wwPDB EM Validation Summary Report (i)

Sep 16, 2026 – 03:09 AM EDT

PDB ID	:	8G7R / pdb_00008g7r
EMDB ID	:	EMD-29821
Title	:	Structure of the Escherichia coli 70S ribosome in complex with A-site tRNAIle(LAU) bound to the cognate AUA codon (Structure III)
Authors	:	Rybak, M.Y.; Gagnon, M.G.
Deposited on	:	2023-02-16
Resolution	:	2.80 Å(reported)
Based on initial model	:	7K00

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:

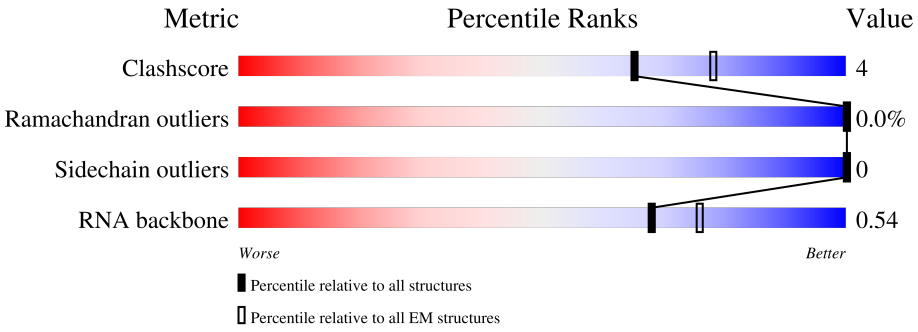
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

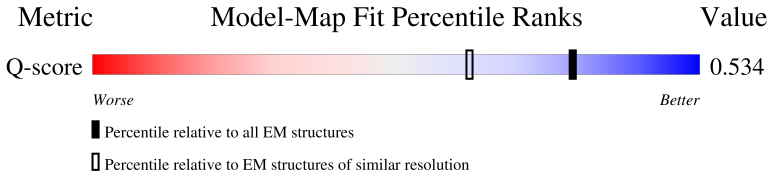
1 Overall quality at a glance

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

The reported resolution of this entry is 2.80 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	11806 (2.30 - 3.30)

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	1542	69% 27%
2	b	241	47% 67% 26% 7%
3	c	233	79% 10% 12%

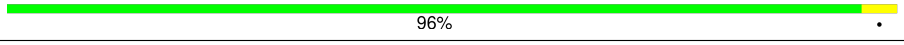
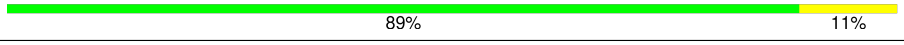
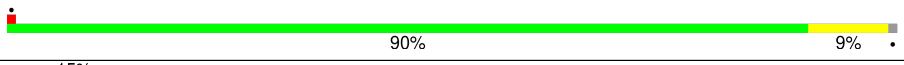
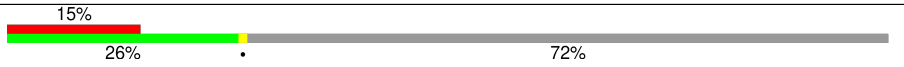
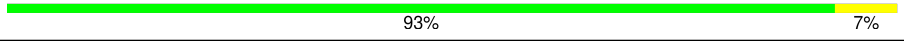
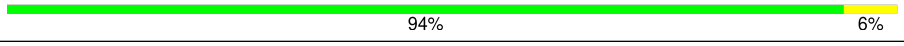
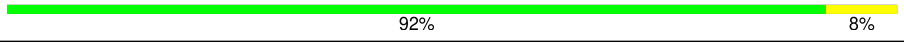
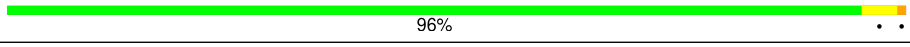
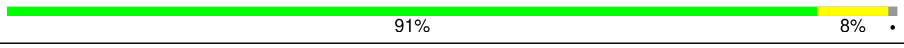
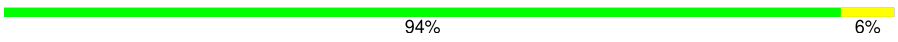
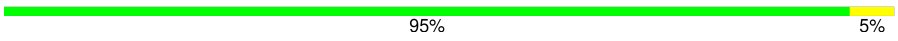
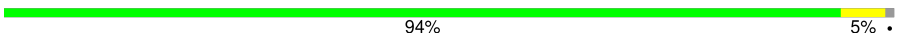
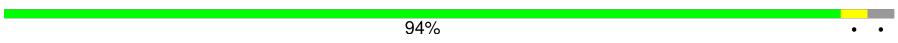
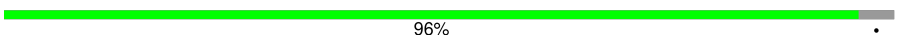
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Mol	Chain	Length	Quality of chain
4	d	206	85% 15%
5	e	167	83% 11% 7%
6	f	131	51% 27% 21%
7	g	156	84% 13%
8	h	130	91% 8%
9	i	130	75% 23%
10	j	103	71% 24% 5%
11	k	129	71% 19% 9%
12	l	124	91% 6%
13	m	118	81% 17%
14	n	101	83% 16%
15	o	89	89% 10%
16	p	82	80% 18%
17	q	84	81% 13% 6%
18	r	75	63% 9% 28%
19	s	92	72% 18% 10%
20	t	87	91% 8%
21	u	71	6% 72% 6% 23%
22	w	76	51% 33% 12%
22	y	76	39% 38% 13% 9%
23	x	77	66% 25% 8%
24	v	27	37% 59%
25	A	2904	77% 20%
26	B	120	79% 18%
27	C	273	92% 7%

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Mol	Chain	Length	Quality of chain
28	D	209	
29	E	201	
30	F	179	
31	G	177	
32	H	149	
33	L	142	
34	M	123	
35	N	144	
36	O	136	
37	P	127	
38	Q	117	
39	R	115	
40	S	118	
41	T	103	
42	U	110	
43	V	100	
44	W	104	
45	X	94	
46	Y	85	
47	Z	78	
48	1	63	
49	2	59	
50	3	70	
51	4	57	
52	5	55	

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Mol	Chain	Length	Quality of chain
53	6	46	
54	7	65	
55	8	38	

2 Entry composition (i)

There are 61 unique types of molecules in this entry. The entry contains 147376 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	1528	32803	14637	6019	10619	1528	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	1754	1110	315	321	8	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	206	1624	1028	305	288	3	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	1643	1026	315	298	4	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	156	1152	717	217	212	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	103	839	530	151	151	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	modified residue	UNP A0A0H3PWX2

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			446	283	85	78		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

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

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

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

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

- Molecule 22 is a RNA chain called Isoleucine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	w	76	Total	C	N	O	P	S	0	0
			1645	740	292	537	75	1		
22	y	76	Total	C	N	O	P	S	0	0
			1644	740	292	536	75	1		

- Molecule 23 is a RNA chain called P-site initiator tRNA.

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

- Molecule 24 is a RNA chain called M-I mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	11	Total	C	N	O	P	0	0
			239	108	49	71	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

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

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

- Molecule 36 is a protein called 50S ribosomal protein L16.

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	82	MS6	MET	modified residue	UNP E6BI61

- Molecule 37 is a protein called 50S ribosomal protein L17.

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

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called Ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	76	Total 582	C 360	N 117	O 104	S 1	0	0

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	60	Total	C	N	O	S	0	0
			468	290	87	85	6		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	5	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

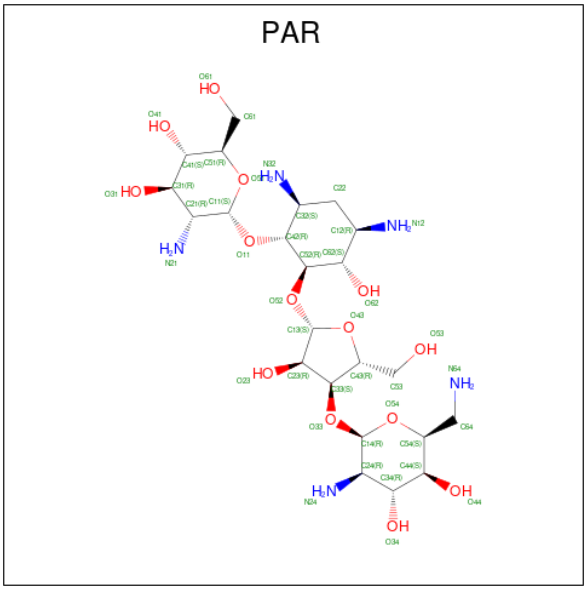
- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
56	a	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	a	91	Total	Mg	0
			91	91	
57	e	2	Total	Mg	0
			2	2	
57	l	1	Total	Mg	0
			1	1	
57	x	2	Total	Mg	0
			2	2	

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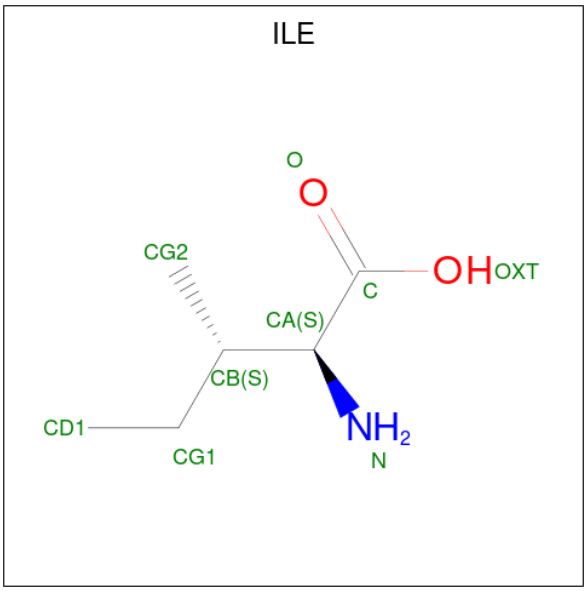
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
57	v	2	Total Mg 2 2	0
57	A	603	Total Mg 603 603	0
57	B	6	Total Mg 6 6	0
57	D	1	Total Mg 1 1	0
57	E	2	Total Mg 2 2	0
57	L	4	Total Mg 4 4	0
57	N	2	Total Mg 2 2	0
57	P	1	Total Mg 1 1	0
57	R	1	Total Mg 1 1	0
57	S	2	Total Mg 2 2	0
57	U	1	Total Mg 1 1	0
57	V	2	Total Mg 2 2	0
57	Y	1	Total Mg 1 1	0
57	4	7	Total Mg 7 7	0
57	8	3	Total Mg 3 3	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
58	a	1	Total K 1 1	0
58	l	1	Total K 1 1	0

- Molecule 59 is ISOLEUCINE (CCD ID: ILE) (formula: $C_6H_{13}NO_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
59	y	1	Total C N O 8 6 1 1	0

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
60	3	1	Total Zn 1 1	0
60	8	1	Total Zn 1 1	0

- Molecule 61 is water.

Mol	Chain	Residues	Atoms	AltConf
61	a	31	Total O 31 31	0
61	k	1	Total O 1 1	0
61	l	2	Total O 2 2	0
61	w	1	Total O 1 1	0
61	A	278	Total O 278 278	0
61	B	3	Total O 3 3	0

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Mol	Chain	Residues	Atoms	AltConf
61	D	2	Total O 2 2	0
61	L	2	Total O 2 2	0
61	T	1	Total O 1 1	0
61	U	2	Total O 2 2	0
61	V	2	Total O 2 2	0
61	Y	1	Total O 1 1	0
61	Z	2	Total O 2 2	0
61	4	3	Total O 3 3	0

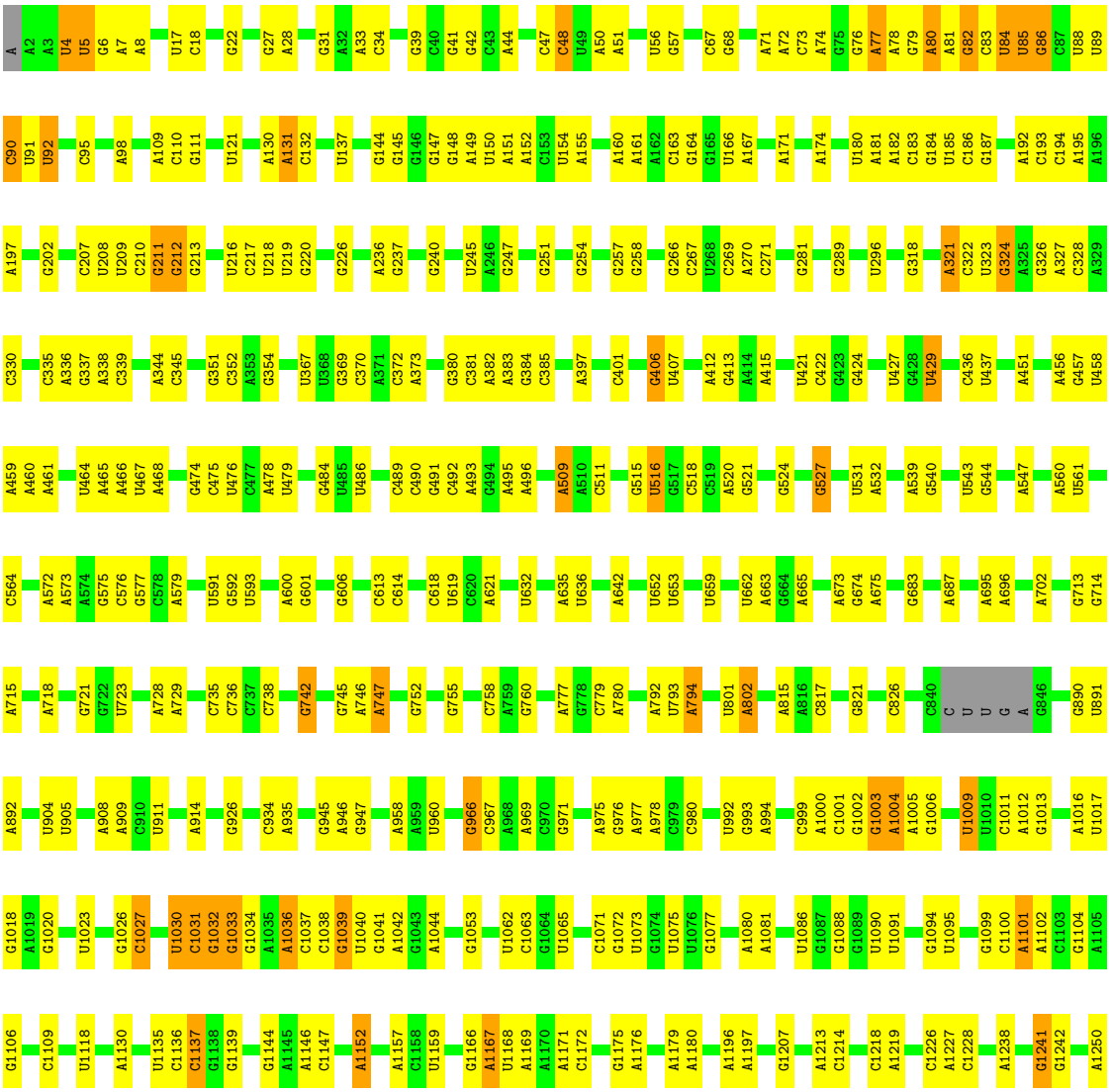
3 Residue-property plots (i)

