wwPDB EM Validation Summary Report (i)

Sep 16, 2026 – 12:40 PM EDT

PDB ID	:	9PIH / pdb_00009pih
EMDB ID	:	EMD-71667
Title	:	E. coli 70S ribosome bound to Doxycycline
Authors	:	Devarkar, S.C.; Lomakin, I.B.; Bunick, C.G.
Deposited on	:	2025-07-10
Resolution	:	2.40 Å(reported)

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:

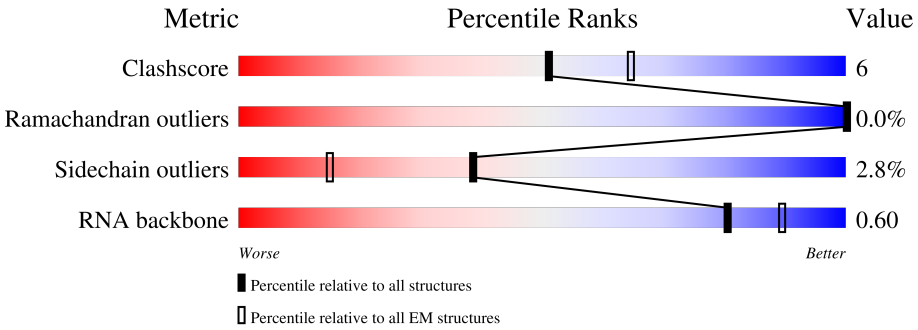
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

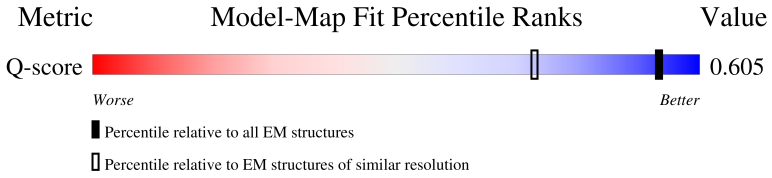
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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.





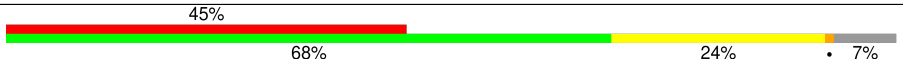
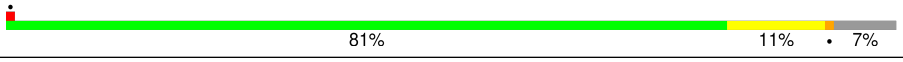
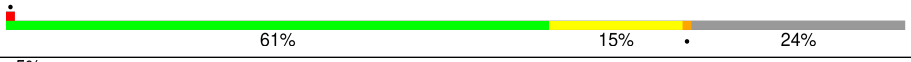
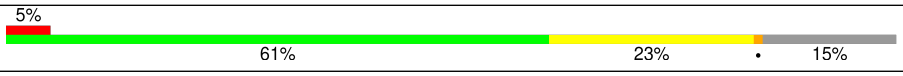
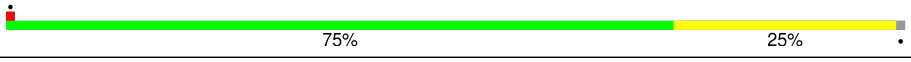
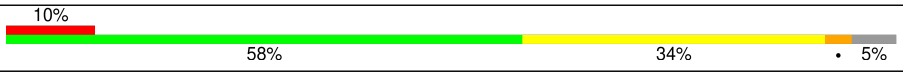
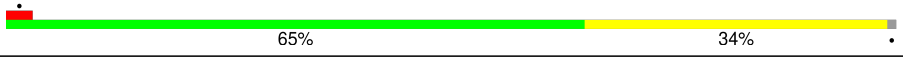
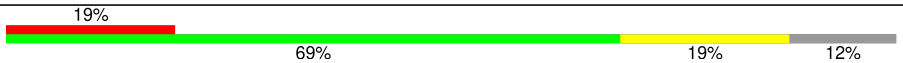
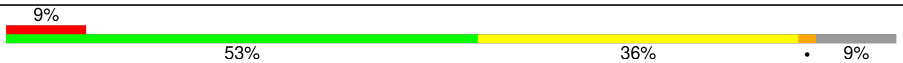
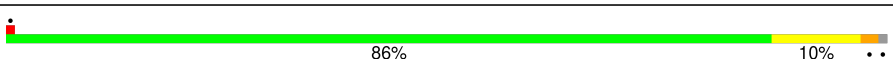
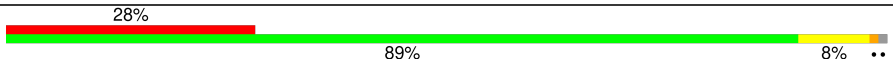
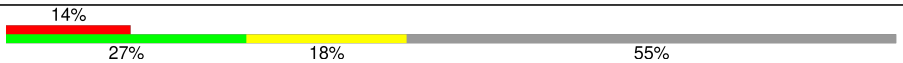
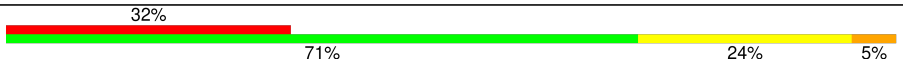
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	0	55	67% 25% 7%
2	1	46	93% 7%
3	2	65	88% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	3	38	
5	4	70	
6	A	1542	
7	B	241	
8	C	233	
9	D	206	
10	E	167	
11	F	135	
12	G	179	
13	H	130	
14	I	130	
15	J	103	
16	K	129	
17	L	124	
18	M	118	
19	N	101	
20	O	89	
21	P	82	
22	Q	84	
23	R	75	
24	S	92	
25	T	87	
26	U	71	
27	X	22	
28	Z	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	a	2904	69% 24% 5%
30	b	120	79% 18%
31	c	273	88% 10%
32	d	209	85% 14%
33	e	201	92% 7%
34	f	179	71% 26%
35	g	177	72% 25%
36	h	149	19% 9% 72%
37	i	142	88% 12%
38	j	123	88% 12%
39	k	144	92% 7%
40	l	136	83% 17%
41	m	127	78% 14% 7%
42	n	117	81% 15%
43	o	115	83% 16%
44	p	118	90% 9%
45	q	103	91% 9%
46	r	110	88% 12%
47	s	100	81% 12% 7%
48	t	104	82% 16%
49	u	94	78% 20%
50	v	85	84% 8% 8%
51	w	78	87% 12%
52	x	63	71% 27%
53	y	59	5% 88% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	z	57	

2 Entry composition (i)

There are 59 unique types of molecules in this entry. The entry contains 141390 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	51	Total	C	N	O	0	0
			417	269	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 6 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1500	Total	C	N	O	P	0	0
			32211	14373	5919	10419	1500		

- Molecule 7 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	153	Total	C	N	O	S	0	0
			1203	750	231	218	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 16 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	K	117	Total	C	N	O	S	0	0
			877	540	174	160	3		

- Molecule 17 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 18 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 21 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 22 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 23 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 24 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 25 is a protein called Small ribosomal subunit protein bS20.

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

- Molecule 26 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 27 is a RNA chain called messenger RNA (mRNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
27	X	10	Total	C	N	O	P	0	0
			211	95	35	71	10		

- Molecule 28 is a RNA chain called P-site tRNA.

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

- Molecule 29 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	2753	Total	C	N	O	P	0	0
			59130	26384	10897	19096	2753		

- Molecule 30 is a RNA chain called 5S ribosomal RNA.

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

- Molecule 31 is a protein called 50S ribosomal protein L2.

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

- Molecule 32 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 33 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 34 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 35 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 36 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 37 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 39 is a protein called Large ribosomal subunit protein uL15.

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

- Molecule 40 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	136	Total	C	N	O	S	0	0
			1075	686	205	178	6		

- Molecule 41 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 42 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 43 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 44 is a protein called 50S ribosomal protein L20.

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

- Molecule 45 is a protein called Ribosomal protein L21.

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

- Molecule 46 is a protein called 50S ribosomal protein L22.

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

- Molecule 47 is a protein called 50S ribosomal protein L23.

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

- Molecule 48 is a protein called 50S ribosomal protein L24.

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

- Molecule 49 is a protein called Large ribosomal subunit protein bL25.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

- Molecule 51 is a protein called 50S ribosomal protein L28.

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

- Molecule 52 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 53 is a protein called 50S ribosomal protein L30.

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

- Molecule 54 is a protein called 50S ribosomal protein L32.

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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	Zn	0
			1	1	

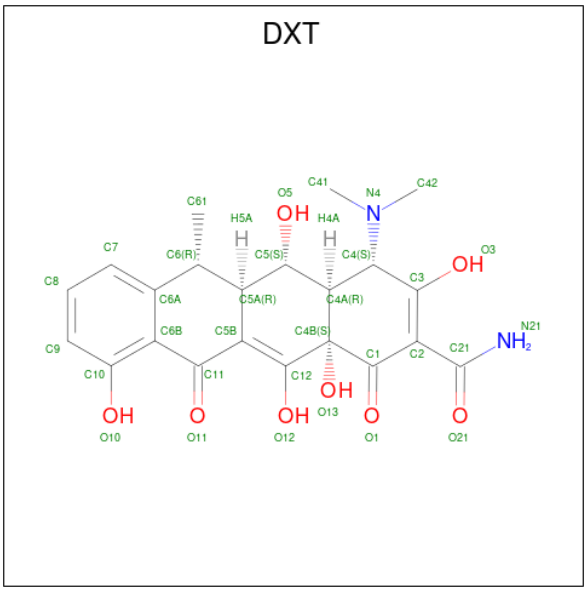
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	A	59	Total Mg 59 59	0
56	a	210	Total Mg 210 210	0
56	b	5	Total Mg 5 5	0
56	p	2	Total Mg 2 2	0

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

Mol	Chain	Residues	Atoms	AltConf
57	A	20	Total K 20 20	0
57	a	71	Total K 71 71	0
57	b	1	Total K 1 1	0

- Molecule 58 is (4S,4AR,5S,5AR,6R,12AS)-4-(DIMETHYLAMINO)-3,5,10,12,12A-PENTAHYDROXY-6-METHYL-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: DXT) (formula: $C_{22}H_{24}N_2O_8$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
58	A	1	Total C N O 32 22 2 8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
58	a	1	Total C N O 32 22 2 8	0
58	a	1	Total C N O 32 22 2 8	0
58	a	1	Total C N O 32 22 2 8	0
58	a	1	Total C N O 32 22 2 8	0
58	r	1	Total C N O 32 22 2 8	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms	AltConf
59	1	4	Total O 4 4	0
59	2	3	Total O 3 3	0
59	3	1	Total O 1 1	0
59	A	88	Total O 88 88	0
59	L	1	Total O 1 1	0
59	T	1	Total O 1 1	0
59	X	1	Total O 1 1	0
59	a	1189	Total O 1189 1189	0
59	b	10	Total O 10 10	0
59	c	6	Total O 6 6	0
59	d	4	Total O 4 4	0
59	e	3	Total O 3 3	0
59	i	1	Total O 1 1	0
59	j	1	Total O 1 1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
59	k	4	Total O 4 4	0
59	l	1	Total O 1 1	0
59	m	2	Total O 2 2	0
59	p	4	Total O 4 4	0
59	q	3	Total O 3 3	0
59	r	3	Total O 3 3	0
59	s	1	Total O 1 1	0
59	u	1	Total O 1 1	0
59	w	1	Total O 1 1	0
59	z	2	Total O 2 2	0

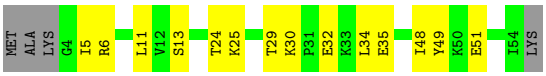
3 Residue-property plots (i)

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

• Molecule 1: 50S ribosomal protein L33

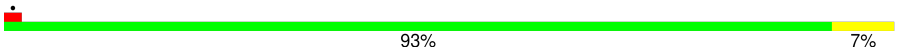
Chain 0:

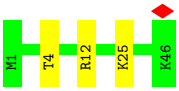




• Molecule 2: 50S ribosomal protein L34

Chain 1:

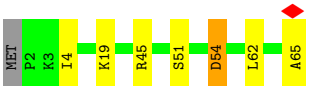




• Molecule 3: 50S ribosomal protein L35

Chain 2:

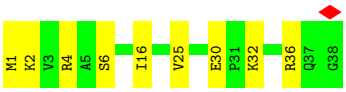




• Molecule 4: 50S ribosomal protein L36

Chain 3:

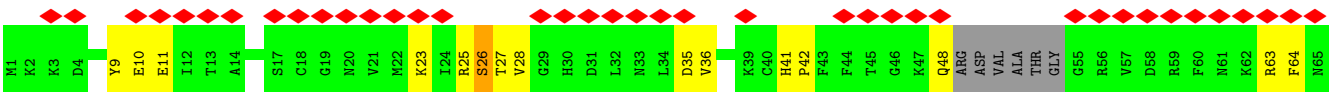




• Molecule 5: 50S ribosomal protein L31

Chain 4:



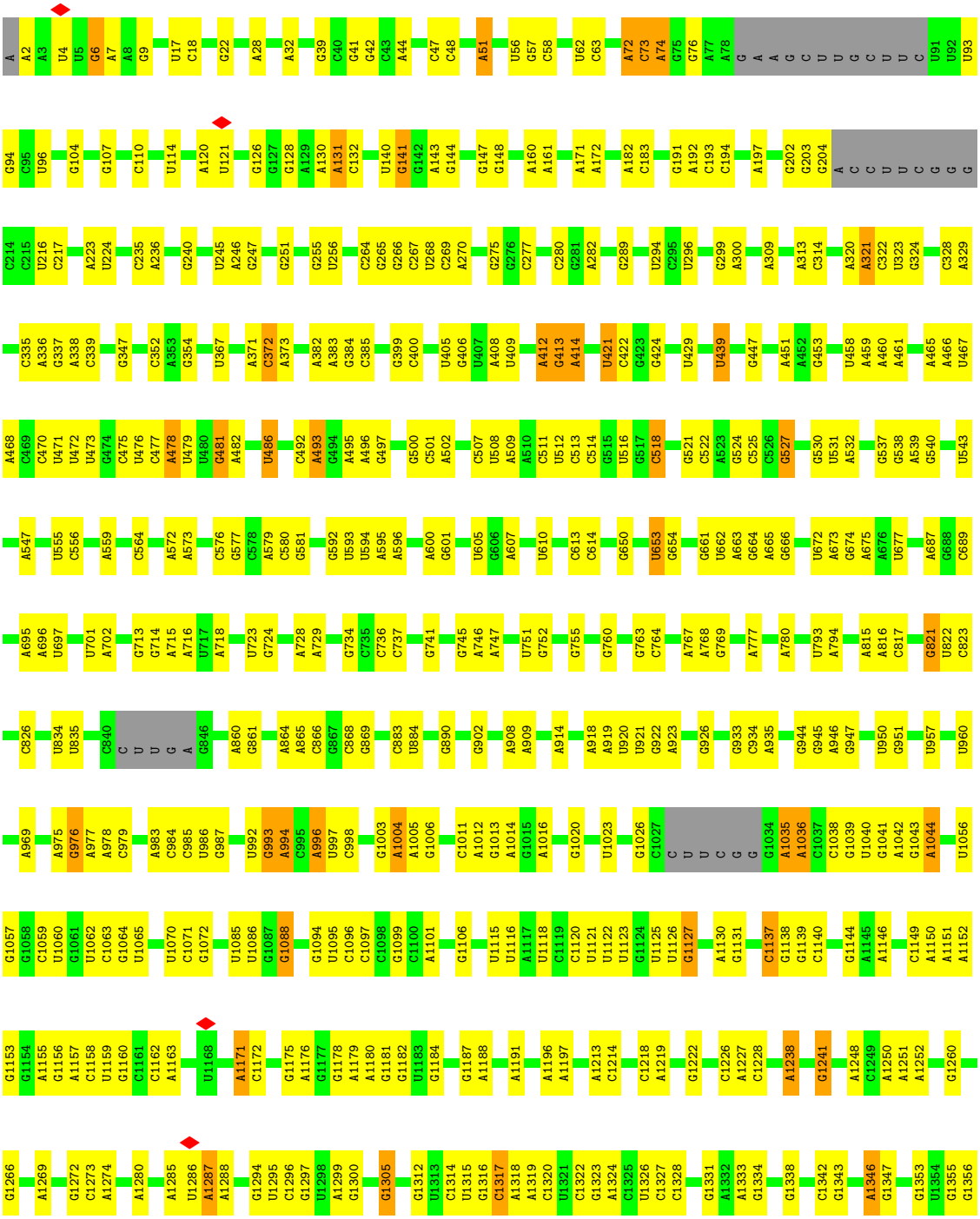


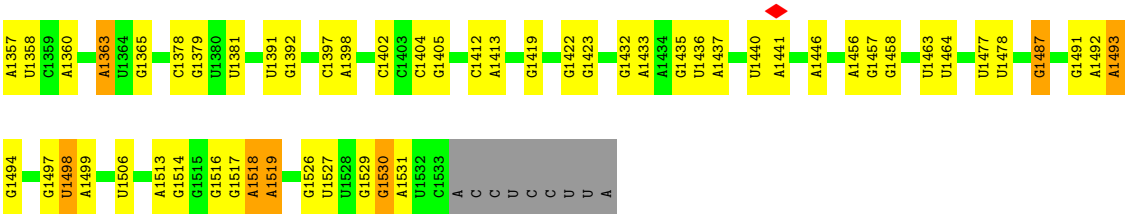


• Molecule 6: 16S ribosomal RNA

Chain A:



