



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 04:33 PM EDT

PDB ID : 5WF0 / pdb_00005wf0
EMDB ID : EMD-8826
Title : 70S ribosome-EF-Tu H84A complex with GTP and near-cognate tRNA (Complex C2)
Authors : Fislage, M.; Frank, J.
Deposited on : 2017-07-11
Resolution : 3.60 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:

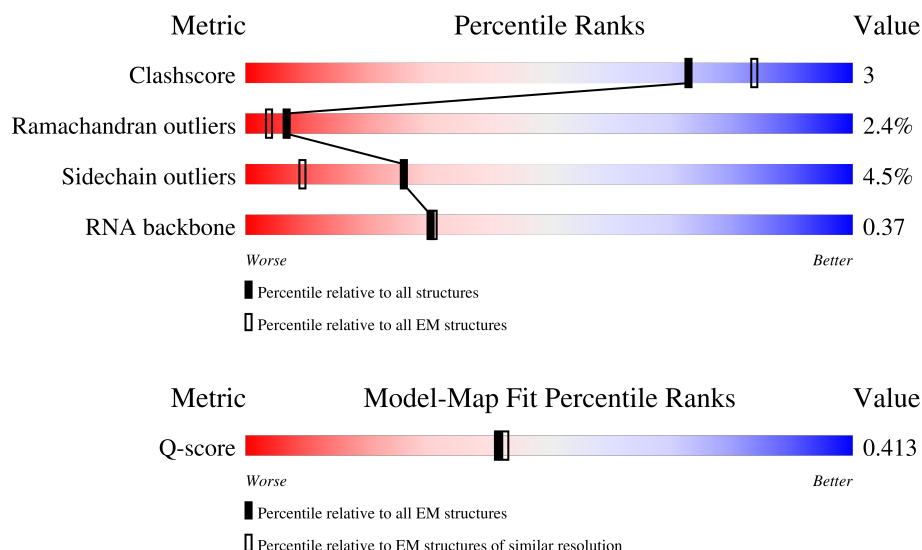
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



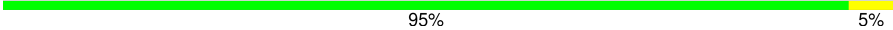
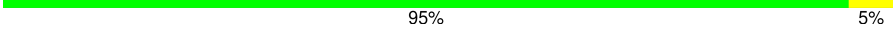
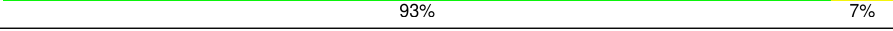
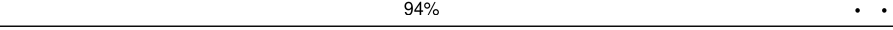
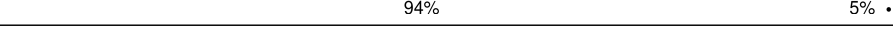
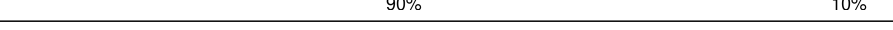
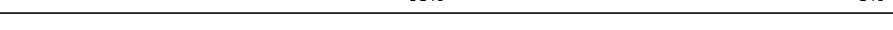
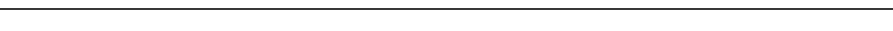
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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% 7% .
5	E	200	 90% 9% .
6	F	177	 93% 6% .
7	G	174	 95% 5% .
8	H	149	 8% 95% 5% .
9	I	141	 16% 80% 17% .
10	J	141	 90% 9% .
11	K	122	 82% 16% ..
12	L	143	 90% 10% .
13	M	136	 93% 7% .
14	N	119	 94% . .
15	O	116	 94% 5% .
16	P	114	 92% 8% .
17	Q	115	 90% 10% .
18	R	102	 88% 11% .
19	S	109	 88% 12% .
20	T	92	 90% 10% .
21	U	102	 88% 11% .
22	V	92	 95% 5% .
23	W	75	 81% 16% .
24	X	77	 96% .
25	Y	60	 93% 7% .
26	Z	56	 96% .
27	0	55	 84% 16% .
28	1	51	 96% .

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Mol	Chain	Length	Quality of chain
29	2	45	
30	3	64	
31	4	38	
32	5	131	
33	6	66	
34	a	1540	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	115	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	

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Mol	Chain	Length	Quality of chain
54	u	65	 72% 22% 6%
55	v	77	 73% 23% •
55	w	77	 51% 36% 10% •
56	x	12	 58% 42%
57	y	76	 51% 41% 8% 96%
58	z	393	 94% 6% 96%

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 154600 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	0	0
			1156	719	218	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		

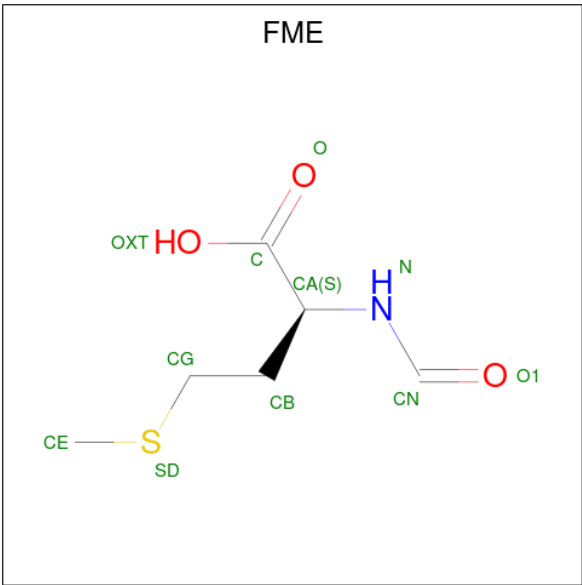
- Molecule 58 is a protein called Elongation factor Tu 2.

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	1001	Total	Mg	0
			1001	1001	
60	B	34	Total	Mg	0
			34	34	
60	D	2	Total	Mg	0
			2	2	
60	E	2	Total	Mg	0
			2	2	
60	L	3	Total	Mg	0
			3	3	
60	M	1	Total	Mg	0
			1	1	
60	N	2	Total	Mg	0
			2	2	
60	Q	2	Total	Mg	0
			2	2	
60	T	1	Total	Mg	0
			1	1	
60	W	2	Total	Mg	0
			2	2	
60	X	2	Total	Mg	0
			2	2	

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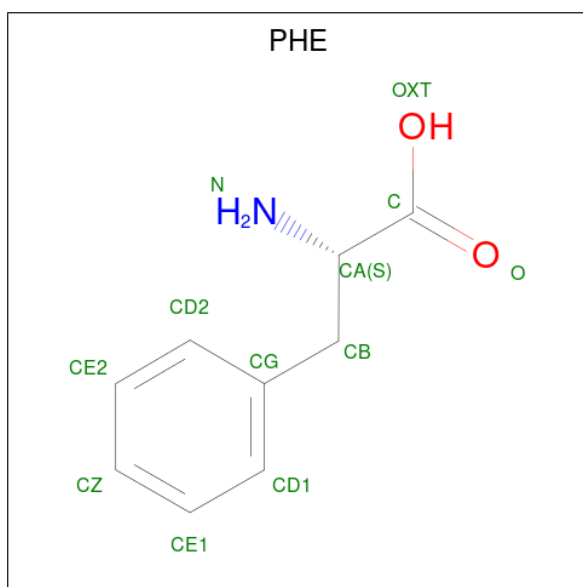
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Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total 1	Mg 1	0
60	4	1	Total 1	Mg 1	0
60	a	402	Total 402	Mg 402	0
60	d	3	Total 3	Mg 3	0
60	g	1	Total 1	Mg 1	0
60	i	2	Total 2	Mg 2	0
60	k	1	Total 1	Mg 1	0
60	m	1	Total 1	Mg 1	0
60	n	1	Total 1	Mg 1	0
60	o	2	Total 2	Mg 2	0
60	t	3	Total 3	Mg 3	0
60	v	8	Total 8	Mg 8	0
60	w	1	Total 1	Mg 1	0
60	x	1	Total 1	Mg 1	0

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

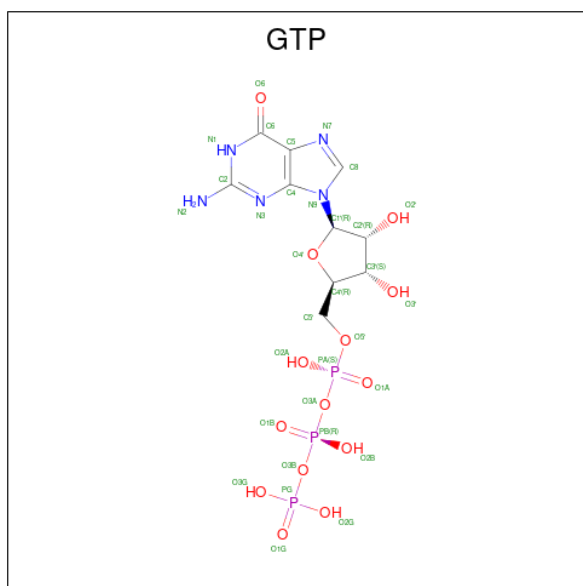
Mol	Chain	Residues	Atoms		AltConf
61	A	4	Total 4	K 4	0
61	a	1	Total 1	K 1	0

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



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

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



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

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	A	463	Total O 463 463	0
64	B	11	Total O 11 11	0
64	C	5	Total O 5 5	0
64	D	1	Total O 1 1	0
64	E	1	Total O 1 1	0
64	G	3	Total O 3 3	0
64	J	2	Total O 2 2	0
64	L	3	Total O 3 3	0
64	M	2	Total O 2 2	0
64	N	4	Total O 4 4	0
64	O	1	Total O 1 1	0
64	Q	2	Total O 2 2	0
64	S	1	Total O 1 1	0
64	W	2	Total O 2 2	0
64	X	1	Total O 1 1	0
64	Z	2	Total O 2 2	0
64	0	1	Total O 1 1	0
64	3	2	Total O 2 2	0
64	a	160	Total O 160 160	0
64	d	1	Total O 1 1	0
64	i	1	Total O 1 1	0
64	s	3	Total O 3 3	0

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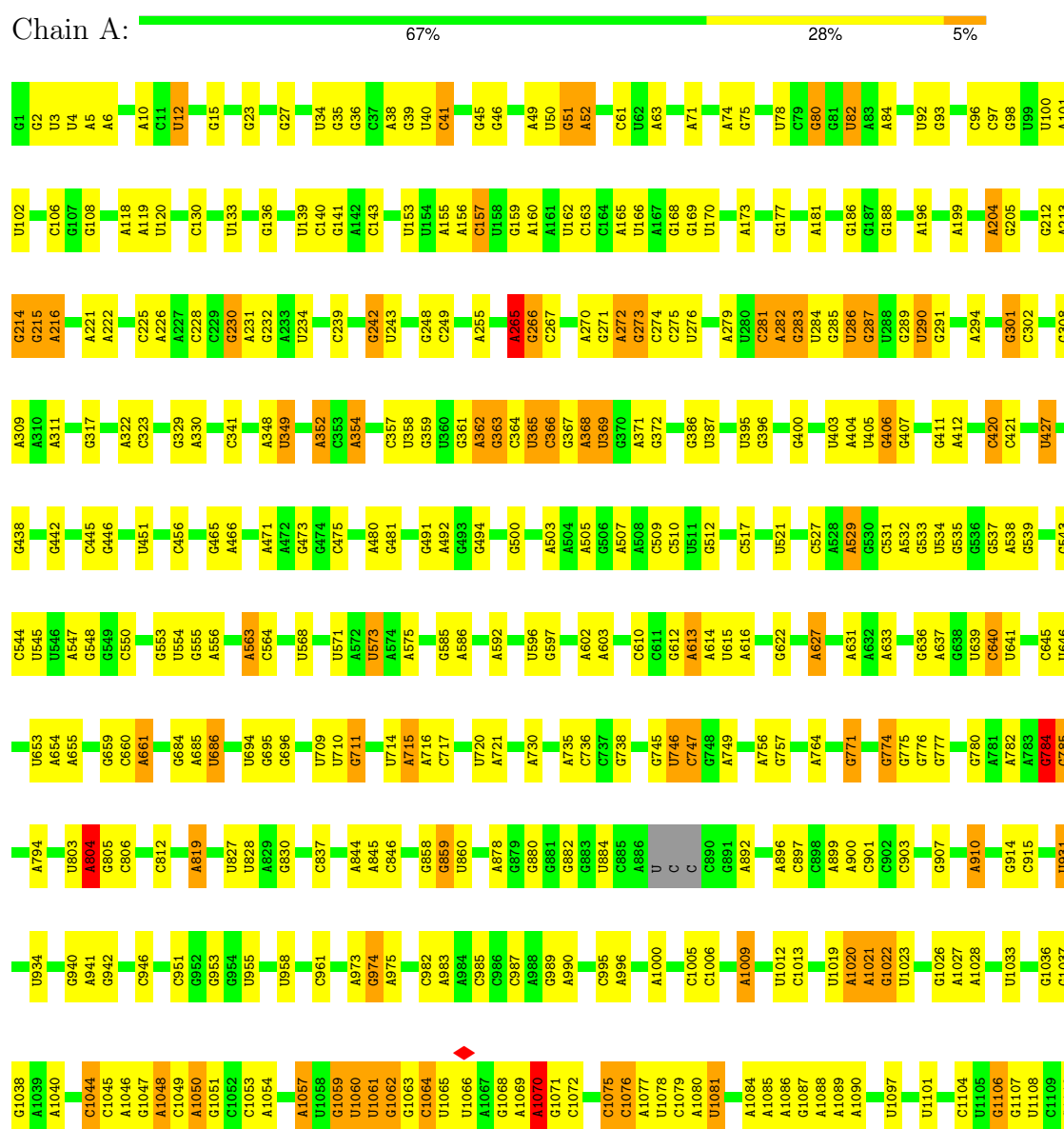
Continued from previous page...

Mol	Chain	Residues	Atoms		AltConf
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	w	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.