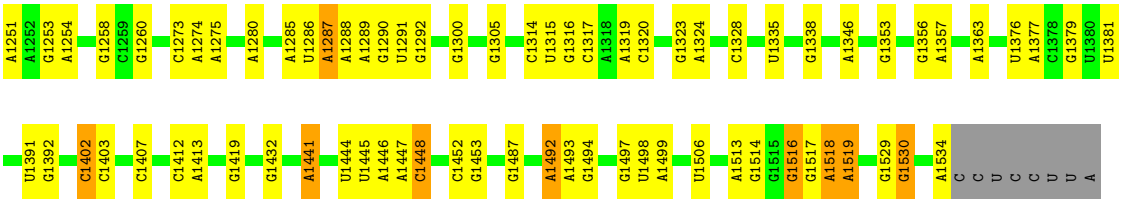
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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:



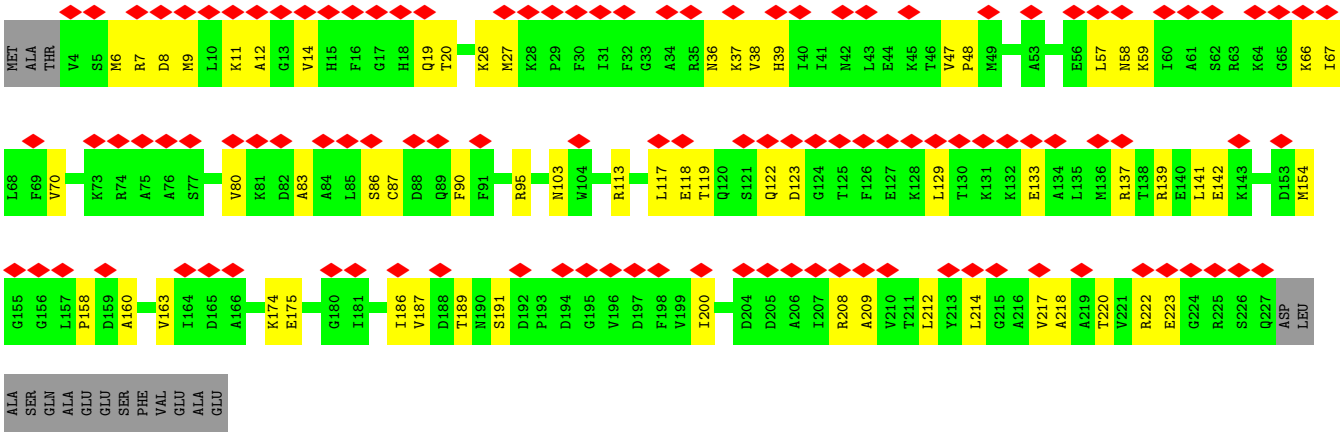




• Molecule 2: 30S ribosomal protein S2

Chain b:

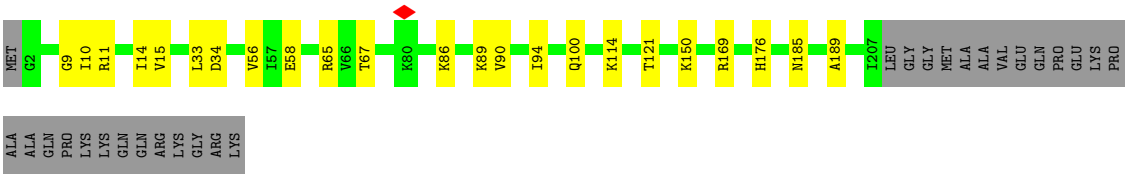




• Molecule 3: 30S ribosomal protein S3

Chain c:

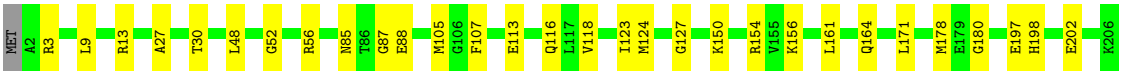




• Molecule 4: 30S ribosomal protein S4

Chain d:

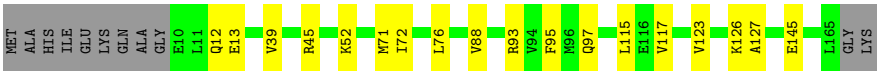




• Molecule 5: 30S ribosomal protein S5

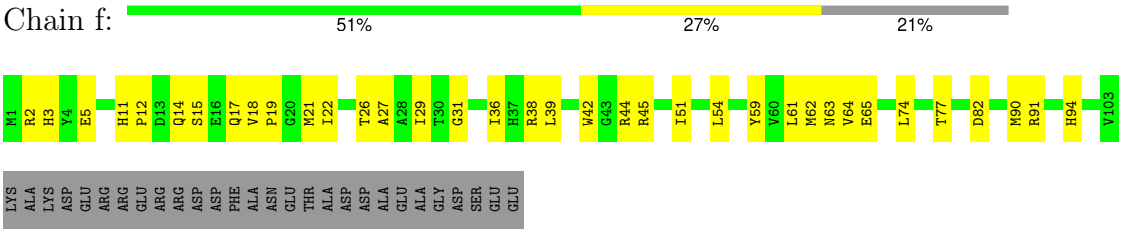
Chain e:





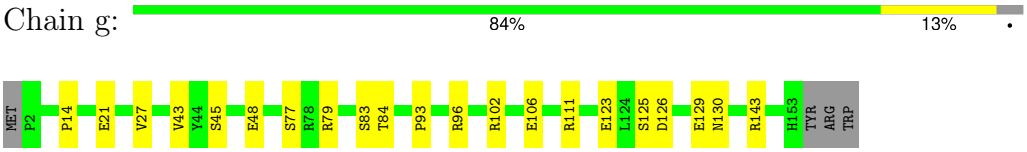
• Molecule 6: 30S ribosomal protein S6

Chain f:



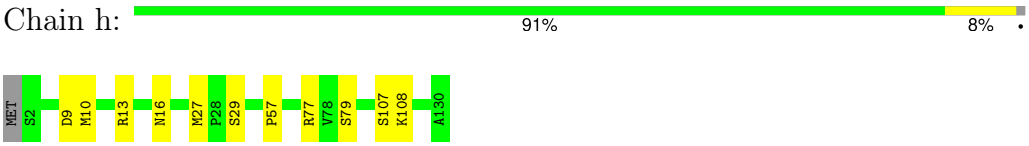
• Molecule 7: 30S ribosomal protein S7

Chain g:



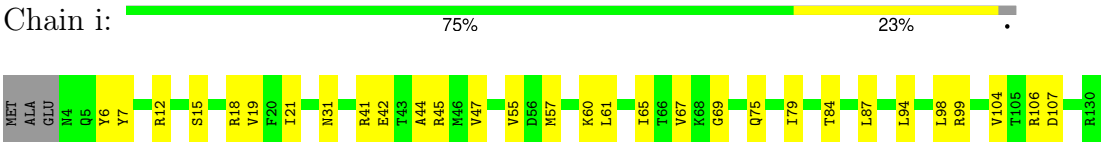
• Molecule 8: 30S ribosomal protein S8

Chain h:



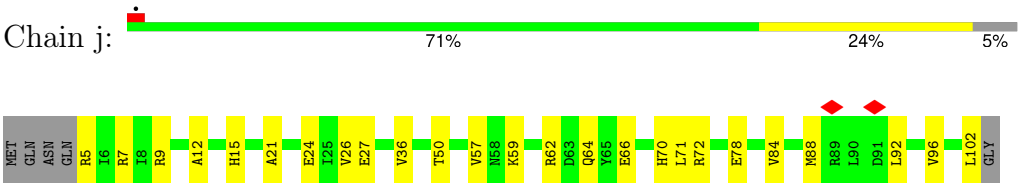
• Molecule 9: 30S ribosomal protein S9

Chain i:



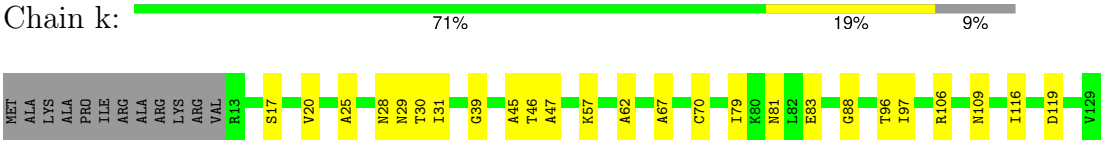
• Molecule 10: 30S ribosomal protein S10

Chain j:



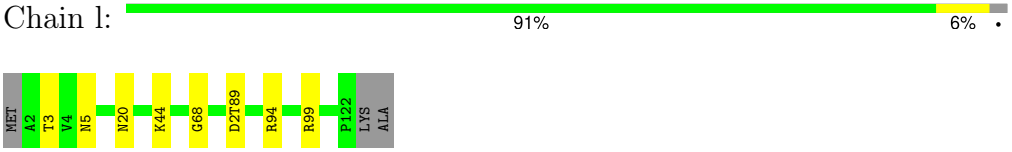
• Molecule 11: 30S ribosomal protein S11

Chain k:



• Molecule 12: 30S ribosomal protein S12

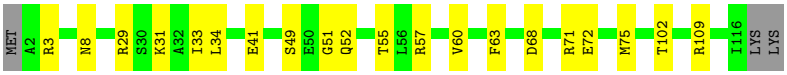
Chain l:



• Molecule 13: 30S ribosomal protein S13

Chain m:

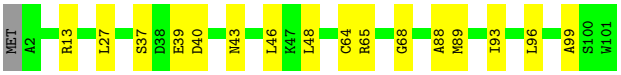




• Molecule 14: 30S ribosomal protein S14

Chain n:

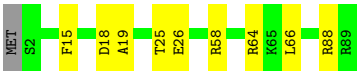




• Molecule 15: 30S ribosomal protein S15

Chain o:

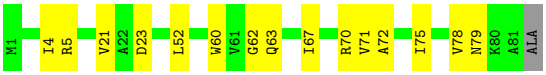




• Molecule 16: 30S ribosomal protein S16

Chain p:





• Molecule 17: 30S ribosomal protein S17

Chain q:

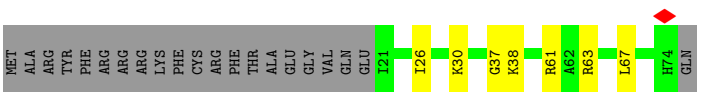




• Molecule 18: 30S ribosomal protein S18

Chain r:

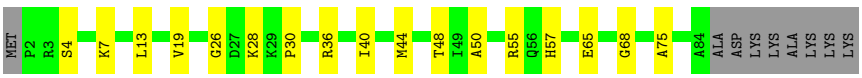




• Molecule 19: 30S ribosomal protein S19

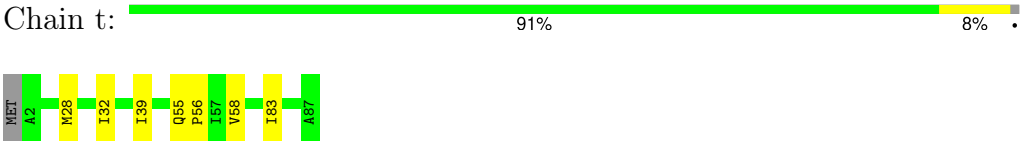
Chain s:





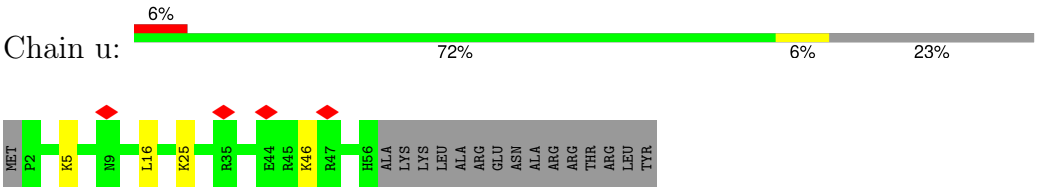
• Molecule 20: 30S ribosomal protein S20

Chain t:



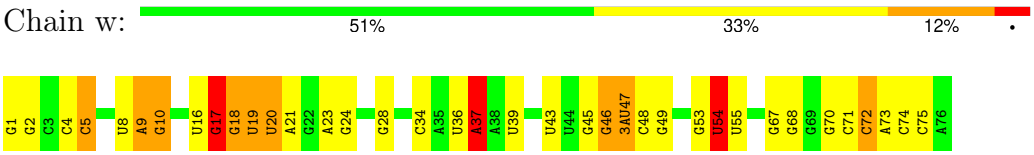
• Molecule 21: 30S ribosomal protein S21

Chain u:



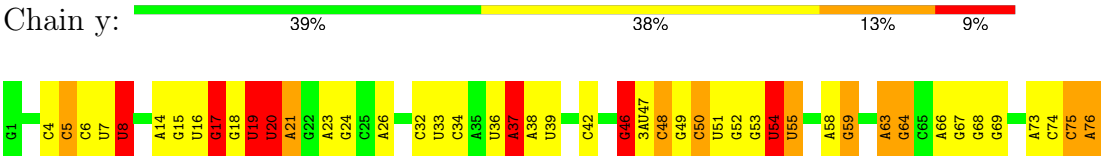
• Molecule 22: Isoleucine tRNA

Chain w:



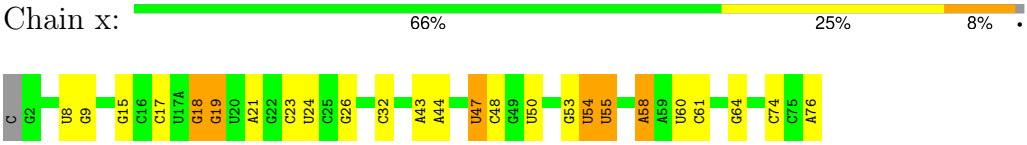
• Molecule 22: Isoleucine tRNA

Chain y:



• Molecule 23: P-site initiator tRNA

Chain x:



