



wwPDB EM Validation Summary Report ⓘ

Sep 15, 2026 – 11:07 PM EDT

PDB ID : 5WE6 / pdb_00005we6
EMDB ID : EMD-8815
Title : 70S ribosome-EF-Tu H84A complex with GTP and cognate tRNA
Authors : Fislage, M.; Frank, J.
Deposited on : 2017-07-07
Resolution : 3.40 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ 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:

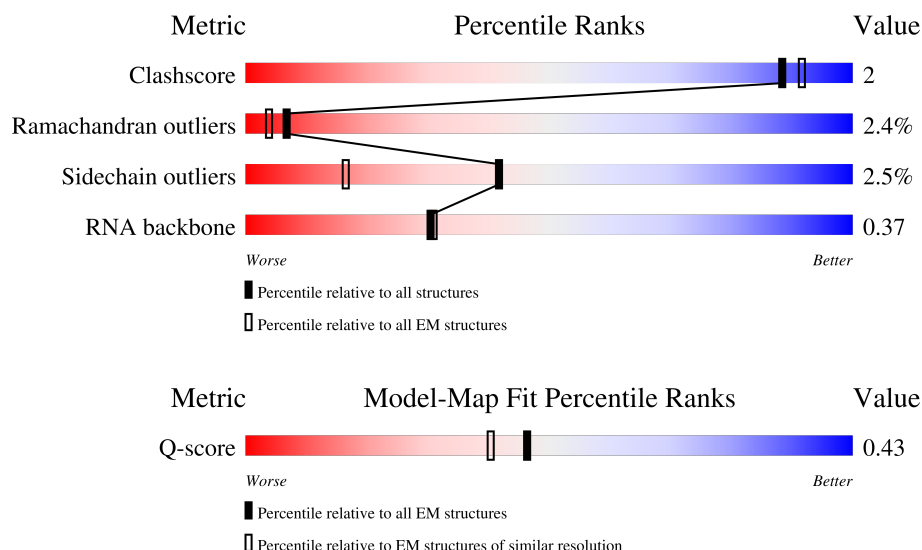
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

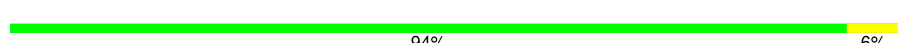
The reported resolution of this entry is 3.40 Å.

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



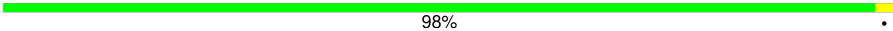
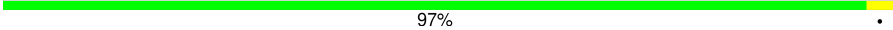
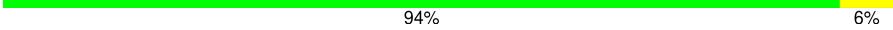
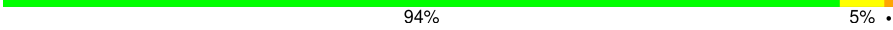
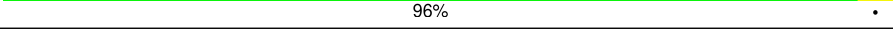
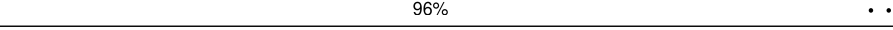
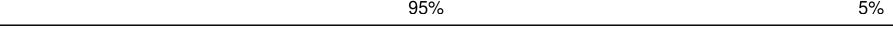
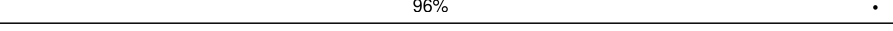
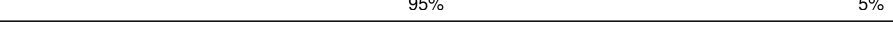
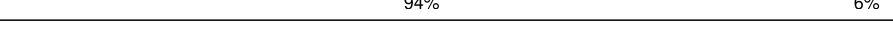
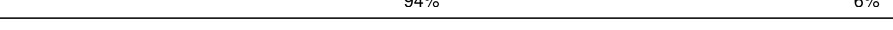
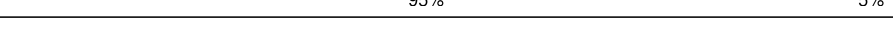
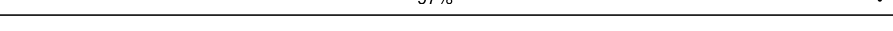
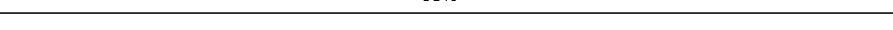
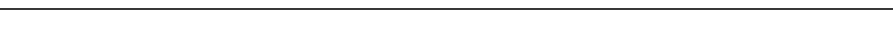
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	