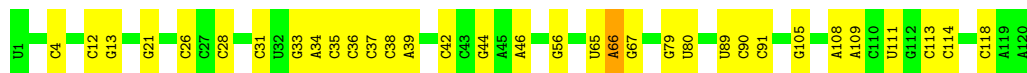
• Molecule 1: 23S rRNA



U2798	A2547	U2423	C2310	G2162	C2055	A1918	A1808	G1715	G1588	U1484	A1395	G1225	A1111
G2799	U2552	C2424	A2311	A2163	G2056	A1919	A1809	A1716	A1569	U1485	A1326	A1226	G1112
G2800	U2553	C2425	C2313	C2164	A2061	A1920	A1810	A1717	A1578	A1490	U1399	G1227	G1115
G2801	U2554	G2428	G2318	A2170	G2060	G1929	G1816	U1720	U1579	G1491	U1400	G1236	G1116
A2802	G2429	G2429	G2319	A2171	A2062	G1930	G1817	G1721	A1580	G1492	U1397	A1287	G1117
G2803	A2430	A2430	G2319	A2173	G2069	A1936	U1818	A1722	G1581	C1493	U1402	G1238	G1118
U2804			G2323	A2173	G2069	A1937	A1836	G1723	C1582		A1403		U1119
C2805	A2435	A2435	G2323	U2180	A2071	A1938	G1826	G1724	U1584	A1496	G1407	G1245	
C2806	U2441	U2441	G2325	U2180	A2071	A1939	A2071	G1725	U1584	A1497	G1407	A1246	G1124
U2807	U2441	U2441	G2325	U2180	A2071	A1939	A2071	G1725	C1585	C1498	A1247	A1247	G1125
G2808	U2441	U2441	G2326	G2186	C2072	U1940	U1834	G1726	C1586	C1499	G1410	G1248	
A2809	U2441	U2441	A2327	G2186	A2077	C1941	G1835	A1727	A1586	U1500			U1130
G2810	G2445	G2445	A2327	U2192	C2077	C1942	G1835	C1728	G1587	G1500			G1131
G2811	G2446	G2446	A2328	U2192	C2078	U1955	U1841	U1729	U1588		G1416	A1263	U1132
G2812	G2447	G2447	A2328	U2198	C2079	U1965	U1841	U1730	U1589	A1504	C1417		U1133
G2813	G2448	U2448	G2330	A2198	A2080	G1842	G1842	G1731	A1590	A1505	C1418	G1256	C1135
G2814	U2449	U2449	G2331	G2204	U2082	C1962	G1847	G1737	A1591	U1506	A1419	C1257	
C2815	U2457	U2457	A2332	A2205	G2083	U1963	G1847	G1738	C1592	U1507	A1420	U1258	
A2816			A2333	C2206	C2086	G1965	U1851	A1739	C1595	A1508	A1419	A1262	G1139
U2817	U2457	U2457	G2334	C2207	C2096	C1965	U1852	A1740	A1596	U1510	A1421		C1140
G2818	U2458	A2469	A2335	C2207	A2097	C1967	U1853	C1741	A1591	U1507	A1420	U1258	U1141
G2819	U2585	G2470	A2336	C2208	U2098	C1967	A1854	U1742	C1592	A1506	G1422		A1142
U2820	U2586	G2470	A2336	C2208	U2098	C1967	A1854	U1742	C1592	A1506	G1422		A1143
A2821			C2342	A2211	U2089	A1970	G1866	G1743	G1605	A1515	G1429	U1273	
G2822	G2603	C2475	C2342	A2212	G2100	U1971	G1867	A1744	A1608	A1516	G1430		G1149
U2823	U2604	A2476	C2350	A2213	A2101	G1972	A1858	A1745	C1609	U1519	A1431	G1300	C1150
G2824	U2605	C2480	G2357	C2214	G2102	U1976	G1862	A1746	A1610	U1520	A1432	A1301	A1151
G2825	U2608	G2481	G2357	G2221	C2103	U1976	G1862	U1747	A1615	G1521	A1433	C1152	C1152
U2826	U2609	U2491	G2361	G2225	U2106	G1980	A1866	C1748	C1616	U1523	A1434	C1305	G1153
G2827	U2613	G2494	G2373	A2226	U2107	U1982	A1866	A1749	C1617	U1524			G1154
A2828	A2614	C2498	A2378	C2226	A2108	A1981	G1869	U1751	A1618	G1528	G1441	C1320	A1155
G2829	U2615	C2499	G2379	G2238	U2109	U1991	A1871	C1752	G1619	A1528	C1447		G1171
A2830	U2623	U2500	G2383	G2239	G2110	G1992	A1872	U1758	G1642	A1529	G1450	A1327	C1172
G2831	G2624	C2501	G2384	G2251	U2111	U1993	A1873	C1764	G1643		C1451	U1329	U1173
U2832	U2629	G2502	U2384	G2251	G2112	C1997	G1875	U1773	U1647	C1533	C1452	G1330	U1174
G2833	U2636	U2504	A2386	U2262	U2113	C1997	A1876	A1773	U1648	A1535	C1453	G1332	A1175
C2834	U2637	U2506	G2391	C2264	U2118	G2004	C1881	A1784	C1675	A1537	G1455	C1345	G1177
A2835	U2638	G2505	A2392	A2273	A2119	A2013	U1882	G1776	A1680	G1542	U1468		C1178
G2836	U2639	U2514	G2399	A2274	G2121	A2020	U1883	U1779	G1651	U1543	U1468	U1382	U1180
U2837	G2642	C2503	G2400	A2274	U2122	A2020	G1884	A1780	A1654	A1544	C1461	C1357	U1181
A2838	U2645	C2516	G2401	A2278	G2127	U2022	C2021	U1781	A1545	A1545			G1182
G2839	U2645	C2516	U2401	G2279	G2127	C2023	C1895	A1783	G1674	G1546	U1466	A1359	U1183
U2840	A2654	C2517	U2402	G2283	U2131	C2032	U1911	A1784	C1675	C1547	U1467	C1363	U1184
C2841	G2655	A2518	C2403	C2283	U2132	U2028	G1903	A1791	U1688	A1548	U1468	C1363	A1189
G2842	U2656	U2518	U2404	A2286	A2134	G2029	U1906	A1791	A1693	A1549	A1469	G1364	G1190
A2843	U2657	G2525	G2405	G2286	G2134	A2030	G1907	A1794	C1366		A1470	A1365	C1193
G2844	G2658	U2529	A2406	A2287	A2031	G2032	G1907	C1795	C1694	A1565	G1471	A1366	G1193
U2845	U2659	G2530	A2407	A2288	G2141	A2033	U1911	U1796	C1695	C1567	G1475	G1368	U1203
C2846	U2660	A2531	U2408	A2296	C2145	A2033	A1912	U1796	A1700	C1568	U1476	C1368	
G2847	G2661	A2531	A2411	A2297	C2146	G2038	A1913	C1800	A1700	U1569	A1477	A1378	G1210
A2848	U2662	G2535	A2412	A2297	A2147	U2039	C1914	A1801	G1710	G1560	G1479	U1379	G1216
G2849	G2663	G2535	A2412	A2297	A2147	U2039	A1914	A1802	G1710	U1560	G1479	A1383	U1217
U2850	G2664	A2542	G2415	A2305	G2157	C2043	A1916	A1803	A1713	C1565	G1482	A1383	G1218
A2851	U2682		G2415	A2309	G2157	C2043	A1916	A1803	U1744	C1567	G1482	A1387	

- Molecule 2: 5S rRNA

Chain B:  72% 27%



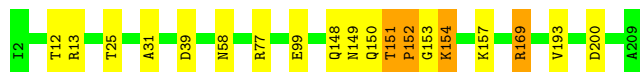
- Molecule 3: 50S ribosomal protein L2

Chain C:  92% 8%



- Molecule 4: 50S ribosomal protein L3

Chain D:  91% 7%



- Molecule 5: 50S ribosomal protein L4

Chain E:  90% 9%

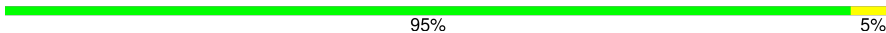


- Molecule 6: 50S ribosomal protein L5

Chain F:  93% 6%

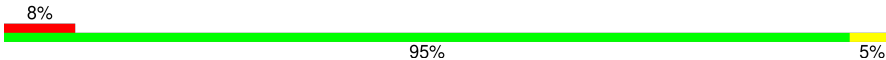


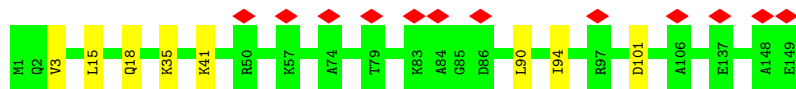
- Molecule 7: 50S ribosomal protein L6

Chain G:  95% 5%

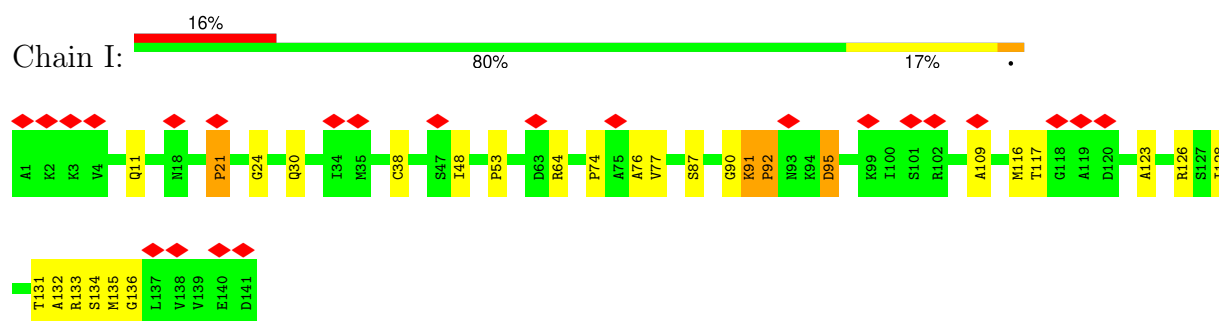


- Molecule 8: 50S ribosomal protein L9

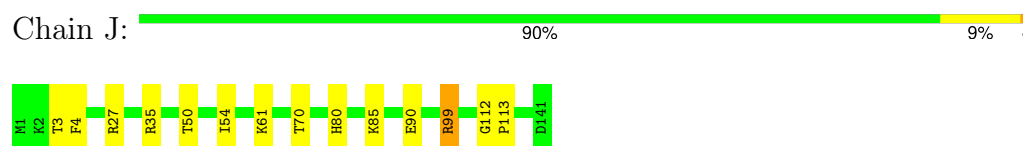
Chain H:  8% 95% 5%



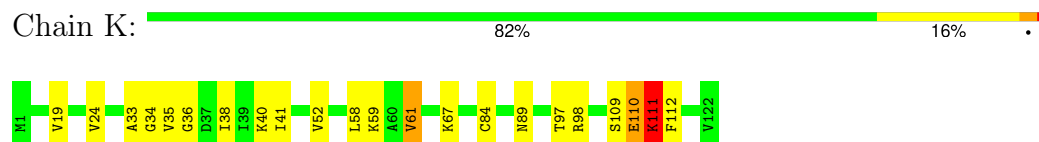
- Molecule 9: 50S ribosomal protein L11



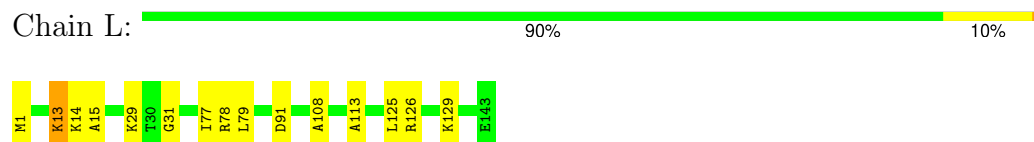
- Molecule 10: 50S ribosomal protein L13



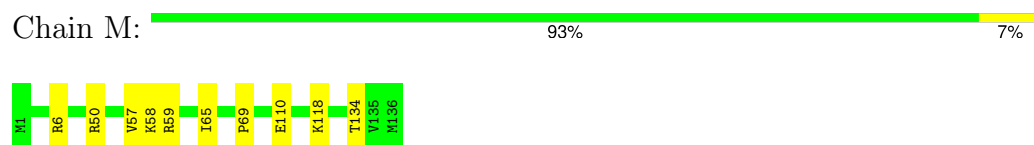
- Molecule 11: 50S ribosomal protein L14



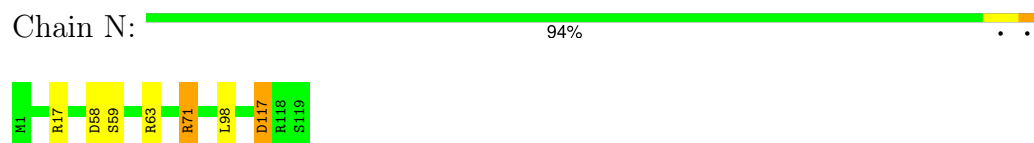
- Molecule 12: 50S ribosomal protein L15



- Molecule 13: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L17



- Molecule 15: 50S ribosomal protein L18





- Molecule 16: 50S ribosomal protein L19

Chain P: 92% 8%



- Molecule 17: 50S ribosomal protein L20

Chain Q: 90% 10%



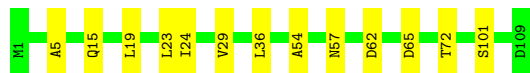
- Molecule 18: 50S ribosomal protein L21

Chain R: 88% 11%



- Molecule 19: 50S ribosomal protein L22

Chain S: 88% 12%



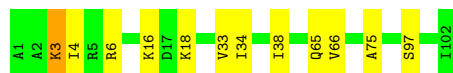
- Molecule 20: 50S ribosomal protein L23

Chain T: 90% 10%



- Molecule 21: 50S ribosomal protein L24

Chain U: 88% 11%



- Molecule 22: 50S ribosomal protein L25

Chain V: 95% 5%



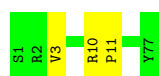
- Molecule 23: 50S ribosomal protein L27

Chain W: 81% 16%



- Molecule 24: 50S ribosomal protein L28

Chain X: 96%



- Molecule 25: 50S ribosomal protein L29

Chain Y: 93% 7%



- Molecule 26: 50S ribosomal protein L30

Chain Z: 96%



- Molecule 27: 50S ribosomal protein L32

Chain 0: 84% 16%



- Molecule 28: 50S ribosomal protein L33

Chain 1: 96%



- Molecule 29: 50S ribosomal protein L34

Chain 2: 80% 20%



- Molecule 30: 50S ribosomal protein L35

Chain 3: 97% .



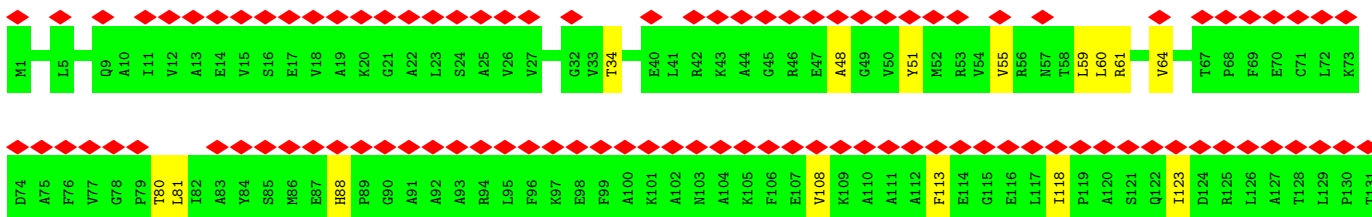
- Molecule 31: 50S ribosomal protein L36 1

Chain 4: 100%

There are no outlier residues recorded for this chain.