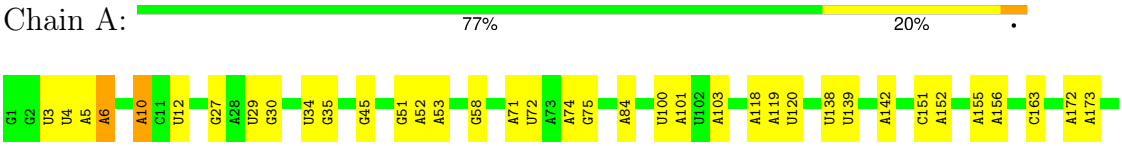
• Molecule 24: M-I mRNA

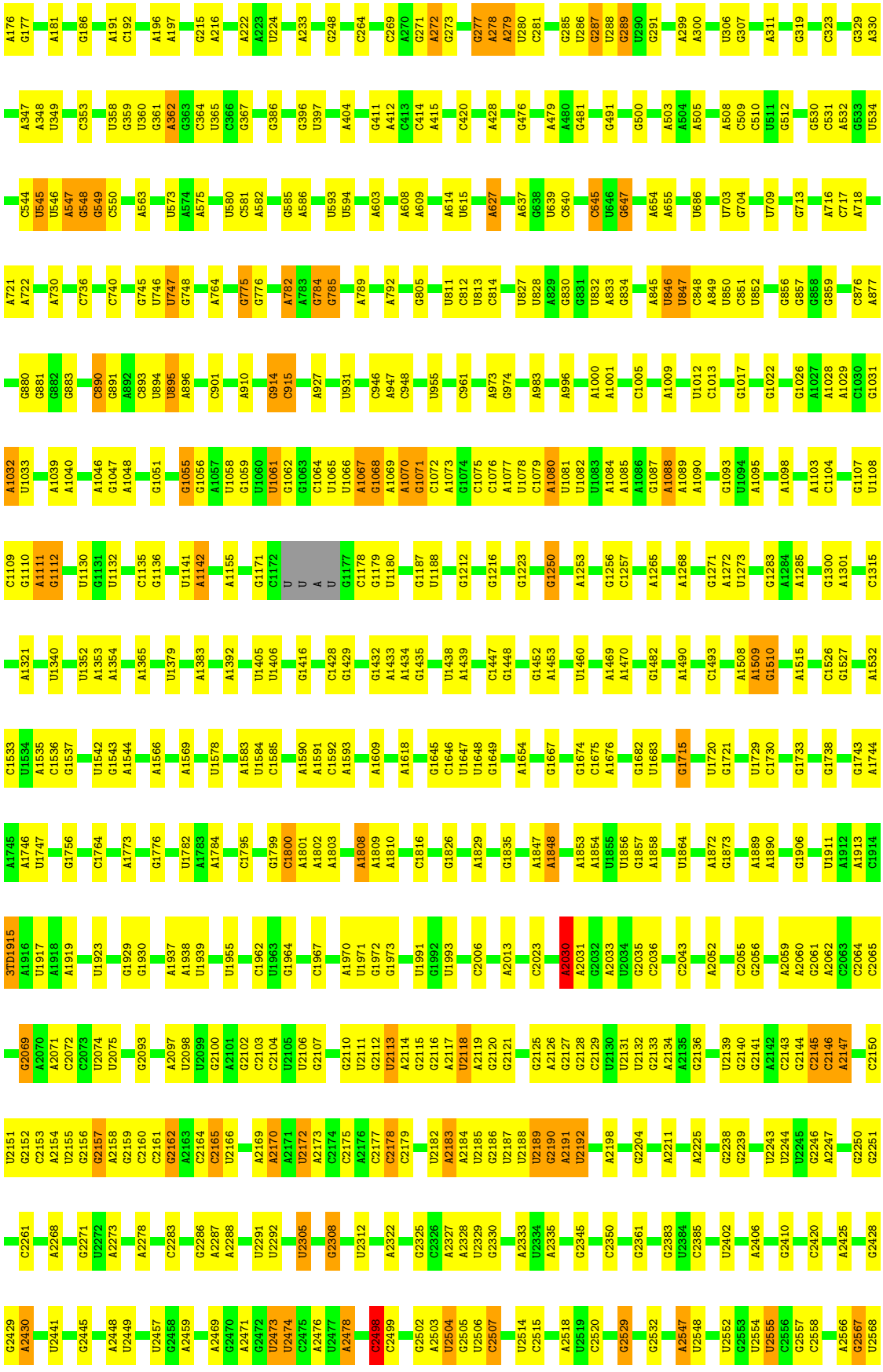
Chain v:

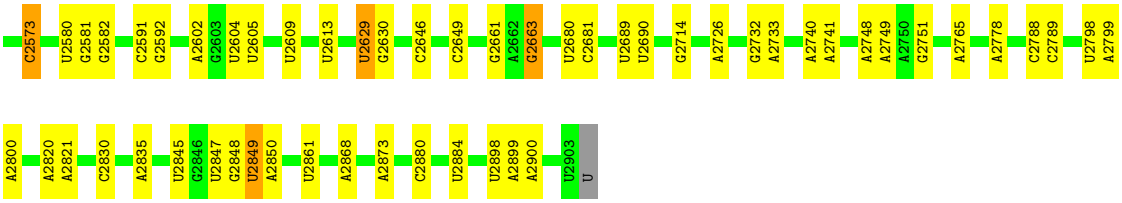


• Molecule 25: 23S Ribosomal RNA

Chain A:



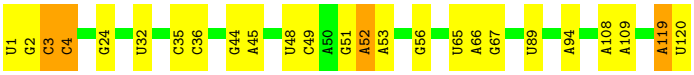




• Molecule 26: 5S Ribosomal RNA

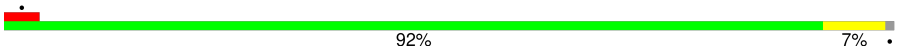
Chain B:

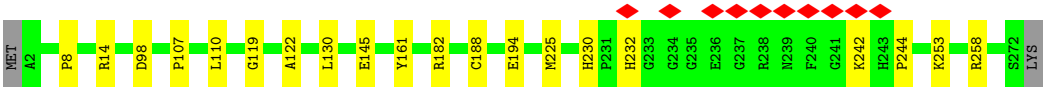




• Molecule 27: 50S ribosomal protein L2

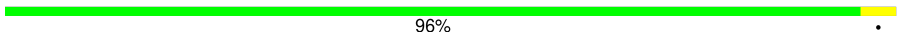
Chain C:





• Molecule 28: 50S ribosomal protein L3

Chain D:

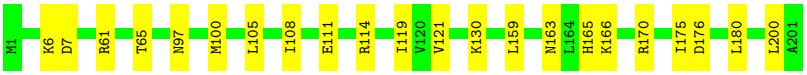




• Molecule 29: 50S ribosomal protein L4

Chain E:





• Molecule 30: 50S ribosomal protein L5

Chain F:

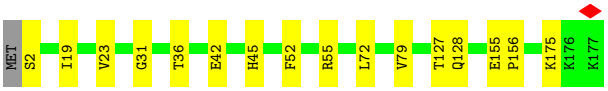




• Molecule 31: 50S ribosomal protein L6

Chain G:

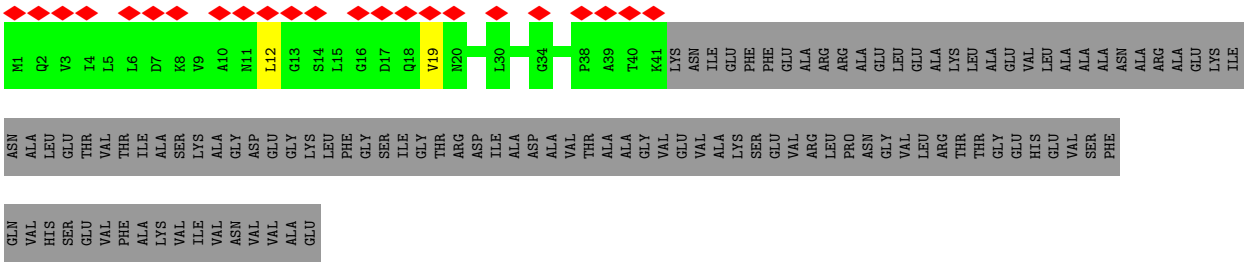




• Molecule 32: 50S ribosomal protein L9

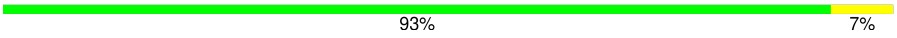
Chain H:





• Molecule 33: 50S ribosomal protein L13

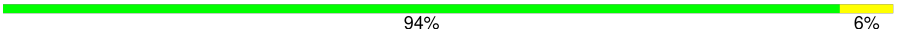
Chain L:

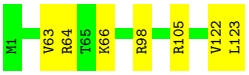




• Molecule 34: 50S ribosomal protein L14

Chain M:

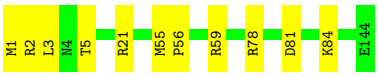




• Molecule 35: 50S ribosomal protein L15

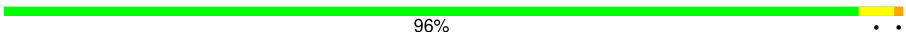
Chain N:





• Molecule 36: 50S ribosomal protein L16

Chain O:

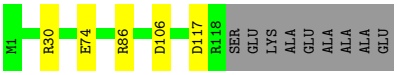




• Molecule 37: 50S ribosomal protein L17

Chain P:





• Molecule 38: 50S ribosomal protein L18

Chain Q:





• Molecule 39: 50S ribosomal protein L19

Chain R:





• Molecule 40: 50S ribosomal protein L20

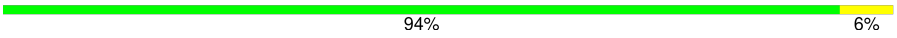
Chain S:

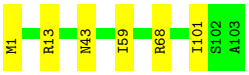




• Molecule 41: Ribosomal protein L21

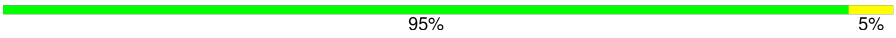
Chain T:

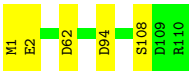




• Molecule 42: 50S ribosomal protein L22

Chain U:

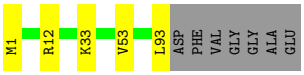




• Molecule 43: 50S ribosomal protein L23

Chain V:

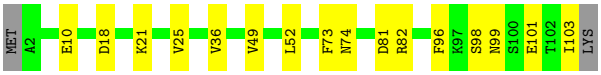




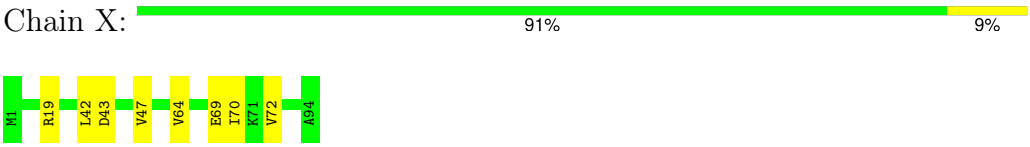
• Molecule 44: 50S ribosomal protein L24

Chain W:

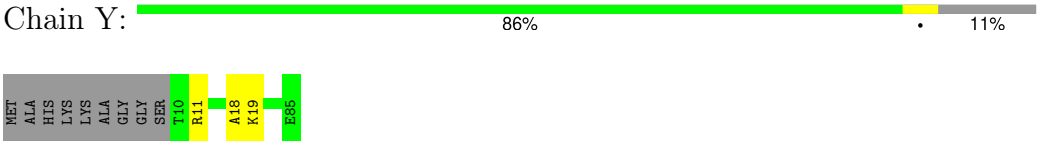




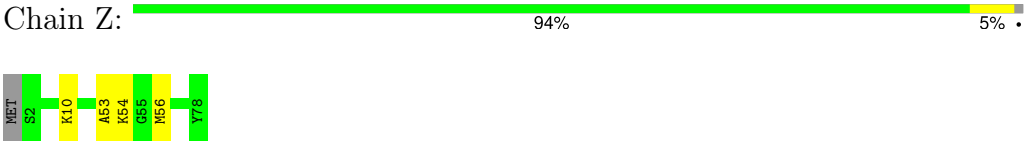
• Molecule 45: 50S ribosomal protein L25



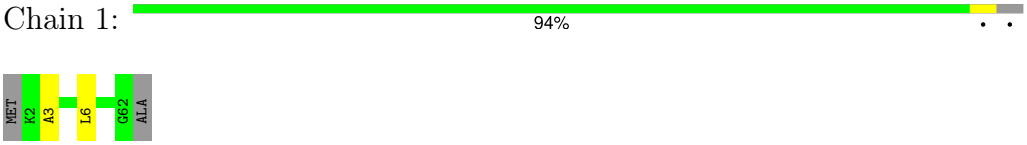
• Molecule 46: 50S ribosomal protein L27



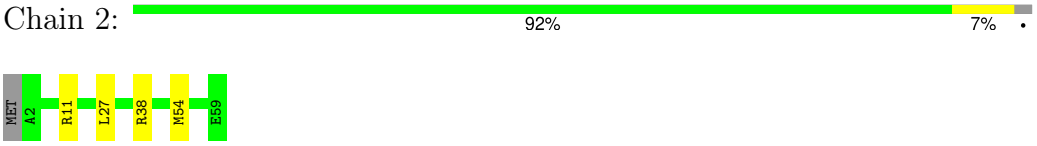
• Molecule 47: 50S ribosomal protein L28



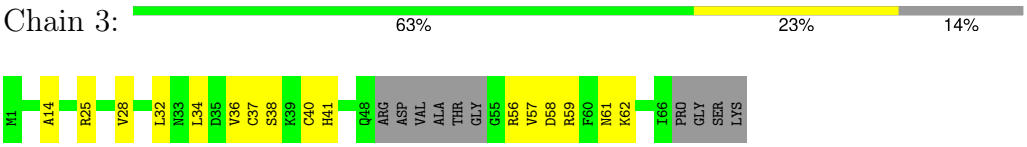
• Molecule 48: 50S ribosomal protein L29



• Molecule 49: 50S ribosomal protein L30



• Molecule 50: 50S ribosomal protein L31



• Molecule 51: 50S ribosomal protein L32

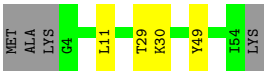




• Molecule 52: 50S ribosomal protein L33

Chain 5:

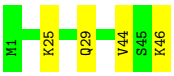




• Molecule 53: 50S ribosomal protein L34

Chain 6:

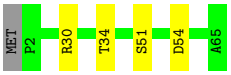




• Molecule 54: 50S ribosomal protein L35

Chain 7:

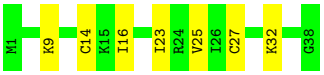




• Molecule 55: 50S ribosomal protein L36

Chain 8:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	466262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.865	Depositor
Minimum map value	-0.587	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PAR, OMC, G7M, 5MU, ZN, MS6, 4SU, 3TD, IAS, OMG, 1MG, T6A, UR3, K, 2MA, D2T, MEQ, MA6, 4OC, 6MZ, M3X, 5MC, OMU, PSU, 2MG, 3AU, H2U, MG, 4D4