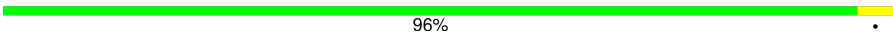
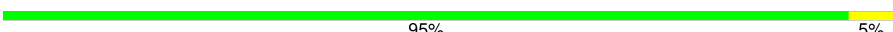
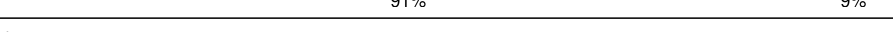
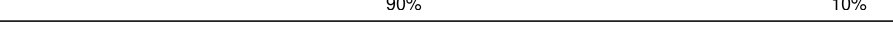
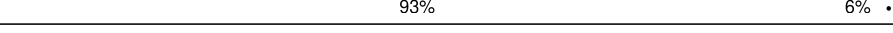
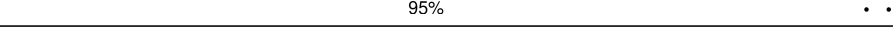
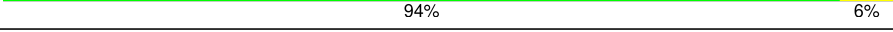
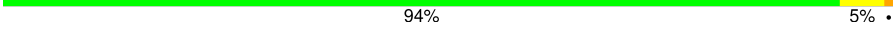
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Mol	Chain	Length	Quality of chain
4	D	208	 95% .
5	E	200	 92% 8% .
6	F	177	 98% ..
7	G	174	 97% .
8	H	149	 10% 94% 6%
9	I	141	 16% 94% 5% .
10	J	141	 92% 8%
11	K	122	 88% 10% .
12	L	142	 . 90% 10%
13	M	136	 96% .
14	N	119	 96% ..
15	O	116	 95% 5%
16	P	114	 . 96% .
17	Q	115	 95% 5%
18	R	102	 94% 6%
19	S	109	 94% 6%
20	T	92	 95% 5%
21	U	102	 97% .
22	V	92	 98% .
23	W	75	 95% 5%
24	X	77	 97% .
25	Y	60	 98% .
26	Z	56	 95% . .
27	0	55	 95% 5%
28	1	51	 96% .

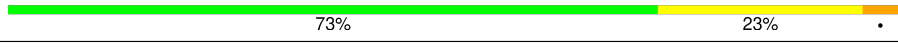
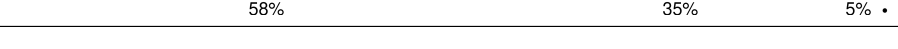
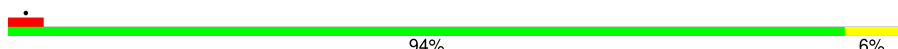
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Mol	Chain	Length	Quality of chain
29	2	45	
30	3	64	
31	4	38	
32	5	131	
33	6	66	
34	a	1539	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	114	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	

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Mol	Chain	Length	Quality of chain
54	u	65	
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	1618	-	-	X	-
1	6MZ	A	2030	-	-	X	-

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 153233 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
			62278	27789	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 731469900
A	1723	G	A	conflict	GB 731469900
A	1847	G	A	conflict	GB 731469900

- 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	-	conflict	GB 1174070234

- 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	142	Total	C	N	O	S	0	0
			1035	644	205	185	1		

- 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.