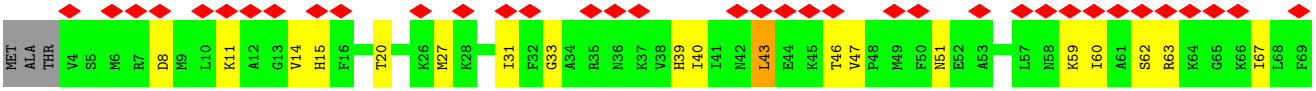


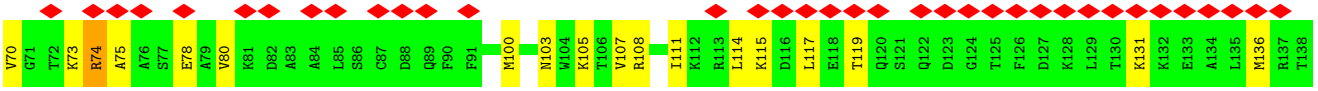


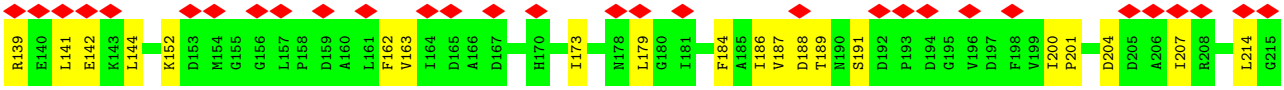
• Molecule 7: 30S ribosomal protein S2

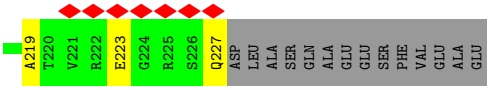
Chain B:







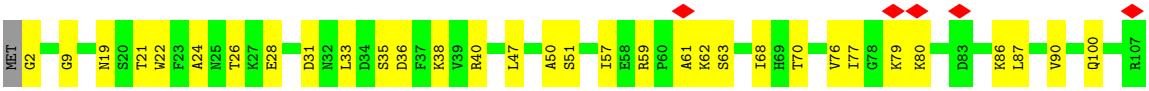


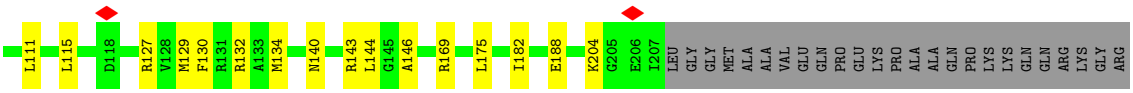


• Molecule 8: Small ribosomal subunit protein uS3

Chain C:





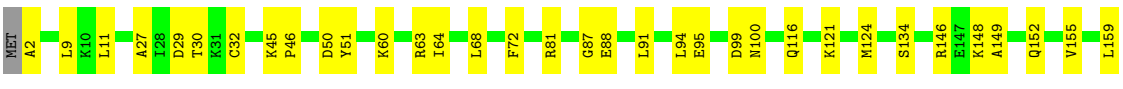


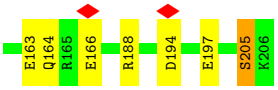


• Molecule 9: Small ribosomal subunit protein uS4

Chain D:







• Molecule 10: Small ribosomal subunit protein uS5

Chain E:

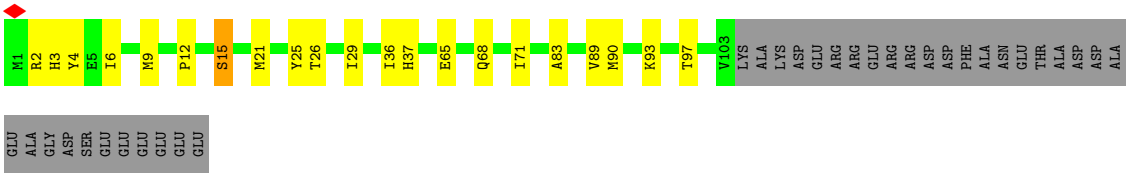




• Molecule 11: Small ribosomal subunit protein bS6

Chain F:

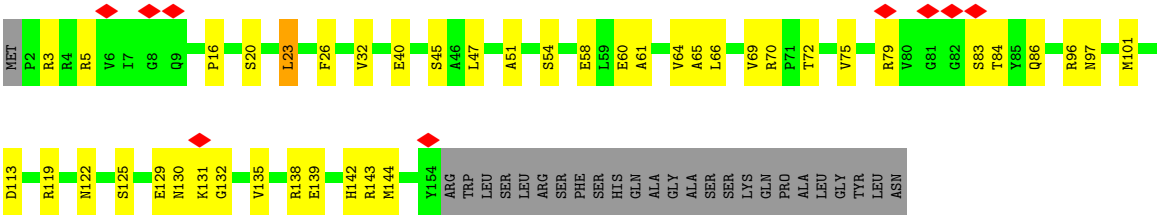




• Molecule 12: Small ribosomal subunit protein uS7

Chain G:

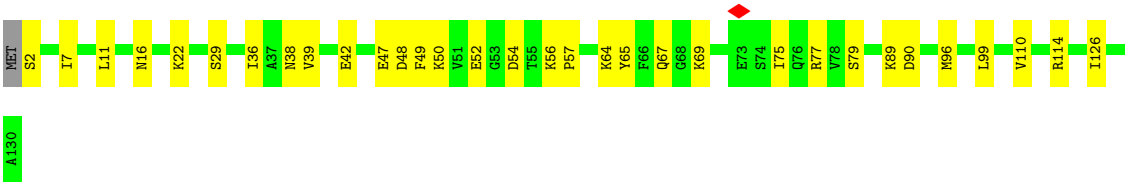




• Molecule 13: Small ribosomal subunit protein uS8

Chain H:

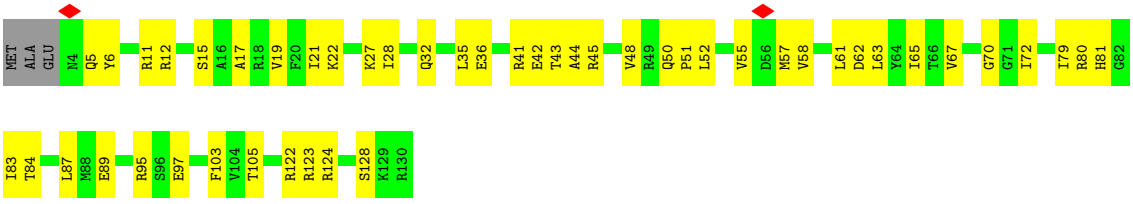




• Molecule 14: Small ribosomal subunit protein uS9

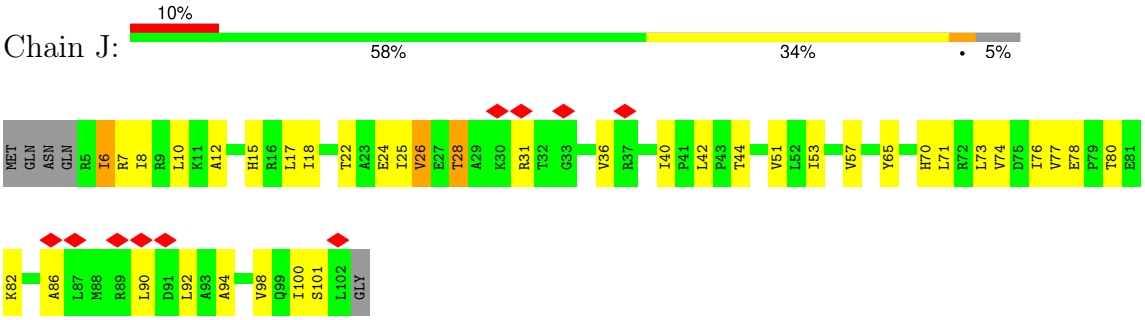
Chain I:





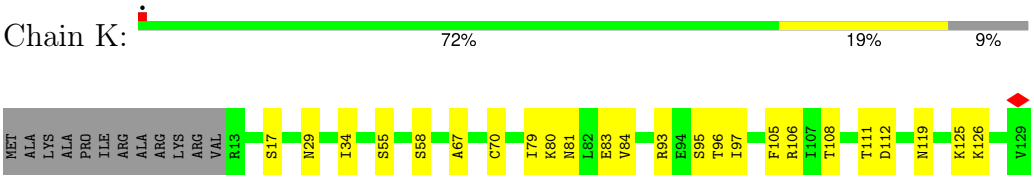
• Molecule 15: Small ribosomal subunit protein uS10

Chain J:



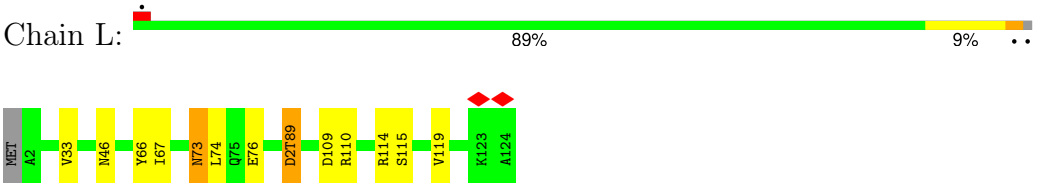
• Molecule 16: 30S ribosomal protein S11

Chain K:



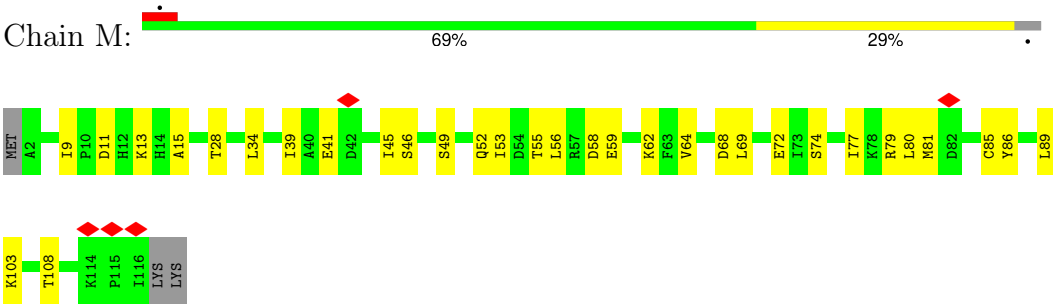
• Molecule 17: Small ribosomal subunit protein uS12

Chain L:



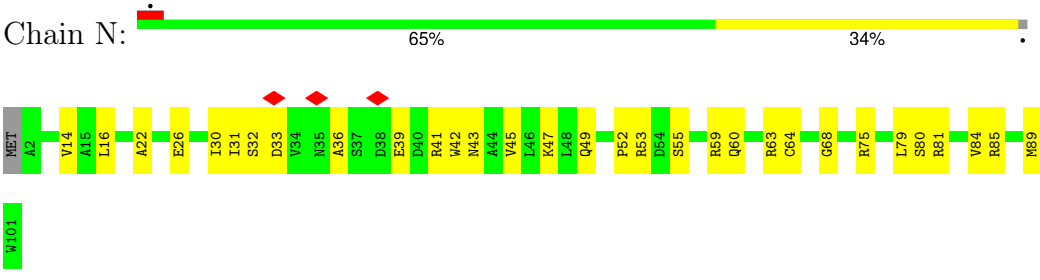
• Molecule 18: Small ribosomal subunit protein uS13

Chain M:



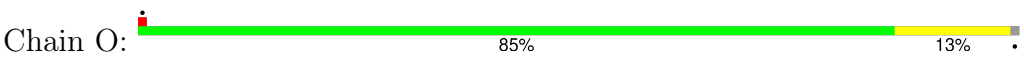
• Molecule 19: Small ribosomal subunit protein uS14

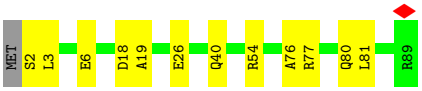
Chain N:



• Molecule 20: Small ribosomal subunit protein uS15

Chain O:





• Molecule 21: Small ribosomal subunit protein bS16

Chain P:

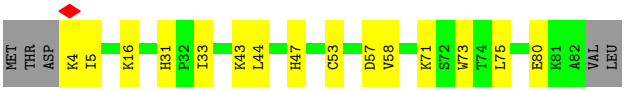




• Molecule 22: Small ribosomal subunit protein uS17

Chain Q:

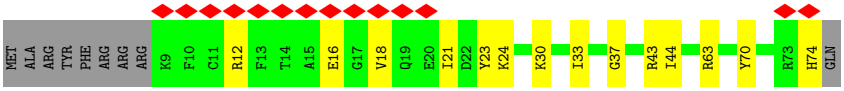




• Molecule 23: Small ribosomal subunit protein bS18

Chain R:

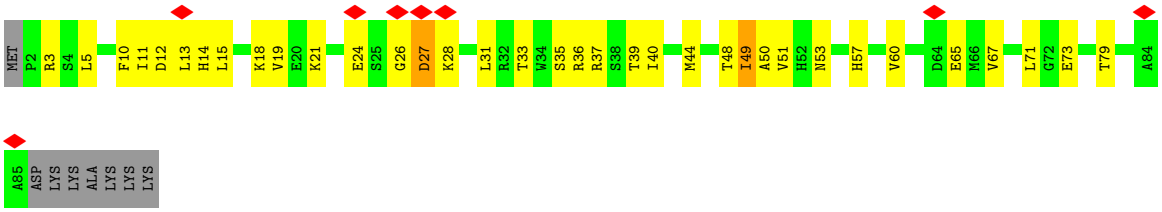




• Molecule 24: Small ribosomal subunit protein uS19

Chain S:

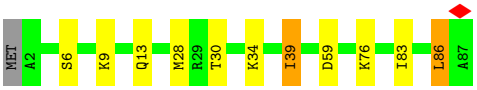




• Molecule 25: Small ribosomal subunit protein bS20

Chain T:

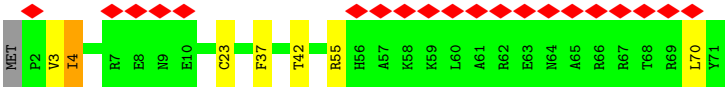




• Molecule 26: Small ribosomal subunit protein bS21

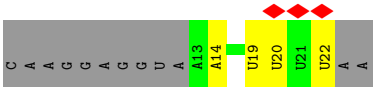
Chain U:





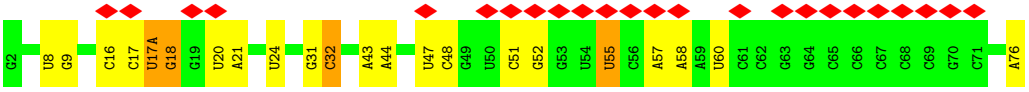
• Molecule 27: messenger RNA (mRNA)





