wwPDB EM Validation Summary Report

Sep 16, 2026 – 05:14 AM EDT

PDB ID	:	5WFS / pdb_00005wfs
EMDB ID	:	EMD-8829
Title	:	70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C4)
Authors	:	Fislage, M.; Frank, J.
Deposited on	:	2017-07-12
Resolution	:	3.00 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 ⓘ 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 ⓘ) were used in the production of this report:

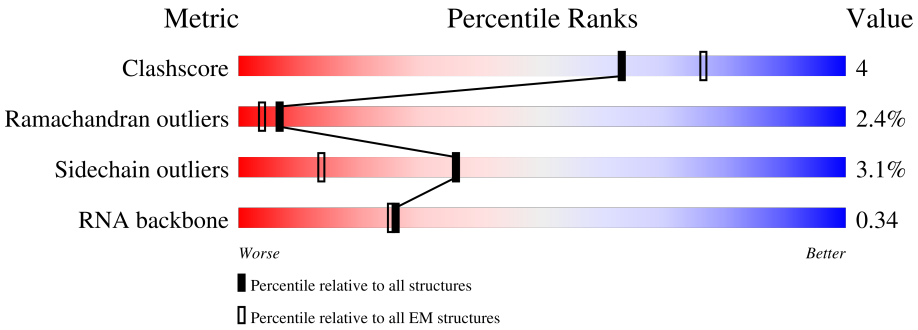
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

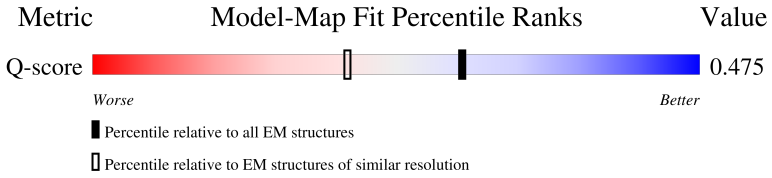
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.00 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	14081 (2.50 - 3.50)

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	2903	59% 33% 7% •
2	B	120	49% 41% 10%
3	C	271	88% 11% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	208	91% 8%
5	E	200	90% 9%
6	F	177	90% 8%
7	G	174	97%
8	H	149	10% 91% 8%
9	I	141	24% 84% 15%
10	J	141	91% 8%
11	K	122	89% 11%
12	L	143	87% 10%
13	M	136	93% 7%
14	N	119	88% 12%
15	O	116	94% 6%
16	P	114	90% 9%
17	Q	115	90% 10%
18	R	102	87% 13%
19	S	109	92% 8%
20	T	92	90% 10%
21	U	102	93% 7%
22	V	92	91% 9%
23	W	75	95% 5%
24	X	77	99%
25	Y	60	95%
26	Z	56	96%
27	0	55	91% 7%
28	1	51	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	2	45	84% 16%
30	3	64	98%
31	4	38	89% 11%
32	5	131	89% 90% 9%
33	6	66	92% 8%
34	a	1540	55% 35% 9%
35	b	218	94% 6%
36	c	206	92% 6%
37	d	205	93% 7%
38	e	157	83% 16%
39	f	100	87% 9%
40	g	151	89% 10%
41	h	129	88% 12%
42	i	127	93% 7%
43	j	98	91% 8%
44	k	116	93% 7%
45	l	121	89% 10%
46	m	115	91% 8%
47	n	101	86% 13%
48	o	88	91% 8%
49	p	82	87% 13%
50	q	80	84% 15%
51	r	65	80% 18%
52	s	79	91% 9%
53	t	85	91% 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
54	u	65	77% 18% 5%
55	v	77	65% 31%
55	w	77	8% 55% 31% 13%
56	x	12	67% 25% 8%
57	y	76	46% 43% 11%
58	z	393	92% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	6MZ	A	2030	-	-	X	-
63	GTP	z	402	-	-	X	-

2 Entry composition (i)

There are 64 unique types of molecules in this entry. The entry contains 155100 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 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	2900	62277	27788	11459	20130	2900	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 216643
A	1723	G	A	conflict	GB 216643
A	1847	G	A	conflict	GB 216643

- Molecule 2 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	B	120	2572	1145	471	836	120	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1199817771

- Molecule 3 is a protein called 50S ribosomal protein L2.

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

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	208	1557	974	287	293	3	0	0

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	200	Total	C	N	O	S	0	0
			1544	969	282	289	4		

- Molecule 6 is a protein called 50S ribosomal protein L5.

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

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	174	Total	C	N	O	S	0	0
			1304	820	239	243	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

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

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	141	Total	C	N	O	S	0	0
			1032	651	179	196	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 11 is a protein called 50S ribosomal protein L14.

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

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 13 is a protein called 50S ribosomal protein L16.

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

- Molecule 14 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

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

- Molecule 16 is a protein called 50S ribosomal protein L19.

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

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	115	Total	C	N	O	0	0
			933	595	190	148		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	102	Total	C	N	O	S	0	0
			810	513	152	143	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	109	Total 845	C 526	N 162	O 154	S 3	0	0

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	92	Total 730	C 461	N 138	O 130	S 1	0	0

- Molecule 21 is a protein called 50S ribosomal protein L24.

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

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	92	Total 739	C 471	N 135	O 131	S 2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	75	Total 572	C 355	N 116	O 100	S 1	0	0

- Molecule 24 is a protein called 50S ribosomal protein L28.

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

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	60	Total 494	C 305	N 96	O 91	S 2	0	0

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	56	Total	C	N	O	S	0	0
			434	273	85	74	2		

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 32 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	5	131	Total	C	N	O	S	0	0
			988	625	175	183	5		

- Molecule 33 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	6	66	Total	C	N	O	S	0	0
			522	323	99	94	6		

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	1	0
			1164	724	221	213	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
45	l	121	Total	C	N	O	S	0	0
			940	581	193	162	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
47	n	101	Total	C	N	O	S	0	0
			810	502	165	140	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP B7MCS2

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	79	Total	C	N	O	S	0	0
			637	408	120	107	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
54	u	65	Total	C	N	O	S	0	0
			544	335	117	91	1		

- Molecule 55 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms						AltConf	Trace
55	v	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		
55	w	77	Total	C	N	O	P	S	0	0
			1644	733	297	536	77	1		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	43	84	12		

- Molecule 57 is a RNA chain called Phe-tRNA-Phe.

Mol	Chain	Residues	Atoms						AltConf	Trace
57	y	76	Total	C	N	O	P	S	0	0
			1632	731	290	533	76	2		

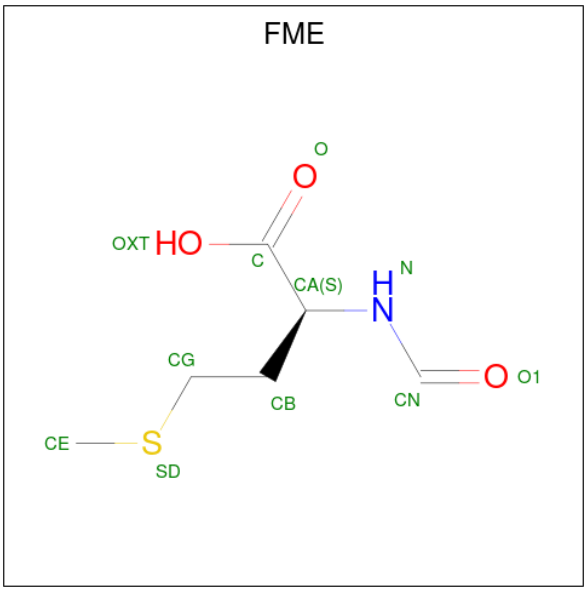
- Molecule 58 is a protein called Elongation factor Tu 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3031	1915	522	581	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	84	ALA	HIS	engineered mutation	UNP A7ZUJ2

- Molecule 59 is N-FORMYLMETHIONINE (CCD ID: FME) (formula: $C_6H_{11}NO_3S$).



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

- Molecule 60 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
60	A	1011	Total	Mg	0
			1011	1011	
60	B	37	Total	Mg	0
			37	37	
60	C	1	Total	Mg	0
			1	1	
60	D	2	Total	Mg	0
			2	2	
60	E	1	Total	Mg	0
			1	1	
60	M	2	Total	Mg	0
			2	2	
60	N	1	Total	Mg	0
			1	1	
60	Q	1	Total	Mg	0
			1	1	
60	T	1	Total	Mg	0
			1	1	
60	W	1	Total	Mg	0
			1	1	
60	0	3	Total	Mg	0
			3	3	

Continued on next page...

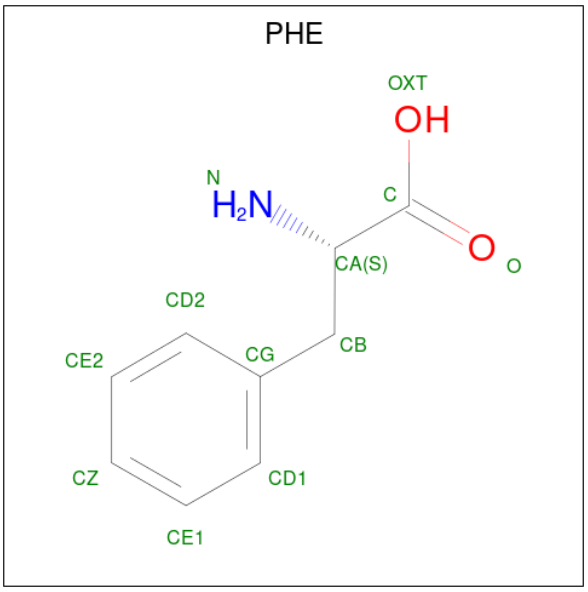
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
60	2	1	Total Mg 1 1	0
60	a	392	Total Mg 392 392	0
60	d	1	Total Mg 1 1	0
60	e	1	Total Mg 1 1	0
60	i	1	Total Mg 1 1	0
60	u	1	Total Mg 1 1	0
60	v	6	Total Mg 6 6	0
60	w	2	Total Mg 2 2	0
60	x	1	Total Mg 1 1	0
60	y	2	Total Mg 2 2	0
60	z	2	Total Mg 2 2	0

- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

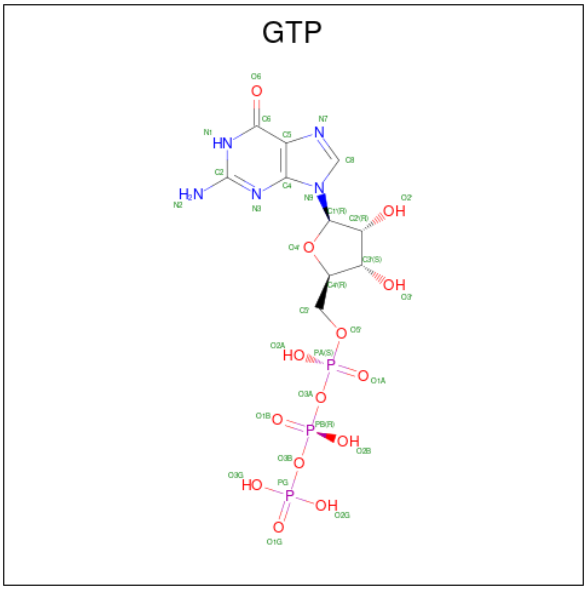
Mol	Chain	Residues	Atoms	AltConf
61	A	6	Total K 6 6	0
61	a	1	Total K 1 1	0

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
62	z	1	11	9	1	1	0

- Molecule 63 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
63	z	1	32	10	5	14	3	0

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	A	828	Total O 828 828	0
64	B	29	Total O 29 29	0
64	C	5	Total O 5 5	0
64	D	6	Total O 6 6	0
64	E	5	Total O 5 5	0
64	J	4	Total O 4 4	0
64	L	5	Total O 5 5	0
64	N	1	Total O 1 1	0
64	O	1	Total O 1 1	0
64	Q	3	Total O 3 3	0
64	R	1	Total O 1 1	0
64	S	3	Total O 3 3	0
64	W	2	Total O 2 2	0
64	X	3	Total O 3 3	0
64	Y	1	Total O 1 1	0
64	0	2	Total O 2 2	0
64	1	1	Total O 1 1	0
64	2	2	Total O 2 2	0
64	3	1	Total O 1 1	0
64	a	253	Total O 253 253	0
64	c	1	Total O 1 1	0
64	i	1	Total O 1 1	0

Continued on next page...

Continued from previous page...

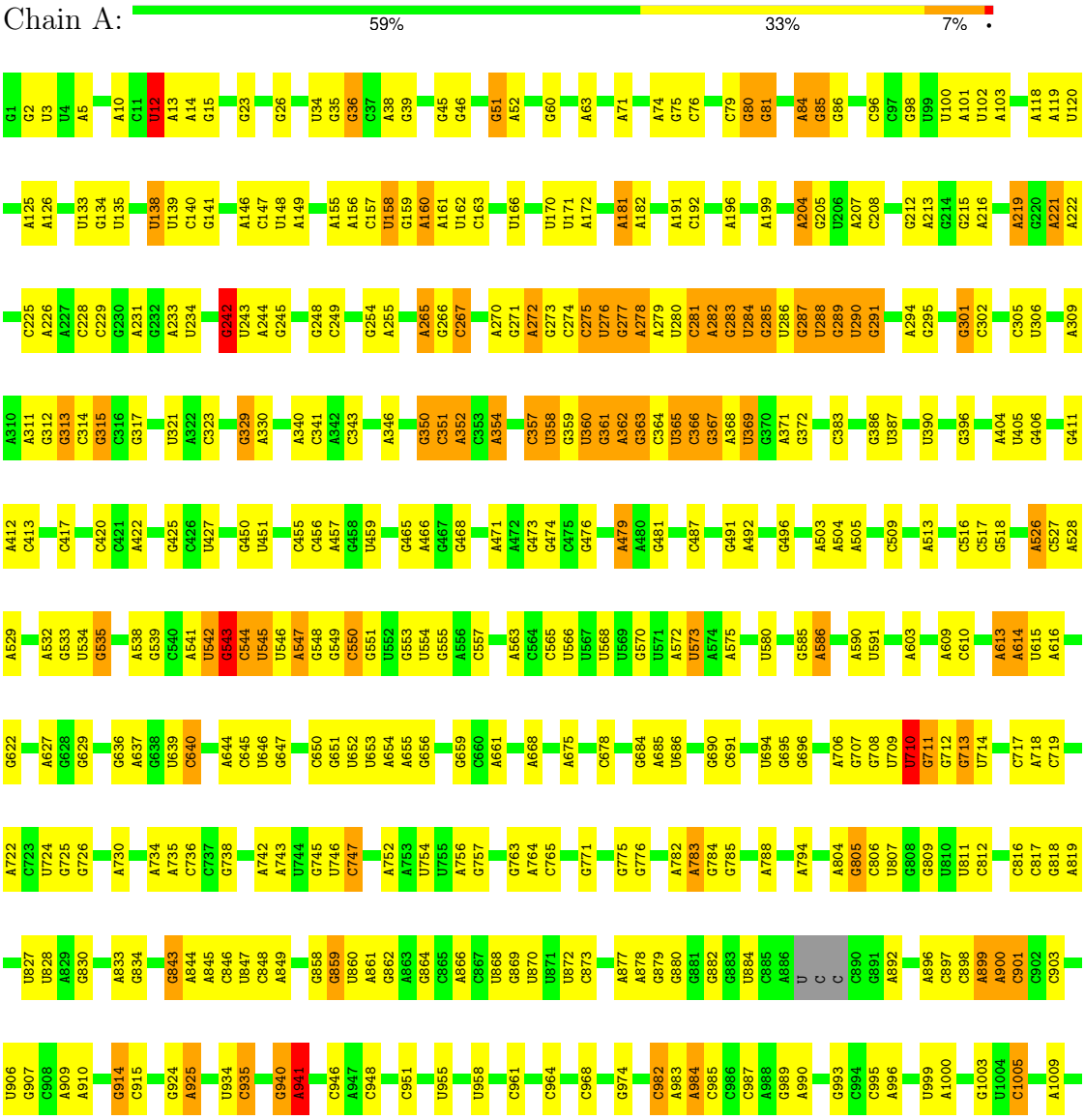
Mol	Chain	Residues	Atoms	AltConf
64	j	1	Total O 1 1	0
64	l	2	Total O 2 2	0
64	m	1	Total O 1 1	0
64	o	1	Total O 1 1	0
64	q	1	Total O 1 1	0
64	s	3	Total O 3 3	0
64	u	1	Total O 1 1	0
64	v	3	Total O 3 3	0
64	w	1	Total O 1 1	0
64	x	1	Total O 1 1	0
64	y	2	Total O 2 2	0