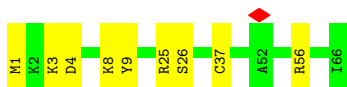
- Molecule 32: 50S ribosomal protein L10

Chain 5: 76%
89% 11%



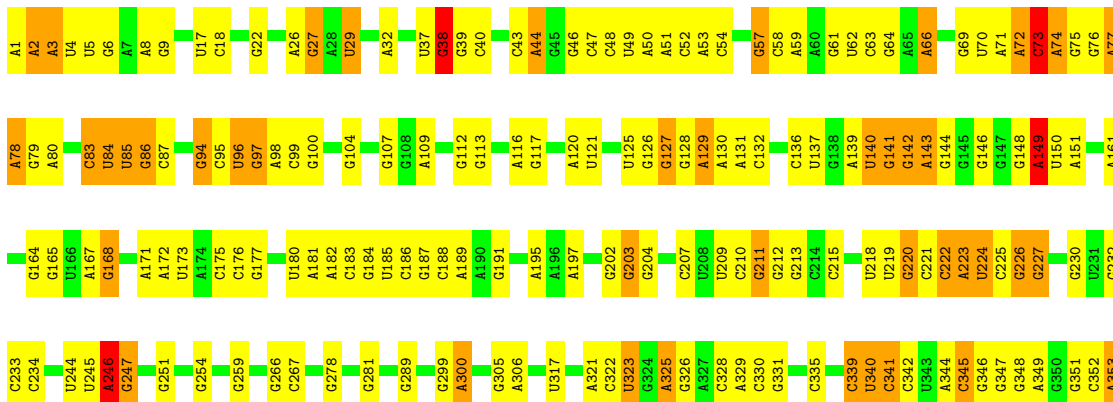
- Molecule 33: 50S ribosomal protein L31

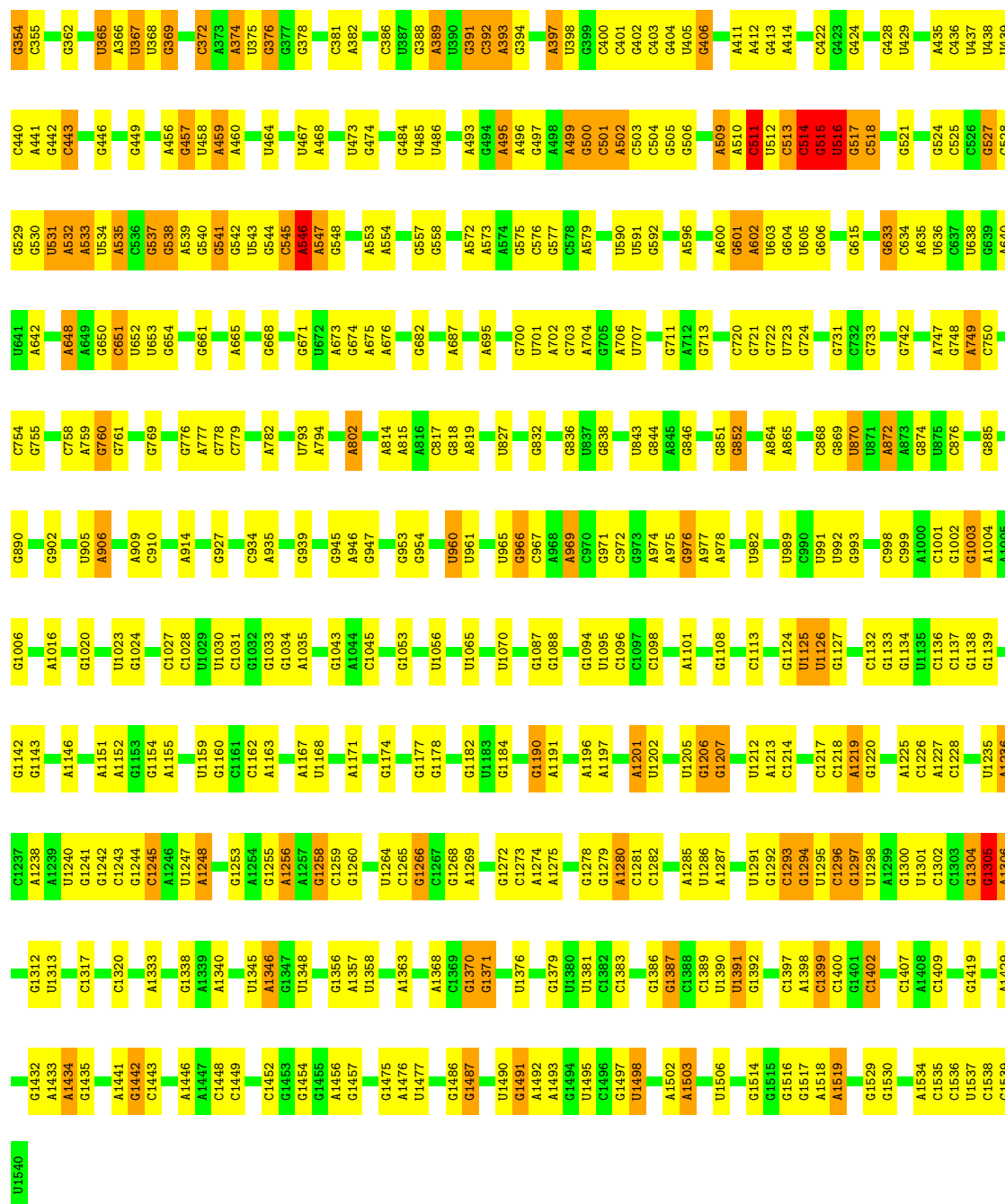
Chain 6: 86% 14%



- Molecule 34: 16S rRNA

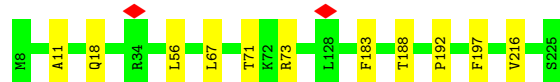
Chain a: 59% 32% 8% .





- Molecule 35: 30S ribosomal protein S2

Chain b: 95%



- Molecule 36: 30S ribosomal protein S3

Chain c: 96%



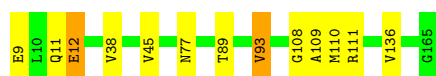
- Molecule 37: 30S ribosomal protein S4

Chain d: 96% .



- Molecule 38: 30S ribosomal protein S5

Chain e: 92% 7% .



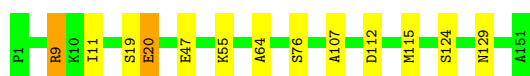
- Molecule 39: 30S ribosomal protein S6

Chain f: 91% 7% .



- Molecule 40: 30S ribosomal protein S7

Chain g: 91% 7% .



- Molecule 41: 30S ribosomal protein S8

Chain h: 93% 7% .



- Molecule 42: 30S ribosomal protein S9

Chain i: 83% 16% .

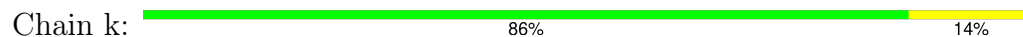


- Molecule 43: 30S ribosomal protein S10

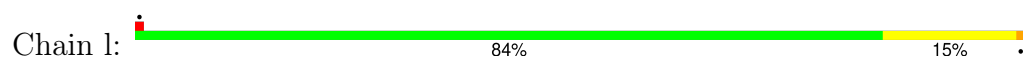
Chain j: 86% 10% .



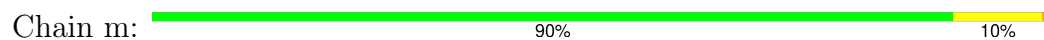
- Molecule 44: 30S ribosomal protein S11



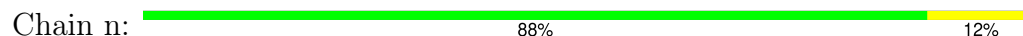
- Molecule 45: 30S ribosomal protein S12



- Molecule 46: 30S ribosomal protein S13



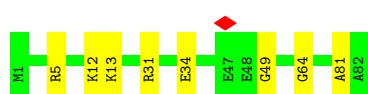
- Molecule 47: 30S ribosomal protein S14



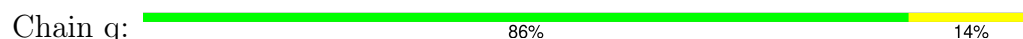
- Molecule 48: 30S ribosomal protein S15



- Molecule 49: 30S ribosomal protein S16

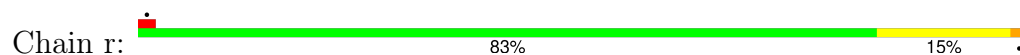


- Molecule 50: 30S ribosomal protein S17

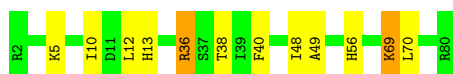
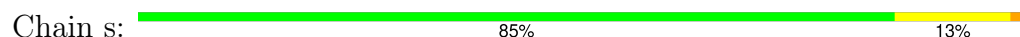




- Molecule 51: 30S ribosomal protein S18



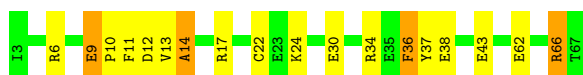
- Molecule 52: 30S ribosomal protein S19



- Molecule 53: 30S ribosomal protein S20



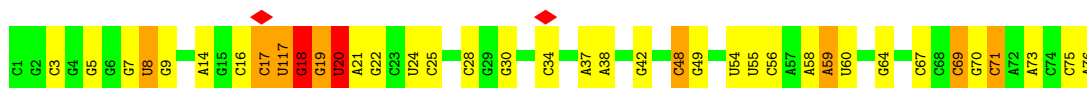
- Molecule 54: 30S ribosomal protein S21



- Molecule 55: tRNA-fMet



- Molecule 55: tRNA-fMet

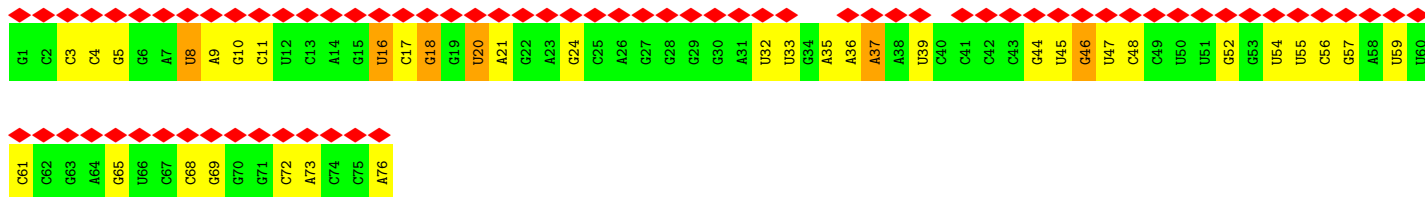


- Molecule 56: mRNA

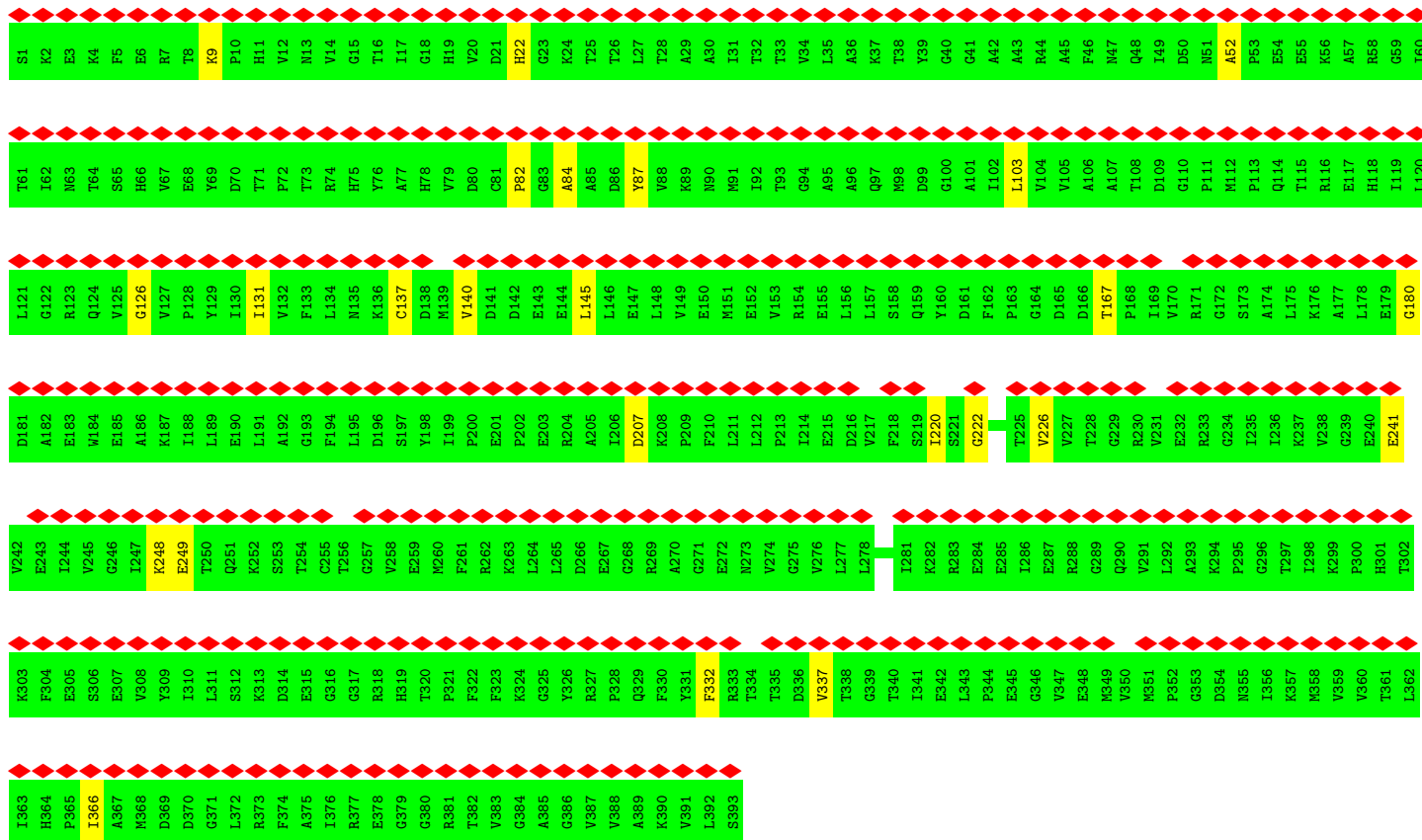




• Molecule 57: Phe-tRNA-Phe



• Molecule 58: Elongation factor Tu 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30623	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	39000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.222	Depositor
Minimum map value	-0.116	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.00371	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: 3TD, FME, H2U, 1MG, 7MG, 5MU, 4SU, 5MC, K, OMC, MG, GTP, PSU, 2MA, UR3, MIA, 6MZ, MA6, 4OC, OMG, 2MG, OMU