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	0.16	0/36450	0.28	0/56856
2	b	0.13	0/1785	0.39	0/2404
3	c	0.14	0/1651	0.32	0/2225
4	d	0.12	0/1665	0.28	0/2227
5	e	0.15	0/1165	0.33	0/1568
6	f	0.13	0/858	0.35	0/1160
7	g	0.14	0/1206	0.33	0/1617
8	h	0.15	0/989	0.30	0/1326
9	i	0.12	0/1034	0.28	0/1375
10	j	0.12	0/796	0.34	0/1077
11	k	0.14	0/884	0.29	0/1191
12	l	0.16	0/945	0.36	0/1268
13	m	0.12	0/900	0.32	0/1204
14	n	0.11	0/817	0.25	0/1088
15	o	0.15	0/722	0.29	0/964
16	p	0.14	0/653	0.39	0/877
17	q	0.15	0/650	0.33	0/871
18	r	0.12	0/453	0.25	0/609
19	s	0.11	0/680	0.26	0/915
20	t	0.16	0/676	0.35	0/895
21	u	0.10	0/467	0.23	0/620
22	w	0.21	0/1550	0.28	0/2411
22	y	0.31	2/1549 (0.1%)	0.31	0/2408
23	x	0.18	0/1725	0.26	0/2689
24	v	0.16	0/269	0.27	0/417
25	A	0.23	1/69147 (0.0%)	0.33	0/107869
26	B	0.18	0/2876	0.31	0/4483
27	C	0.19	0/2121	0.32	0/2852
28	D	0.22	0/1576	0.35	0/2119
29	E	0.16	0/1571	0.31	0/2113
30	F	0.12	0/1434	0.29	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	G	0.14	0/1343	0.30	0/1816
32	H	0.11	0/306	0.34	0/413
33	L	0.20	0/1152	0.32	0/1551
34	M	0.20	0/955	0.36	0/1279
35	N	0.18	0/1061	0.29	0/1412
36	O	0.20	0/1073	0.32	0/1433
37	P	0.21	0/958	0.33	0/1281
38	Q	0.15	0/902	0.32	0/1209
39	R	0.18	0/929	0.28	0/1242
40	S	0.22	0/960	0.28	0/1278
41	T	0.19	0/829	0.34	0/1107
42	U	0.19	0/864	0.29	0/1156
43	V	0.16	0/744	0.31	0/994
44	W	0.19	0/787	0.51	2/1051 (0.2%)
45	X	0.18	0/766	0.29	0/1025
46	Y	0.18	0/589	0.40	0/779
47	Z	0.19	0/635	0.31	0/848
48	1	0.15	0/496	0.24	0/660
49	2	0.18	0/453	0.32	0/605
50	3	0.10	0/475	0.30	0/633
51	4	0.20	0/440	0.33	0/588
52	5	0.16	0/424	0.33	0/565
53	6	0.22	0/380	0.30	0/498
54	7	0.21	0/513	0.32	0/676
55	8	0.22	0/303	0.40	0/397
All	All	0.20	3/157601 (0.0%)	0.31	2/236120 (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
36	O	0	1
54	7	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	76	A	C6-N6	7.01	1.48	1.33
22	y	37	T6A	O3'-P	5.03	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2552	OMU	O3'-P	5.02	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	W	98	SER	CA-C-N	6.47	133.90	121.54
44	W	98	SER	C-N-CA	6.47	133.90	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	7	30	ARG	Peptide
36	O	81	4D4	Mainchain

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	32803	0	16528	247	0
2	b	1754	0	1782	43	0
3	c	1624	0	1696	15	0
4	d	1643	0	1707	23	0
5	e	1152	0	1196	10	0
6	f	839	0	833	29	0
7	g	1191	0	1244	15	0
8	h	979	0	1031	8	0
9	i	1022	0	1070	23	0
10	j	786	0	828	14	0
11	k	877	0	884	14	0
12	l	942	0	999	5	0
13	m	891	0	952	14	0
14	n	805	0	844	11	0
15	o	714	0	734	7	0
16	p	643	0	661	10	0
17	q	641	0	682	7	0
18	r	446	0	472	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	s	663	0	688	11	0
20	t	670	0	719	5	0
21	u	460	0	486	4	0
22	w	1645	0	834	14	0
22	y	1644	0	833	42	0
23	x	1625	0	829	13	0
24	v	239	0	120	0	0
25	A	62252	0	31333	274	0
26	B	2572	0	1301	11	0
27	C	2082	0	2154	17	0
28	D	1566	0	1618	6	0
29	E	1552	0	1619	14	0
30	F	1410	0	1444	20	0
31	G	1323	0	1371	10	0
32	H	303	0	327	2	0
33	L	1129	0	1162	7	0
34	M	946	0	1023	9	0
35	N	1052	0	1127	8	0
36	O	1075	0	1146	3	0
37	P	945	0	989	4	0
38	Q	892	0	923	7	0
39	R	917	0	962	8	0
40	S	947	0	1019	8	0
41	T	816	0	839	4	0
42	U	857	0	922	3	0
43	V	738	0	807	4	0
44	W	779	0	831	8	0
45	X	753	0	780	5	0
46	Y	582	0	599	3	0
47	Z	625	0	652	3	0
48	1	495	0	526	1	0
49	2	449	0	488	2	0
50	3	468	0	460	12	0
51	4	434	0	445	0	0
52	5	417	0	451	3	0
53	6	377	0	418	2	0
54	7	504	0	572	2	0
55	8	302	0	340	5	0
56	a	42	0	45	0	0
57	4	7	0	0	0	0
57	8	3	0	0	0	0
57	A	603	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B	6	0	0	0	0
57	D	1	0	0	0	0
57	E	2	0	0	0	0
57	L	4	0	0	0	0
57	N	2	0	0	0	0
57	P	1	0	0	0	0
57	R	1	0	0	0	0
57	S	2	0	0	0	0
57	U	1	0	0	0	0
57	V	2	0	0	0	0
57	Y	1	0	0	0	0
57	a	91	0	0	0	0
57	e	2	0	0	0	0
57	l	1	0	0	0	0
57	v	2	0	0	0	0
57	x	2	0	0	0	0
58	a	1	0	0	0	0
58	l	1	0	0	0	0
59	y	8	0	10	0	0
60	3	1	0	0	0	0
60	8	1	0	0	0	0
61	4	3	0	0	0	0
61	A	278	0	0	2	0
61	B	3	0	0	0	0
61	D	2	0	0	0	0
61	L	2	0	0	0	0
61	T	1	0	0	0	0
61	U	2	0	0	0	0
61	V	2	0	0	0	0
61	Y	1	0	0	0	0
61	Z	2	0	0	0	0
61	a	31	0	0	0	0
61	k	1	0	0	0	0
61	l	2	0	0	0	0
61	w	1	0	0	0	0
All	All	147376	0	97355	943	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 4.

The worst 5 of 943 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:1093:G:N2	25:A:1098:A:H62	1.38	1.19
25:A:1093:G:H21	25:A:1098:A:N6	1.43	1.17
1:a:1088:G:N2	1:a:1167:A:H61	1.49	1.07
1:a:1088:G:H21	1:a:1167:A:N6	1.53	1.05
22:y:15:G:N2	22:y:48:C:H42	1.61	0.98

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	222/241 (92%)	203 (91%)	19 (9%)	0	100	100
3	c	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
4	d	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	e	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	f	101/131 (77%)	95 (94%)	6 (6%)	0	100	100
7	g	150/156 (96%)	142 (95%)	8 (5%)	0	100	100
8	h	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	i	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
10	j	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	38
11	k	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
12	l	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
13	m	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	n	98/101 (97%)	98 (100%)	0	0	100	100
15	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	p	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
17	q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	52/75 (69%)	48 (92%)	4 (8%)	0	100	100
19	s	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
20	t	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	u	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
27	C	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
28	D	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
29	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
30	F	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
31	G	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
32	H	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
33	L	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	M	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
35	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
36	O	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
37	P	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
38	Q	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
39	R	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
40	S	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
41	T	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
42	U	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
43	V	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
44	W	100/104 (96%)	94 (94%)	5 (5%)	1 (1%)	12	38
45	X	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	Y	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
47	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
48	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
49	2	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	3	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
51	4	53/57 (93%)	53 (100%)	0	0	100	100
52	5	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
53	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	7	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5446/5886 (92%)	5223 (96%)	221 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	j	57	VAL
44	W	99	ASN

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	186/199 (94%)	186 (100%)	0	100	100
3	c	170/190 (90%)	170 (100%)	0	100	100
4	d	172/173 (99%)	172 (100%)	0	100	100
5	e	119/126 (94%)	119 (100%)	0	100	100
6	f	90/112 (80%)	90 (100%)	0	100	100
7	g	125/129 (97%)	125 (100%)	0	100	100
8	h	104/105 (99%)	104 (100%)	0	100	100
9	i	105/107 (98%)	105 (100%)	0	100	100
10	j	86/90 (96%)	86 (100%)	0	100	100
11	k	89/98 (91%)	89 (100%)	0	100	100
12	l	101/103 (98%)	101 (100%)	0	100	100
13	m	93/96 (97%)	93 (100%)	0	100	100
14	n	83/84 (99%)	83 (100%)	0	100	100
15	o	76/77 (99%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	73/78 (94%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	r	47/65 (72%)	47 (100%)	0	100	100
19	s	72/79 (91%)	72 (100%)	0	100	100
20	t	65/66 (98%)	65 (100%)	0	100	100
21	u	48/61 (79%)	48 (100%)	0	100	100
27	C	216/218 (99%)	216 (100%)	0	100	100
28	D	163/163 (100%)	163 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/150 (99%)	148 (100%)	0	100	100
31	G	137/138 (99%)	137 (100%)	0	100	100
32	H	32/114 (28%)	32 (100%)	0	100	100
33	L	116/116 (100%)	116 (100%)	0	100	100
34	M	104/104 (100%)	104 (100%)	0	100	100
35	N	103/103 (100%)	103 (100%)	0	100	100
36	O	107/107 (100%)	107 (100%)	0	100	100
37	P	98/103 (95%)	98 (100%)	0	100	100
38	Q	86/87 (99%)	86 (100%)	0	100	100
39	R	99/100 (99%)	99 (100%)	0	100	100
40	S	89/90 (99%)	89 (100%)	0	100	100
41	T	84/84 (100%)	84 (100%)	0	100	100
42	U	93/93 (100%)	93 (100%)	0	100	100
43	V	80/84 (95%)	80 (100%)	0	100	100
44	W	83/85 (98%)	83 (100%)	0	100	100
45	X	78/78 (100%)	78 (100%)	0	100	100
46	Y	58/63 (92%)	58 (100%)	0	100	100
47	Z	67/68 (98%)	67 (100%)	0	100	100
48	1	54/55 (98%)	54 (100%)	0	100	100
49	2	48/49 (98%)	48 (100%)	0	100	100
50	3	53/62 (86%)	53 (100%)	0	100	100
51	4	46/48 (96%)	46 (100%)	0	100	100
52	5	46/49 (94%)	46 (100%)	0	100	100
53	6	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	7	51/52 (98%)	51 (100%)	0	100	100
55	8	34/34 (100%)	34 (100%)	0	100	100
All	All	4545/4803 (95%)	4545 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 54 such sidechains are listed below:

Mol	Chain	Res	Type
27	C	134	ASN
29	E	165	HIS
44	W	45	HIS
27	C	232	HIS
28	D	49	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1542 (98%)	193 (12%)	0
22	w	75/76 (98%)	20 (26%)	0
22	y	75/76 (98%)	22 (29%)	0
23	x	75/77 (97%)	9 (12%)	0
24	v	10/27 (37%)	1 (10%)	0
25	A	2897/2904 (99%)	366 (12%)	13 (0%)
26	B	119/120 (99%)	15 (12%)	2 (1%)
All	All	4777/4822 (99%)	626 (13%)	15 (0%)

5 of 626 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	7	A
1	a	8	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	1583	A

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Mol	Chain	Res	Type
26	B	3	C
25	A	2097	A
26	B	66	A
25	A	2473	U