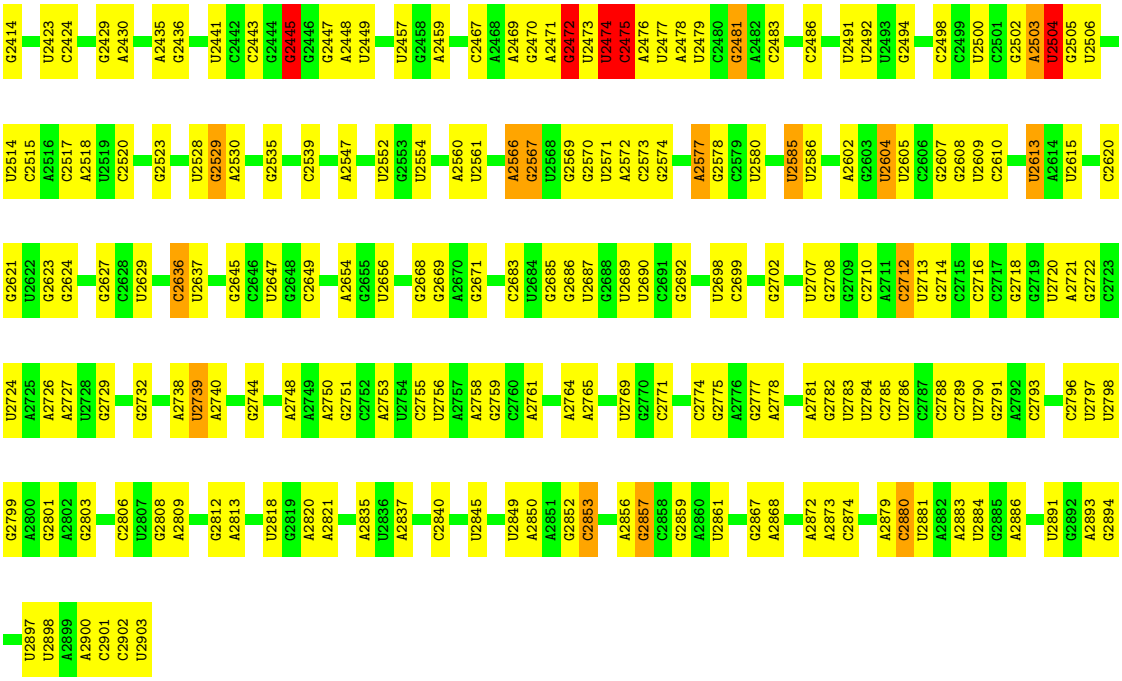
3 Residue-property plots (i)

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: 23S rRNA

Chain A:

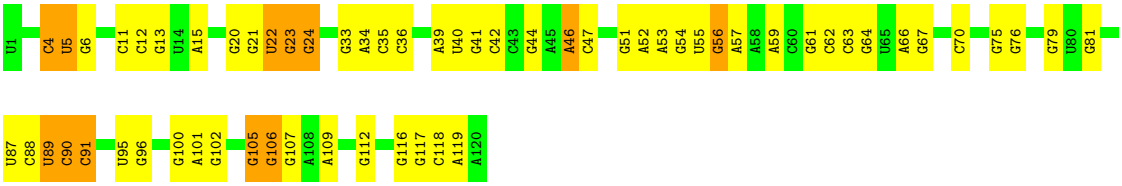




• Molecule 2: 5S rRNA

Chain B:

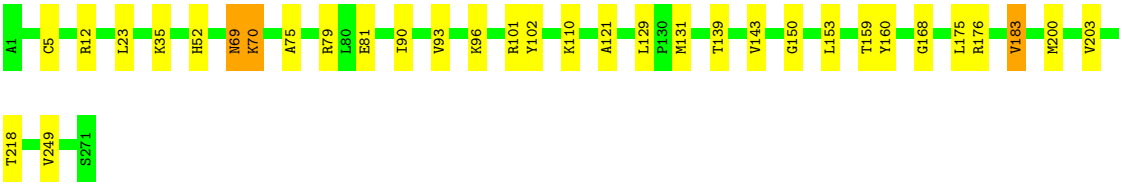




• Molecule 3: 50S ribosomal protein L2

Chain C:

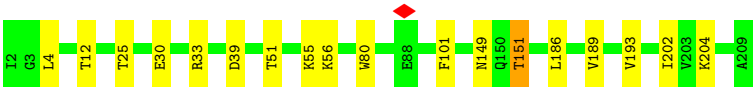




• Molecule 4: 50S ribosomal protein L3

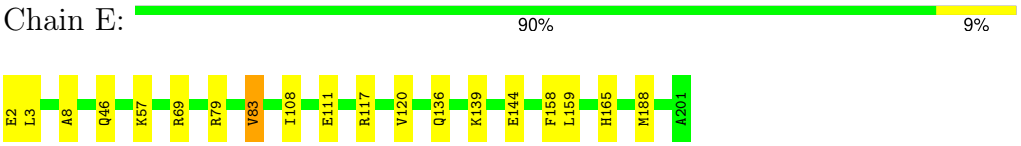
Chain D:





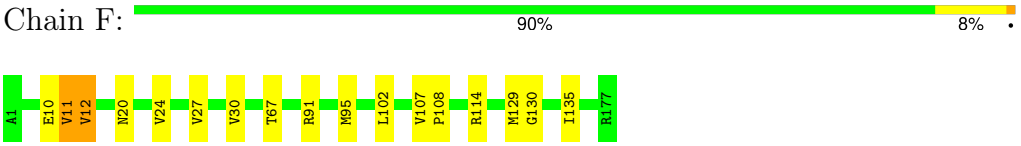
• Molecule 5: 50S ribosomal protein L4

Chain E:



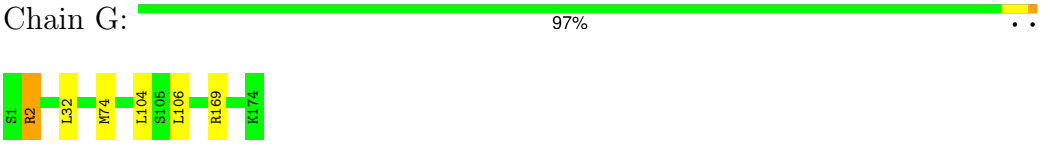
• Molecule 6: 50S ribosomal protein L5

Chain F:



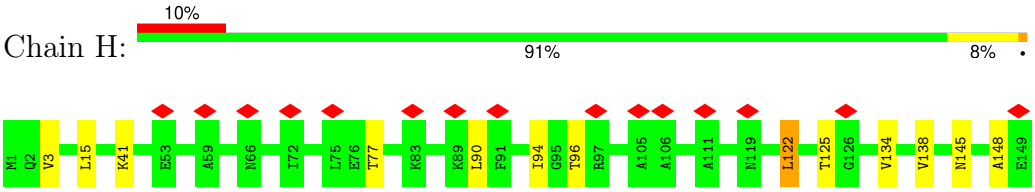
• Molecule 7: 50S ribosomal protein L6

Chain G:



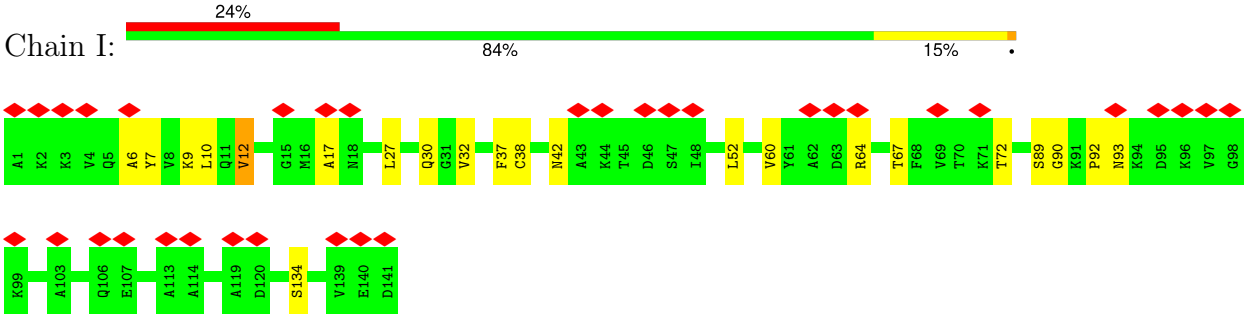
• Molecule 8: 50S ribosomal protein L9

Chain H:



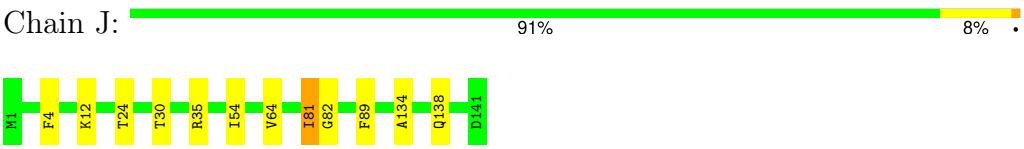
• Molecule 9: 50S ribosomal protein L11

Chain I:



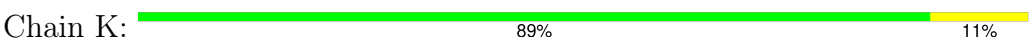
• Molecule 10: 50S ribosomal protein L13

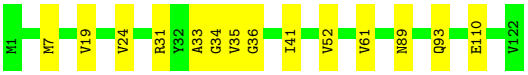
Chain J:



• Molecule 11: 50S ribosomal protein L14

Chain K:





• Molecule 12: 50S ribosomal protein L15

Chain L:





• Molecule 13: 50S ribosomal protein L16

Chain M:

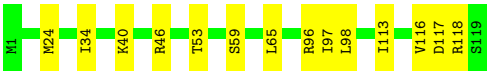




• Molecule 14: 50S ribosomal protein L17

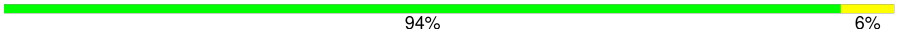
Chain N:





• Molecule 15: 50S ribosomal protein L18

Chain O:

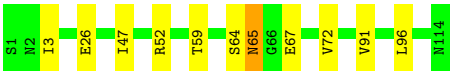




• Molecule 16: 50S ribosomal protein L19

Chain P:





• Molecule 17: 50S ribosomal protein L20

Chain Q:

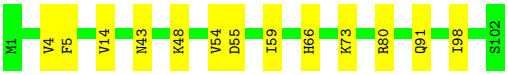




• Molecule 18: 50S ribosomal protein L21

Chain R:

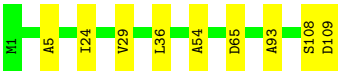




• Molecule 19: 50S ribosomal protein L22

Chain S:





• Molecule 20: 50S ribosomal protein L23

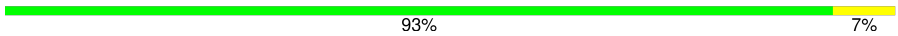
Chain T:





• Molecule 21: 50S ribosomal protein L24

Chain U:





• Molecule 22: 50S ribosomal protein L25

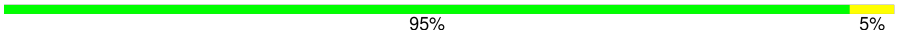
Chain V:





• Molecule 23: 50S ribosomal protein L27

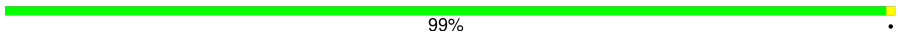
Chain W:





• Molecule 24: 50S ribosomal protein L28

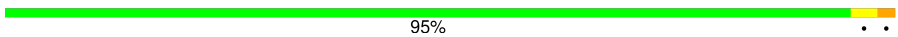
Chain X:





• Molecule 25: 50S ribosomal protein L29

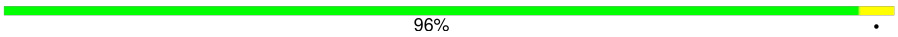
Chain Y:

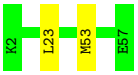




• Molecule 26: 50S ribosomal protein L30

Chain Z:





• Molecule 27: 50S ribosomal protein L32

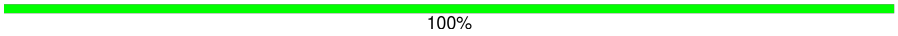
Chain 0:





• Molecule 28: 50S ribosomal protein L33

Chain 1:

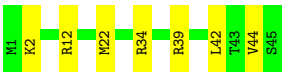


There are no outlier residues recorded for this chain.

• Molecule 29: 50S ribosomal protein L34

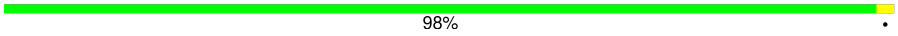
Chain 2:





• Molecule 30: 50S ribosomal protein L35

Chain 3:





• Molecule 31: 50S ribosomal protein L36 1

Chain 4:

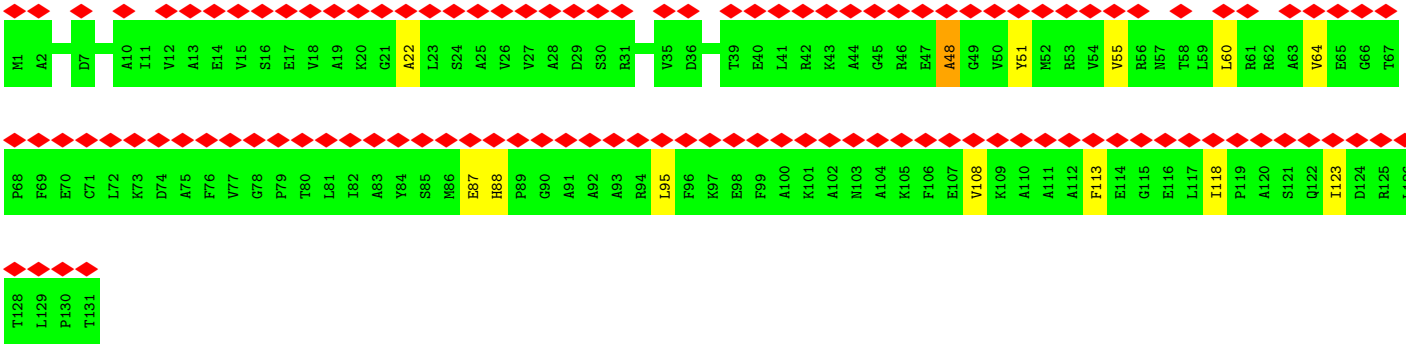




• Molecule 32: 50S ribosomal protein L10

Chain 5:

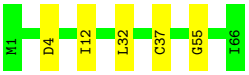




• Molecule 33: 50S ribosomal protein L31

Chain 6:

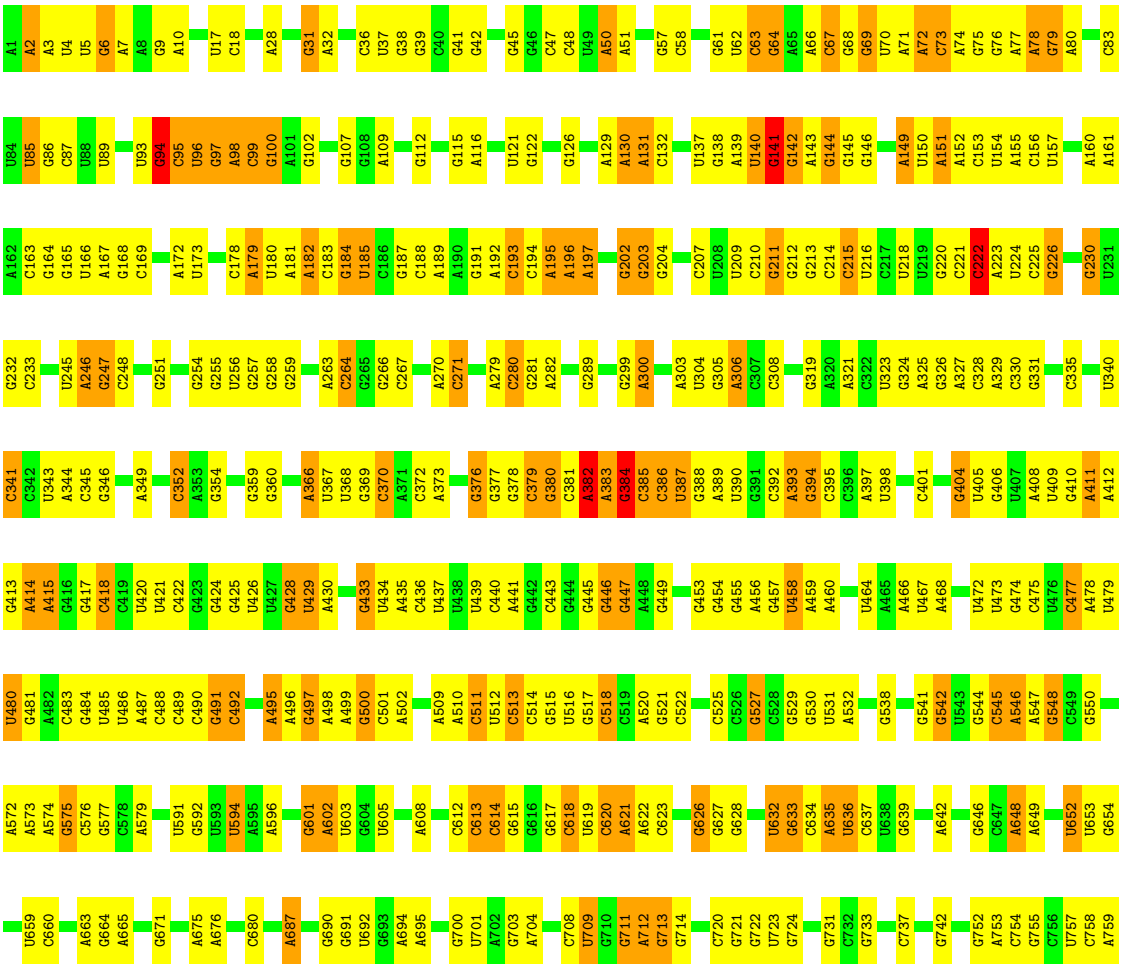


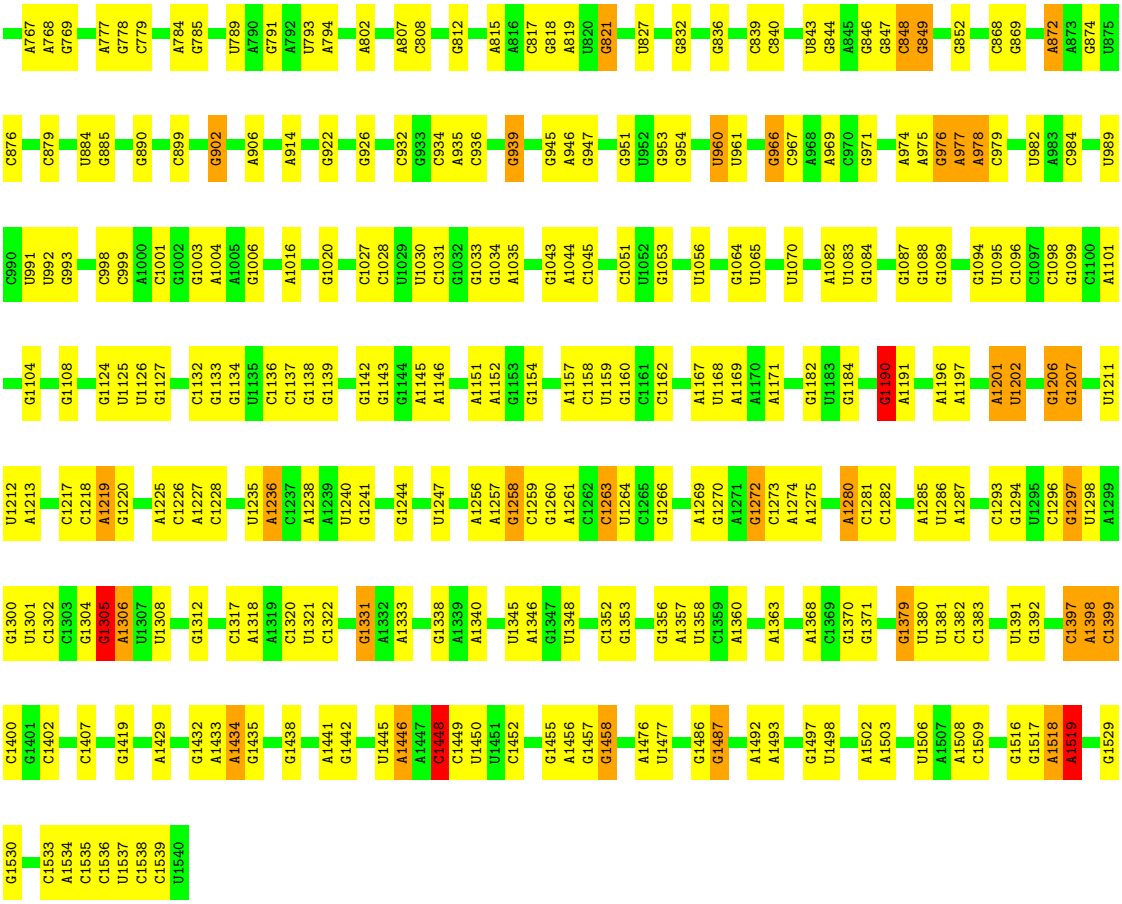


• Molecule 34: 16S rRNA

Chain a:

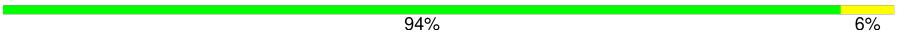


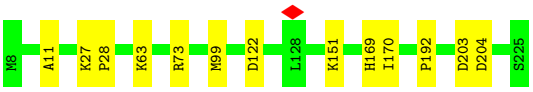




• Molecule 35: 30S ribosomal protein S2

Chain b:

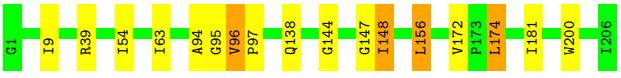




• Molecule 36: 30S ribosomal protein S3

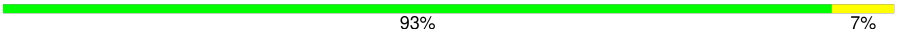
Chain c:





• Molecule 37: 30S ribosomal protein S4

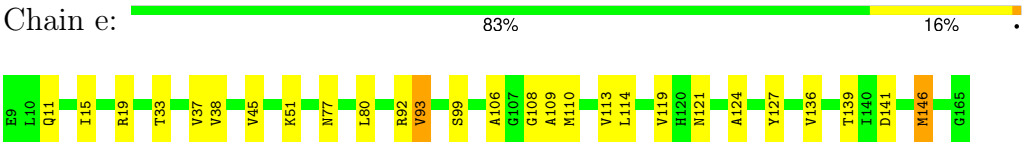
Chain d:





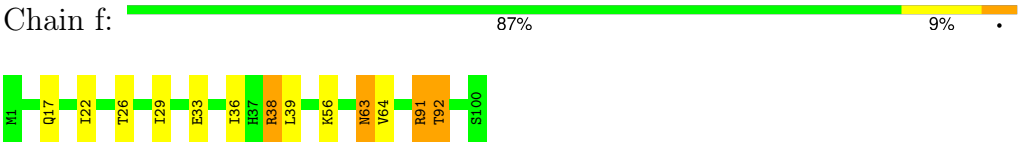
• Molecule 38: 30S ribosomal protein S5

Chain e:



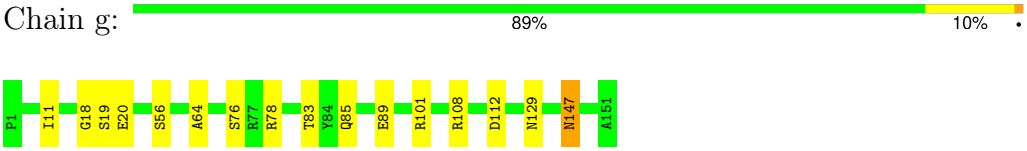
• Molecule 39: 30S ribosomal protein S6

Chain f:



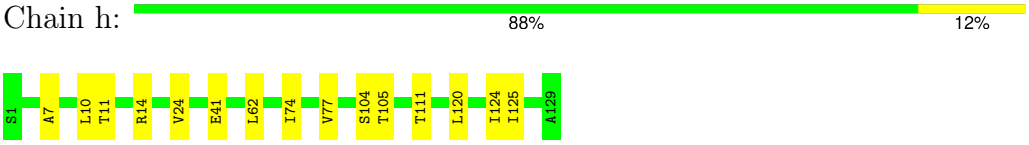
• Molecule 40: 30S ribosomal protein S7

Chain g:



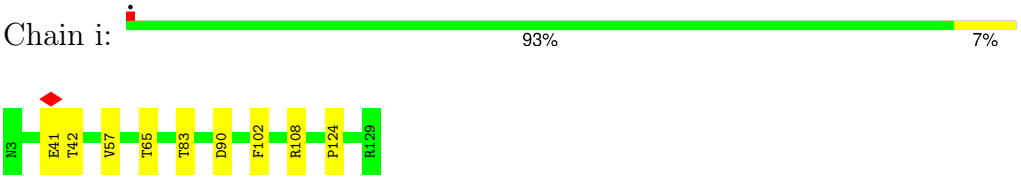
• Molecule 41: 30S ribosomal protein S8

Chain h:



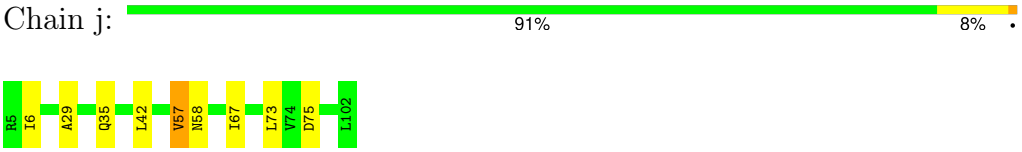
• Molecule 42: 30S ribosomal protein S9

Chain i:



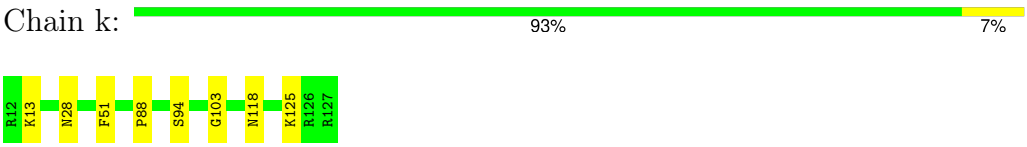
• Molecule 43: 30S ribosomal protein S10

Chain j:



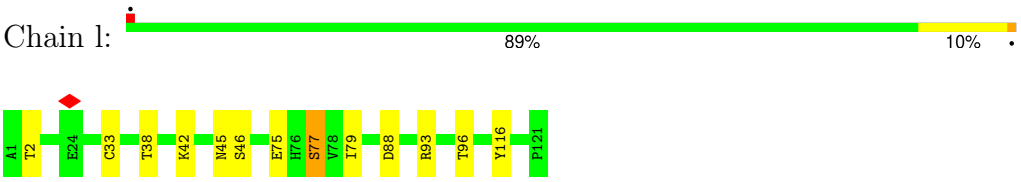
• Molecule 44: 30S ribosomal protein S11

Chain k:



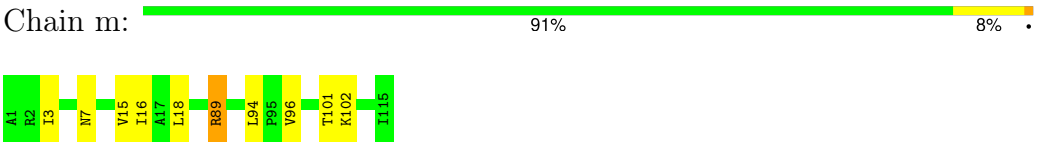
• Molecule 45: 30S ribosomal protein S12

Chain l:



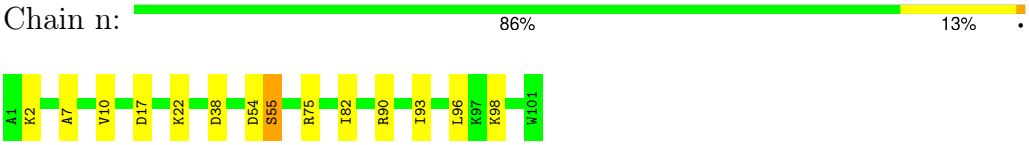
• Molecule 46: 30S ribosomal protein S13

Chain m:



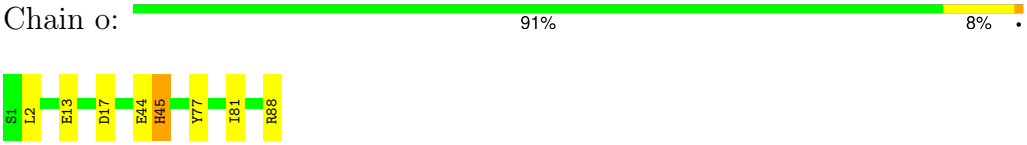
• Molecule 47: 30S ribosomal protein S14

Chain n:



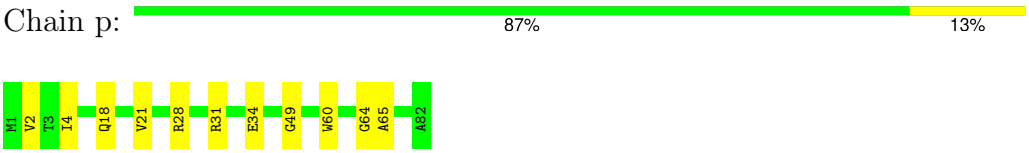
• Molecule 48: 30S ribosomal protein S15

Chain o:



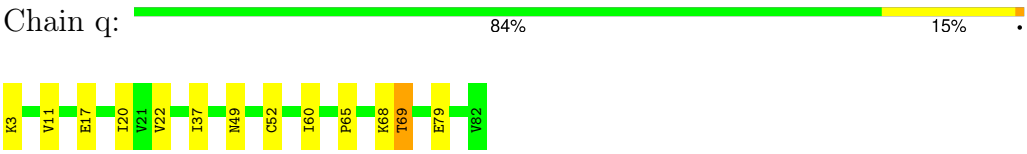
• Molecule 49: 30S ribosomal protein S16

Chain p:



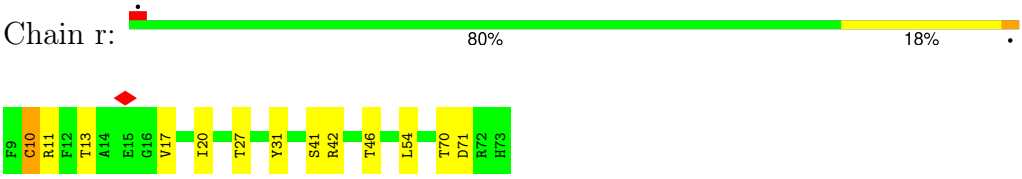
• Molecule 50: 30S ribosomal protein S17

Chain q:



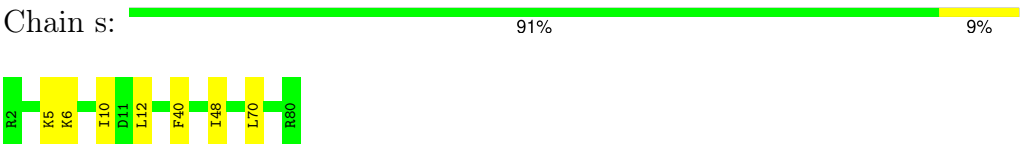
• Molecule 51: 30S ribosomal protein S18

Chain r:



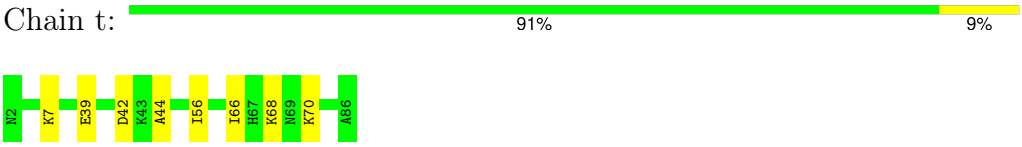
• Molecule 52: 30S ribosomal protein S19

Chain s:



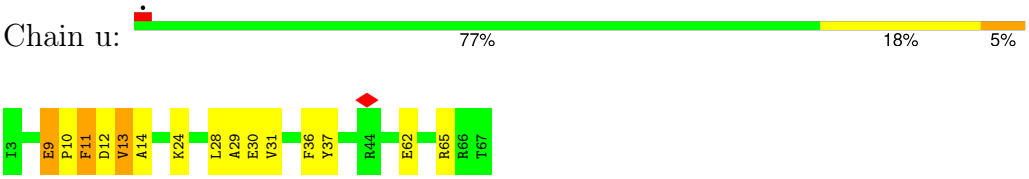
• Molecule 53: 30S ribosomal protein S20

Chain t:



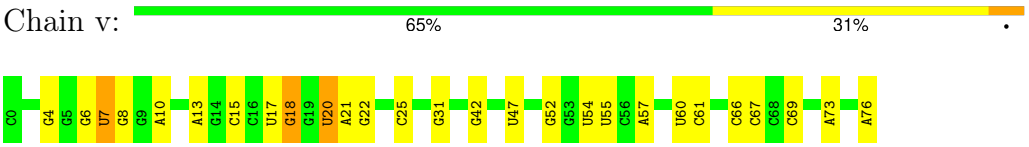
• Molecule 54: 30S ribosomal protein S21

Chain u:



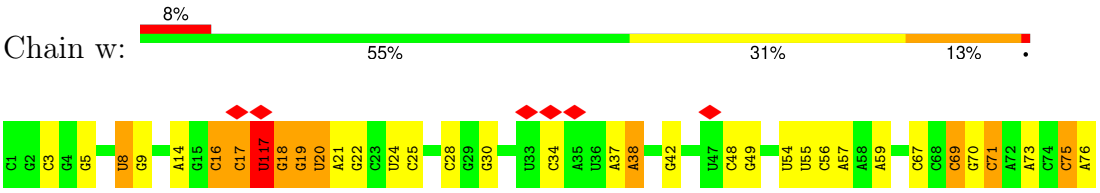
• Molecule 55: tRNA-fMet

Chain v:



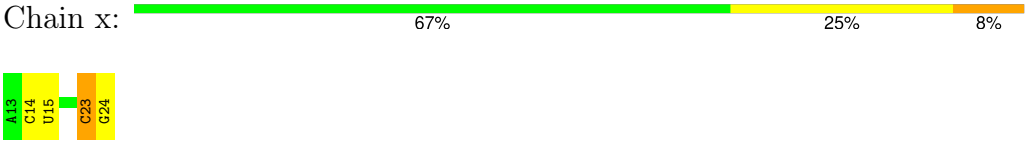
• Molecule 55: tRNA-fMet

Chain w:



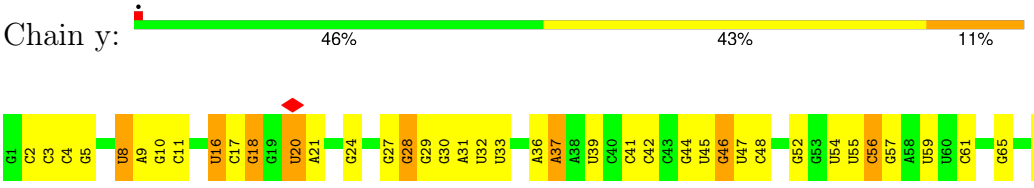
• Molecule 56: mRNA

Chain x:



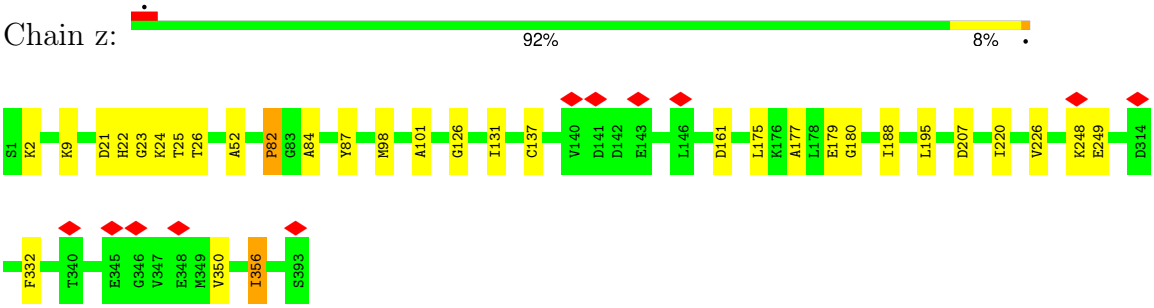
• Molecule 57: Phe-tRNA-Phe

Chain y:



• Molecule 58: Elongation factor Tu 2

Chain z:


92%
8%
S1
K2
K9
D21
H22
G23
K24
T25
T26
A52
P82
G83
A84
Y87
M98
A101
G126
I131
C137
V140
D141
D142
E143
L146
D161
L175
K176
A177
L178
E179
G180
I188
L195
D207
I220
V226
K248
E249
D314
F332
T340
E345
G346
V347
E348
M349
V350
I356
S393

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	58475	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	67	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.288	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.00532	Depositor
Map size (Å)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.98, 0.98, 0.98	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OMG, OMC, 3TD, MG, 7MG, MIA, 1MG, GTP, H2U, FME, PSU, MA6, K, 5MU, UR3, 2MA, 6MZ, OMU, 4SU, 2MG, 5MC, 4OC

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	0.38	0/69174	0.76	48/107907 (0.0%)
2	B	0.39	0/2876	0.77	0/4483
3	C	0.50	0/2121	0.78	0/2852
4	D	0.49	0/1578	0.77	2/2124 (0.1%)
5	E	0.49	0/1563	0.82	0/2103
6	F	0.55	0/1434	0.82	0/1926
7	G	0.53	0/1324	0.74	0/1794
8	H	0.62	0/1122	0.81	0/1515
9	I	0.69	0/1046	0.92	0/1410
10	J	0.49	0/1143	0.80	0/1540
11	K	0.50	0/947	0.76	0/1268
12	L	0.51	0/1052	0.88	0/1401
13	M	0.49	0/1093	0.79	0/1460
14	N	0.53	0/964	0.86	0/1289
15	O	0.52	0/902	0.84	0/1209
16	P	0.48	0/929	0.75	0/1242
17	Q	0.49	0/946	0.88	0/1260
18	R	0.48	0/823	0.70	0/1100
19	S	0.49	0/852	0.83	0/1142
20	T	0.50	0/736	0.76	0/984
21	U	0.47	0/787	0.73	0/1051
22	V	0.49	0/752	0.74	0/1008
23	W	0.47	0/579	0.68	0/767
24	X	0.48	0/635	0.72	0/848
25	Y	0.53	0/495	0.87	0/658
26	Z	0.52	0/438	0.78	0/586
27	0	0.45	0/440	0.81	0/588
28	1	0.49	0/424	0.69	0/565
29	2	0.52	0/370	0.97	0/487
30	3	0.46	0/513	0.84	0/676
31	4	0.46	0/303	0.75	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	5	0.67	0/1001	0.84	0/1350
33	6	0.57	0/531	0.79	0/709
34	a	0.39	0/36725	0.76	25/57285 (0.0%)
35	b	0.55	0/1735	0.79	0/2338
36	c	0.53	0/1651	0.80	0/2225
37	d	0.60	0/1665	0.82	0/2227
38	e	0.52	0/1180	0.84	0/1587
39	f	0.56	0/835	0.81	2/1128 (0.2%)
40	g	0.53	0/1195	0.82	0/1602
41	h	0.52	0/989	0.80	0/1326
42	i	0.56	0/1034	0.76	0/1375
43	j	0.55	0/796	0.74	0/1077
44	k	0.54	0/885	0.78	0/1195
45	l	0.56	0/954	0.78	0/1282
46	m	0.56	0/900	0.84	0/1204
47	n	0.53	0/822	0.79	0/1095
48	o	0.50	0/722	0.83	0/964
49	p	0.56	0/659	0.78	0/884
50	q	0.56	0/657	0.76	0/881
51	r	0.60	0/544	0.80	0/731
52	s	0.55	0/652	0.75	0/877
53	t	0.54	0/671	0.88	0/888
54	u	0.64	0/550	0.92	0/728
55	v	0.41	1/1747 (0.1%)	0.74	0/2721
55	w	0.40	0/1747	0.98	5/2721 (0.2%)
56	x	0.37	0/280	0.77	0/433
57	y	0.40	0/1607	0.73	1/2501 (0.0%)
58	z	0.57	0/3086	0.78	0/4175
All	All	0.43	1/164181 (0.0%)	0.77	83/245149 (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
1	A	0	1
34	a	0	2
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	7	4SU	O3'-P	5.46	1.61	1.56

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	117	U	O3'-P-O5'	23.50	139.25	104.00
55	w	117	U	P-O3'-C3'	22.09	153.34	120.20
34	a	1399	C	C2'-C3'-O3'	10.11	124.67	109.50
34	a	1305	G	C2'-C3'-O3'	9.84	124.27	109.50
1	A	301	G	C4'-C3'-O3'	9.44	123.55	109.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1054	A	Sidechain
34	a	141	G	Sidechain
34	a	222	C	Sidechain

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	62277	0	31337	505	0
2	B	2572	0	1302	19	0
3	C	2082	0	2157	12	0
4	D	1557	0	1604	5	0
5	E	1544	0	1607	5	0
6	F	1410	0	1447	7	0
7	G	1304	0	1348	3	0
8	H	1111	0	1148	2	0
9	I	1032	0	1088	8	0
10	J	1120	0	1151	7	0
11	K	938	0	1012	3	0
12	L	1043	0	1123	7	0
13	M	1074	0	1157	5	0
14	N	951	0	994	4	0
15	O	892	0	923	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	P	917	0	965	6	0
17	Q	933	0	1006	7	0
18	R	810	0	834	6	0
19	S	845	0	909	4	0
20	T	730	0	795	2	0
21	U	779	0	834	1	0
22	V	739	0	763	3	0
23	W	572	0	593	2	0
24	X	625	0	655	0	0
25	Y	494	0	530	1	0
26	Z	434	0	477	2	0
27	0	434	0	448	5	0
28	1	417	0	451	0	0
29	2	367	0	405	6	0
30	3	504	0	574	0	0
31	4	302	0	343	5	0
32	5	988	0	1025	3	0
33	6	522	0	524	1	0
34	a	33050	0	16652	300	0
35	b	1704	0	1732	3	0
36	c	1624	0	1699	8	0
37	d	1643	0	1710	5	0
38	e	1164	0	1212	11	0
39	f	817	0	808	15	0
40	g	1181	0	1240	5	0
41	h	979	0	1034	9	0
42	i	1022	0	1070	1	0
43	j	786	0	828	3	0
44	k	869	0	878	0	0
45	l	940	0	1001	3	0
46	m	891	0	955	5	0
47	n	810	0	852	5	0
48	o	714	0	737	2	0
49	p	649	0	666	5	0
50	q	648	0	691	4	0
51	r	535	0	552	4	0
52	s	637	0	665	3	0
53	t	665	0	714	1	0
54	u	544	0	579	4	0
55	v	1644	0	840	1	0
55	w	1644	0	840	14	0
56	x	252	0	130	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	y	1632	0	843	8	0
58	z	3031	0	3052	19	0
59	A	10	0	10	0	0
60	0	3	0	0	0	0
60	2	1	0	0	0	0
60	A	1011	0	0	0	0
60	B	37	0	0	0	0
60	C	1	0	0	0	0
60	D	2	0	0	0	0
60	E	1	0	0	0	0
60	M	2	0	0	0	0
60	N	1	0	0	0	0
60	Q	1	0	0	0	0
60	T	1	0	0	0	0
60	W	1	0	0	0	0
60	a	392	0	0	0	0
60	d	1	0	0	0	0
60	e	1	0	0	0	0
60	i	1	0	0	0	0
60	u	1	0	0	0	0
60	v	6	0	0	0	0
60	w	2	0	0	0	0
60	x	1	0	0	0	0
60	y	2	0	0	0	0
60	z	2	0	0	0	0
61	A	6	0	0	0	0
61	a	1	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	12	16	0
64	0	2	0	0	0	0
64	1	1	0	0	0	0
64	2	2	0	0	0	0
64	3	1	0	0	0	0
64	A	828	0	0	0	0
64	B	29	0	0	0	0
64	C	5	0	0	0	0
64	D	6	0	0	0	0
64	E	5	0	0	0	0
64	J	4	0	0	0	0
64	L	5	0	0	0	0
64	N	1	0	0	0	0
64	O	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	Q	3	0	0	0	0
64	R	1	0	0	0	0
64	S	3	0	0	0	0
64	W	2	0	0	0	0
64	X	3	0	0	0	0
64	Y	1	0	0	0	0
64	a	253	0	0	1	0
64	c	1	0	0	0	0
64	i	1	0	0	0	0
64	j	1	0	0	0	0
64	l	2	0	0	0	0
64	m	1	0	0	0	0
64	o	1	0	0	0	0
64	q	1	0	0	0	0
64	s	3	0	0	0	0
64	u	1	0	0	0	0
64	v	3	0	0	0	0
64	w	1	0	0	0	0
64	x	1	0	0	0	0
64	y	2	0	0	0	0
All	All	155100	0	103539	1030	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 1030 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)
34:a:182:A:N1	34:a:185:U:O4	1.63	1.31
1:A:1105:U:N3	1:A:1106:G:N9	1.79	1.28
1:A:1021:A:N1	1:A:1141:U:O4	1.70	1.24
1:A:1054:A:N6	1:A:1106:G:N7	1.91	1.18
1:A:1915:3TD:C1'	1:A:1915:3TD:O4'	1.66	1.18

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
3	C	269/271 (99%)	239 (89%)	27 (10%)	3 (1%)	11 43
4	D	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	24 60
5	E	198/200 (99%)	178 (90%)	18 (9%)	2 (1%)	12 45
6	F	175/177 (99%)	157 (90%)	16 (9%)	2 (1%)	11 43
7	G	172/174 (99%)	158 (92%)	14 (8%)	0	100 100
8	H	147/149 (99%)	128 (87%)	15 (10%)	4 (3%)	4 22
9	I	139/141 (99%)	109 (78%)	23 (16%)	7 (5%)	1 10
10	J	139/141 (99%)	130 (94%)	8 (6%)	1 (1%)	18 53
11	K	120/122 (98%)	106 (88%)	10 (8%)	4 (3%)	3 17
12	L	141/143 (99%)	117 (83%)	18 (13%)	6 (4%)	2 12
13	M	134/136 (98%)	128 (96%)	5 (4%)	1 (1%)	18 53
14	N	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	7 32
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14 48
16	P	112/114 (98%)	99 (88%)	12 (11%)	1 (1%)	14 48
17	Q	113/115 (98%)	111 (98%)	2 (2%)	0	100 100
18	R	100/102 (98%)	85 (85%)	12 (12%)	3 (3%)	3 19
19	S	107/109 (98%)	100 (94%)	6 (6%)	1 (1%)	14 48
20	T	90/92 (98%)	81 (90%)	7 (8%)	2 (2%)	5 26
21	U	100/102 (98%)	87 (87%)	9 (9%)	4 (4%)	2 14
22	V	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	11 43
23	W	73/75 (97%)	68 (93%)	5 (7%)	0	100 100
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100 100
25	Y	58/60 (97%)	54 (93%)	3 (5%)	1 (2%)	7 32
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100 100
27	0	53/55 (96%)	44 (83%)	8 (15%)	1 (2%)	6 30

