



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 08:57 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:

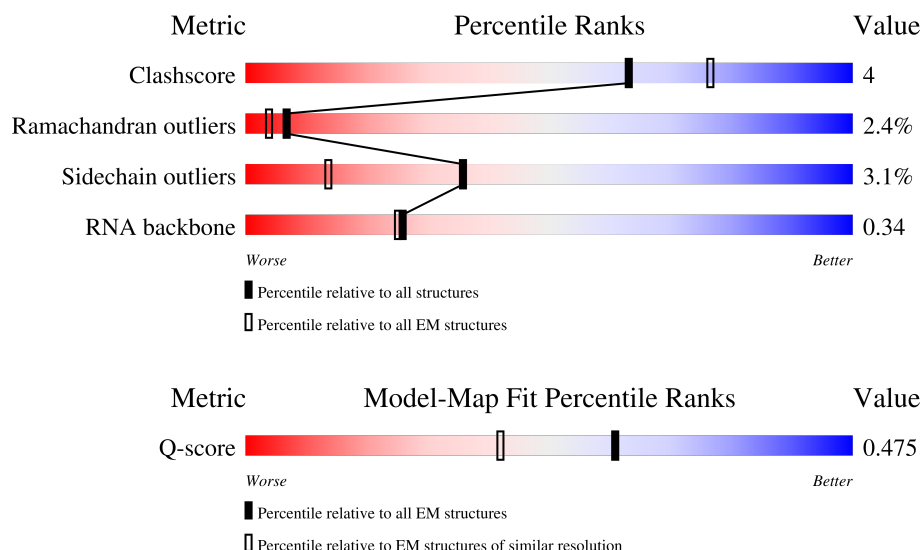
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 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.



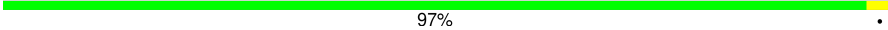
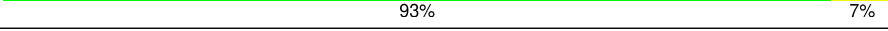
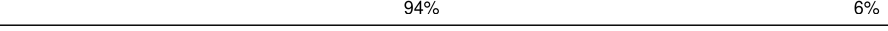
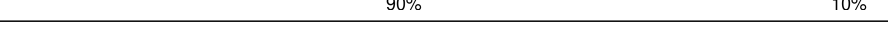
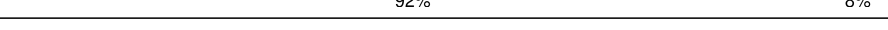
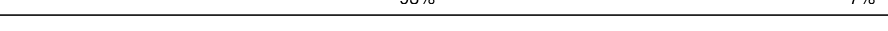
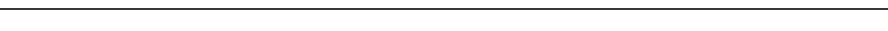
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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 $\leq 5\%$. 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	
2	B	120	
3	C	271	

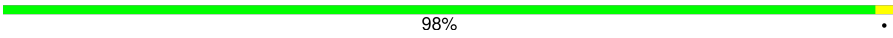
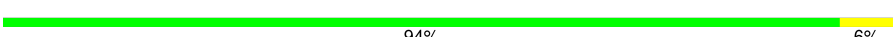
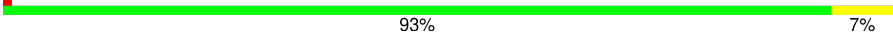
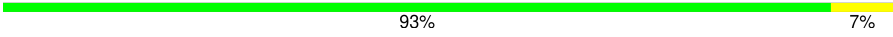
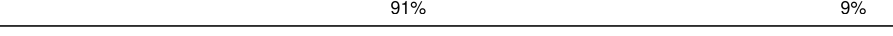
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Mol	Chain	Length	Quality of chain
4	D	208	 91% 8%
5	E	200	 90% 9%
6	F	177	 90% 8% .
7	G	174	 97% . .
8	H	149	 10% 91% 8% .
9	I	141	 24% 84% 15% .
10	J	141	 91% 8% .
11	K	122	 89% 11%
12	L	143	 87% 10% .
13	M	136	 93% 7%
14	N	119	 88% 12%
15	O	116	 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%

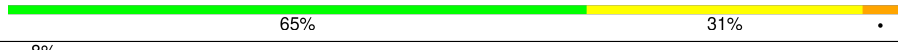
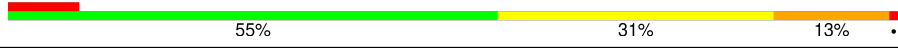
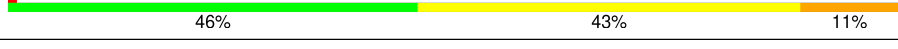
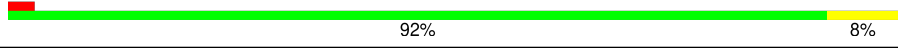
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Mol	Chain	Length	Quality of chain
29	2	45	 84% 16%
30	3	64	 98% .
31	4	38	 89% 11%
32	5	131	 89% 9% .
33	6	66	 92% 8%
34	a	1540	 55% 35% 9% .
35	b	218	 94% 6%
36	c	206	 92% 6% .
37	d	205	 93% 7%
38	e	157	 83% 16% .
39	f	100	 87% 9% .
40	g	151	 89% 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%

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Mol	Chain	Length	Quality of chain
54	u	65	
55	v	77	
55	w	77	
56	x	12	
57	y	76	
58	z	393	

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

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
1	A	2900	Total	C	N	O	P	0	0
			62277	27788	11459	20130	2900		

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
2	B	120	Total	C	N	O	P	0	0
			2572	1145	471	836	120		

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
3	C	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

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

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

- 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	C	N	O	S	0	0
			845	526	162	154	3		

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

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

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

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

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

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

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

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

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

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

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

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

- 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	S	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 1644	C 733	N 297	O 536	P 77	S 1	0	0
55	w	77	Total 1644	C 733	N 297	O 536	P 77	S 1	0	0

- 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		

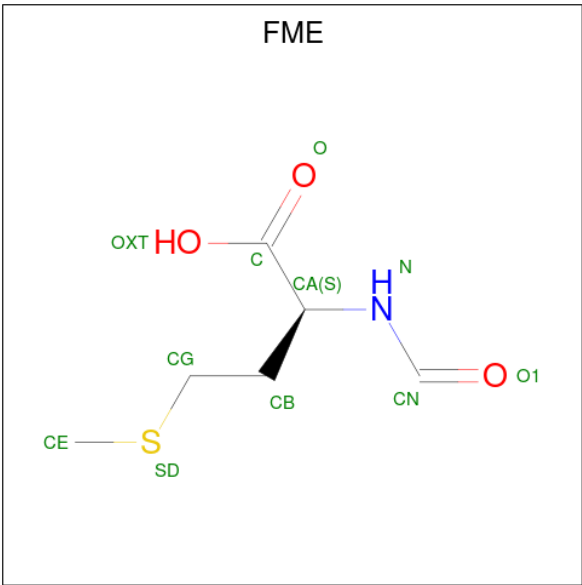
- Molecule 58 is a protein called Elongation factor Tu 2.

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: C₆H₁₁NO₃S).



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	

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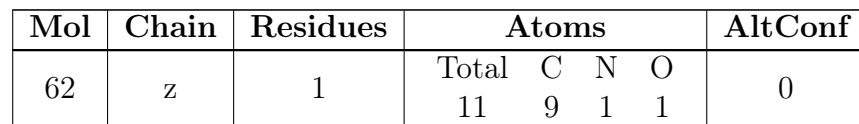
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Mol	Chain	Residues	Atoms		AltConf
60	2	1	Total 1	Mg 1	0
60	a	392	Total 392	Mg 392	0
60	d	1	Total 1	Mg 1	0
60	e	1	Total 1	Mg 1	0
60	i	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	6	Total 6	Mg 6	0
60	w	2	Total 2	Mg 2	0
60	x	1	Total 1	Mg 1	0
60	y	2	Total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

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

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

- Molecule 62 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



-
- The image displays the chemical structure of Guanosine Triphosphate (GTP). It consists of a guanine base (a purine ring system with an amino group at C6) linked to a ribose sugar, which is in turn linked to a chain of three phosphate groups. The structure is labeled with atom names and numbers, and the phosphate groups are color-coded: the gamma phosphate is red, the beta phosphate is orange, and the alpha phosphate is purple. The ribose sugar is shown in a chair conformation with hydroxyl groups at the 2' and 3' positions.

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

- 

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

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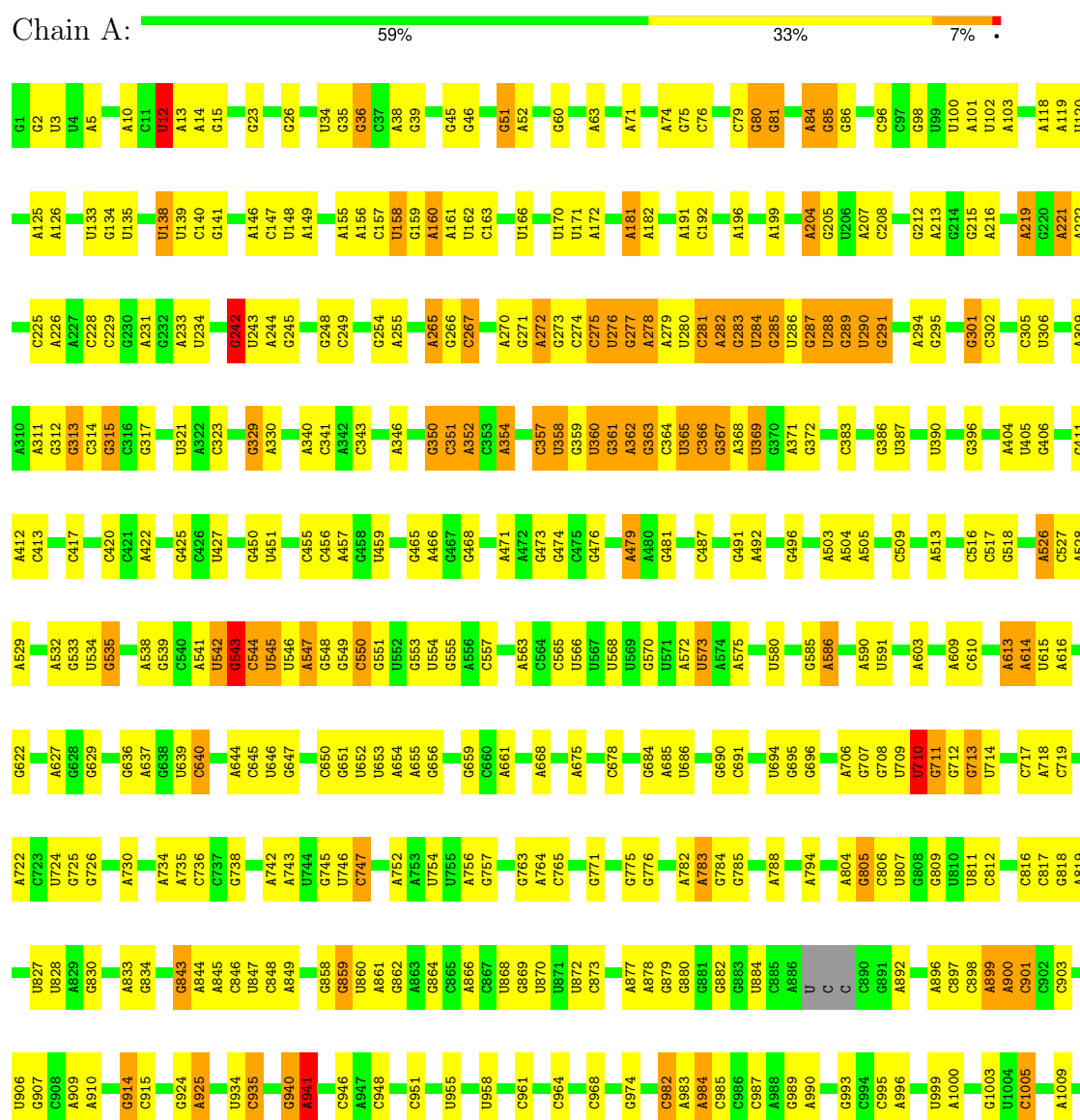
Continued from previous page...