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

66 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
25	2MA	A	2503	57,25	22,25,26	1.46	5 (22%)	32,37,40	2.27	9 (28%)
22	OMG	y	17	22	23,26,27	1.18	3 (13%)	32,38,41	2.01	6 (18%)
25	5MU	A	1939	25	19,22,23	1.39	4 (21%)	27,32,35	2.12	6 (22%)
12	D2T	l	89	12	8,9,10	1.75	1 (12%)	6,11,13	2.48	2 (33%)
22	T6A	w	37	22	31,34,35	1.41	6 (19%)	43,49,52	1.90	11 (25%)
22	T6A	y	37	22	31,34,35	1.41	4 (12%)	43,49,52	1.98	10 (23%)
25	1MG	A	745	25	23,26,27	1.15	3 (13%)	33,39,42	1.74	5 (15%)
22	OMG	w	17	22	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
25	PSU	A	955	25	18,21,22	1.46	3 (16%)	21,30,33	2.15	4 (19%)
23	PSU	x	55	23	18,21,22	1.39	2 (11%)	21,30,33	2.06	3 (14%)
25	5MU	A	747	25	19,22,23	1.43	6 (31%)	27,32,35	2.08	6 (22%)
25	6MZ	A	1618	25	22,25,26	1.40	5 (22%)	29,36,39	2.20	9 (31%)
25	2MG	A	1835	25	23,26,27	1.26	3 (13%)	33,38,41	2.20	7 (21%)
25	PSU	A	1911	25	18,21,22	1.42	3 (16%)	21,30,33	2.13	4 (19%)
25	6MZ	A	2030	25	22,25,26	1.43	5 (22%)	29,36,39	2.23	10 (34%)
25	OMU	A	2552	57,25	19,22,23	1.31	3 (15%)	25,31,34	1.88	5 (20%)
22	M3X	w	34	24,22	24,30,31	2.19	4 (16%)	24,41,44	1.00	2 (8%)
22	5MU	y	54	22	19,22,23	1.43	5 (26%)	27,32,35	2.13	8 (29%)
22	M3X	y	34	22	24,30,31	2.23	3 (12%)	24,41,44	0.99	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
25	3TD	A	1915	25	19,22,23	4.18	7 (36%)	23,32,35	1.79	3 (13%)
25	G7M	A	2069	57,25	23,26,27	1.58	3 (13%)	34,39,42	1.75	5 (14%)
23	5MC	x	32	23	19,22,23	1.42	3 (15%)	26,32,35	1.31	4 (15%)
36	4D4	O	81	36	9,11,12	2.60	3 (33%)	7,13,15	0.98	0
22	4SU	y	8	22	18,21,22	1.87	4 (22%)	25,30,33	2.38	5 (20%)
25	PSU	A	2605	25	18,21,22	1.43	4 (22%)	21,30,33	2.09	4 (19%)
1	UR3	a	1498	1	19,22,23	0.96	0	26,32,35	1.82	3 (11%)
1	5MC	a	1407	1	19,22,23	1.54	3 (15%)	26,32,35	1.17	3 (11%)
22	G7M	w	46	22	23,26,27	1.53	3 (13%)	34,39,42	1.74	5 (14%)
25	2MG	A	2445	57,25	23,26,27	1.29	3 (13%)	33,38,41	2.22	5 (15%)
28	MEQ	D	150	28	8,9,10	0.52	0	5,10,12	0.33	0
1	G7M	a	527	1	23,26,27	1.57	3 (13%)	34,39,42	1.76	5 (14%)
1	4OC	a	1402	1,57	20,23,24	0.74	0	25,32,35	1.00	1 (4%)
22	H2U	y	19	22	18,21,22	1.02	2 (11%)	19,30,33	0.81	1 (5%)
25	PSU	A	746	25	18,21,22	1.44	5 (27%)	21,30,33	2.17	5 (23%)
23	5MU	x	54	23	19,22,23	1.39	6 (31%)	27,32,35	2.10	6 (22%)
11	IAS	k	119	11	6,7,8	0.95	0	3,8,10	1.46	1 (33%)
1	PSU	a	516	1	18,21,22	1.41	4 (22%)	21,30,33	2.07	4 (19%)
22	H2U	w	19	22	18,21,22	1.02	2 (11%)	19,30,33	0.82	1 (5%)
22	G7M	y	46	22	23,26,27	1.53	3 (13%)	34,39,42	1.71	5 (14%)
22	PSU	y	55	22	18,21,22	1.35	2 (11%)	21,30,33	2.04	3 (14%)
25	PSU	A	2604	25	18,21,22	1.43	3 (16%)	21,30,33	2.17	4 (19%)
22	PSU	w	55	22	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
25	PSU	A	2504	25	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
25	PSU	A	2457	25	18,21,22	1.43	4 (22%)	21,30,33	2.16	5 (23%)
25	H2U	A	2449	25	18,21,22	1.16	2 (11%)	19,30,33	0.78	0
1	2MG	a	1516	1	23,26,27	1.26	3 (13%)	33,38,41	2.24	7 (21%)
25	OMG	A	2251	57,25,23	23,26,27	1.21	3 (13%)	32,38,41	2.08	7 (21%)
22	PSU	w	39	22	18,21,22	1.36	2 (11%)	21,30,33	2.07	3 (14%)
25	5MC	A	1962	25	19,22,23	1.45	3 (15%)	26,32,35	1.09	2 (7%)
22	PSU	y	39	22	18,21,22	1.46	3 (16%)	21,30,33	1.79	3 (14%)
22	4SU	w	8	22	18,21,22	1.84	4 (22%)	25,30,33	2.26	4 (16%)
1	MA6	a	1518	1	23,26,27	1.44	3 (13%)	33,38,41	2.48	13 (39%)
22	3AU	w	47	22	24,28,29	2.70	9 (37%)	30,40,43	1.37	4 (13%)
25	PSU	A	1917	25	18,21,22	1.40	3 (16%)	21,30,33	2.03	3 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
22	H2U	w	20	22	18,21,22	1.03	2 (11%)	19,30,33	0.86	1 (5%)
25	OMC	A	2498	57,25	19,22,23	0.82	0	25,31,34	0.98	1 (4%)
22	H2U	y	20	22	18,21,22	0.98	2 (11%)	19,30,33	0.86	1 (5%)
1	MA6	a	1519	1	23,26,27	1.45	5 (21%)	33,38,41	2.50	14 (42%)
22	5MU	w	54	22	19,22,23	1.42	6 (31%)	27,32,35	2.23	6 (22%)
1	5MC	a	967	1	19,22,23	1.54	3 (15%)	26,32,35	1.14	2 (7%)
1	2MG	a	966	1	23,26,27	1.25	4 (17%)	33,38,41	2.23	8 (24%)
23	4SU	x	8	23	18,21,22	1.83	4 (22%)	25,30,33	2.24	5 (20%)
25	PSU	A	2580	25	18,21,22	1.43	5 (27%)	21,30,33	2.21	4 (19%)
36	MS6	O	82	36	5,7,8	0.54	0	2,7,9	1.23	0
1	2MG	a	1207	1	23,26,27	1.27	4 (17%)	33,38,41	2.19	6 (18%)
22	3AU	y	47	22	24,28,29	2.72	9 (37%)	30,40,43	1.40	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	2MA	A	2503	57,25	-	2/7/25/26	0/3/3/3
22	OMG	y	17	22	-	0/9/27/28	0/3/3/3
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
12	D2T	l	89	12	-	2/7/12/14	-
22	T6A	w	37	22	-	2/23/41/42	0/3/3/3
22	T6A	y	37	22	-	9/23/41/42	0/3/3/3
25	1MG	A	745	25	-	0/7/25/26	0/3/3/3
22	OMG	w	17	22	-	0/9/27/28	0/3/3/3
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
23	PSU	x	55	23	-	0/7/25/26	0/2/2/2
25	5MU	A	747	25	-	2/7/25/26	0/2/2/2
25	6MZ	A	1618	25	-	0/9/27/28	0/3/3/3
25	2MG	A	1835	25	-	0/9/27/28	0/3/3/3
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	6MZ	A	2030	25	-	2/9/27/28	0/3/3/3
25	OMU	A	2552	57,25	-	2/9/27/28	0/2/2/2
22	M3X	w	34	24,22	-	10/17/37/38	0/2/2/2
22	5MU	y	54	22	-	1/7/25/26	0/2/2/2
22	M3X	y	34	22	-	6/17/37/38	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	3TD	A	1915	25	-	0/7/25/26	0/2/2/2
25	G7M	A	2069	57,25	-	1/7/25/26	0/3/3/3
23	5MC	x	32	23	-	1/7/25/26	0/2/2/2
36	4D4	O	81	36	-	0/11/12/14	-
22	4SU	y	8	22	-	1/7/25/26	0/2/2/2
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
22	G7M	w	46	22	-	0/7/25/26	0/3/3/3
25	2MG	A	2445	57,25	-	0/9/27/28	0/3/3/3
28	MEQ	D	150	28	-	3/8/9/11	-
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
1	4OC	a	1402	1,57	-	2/9/29/30	0/2/2/2
22	H2U	y	19	22	-	3/7/38/39	0/2/2/2
25	PSU	A	746	25	-	1/7/25/26	0/2/2/2
23	5MU	x	54	23	-	0/7/25/26	0/2/2/2
11	IAS	k	119	11	-	0/7/7/8	-
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
22	H2U	w	19	22	-	3/7/38/39	0/2/2/2
22	G7M	y	46	22	-	2/7/25/26	0/3/3/3
22	PSU	y	55	22	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
22	PSU	w	55	22	-	0/7/25/26	0/2/2/2
25	PSU	A	2504	25	-	2/7/25/26	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
25	OMG	A	2251	57,25,23	-	0/9/27/28	0/3/3/3
22	PSU	w	39	22	-	2/7/25/26	0/2/2/2
25	5MC	A	1962	25	-	0/7/25/26	0/2/2/2
22	PSU	y	39	22	-	3/7/25/26	0/2/2/2
22	4SU	w	8	22	-	0/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/11/29/30	0/3/3/3
22	3AU	w	47	22	-	4/16/34/35	0/2/2/2
25	PSU	A	1917	25	-	2/7/25/26	0/2/2/2
22	H2U	w	20	22	-	1/7/38/39	0/2/2/2
25	OMC	A	2498	57,25	-	3/9/27/28	0/2/2/2
22	H2U	y	20	22	-	3/7/38/39	0/2/2/2
1	MA6	a	1519	1	-	5/11/29/30	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	5MU	w	54	22	-	0/7/25/26	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
23	4SU	x	8	23	-	0/7/25/26	0/2/2/2
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
36	MS6	O	82	36	-	2/4/6/8	-
1	2MG	a	1207	1	-	0/9/27/28	0/3/3/3
22	3AU	y	47	22	-	4/16/34/35	0/2/2/2

The worst 5 of 222 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	12.32	1.48	1.35
25	A	1915	3TD	C2-N1	9.73	1.49	1.37
22	y	34	M3X	C2-N2	8.86	1.47	1.34
22	w	34	M3X	C2-N2	8.53	1.47	1.34
22	y	47	3AU	C2-N1	6.50	1.47	1.38

The worst 5 of 299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	A	2503	2MA	C5-C4-N3	-7.85	118.91	127.18
1	a	1498	UR3	C4-N3-C2	-7.27	118.73	124.58
25	A	2445	2MG	C2-N3-C4	7.27	121.09	112.00
1	a	1516	2MG	C2-N3-C4	7.25	121.06	112.00
25	A	1835	2MG	C2-N3-C4	7.21	121.02	112.00

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
1	a	1519	MA6	N1-C6-N6-C9

There are no ring outliers.

21 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	y	17	OMG	2	0
22	w	37	T6A	2	0
22	y	37	T6A	5	0
22	w	17	OMG	1	0
23	x	55	PSU	1	0
25	A	2030	6MZ	1	0
22	y	54	5MU	2	0
25	A	1915	3TD	1	0
22	y	8	4SU	2	0
1	a	1402	4OC	1	0
22	y	19	H2U	1	0
23	x	54	5MU	1	0
1	a	516	PSU	1	0
22	y	46	G7M	1	0
22	y	55	PSU	2	0
1	a	1516	2MG	1	0
1	a	1518	MA6	1	0
25	A	2498	OMC	1	0
22	y	20	H2U	1	0
1	a	1519	MA6	1	0
22	w	54	5MU	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 740 ligands modelled in this entry, 738 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	ILE	y	101	-	6,7,8	0.55	0	4,8,10	1.10	0
56	PAR	a	1601	-	44,45,45	3.17	12 (27%)	63,67,67	1.08	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
59	ILE	y	101	-	-	1/7/8/10	-
56	PAR	a	1601	-	-	5/18/94/94	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	a	1601	PAR	C23-C33	-12.11	1.26	1.53
56	a	1601	PAR	C13-C23	10.88	1.66	1.52
56	a	1601	PAR	O43-C13	-7.07	1.29	1.41
56	a	1601	PAR	O43-C43	4.67	1.55	1.45
56	a	1601	PAR	C31-C21	-4.14	1.48	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	a	1601	PAR	C14-O33-C33	-2.97	110.94	117.98
56	a	1601	PAR	O11-C42-C32	-2.14	104.07	109.18
56	a	1601	PAR	C13-O52-C52	-2.13	112.92	117.98

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
56	a	1601	PAR	O43-C43-C53-O53
56	a	1601	PAR	C33-C43-C53-O53
56	a	1601	PAR	O51-C51-C61-O61
56	a	1601	PAR	O54-C14-O33-C33
56	a	1601	PAR	C52-C42-O11-C11

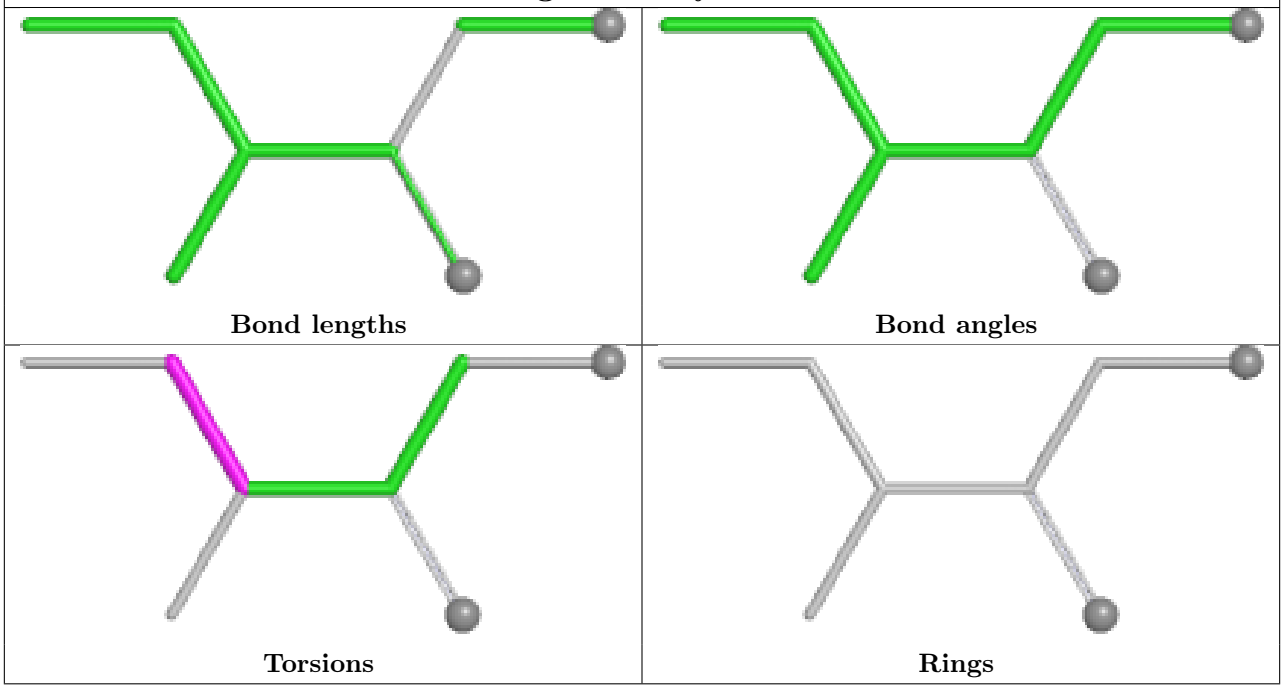
There are no ring outliers.

No monomer is involved in short contacts.