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	1539	Total	C	N	O	P	0	0
			33028	14738	6052	10699	1539		

- 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	114	Total	C	N	O	S	0	0
			883	546	178	156	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 P0AG59

- 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	42	85	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		

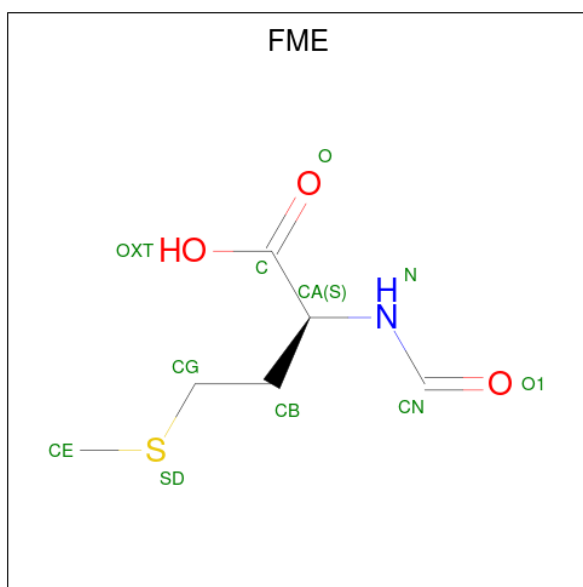
- Molecule 58 is a protein called Elongation factor Tu 2.

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

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	47	ASN	ASP	conflict	UNP P0CE48
z	84	ALA	HIS	engineered mutation	UNP P0CE48

- 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	404	Total	Mg	0
			404	404	
60	B	6	Total	Mg	0
			6	6	
60	C	2	Total	Mg	0
			2	2	
60	D	1	Total	Mg	0
			1	1	
60	E	1	Total	Mg	0
			1	1	
60	J	1	Total	Mg	0
			1	1	
60	L	1	Total	Mg	0
			1	1	
60	N	3	Total	Mg	0
			3	3	
60	O	1	Total	Mg	0
			1	1	
60	S	1	Total	Mg	0
			1	1	
60	T	2	Total	Mg	0
			2	2	

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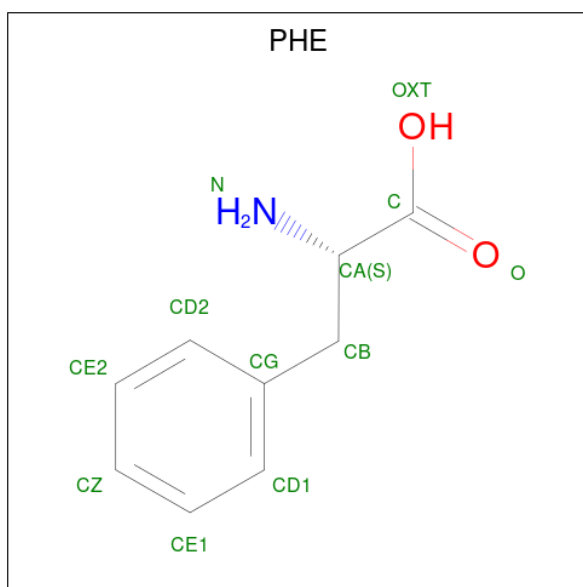
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Mol	Chain	Residues	Atoms		AltConf
60	0	3	Total 3	Mg 3	0
60	3	2	Total 2	Mg 2	0
60	4	1	Total 1	Mg 1	0
60	a	221	Total 221	Mg 221	0
60	e	1	Total 1	Mg 1	0
60	i	1	Total 1	Mg 1	0
60	t	1	Total 1	Mg 1	0
60	u	1	Total 1	Mg 1	0
60	v	2	Total 2	Mg 2	0
60	y	4	Total 4	Mg 4	0
60	z	2	Total 2	Mg 2	0