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

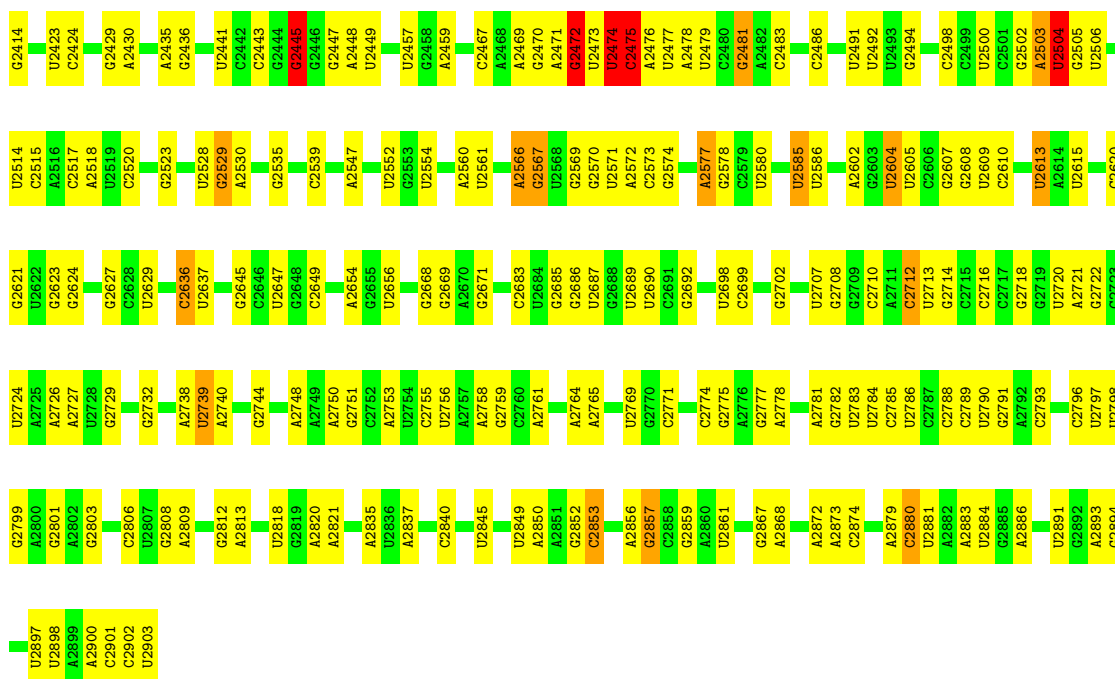
3 Residue-property plots

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

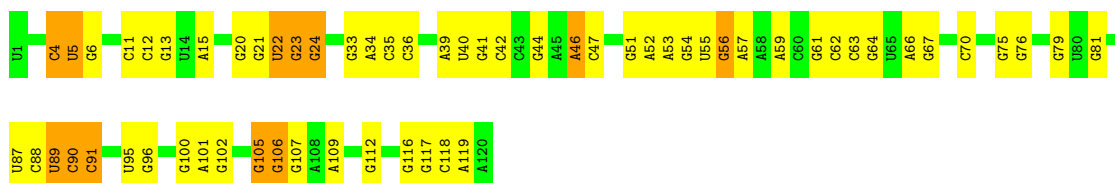


G2315	U2202	A2094	G2004	G1907	A1808	U1693	A1571	A1490	G1288	G1154	A1077	U1012
G2319	U2203	A2095	A2013	U1911	A1809	U1694	A1572	G1491	C1289	A1165	U1078	C1013
U2320	G2204	A2097	A2096	U1912	G1810	G1695	U1578	G1492	C1297	A1084	C1079	U1015
U2321	U2098	A1913	U2016	A1913	U1812	U1579	A1579	A1494	G1300	G1168	A1085	U1019
A2322	C2208	U2099	U2016	C1914	G1816	G1703	A1580	A1495	A1301	A1169	A1086	A1020
G2323	A2211	G2100	A2020	A1916	G1817	G1715	G1581	C1498	C1306	C1170	A1087	A1021
U2324	G2102	U1917	C2021	U1917	U1818	U1716	A1583	C1582	C1072	G1171	A1088	G1022
G2325	C2214	A1819	C2023	A1819	A1819	A1717	U1584	G1418	A1321	U1173	A1089	U1023
A2327	U2106	U1923	G2024	U1923	C1830	G1721	C1585	A1502	U1318	U1174	G1024	G1024
U2328	G2107	C1924	C2025	C1924	A1503	A1722	U1589	A1504	U1319	A1175	G1025	G1025
U2329	A2108	G1831	U2026	C1925	C1832	G1723	U1590	A1505	G1320	U1176	A1095	G1026
G2330	U2109	U1926	G2027	U1926	C1833	G1724	A1591	C1507	A1321	G1178	A1096	A1027
G2331	G2223	A1927	U2028	A1927	U1834	G1725	C1592	A1508	A1327	U1179	U1097	U1028
A2332	U2110	A1928	G2029	A1928	G1835	G1726	U1599	A1509	A1328	U1180	U1101	A1032
C2333	G2225	U1835	A2030	G1929	U1835	G1727	C1600	G1510	U1329	U1181	C1102	U1033
A2333	G2226	G1835	A2031	G1930	G1839	A1727	U1599	G1510	C1330	G1182	A1103	G1034
G2336	G2238	U2113	G2032	U1931	G1842	U1728	C1600	G1514	G1343	U1184	C1104	U1035
G2337	G2239	A2119	A2033	A1932	G1847	U1729	A1603	A1515	C1345	G1190	G1106	U1036
G2345	G2246	G2120	C2036	A1936	G1847	G1732	C1607	G1519	G1346	U1195	U1108	A1040
A2346	A2247	G2121	G2038	A1937	U1851	G1733	A1608	A1522	C1350	G1195	C1109	G1041
C2347	G2251	G2127	U2039	U1938	U1852	G1735	A1609	U1523	C1351	G1110	G1042	G1042
G2350	C2263	U2131	A2042	U1940	A1853	G1738	A1610	G1524	U1203	A1111	C1043	C1043
G2351	G2263	U2132	C2043	C1941	G1857	G1739	C1612	A1528	C1352	U1204	G1112	C1044
A2352	A2267	G2133	G2043	C1942	A1858	U1943	G1613	G1529	A1353	U1113	C1045	C1045
U2356	A2268	A2134	G2049	U1943	A1858	G1740	G1613	G1529	A1353	A1205	U1113	C1045
G2357	C2050	U1944	C2050	U1944	G1860	U1944	A1614	C1533	G1360	C1114	C1114	A1046
G2361	A2273	G2141	A2051	G1945	G1863	G1750	G1615	C1533	G1361	U1211	G1115	G1047
G2362	A2274	C2145	C2055	U1955	A1866	A1754	A1616	U1534	C1362	G1218	G1116	A1048
G2373	A2278	C2146	G2056	U1955	G1867	A1754	C1617	U1534	G1363	G1218	C1117	C1049
C2374	C2283	A2147	C2056	C1962	C1870	G1764	G1619	C1535	A1365	A1230	C1118	A1050
A2377	G2286	G2157	A2059	U1963	A1871	A1773	G1622	C1536	G1368	U1231	U1119	G1051
A2378	G2286	G2157	G2060	G1964	A1872	G1776	G1642	C1537	U1369	G1236	G1120	C1052
G2383	A2287	A2163	A2062	A1966	G1873	U1776	G1643	G1538	C1370	G1124	G1055	A1054
U2384	C2163	C2063	C2063	C1967	G1874	G1776	G1643	U1541	G1371	U1240	G1056	G1056
C2385	C2164	C2164	C2064	G1968	C1875	U1779	C1644	U1542	A1469	A1246	A1129	U1058
G2391	A2170	A1969	G2067	A1970	A1876	U1780	C1644	G1543	A1378	A1247	U1130	G1059
A2392	A2171	U1971	U2068	G1970	G1877	U1781	U1647	A1545	U1379	G1247	G1131	U1060
G2392	U2172	G1878	G2069	G1971	C1879	U1782	U1648	U1545	C1386	G1248	U1132	U1061
U2396	A2173	U1880	A2070	G1972	U1880	A1783	G1649	G1546	A1387	U1249	U1132	G1062
G2396	A2173	C1881	A2071	U1976	C1881	A1784	A1650	G1555	G1475	G1250	G1135	G1063
U2401	G2186	U1976	C2071	U1976	G1651	G1791	G1651	C1556	A1476	A1253	G1136	C1064
U2402	U2187	U1982	C2072	U1982	A1791	G1792	A1654	C1557	A1477	A1254	U1065	U1065
C2403	U2188	G1792	U2074	C1793	A1884	C1793	A1654	U1558	G1479	U1255	G1139	U1066
U2404	U2189	U1991	U2075	U1991	A1885	U1794	A1668	C1559	C1472	G1256	C1139	A1067
A2404	G2190	A1890	G1992	C1795	A1890	C1795	A1668	G1560	U1481	U1396	U1141	U1068
G2405	A2191	U1993	U2076	U1993	A1890	U1796	A1672	U1563	G1476	A1268	A1142	A1069
A2406	G2306	G1982	A2077	U1993	G1896	U1796	G1673	C1564	U1482	A1269	A1143	A1070
G2407	G2307	G1992	C2078	C1997	G1896	G1799	G1674	C1565	U1483	C1270	A1144	G1071
U2408	G2308	C1997	U2079	C1997	C1902	U1799	G1675	A1566	U1484	G1271	C1072	C1072
G2409	A2309	A1998	A2080	A1998	C1902	A1801	C1675	U1566	U1485	U1272	G1149	A1073
G2410	A2311	U1801	U2092	C2000	C1905	A1802	A1678	A1569	A1403	U1273	G1150	G1074
			U2092		C1905	A1802	A1678	A1569	G1407	A1151	C1151	C1075