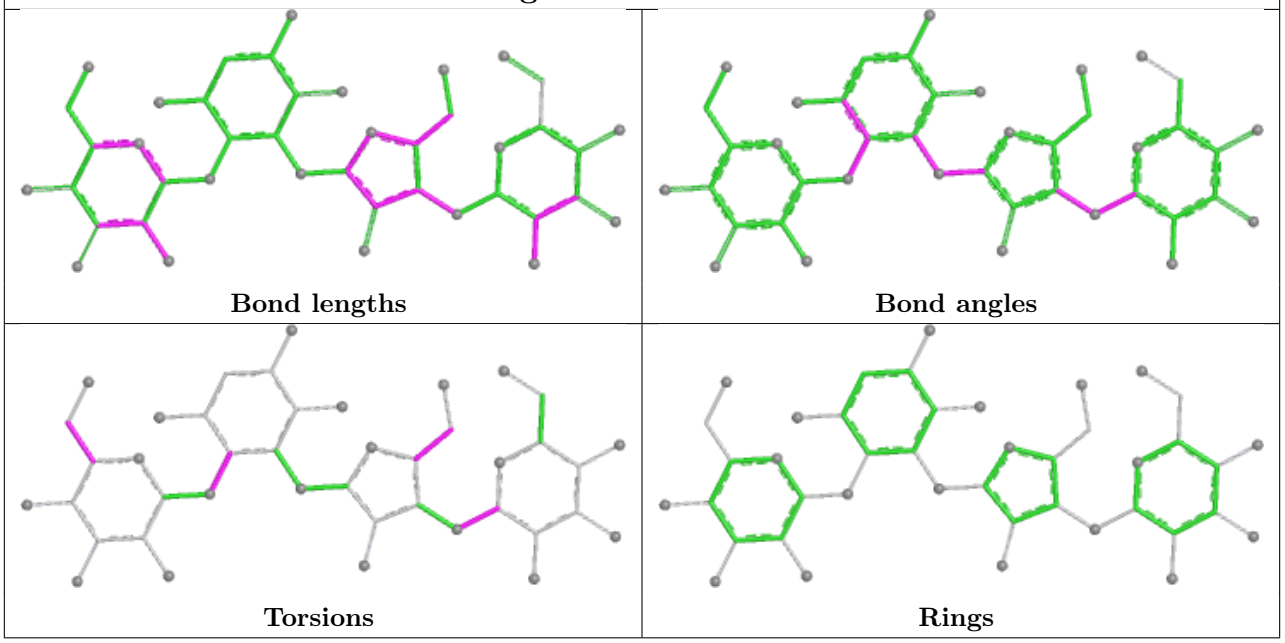
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ILE y 101



Ligand PAR a 1601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

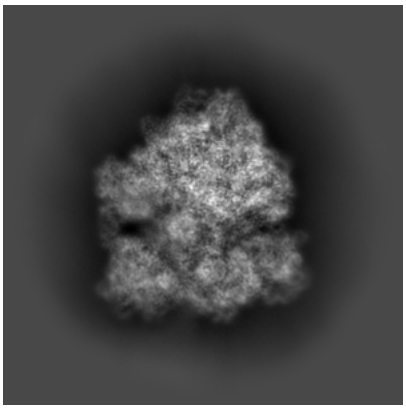
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-29821. These allow visual inspection of the internal detail of the map and identification of artifacts.

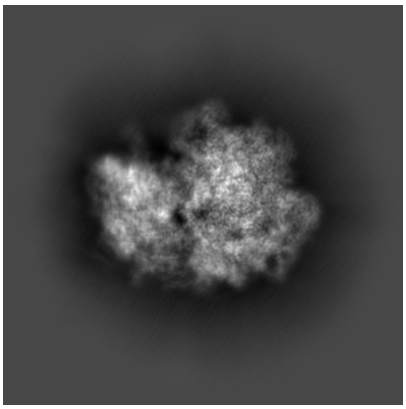
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

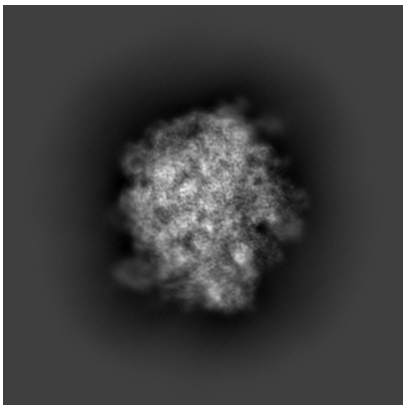
6.1.1 Primary map



X

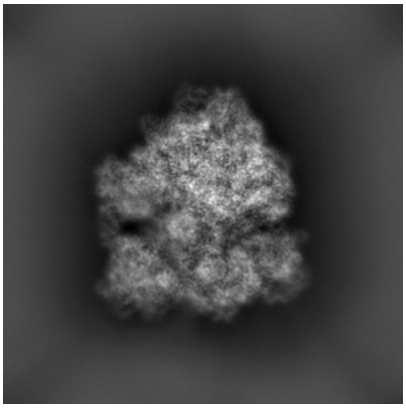


Y

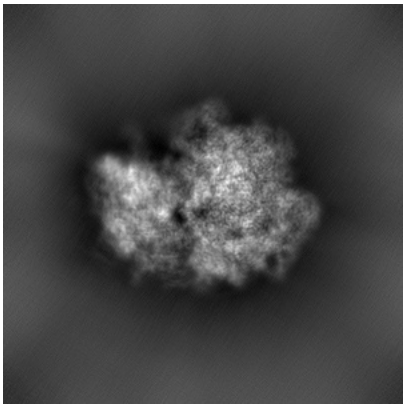


Z

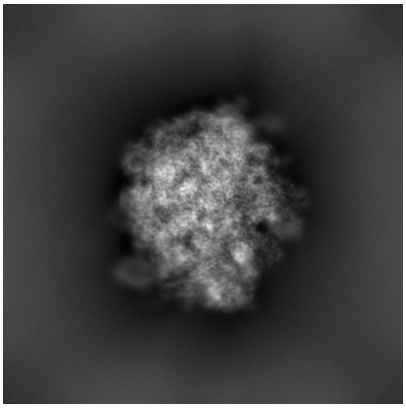
6.1.2 Raw map



X



Y

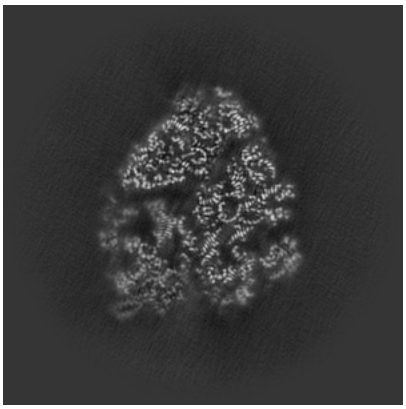


Z

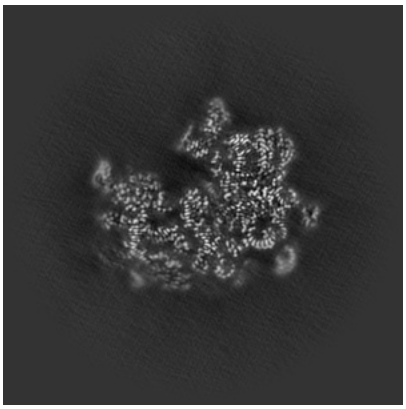
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

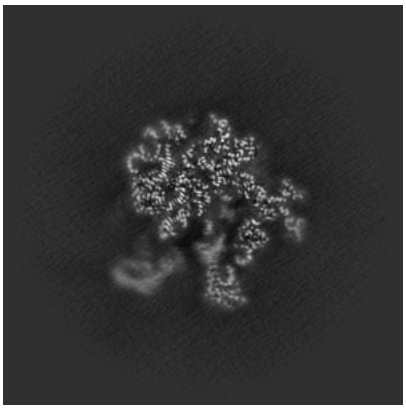
6.2.1 Primary map



X Index: 256

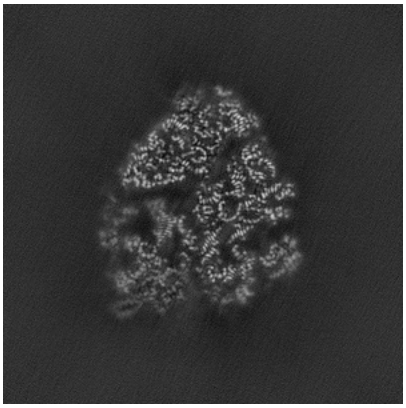


Y Index: 256

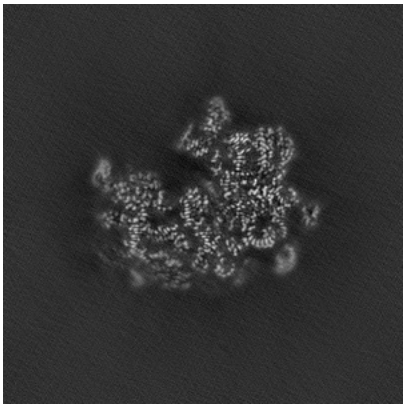


Z Index: 256

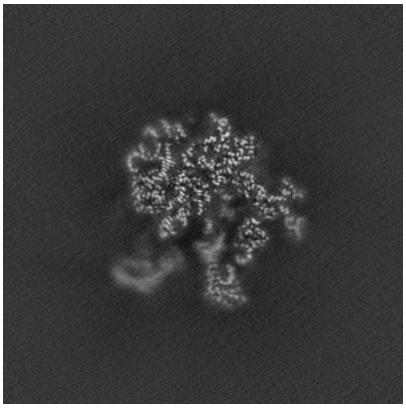
6.2.2 Raw map



X Index: 256



Y Index: 256

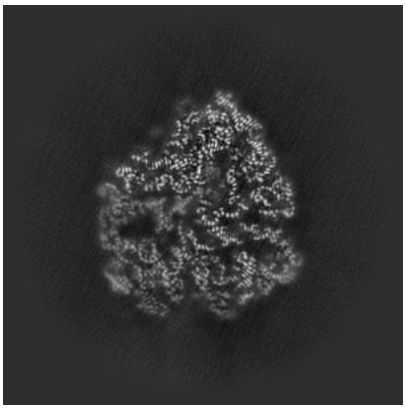


Z Index: 256

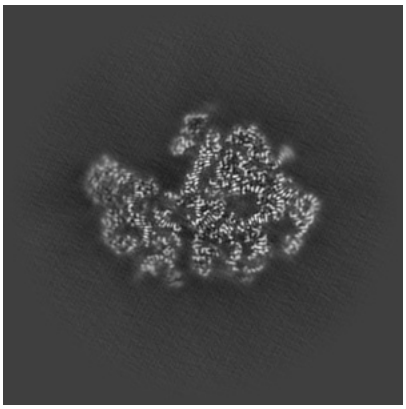
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

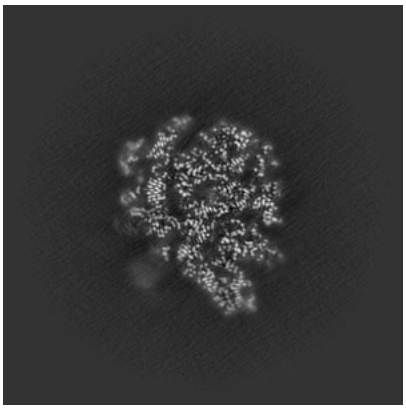
6.3.1 Primary map



X Index: 265

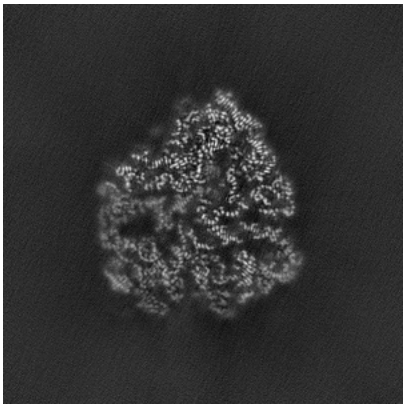


Y Index: 278

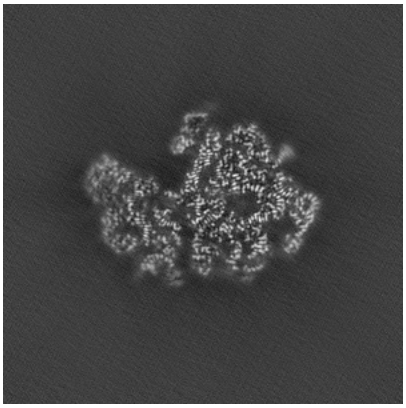


Z Index: 299

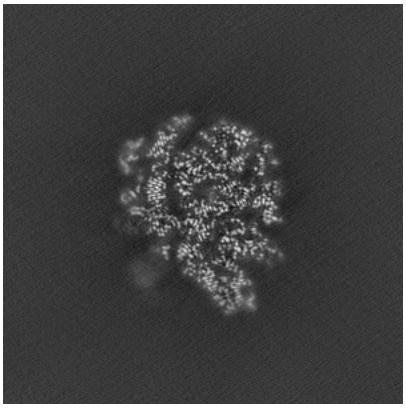
6.3.2 Raw map



X Index: 265



Y Index: 278

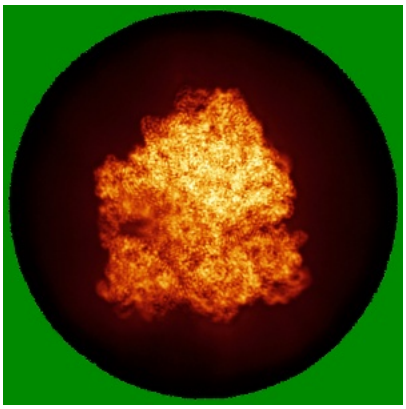


Z Index: 299

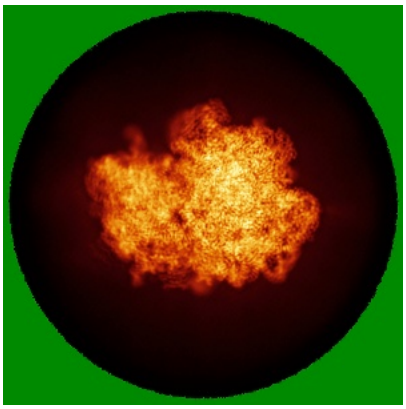
The images above show the largest variance slices of the map in three orthogonal directions.