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	0.37	0/69174	0.71	32/107907 (0.0%)
2	B	0.37	0/2876	0.68	2/4483 (0.0%)
3	C	0.51	0/2121	0.75	0/2852
4	D	0.52	0/1578	0.78	1/2124 (0.0%)
5	E	0.50	0/1563	0.81	0/2103
6	F	0.54	0/1434	0.82	0/1926
7	G	0.54	0/1324	0.75	0/1794
8	H	0.57	0/1122	0.76	0/1515
9	I	0.70	0/1046	0.97	3/1410 (0.2%)
10	J	0.52	0/1143	0.81	2/1540 (0.1%)
11	K	0.52	0/947	0.74	0/1268
12	L	0.52	0/1052	0.86	0/1401
13	M	0.49	0/1093	0.80	0/1460
14	N	0.55	0/964	0.87	0/1289
15	O	0.55	0/902	0.88	0/1209
16	P	0.50	0/929	0.74	0/1242
17	Q	0.52	0/946	0.93	0/1260
18	R	0.50	0/823	0.78	2/1100 (0.2%)
19	S	0.50	0/852	0.82	0/1142
20	T	0.54	0/736	0.79	0/984
21	U	0.51	0/787	0.77	0/1051
22	V	0.51	0/752	0.75	0/1008
23	W	0.45	0/579	0.69	0/767
24	X	0.48	0/635	0.71	0/848
25	Y	0.53	0/495	0.86	0/658
26	Z	0.54	0/438	0.86	0/586
27	0	0.48	0/440	0.80	0/588
28	1	0.48	0/424	0.69	0/565
29	2	0.55	0/370	0.94	0/487
30	3	0.47	0/513	0.83	0/676
31	4	0.46	0/303	0.73	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.66	0/1001	0.85	0/1350
33	6	0.57	0/531	0.83	0/709
34	a	0.37	0/36725	0.73	26/57285 (0.0%)
35	b	0.57	0/1735	0.81	0/2338
36	c	0.54	0/1651	0.79	0/2225
37	d	0.55	0/1665	0.83	0/2227
38	e	0.54	0/1169	0.83	0/1573
39	f	0.57	0/835	0.82	0/1128
40	g	0.54	0/1195	0.83	0/1602
41	h	0.52	0/989	0.84	1/1326 (0.1%)
42	i	0.56	0/1034	0.77	0/1375
43	j	0.58	0/796	0.75	0/1077
44	k	0.54	0/885	0.80	0/1195
45	l	0.58	0/954	0.80	1/1282 (0.1%)
46	m	0.58	0/900	0.86	0/1204
47	n	0.56	0/822	0.81	0/1095
48	o	0.52	0/722	0.88	0/964
49	p	0.55	0/659	0.82	0/884
50	q	0.56	0/657	0.72	0/881
51	r	0.57	0/544	0.79	0/731
52	s	0.56	0/652	0.76	0/877
53	t	0.55	0/671	0.90	0/888
54	u	0.66	0/550	0.94	0/728
55	v	0.40	1/1747 (0.1%)	0.70	0/2721
55	w	0.42	1/1747 (0.1%)	0.87	7/2721 (0.3%)
56	x	0.40	0/280	0.78	0/433
57	y	0.39	0/1607	0.71	0/2501
58	z	0.57	0/3086	0.76	0/4175
All	All	0.43	2/164170 (0.0%)	0.74	77/245135 (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
34	a	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-6.40	1.51	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	7	4SU	O3'-P	5.15	1.61	1.56

The worst 5 of 77 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	O3'-P-O5'	16.31	128.46	104.00
55	w	117	U	P-O3'-C3'	11.04	136.76	120.20
1	A	242	G	C2'-C3'-O3'	10.92	125.88	109.50
34	a	1305	G	C2'-C3'-O3'	9.76	124.15	109.50
1	A	1022	G	C2'-C3'-O3'	9.27	123.40	109.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
34	a	502	A	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	31338	328	0
2	B	2572	0	1302	3	0
3	C	2082	0	2157	7	0
4	D	1557	0	1604	6	0
5	E	1544	0	1607	6	0
6	F	1410	0	1447	6	0
7	G	1304	0	1348	3	0
8	H	1111	0	1148	1	0
9	I	1032	0	1088	21	0
10	J	1120	0	1151	5	0
11	K	938	0	1012	11	0
12	L	1043	0	1123	7	0
13	M	1074	0	1157	1	0
14	N	951	0	994	3	0
15	O	892	0	923	2	0
16	P	917	0	965	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	Q	933	0	1006	8	0
18	R	810	0	834	5	0
19	S	845	0	909	4	0
20	T	730	0	795	1	0
21	U	779	0	834	2	0
22	V	739	0	763	1	0
23	W	572	0	593	9	0
24	X	625	0	655	3	0
25	Y	494	0	530	1	0
26	Z	434	0	477	1	0
27	0	434	0	448	8	0
28	1	417	0	451	0	0
29	2	367	0	405	4	0
30	3	504	0	574	0	0
31	4	302	0	343	0	0
32	5	988	0	1025	4	0
33	6	522	0	524	2	0
34	a	33050	0	16655	296	0
35	b	1704	0	1732	2	0
36	c	1624	0	1699	3	0
37	d	1643	0	1710	4	0
38	e	1156	0	1199	3	0
39	f	817	0	808	6	0
40	g	1181	0	1240	4	0
41	h	979	0	1034	2	0
42	i	1022	0	1070	19	0
43	j	786	0	828	7	0
44	k	869	0	878	2	0
45	l	940	0	1001	5	0
46	m	891	0	955	2	0
47	n	810	0	852	0	0
48	o	714	0	736	13	0
49	p	649	0	666	2	0
50	q	648	0	691	1	0
51	r	535	0	552	2	0
52	s	637	0	665	6	0
53	t	665	0	714	14	0
54	u	544	0	579	6	0
55	v	1644	0	840	1	0
55	w	1644	0	840	13	0
56	x	252	0	130	2	0
57	y	1632	0	843	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	z	3031	0	3052	5	0
59	A	10	0	10	0	0
60	0	1	0	0	0	0
60	4	1	0	0	0	0
60	A	1001	0	0	0	0
60	B	34	0	0	0	0
60	D	2	0	0	0	0
60	E	2	0	0	0	0
60	L	3	0	0	0	0
60	M	1	0	0	0	0
60	N	2	0	0	0	0
60	Q	2	0	0	0	0
60	T	1	0	0	0	0
60	W	2	0	0	0	0
60	X	2	0	0	0	0
60	a	402	0	0	0	0
60	d	3	0	0	0	0
60	g	1	0	0	0	0
60	i	2	0	0	0	0
60	k	1	0	0	0	0
60	m	1	0	0	0	0
60	n	1	0	0	0	0
60	o	2	0	0	0	0
60	t	3	0	0	0	0
60	v	8	0	0	0	0
60	w	1	0	0	0	0
60	x	1	0	0	0	0
61	A	4	0	0	0	0
61	a	1	0	0	0	0
62	z	11	0	8	0	0
63	z	32	0	12	0	0
64	0	1	0	0	0	0
64	3	2	0	0	0	0
64	A	463	0	0	0	0
64	B	11	0	0	0	0
64	C	5	0	0	0	0
64	D	1	0	0	0	0
64	E	1	0	0	0	0
64	G	3	0	0	0	0
64	J	2	0	0	0	0
64	L	3	0	0	0	0
64	M	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
64	N	4	0	0	0	0
64	O	1	0	0	0	0
64	Q	2	0	0	0	0
64	S	1	0	0	0	0
64	W	2	0	0	0	0
64	X	1	0	0	0	0
64	Z	2	0	0	0	0
64	a	160	0	0	1	0
64	d	1	0	0	0	0
64	i	1	0	0	0	0
64	s	3	0	0	0	0
64	t	1	0	0	0	0
64	u	1	0	0	0	0
64	w	2	0	0	0	0
All	All	154600	0	103529	799	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 3.

The worst 5 of 799 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:514:C:O2	34:a:538:G:N2	1.62	1.30
1:A:627:A:OP1	12:L:78:ARG:NH1	1.71	1.22
1:A:2013:A:N1	1:A:2613:U:O4	1.71	1.21
1:A:714:U:OP2	48:o:88:ARG:NH1	1.76	1.19
34:a:502:A:H61	34:a:544:G:N2	1.43	1.17

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%)	241 (90%)	26 (10%)	2 (1%)	18	51
4	D	206/208 (99%)	187 (91%)	15 (7%)	4 (2%)	6	33
5	E	198/200 (99%)	181 (91%)	13 (7%)	4 (2%)	6	32
6	F	175/177 (99%)	158 (90%)	17 (10%)	0	100	100
7	G	172/174 (99%)	156 (91%)	15 (9%)	1 (1%)	21	54
8	H	147/149 (99%)	126 (86%)	18 (12%)	3 (2%)	6	32
9	I	139/141 (99%)	110 (79%)	24 (17%)	5 (4%)	2	22
10	J	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
11	K	120/122 (98%)	104 (87%)	12 (10%)	4 (3%)	3	24
12	L	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	4	26
13	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	5	30
14	N	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	7	35
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14	46
16	P	112/114 (98%)	100 (89%)	12 (11%)	0	100	100
17	Q	113/115 (98%)	110 (97%)	3 (3%)	0	100	100
18	R	100/102 (98%)	83 (83%)	13 (13%)	4 (4%)	2	20
19	S	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	14	46
20	T	90/92 (98%)	77 (86%)	11 (12%)	2 (2%)	5	30
21	U	100/102 (98%)	84 (84%)	12 (12%)	4 (4%)	2	20
22	V	90/92 (98%)	84 (93%)	5 (6%)	1 (1%)	11	43
23	W	73/75 (97%)	65 (89%)	7 (10%)	1 (1%)	9	38
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
25	Y	58/60 (97%)	55 (95%)	2 (3%)	1 (2%)	7	35
26	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
27	0	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	33
28	1	49/51 (96%)	41 (84%)	6 (12%)	2 (4%)	2	19
29	2	43/45 (96%)	42 (98%)	1 (2%)	0	100	100
30	3	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
31	4	36/38 (95%)	32 (89%)	4 (11%)	0	100	100
32	5	129/131 (98%)	98 (76%)	21 (16%)	10 (8%)	1	8
33	6	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	7	36
35	b	216/218 (99%)	187 (87%)	25 (12%)	4 (2%)	6	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	c	204/206 (99%)	184 (90%)	14 (7%)	6 (3%)	3	26
37	d	203/205 (99%)	181 (89%)	20 (10%)	2 (1%)	12	45
38	e	155/157 (99%)	129 (83%)	23 (15%)	3 (2%)	6	33
39	f	98/100 (98%)	84 (86%)	12 (12%)	2 (2%)	6	32
40	g	149/151 (99%)	132 (89%)	12 (8%)	5 (3%)	3	23
41	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
42	i	125/127 (98%)	96 (77%)	24 (19%)	5 (4%)	2	20
43	j	96/98 (98%)	73 (76%)	16 (17%)	7 (7%)	1	10
44	k	114/116 (98%)	100 (88%)	9 (8%)	5 (4%)	2	18
45	l	119/121 (98%)	98 (82%)	14 (12%)	7 (6%)	1	13
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	6	34
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	1	15
48	o	86/88 (98%)	79 (92%)	3 (4%)	4 (5%)	2	17
49	p	80/82 (98%)	69 (86%)	8 (10%)	3 (4%)	2	21
50	q	78/80 (98%)	71 (91%)	4 (5%)	3 (4%)	2	21
51	r	63/65 (97%)	52 (82%)	7 (11%)	4 (6%)	1	12
52	s	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	9	39
53	t	83/85 (98%)	73 (88%)	7 (8%)	3 (4%)	2	22
54	u	63/65 (97%)	41 (65%)	13 (21%)	9 (14%)	0	3
58	z	391/393 (100%)	348 (89%)	32 (8%)	11 (3%)	4	26
All	All	6218/6322 (98%)	5461 (88%)	605 (10%)	152 (2%)	7	29

5 of 152 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	L	31	GLY
18	R	51	VAL
20	T	37	ASP
21	U	6	ARG
32	5	123	ILE

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%)	205 (95%)	11 (5%)	21	49
4	D	163/163 (100%)	152 (93%)	11 (7%)	15	42
5	E	164/164 (100%)	156 (95%)	8 (5%)	22	49
6	F	148/148 (100%)	141 (95%)	7 (5%)	23	50
7	G	135/135 (100%)	132 (98%)	3 (2%)	45	65
8	H	114/114 (100%)	111 (97%)	3 (3%)	40	62
9	I	109/109 (100%)	102 (94%)	7 (6%)	16	43
10	J	115/115 (100%)	107 (93%)	8 (7%)	14	41
11	K	103/103 (100%)	93 (90%)	10 (10%)	8	31
12	L	102/102 (100%)	96 (94%)	6 (6%)	18	45
13	M	109/109 (100%)	104 (95%)	5 (5%)	24	51
14	N	99/99 (100%)	96 (97%)	3 (3%)	36	59
15	O	86/86 (100%)	83 (96%)	3 (4%)	32	57
16	P	99/99 (100%)	95 (96%)	4 (4%)	28	54
17	Q	88/88 (100%)	85 (97%)	3 (3%)	32	57
18	R	84/84 (100%)	81 (96%)	3 (4%)	31	56
19	S	92/92 (100%)	86 (94%)	6 (6%)	15	43
20	T	79/79 (100%)	74 (94%)	5 (6%)	16	44
21	U	83/83 (100%)	78 (94%)	5 (6%)	17	45
22	V	77/77 (100%)	75 (97%)	2 (3%)	40	62
23	W	57/57 (100%)	52 (91%)	5 (9%)	9	33
24	X	67/67 (100%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	54 (98%)	1 (2%)	51	68
26	Z	47/47 (100%)	46 (98%)	1 (2%)	47	65
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%)	33 (89%)	4 (11%)	6	28
30	3	51/51 (100%)	49 (96%)	2 (4%)	28	54
31	4	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	5	100/100 (100%)	99 (99%)	1 (1%)	68	75
33	6	59/59 (100%)	53 (90%)	6 (10%)	7	30
35	b	180/180 (100%)	177 (98%)	3 (2%)	53	69
36	c	170/170 (100%)	169 (99%)	1 (1%)	78	79
37	d	172/172 (100%)	168 (98%)	4 (2%)	44	64
38	e	119/119 (100%)	113 (95%)	6 (5%)	22	49
39	f	87/87 (100%)	84 (97%)	3 (3%)	32	57
40	g	124/124 (100%)	117 (94%)	7 (6%)	19	47
41	h	104/104 (100%)	99 (95%)	5 (5%)	23	50
42	i	105/105 (100%)	102 (97%)	3 (3%)	37	60
43	j	86/86 (100%)	83 (96%)	3 (4%)	32	57
44	k	89/89 (100%)	81 (91%)	8 (9%)	9	33
45	l	102/102 (100%)	96 (94%)	6 (6%)	18	45
46	m	93/93 (100%)	86 (92%)	7 (8%)	12	39
47	n	83/83 (100%)	76 (92%)	7 (8%)	10	35
48	o	76/76 (100%)	74 (97%)	2 (3%)	40	62
49	p	65/65 (100%)	63 (97%)	2 (3%)	35	59
50	q	74/74 (100%)	68 (92%)	6 (8%)	11	36
51	r	56/56 (100%)	52 (93%)	4 (7%)	13	40
52	s	70/70 (100%)	65 (93%)	5 (7%)	13	40
53	t	65/65 (100%)	57 (88%)	8 (12%)	4	23
54	u	55/55 (100%)	50 (91%)	5 (9%)	9	33
58	z	325/325 (100%)	322 (99%)	3 (1%)	70	76
All	All	5164/5164 (100%)	4933 (96%)	231 (4%)	26	51

