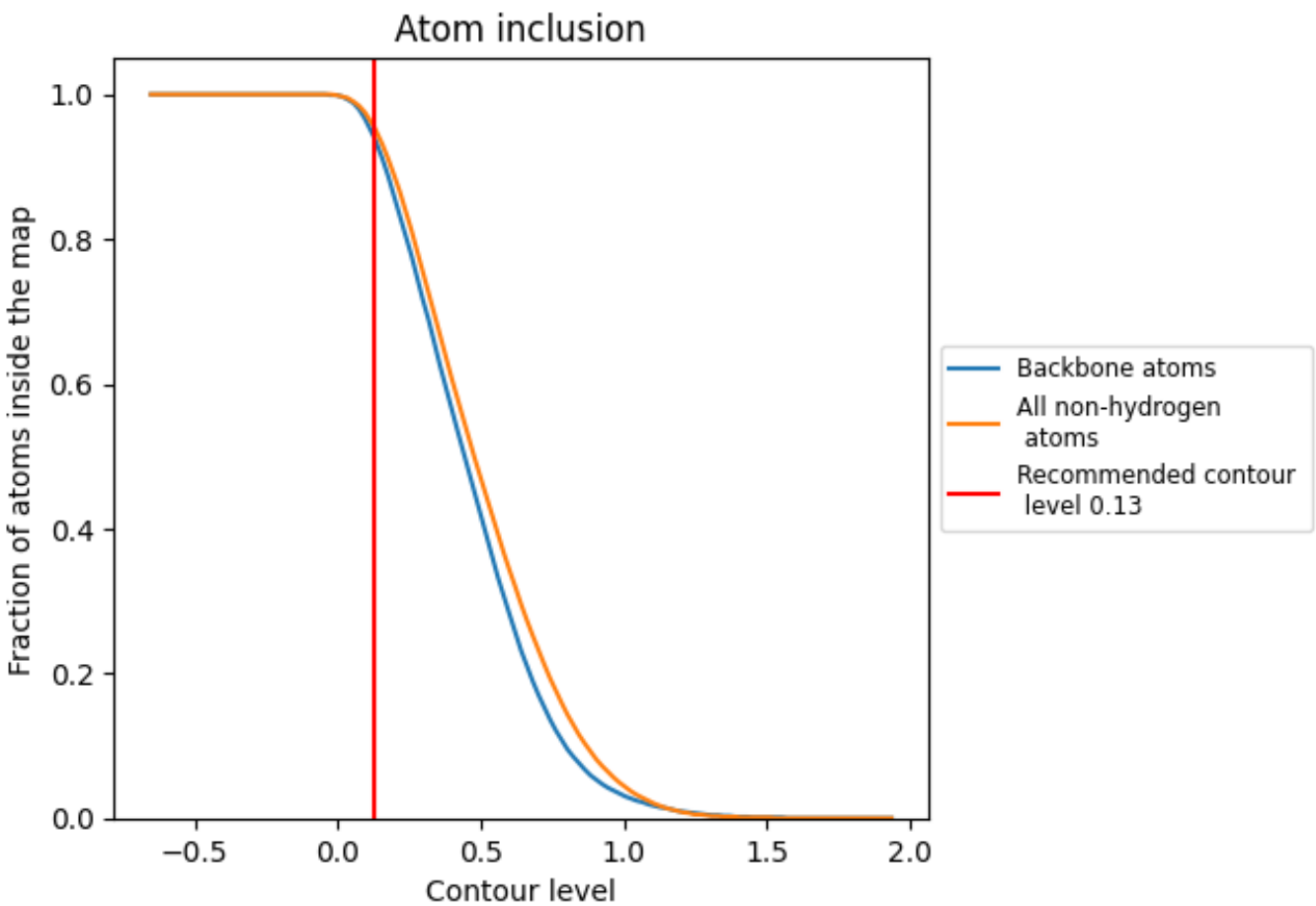
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.13).

9.4 Atom inclusion (i)



At the recommended contour level, 94% 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 (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9530	0.5540
1	0.9400	0.5510
2	0.9650	0.5970
3	0.6260	0.3590
4	0.9530	0.6000
5	0.9160	0.5740
6	0.9770	0.6280
7	0.9740	0.6250
8	0.9660	0.6130
A	0.9820	0.5940
B	0.9930	0.5490
C	0.9670	0.6160
D	0.9520	0.5970
E	0.9550	0.5930
F	0.8470	0.4200
G	0.9210	0.5460
H	0.8300	0.4700
I	0.7570	0.3780
J	0.5910	0.2800
L	0.9700	0.6100
M	0.9450	0.6070
N	0.9580	0.6040
O	0.9620	0.6120
P	0.9740	0.6140
Q	0.9300	0.5380
R	0.9410	0.5960
S	0.9710	0.6140
T	0.9450	0.5910
U	0.9460	0.6010
V	0.9550	0.5890
W	0.9080	0.5380
X	0.9390	0.5660
Y	0.9640	0.6110
Z	0.9500	0.6000
a	0.9850	0.5280

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Chain	Atom inclusion	Q-score
b	0.8260	0.4270
c	0.8690	0.4920
d	0.9050	0.5200
e	0.9340	0.5480
f	0.8420	0.4360
g	0.7780	0.3900
h	0.9130	0.5340
i	0.8450	0.4190
j	0.7810	0.4300
k	0.8720	0.4880
l	0.9220	0.5770
m	0.8220	0.3860
n	0.8630	0.4490
o	0.9240	0.5310
p	0.9510	0.5590
q	0.9250	0.5370
r	0.8590	0.4930
s	0.7900	0.3740
t	0.9380	0.5330
u	0.8190	0.4520
v	0.9110	0.4210
w	0.9620	0.5830
x	0.8620	0.5130