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

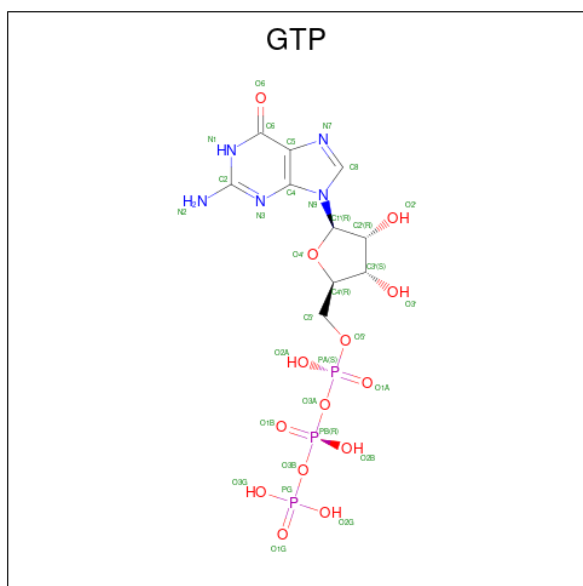
Mol	Chain	Residues	Atoms		AltConf
61	A	7	Total 7	K 7	0
61	v	1	Total 1	K 1	0

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



Mol	Chain	Residues	Atoms				AltConf
62	y	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	

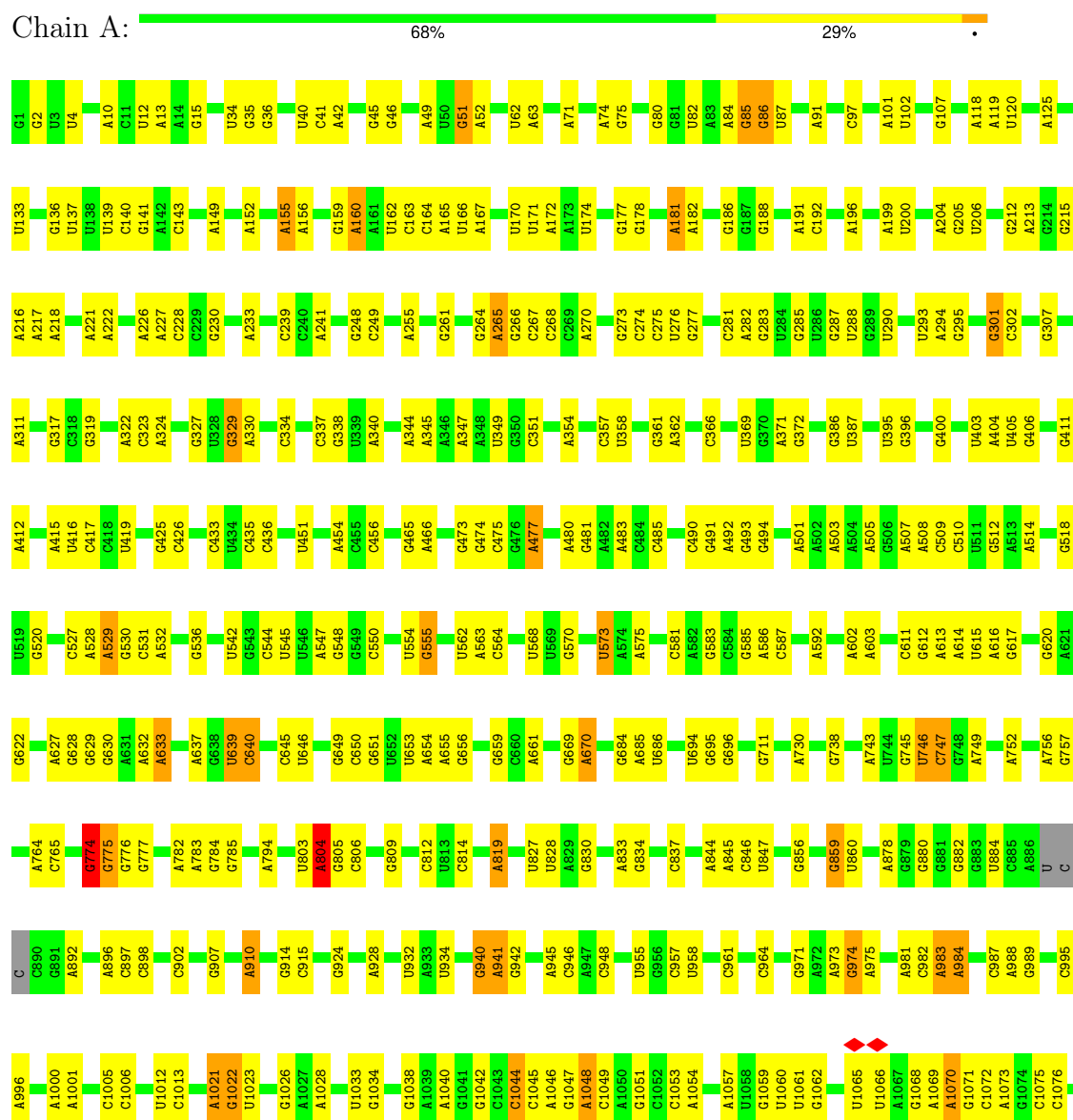
- Molecule 64 is water.