5 of 231 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
23	W	15	LYS
53	t	63	LYS
38	e	12	GLU
53	t	43	LYS
49	p	34	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
48	o	19	ASN
58	z	355	ASN
48	o	36	ASN
53	t	47	GLN
16	P	6	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2897/2903 (99%)	732 (25%)	74 (2%)
2	B	119/120 (99%)	25 (21%)	5 (4%)
34	a	1539/1540 (99%)	466 (30%)	0
55	v	76/77 (98%)	18 (23%)	0
55	w	76/77 (98%)	34 (44%)	0
56	x	11/12 (91%)	3 (27%)	0
57	y	75/76 (98%)	30 (40%)	0
All	All	4793/4805 (99%)	1308 (27%)	79 (1%)

5 of 1308 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	3	U
1	A	4	U
1	A	5	A
1	A	6	A

5 of 79 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1940	U
1	A	2798	U
1	A	2238	G
1	A	2402	U
2	B	56	G

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$
1	PSU	A	2605	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
1	PSU	A	2580	1	18,21,22	1.44	2 (11%)	21,30,33	2.03	5 (23%)
1	PSU	A	2604	60,1	18,21,22	1.43	2 (11%)	21,30,33	1.95	4 (19%)
1	PSU	A	2457	1	18,21,22	1.44	2 (11%)	21,30,33	2.12	5 (23%)
57	4SU	y	8	57	18,21,22	1.82	5 (27%)	25,30,33	2.37	7 (28%)
55	5MU	v	54	55	19,22,23	1.49	4 (21%)	27,32,35	1.97	7 (25%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.02	11 (40%)
34	UR3	a	1498	34	19,22,23	1.13	2 (10%)	26,32,35	1.97	5 (19%)
34	4OC	a	1402	34	20,23,24	0.84	0	25,32,35	1.33	5 (20%)
1	PSU	A	746	60,1	18,21,22	1.40	2 (11%)	21,30,33	2.05	5 (23%)
34	7MG	a	527	34,60	23,26,27	1.42	3 (13%)	27,39,42	2.55	7 (25%)
1	3TD	A	1915	1	19,22,23	7.09	13 (68%)	23,32,35	1.95	5 (21%)
57	MIA	y	37	57	28,31,32	2.39	8 (28%)	38,44,47	2.88	17 (44%)
57	PSU	y	32	57	18,21,22	1.35	2 (11%)	21,30,33	2.10	5 (23%)
34	PSU	a	516	34	18,21,22	1.36	2 (11%)	21,30,33	2.12	5 (23%)
1	OMG	A	2251	55,1	23,26,27	1.26	3 (13%)	32,38,41	1.99	6 (18%)
1	H2U	A	2449	1	18,21,22	0.94	2 (11%)	19,30,33	1.61	4 (21%)
1	2MA	A	2503	60,1	22,25,26	1.59	5 (22%)	32,37,40	2.22	9 (28%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.40	3 (15%)
1	2MG	A	2445	1	23,26,27	1.26	4 (17%)	33,38,41	2.35	10 (30%)
1	PSU	A	955	1	18,21,22	1.42	2 (11%)	21,30,33	2.08	4 (19%)
57	PSU	y	55	57	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
34	2MG	a	966	34	23,26,27	1.30	4 (17%)	33,38,41	2.64	9 (27%)
55	H2U	w	20	55	18,21,22	0.81	0	19,30,33	1.34	3 (15%)
34	5MC	a	1407	34	19,22,23	1.98	2 (10%)	26,32,35	1.60	5 (19%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
57	7MG	y	46	57	23,26,27	1.42	3 (13%)	27,39,42	2.48	7 (25%)
34	2MG	a	1207	34	23,26,27	1.27	3 (13%)	33,38,41	2.82	10 (30%)
1	PSU	A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.15	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	A	1835	1	23,26,27	1.36	4 (17%)	33,38,41	2.24	7 (21%)
1	6MZ	A	2030	60,1	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
34	MA6	a	1518	34	23,26,27	1.77	5 (21%)	33,38,41	2.37	11 (33%)
1	1MG	A	745	1	23,26,27	1.41	3 (13%)	33,39,42	2.00	7 (21%)
1	7MG	A	2069	1	23,26,27	1.46	3 (13%)	27,39,42	2.52	11 (40%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.50	2 (10%)
57	5MU	y	54	57	19,22,23	1.47	4 (21%)	27,32,35	2.04	8 (29%)
34	2MG	a	1516	34	23,26,27	1.26	4 (17%)	33,38,41	2.33	10 (30%)
1	6MZ	A	1618	1	22,25,26	1.53	4 (18%)	29,36,39	2.30	11 (37%)
1	5MU	A	1939	1	19,22,23	1.47	4 (21%)	27,32,35	2.10	8 (29%)
1	5MC	A	1962	1	19,22,23	2.00	2 (10%)	26,32,35	1.52	4 (15%)
34	MA6	a	1519	34	23,26,27	1.73	5 (21%)	33,38,41	2.49	16 (48%)
55	PSU	v	55	55	18,21,22	1.37	3 (16%)	21,30,33	2.00	4 (19%)
55	4SU	v	7	55	18,21,22	1.81	4 (22%)	25,30,33	2.34	6 (24%)
1	PSU	A	1917	1	18,21,22	1.44	2 (11%)	21,30,33	2.07	5 (23%)
1	OMC	A	2498	60,1	19,22,23	0.86	0	25,31,34	1.25	2 (8%)
55	4SU	w	8	55	18,21,22	1.82	5 (27%)	25,30,33	2.26	6 (24%)
55	PSU	w	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.07	5 (23%)
34	5MC	a	967	34	19,22,23	2.05	2 (10%)	26,32,35	1.51	4 (15%)
1	5MC	A	747	1	19,22,23	1.97	2 (10%)	26,32,35	1.59	4 (15%)
57	PSU	y	39	57	18,21,22	1.41	2 (11%)	21,30,33	2.00	4 (19%)
1	OMU	A	2552	1	19,22,23	1.30	3 (15%)	25,31,34	2.03	8 (32%)
55	H2U	v	20	55,60	18,21,22	0.83	1 (5%)	19,30,33	1.57	3 (15%)

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	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2604	60,1	-	0/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
1	PSU	A	746	60,1	-	1/7/25/26	0/2/2/2
34	7MG	a	527	34,60	-	2/7/37/38	0/3/3/3
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
57	MIA	y	37	57	-	4/15/33/34	0/3/3/3
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
34	PSU	a	516	34	-	3/7/25/26	0/2/2/2
1	OMG	A	2251	55,1	-	0/9/27/28	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	2MA	A	2503	60,1	-	2/7/25/26	0/3/3/3
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	2MG	A	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
57	PSU	y	55	57	-	2/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/9/27/28	0/3/3/3
55	H2U	w	20	55	-	2/7/38/39	0/2/2/2
34	5MC	a	1407	34	-	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	2MG	a	1207	34	-	2/9/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
1	6MZ	A	2030	60,1	-	3/9/27/28	0/3/3/3
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
1	1MG	A	745	1	-	0/7/25/26	0/3/3/3
1	7MG	A	2069	1	-	2/7/37/38	0/3/3/3
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3
1	6MZ	A	1618	1	-	5/9/27/28	0/3/3/3
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	4/11/29/30	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	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	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	OMC	A	2498	60,1	-	1/9/27/28	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	2/9/27/28	0/2/2/2
55	H2U	v	20	55,60	-	0/7/38/39	0/2/2/2

The worst 5 of 157 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.59	1.66	1.43
1	A	1915	3TD	C6-C5	15.85	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.27	1.34	1.53
1	A	1915	3TD	C2-N1	8.55	1.47	1.37
34	a	967	5MC	C5-C4	7.75	1.50	1.44

The worst 5 of 336 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	1207	2MG	C2-N3-C4	8.47	122.60	112.00
34	a	527	7MG	N9-C4-N3	8.41	137.79	125.46
34	a	966	2MG	C2-N3-C4	8.32	122.41	112.00
57	y	37	MIA	C5-C4-N3	-8.20	118.54	127.18
57	y	46	7MG	N9-C4-N3	8.18	137.45	125.46

There are no chirality outliers.

5 of 83 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1618	6MZ	C5-C6-N6-C9
1	A	1618	6MZ	N1-C6-N6-C9
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	O4'-C1'-C5-C6
1	A	1915	3TD	C3'-C4'-C5'-O5'

There are no ring outliers.

8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a	1498	UR3	1	0
1	A	1915	3TD	1	0
34	a	516	PSU	1	0
55	w	20	H2U	1	0
1	A	2504	PSU	1	0
1	A	2030	6MZ	4	0
1	A	1618	6MZ	8	0
1	A	2498	OMC	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1488 ligands modelled in this entry, 1485 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	-	33,34,34	1.21	3 (9%)	50,54,54	1.75	8 (16%)
62	PHE	z	401	-	10,11,12	0.46	0	8,13,15	0.16	0
59	FME	A	3001	-	8,9,10	0.51	0	8,9,11	0.97	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	-	-	1/22/38/38	0/3/3/3
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
59	FME	A	3001	-	-	1/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	C5-C4	3.30	1.47	1.38
63	z	402	GTP	C5-N7	-2.11	1.34	1.39
63	z	402	GTP	C6-N1	-2.06	1.35	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GTP	C5-C4-N3	-6.16	118.58	128.39
63	z	402	GTP	C2-N3-C4	5.19	121.24	112.30
63	z	402	GTP	N9-C4-N3	4.62	135.19	125.95
63	z	402	GTP	C6-C5-N7	3.31	136.31	130.29
63	z	402	GTP	C4-C5-N7	-2.60	106.55	110.67

There are no chirality outliers.

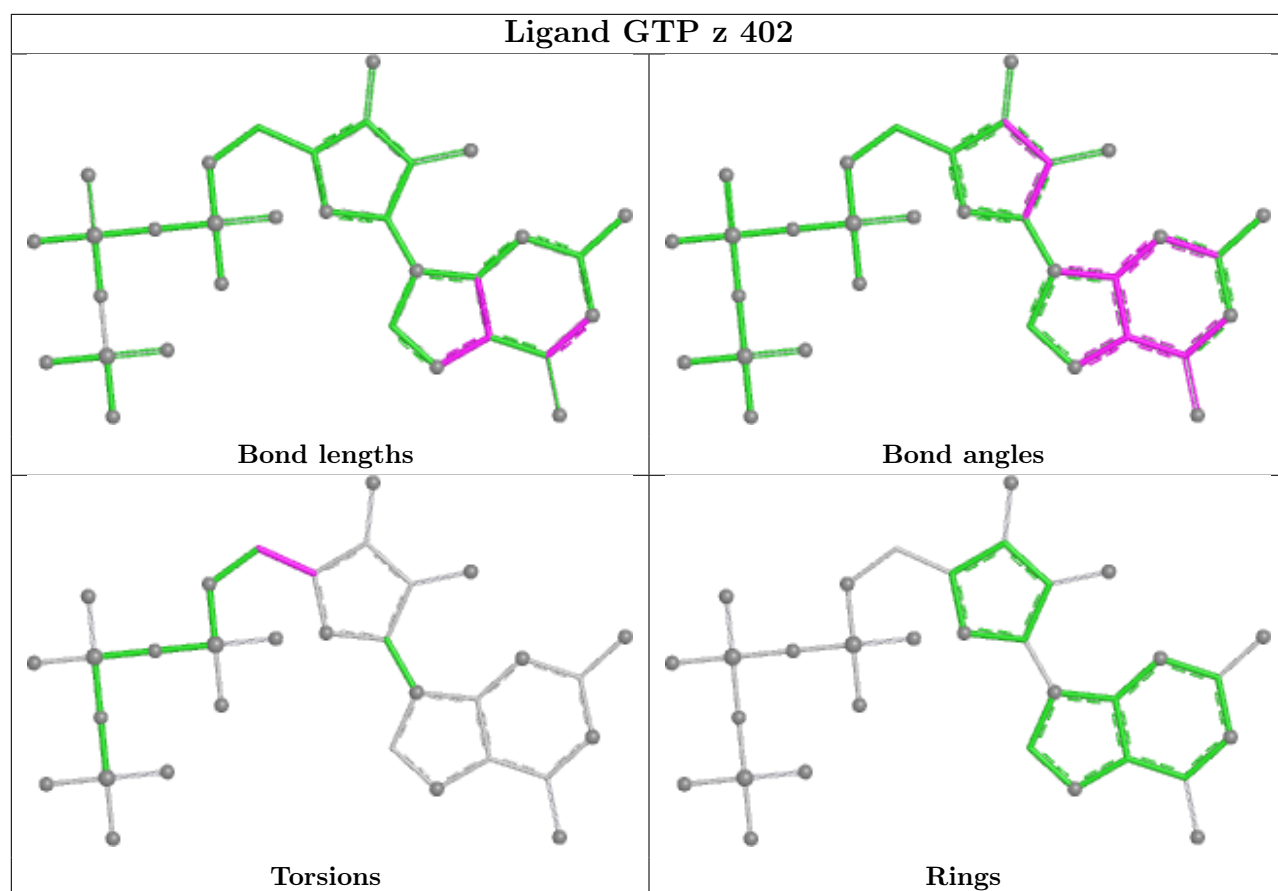
All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
59	A	3001	FME	O-C-CA-CB
62	z	401	PHE	O-C-CA-CB
63	z	402	GTP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

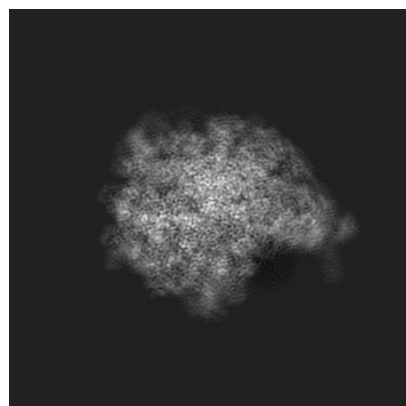
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8826. These allow visual inspection of the internal detail of the map and identification of artifacts.