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
28	1	49/51 (96%)	43 (88%)	6 (12%)	0	100 100
29	2	43/45 (96%)	40 (93%)	2 (5%)	1 (2%)	5 25
30	3	62/64 (97%)	59 (95%)	3 (5%)	0	100 100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100 100
32	5	129/131 (98%)	99 (77%)	21 (16%)	9 (7%)	1 4
33	6	64/66 (97%)	58 (91%)	4 (6%)	2 (3%)	3 19
35	b	216/218 (99%)	186 (86%)	25 (12%)	5 (2%)	5 25
36	c	204/206 (99%)	183 (90%)	15 (7%)	6 (3%)	3 20
37	d	203/205 (99%)	183 (90%)	17 (8%)	3 (2%)	8 35
38	e	156/157 (99%)	133 (85%)	21 (14%)	2 (1%)	9 38
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	2 13
40	g	149/151 (99%)	131 (88%)	11 (7%)	7 (5%)	2 11
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100 100
42	i	125/127 (98%)	97 (78%)	24 (19%)	4 (3%)	3 18
43	j	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	1 9
44	k	114/116 (98%)	97 (85%)	11 (10%)	6 (5%)	1 9
45	l	119/121 (98%)	93 (78%)	19 (16%)	7 (6%)	1 7
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	6 31
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	1 10
48	o	86/88 (98%)	79 (92%)	4 (5%)	3 (4%)	3 16
49	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	4 23
50	q	78/80 (98%)	67 (86%)	7 (9%)	4 (5%)	1 10
51	r	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2 11
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100 100
53	t	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	4 24
54	u	63/65 (97%)	41 (65%)	12 (19%)	10 (16%)	0 0
58	z	391/393 (100%)	357 (91%)	22 (6%)	12 (3%)	3 19
All	All	6219/6322 (98%)	5486 (88%)	581 (9%)	152 (2%)	7 24

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	70	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	E	83	VAL
6	F	11	VAL
11	K	89	ASN
16	P	65	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
3	C	216/216 (100%)	206 (95%)	10 (5%)	24 58
4	D	163/163 (100%)	153 (94%)	10 (6%)	17 49
5	E	164/164 (100%)	153 (93%)	11 (7%)	15 46
6	F	148/148 (100%)	143 (97%)	5 (3%)	32 66
7	G	135/135 (100%)	133 (98%)	2 (2%)	57 80
8	H	114/114 (100%)	108 (95%)	6 (5%)	20 54
9	I	109/109 (100%)	102 (94%)	7 (6%)	16 48
10	J	115/115 (100%)	112 (97%)	3 (3%)	40 72
11	K	103/103 (100%)	99 (96%)	4 (4%)	28 62
12	L	102/102 (100%)	93 (91%)	9 (9%)	9 35
13	M	109/109 (100%)	108 (99%)	1 (1%)	70 85
14	N	99/99 (100%)	94 (95%)	5 (5%)	21 55
15	O	86/86 (100%)	85 (99%)	1 (1%)	63 82
16	P	99/99 (100%)	96 (97%)	3 (3%)	36 69
17	Q	88/88 (100%)	84 (96%)	4 (4%)	24 59
18	R	84/84 (100%)	82 (98%)	2 (2%)	43 73
19	S	92/92 (100%)	91 (99%)	1 (1%)	65 83
20	T	79/79 (100%)	76 (96%)	3 (4%)	29 63
21	U	83/83 (100%)	82 (99%)	1 (1%)	63 82
22	V	77/77 (100%)	76 (99%)	1 (1%)	61 81

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
23	W	57/57 (100%)	56 (98%)	1 (2%)	51 77
24	X	67/67 (100%)	66 (98%)	1 (2%)	57 80
25	Y	55/55 (100%)	54 (98%)	1 (2%)	51 77
26	Z	47/47 (100%)	47 (100%)	0	100 100
27	0	46/46 (100%)	46 (100%)	0	100 100
28	1	46/46 (100%)	46 (100%)	0	100 100
29	2	37/37 (100%)	36 (97%)	1 (3%)	39 71
30	3	51/51 (100%)	50 (98%)	1 (2%)	48 76
31	4	34/34 (100%)	34 (100%)	0	100 100
32	5	100/100 (100%)	100 (100%)	0	100 100
33	6	59/59 (100%)	58 (98%)	1 (2%)	53 78
35	b	180/180 (100%)	178 (99%)	2 (1%)	65 83
36	c	170/170 (100%)	167 (98%)	3 (2%)	51 77
37	d	172/172 (100%)	167 (97%)	5 (3%)	37 70
38	e	120/119 (101%)	109 (91%)	11 (9%)	8 33
39	f	87/87 (100%)	84 (97%)	3 (3%)	32 66
40	g	124/124 (100%)	120 (97%)	4 (3%)	34 67
41	h	104/104 (100%)	102 (98%)	2 (2%)	50 76
42	i	105/105 (100%)	102 (97%)	3 (3%)	37 70
43	j	86/86 (100%)	85 (99%)	1 (1%)	63 82
44	k	89/89 (100%)	87 (98%)	2 (2%)	45 74
45	l	102/102 (100%)	99 (97%)	3 (3%)	37 70
46	m	93/93 (100%)	92 (99%)	1 (1%)	65 83
47	n	83/83 (100%)	81 (98%)	2 (2%)	43 73
48	o	76/76 (100%)	74 (97%)	2 (3%)	40 72
49	p	65/65 (100%)	63 (97%)	2 (3%)	35 68
50	q	74/74 (100%)	71 (96%)	3 (4%)	27 61
51	r	56/56 (100%)	52 (93%)	4 (7%)	13 43
52	s	70/70 (100%)	67 (96%)	3 (4%)	26 60
53	t	65/65 (100%)	61 (94%)	4 (6%)	16 49
54	u	55/55 (100%)	53 (96%)	2 (4%)	31 65

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
58	z	325/325 (100%)	322 (99%)	3 (1%)	70 85
All	All	5165/5164 (100%)	5005 (97%)	160 (3%)	36 68

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
38	e	146	MET
50	q	52	CYS
40	g	11	ILE
44	k	125	LYS
52	s	12	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
40	g	129	ASN
53	t	47	GLN
42	i	125	GLN
46	m	99	GLN
58	z	329	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	830 (28%)	91 (3%)
2	B	119/120 (99%)	46 (38%)	7 (5%)
34	a	1539/1540 (99%)	498 (32%)	0
55	v	76/77 (98%)	24 (31%)	0
55	w	76/77 (98%)	33 (43%)	0
56	x	11/12 (91%)	4 (36%)	0
57	y	75/76 (98%)	31 (41%)	0
All	All	4793/4805 (99%)	1466 (30%)	98 (2%)

5 of 1466 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	5	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	10	A
1	A	12	U

5 of 98 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1538	G
1	A	2192	U
1	A	1607	C
1	A	1884	G
1	A	2401	U

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	5MC	A	747	1	19,22,23	1.84	3 (15%)	26,32,35	1.66	6 (23%)
34	MA6	a	1519	34	23,26,27	1.70	6 (26%)	33,38,41	2.34	12 (36%)
1	PSU	A	955	1	18,21,22	1.41	3 (16%)	21,30,33	2.10	4 (19%)
34	7MG	a	527	34	23,26,27	1.45	4 (17%)	27,39,42	2.48	7 (25%)
34	5MC	a	1407	34	19,22,23	1.68	2 (10%)	26,32,35	1.31	4 (15%)
1	PSU	A	2604	1	18,21,22	1.42	3 (16%)	21,30,33	1.99	4 (19%)
55	4SU	v	7	55	18,21,22	1.75	4 (22%)	25,30,33	2.42	5 (20%)
57	4SU	y	8	57	18,21,22	1.81	5 (27%)	25,30,33	2.37	7 (28%)
34	UR3	a	1498	34	19,22,23	1.09	2 (10%)	26,32,35	1.99	5 (19%)
57	MIA	y	37	57	28,31,32	2.44	7 (25%)	38,44,47	2.92	15 (39%)
34	5MC	a	967	34	19,22,23	1.84	2 (10%)	26,32,35	1.26	3 (11%)
1	OMG	A	2251	1,55,60	23,26,27	1.27	3 (13%)	32,38,41	1.94	7 (21%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.58	2 (10%)
1	7MG	A	2069	1,60	23,26,27	1.49	4 (17%)	27,39,42	2.54	10 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	PSU	a	516	34	18,21,22	1.44	2 (11%)	21,30,33	2.08	5 (23%)
1	2MA	A	2503	1,60	22,25,26	1.51	5 (22%)	32,37,40	2.25	9 (28%)
55	4SU	w	8	55	18,21,22	1.81	5 (27%)	25,30,33	2.22	5 (20%)
1	OMC	A	2498	1,60	19,22,23	0.88	1 (5%)	25,31,34	1.23	2 (8%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.39	4 (21%)
55	5MU	v	54	55	19,22,23	1.49	5 (26%)	27,32,35	1.91	8 (29%)
1	PSU	A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
34	2MG	a	1207	34,60	23,26,27	1.24	3 (13%)	33,38,41	3.00	10 (30%)
1	PSU	A	2580	1	18,21,22	1.50	3 (16%)	21,30,33	2.07	5 (23%)
1	6MZ	A	2030	1	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
1	PSU	A	2605	1,60	18,21,22	1.42	2 (11%)	21,30,33	2.21	4 (19%)
1	2MG	A	2445	1	23,26,27	1.32	5 (21%)	33,38,41	2.29	8 (24%)
1	6MZ	A	1618	1	22,25,26	1.54	4 (18%)	29,36,39	2.29	10 (34%)
1	3TD	A	1915	1,60	19,22,23	7.04	13 (68%)	23,32,35	2.05	4 (17%)
1	PSU	A	2457	1	18,21,22	1.55	3 (16%)	21,30,33	2.00	5 (23%)
34	2MG	a	1516	34	23,26,27	1.27	5 (21%)	33,38,41	2.42	12 (36%)
55	H2U	v	20	55	18,21,22	0.91	1 (5%)	19,30,33	1.63	4 (21%)
57	PSU	y	55	57	18,21,22	1.40	2 (11%)	21,30,33	2.05	5 (23%)
1	2MG	A	1835	1	23,26,27	1.28	3 (13%)	33,38,41	2.18	7 (21%)
57	5MU	y	54	57	19,22,23	1.41	4 (21%)	27,32,35	2.12	8 (29%)
1	PSU	A	746	1,60	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
1	5MU	A	1939	1	19,22,23	1.38	5 (26%)	27,32,35	2.04	8 (29%)
1	PSU	A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.09	4 (19%)
1	1MG	A	745	1	23,26,27	1.29	3 (13%)	33,39,42	1.97	7 (21%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.48	4 (21%)
57	PSU	y	39	57	18,21,22	1.45	2 (11%)	21,30,33	2.01	4 (19%)
55	PSU	w	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.06	5 (23%)
1	5MC	A	1962	1	19,22,23	1.49	2 (10%)	26,32,35	1.24	3 (11%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.08	11 (40%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	21,30,33	1.94	4 (19%)
57	7MG	y	46	57	23,26,27	1.43	4 (17%)	27,39,42	2.47	7 (25%)
34	4OC	a	1402	34,60	20,23,24	0.81	0	25,32,35	1.34	5 (20%)
34	2MG	a	966	34	23,26,27	1.28	3 (13%)	33,38,41	2.65	10 (30%)
34	MA6	a	1518	34	23,26,27	1.83	6 (26%)	33,38,41	2.19	10 (30%)
57	PSU	y	32	57	18,21,22	1.36	2 (11%)	21,30,33	2.05	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	H2U	A	2449	1	18,21,22	1.03	2 (11%)	19,30,33	1.49	3 (15%)
1	OMU	A	2552	1,60	19,22,23	1.39	2 (10%)	25,31,34	2.25	8 (32%)
55	PSU	v	55	55,60	18,21,22	1.38	3 (16%)	21,30,33	1.98	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
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	3/11/29/30	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	2/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
57	MIA	y	37	57	-	5/15/33/34	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	OMG	A	2251	1,55,60	-	0/9/27/28	0/3/3/3
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
1	7MG	A	2069	1,60	-	2/7/37/38	0/3/3/3
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
1	2MA	A	2503	1,60	-	0/7/25/26	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34,60	-	0/9/27/28	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	3/9/27/28	0/3/3/3
1	PSU	A	2605	1,60	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
1	6MZ	A	1618	1	-	3/9/27/28	0/3/3/3
1	3TD	A	1915	1,60	-	3/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	1/7/25/26	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	PSU	A	746	1,60	-	4/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
57	PSU	y	39	57	-	2/7/25/26	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
34	4OC	a	1402	34,60	-	2/9/29/30	0/2/2/2
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	OMU	A	2552	1,60	-	2/9/27/28	0/2/2/2
55	PSU	v	55	55,60	-	2/7/25/26	0/2/2/2

The worst 5 of 170 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.11	1.66	1.43
1	A	1915	3TD	C6-C5	16.03	1.53	1.35
1	A	1915	3TD	C2'-C1'	-14.45	1.34	1.53
1	A	1915	3TD	C2-N1	8.02	1.47	1.37
57	y	37	MIA	C13-C14	7.18	1.53	1.32

The worst 5 of 327 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	1207	2MG	N1-C2-N2	8.86	125.60	116.56
57	y	37	MIA	C5-C4-N3	-8.39	118.34	127.18
34	a	966	2MG	C2-N3-C4	8.31	122.39	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	y	37	MIA	C12-C13-C14	-8.22	112.26	127.01
34	a	1207	2MG	C2-N3-C4	8.15	122.19	112.00

There are no chirality outliers.