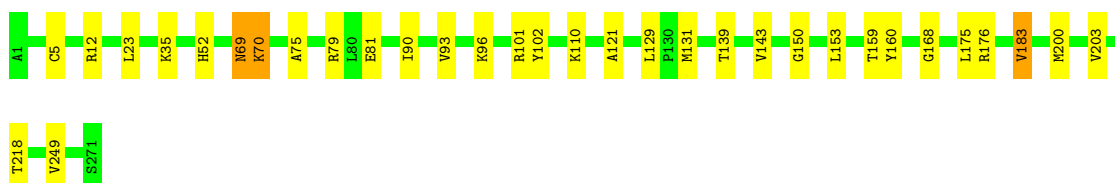
• Molecule 2: 5S rRNA

Chain B: 49% 41% 10%



• Molecule 3: 50S ribosomal protein L2

Chain C: 88% 11%



• Molecule 4: 50S ribosomal protein L3

Chain D: 91% 8%



• Molecule 5: 50S ribosomal protein L4

Chain E:  90% 9%

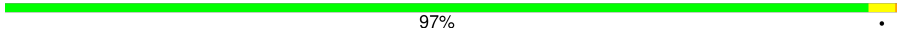


- Molecule 6: 50S ribosomal protein L5

Chain F:  90% 8%

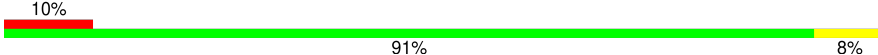


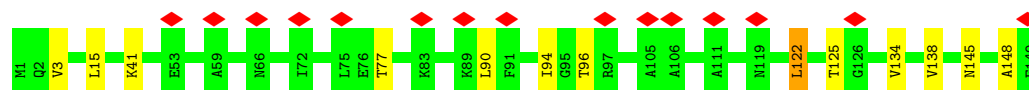
- Molecule 7: 50S ribosomal protein L6

Chain G:  97%



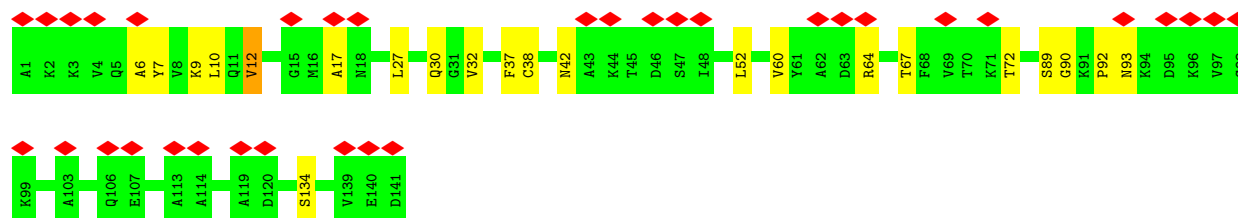
- Molecule 8: 50S ribosomal protein L9

Chain H:  10% 91% 8%



- Molecule 9: 50S ribosomal protein L11

Chain I:  24% 84% 15%



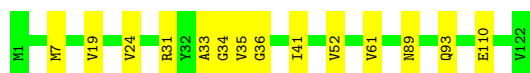
- Molecule 10: 50S ribosomal protein L13

Chain J:  91% 8%

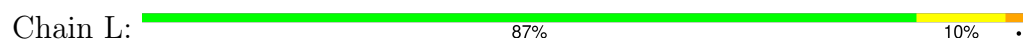


- Molecule 11: 50S ribosomal protein L14

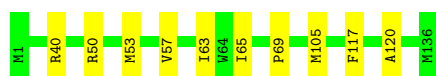
Chain K:  89% 11%



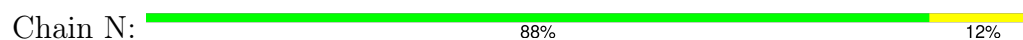
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



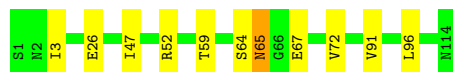
- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18



- Molecule 16: 50S ribosomal protein L19



- Molecule 17: 50S ribosomal protein L20

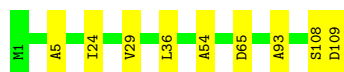


- Molecule 18: 50S ribosomal protein L21





- Molecule 19: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24



- Molecule 22: 50S ribosomal protein L25



- Molecule 23: 50S ribosomal protein L27



- Molecule 24: 50S ribosomal protein L28



- Molecule 25: 50S ribosomal protein L29





- Molecule 26: 50S ribosomal protein L30

Chain Z: 96% .



- Molecule 27: 50S ribosomal protein L32

Chain 0: 91% 7% .



- Molecule 28: 50S ribosomal protein L33

Chain 1: 100%

There are no outlier residues recorded for this chain.

- Molecule 29: 50S ribosomal protein L34

Chain 2: 84% 16%



- Molecule 30: 50S ribosomal protein L35

Chain 3: 98% .



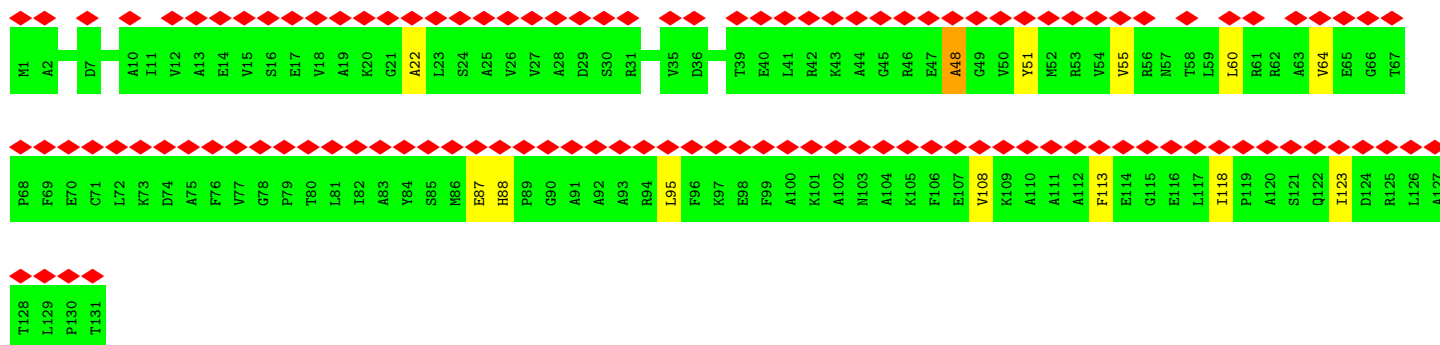
- Molecule 31: 50S ribosomal protein L36 1

Chain 4: 89% 11%



- Molecule 32: 50S ribosomal protein L10

Chain 5: 89% 90% 9% .



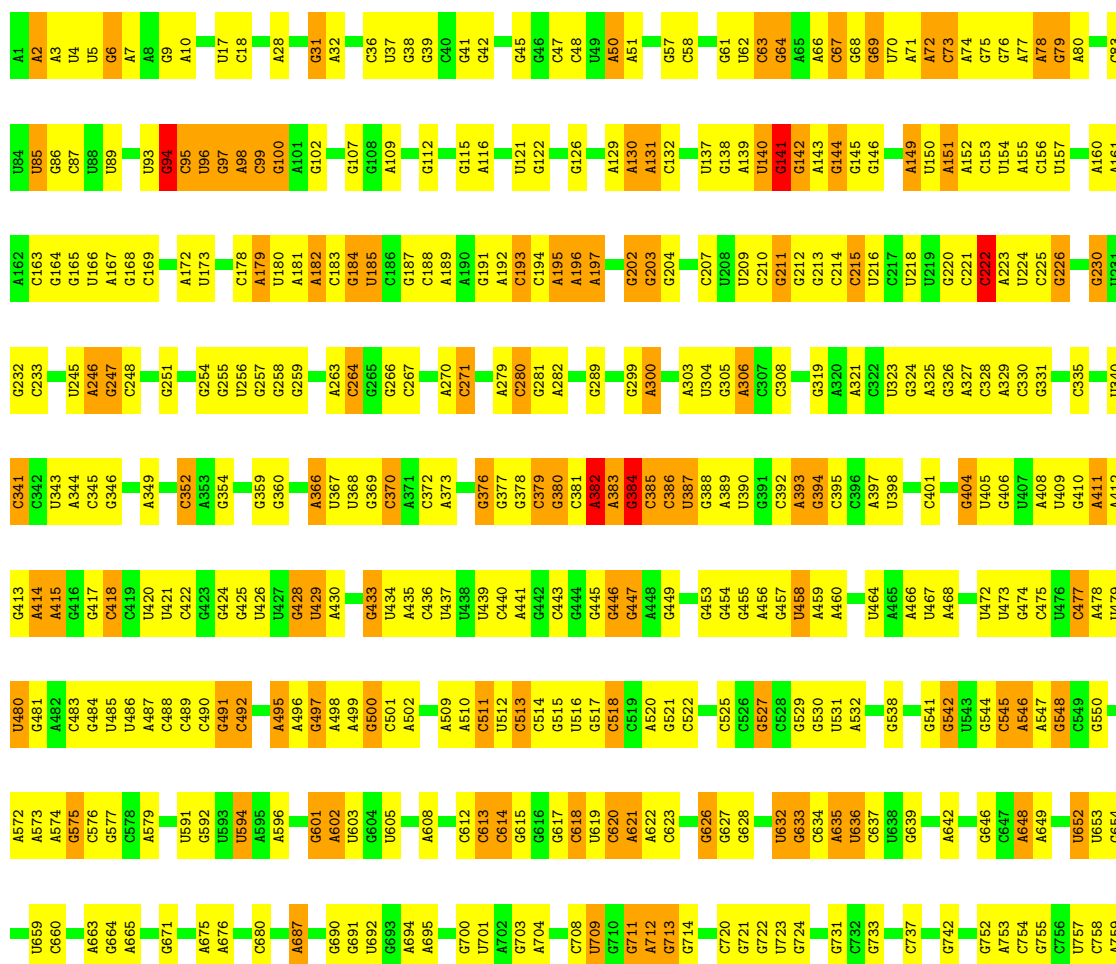
- Molecule 33: 50S ribosomal protein L31

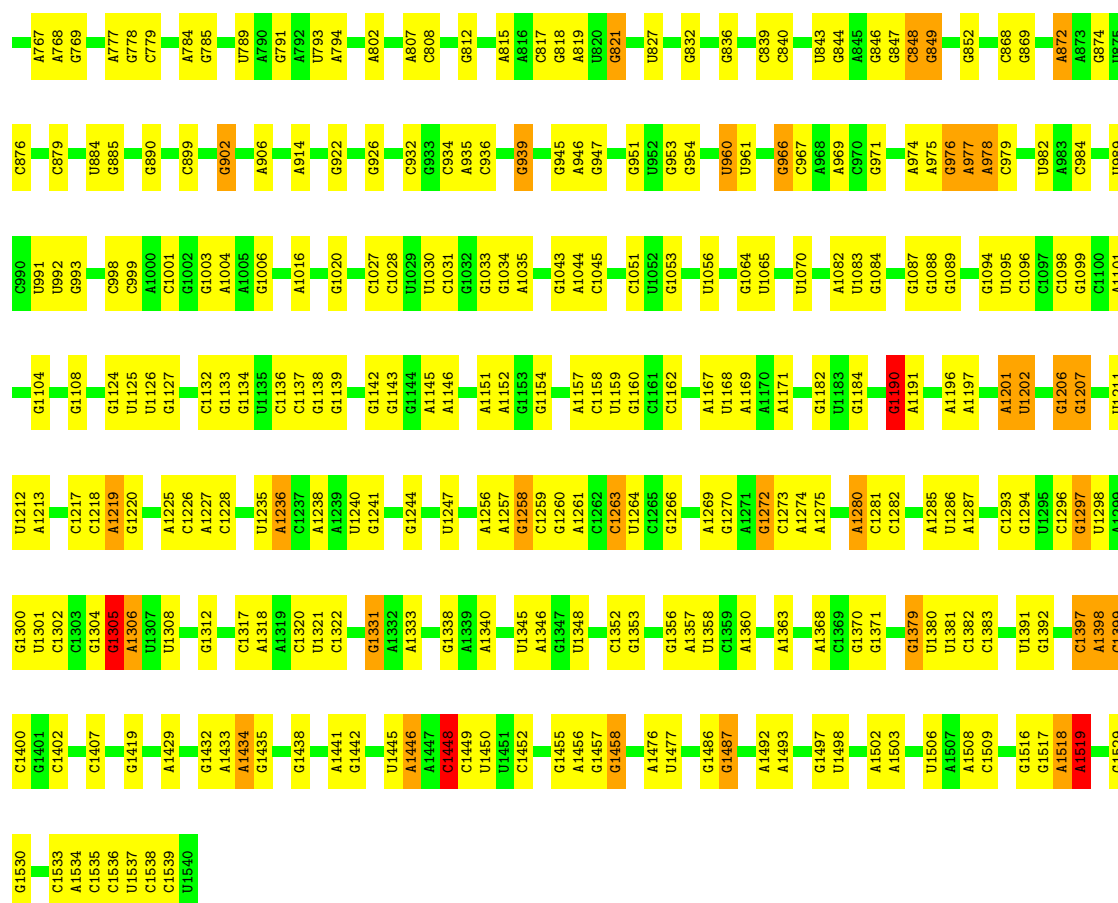
Chain 6:



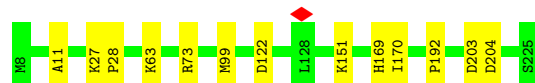
- Molecule 34: 16S rRNA

Chain a:





• Molecule 35: 30S ribosomal protein S2



• Molecule 36: 30S ribosomal protein S3



• Molecule 37: 30S ribosomal protein S4



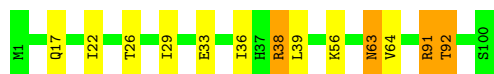
• Molecule 38: 30S ribosomal protein S5

Chain e:  83% 16%



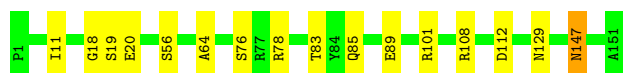
- Molecule 39: 30S ribosomal protein S6

Chain f:  87% 9%



- Molecule 40: 30S ribosomal protein S7

Chain g:  89% 10%



- Molecule 41: 30S ribosomal protein S8

Chain h:  88% 12%



- Molecule 42: 30S ribosomal protein S9

Chain i:  93% 7%

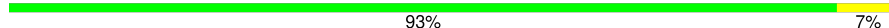


- Molecule 43: 30S ribosomal protein S10

Chain j:  91% 8%

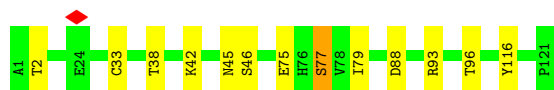
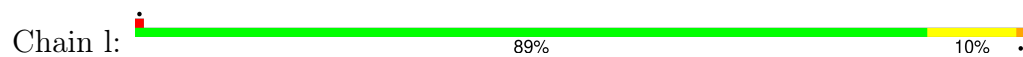


- Molecule 44: 30S ribosomal protein S11

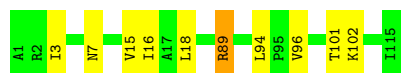
Chain k:  93% 7%



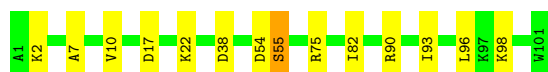
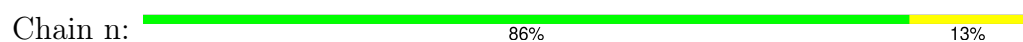
- Molecule 45: 30S ribosomal protein S12



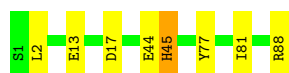
- Molecule 46: 30S ribosomal protein S13



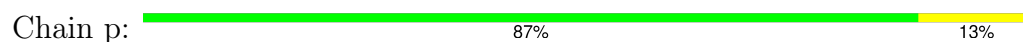
- Molecule 47: 30S ribosomal protein S14



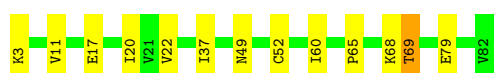
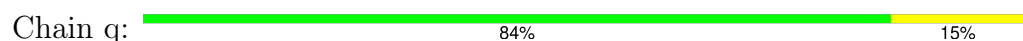
- Molecule 48: 30S ribosomal protein S15



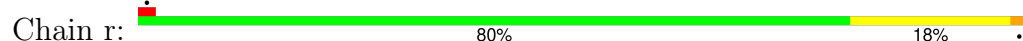
- Molecule 49: 30S ribosomal protein S16



- Molecule 50: 30S ribosomal protein S17



- Molecule 51: 30S ribosomal protein S18



- Molecule 52: 30S ribosomal protein S19

Chain s:  91% 9%



- Molecule 53: 30S ribosomal protein S20

Chain t:  91% 9%



- Molecule 54: 30S ribosomal protein S21

Chain u:  77% 18% 5%



- Molecule 55: tRNA-fMet

Chain v:  65% 31% .



- Molecule 55: tRNA-fMet

Chain w:  8% 55% 31% 13% .



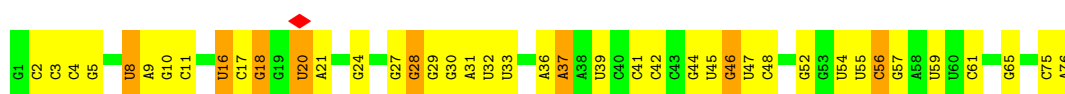
- Molecule 56: mRNA

Chain x:  67% 25% 8%



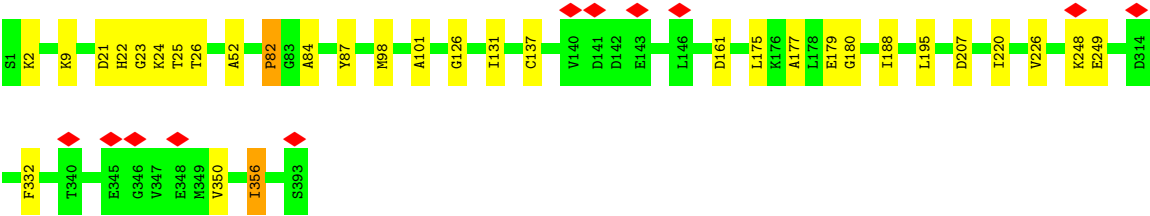
- Molecule 57: Phe-tRNA-Phe

Chain y:  46% 43% 11%



- Molecule 58: Elongation factor Tu 2

Chain z:  92% 8%



4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

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

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(°)	Ideal(°)
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

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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

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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

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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 ⓘ

5.3.1 Protein backbone ⓘ

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

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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

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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 ⓘ

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

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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

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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 ⓘ

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

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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 ⓘ

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	$\# Z > 2$
57	7MG	y	46	57	23,26,27	1.43	4 (17%)	27,39,42	2.47	7 (25%)
1	2MG	A	1835	1	23,26,27	1.28	3 (13%)	33,38,41	2.18	7 (21%)
1	PSU	A	1917	1	18,21,22	1.41	2 (11%)	21,30,33	2.09	4 (19%)
1	PSU	A	2605	60,1	18,21,22	1.42	2 (11%)	21,30,33	2.21	4 (19%)
1	5MC	A	1962	1	19,22,23	1.49	2 (10%)	26,32,35	1.24	3 (11%)
1	PSU	A	2457	1	18,21,22	1.55	3 (16%)	21,30,33	2.00	5 (23%)
57	PSU	y	55	57	18,21,22	1.40	2 (11%)	21,30,33	2.05	5 (23%)
34	2MG	a	1516	34	23,26,27	1.27	5 (21%)	33,38,41	2.42	12 (36%)
34	4OC	a	1402	60,34	20,23,24	0.81	0	25,32,35	1.34	5 (20%)
1	PSU	A	955	1	18,21,22	1.41	3 (16%)	21,30,33	2.10	4 (19%)
1	2MG	A	2445	1	23,26,27	1.32	5 (21%)	33,38,41	2.29	8 (24%)
34	5MC	a	1407	34	19,22,23	1.68	2 (10%)	26,32,35	1.31	4 (15%)
57	PSU	y	39	57	18,21,22	1.45	2 (11%)	21,30,33	2.01	4 (19%)
34	7MG	a	527	34	23,26,27	1.45	4 (17%)	27,39,42	2.48	7 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
55	PSU	w	55	55	18,21,22	1.34	2 (11%)	21,30,33	2.06	5 (23%)
1	2MA	A	2503	60,1	22,25,26	1.51	5 (22%)	32,37,40	2.25	9 (28%)
57	PSU	y	32	57	18,21,22	1.36	2 (11%)	21,30,33	2.05	5 (23%)
34	2MG	a	1207	60,34	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%)
57	4SU	y	8	57	18,21,22	1.81	5 (27%)	25,30,33	2.37	7 (28%)
1	OMG	A	2251	60,1,55	23,26,27	1.27	3 (13%)	32,38,41	1.94	7 (21%)
34	PSU	a	516	34	18,21,22	1.44	2 (11%)	21,30,33	2.08	5 (23%)
57	5MU	y	54	57	19,22,23	1.41	4 (21%)	27,32,35	2.12	8 (29%)
34	5MC	a	967	34	19,22,23	1.84	2 (10%)	26,32,35	1.26	3 (11%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.39	4 (21%)
1	5MC	A	747	1	19,22,23	1.84	3 (15%)	26,32,35	1.66	6 (23%)
1	OMU	A	2552	60,1	19,22,23	1.39	2 (10%)	25,31,34	2.25	8 (32%)
1	3TD	A	1915	60,1	19,22,23	7.04	13 (68%)	23,32,35	2.05	4 (17%)
55	4SU	v	7	55	18,21,22	1.75	4 (22%)	25,30,33	2.42	5 (20%)
1	6MZ	A	1618	1	22,25,26	1.54	4 (18%)	29,36,39	2.29	10 (34%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.08	11 (40%)
1	5MU	A	1939	1	19,22,23	1.38	5 (26%)	27,32,35	2.04	8 (29%)
34	UR3	a	1498	34	19,22,23	1.09	2 (10%)	26,32,35	1.99	5 (19%)
1	PSU	A	1911	1	18,21,22	1.39	2 (11%)	21,30,33	2.08	4 (19%)
34	MA6	a	1519	34	23,26,27	1.70	6 (26%)	33,38,41	2.34	12 (36%)
1	PSU	A	746	60,1	18,21,22	1.41	3 (16%)	21,30,33	2.06	4 (19%)
1	6MZ	A	2030	1	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	21,30,33	1.94	4 (19%)
1	PSU	A	2604	1	18,21,22	1.42	3 (16%)	21,30,33	1.99	4 (19%)
1	OMC	A	2498	60,1	19,22,23	0.88	1 (5%)	25,31,34	1.23	2 (8%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.48	4 (21%)
55	H2U	w	20	55	18,21,22	0.82	1 (5%)	19,30,33	1.58	2 (10%)
55	4SU	w	8	55	18,21,22	1.81	5 (27%)	25,30,33	2.22	5 (20%)
55	H2U	v	20	55	18,21,22	0.91	1 (5%)	19,30,33	1.63	4 (21%)
57	MIA	y	37	57	28,31,32	2.44	7 (25%)	38,44,47	2.92	15 (39%)
55	PSU	v	55	60,55	18,21,22	1.38	3 (16%)	21,30,33	1.98	5 (23%)
1	1MG	A	745	1	23,26,27	1.29	3 (13%)	33,39,42	1.97	7 (21%)
1	H2U	A	2449	1	18,21,22	1.03	2 (11%)	19,30,33	1.49	3 (15%)
55	5MU	v	54	55	19,22,23	1.49	5 (26%)	27,32,35	1.91	8 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	7MG	A	2069	60,1	23,26,27	1.49	4 (17%)	27,39,42	2.54	10 (37%)
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%)

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
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2605	60,1	-	0/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	1/7/25/26	0/2/2/2
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
34	4OC	a	1402	60,34	-	2/9/29/30	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
57	PSU	y	39	57	-	2/7/25/26	0/2/2/2
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	2MA	A	2503	60,1	-	0/7/25/26	0/3/3/3
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
34	2MG	a	1207	60,34	-	0/9/27/28	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	OMG	A	2251	60,1,55	-	0/9/27/28	0/3/3/3
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	60,1	-	2/9/27/28	0/2/2/2
1	3TD	A	1915	60,1	-	3/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	A	1618	1	-	3/9/27/28	0/3/3/3
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	1/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
1	PSU	A	1911	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	746	60,1	-	4/7/25/26	0/2/2/2
1	6MZ	A	2030	1	-	3/9/27/28	0/3/3/3
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	2/7/25/26	0/2/2/2
1	OMC	A	2498	60,1	-	0/9/27/28	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
55	H2U	v	20	55	-	5/7/38/39	0/2/2/2
57	MIA	y	37	57	-	5/15/33/34	0/3/3/3
55	PSU	v	55	60,55	-	2/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	7MG	A	2069	60,1	-	2/7/37/38	0/3/3/3
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