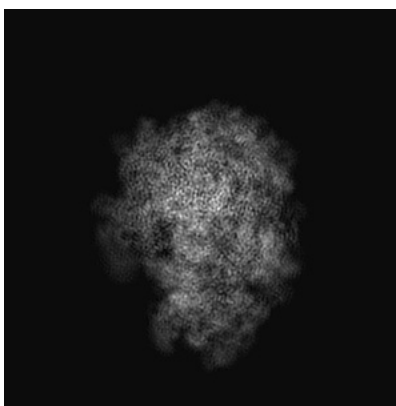
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

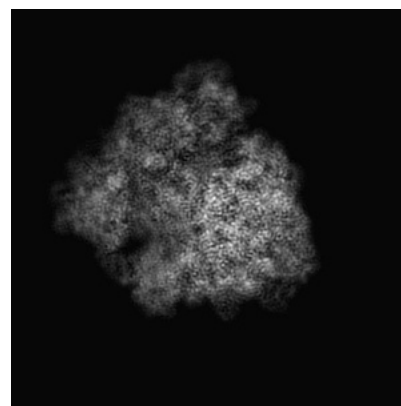
6.1.1 Primary map



X

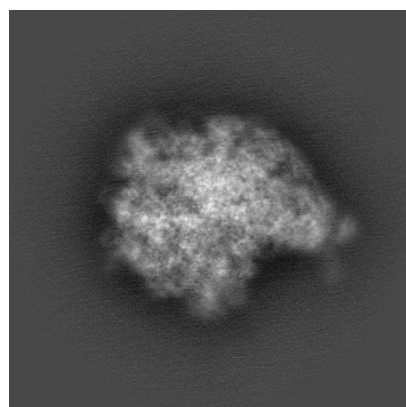


Y

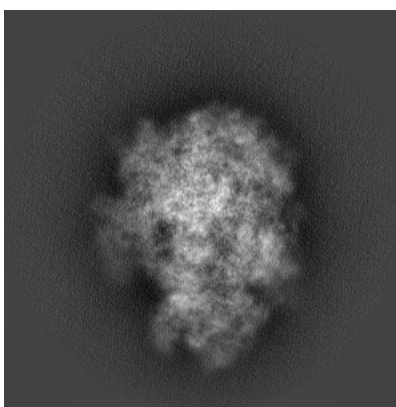


Z

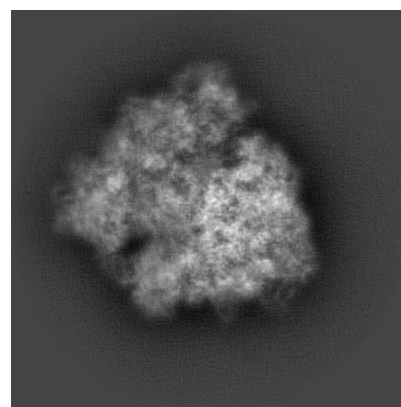
6.1.2 Raw map



X



Y

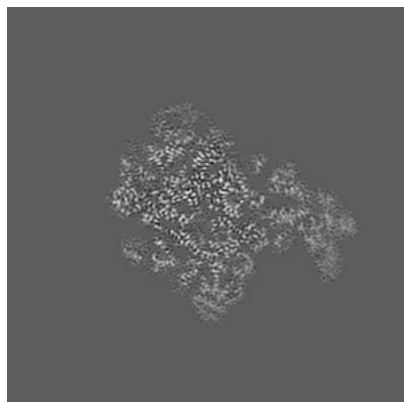


Z

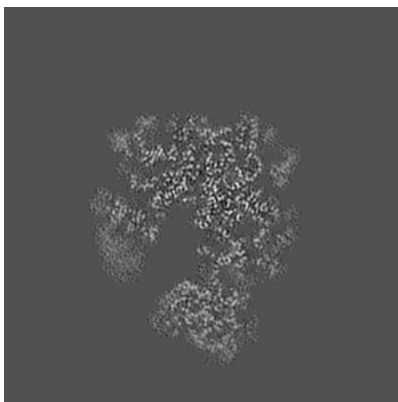
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

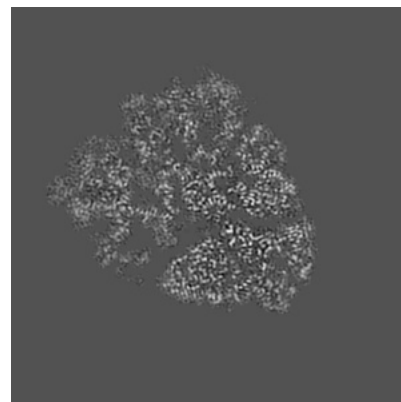
6.2.1 Primary map



X Index: 199

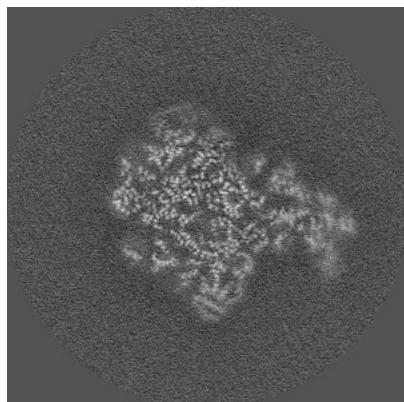


Y Index: 199

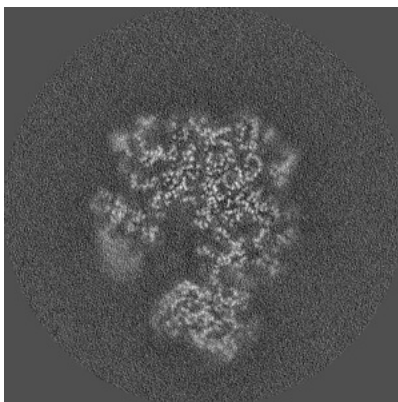


Z Index: 199

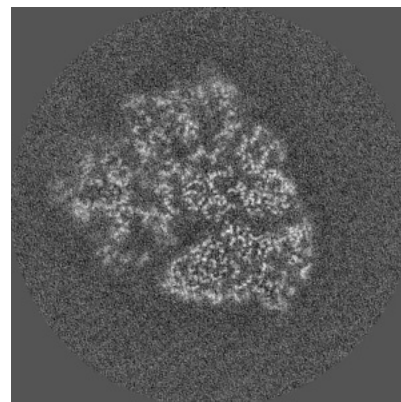
6.2.2 Raw map



X Index: 199



Y Index: 199

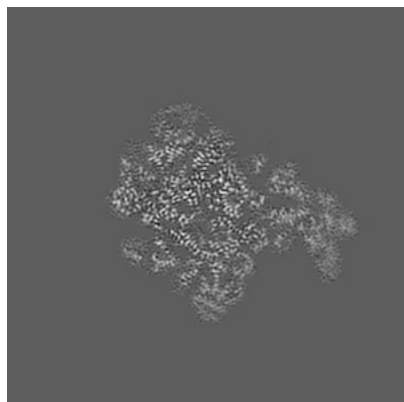


Z Index: 199

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

6.3 Largest variance slices [i](#)

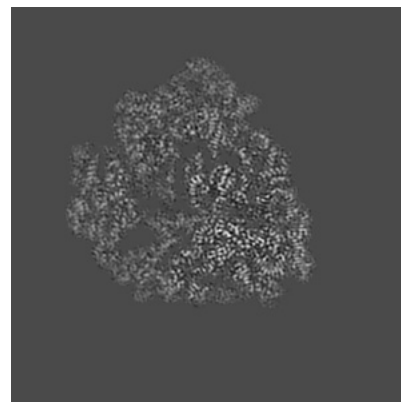
6.3.1 Primary map



X Index: 199

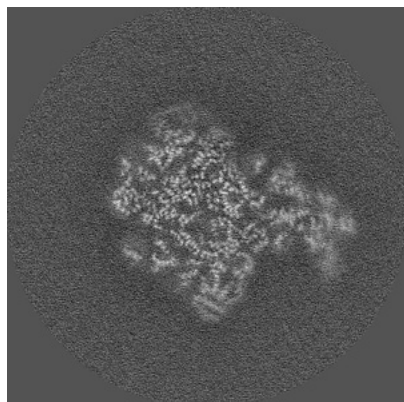


Y Index: 207

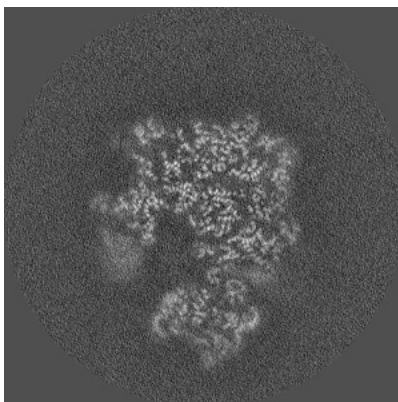


Z Index: 190

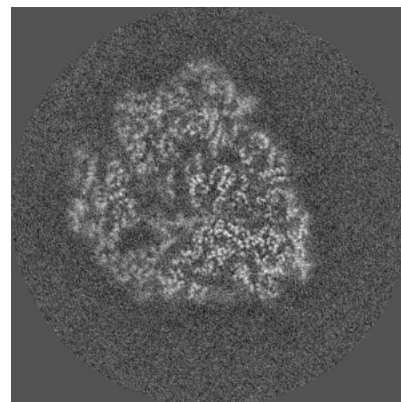
6.3.2 Raw map



X Index: 199



Y Index: 207

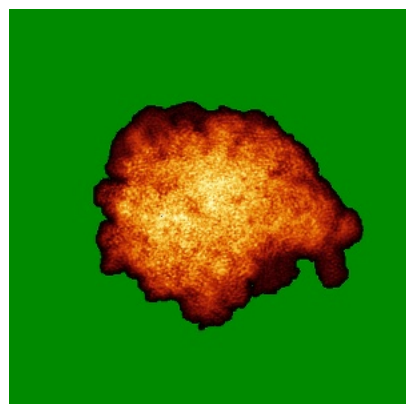


Z Index: 190

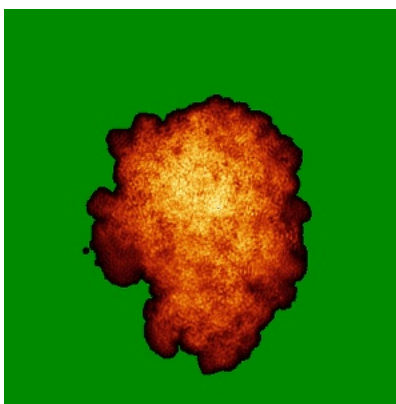
The images above show the largest variance slices of the map in three orthogonal directions.

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

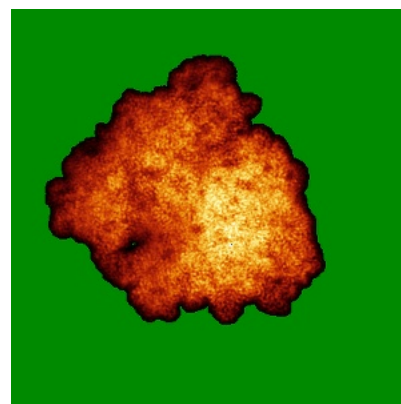
6.4.1 Primary map



X

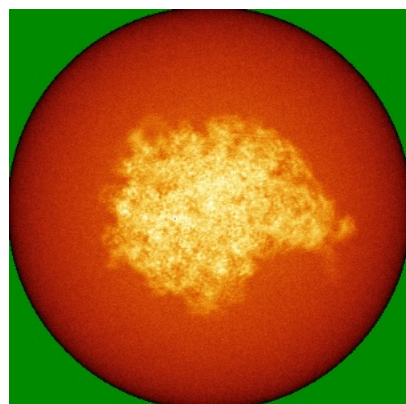


Y

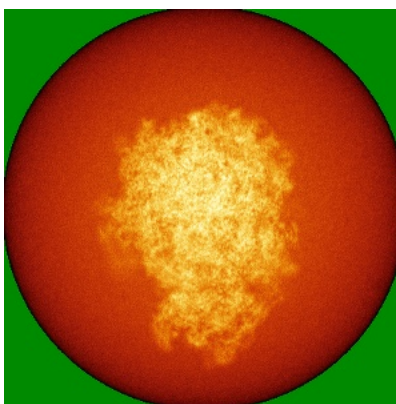


Z

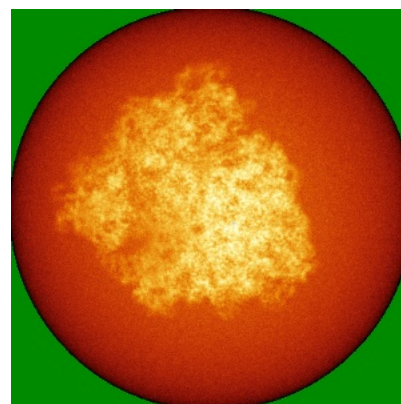
6.4.2 Raw map



X



Y

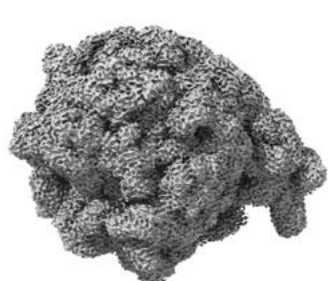


Z

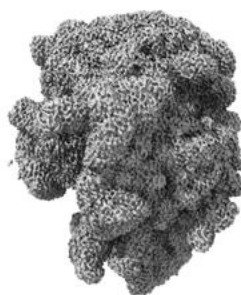
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

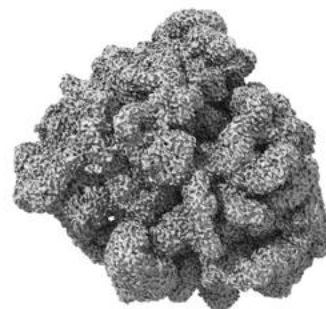
6.5.1 Primary map



X



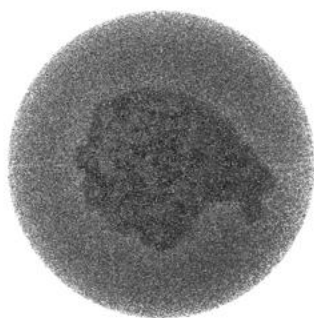
Y



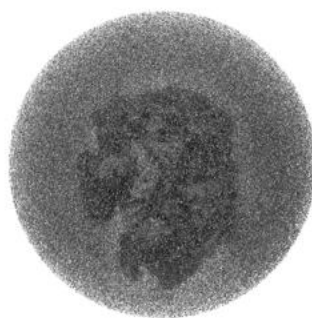
Z

The images above show the 3D surface view of the map at the recommended contour level 0.00371. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

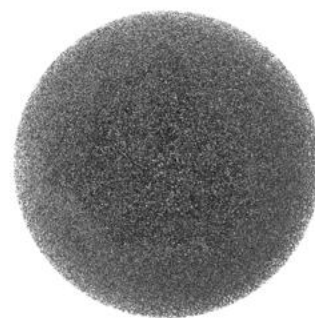
6.5.2 Raw map



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.