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

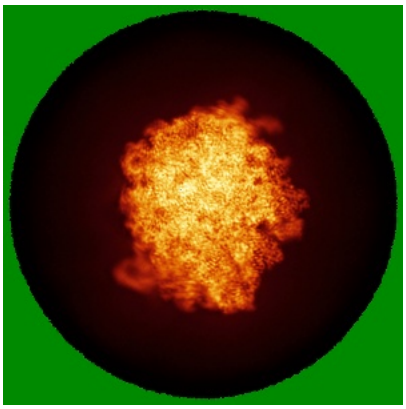
6.4.1 Primary map



X

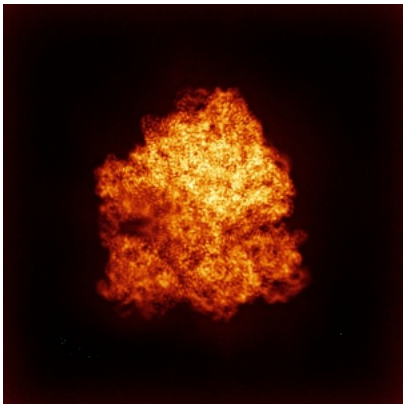


Y

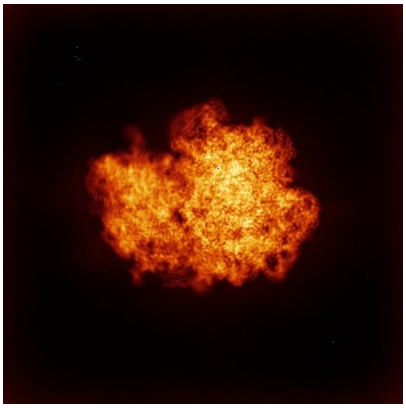


Z

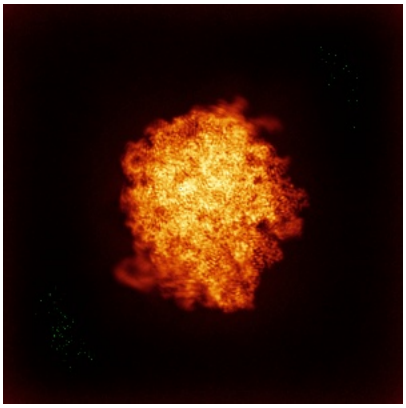
6.4.2 Raw map



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)

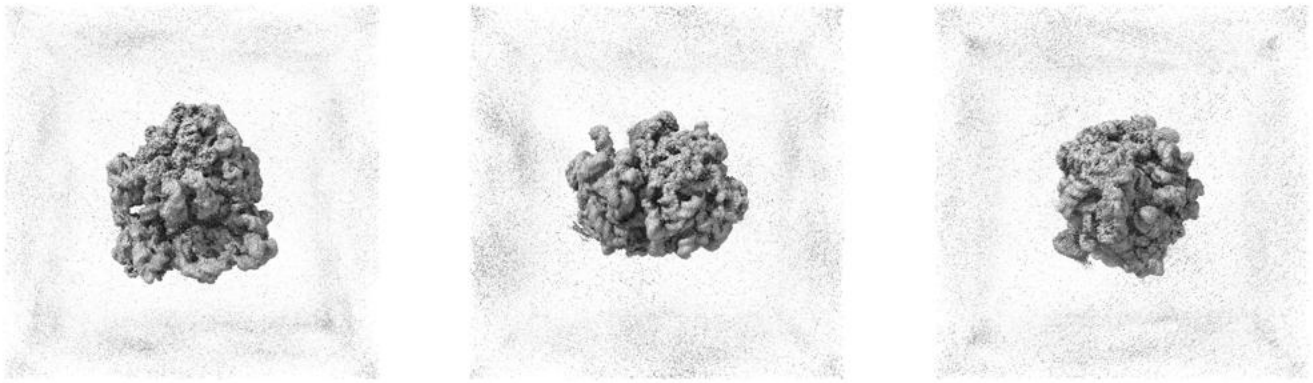
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

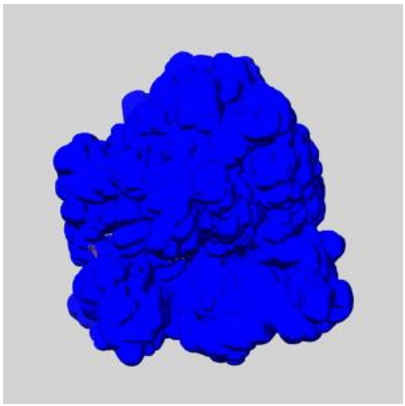
6.6 Mask visualisation

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

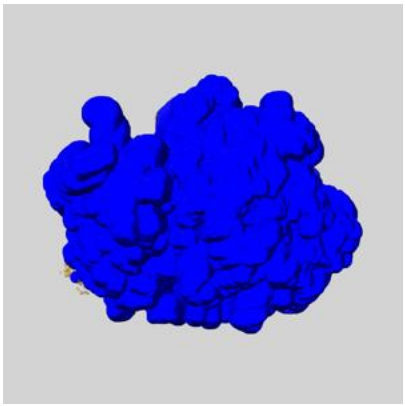
A mask typically either:

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

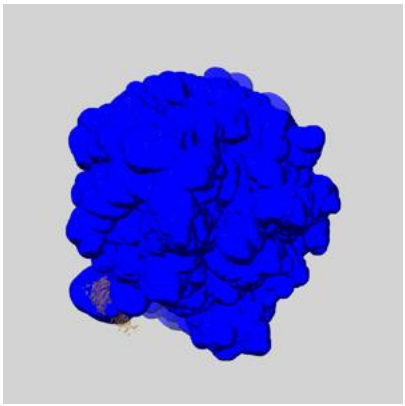
6.6.1 emd_29821_msk_1.map



X



Y

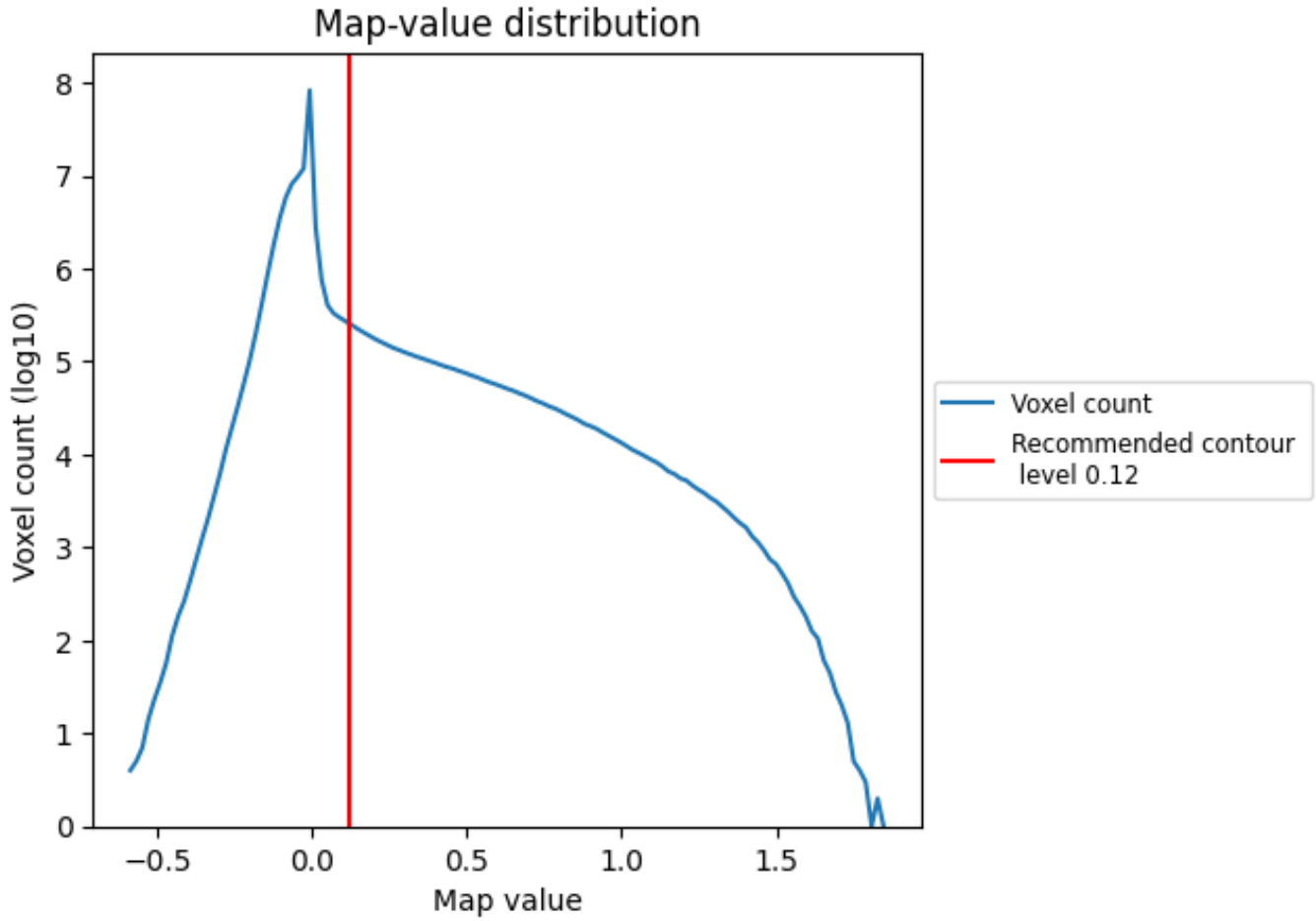


Z

7 Map analysis

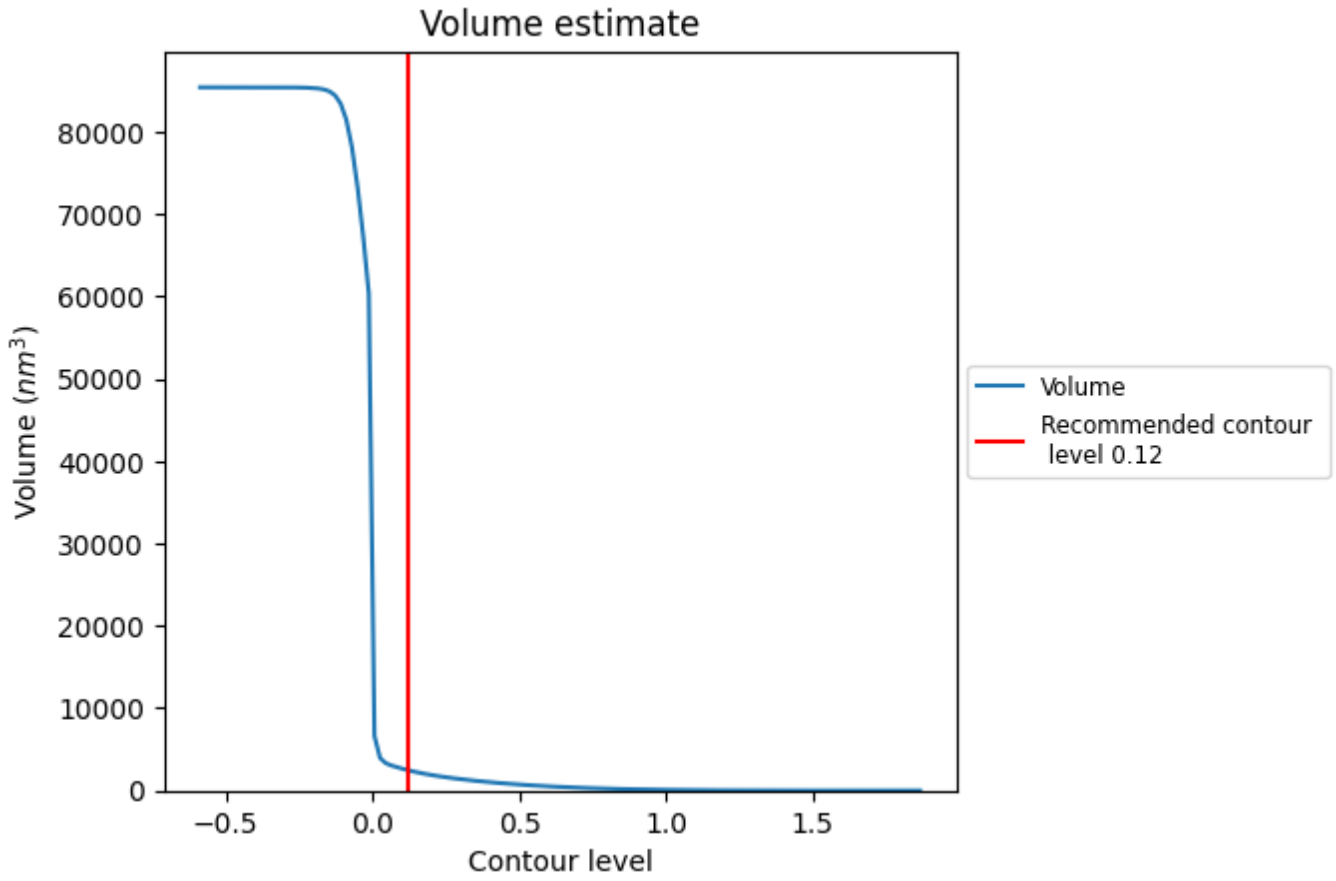
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

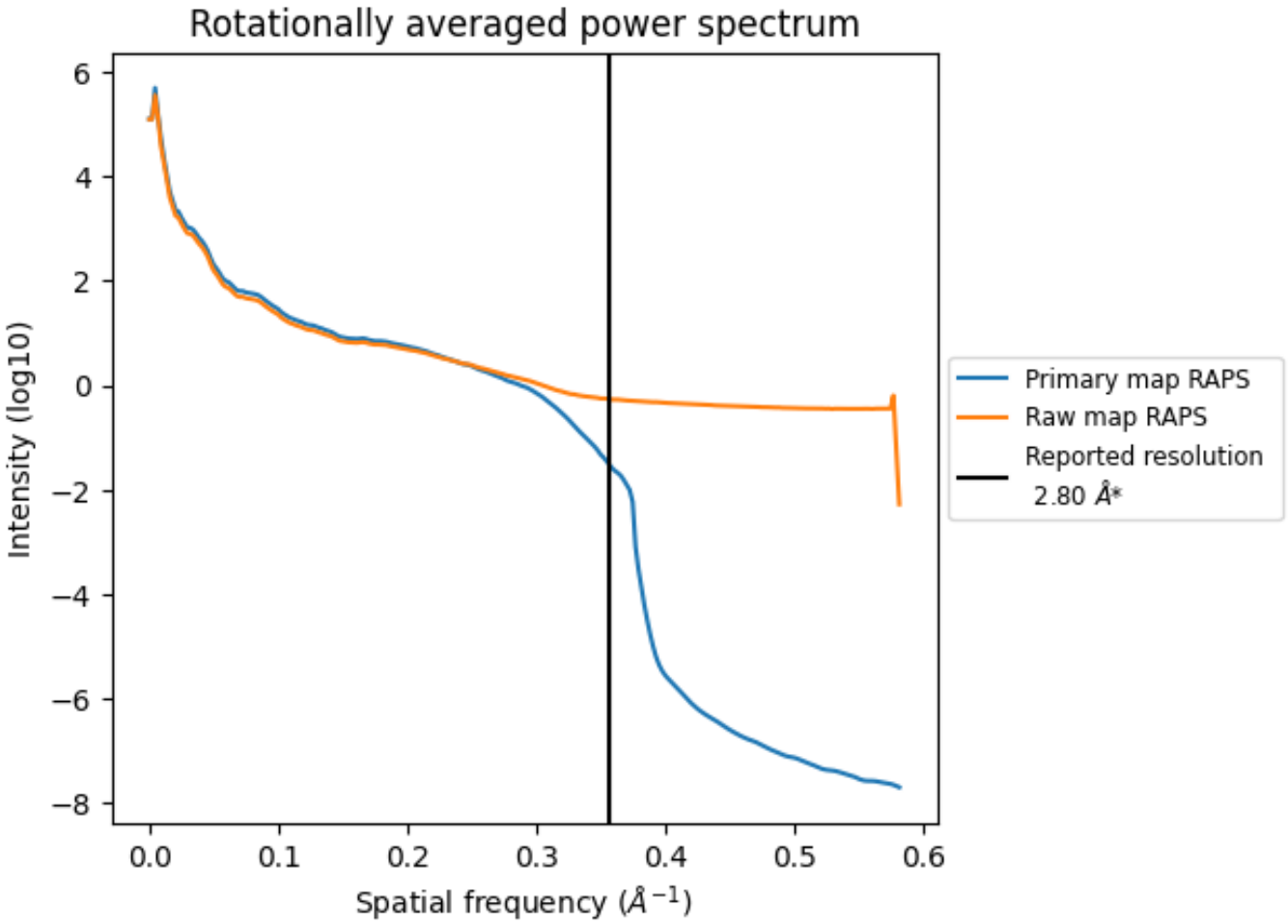
7.2 Volume estimate (i)