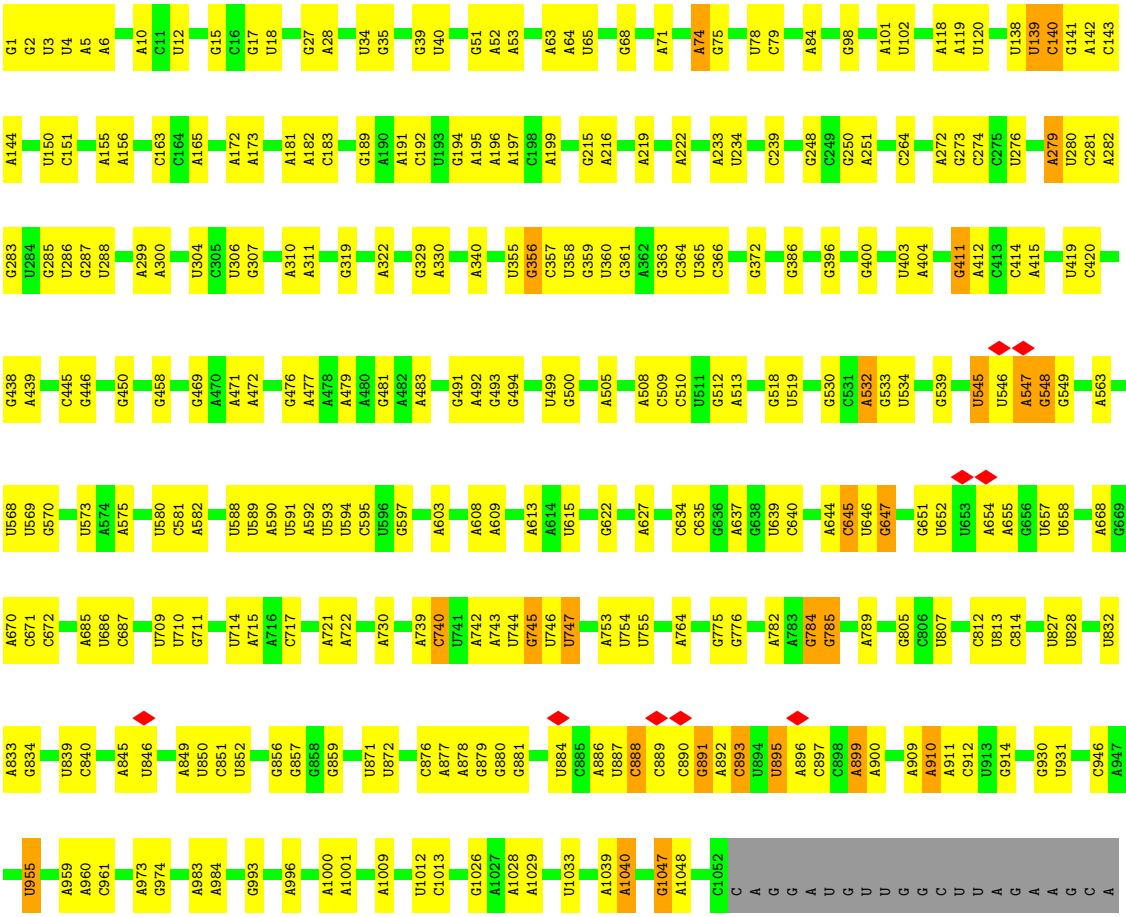
• Molecule 28: P-site tRNA

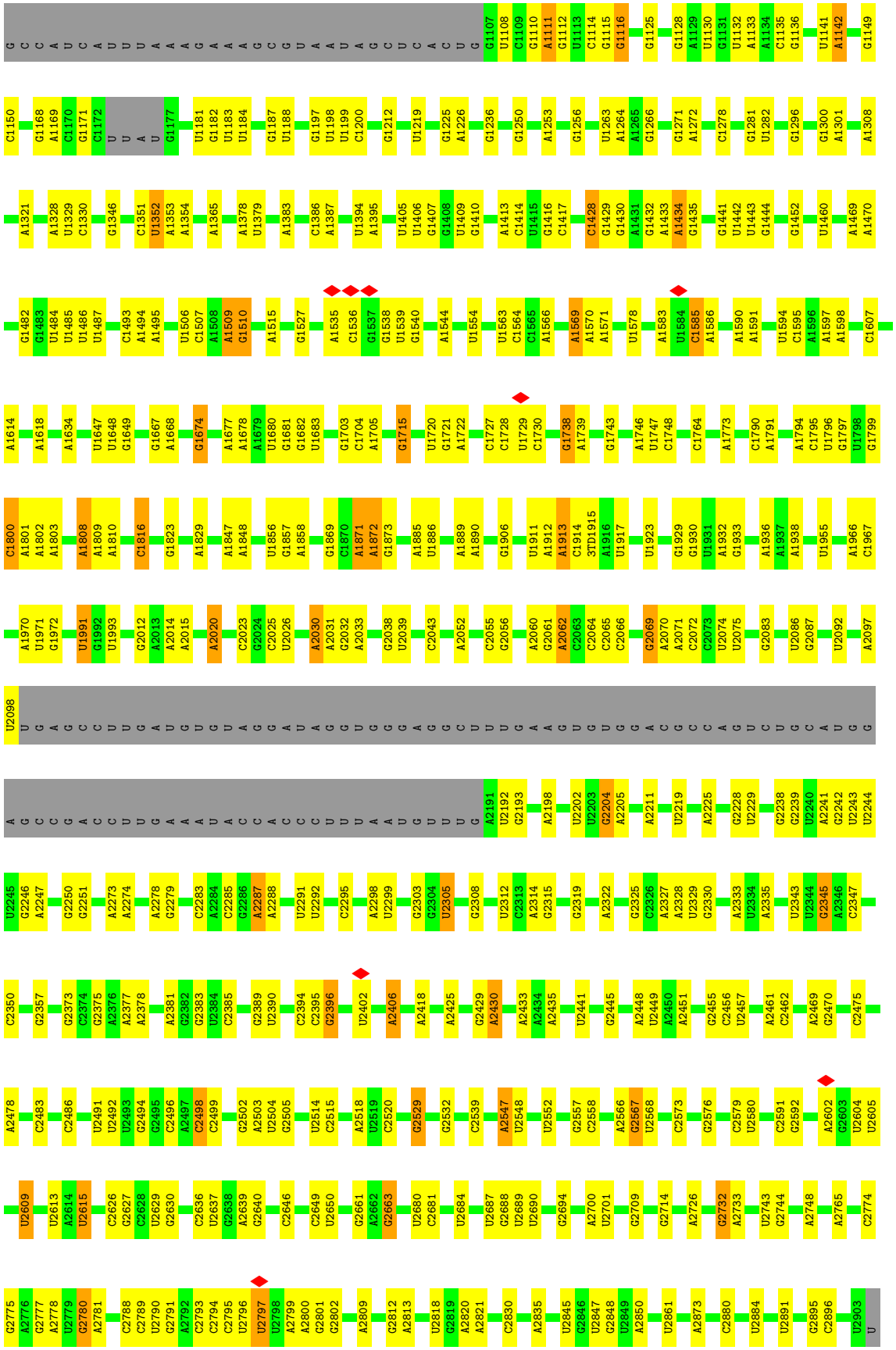




• Molecule 29: 23S ribosomal RNA

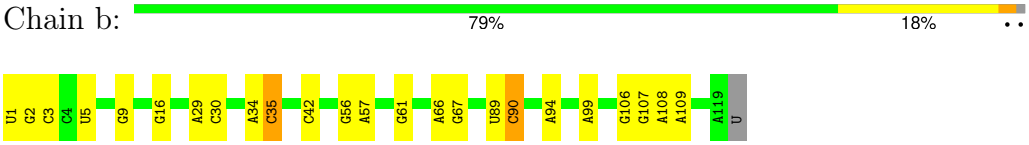






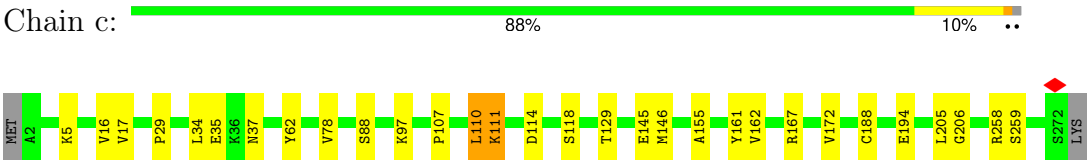
• Molecule 30: 5S ribosomal RNA

Chain b:



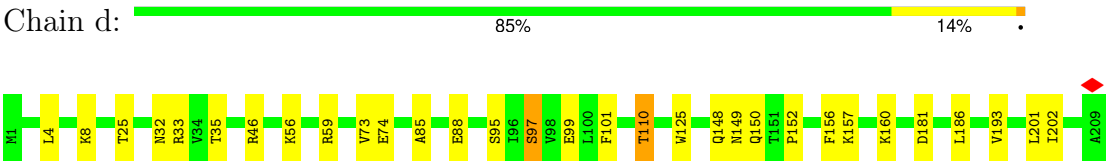
• Molecule 31: 50S ribosomal protein L2

Chain c:



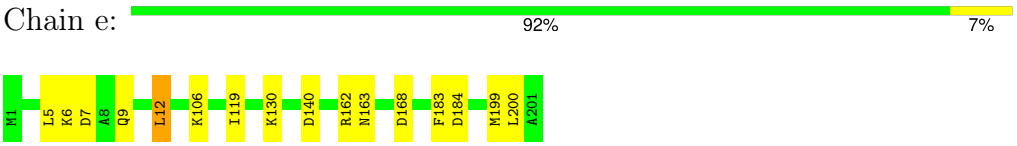
• Molecule 32: 50S ribosomal protein L3

Chain d:



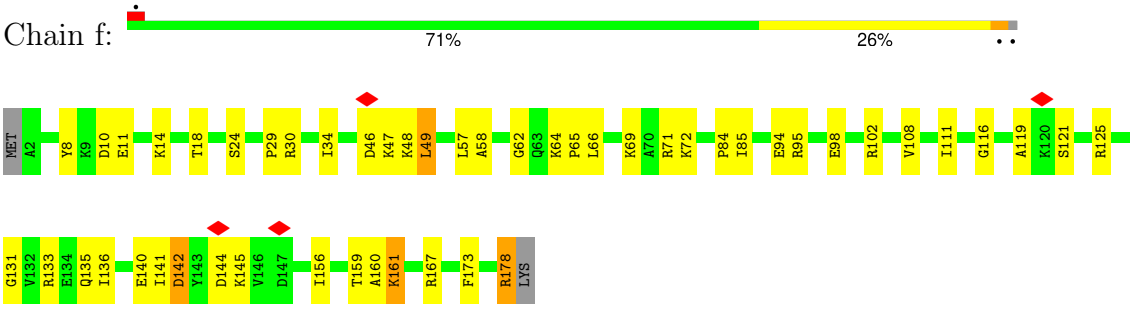
• Molecule 33: Large ribosomal subunit protein uL4

Chain e:



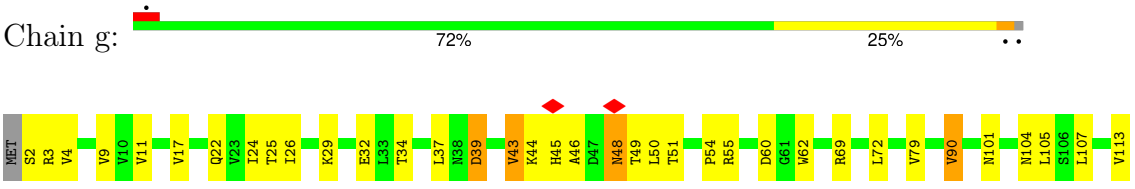
• Molecule 34: Large ribosomal subunit protein uL5

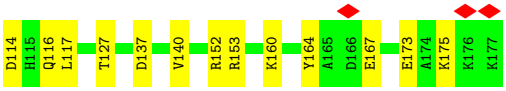
Chain f:



• Molecule 35: Large ribosomal subunit protein uL6

Chain g:

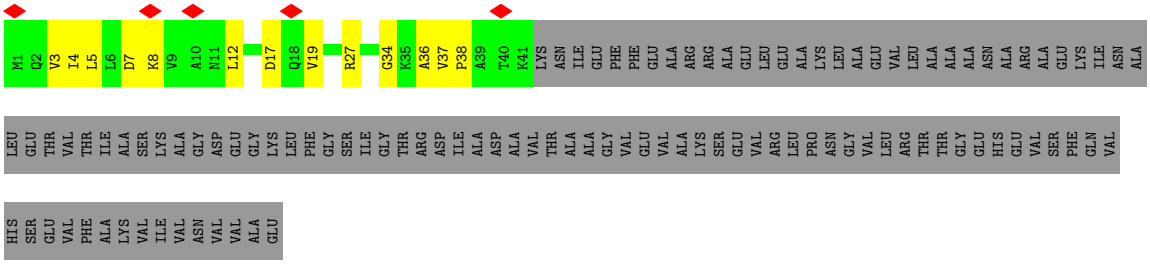




• Molecule 36: Large ribosomal subunit protein bL9

Chain h:

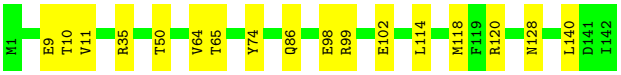




• Molecule 37: Large ribosomal subunit protein uL13

Chain i:





• Molecule 38: Large ribosomal subunit protein uL14

Chain j:

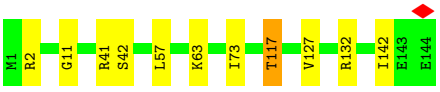




• Molecule 39: Large ribosomal subunit protein uL15

Chain k:

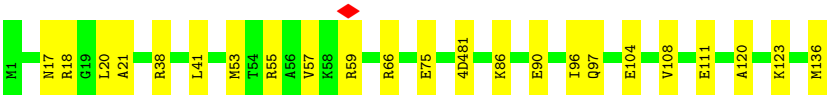




• Molecule 40: 50S ribosomal protein L16

Chain l:

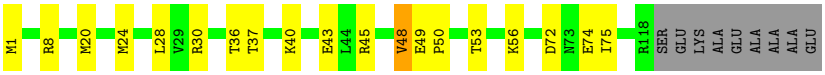




• Molecule 41: Large ribosomal subunit protein bL17

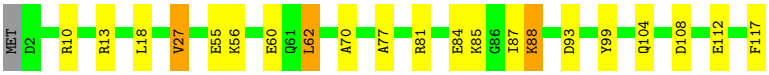
Chain m:





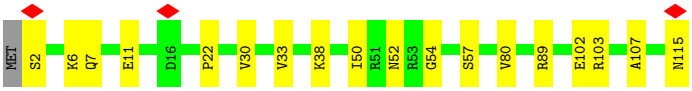
• Molecule 42: Large ribosomal subunit protein uL18





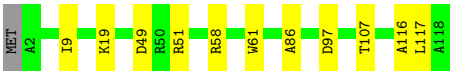
• Molecule 43: Large ribosomal subunit protein bL19





• Molecule 44: 50S ribosomal protein L20





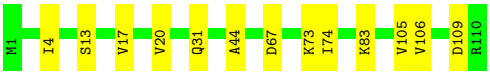
• Molecule 45: Ribosomal protein L21





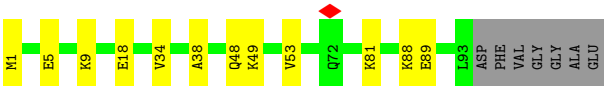
• Molecule 46: 50S ribosomal protein L22





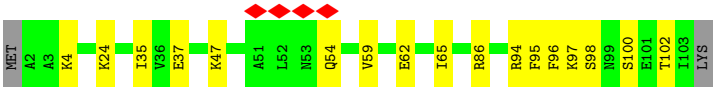
• Molecule 47: 50S ribosomal protein L23





• Molecule 48: 50S ribosomal protein L24

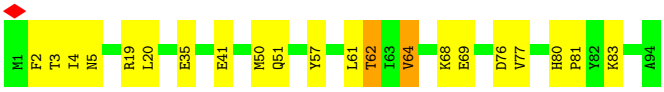




• Molecule 49: Large ribosomal subunit protein bL25

Chain u:

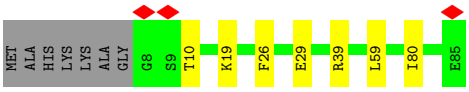




• Molecule 50: 50S ribosomal protein L27

Chain v:

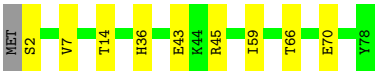




• Molecule 51: 50S ribosomal protein L28

Chain w:

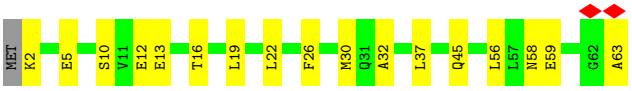




• Molecule 52: Large ribosomal subunit protein uL29

Chain x:

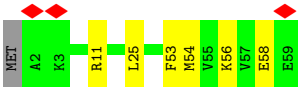




• Molecule 53: 50S ribosomal protein L30

Chain y:

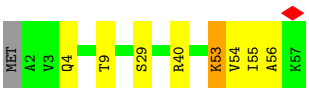




• Molecule 54: 50S ribosomal protein L32

Chain z:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	248202	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.670	Depositor
Minimum map value	-0.213	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	470.80002, 470.80002, 470.80002	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: D2T, H2U, 5MC, MA6, 4SU, K, 4OC, OMC, MG, 1MG, 3TD, PSU, UR3, 2MA, DXT, ZN, G7M, 4D4, OMU, MEQ, 6MZ, 2MG, OMG, 5MU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	0	0.32	0/424	0.36	0/565
2	1	0.36	0/380	0.33	0/498
3	2	0.35	0/513	0.35	0/676
4	3	0.35	0/303	0.35	0/397
5	4	0.14	0/488	0.30	0/649
6	A	0.32	0/35787	0.28	0/55816
7	B	0.17	0/1784	0.33	0/2403
8	C	0.22	0/1651	0.31	0/2225
9	D	0.23	0/1665	0.30	0/2227
10	E	0.28	0/1165	0.32	0/1568
11	F	0.23	0/858	0.34	0/1160
12	G	0.21	0/1219	0.33	0/1635
13	H	0.26	0/989	0.33	0/1326
14	I	0.22	0/1034	0.39	0/1375
15	J	0.22	0/796	0.40	0/1077
16	K	0.25	0/893	0.36	0/1205
17	L	0.28	0/960	0.32	0/1286
18	M	0.19	0/900	0.30	0/1204
19	N	0.23	0/817	0.41	0/1088
20	O	0.25	0/722	0.29	0/964
21	P	0.27	0/653	0.34	0/877
22	Q	0.25	0/650	0.32	0/871
23	R	0.25	0/553	0.37	0/742
24	S	0.19	0/685	0.34	0/922
25	T	0.24	0/676	0.27	0/895
26	U	0.18	0/597	0.25	0/792
27	X	0.50	0/235	0.63	0/363
28	Z	0.20	0/1725	0.26	0/2689
29	a	0.43	0/65651	0.34	0/102413
30	b	0.31	0/2850	0.26	0/4444
31	c	0.35	0/2121	0.36	0/2852

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	d	0.34	0/1576	0.32	0/2119
33	e	0.31	0/1571	0.32	0/2113
34	f	0.21	0/1434	0.33	0/1926
35	g	0.27	0/1343	0.43	0/1816
36	h	0.27	0/306	0.54	0/413
37	i	0.34	0/1152	0.30	0/1551
38	j	0.33	0/955	0.32	0/1279
39	k	0.33	0/1062	0.31	0/1413
40	l	0.31	0/1081	0.33	0/1443
41	m	0.35	0/958	0.46	0/1281
42	n	0.27	0/902	0.41	0/1209
43	o	0.32	0/929	0.29	0/1242
44	p	0.37	0/960	0.33	0/1278
45	q	0.32	0/829	0.41	0/1107
46	r	0.34	0/864	0.32	0/1156
47	s	0.30	0/744	0.38	0/994
48	t	0.28	0/787	0.43	0/1051
49	u	0.28	0/766	0.36	0/1025
50	v	0.34	0/593	0.31	0/785
51	w	0.35	0/635	0.34	0/848
52	x	0.25	0/502	0.29	0/667
53	y	0.30	0/453	0.32	0/605
54	z	0.35	0/450	0.32	0/599
All	All	0.36	0/150596	0.33	0/225124

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	0	417	0	451	11	0
2	1	377	0	418	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	2	504	0	572	7	0
4	3	302	0	340	10	0
5	4	480	0	482	12	0
6	A	32211	0	16229	298	0
7	B	1753	0	1780	36	0
8	C	1624	0	1696	29	0
9	D	1643	0	1707	25	0
10	E	1152	0	1196	14	0
11	F	839	0	833	11	0
12	G	1203	0	1254	25	0
13	H	979	0	1031	19	0
14	I	1022	0	1070	33	0
15	J	786	0	828	32	0
16	K	877	0	887	14	0
17	L	957	0	1017	10	0
18	M	891	0	952	20	0
19	N	805	0	844	25	0
20	O	714	0	734	9	0
21	P	643	0	661	10	0
22	Q	641	0	682	9	0
23	R	544	0	565	8	0
24	S	668	0	693	25	0
25	T	670	0	719	8	0
26	U	589	0	629	5	0
27	X	211	0	106	0	0
28	Z	1625	0	829	11	0
29	a	59130	0	29758	383	0
30	b	2549	0	1291	17	0
31	c	2082	0	2154	19	0
32	d	1566	0	1618	20	0
33	e	1552	0	1619	10	0
34	f	1410	0	1444	34	0
35	g	1323	0	1371	28	0
36	h	303	0	327	10	0
37	i	1129	0	1162	12	0
38	j	946	0	1023	9	0
39	k	1053	0	1129	8	0
40	l	1075	0	1154	14	0
41	m	945	0	989	12	0
42	n	892	0	923	16	0
43	o	917	0	962	10	0
44	p	947	0	1019	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	q	816	0	839	7	0
46	r	857	0	922	6	0
47	s	738	0	807	11	0
48	t	779	0	831	12	0
49	u	753	0	780	15	0
50	v	586	0	596	3	0
51	w	625	0	652	5	0
52	x	501	0	531	9	0
53	y	449	0	488	4	0
54	z	444	0	458	5	0
55	3	1	0	0	0	0
56	A	59	0	0	0	0
56	a	210	0	0	0	0
56	b	5	0	0	0	0
56	p	2	0	0	0	0
57	A	20	0	0	0	0
57	a	71	0	0	0	0
57	b	1	0	0	0	0
58	A	32	0	21	0	0
58	a	128	0	84	5	0
58	r	32	0	21	1	0
59	1	4	0	0	0	0
59	2	3	0	0	0	0
59	3	1	0	0	1	0
59	A	88	0	0	2	0
59	L	1	0	0	0	0
59	T	1	0	0	0	0
59	X	1	0	0	0	0
59	a	1189	0	0	15	0
59	b	10	0	0	0	0
59	c	6	0	0	0	0
59	d	4	0	0	0	0
59	e	3	0	0	0	0
59	i	1	0	0	0	0
59	j	1	0	0	0	0
59	k	4	0	0	0	0
59	l	1	0	0	0	0
59	m	2	0	0	0	0
59	p	4	0	0	0	0
59	q	3	0	0	1	0
59	r	3	0	0	0	0
59	s	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	u	1	0	0	0	0
59	w	1	0	0	1	0
59	z	2	0	0	0	0
All	All	141390	0	94178	1264	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 1264 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)
6:A:76:G:H1	6:A:93:U:H3	1.21	0.85
29:a:881:G:H1	29:a:895:U:H3	0.87	0.81
14:I:19:VAL:HG12	14:I:65:ILE:HG12	1.66	0.78
18:M:34:LEU:HD23	18:M:41:GLU:HA	1.67	0.77
15:J:8:ILE:HD12	15:J:100:ILE:HD12	1.67	0.76

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	
1	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	61 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	56/70 (80%)	54 (96%)	2 (4%)	0	100	100
7	B	222/241 (92%)	211 (95%)	11 (5%)	0	100	100
8	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	D	203/206 (98%)	200 (98%)	3 (2%)	0	100	100
10	E	154/167 (92%)	147 (96%)	7 (4%)	0	100	100
11	F	101/135 (75%)	98 (97%)	3 (3%)	0	100	100
12	G	151/179 (84%)	140 (93%)	11 (7%)	0	100	100
13	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	I	125/130 (96%)	121 (97%)	4 (3%)	0	100	100
15	J	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	20
16	K	115/129 (89%)	109 (95%)	6 (5%)	0	100	100
17	L	120/124 (97%)	114 (95%)	6 (5%)	0	100	100
18	M	113/118 (96%)	107 (95%)	6 (5%)	0	100	100
19	N	98/101 (97%)	95 (97%)	3 (3%)	0	100	100
20	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
21	P	79/82 (96%)	73 (92%)	6 (8%)	0	100	100
22	Q	77/84 (92%)	76 (99%)	1 (1%)	0	100	100
23	R	64/75 (85%)	60 (94%)	4 (6%)	0	100	100
24	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
25	T	84/87 (97%)	84 (100%)	0	0	100	100
26	U	68/71 (96%)	67 (98%)	1 (2%)	0	100	100
31	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
32	d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	37
33	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
34	f	175/179 (98%)	164 (94%)	11 (6%)	0	100	100
35	g	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
36	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
37	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
38	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
39	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
40	l	133/136 (98%)	130 (98%)	3 (2%)	0	100	100
41	m	116/127 (91%)	111 (96%)	5 (4%)	0	100	100
42	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
43	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	p	115/118 (98%)	115 (100%)	0	0	100	100
45	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
46	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
47	s	91/100 (91%)	87 (96%)	4 (4%)	0	100	100
48	t	100/104 (96%)	95 (95%)	5 (5%)	0	100	100
49	u	92/94 (98%)	88 (96%)	4 (4%)	0	100	100
50	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
51	w	75/78 (96%)	75 (100%)	0	0	100	100
52	x	60/63 (95%)	57 (95%)	3 (5%)	0	100	100
53	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
54	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
All	All	5484/5913 (93%)	5288 (96%)	194 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	d	149	ASN
15	J	57	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	46/49 (94%)	46 (100%)	0	100	100
2	1	38/38 (100%)	38 (100%)	0	100	100
3	2	51/52 (98%)	49 (96%)	2 (4%)	28	48
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	55/62 (89%)	54 (98%)	1 (2%)	51	73
7	B	186/199 (94%)	179 (96%)	7 (4%)	29	49
8	C	170/190 (90%)	164 (96%)	6 (4%)	32	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	D	172/173 (99%)	167 (97%)	5 (3%)	37	60
10	E	119/126 (94%)	116 (98%)	3 (2%)	42	64
11	F	90/116 (78%)	88 (98%)	2 (2%)	45	67
12	G	126/147 (86%)	119 (94%)	7 (6%)	19	33
13	H	104/105 (99%)	103 (99%)	1 (1%)	68	84
14	I	105/107 (98%)	102 (97%)	3 (3%)	37	60
15	J	86/90 (96%)	80 (93%)	6 (7%)	14	24
16	K	90/99 (91%)	87 (97%)	3 (3%)	33	55
17	L	102/103 (99%)	98 (96%)	4 (4%)	28	48
18	M	93/96 (97%)	90 (97%)	3 (3%)	34	56
19	N	83/84 (99%)	82 (99%)	1 (1%)	63	81
20	O	76/77 (99%)	76 (100%)	0	100	100
21	P	65/65 (100%)	64 (98%)	1 (2%)	57	77
22	Q	73/78 (94%)	73 (100%)	0	100	100
23	R	57/65 (88%)	55 (96%)	2 (4%)	32	53
24	S	72/79 (91%)	67 (93%)	5 (7%)	14	24
25	T	65/66 (98%)	62 (95%)	3 (5%)	24	41
26	U	60/61 (98%)	57 (95%)	3 (5%)	22	38
31	c	216/218 (99%)	213 (99%)	3 (1%)	59	79
32	d	163/163 (100%)	160 (98%)	3 (2%)	51	73
33	e	165/165 (100%)	161 (98%)	4 (2%)	43	65
34	f	148/150 (99%)	140 (95%)	8 (5%)	20	35
35	g	137/138 (99%)	126 (92%)	11 (8%)	11	19
36	h	32/114 (28%)	32 (100%)	0	100	100
37	i	116/116 (100%)	114 (98%)	2 (2%)	53	74
38	j	104/104 (100%)	104 (100%)	0	100	100
39	k	103/103 (100%)	100 (97%)	3 (3%)	37	60
40	l	108/108 (100%)	106 (98%)	2 (2%)	50	71
41	m	98/103 (95%)	97 (99%)	1 (1%)	68	84
42	n	86/87 (99%)	82 (95%)	4 (5%)	23	41
43	o	99/100 (99%)	99 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
44	p	89/90 (99%)	87 (98%)	2 (2%)	45	67
45	q	84/84 (100%)	82 (98%)	2 (2%)	43	65
46	r	93/93 (100%)	90 (97%)	3 (3%)	34	56
47	s	80/84 (95%)	80 (100%)	0	100	100
48	t	83/85 (98%)	80 (96%)	3 (4%)	31	52
49	u	78/78 (100%)	76 (97%)	2 (3%)	40	63
50	v	58/63 (92%)	57 (98%)	1 (2%)	53	74
51	w	67/68 (98%)	66 (98%)	1 (2%)	57	77
52	x	54/55 (98%)	52 (96%)	2 (4%)	30	51
53	y	48/49 (98%)	48 (100%)	0	100	100
54	z	47/48 (98%)	46 (98%)	1 (2%)	47	69
All	All	4574/4827 (95%)	4448 (97%)	126 (3%)	38	60

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
24	S	27	ASP
44	p	107	THR
32	d	95	SER
44	p	9	ILE
48	t	65	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
31	c	134	ASN
35	g	38	ASN
46	r	9	HIS
34	f	127	ASN
35	g	48	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	X	9/22 (40%)	4 (44%)	0
28	Z	75/76 (98%)	7 (9%)	1 (1%)

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
29	a	2749/2904 (94%)	285 (10%)	0
30	b	118/120 (98%)	9 (7%)	0
6	A	1495/1542 (96%)	171 (11%)	2 (0%)
All	All	4446/4664 (95%)	476 (10%)	3 (0%)

5 of 476 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	4	U
6	A	6	G
6	A	9	G
6	A	22	G
6	A	32	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	1035	A
6	A	1440	U
28	Z	17(A)	U