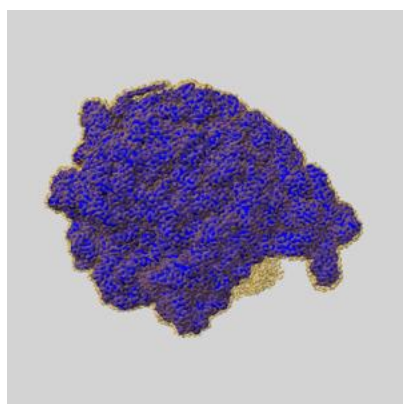
6.6 Mask visualisation [i](#)

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

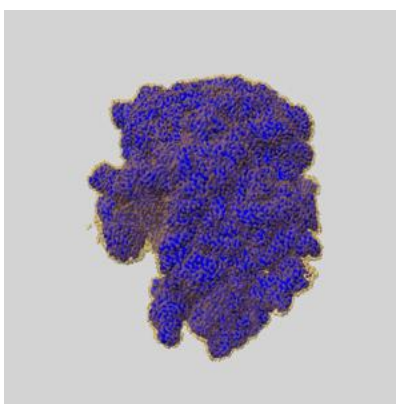
A mask typically either:

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

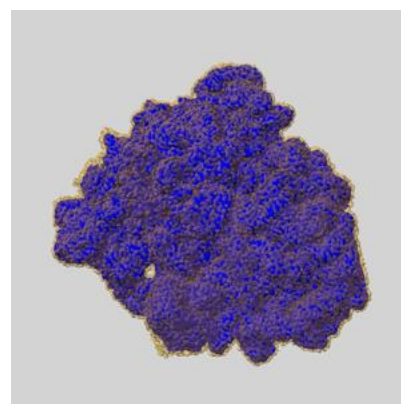
6.6.1 emd_8826_msk_1.map [i](#)



X



Y

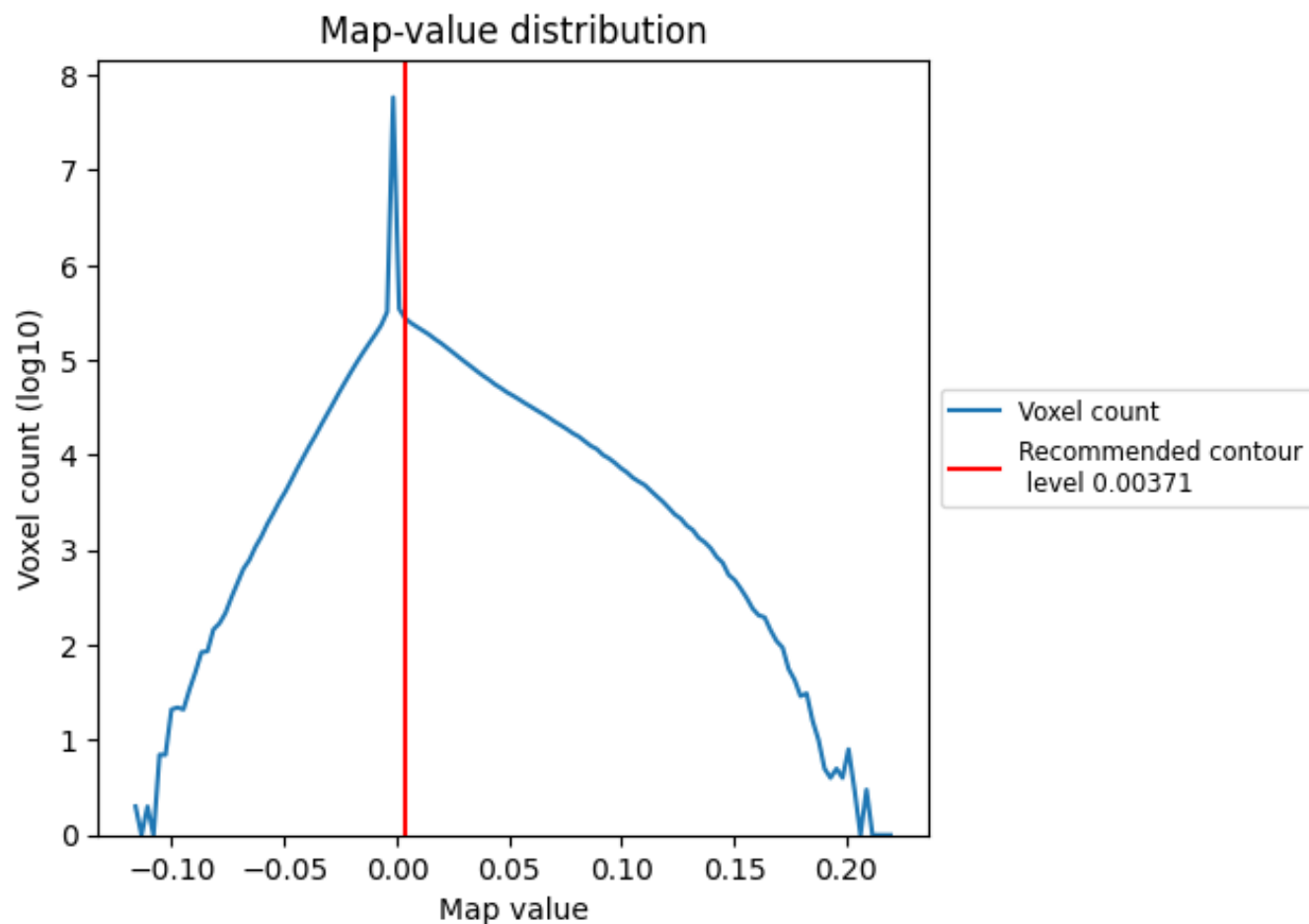


Z

7 Map analysis [i](#)

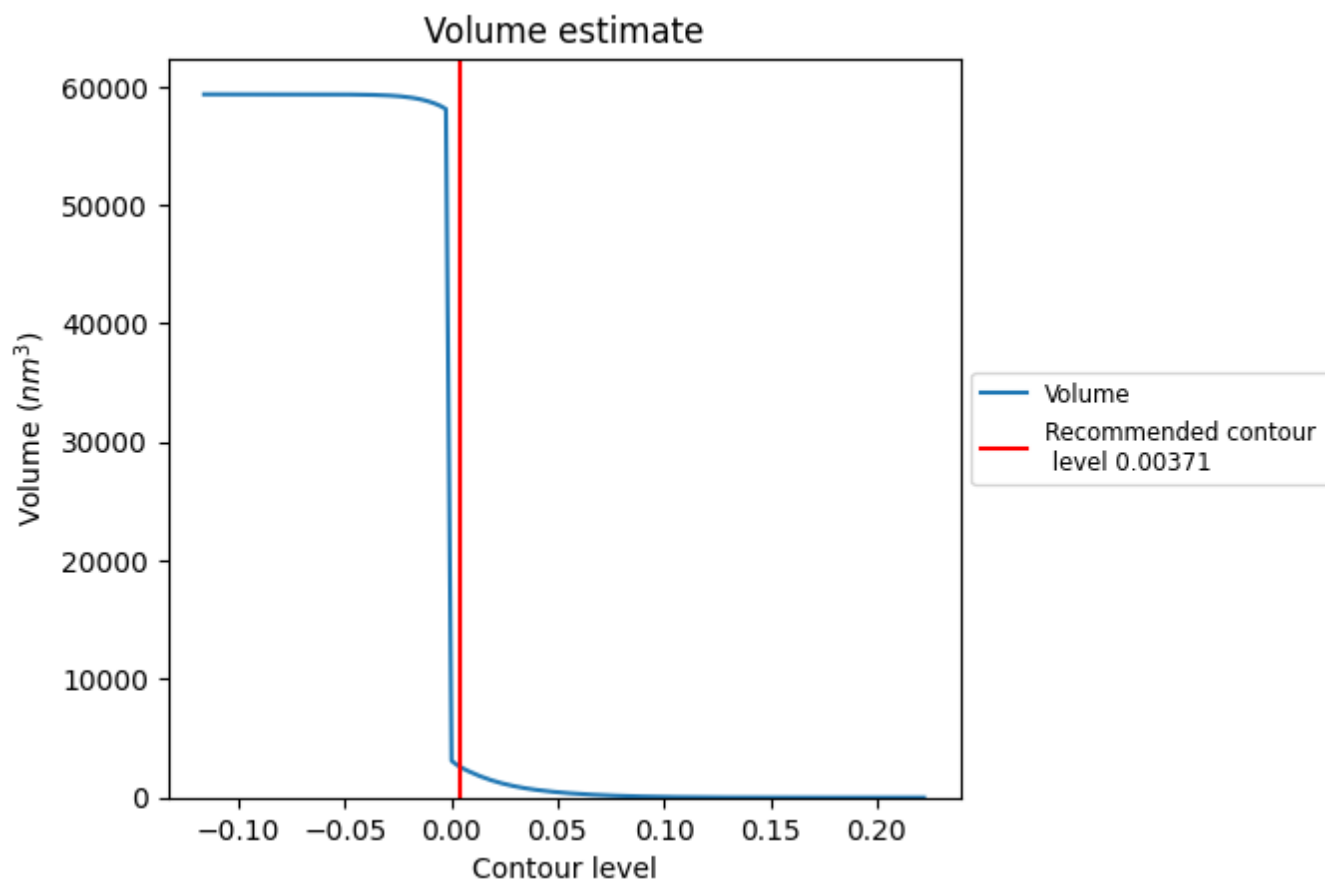
This section contains the results of statistical analysis of the map.

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.

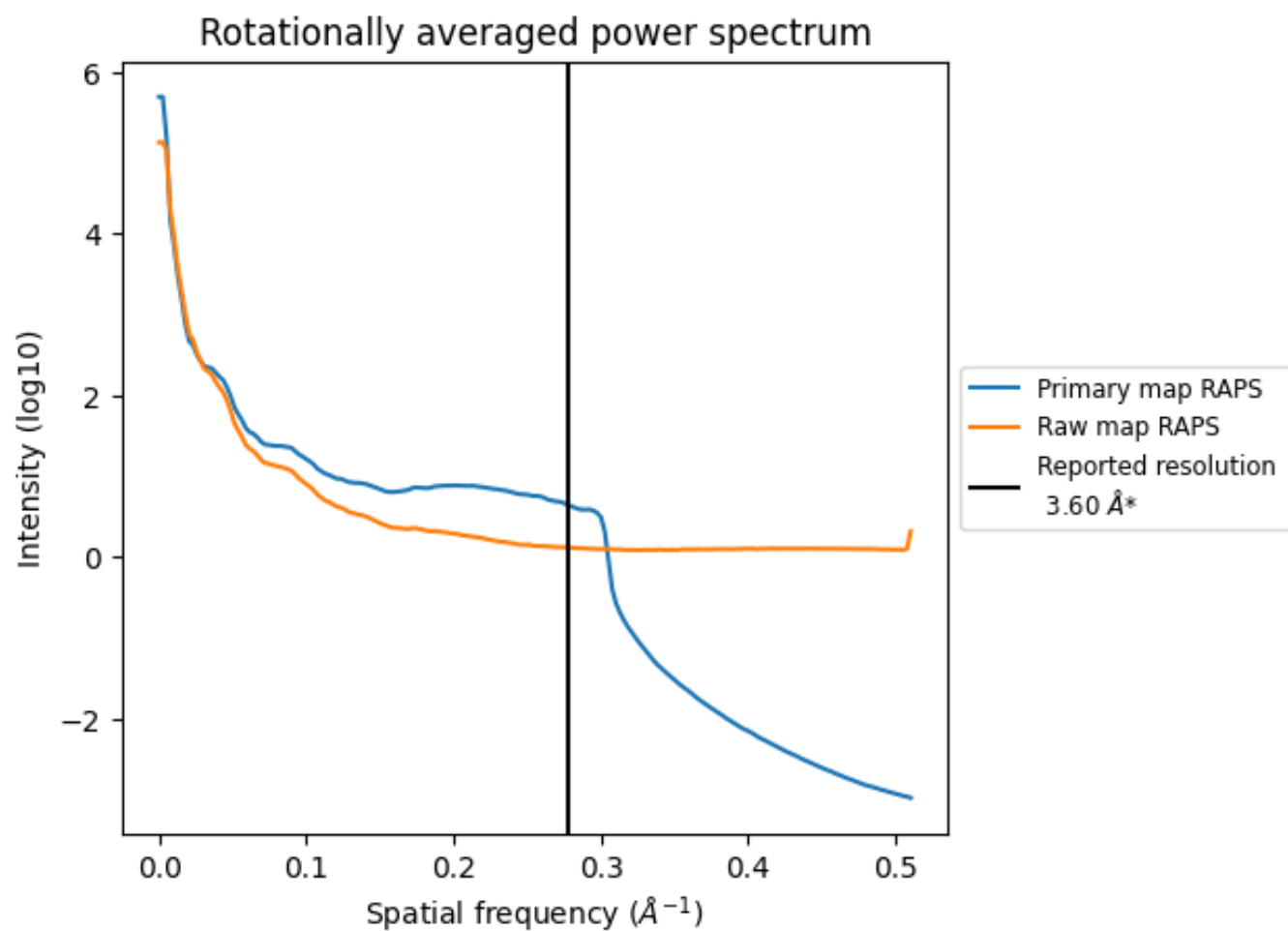
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2650 nm³; this corresponds to an approximate mass of 2393 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 ⓘ