5 of 79 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	746	PSU	C2'-C1'-C5-C4
1	A	746	PSU	O4'-C1'-C5-C6
1	A	2030	6MZ	C4'-C5'-O5'-P
1	A	2030	6MZ	C3'-C4'-C5'-O5'
1	A	2069	7MG	O4'-C4'-C5'-O5'

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	1519	MA6	1	0
1	A	2604	PSU	1	0
34	a	1207	2MG	1	0
1	A	2030	6MZ	10	0
1	A	2445	2MG	1	0
1	A	1618	6MZ	1	0
1	A	1915	3TD	2	0
1	A	1939	5MU	1	0
1	A	2504	PSU	1	0
34	a	1518	MA6	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 1481 ligands modelled in this entry, 1478 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
59	FME	A	3001	-	8,9,10	0.52	0	8,9,11	1.03	0
62	PHE	z	401	-	10,11,12	0.39	0	8,13,15	0.19	0
63	GTP	z	402	60	33,34,34	1.17	3 (9%)	50,54,54	1.74	7 (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
59	FME	A	3001	-	-	0/7/9/11	-
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
63	GTP	z	402	60	-	7/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C5-C4	3.08	1.47	1.38
63	z	402	GTP	C6-N1	-2.68	1.33	1.38
63	z	402	GTP	C5-N7	-2.14	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	z	402	GTP	C5-C4-N3	-6.33	118.31	128.39
63	z	402	GTP	C2-N3-C4	5.18	121.22	112.30
63	z	402	GTP	N9-C4-N3	4.80	135.55	125.95
63	z	402	GTP	C6-C5-N7	3.10	135.93	130.29
63	z	402	GTP	C4-C5-N7	-2.40	106.86	110.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
62	z	401	PHE	O-C-CA-CB
63	z	402	GTP	C5'-O5'-PA-O3A
63	z	402	GTP	C5'-O5'-PA-O1A
63	z	402	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
63	z	402	GTP	C3'-C4'-C5'-O5'

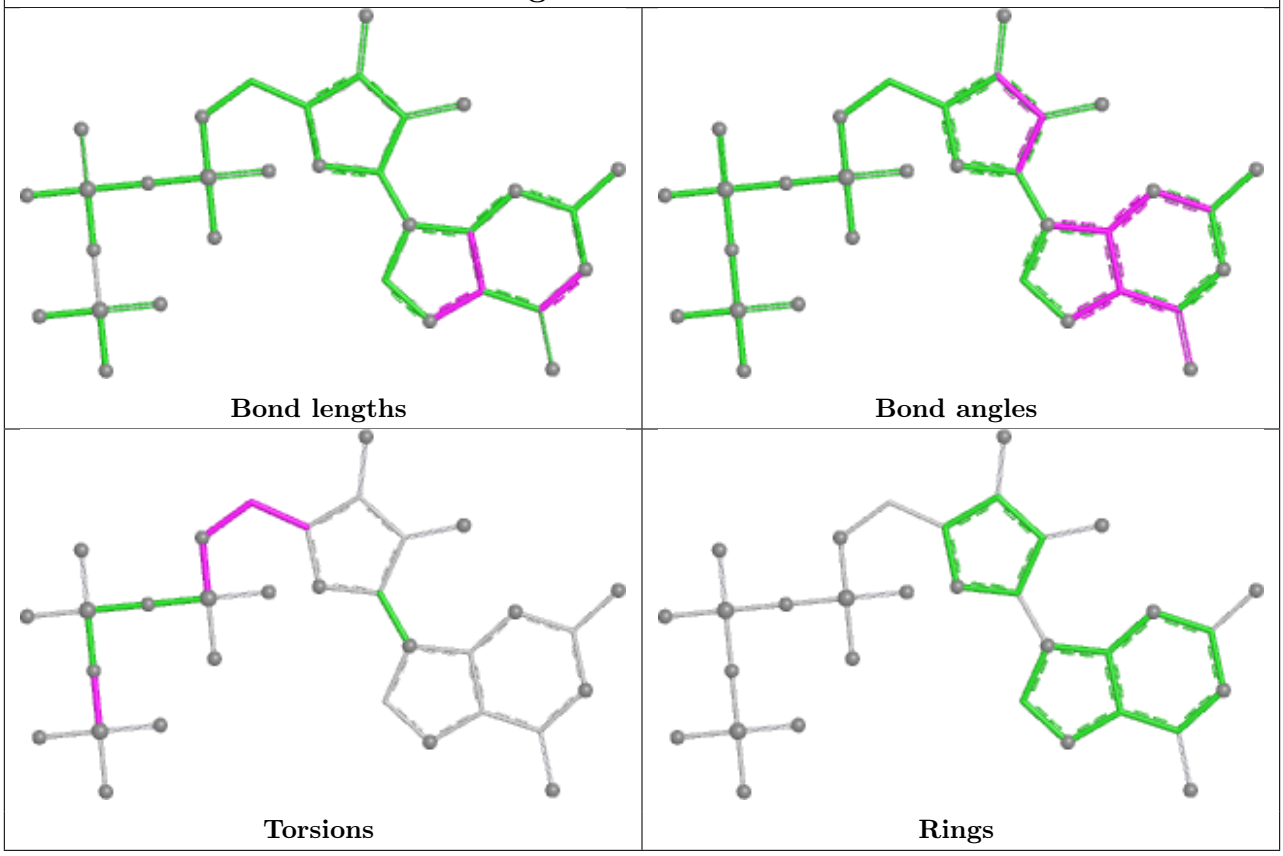
There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
63	z	402	GTP	16	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 GTP z 402



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.

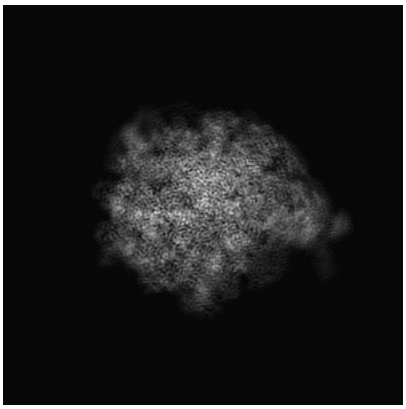
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-8829. These allow visual inspection of the internal detail of the map and identification of artifacts.

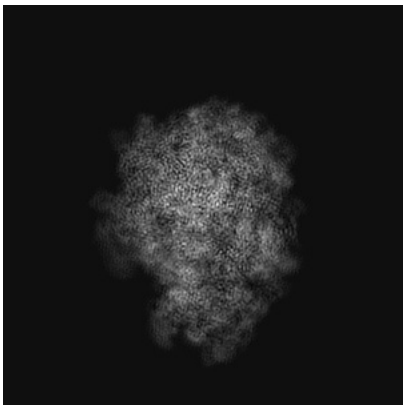
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

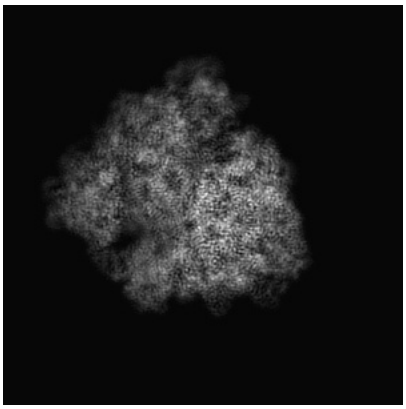
6.1.1 Primary map



X

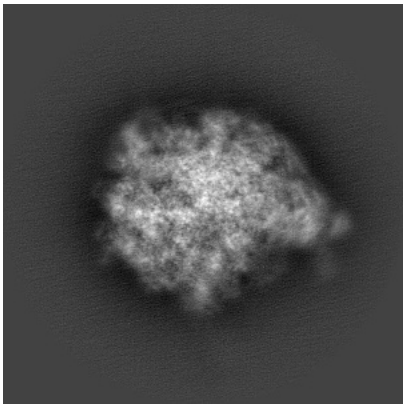


Y

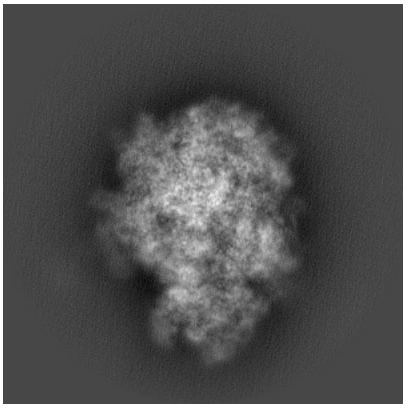


Z

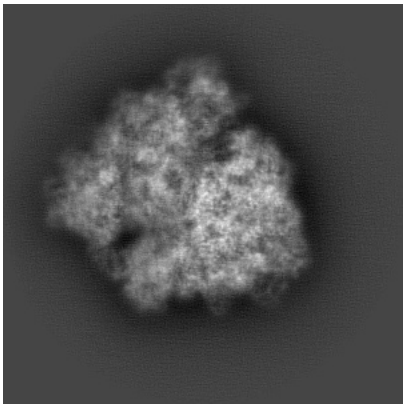
6.1.2 Raw map



X



Y

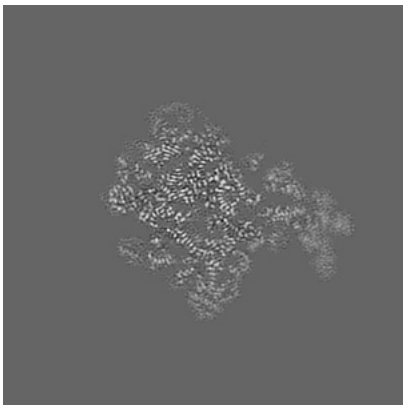


Z

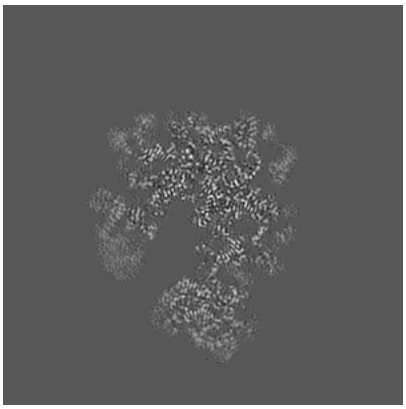
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

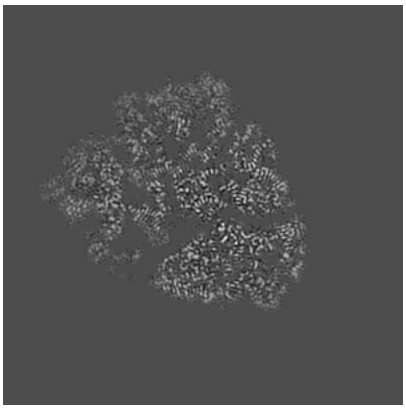
6.2.1 Primary map



X Index: 199

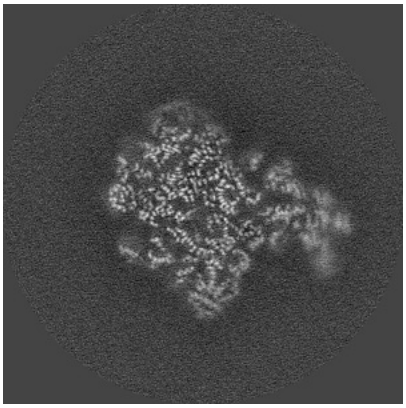


Y Index: 199

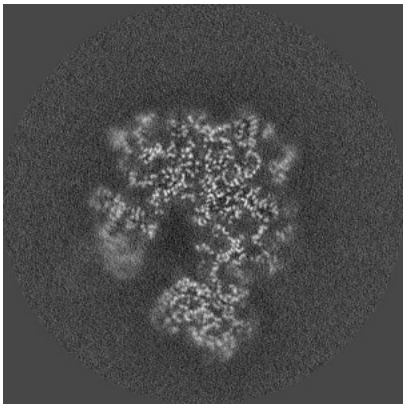


Z Index: 199

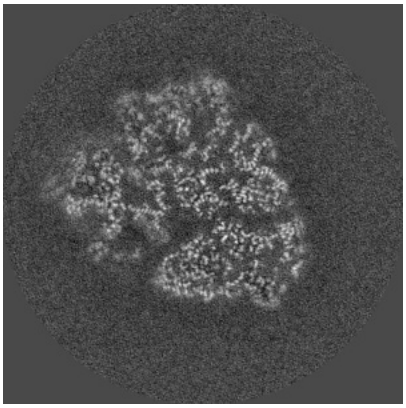
6.2.2 Raw map



X Index: 199



Y Index: 199

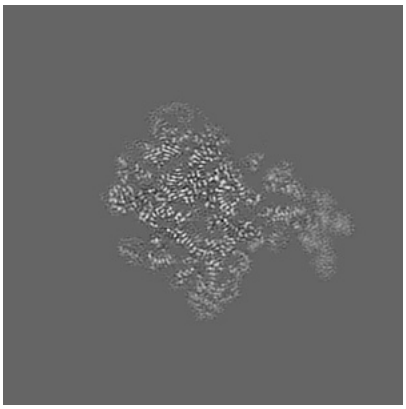


Z Index: 199

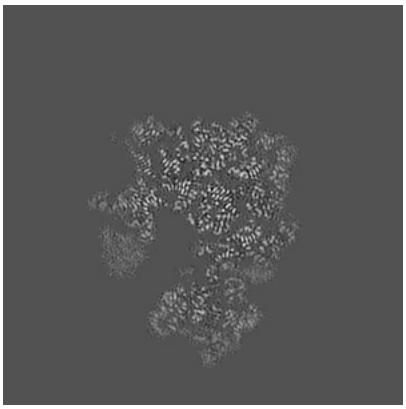
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

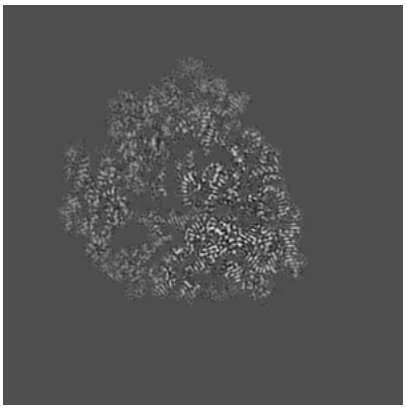
6.3.1 Primary map



X Index: 199

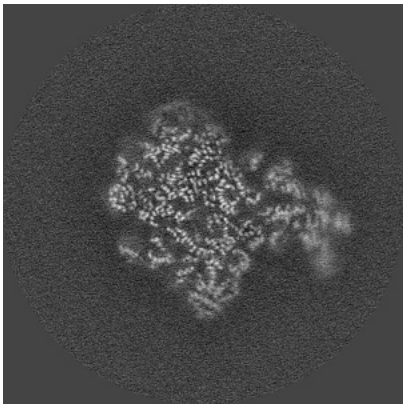


Y Index: 207

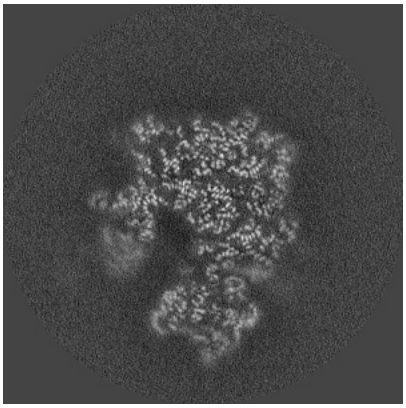


Z Index: 190

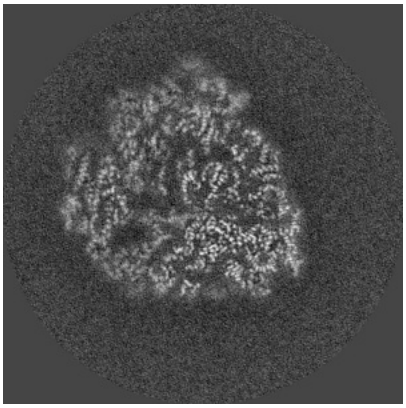
6.3.2 Raw map



X Index: 199



Y Index: 207

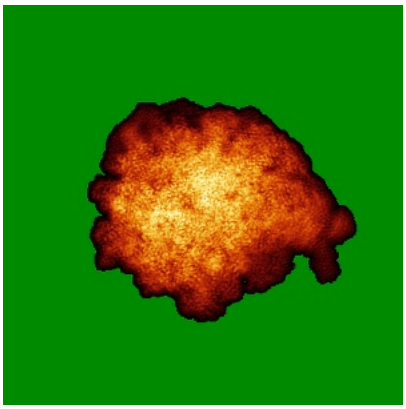


Z Index: 190

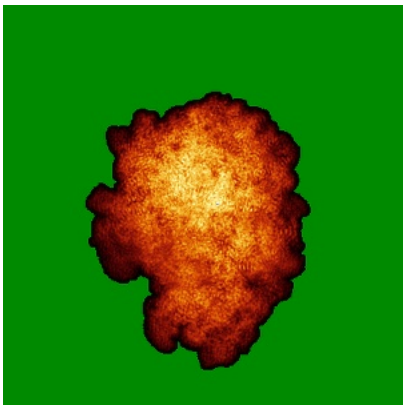
The images above show the largest variance slices of the map in three orthogonal directions.