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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
1	A	2445	2MG	1	0
34	a	1207	2MG	1	0
1	A	1915	3TD	2	0
1	A	1618	6MZ	1	0
1	A	1939	5MU	1	0
34	a	1519	MA6	1	0
1	A	2030	6MZ	10	0
1	A	2504	PSU	1	0
1	A	2604	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	$\# Z > 2$
63	GTP	z	402	60	33,34,34	1.17	3 (9%)	50,54,54	1.74	7 (14%)
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

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
63	GTP	z	402	60	-	7/22/38/38	0/3/3/3
59	FME	A	3001	-	-	0/7/9/11	-
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1

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(°)	Ideal(°)
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

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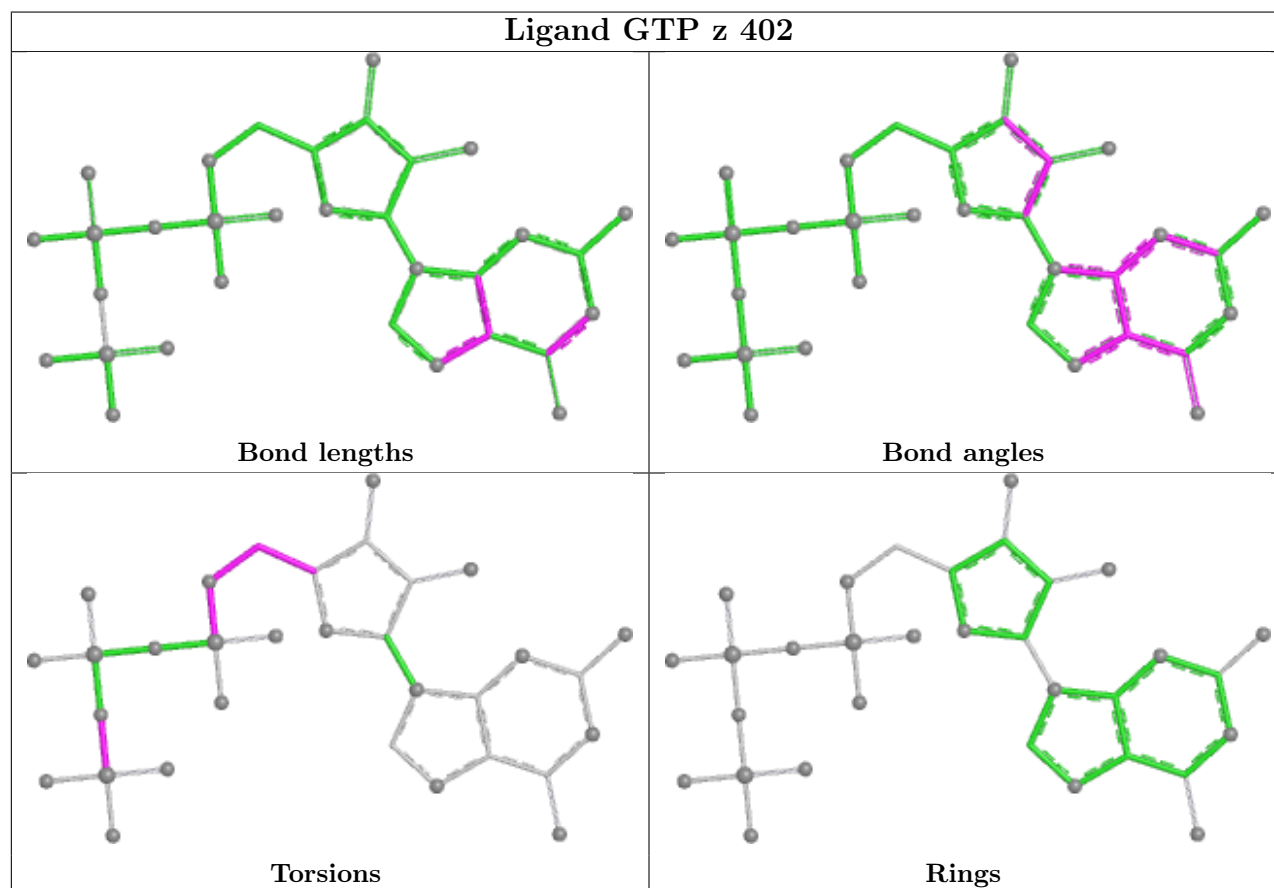
Mol	Chain	Res	Type	Atoms
63	z	402	GTP	C3'-C4'-C5'-O5'

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 than 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.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

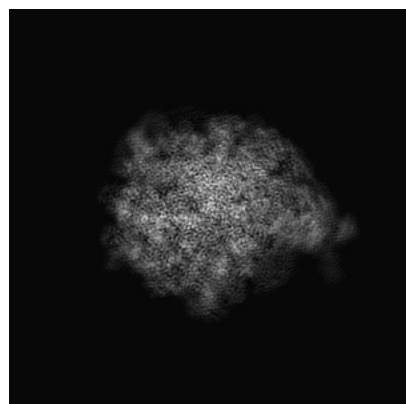
6 Map visualisation [i](#)

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

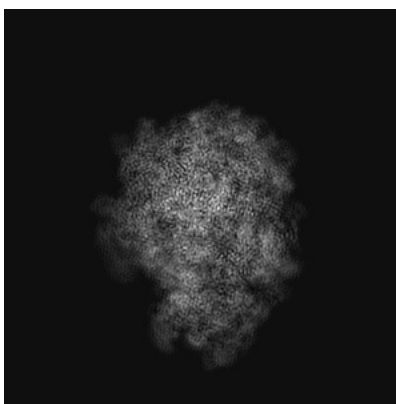
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

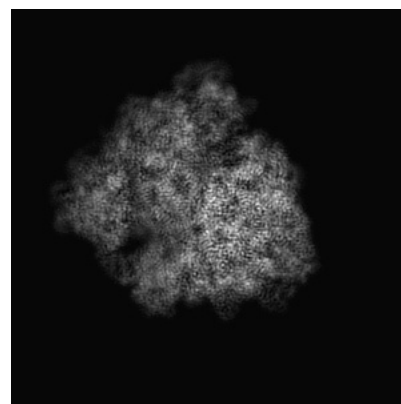
6.1.1 Primary map



X

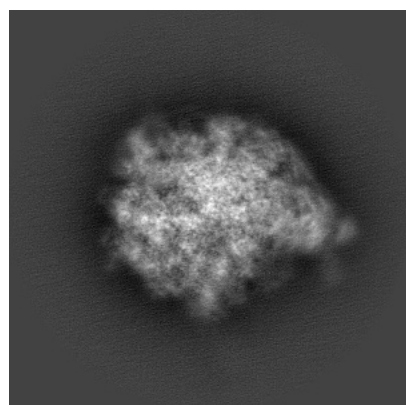


Y

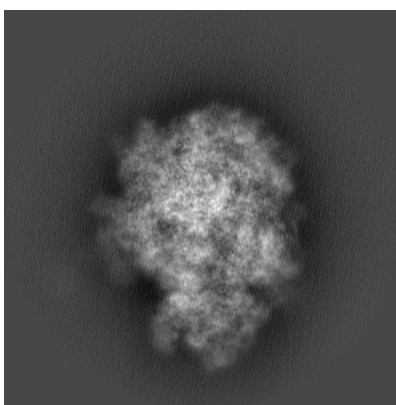


Z

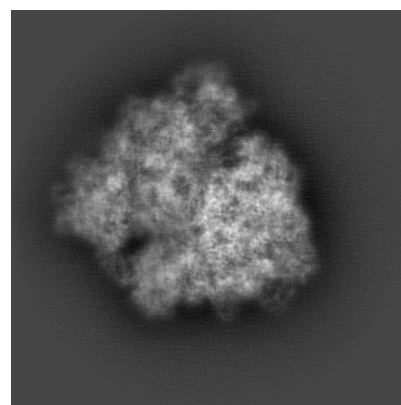
6.1.2 Raw map



X



Y

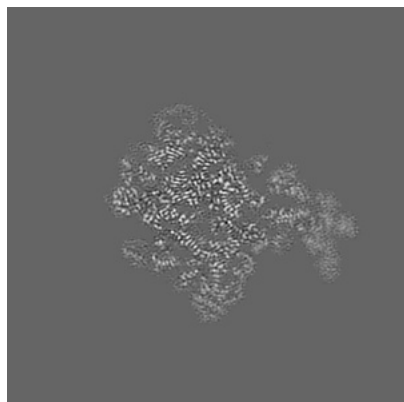


Z

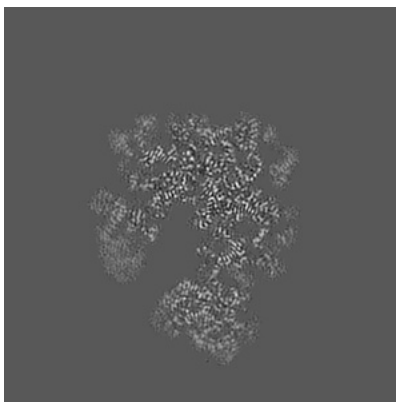
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

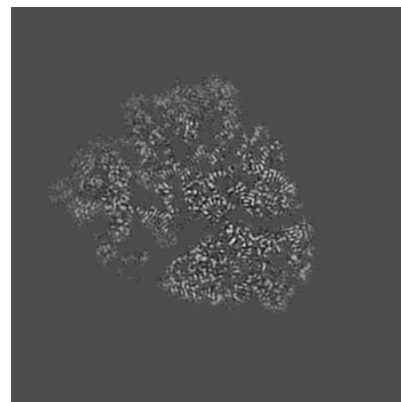
6.2.1 Primary map



X Index: 199

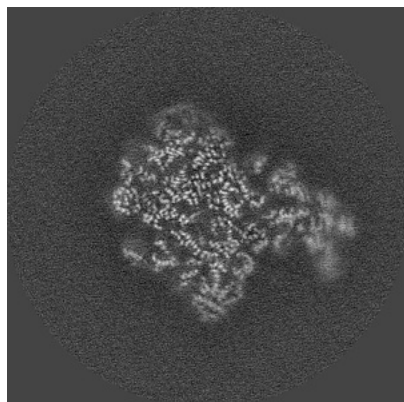


Y Index: 199

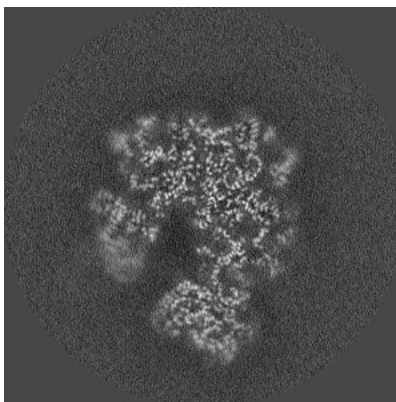


Z Index: 199

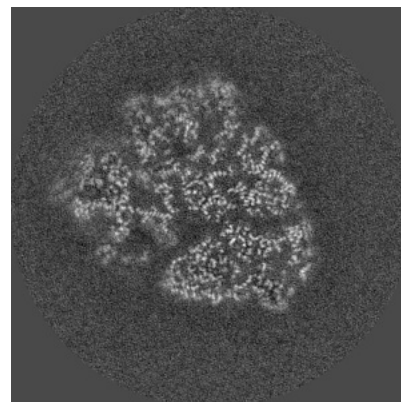
6.2.2 Raw map



X Index: 199



Y Index: 199

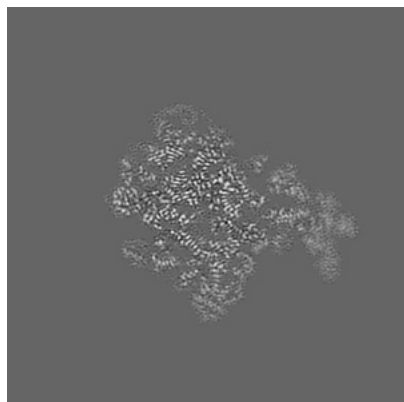


Z Index: 199

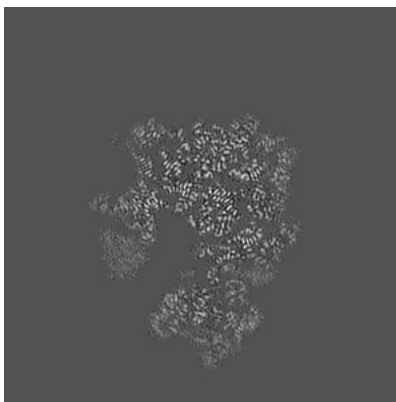
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