Mol	Chain	Residues	Atoms		AltConf
64	A	83	Total 83	O 83	0
64	B	3	Total 3	O 3	0
64	C	3	Total 3	O 3	0
64	E	1	Total 1	O 1	0
64	L	1	Total 1	O 1	0
64	Q	1	Total 1	O 1	0
64	U	1	Total 1	O 1	0
64	W	3	Total 3	O 3	0
64	X	2	Total 2	O 2	0
64	Z	2	Total 2	O 2	0
64	0	1	Total 1	O 1	0
64	2	1	Total 1	O 1	0
64	a	46	Total 46	O 46	0
64	k	1	Total 1	O 1	0
64	q	2	Total 2	O 2	0
64	s	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



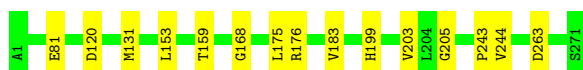
G2715	G2553	G2445	G2332	A2212	C2103	G1992	G1857	G1725	A1593	G1482	A1321	C1196	C1079
G2716	U2554	G2446	A2333	U2219	C2104	U1993	A1858	G1726	U1594	G1483	A1322	G1197	A1084
U2720	A2566	G2447	U2334	U2220	U2105	C1997	G1867	A1727	C1607	U1485	A1328	U1203	A1085
A2721	G2567	A2448	A2336	A2225	U2106	G2004	C1868	C1728	A1608	U1486	G1329	A1204	A1086
G2722	U2568	U2449	A2336	G2225	G2110	A2013	C1870	U1730	A1609	U1487	G1331	A1205	A1087
A2726	A2572	U2457	C2342	G2238	G2111	A2013	A1871	G1731	A1610	G1206	G1341	G1207	A1088
A2733	C2573	G2464	G2345	G2239	G2112	A2020	C1874	G1738	G1613	C1208	G1345	C1208	A1089
U2743	G2578	A2469	C2350	U2243	G2116	A2020	C1874	G1739	A1614	U1209	G1346	U1209	A1090
G2744	C2579	G2470	U2356	G2250	A2117	U2022	U1882	U1740	A1615	G1210	G1351	U1211	U1097
A2748	U2585	U2475	G2357	G2251	A2118	C2023	U1883	U1741	A1616	G1212	U1352	G1212	C1104
A2749	U2586	A2476	A2358	U2262	G2120	G2029	G1884	U1742	C1617	G1218	A1365	U1218	U1106
A2750	G2587	G2477	A2359	U2263	G2121	A2031	A1890	A1755	G1619	U1219	A1366	U1219	G1106
G2751	U2588	A2478	G2360	C2264	U2122	G2032	C1895	U1758	G1622	G1227	A1367	G1227	G1110
C2752	G2602	C2480	G2361	C2264	G2127	A2033	C1895	C1764	G1627	G1232	G1370	G1232	U1112
A2753	G2603	A2481	A2377	A2268	G2128	G2038	C1905	A1773	G1633	G1236	A1378	A1237	U1113
U2754	U2604	G2484	A2378	A2273	C2129	U2039	G1906	G1776	C1639	G1238	U1379	G1238	C1117
A2758	U2605	C2485	G2383	A2274	U2130	G2046	A1913	U1779	C1646	A1244	A1383	G1245	G1124
A2764	G2608	U2491	U2384	C2275	U2131	G2046	C1914	U1780	U1647	G1246	A1383	G1246	G1124
A2765	U2609	G2494	A2386	A2278	U2132	G2049	3TD1915	U1781	U1648	A1247	A1383	A1247	U1130