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

42 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	$\#\|Z\| > 2$
6	MA6	A	1518	6	23,26,27	0.27	0	33,38,41	0.64	1 (3%)
32	MEQ	d	150	32	8,9,10	0.85	0	5,10,12	0.66	0
29	6MZ	a	2030	29	22,25,26	2.32	8 (36%)	29,36,39	2.47	13 (44%)
29	OMG	a	2251	29,57,28	23,26,27	0.64	0	32,38,41	0.47	0
29	5MU	a	1939	29,57	19,22,23	0.74	0	27,32,35	0.51	0
6	UR3	A	1498	6	19,22,23	2.64	8 (42%)	26,32,35	1.62	3 (11%)
6	5MC	A	1407	6	19,22,23	0.73	0	26,32,35	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
29	H2U	a	2449	29	18,21,22	0.66	0	19,30,33	1.00	1 (5%)
28	4SU	Z	8	28	18,21,22	3.87	8 (44%)	25,30,33	2.40	5 (20%)
29	G7M	a	2069	29,57	23,26,27	2.60	8 (34%)	34,39,42	2.48	12 (35%)
29	PSU	a	2605	29	18,21,22	1.06	2 (11%)	21,30,33	2.07	4 (19%)
6	2MG	A	1516	6	23,26,27	0.57	0	33,38,41	0.65	0
29	PSU	a	746	29,56	18,21,22	1.08	2 (11%)	21,30,33	1.83	3 (14%)
28	5MU	Z	54	28	19,22,23	0.38	0	27,32,35	0.55	0
29	PSU	a	2457	29	18,21,22	1.12	2 (11%)	21,30,33	2.28	5 (23%)
17	D2T	L	89	17	8,9,10	1.84	2 (25%)	6,11,13	1.60	2 (33%)
29	OMC	a	2498	29,56	19,22,23	0.78	1 (5%)	25,31,34	0.82	1 (4%)
29	OMU	a	2552	29,57	19,22,23	2.79	6 (31%)	25,31,34	1.93	5 (20%)
29	2MG	a	2445	29	23,26,27	0.75	0	33,38,41	0.48	0
40	4D4	l	81	40	9,11,12	2.05	2 (22%)	7,13,15	1.86	3 (42%)
29	PSU	a	955	29	18,21,22	1.05	2 (11%)	21,30,33	2.13	5 (23%)
6	4OC	A	1402	6	20,23,24	3.11	8 (40%)	25,32,35	0.95	2 (8%)
28	PSU	Z	55	28	18,21,22	1.14	1 (5%)	21,30,33	1.92	5 (23%)
6	G7M	A	527	6	23,26,27	2.61	9 (39%)	34,39,42	2.41	11 (32%)
29	PSU	a	1917	29	18,21,22	1.05	1 (5%)	21,30,33	1.99	4 (19%)
6	5MC	A	967	6	19,22,23	0.67	0	26,32,35	0.66	0
29	2MG	a	1835	29	23,26,27	0.66	0	33,38,41	0.47	0
29	PSU	a	2504	29,57	18,21,22	1.07	2 (11%)	21,30,33	1.88	4 (19%)
29	2MA	a	2503	29,57,56	22,25,26	0.85	1 (4%)	32,37,40	1.20	4 (12%)
29	PSU	a	2604	29	18,21,22	1.11	2 (11%)	21,30,33	2.10	5 (23%)
6	PSU	A	516	6,56	18,21,22	1.05	2 (11%)	21,30,33	1.97	6 (28%)
6	2MG	A	966	6	23,26,27	0.53	0	33,38,41	0.49	0
28	5MC	Z	32	28	19,22,23	0.69	0	26,32,35	0.78	1 (3%)
6	2MG	A	1207	6	23,26,27	0.51	0	33,38,41	0.50	0
29	5MU	a	747	29	19,22,23	0.69	0	27,32,35	0.78	2 (7%)
29	PSU	a	1911	29	18,21,22	1.08	1 (5%)	21,30,33	1.99	4 (19%)
29	1MG	a	745	29	23,26,27	2.78	8 (34%)	33,39,42	1.75	9 (27%)
6	MA6	A	1519	6	23,26,27	0.26	0	33,38,41	0.64	1 (3%)
29	3TD	a	1915	29	19,22,23	4.11	7 (36%)	23,32,35	1.86	4 (17%)
29	6MZ	a	1618	29	22,25,26	2.28	7 (31%)	29,36,39	2.44	9 (31%)
29	5MC	a	1962	29,57	19,22,23	0.82	0	26,32,35	0.59	0
29	PSU	a	2580	29	18,21,22	1.11	3 (16%)	21,30,33	2.16	5 (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
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
32	MEQ	d	150	32	-	2/8/9/11	-
29	6MZ	a	2030	29	-	2/9/27/28	0/3/3/3
29	OMG	a	2251	29,57,28	-	1/9/27/28	0/3/3/3
29	5MU	a	1939	29,57	-	0/7/25/26	0/2/2/2
6	UR3	A	1498	6	-	0/7/25/26	0/2/2/2
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
29	H2U	a	2449	29	-	0/7/38/39	0/2/2/2
28	4SU	Z	8	28	-	0/7/25/26	0/2/2/2
29	G7M	a	2069	29,57	-	2/7/25/26	0/3/3/3
29	PSU	a	2605	29	-	0/7/25/26	0/2/2/2
6	2MG	A	1516	6	-	0/9/27/28	0/3/3/3
29	PSU	a	746	29,56	-	2/7/25/26	0/2/2/2
28	5MU	Z	54	28	-	0/7/25/26	0/2/2/2
29	PSU	a	2457	29	-	0/7/25/26	0/2/2/2
17	D2T	L	89	17	-	4/7/12/14	-
29	OMC	a	2498	29,56	-	0/9/27/28	0/2/2/2
29	OMU	a	2552	29,57	-	2/9/27/28	0/2/2/2
29	2MG	a	2445	29	-	2/9/27/28	0/3/3/3
40	4D4	l	81	40	-	4/11/12/14	-
29	PSU	a	955	29	-	0/7/25/26	0/2/2/2
6	4OC	A	1402	6	-	1/9/29/30	0/2/2/2
28	PSU	Z	55	28	-	0/7/25/26	0/2/2/2
6	G7M	A	527	6	-	3/7/25/26	0/3/3/3
29	PSU	a	1917	29	-	0/7/25/26	0/2/2/2
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
29	2MG	a	1835	29	-	2/9/27/28	0/3/3/3
29	PSU	a	2504	29,57	-	1/7/25/26	0/2/2/2
29	2MA	a	2503	29,57,56	-	2/7/25/26	0/3/3/3
29	PSU	a	2604	29	-	0/7/25/26	0/2/2/2
6	PSU	A	516	6,56	-	0/7/25/26	0/2/2/2
6	2MG	A	966	6	-	0/9/27/28	0/3/3/3
28	5MC	Z	32	28	-	0/7/25/26	0/2/2/2
6	2MG	A	1207	6	-	0/9/27/28	0/3/3/3
29	5MU	a	747	29	-	1/7/25/26	0/2/2/2
29	PSU	a	1911	29	-	0/7/25/26	0/2/2/2
29	1MG	a	745	29	-	0/7/25/26	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MA6	A	1519	6	-	0/11/29/30	0/3/3/3
29	3TD	a	1915	29	-	0/7/25/26	0/2/2/2
29	6MZ	a	1618	29	-	0/9/27/28	0/3/3/3
29	5MC	a	1962	29,57	-	2/7/25/26	0/2/2/2
29	PSU	a	2580	29	-	0/7/25/26	0/2/2/2

The worst 5 of 103 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	1915	3TD	C6-C5	12.77	1.49	1.35
29	a	1915	3TD	C2-N1	9.21	1.48	1.37
28	Z	8	4SU	C4-N3	8.69	1.46	1.37
29	a	1618	6MZ	C6-N6	7.61	1.42	1.34
29	a	745	1MG	C2-N3	7.39	1.45	1.33

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	Z	8	4SU	C4-N3-C2	-8.13	119.52	127.31
29	a	2069	G7M	C1'-N9-C4	6.53	145.76	126.49
6	A	527	G7M	C1'-N9-C4	6.33	145.17	126.49
29	a	2069	G7M	C1'-N9-C8	-6.13	106.05	126.74
29	a	2552	OMU	C4-N3-C2	-5.97	119.20	126.61

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
17	L	89	D2T	CA-CB-CG-OD1
17	L	89	D2T	CA-CB-CG-OD2
29	a	2251	OMG	C1'-C2'-O2'-CM2
29	a	2445	2MG	C3'-C4'-C5'-O5'
32	d	150	MEQ	OE1-CD-CG-CB

There are no ring outliers.

13 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1518	MA6	3	0
32	d	150	MEQ	1	0
29	a	2030	6MZ	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
29	a	2251	OMG	1	0
6	A	1498	UR3	2	0
6	A	1516	2MG	1	0
17	L	89	D2T	2	0
29	a	2498	OMC	1	0
29	a	955	PSU	1	0
28	Z	55	PSU	1	0
28	Z	32	5MC	1	0
29	a	745	1MG	1	0
6	A	1519	MA6	4	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 375 ligands modelled in this entry, 369 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
58	DXT	a	3218	56	34,35,35	0.95	1 (2%)	42,57,57	1.19	6 (14%)
58	DXT	A	1676	56	34,35,35	0.92	1 (2%)	42,57,57	0.96	3 (7%)
58	DXT	a	3238	-	34,35,35	0.86	0	42,57,57	1.54	9 (21%)
58	DXT	a	3213	56	34,35,35	0.79	0	42,57,57	1.02	4 (9%)
58	DXT	r	201	56	34,35,35	0.85	0	42,57,57	1.00	2 (4%)
58	DXT	a	3245	56	34,35,35	0.88	0	42,57,57	1.30	6 (14%)

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
58	DXT	a	3218	56	-	3/8/74/74	0/4/4/4
58	DXT	A	1676	56	-	4/8/74/74	0/4/4/4
58	DXT	a	3238	-	-	5/8/74/74	0/4/4/4
58	DXT	a	3213	56	-	3/8/74/74	0/4/4/4
58	DXT	r	201	56	-	4/8/74/74	0/4/4/4
58	DXT	a	3245	56	-	5/8/74/74	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	a	3218	DXT	C4B-C12	-2.22	1.50	1.52
58	A	1676	DXT	C2-C3	-2.10	1.35	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
58	a	3238	DXT	C21-C2-C1	-5.58	114.36	120.97
58	a	3245	DXT	C11-C5B-C12	-4.55	115.20	118.80
58	a	3238	DXT	C11-C5B-C12	-3.40	116.11	118.80
58	a	3218	DXT	C21-C2-C1	-3.36	117.00	120.97
58	a	3218	DXT	C11-C5B-C12	-3.30	116.19	118.80

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	A	1676	DXT	C3-C4-N4-C41
58	A	1676	DXT	C3-C4-N4-C42
58	A	1676	DXT	C4A-C4-N4-C41
58	a	3213	DXT	C1-C2-C21-O21
58	a	3213	DXT	C1-C2-C21-N21

There are no ring outliers.

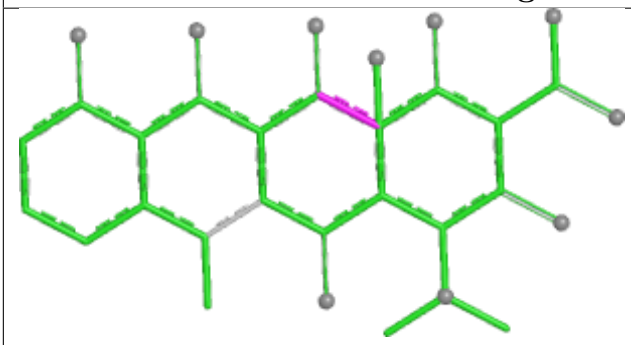
3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	a	3238	DXT	3	0
58	r	201	DXT	1	0
58	a	3245	DXT	2	0

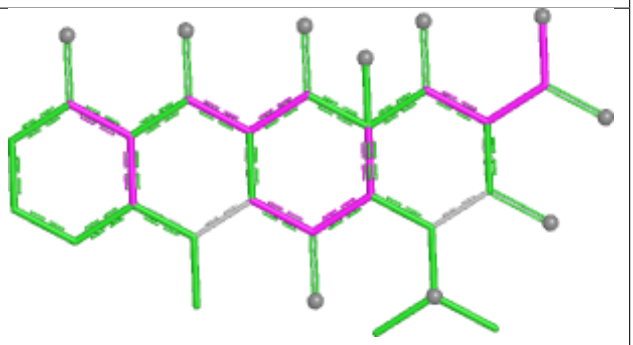
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