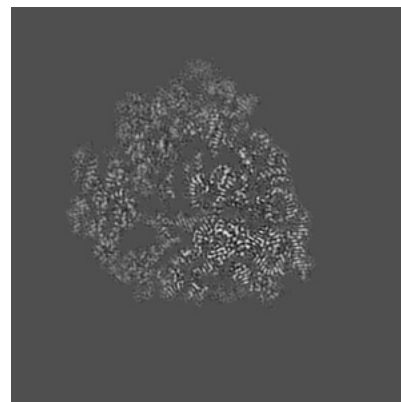
6.3.1 Primary map



X Index: 199

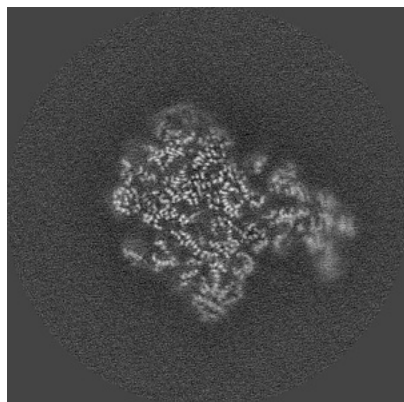


Y Index: 207

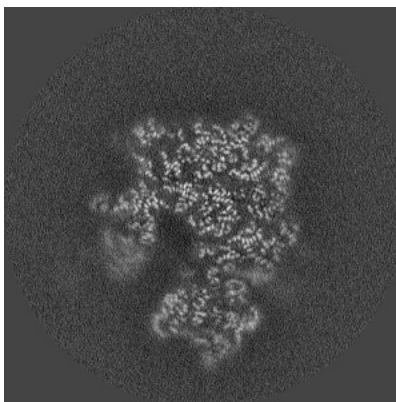


Z Index: 190

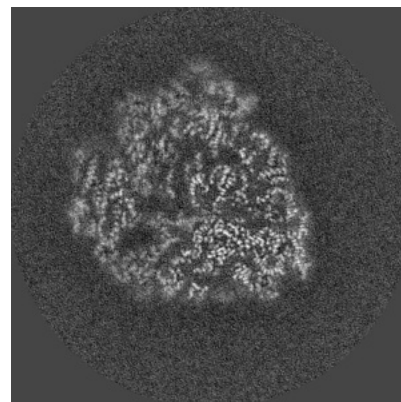
6.3.2 Raw map



X Index: 199



Y Index: 207

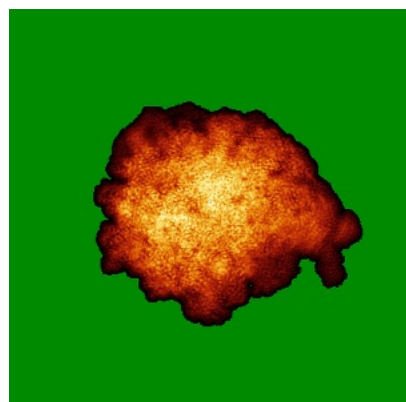


Z Index: 190

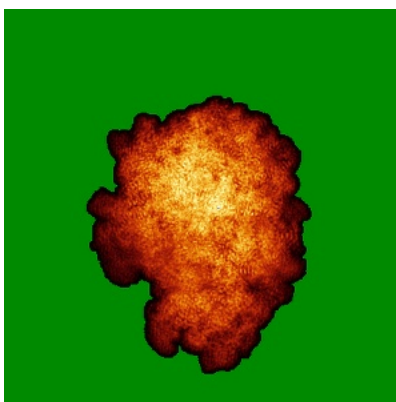
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

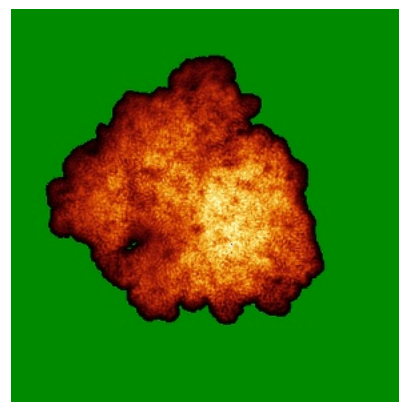
6.4.1 Primary map



X

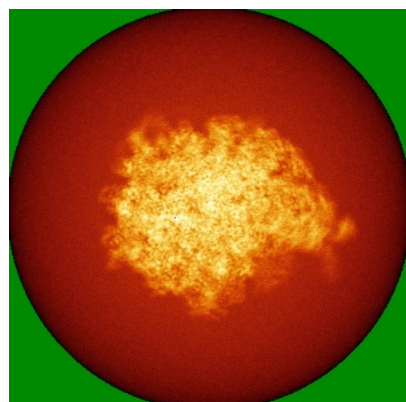


Y

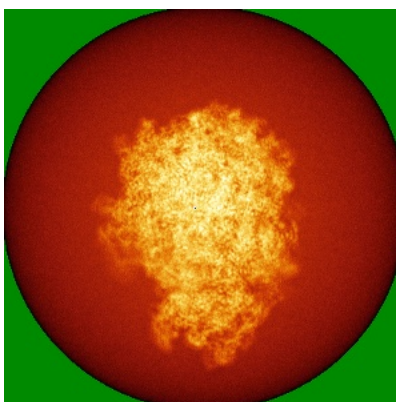


Z

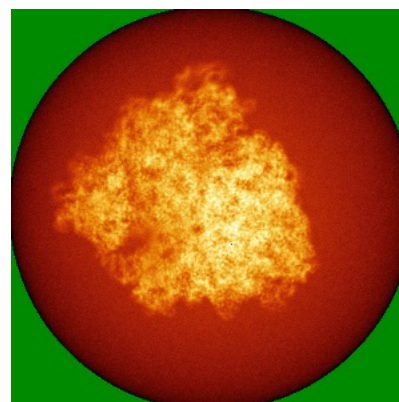
6.4.2 Raw map



X



Y

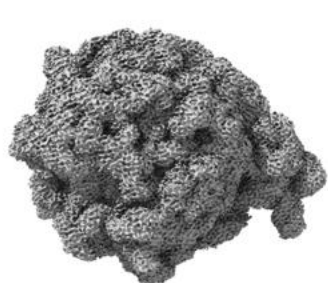


Z

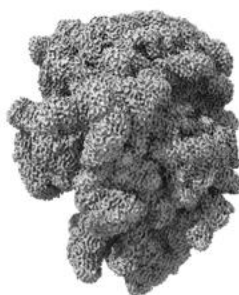
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

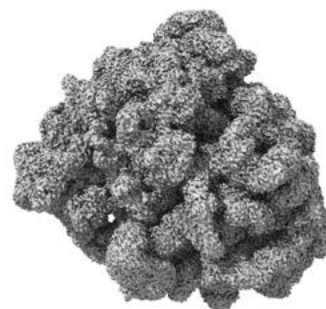
6.5.1 Primary map



X



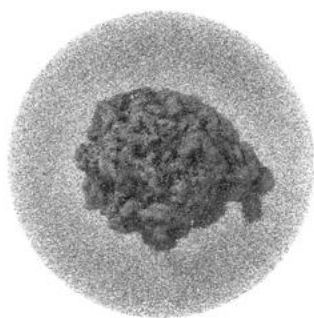
Y



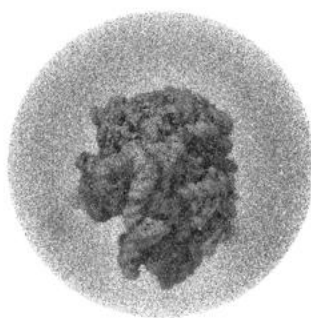
Z

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.

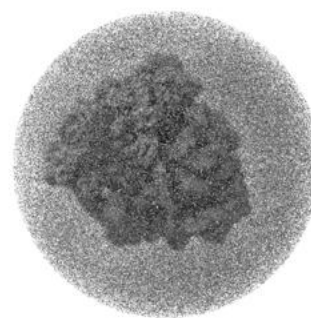
6.5.2 Raw map



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.

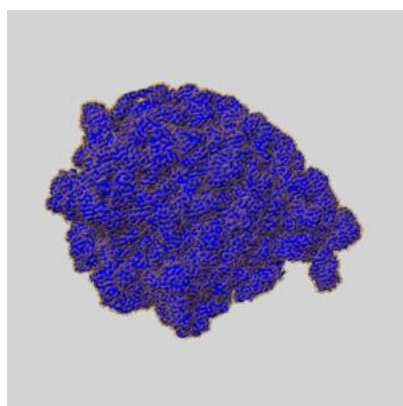
6.6 Mask visualisation [i](#)

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

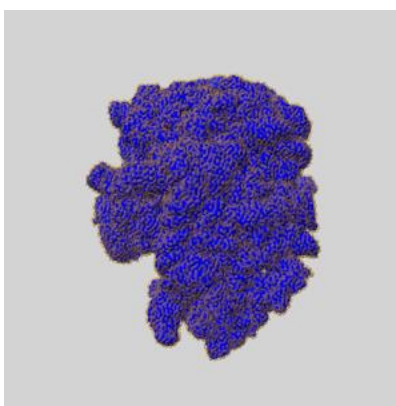
A mask typically either:

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

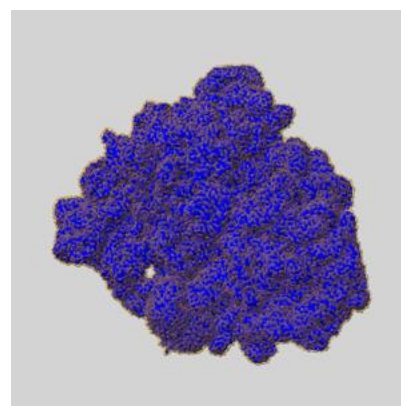
6.6.1 emd_8829_msk_1.map [i](#)