A2778	U2613	G2499	A2387	G2279	U2133	G2049	A1916	U1782	G1649	G1248	G1399	G1248	G1131
A2781	A2614	C2498	A2388	G2282	G2140	C2055	U1917	A1783	G1659	U1249	G1416	G1249	U1132
U2790	U2615	U2500	U2389	C2283	G2141	G2056	A1918	A1784	G1660	G1250	A1419	G1250	C1135
G2791	C2620	U2501	U2393	G2286	C2145	A2060	G1929	A1789	G1666	C1251	A1420	C1251	G1139
G2791	U2522	A2502	G2399	A2287	A2147	G2061	U1930	C1790	G1667	G1252	A1420	G1252	U1140
U2794	G2504	U2504	G2400	A2288	U2148	A2062	U1931	A1791	A1688	A1253	G1425	A1253	G1141
U2797	G2505	G2505	C2295	C2295	C2150	C2063	A1794	C1795	A1669	G1256	C1428	G1256	A1142
U2797	U2506	U2506	A2298	A2298	C2153	G2069	A1937	U1796	G1674	A1265	G1429	A1265	A1143
G2799	A2518	A2518	U2404	U2305	G2157	A2070	A1938	C1800	C1675	A1268	A1430	A1268	A1144
A2800	U2521	U2521	G2405	U2305	G2157	A2071	U1939	A1801	C1685	G1271	A1431	A1271	G1171
G2803	U2522	U2522	A2407	C2072	C2162	C2072	C1941	A1802	C1685	U1272	A1432	U1272	C1172
G2808	G2525	G2525	U2408	A2309	G2163	A2077	U1943	A1803	U1693	U1173	A1433	U1173	U1173
A2809	G2526	G2526	A2311	C2310	C2164	C2078	U1944	A1808	G1694	U1274	C1454	A1274	A1174
A2813	G2529	G2529	G2315	U2079	U2172	A2080	U1955	A1809	A1698	A1275	U1458	A1275	U1175
A2814	G2532	G2532	G2316	A2086	A2173	U2086	C1962	A1810	A1566	G1281	U1459	G1281	U1176
U2818	U2533	U2533	G2318	U2087	G2166	U2087	C1965	C1816	A1569	G1288	U1460	G1288	C1177
G2819	A2534	A2534	G2319	U2092	U2191	U2092	C1967	C1833	G1710	G1297	A1461	G1297	U1181
A2820	G2535	G2535	U2321	G2093	U2192	G2093	C1967	U1834	U1714	U1466	U1466	U1466	G1182
G2822	C2539	C2539	G2323	C2096	A2198	C2096	A1970	G1835	G1715	U1467	U1467	U1467	U1183
A2826	G2429	A2430	U2324	C2097	A2199	U2097	U1971	G1842	U1716	U1468	U1468	G1300	U1184
A2834	U2698	A2542	G2325	U2098	G2204	U2098	G1972	G1847	A1717	A1301	G1471	A1301	U1184
A2835	C2699	A2547	A2327	U2099	G2204	U2099	U1982	G1847	A1717	G1314	G1471	A1301	U1184
	C2710	U2552	A2328	A2101	U2210	G2100	U1982	A1853	G1721	G1475	G1475	G1314	A1189
	G2714		G2331	G2102	A2211	G2102	U1991		G1724	U1476	U1476	C1320	G1190