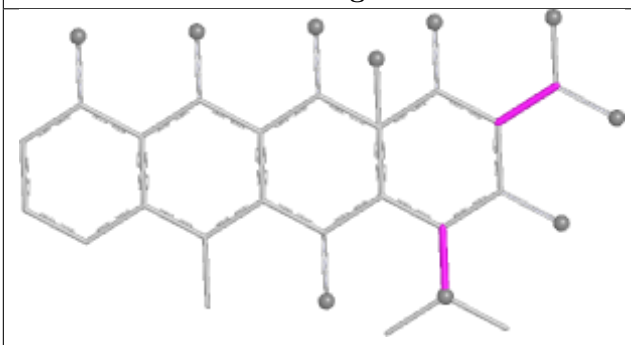
Ligand DXT a 3218



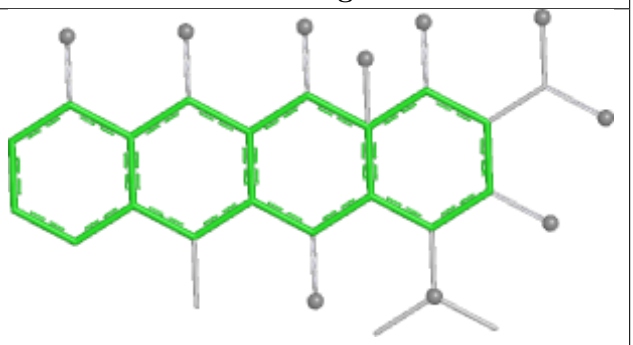
Bond lengths



Bond angles

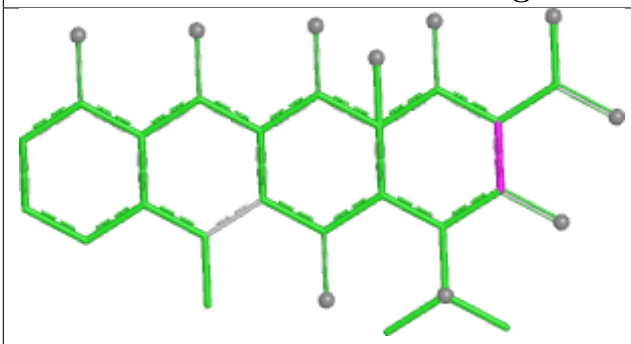


Torsions

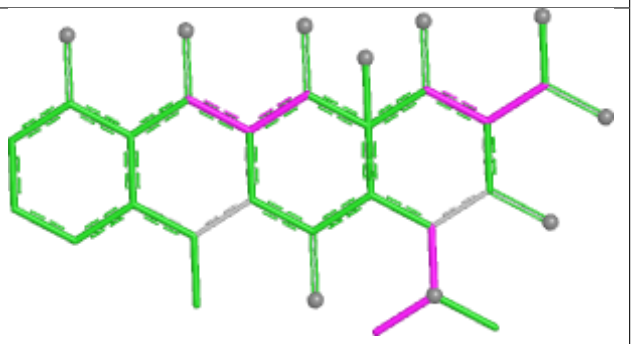


Rings

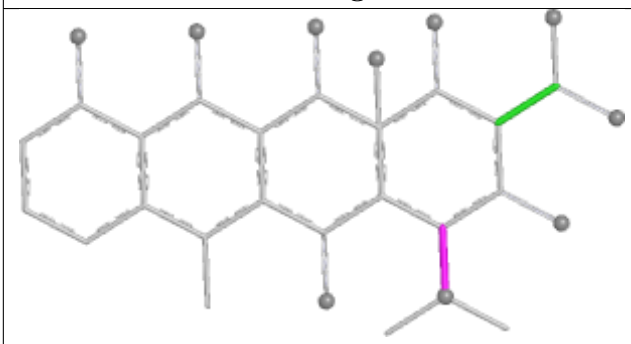
Ligand DXT A 1676



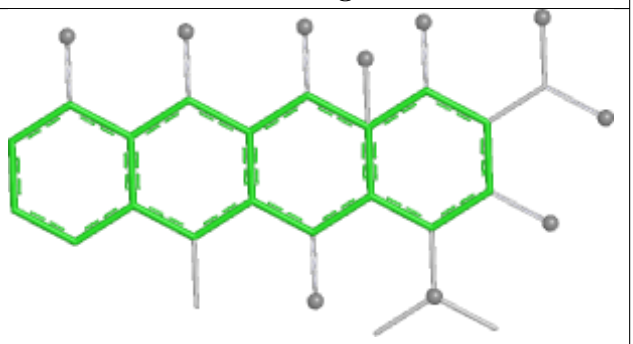
Bond lengths



Bond angles

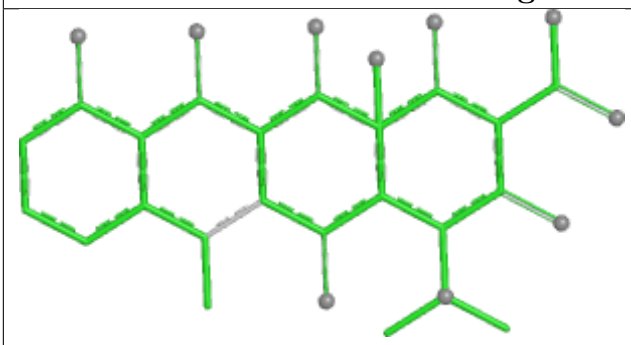


Torsions

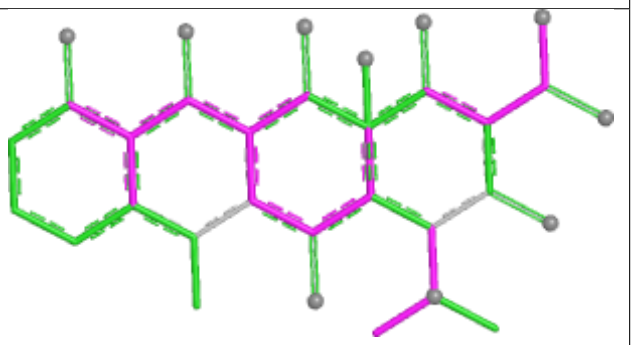


Rings

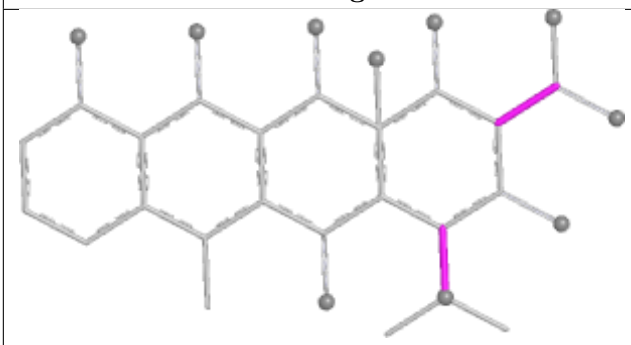
Ligand DXT a 3238



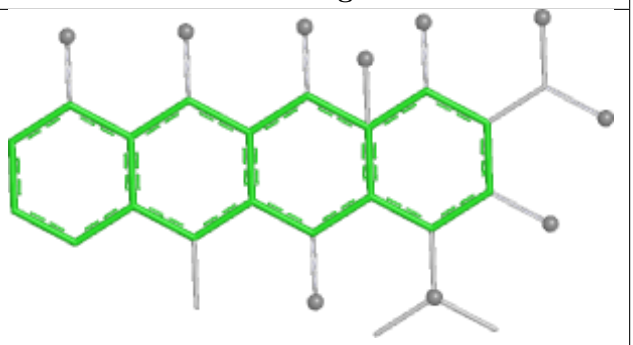
Bond lengths



Bond angles

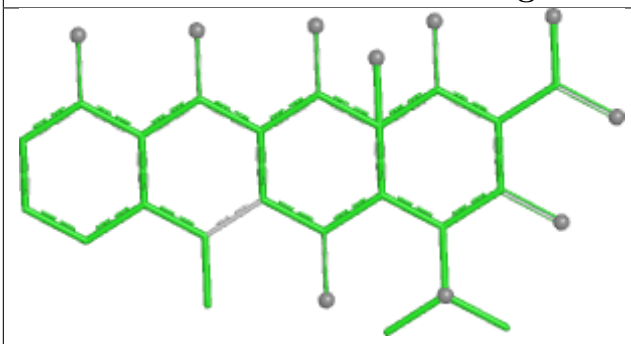


Torsions

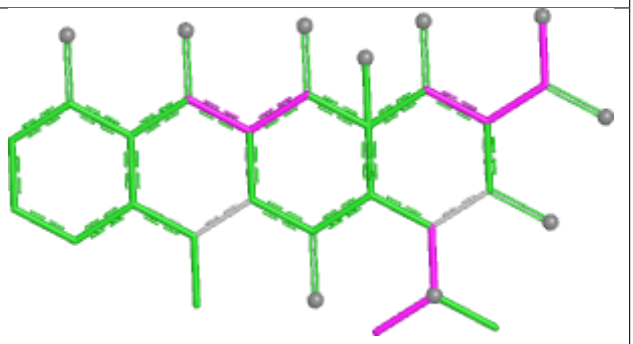


Rings

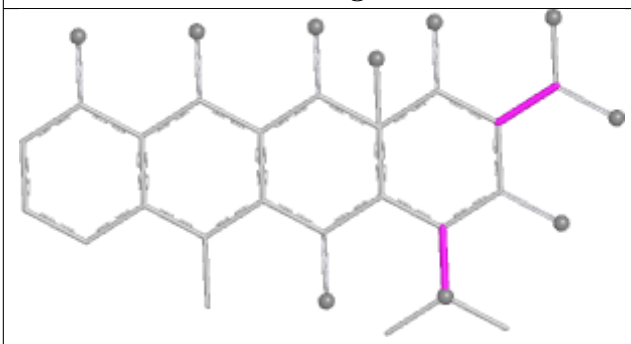
Ligand DXT a 3213



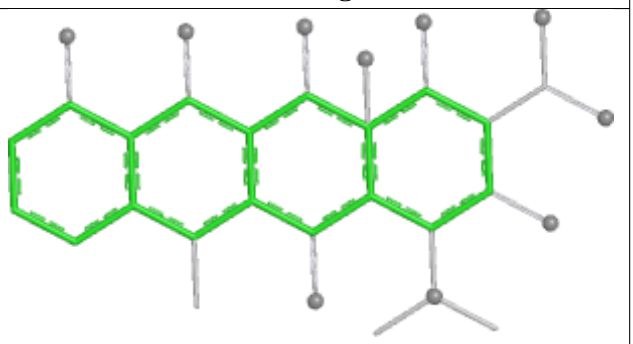
Bond lengths



Bond angles

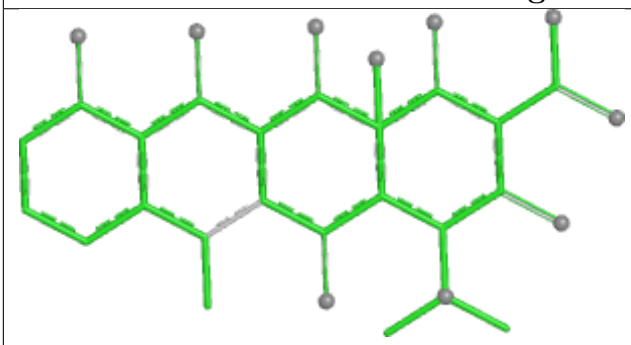


Torsions

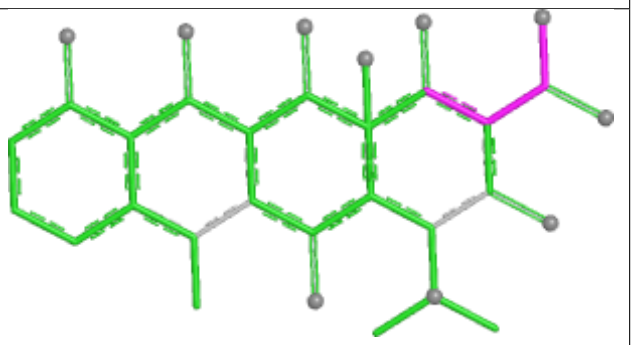


Rings

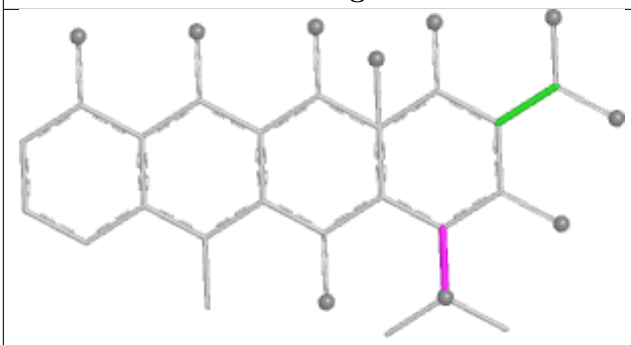
Ligand DXT r 201



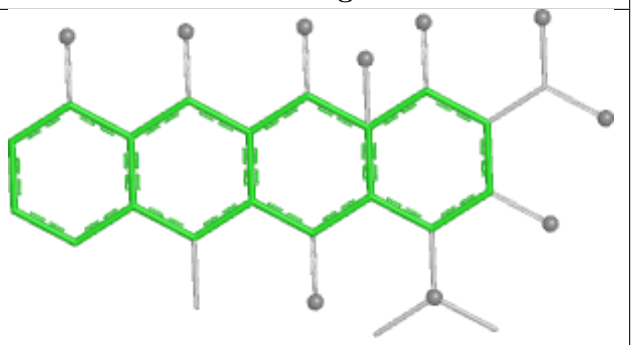
Bond lengths



Bond angles

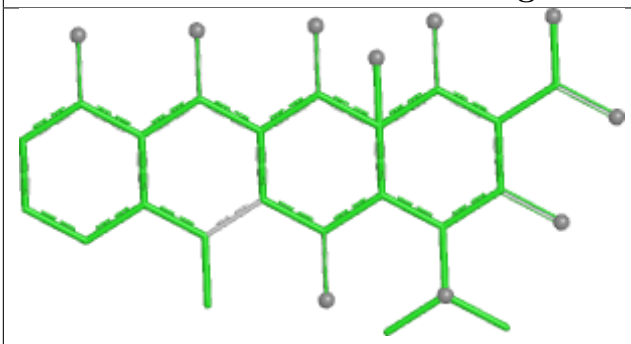


Torsions

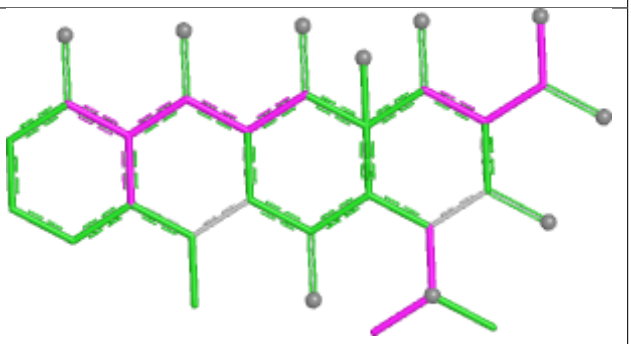


Rings

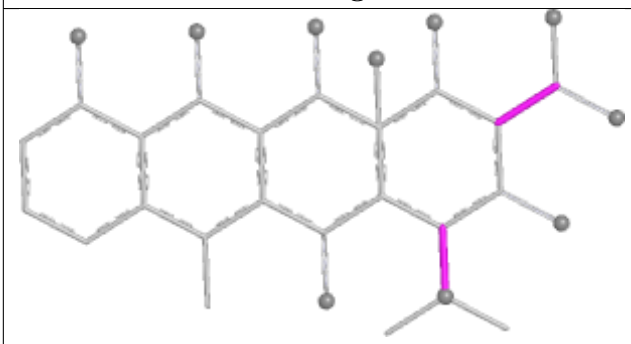
Ligand DXT a 3245



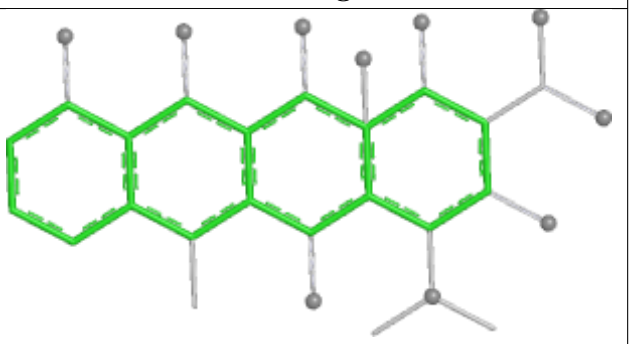
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

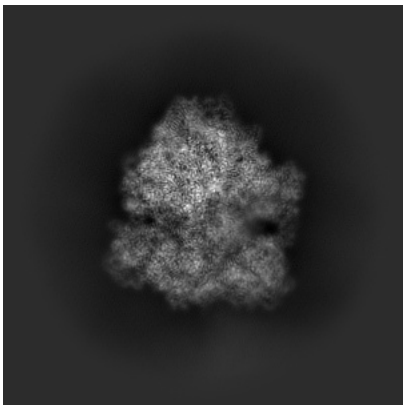
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-71667. These allow visual inspection of the internal detail of the map and identification of artifacts.

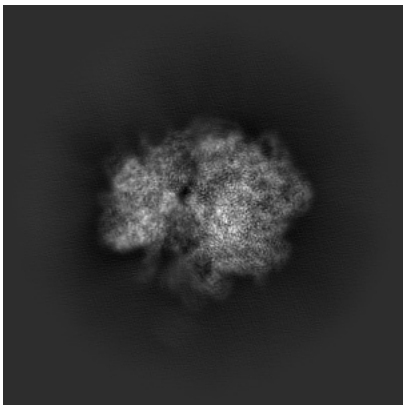
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

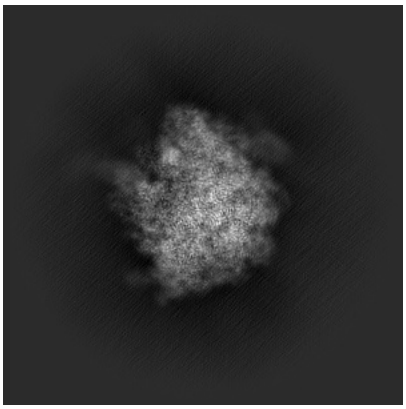
6.1.1 Primary map



X

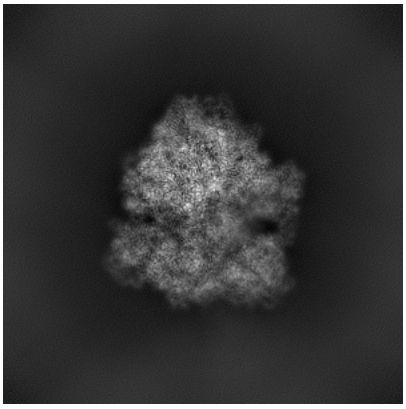


Y

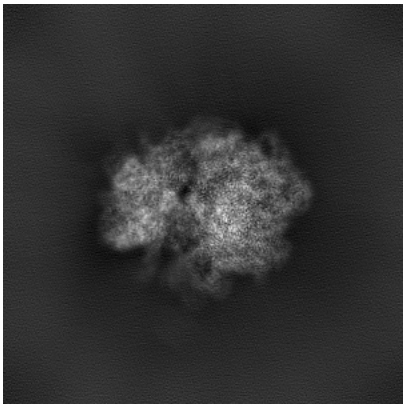


Z

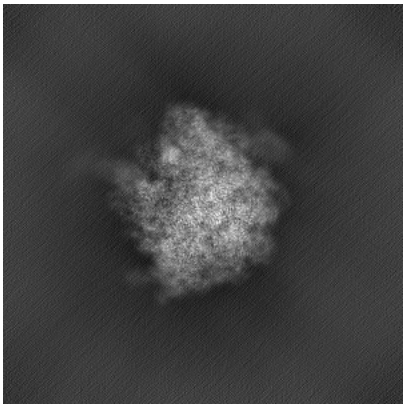
6.1.2 Raw map



X



Y

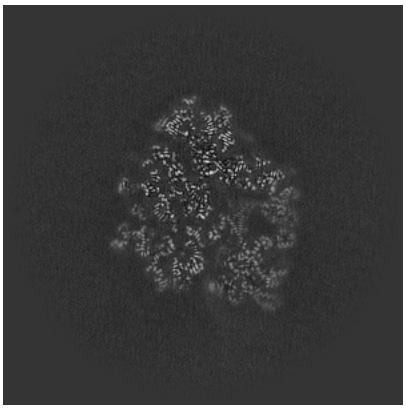


Z

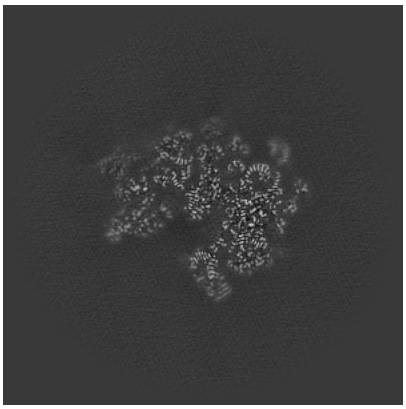
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

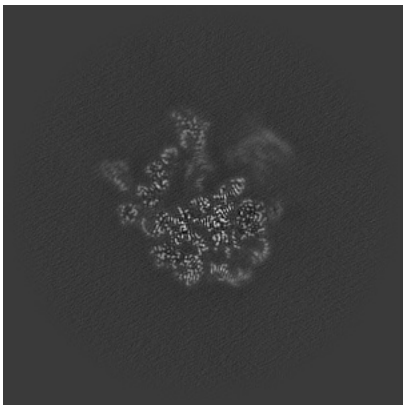
6.2.1 Primary map



X Index: 220

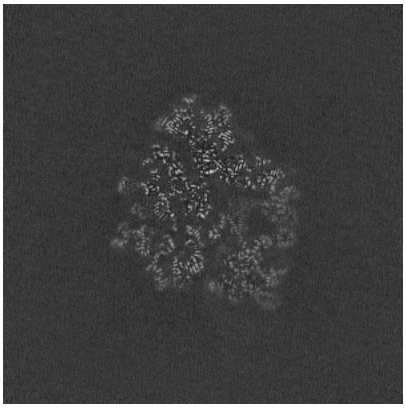


Y Index: 220

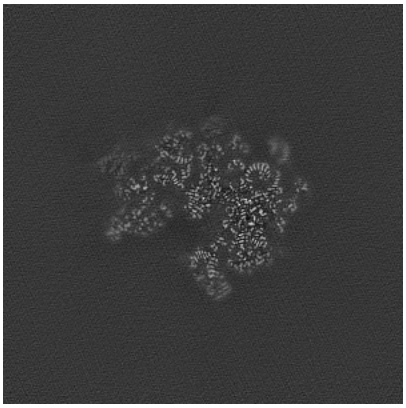


Z Index: 220

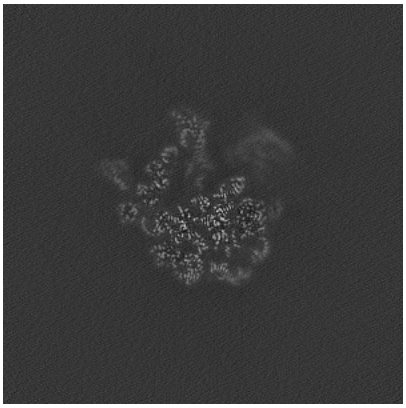
6.2.2 Raw map



X Index: 220



Y Index: 220

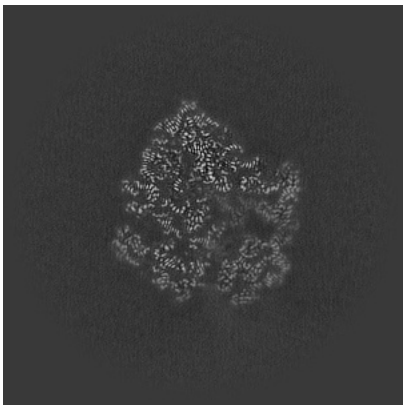


Z Index: 220

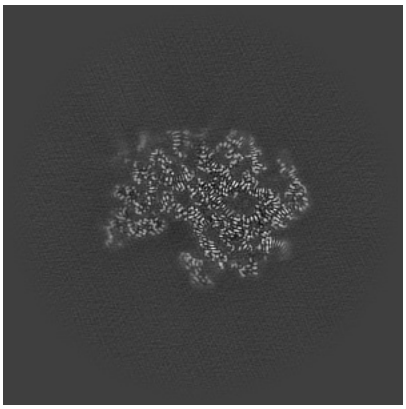
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