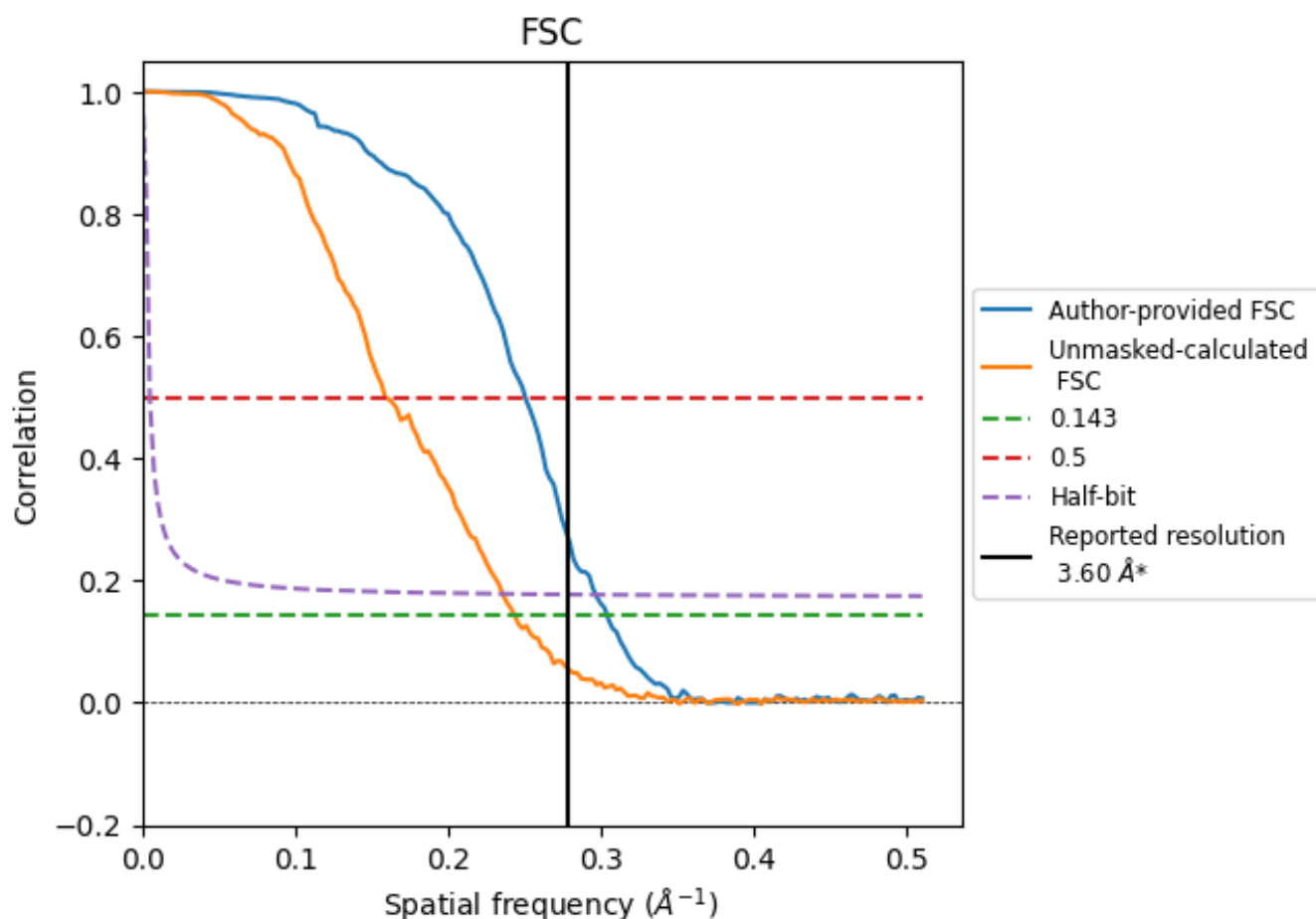


*Reported resolution corresponds to spatial frequency of $0.278 \text{ \AA}^{-1}$

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

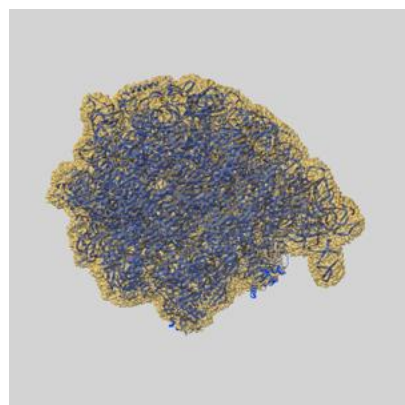
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.29	3.99	3.37
Unmasked-calculated*	4.10	6.29	4.24

*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 4.10 differs from the reported value 3.6 by more than 10 %

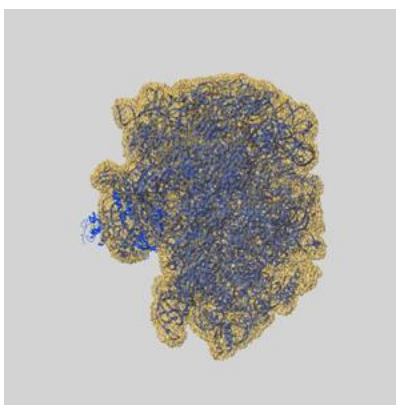
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8826 and PDB model 5WF0. Per-residue inclusion information can be found in section 3 on page 20.

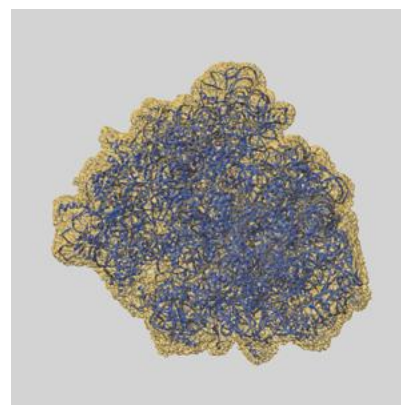
9.1 Map-model overlay [i](#)



X



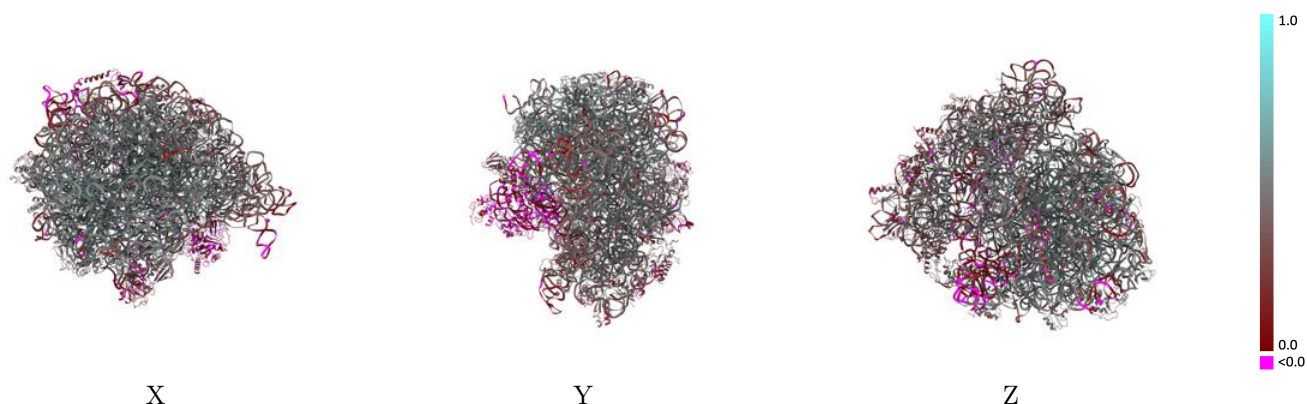
Y



Z

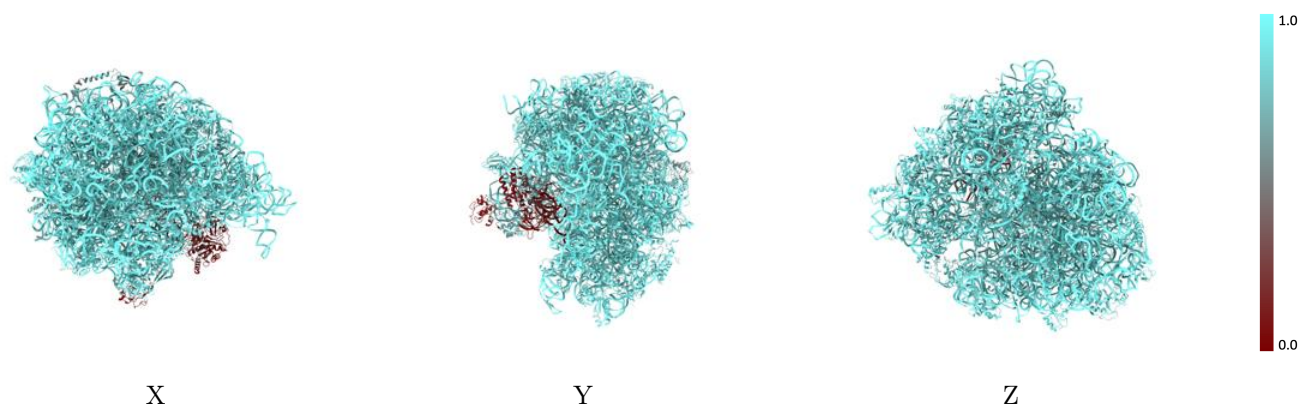
The images above show the 3D surface view of the map at the recommended contour level 0.00371 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



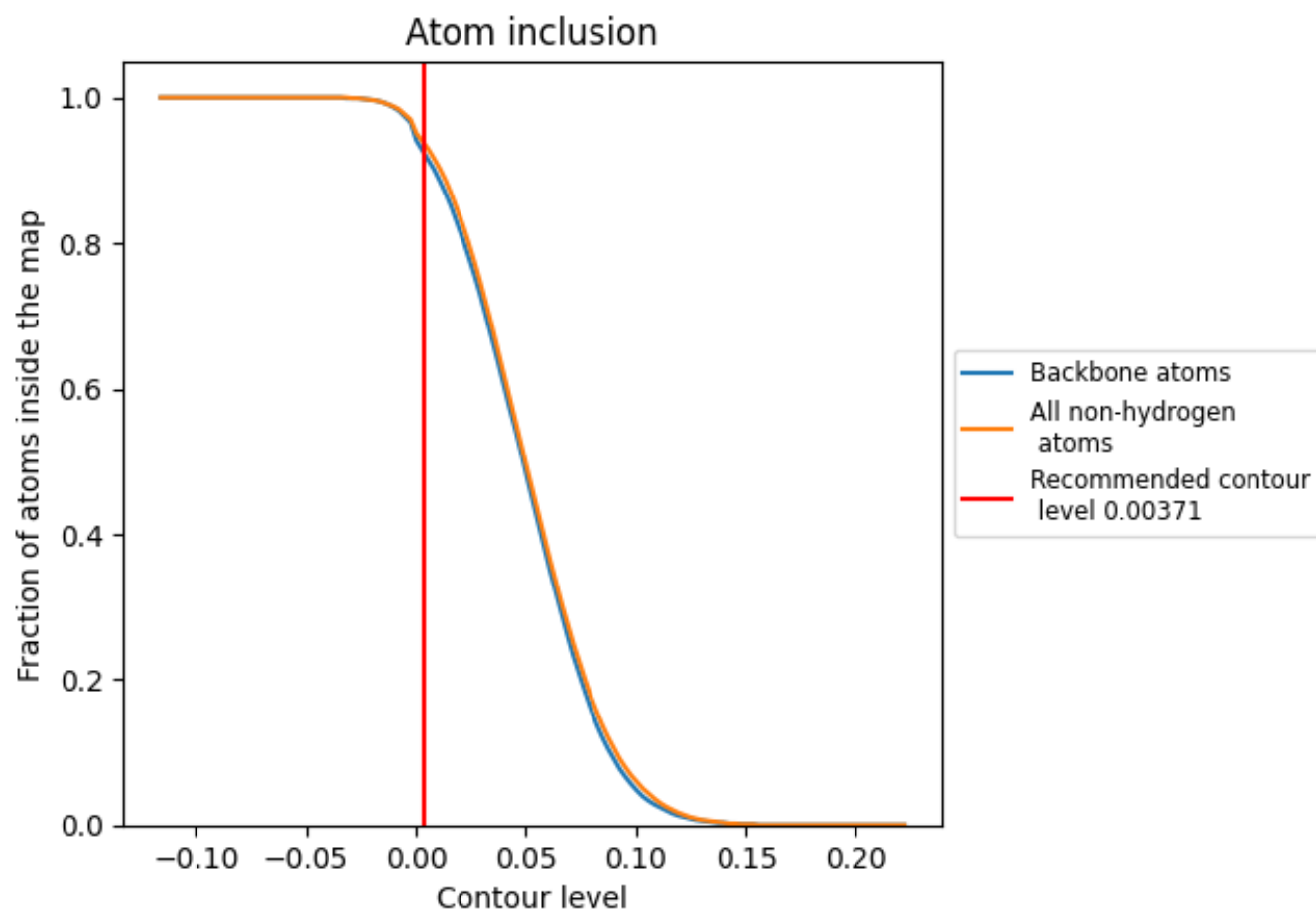
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00371).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 94% 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 (0.00371) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9370	 0.4130
0	 0.9550	 0.4680
1	 0.9630	 0.4550
2	 0.9800	 0.5340
3	 0.9740	 0.5360
4	 0.9690	 0.5040
5	 0.1960	 0.0000
6	 0.9060	 0.2600
A	 0.9840	 0.4570
B	 0.9920	 0.4280
C	 0.9600	 0.5020
D	 0.9620	 0.4850
E	 0.9550	 0.4560
F	 0.9420	 0.3720
G	 0.9410	 0.3460
H	 0.7500	 0.1730
I	 0.6790	 0.0210
J	 0.9630	 0.4730
K	 0.9550	 0.4780
L	 0.9670	 0.4740
M	 0.9640	 0.4860
N	 0.9730	 0.5000
O	 0.9700	 0.4120
P	 0.9610	 0.4690
Q	 0.9780	 0.5090
R	 0.9550	 0.4510
S	 0.9640	 0.4960
T	 0.9610	 0.4470
U	 0.9750	 0.4220
V	 0.9420	 0.4060
W	 0.9590	 0.5090
X	 0.9690	 0.4850
Y	 0.9340	 0.3890
Z	 0.9670	 0.4970
a	 0.9880	 0.4270



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	 0.9110	 0.3010
c	 0.9370	 0.3800
d	 0.9380	 0.3590
e	 0.9590	 0.4440
f	 0.9370	 0.3760
g	 0.9200	 0.3330
h	 0.9510	 0.4390
i	 0.9350	 0.3430
j	 0.9330	 0.3240
k	 0.9550	 0.4270
l	 0.9380	 0.4240
m	 0.9340	 0.3490
n	 0.9490	 0.3720
o	 0.9570	 0.4110
p	 0.9300	 0.3780
q	 0.9380	 0.4060
r	 0.9260	 0.3890
s	 0.9440	 0.3650
t	 0.9480	 0.3790
u	 0.8260	 0.2460
v	 0.9690	 0.3980
w	 0.8240	 0.0890
x	 0.9250	 0.3220
y	 0.1160	 -0.0070
z	 0.1170	 -0.0010