• Molecule 2: 5S rRNA



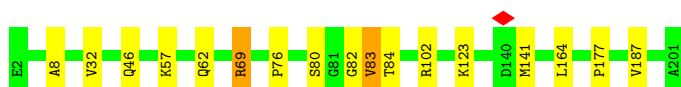
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3



• Molecule 5: 50S ribosomal protein L4



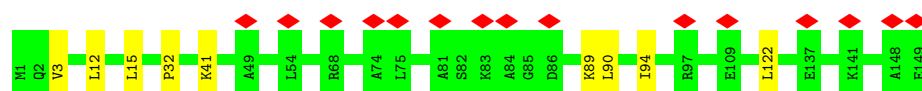
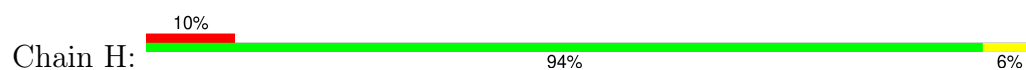
• Molecule 6: 50S ribosomal protein L5



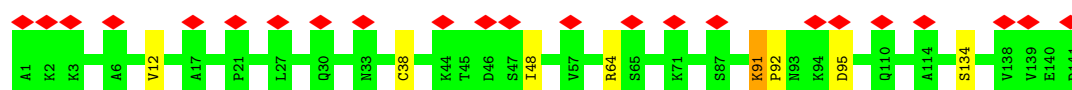
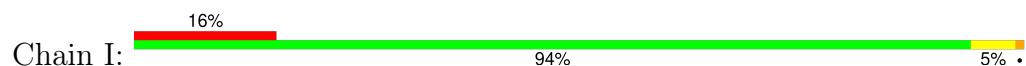
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L9



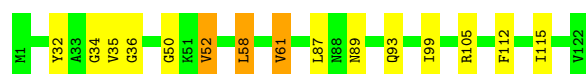
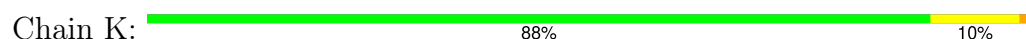
- Molecule 9: 50S ribosomal protein L11



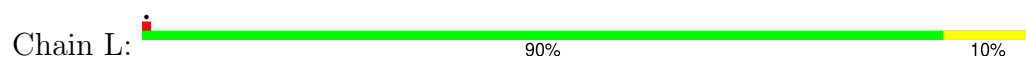
- Molecule 10: 50S ribosomal protein L13



- Molecule 11: 50S ribosomal protein L14



- Molecule 12: 50S ribosomal protein L15



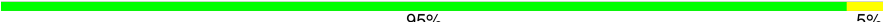
- Molecule 13: 50S ribosomal protein L16



- Molecule 14: 50S ribosomal protein L17



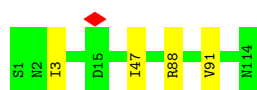
- Molecule 15: 50S ribosomal protein L18

Chain O:  95% 5%



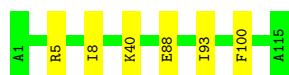
- Molecule 16: 50S ribosomal protein L19

Chain P:  96% 4%



- Molecule 17: 50S ribosomal protein L20

Chain Q:  95% 5%



- Molecule 18: 50S ribosomal protein L21

Chain R:  94% 6%



- Molecule 19: 50S ribosomal protein L22

Chain S:  94% 6%



- Molecule 20: 50S ribosomal protein L23

Chain T:  95% 5%

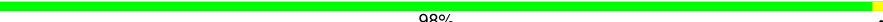


- Molecule 21: 50S ribosomal protein L24

Chain U:  97% 3%

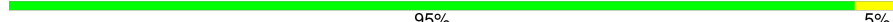


- Molecule 22: 50S ribosomal protein L25

Chain V:  98% .