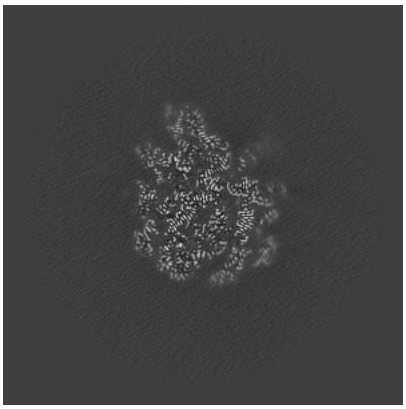
6.3.1 Primary map



X Index: 213

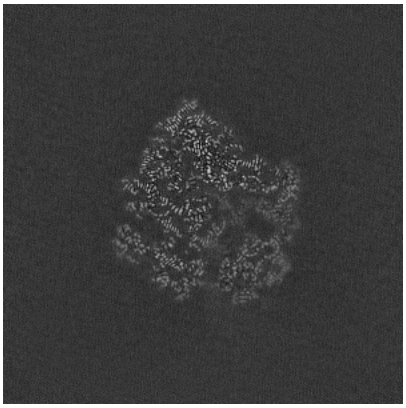


Y Index: 206

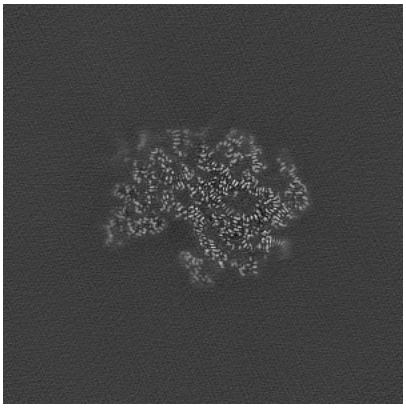


Z Index: 255

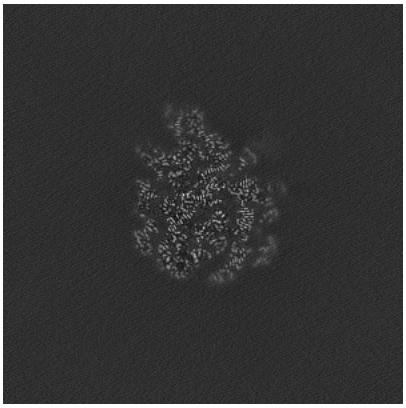
6.3.2 Raw map



X Index: 214



Y Index: 206

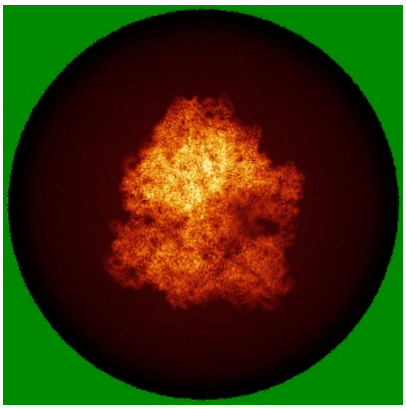


Z Index: 256

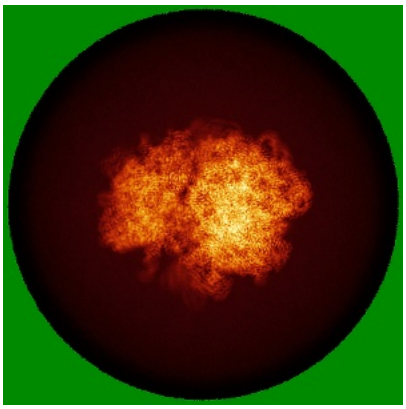
The images above show the largest variance slices of the map in three orthogonal directions.

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

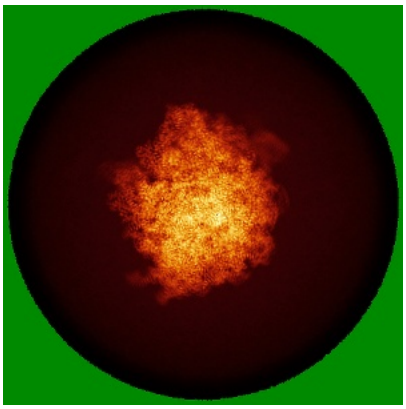
6.4.1 Primary map



X

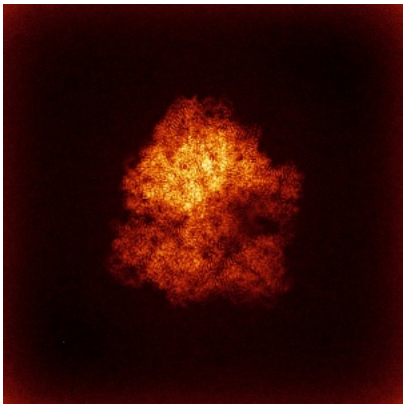


Y

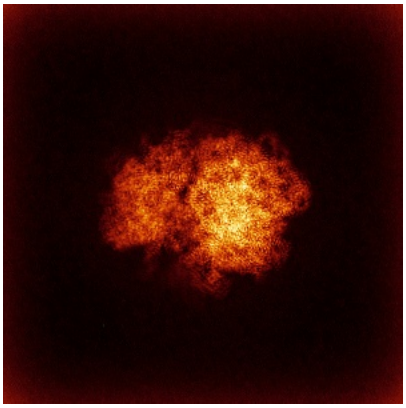


Z

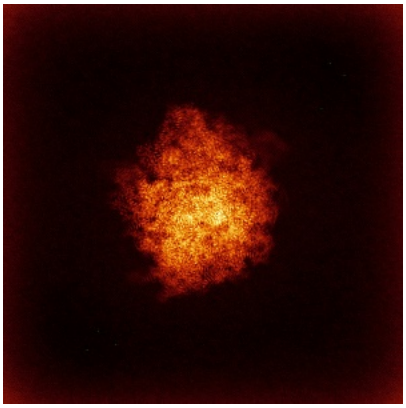
6.4.2 Raw map



X



Y

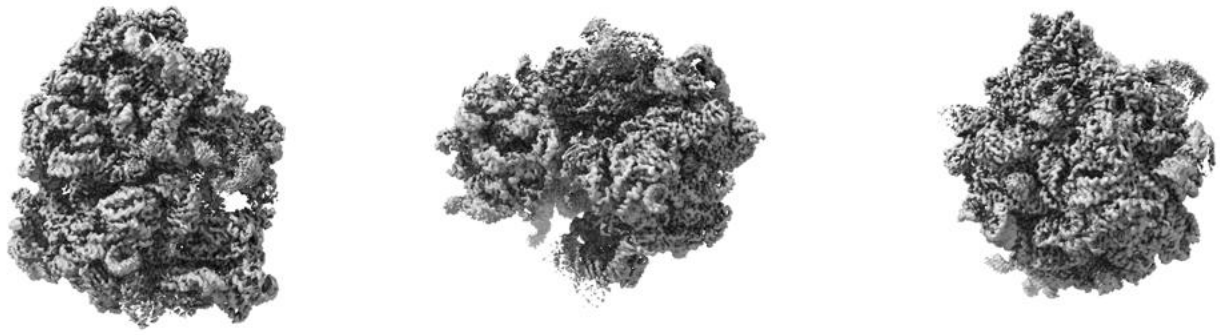


Z

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 0.07. 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.

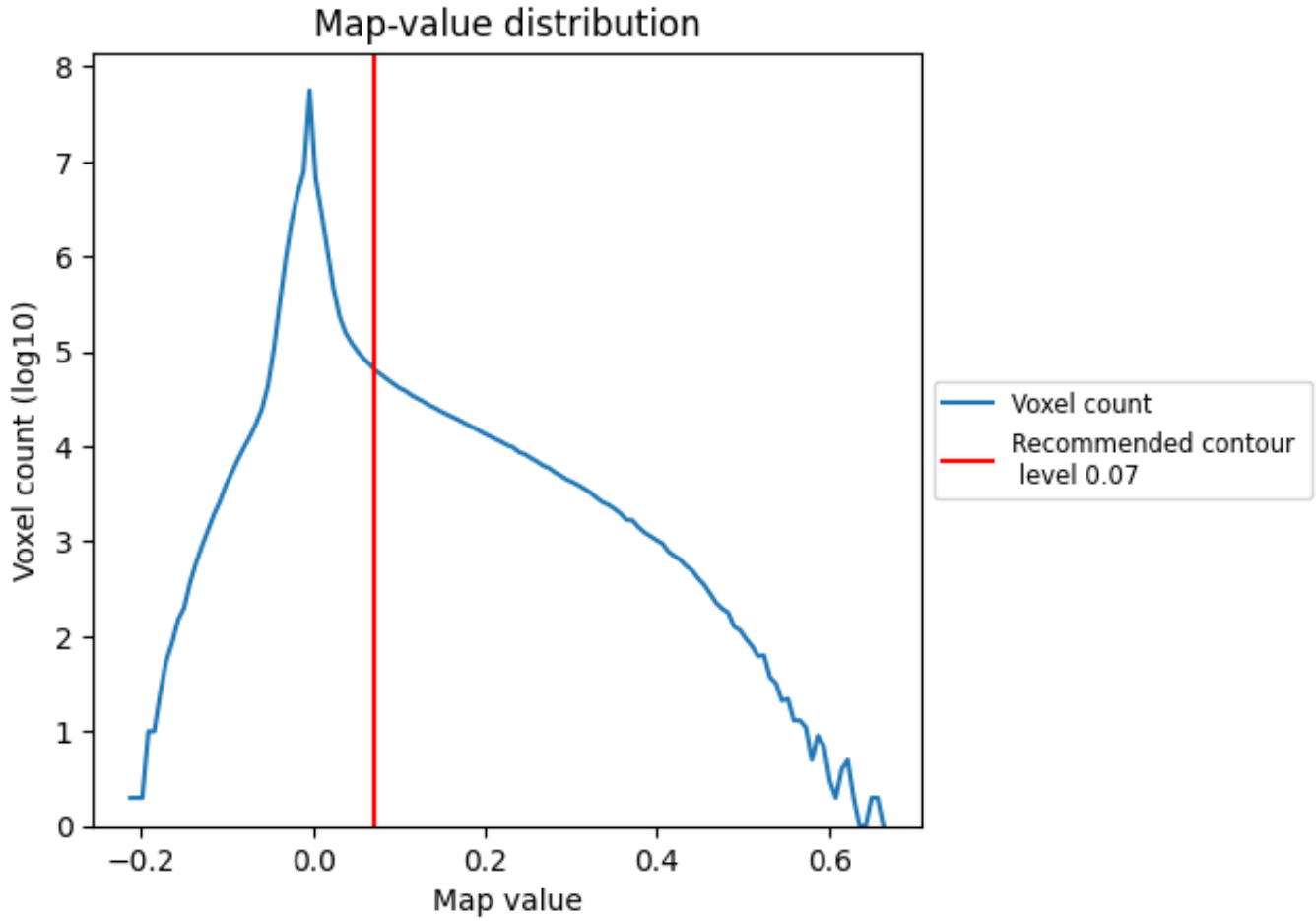
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

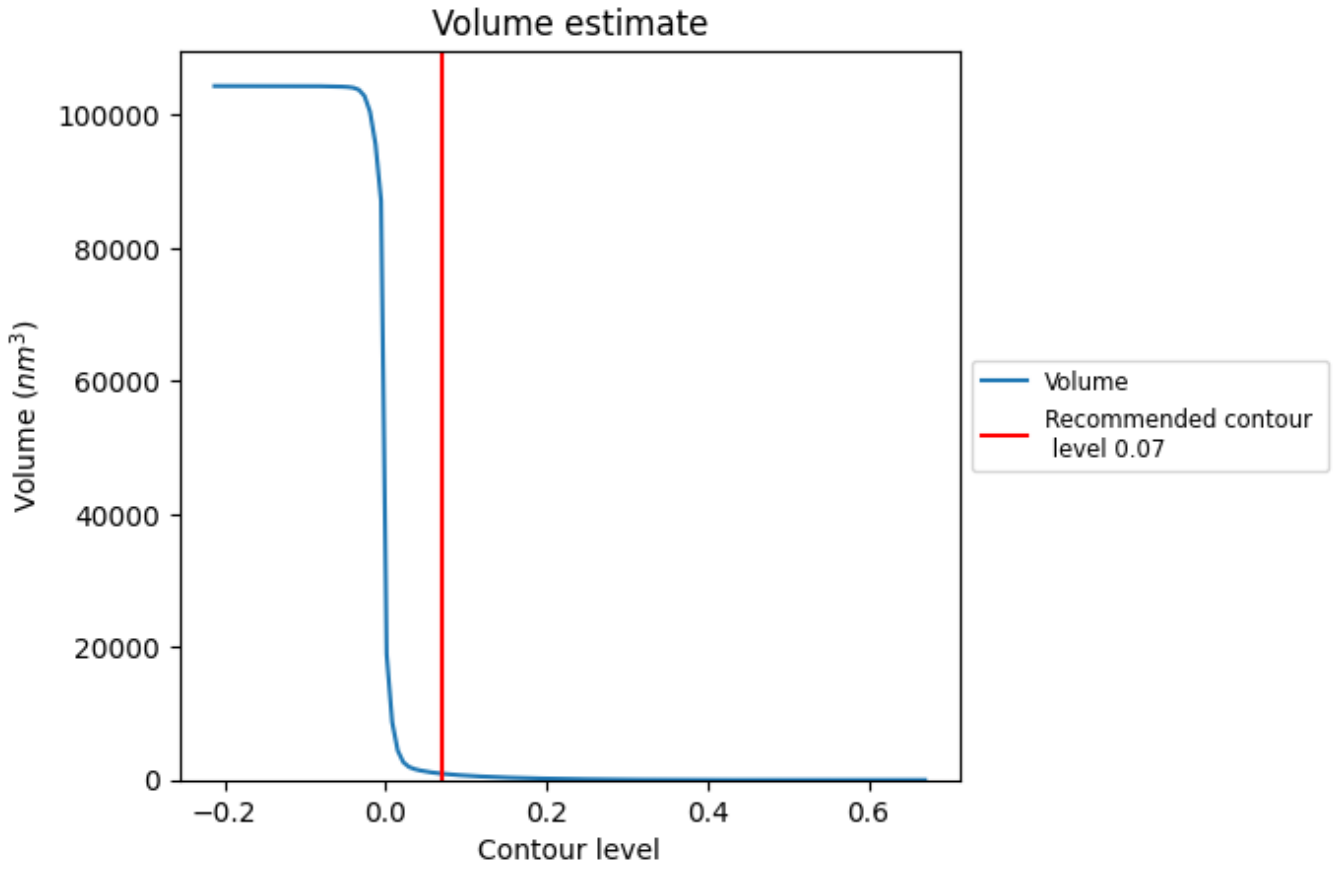
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