X



Y

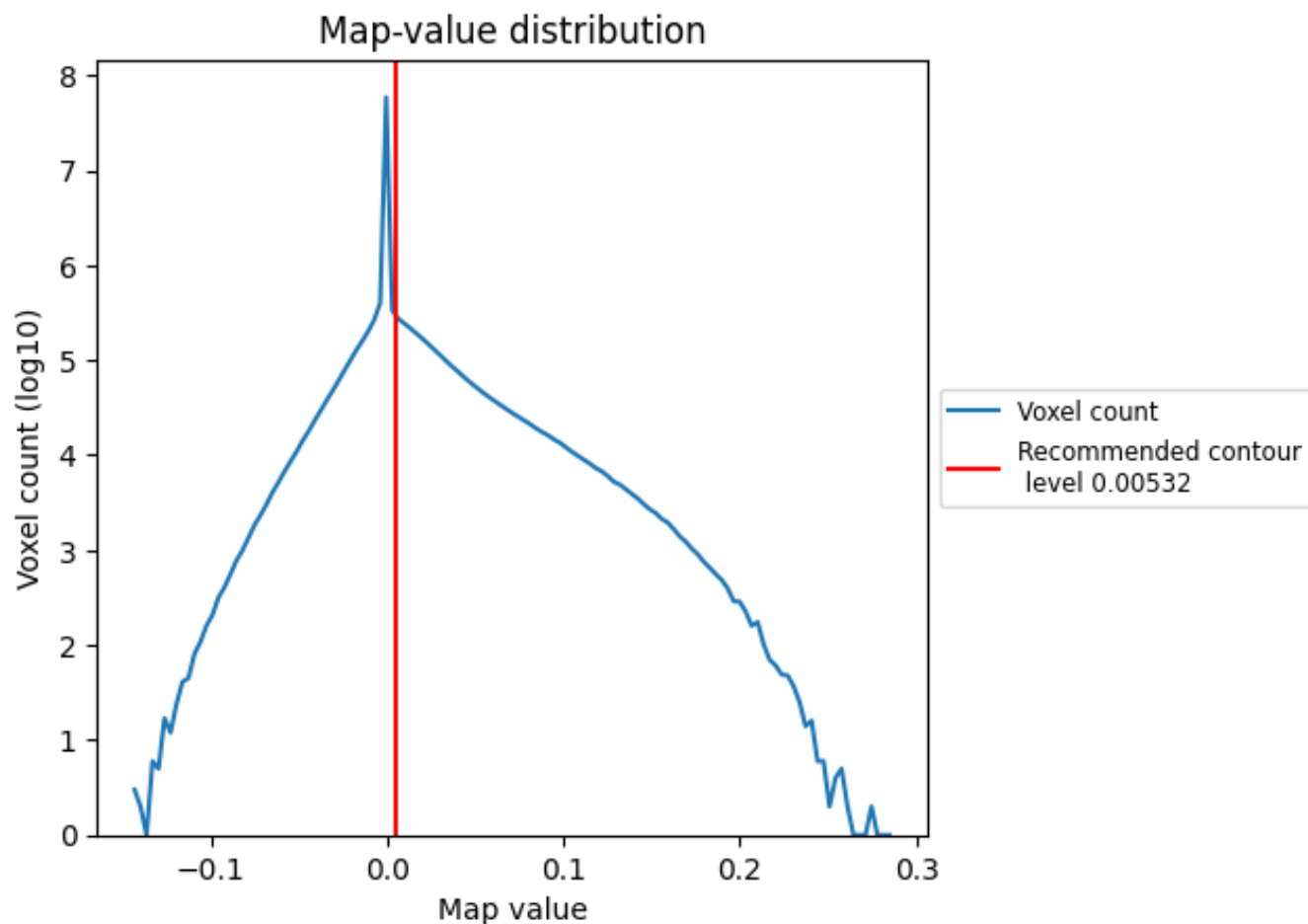


Z

7 Map analysis [i](#)

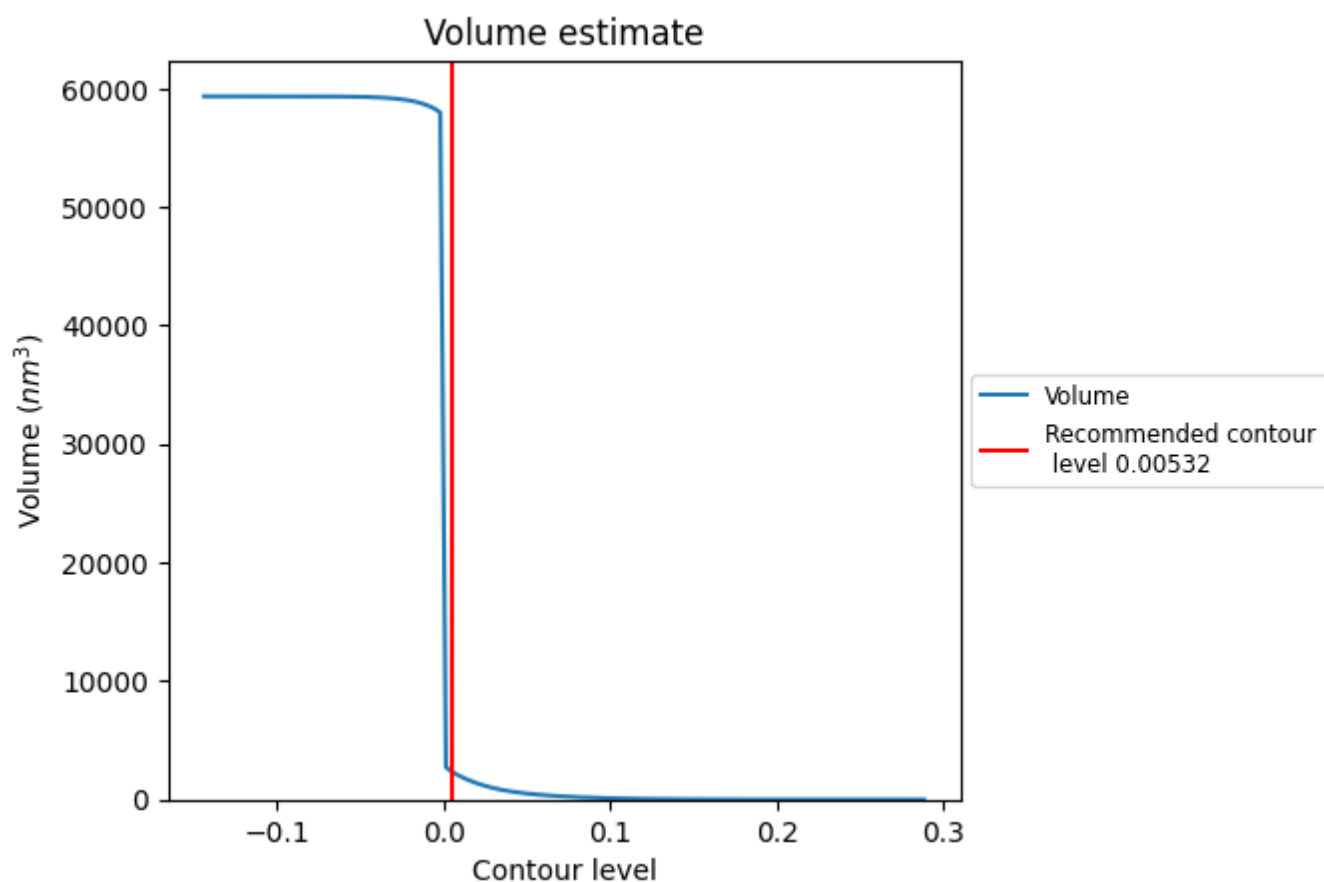
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

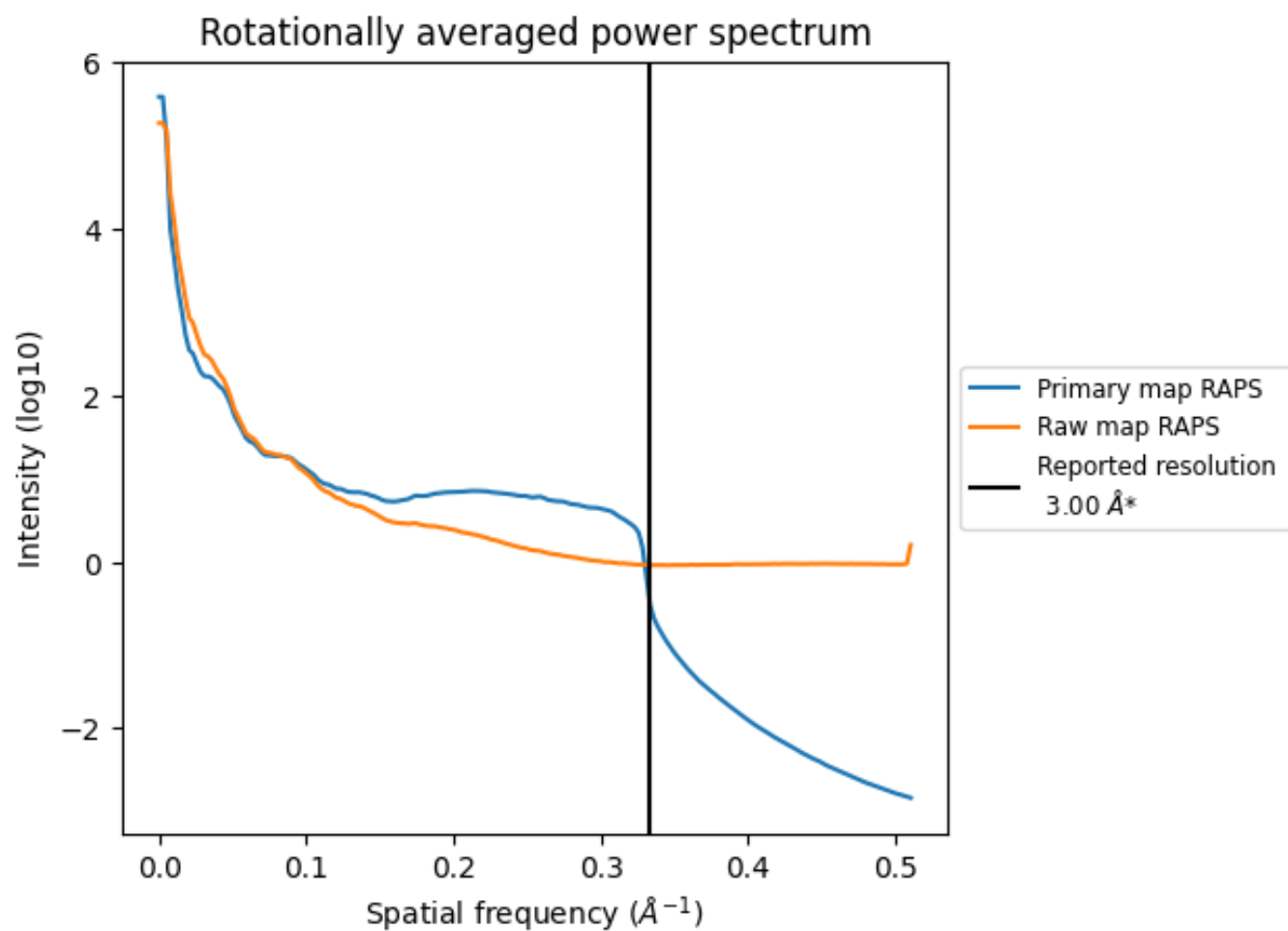
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2339 nm³; 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 ⓘ