The volume at the recommended contour level is 2483 nm^3; this corresponds to an approximate mass of 2243 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)

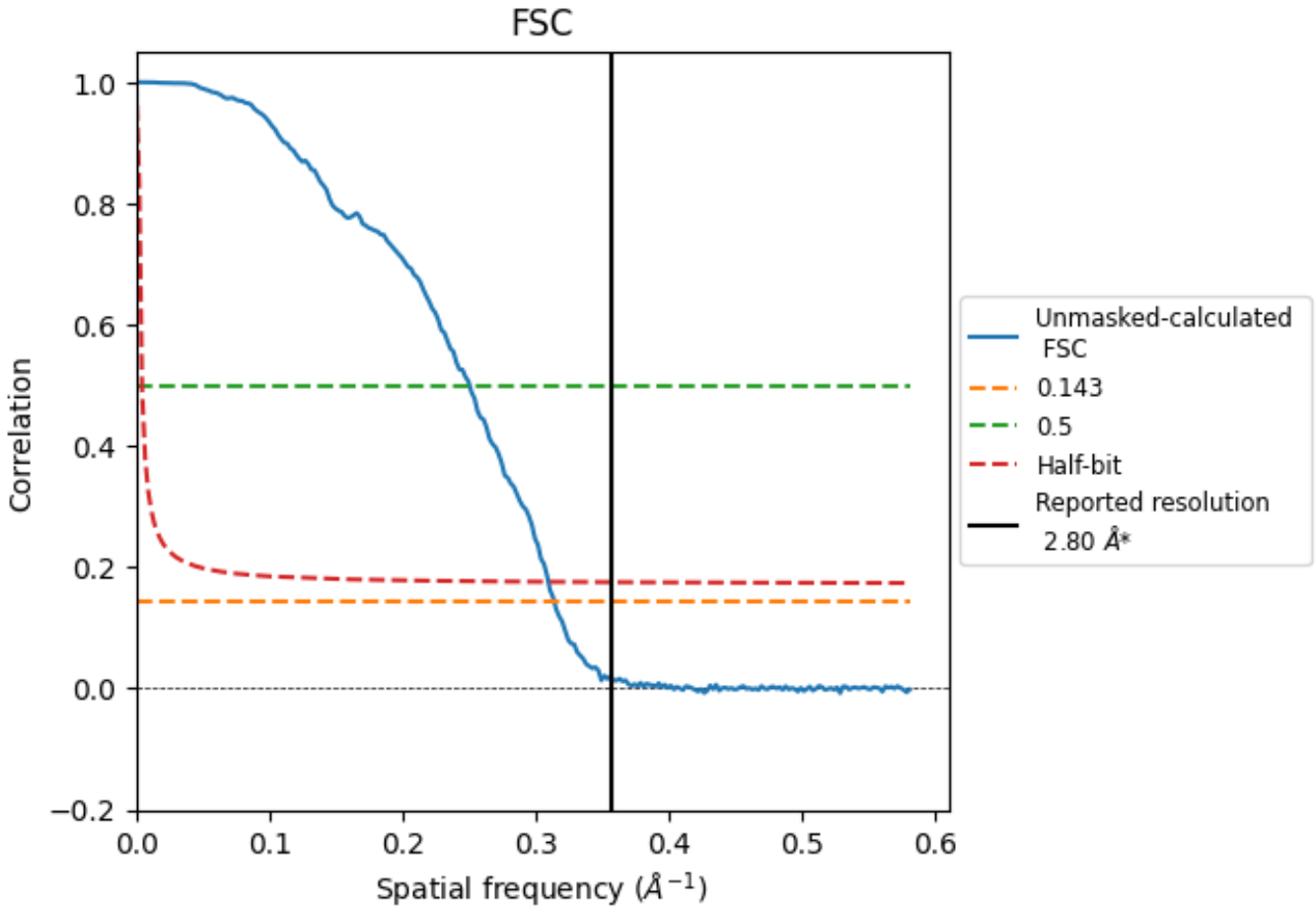


*Reported resolution corresponds to spatial frequency of 0.357 Å^{-1}

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 0.357 Å^{-1}

8.2 Resolution estimates (i)

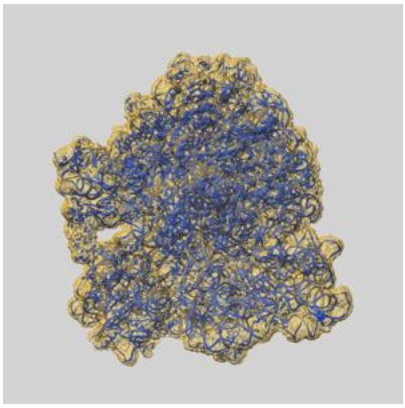
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.99	3.23

*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 3.18 differs from the reported value 2.8 by more than 10 %

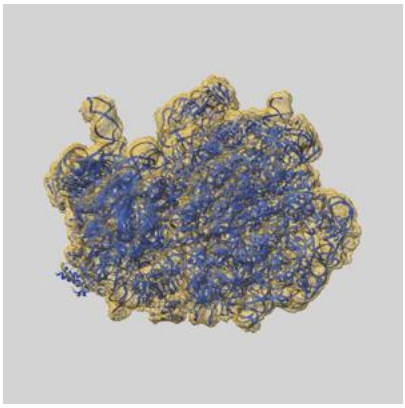
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-29821 and PDB model 8G7R. Per-residue inclusion information can be found in section 3 on page 18.

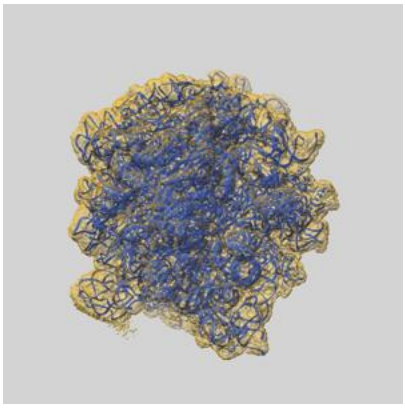
9.1 Map-model overlay



X



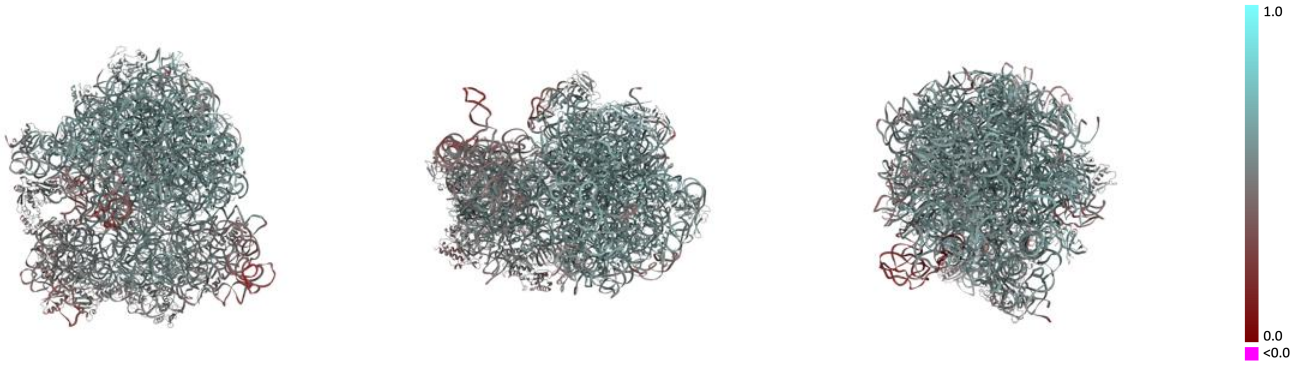
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

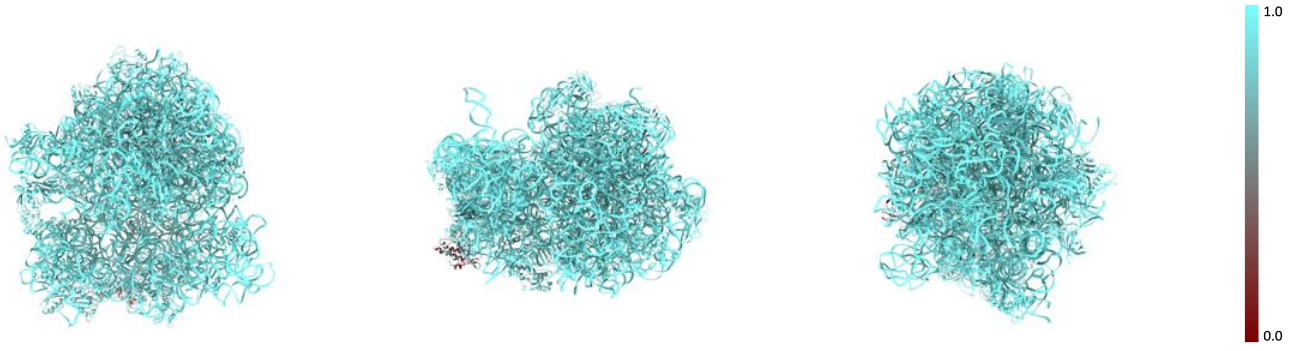
9.2 Q-score mapped to coordinate model



X Y Z

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

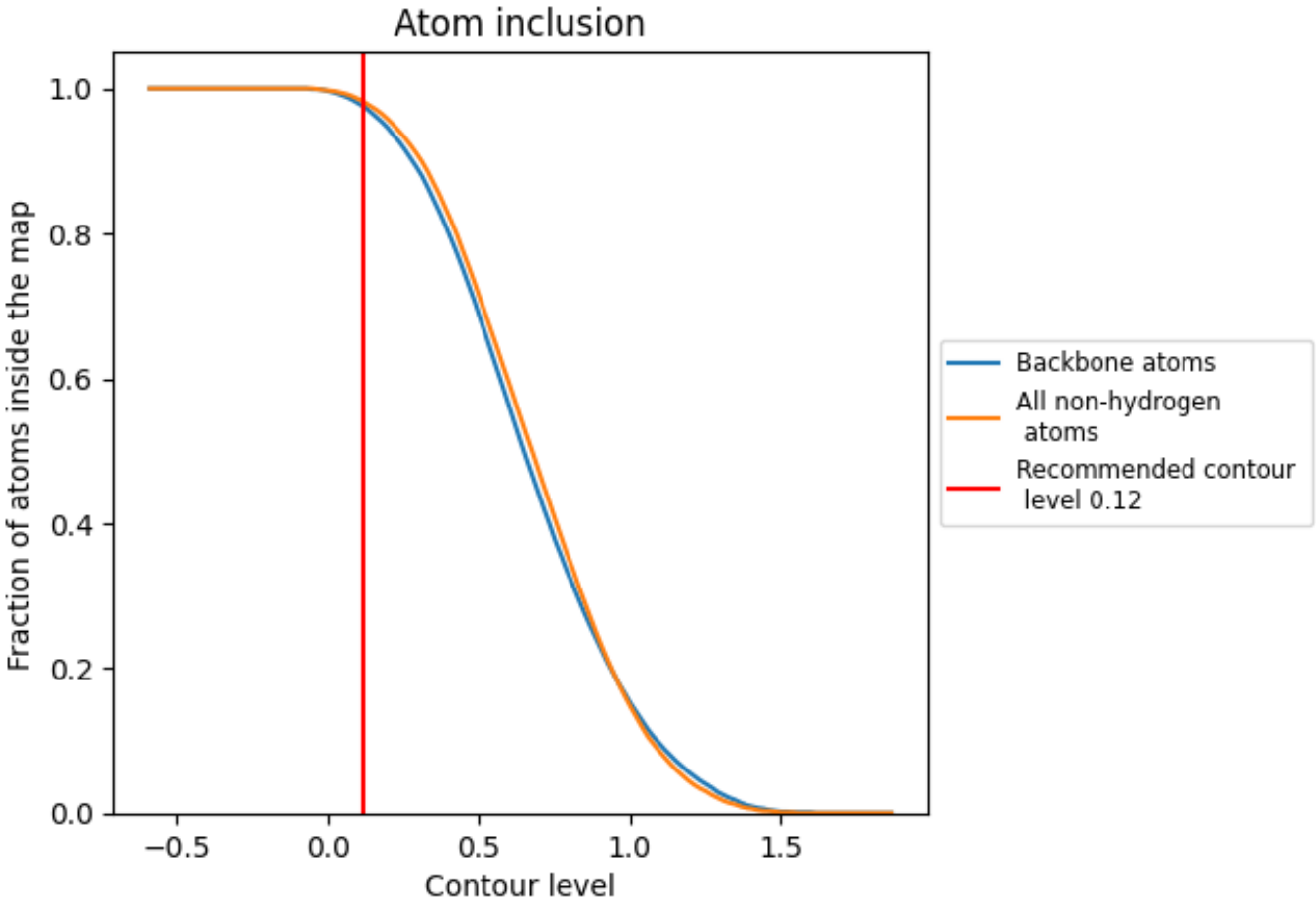
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9820	0.5340
1	0.9900	0.5200
2	0.9860	0.5690
3	0.9570	0.4440
4	0.9950	0.5910
5	0.9780	0.5640
6	0.9830	0.6030
7	0.9880	0.6040
8	0.9900	0.5770
A	0.9990	0.5640
B	0.9980	0.5310
C	0.9480	0.5780
D	0.9960	0.5880
E	0.9720	0.5420
F	0.9860	0.4840
G	0.9820	0.5160
H	0.4100	0.3960
L	0.9950	0.5880
M	0.9880	0.5880
N	0.9880	0.5790
O	0.9820	0.5900
P	0.9980	0.6020
Q	0.9940	0.5280
R	0.9850	0.5780
S	0.9960	0.5960
T	0.9770	0.5710
U	0.9890	0.5760
V	0.9780	0.5490
W	0.9940	0.5310
X	0.9840	0.5550
Y	0.9810	0.5840
Z	0.9850	0.5780
a	0.9980	0.5050
b	0.4140	0.3940
c	0.9350	0.5040



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
d	0.9650	0.4770
e	0.9810	0.5340
f	0.9070	0.4430
g	0.9710	0.4350
h	0.9810	0.5200
i	0.9840	0.4610
j	0.8870	0.4450
k	0.9750	0.4900
l	0.9800	0.5600
m	0.9830	0.4720
n	0.9740	0.4910
o	0.9810	0.4790
p	0.9840	0.4920
q	0.9840	0.5050
r	0.9180	0.4850
s	0.9910	0.4720
t	0.9880	0.4500
u	0.7180	0.4540
v	1.0000	0.5510
w	0.9760	0.4850
x	0.9930	0.4960
y	0.9550	0.2960