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

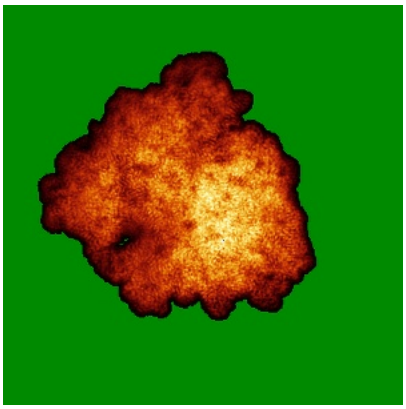
6.4.1 Primary map



X

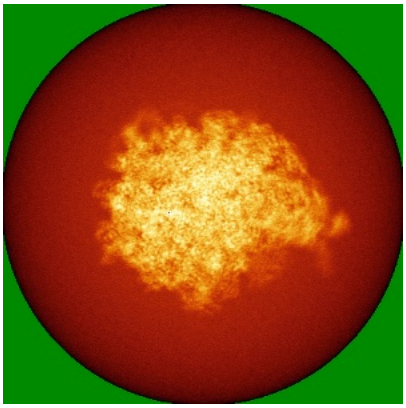


Y

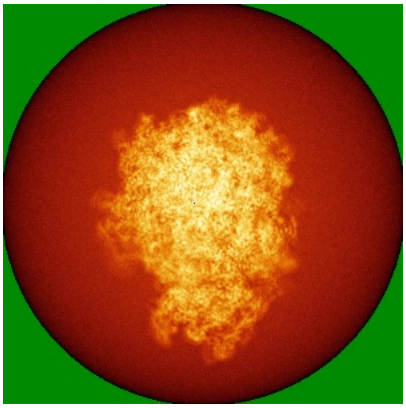


Z

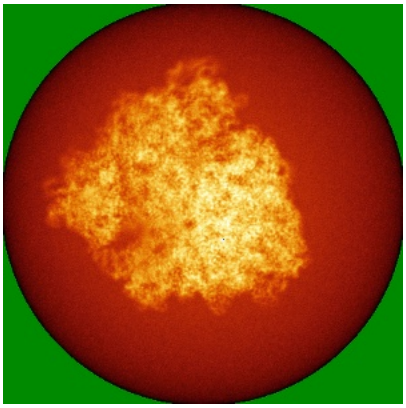
6.4.2 Raw map



X



Y

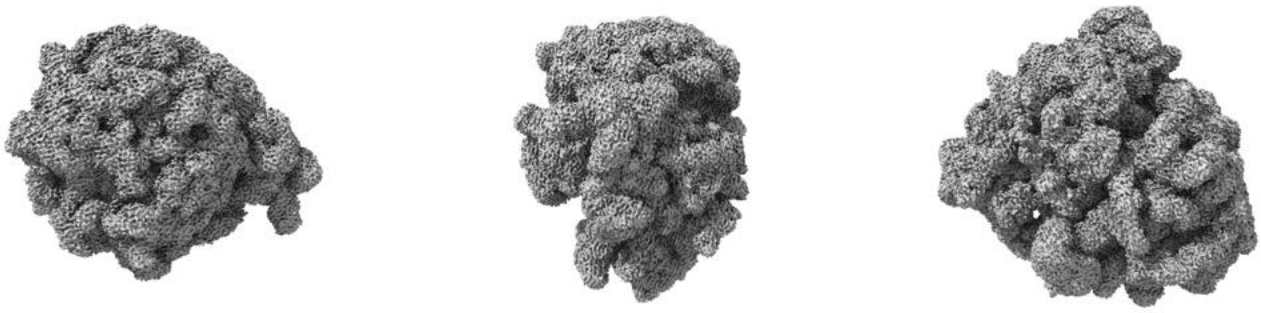


Z

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)

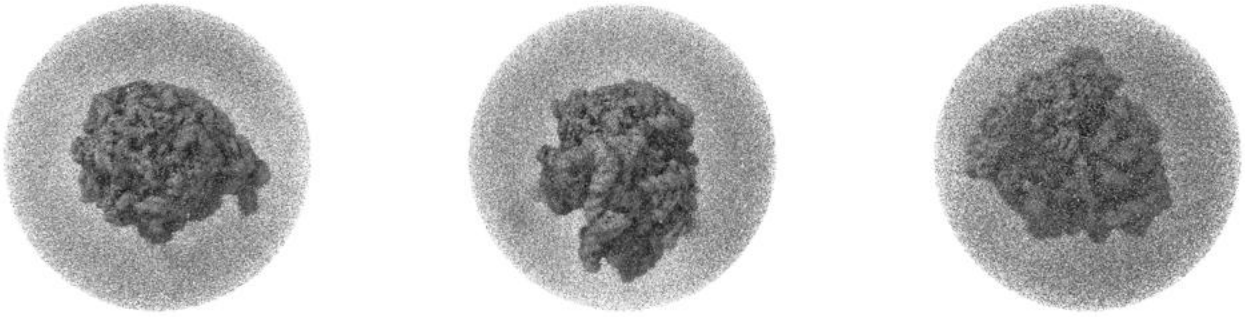
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00532. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

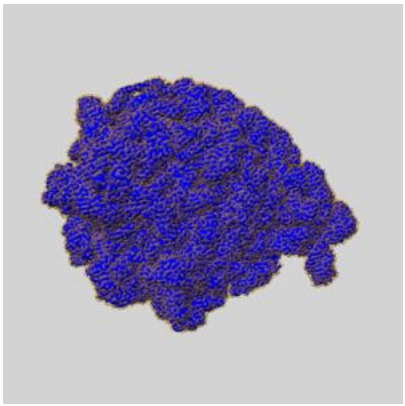
6.6 Mask visualisation (i)

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

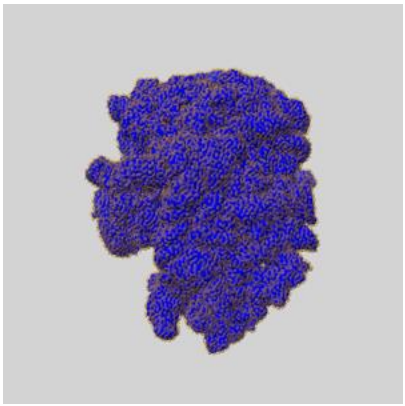
A mask typically either:

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

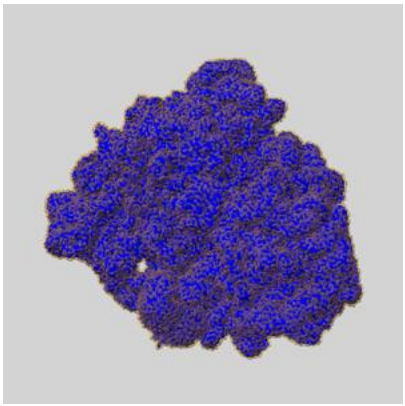
6.6.1 emd_8829_msk_1.map (i)



X



Y

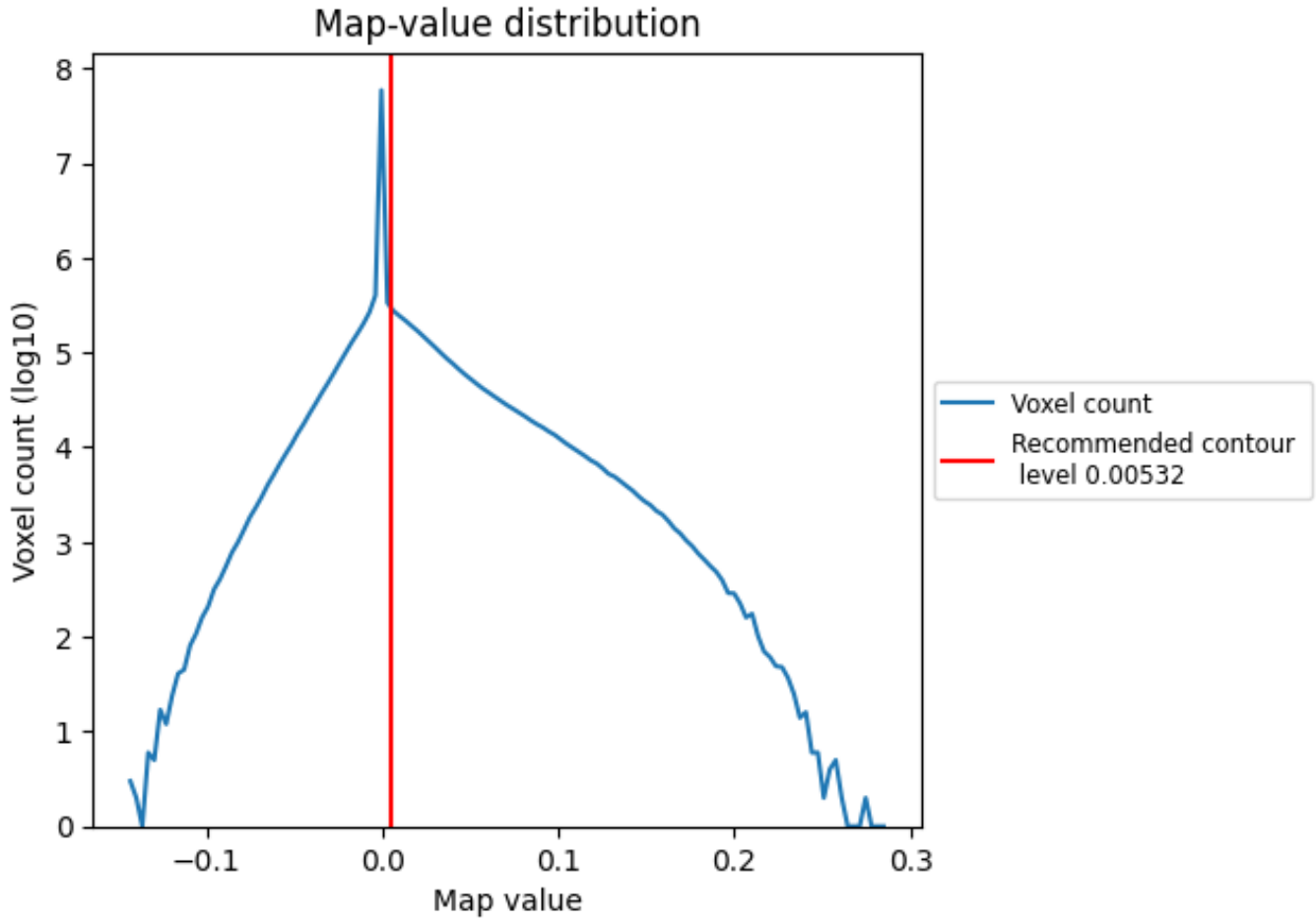


Z

7 Map analysis

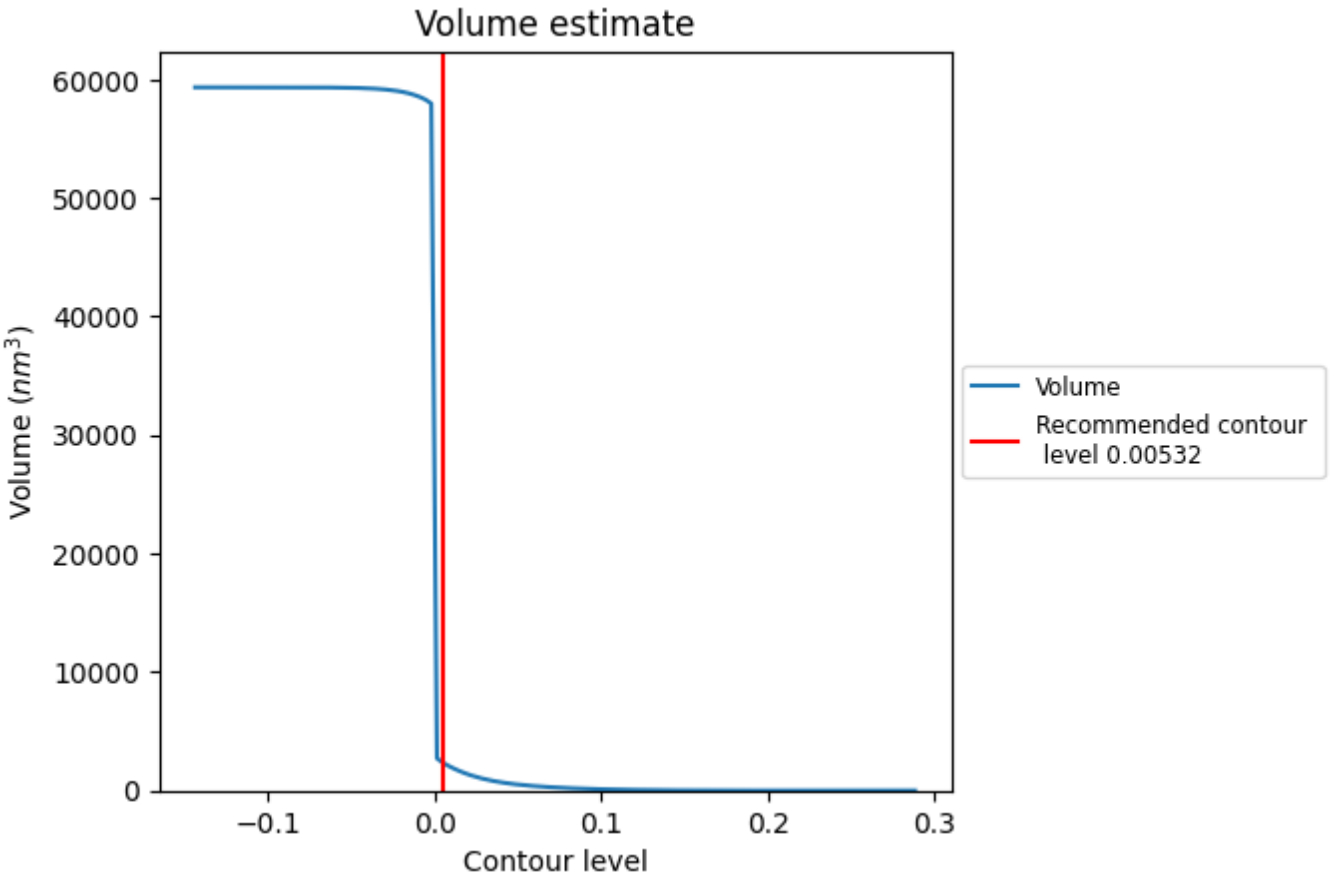
This section contains the results of statistical analysis of the map.

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.