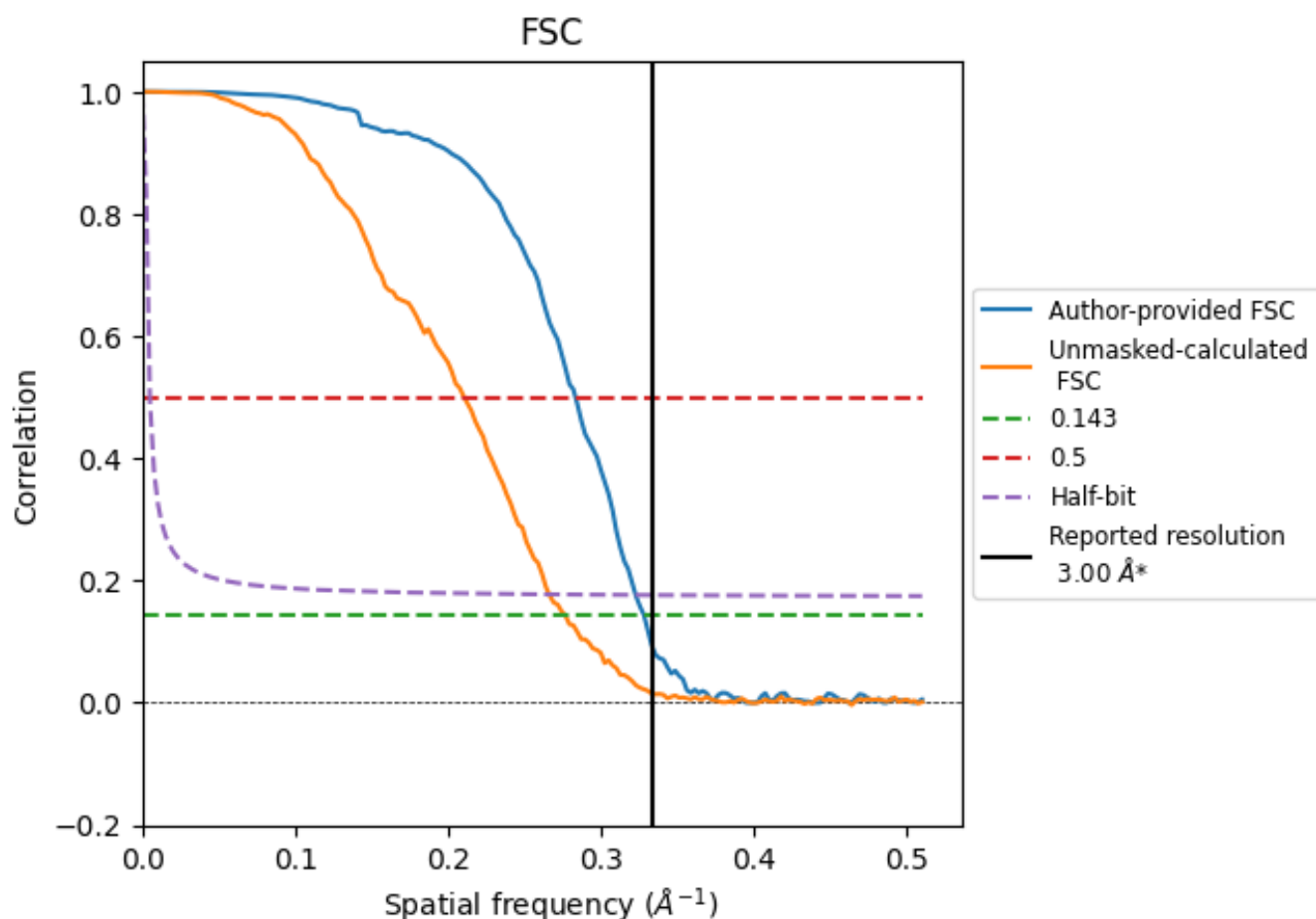


*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

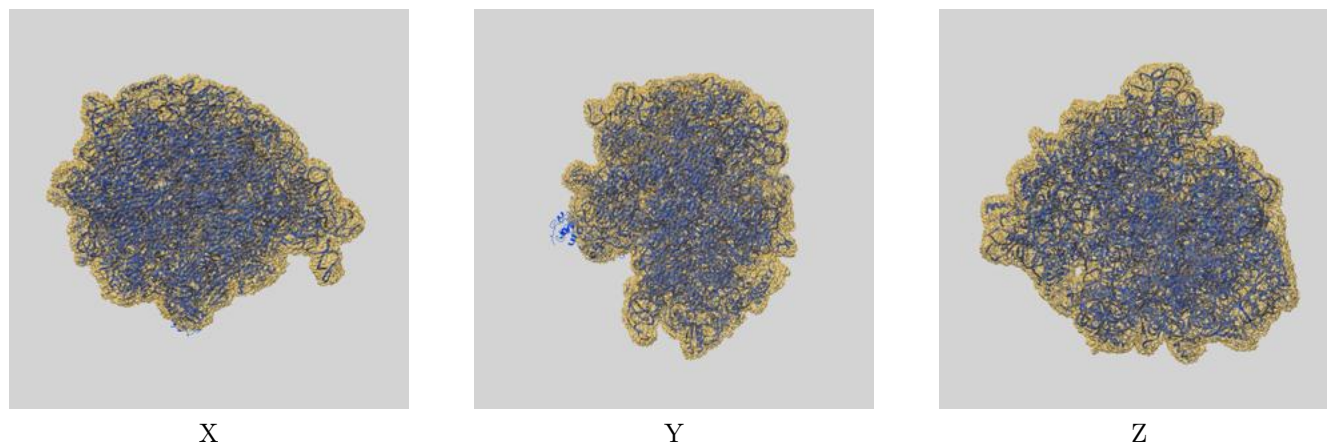
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	3.05	3.53	3.10
Unmasked-calculated*	3.61	4.75	3.76

*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 [i](#)

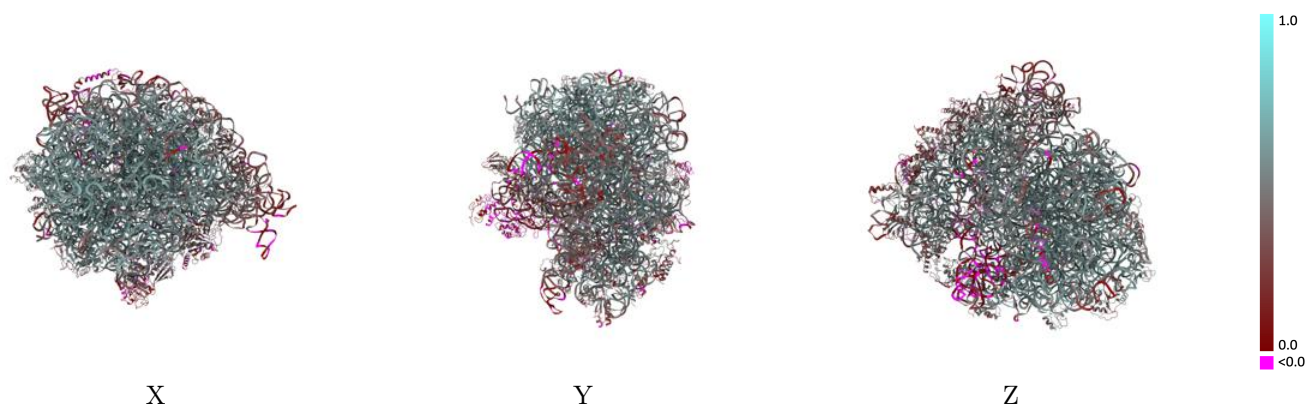
This section contains information regarding the fit between EMDB map EMD-8829 and PDB model 5WFS. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



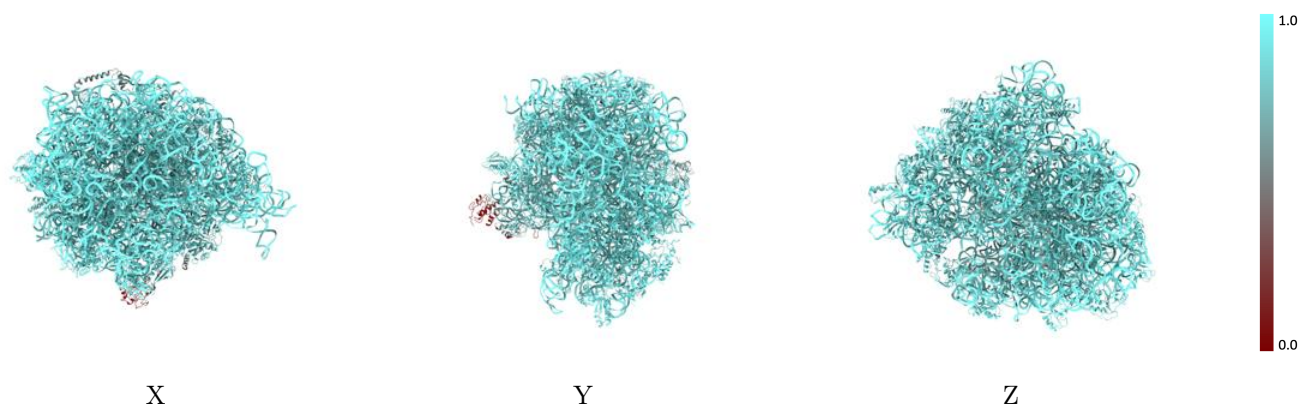
The images above show the 3D surface view of the map at the recommended contour level 0.00532 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



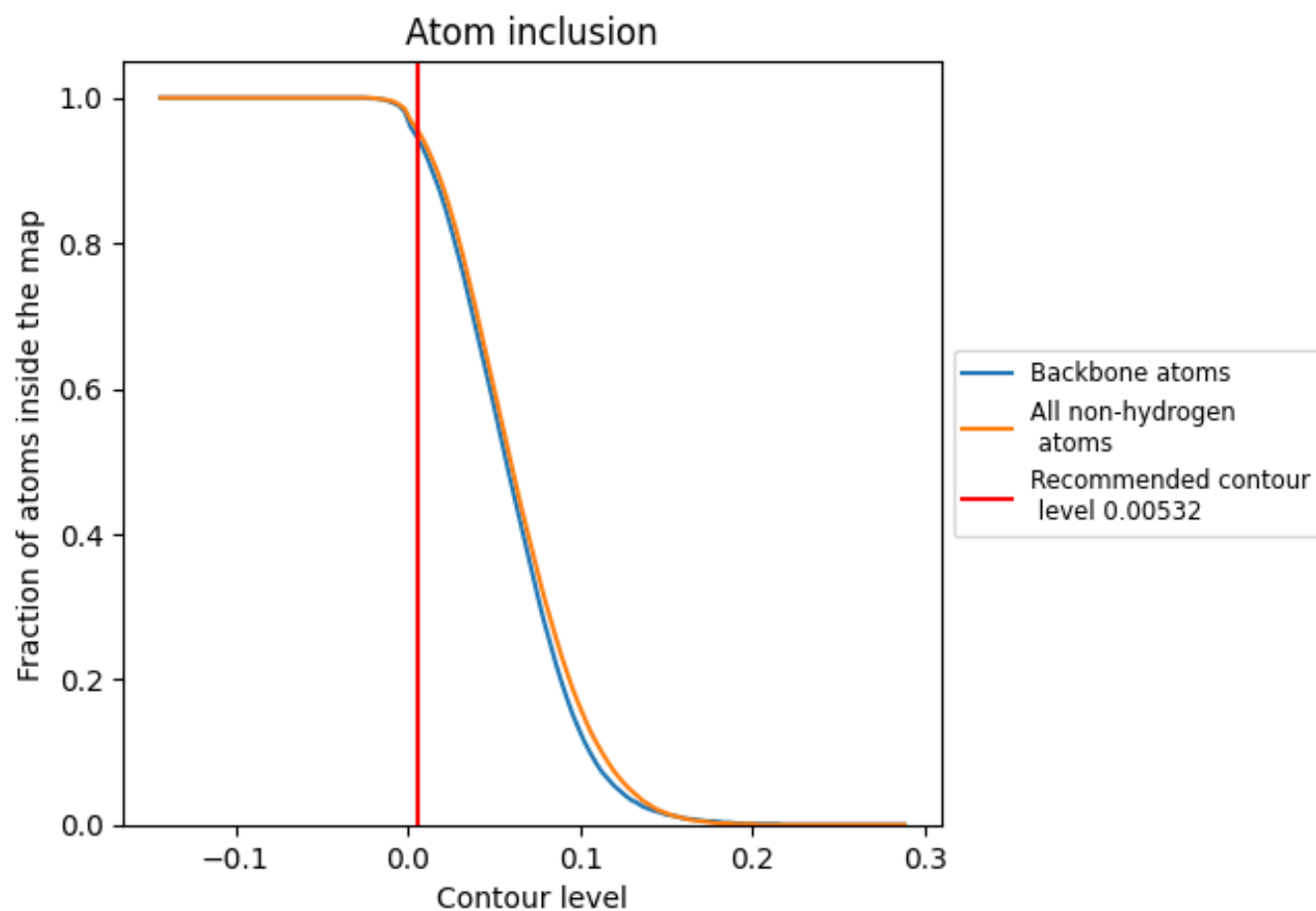
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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



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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