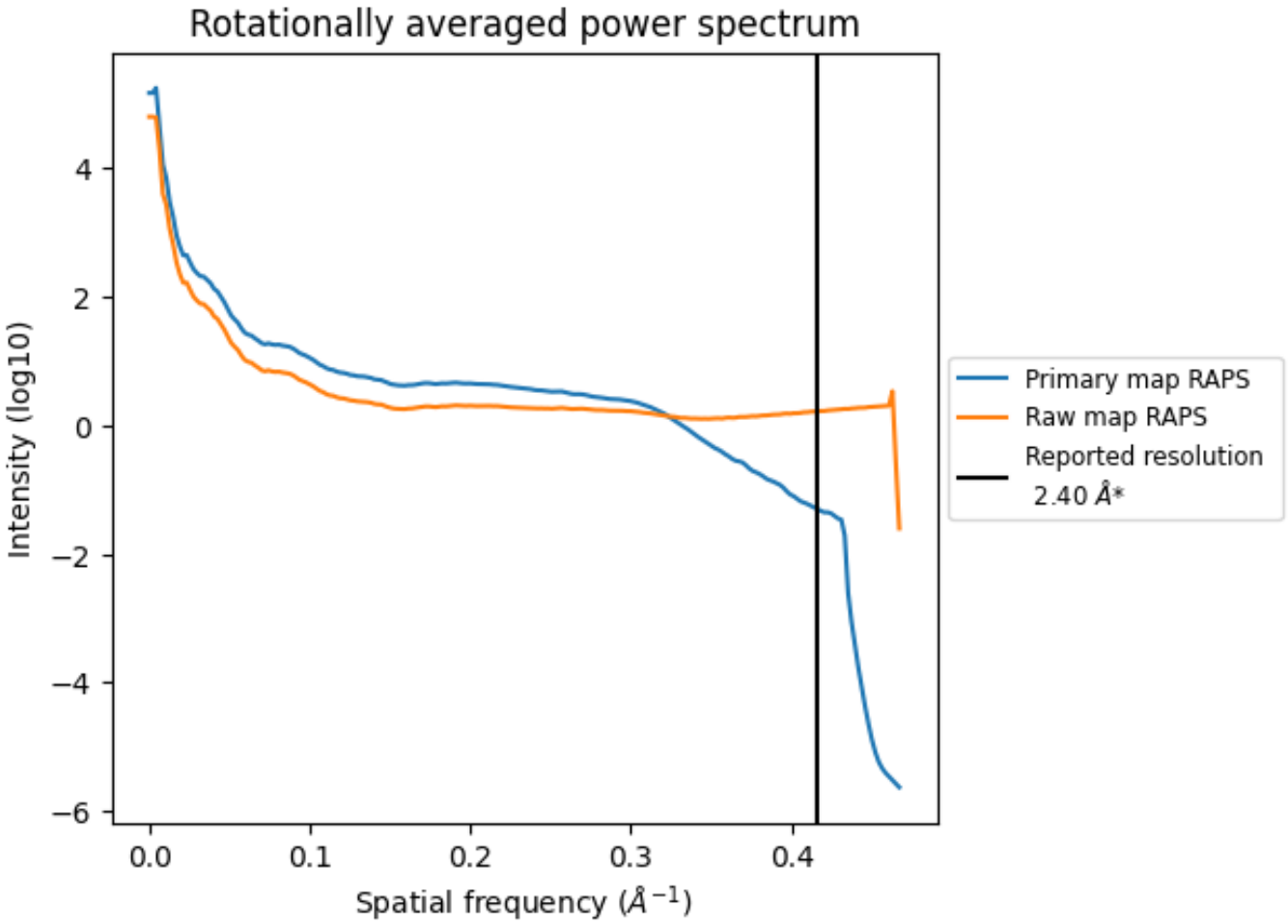
7.2 Volume estimate (i)



The volume at the recommended contour level is 946 nm^3; this corresponds to an approximate mass of 855 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)

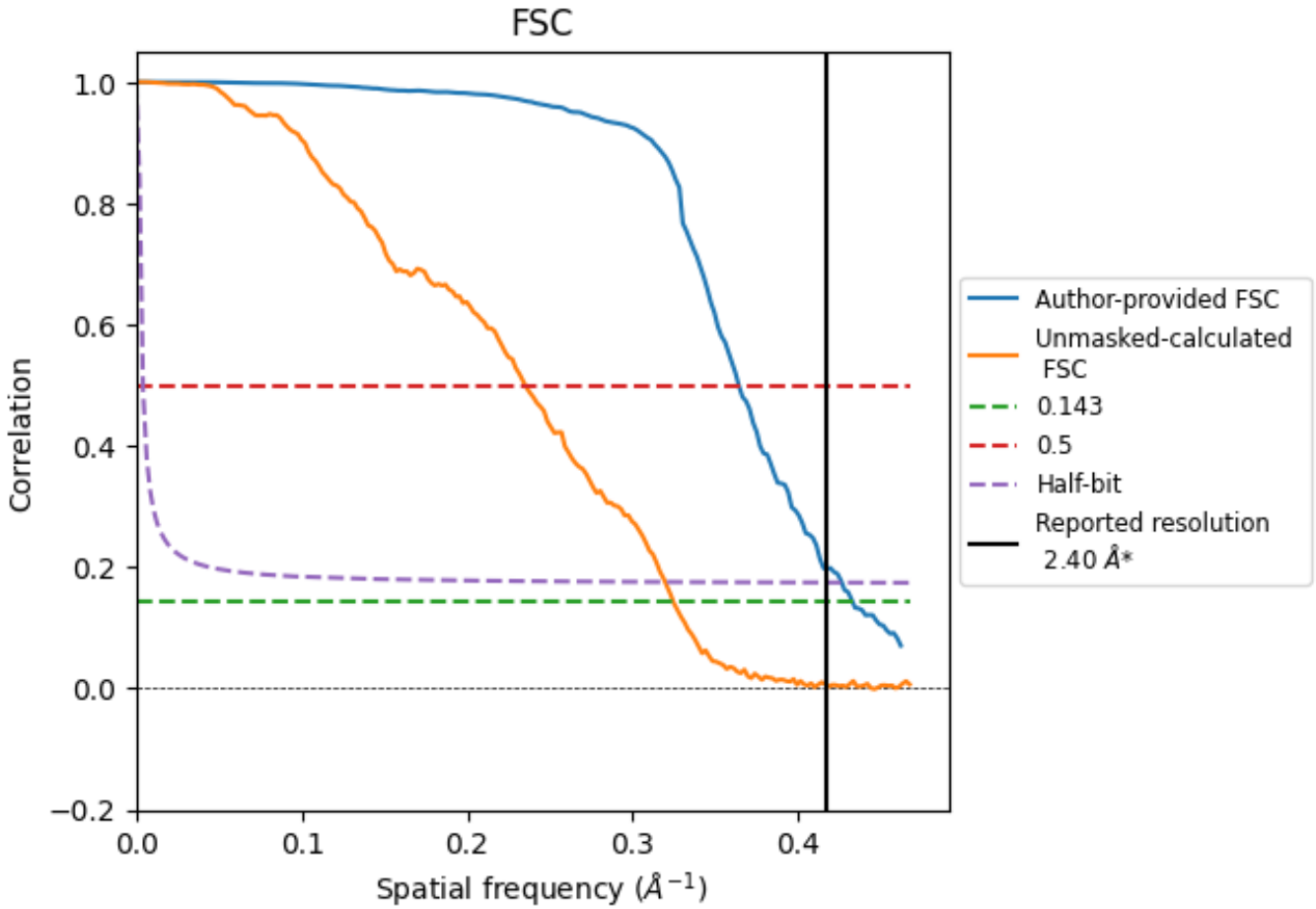


*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.417 Å^{-1}

8.2 Resolution estimates (i)

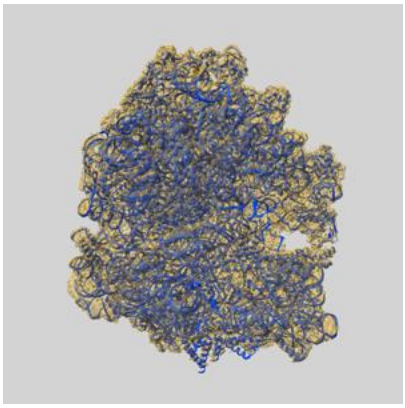
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.31	2.75	2.35
Unmasked-calculated*	3.08	4.25	3.13

*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 3.08 differs from the reported value 2.4 by more than 10 %

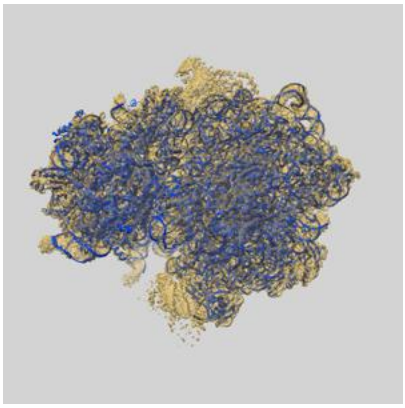
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-71667 and PDB model 9PIH. Per-residue inclusion information can be found in section 3 on page 17.

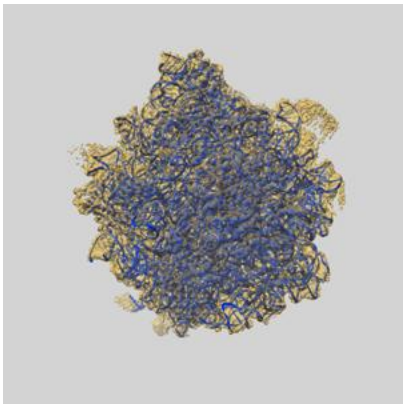
9.1 Map-model overlay



X



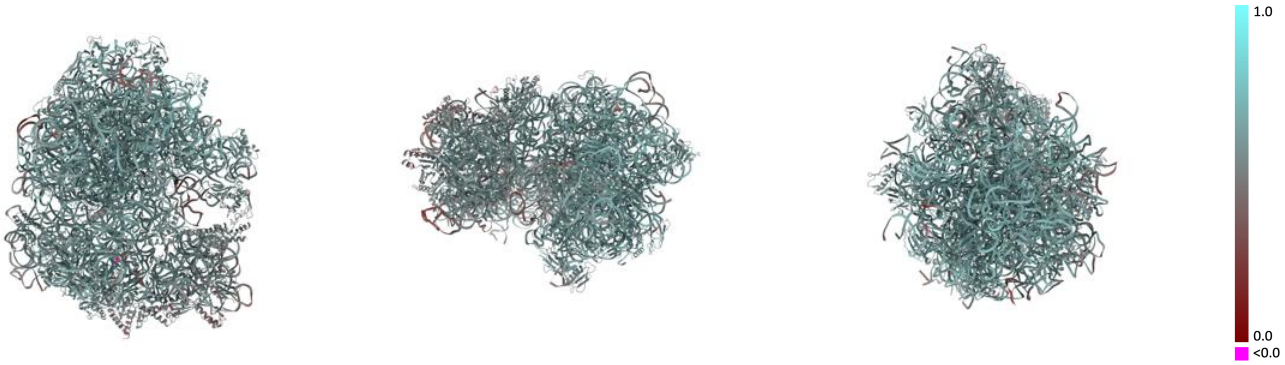
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

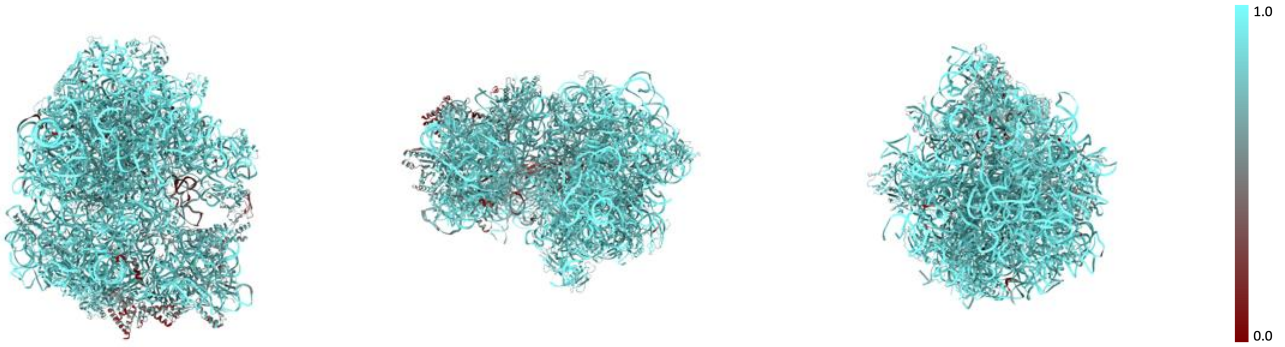
9.2 Q-score mapped to coordinate model (i)



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.

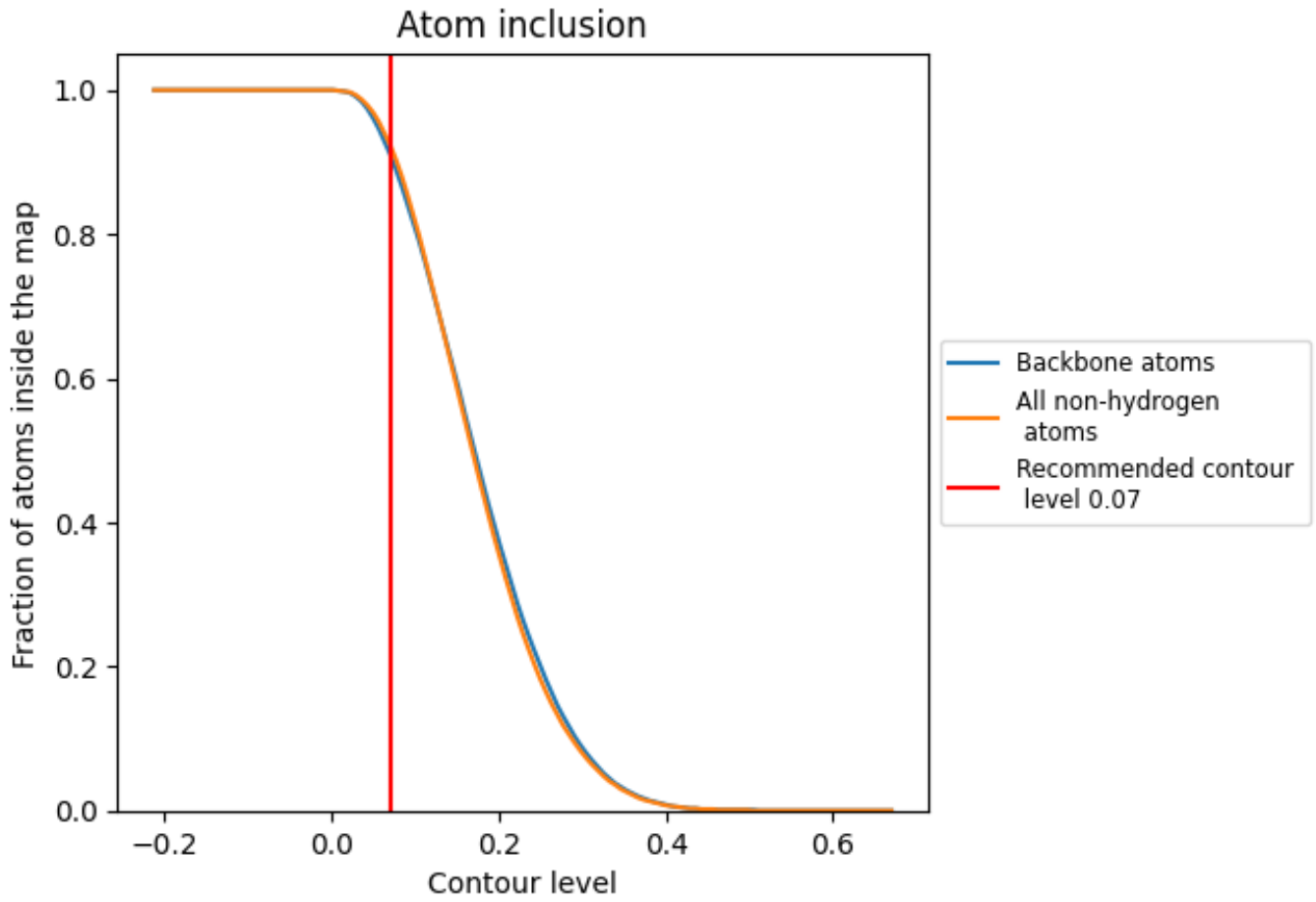
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9240	0.6050
0	0.8660	0.6140
1	0.9490	0.6600
2	0.9590	0.6500
3	0.9080	0.6270
4	0.3460	0.4780
A	0.9660	0.5890
B	0.4050	0.4960
C	0.7740	0.5530
D	0.8310	0.5740
E	0.8910	0.6050
F	0.8140	0.5460
G	0.7140	0.5240
H	0.8780	0.6000
I	0.7850	0.5290
J	0.6950	0.5040
K	0.8270	0.5750
L	0.8620	0.6050
M	0.7390	0.5260
N	0.7830	0.5540
O	0.8650	0.5820
P	0.8820	0.5950
Q	0.8400	0.5950
R	0.6790	0.5180
S	0.7300	0.5150
T	0.8660	0.5790
U	0.5400	0.5230
X	0.5740	0.4570
Z	0.5620	0.5270
a	0.9800	0.6280
b	0.9740	0.5930
c	0.9360	0.6510
d	0.9400	0.6420
e	0.9050	0.6170
f	0.7980	0.5380



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
g	0.8170	0.5540
h	0.7170	0.5510
i	0.9290	0.6380
j	0.9090	0.6380
k	0.9320	0.6340
l	0.9010	0.6330
m	0.9630	0.6440
n	0.8840	0.5800
o	0.8860	0.6280
p	0.9590	0.6490
q	0.9120	0.6250
r	0.9190	0.6350
s	0.8890	0.6010
t	0.8630	0.5880
u	0.8690	0.5960
v	0.9070	0.6430
w	0.9180	0.6280
x	0.8690	0.5710
y	0.8950	0.6170
z	0.9040	0.6350