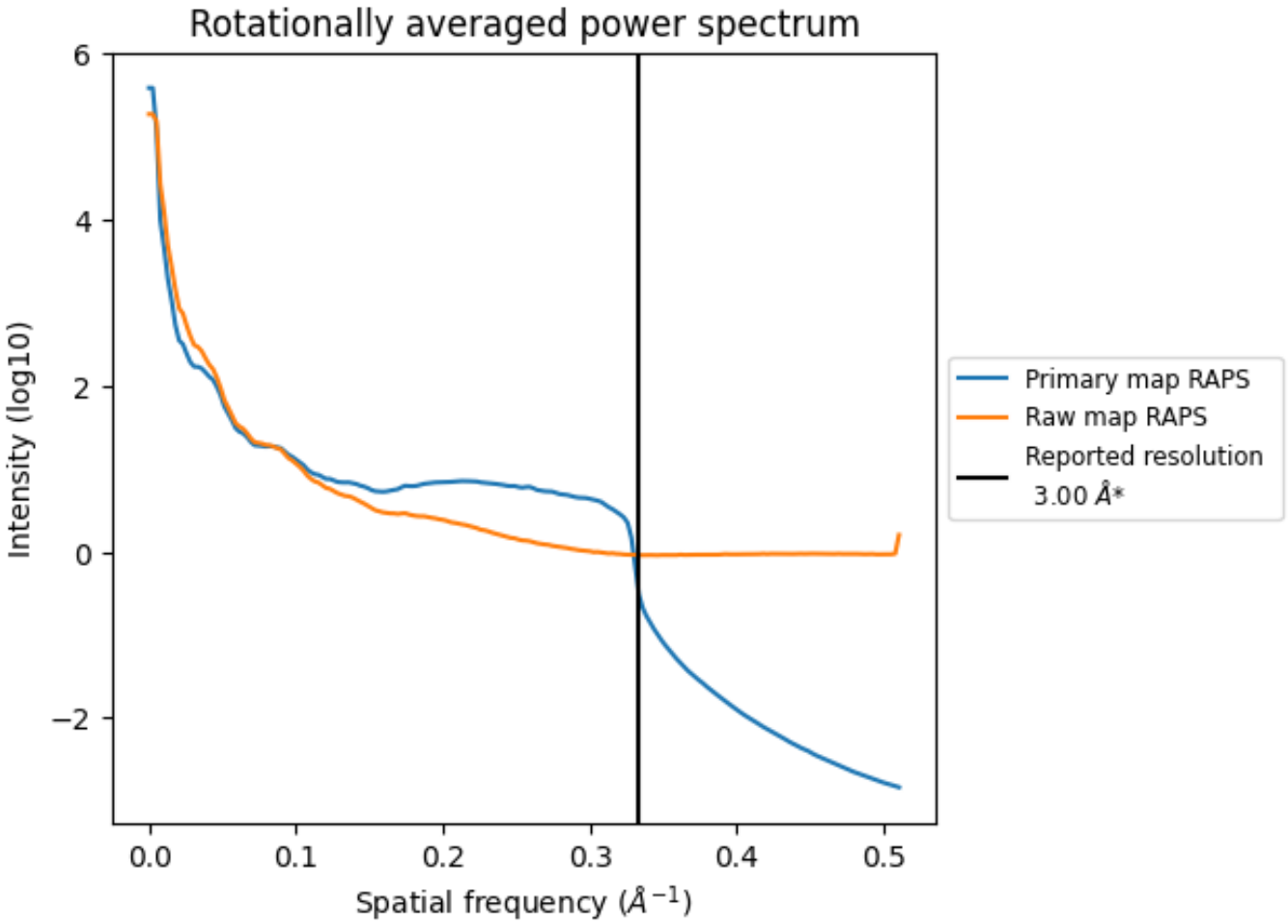
7.2 Volume estimate (i)



The volume at the recommended contour level is 2339 nm^3; this corresponds to an approximate mass of 2113 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)

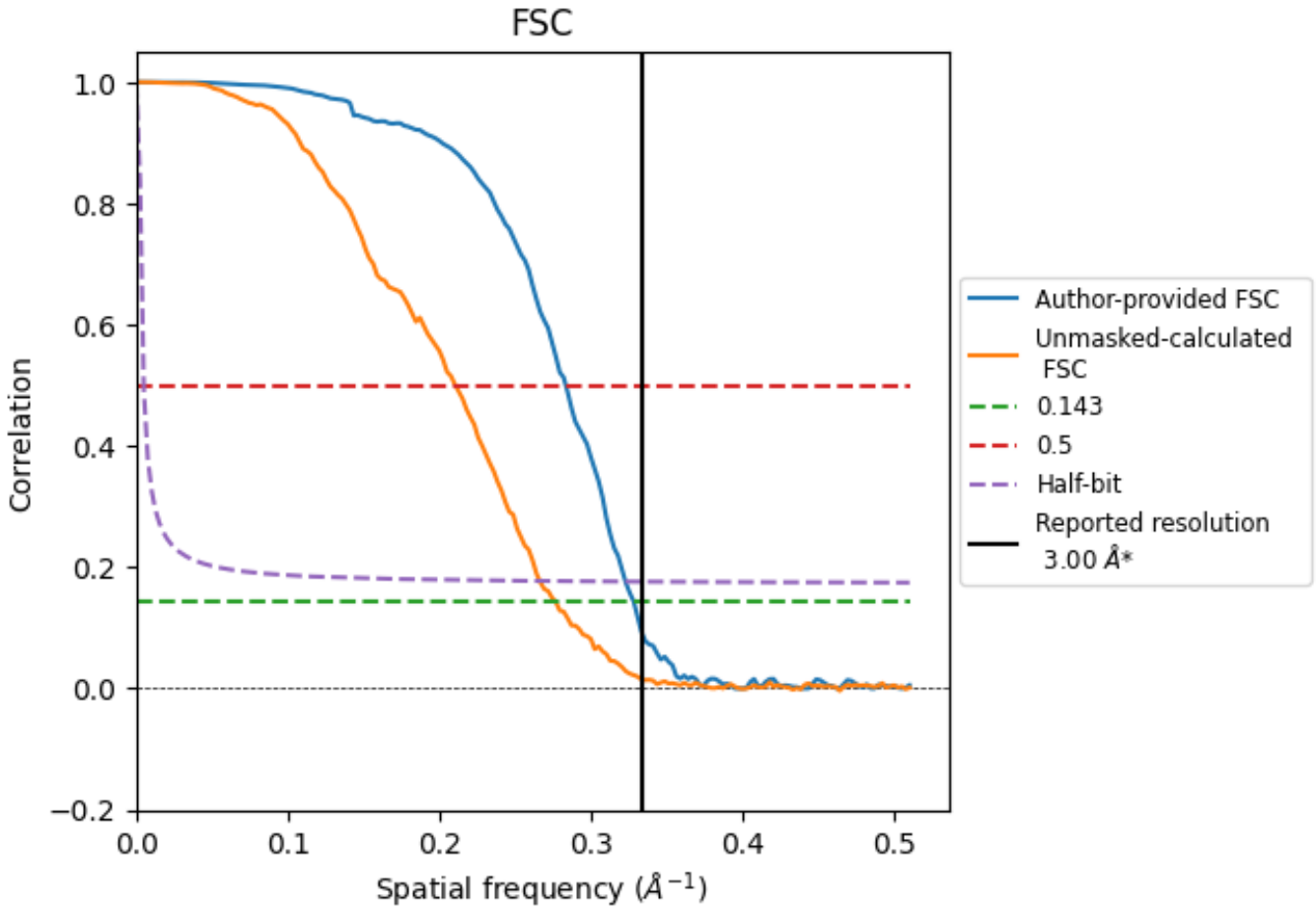


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

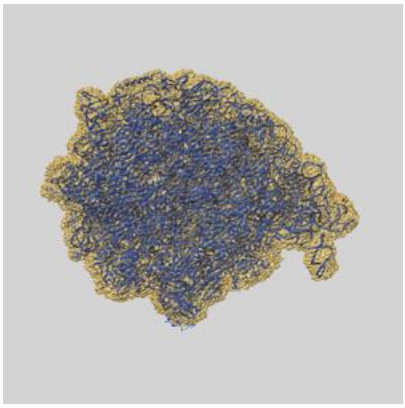
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.05	3.53	3.10
Unmasked-calculated*	3.61	4.75	3.76

*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 3.61 differs from the reported value 3.0 by more than 10 %

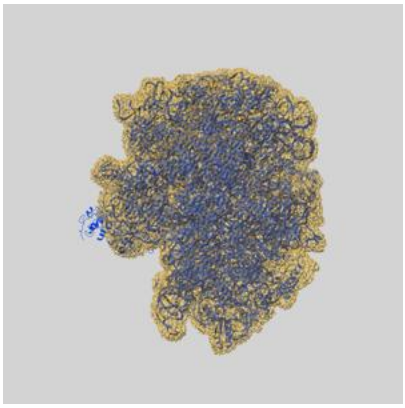
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-8829 and PDB model 5WFS. Per-residue inclusion information can be found in section 3 on page 20.

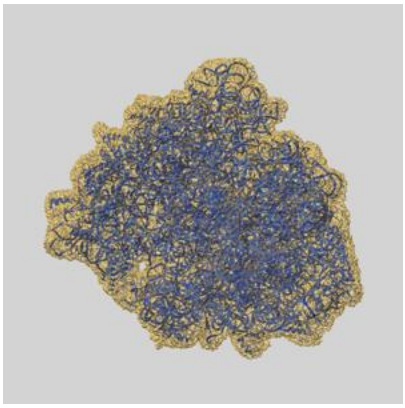
9.1 Map-model overlay



X



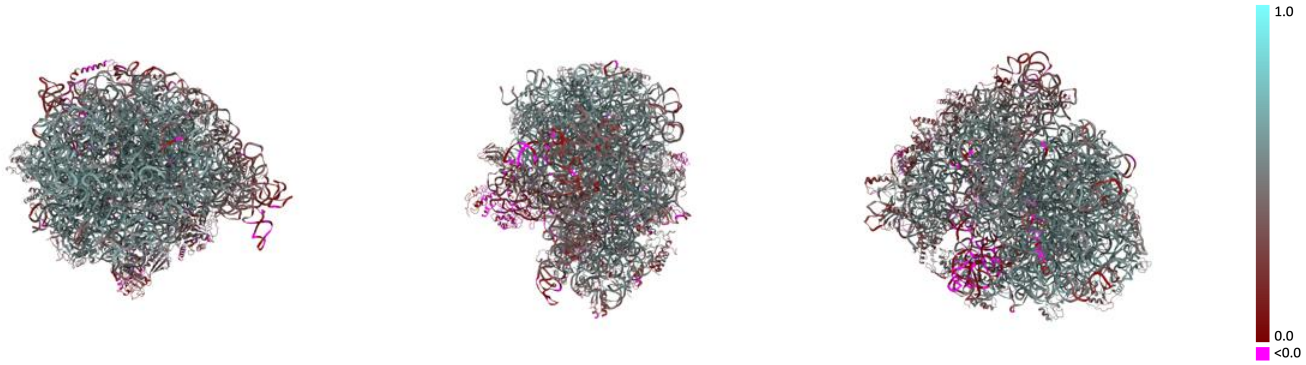
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00532 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.

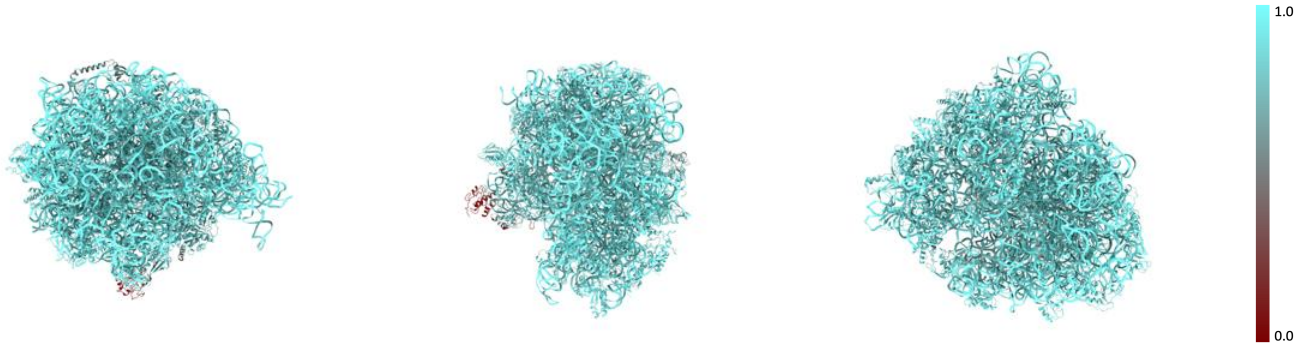
9.2 Q-score mapped to coordinate model



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.

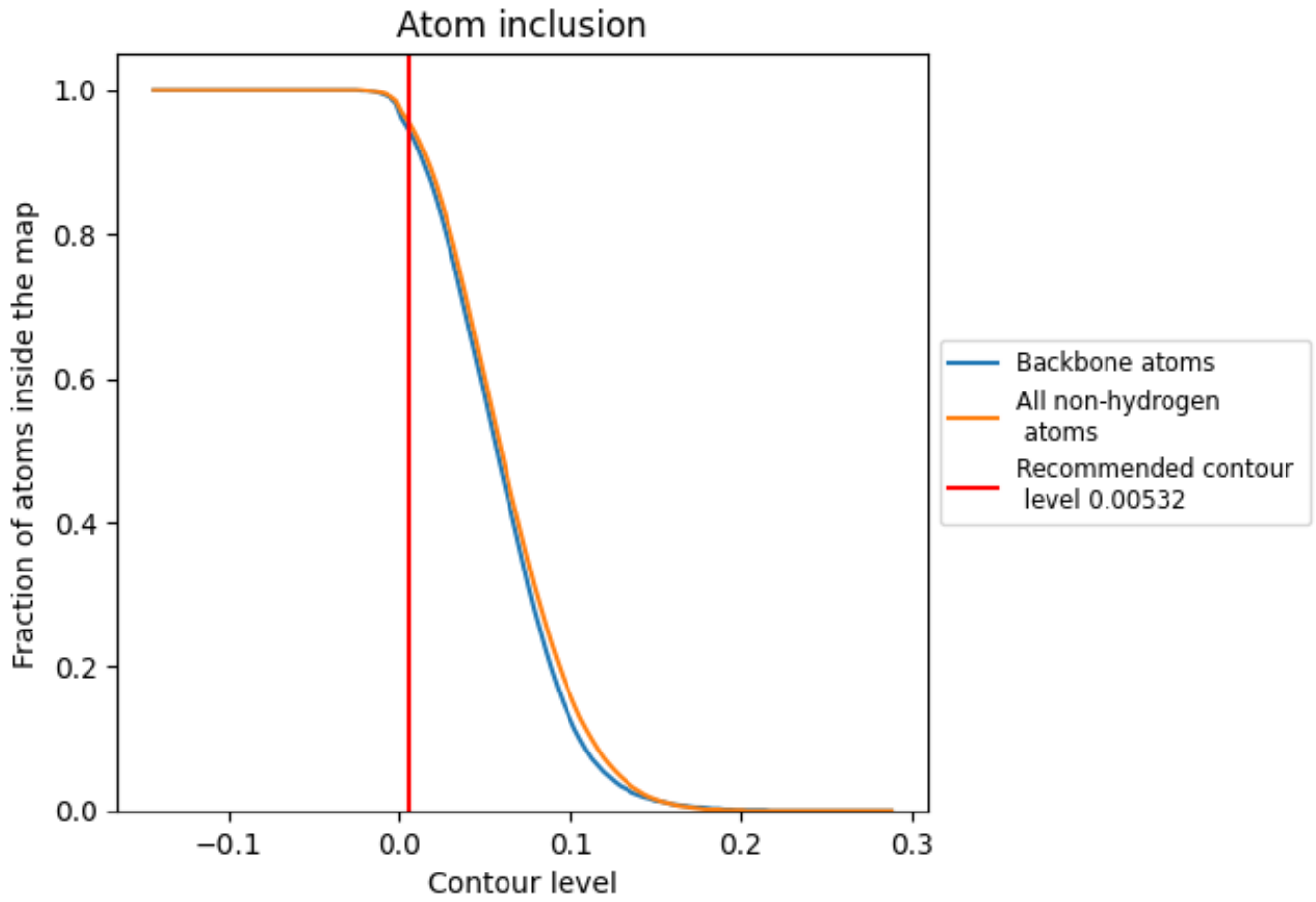
9.3 Atom inclusion mapped to coordinate model



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 (0.00532).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.00532) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9570	0.4750
0	0.9620	0.5080
1	0.9240	0.4640
2	0.9880	0.5860
3	0.9840	0.5760
4	0.9520	0.4940
5	0.1120	-0.0200
6	0.8880	0.3120
A	0.9870	0.5350
B	0.9940	0.5140
C	0.9740	0.5550
D	0.9660	0.5260
E	0.9690	0.5080
F	0.9360	0.4310
G	0.9370	0.3790
H	0.7350	0.2180
I	0.6190	0.0210
J	0.9650	0.5270
K	0.9520	0.5180
L	0.9650	0.5170
M	0.9690	0.5180
N	0.9860	0.5530
O	0.9680	0.4480
P	0.9570	0.5080
Q	0.9560	0.5500
R	0.9390	0.4830
S	0.9520	0.5230
T	0.9340	0.4560
U	0.9450	0.4450
V	0.9490	0.4600
W	0.9640	0.5480
X	0.9550	0.5170
Y	0.9380	0.4430
Z	0.9650	0.5020
a	0.9870	0.4800



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	0.8950	0.3360
c	0.9420	0.4360
d	0.8990	0.2860
e	0.9530	0.4820
f	0.9230	0.4070
g	0.9160	0.3700
h	0.9490	0.4840
i	0.9220	0.3850
j	0.8960	0.3370
k	0.9460	0.4300
l	0.9080	0.4010
m	0.9440	0.4280
n	0.9500	0.4390
o	0.9410	0.4440
p	0.8930	0.2610
q	0.9150	0.3710
r	0.8970	0.4030
s	0.9520	0.4260
t	0.9200	0.3290
u	0.8210	0.2580
v	0.9720	0.4880
w	0.7450	0.0740
x	0.9840	0.4960
y	0.9160	0.2870
z	0.8290	0.2520