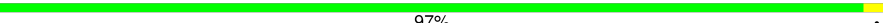


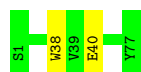
- Molecule 23: 50S ribosomal protein L27

Chain W:  95% 5%



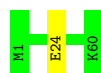
- Molecule 24: 50S ribosomal protein L28

Chain X:  97% .



- Molecule 25: 50S ribosomal protein L29

Chain Y:  98% .



- Molecule 26: 50S ribosomal protein L30

Chain Z:  95% . .

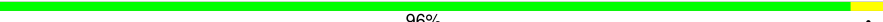


- Molecule 27: 50S ribosomal protein L32

Chain 0:  95% 5%

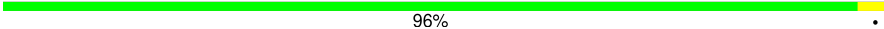


- Molecule 28: 50S ribosomal protein L33

Chain 1:  96% .

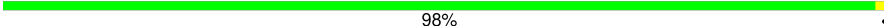


- Molecule 29: 50S ribosomal protein L34

Chain 2:  96%

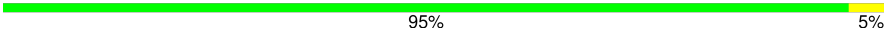


- Molecule 30: 50S ribosomal protein L35

Chain 3:  98%



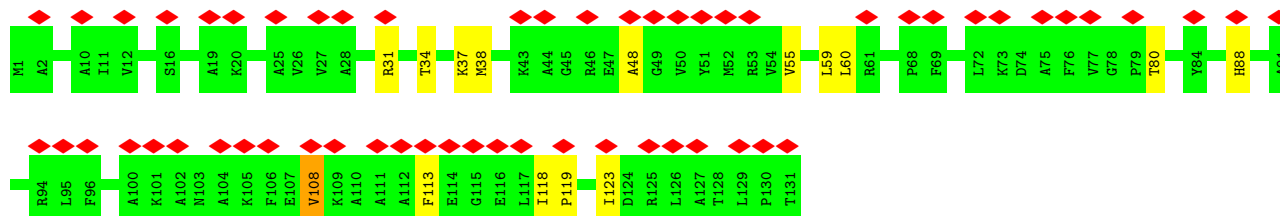
- Molecule 31: 50S ribosomal protein L36

Chain 4:  95%

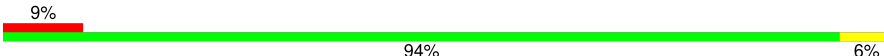


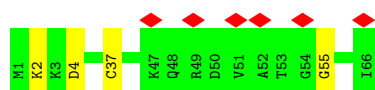
- Molecule 32: 50S ribosomal protein L10

Chain 5:  44% 89% 11%



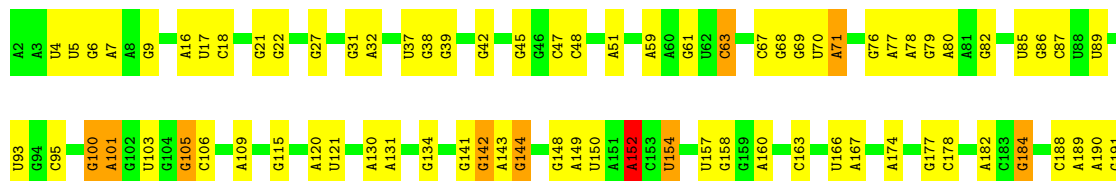
- Molecule 33: 50S ribosomal protein L31

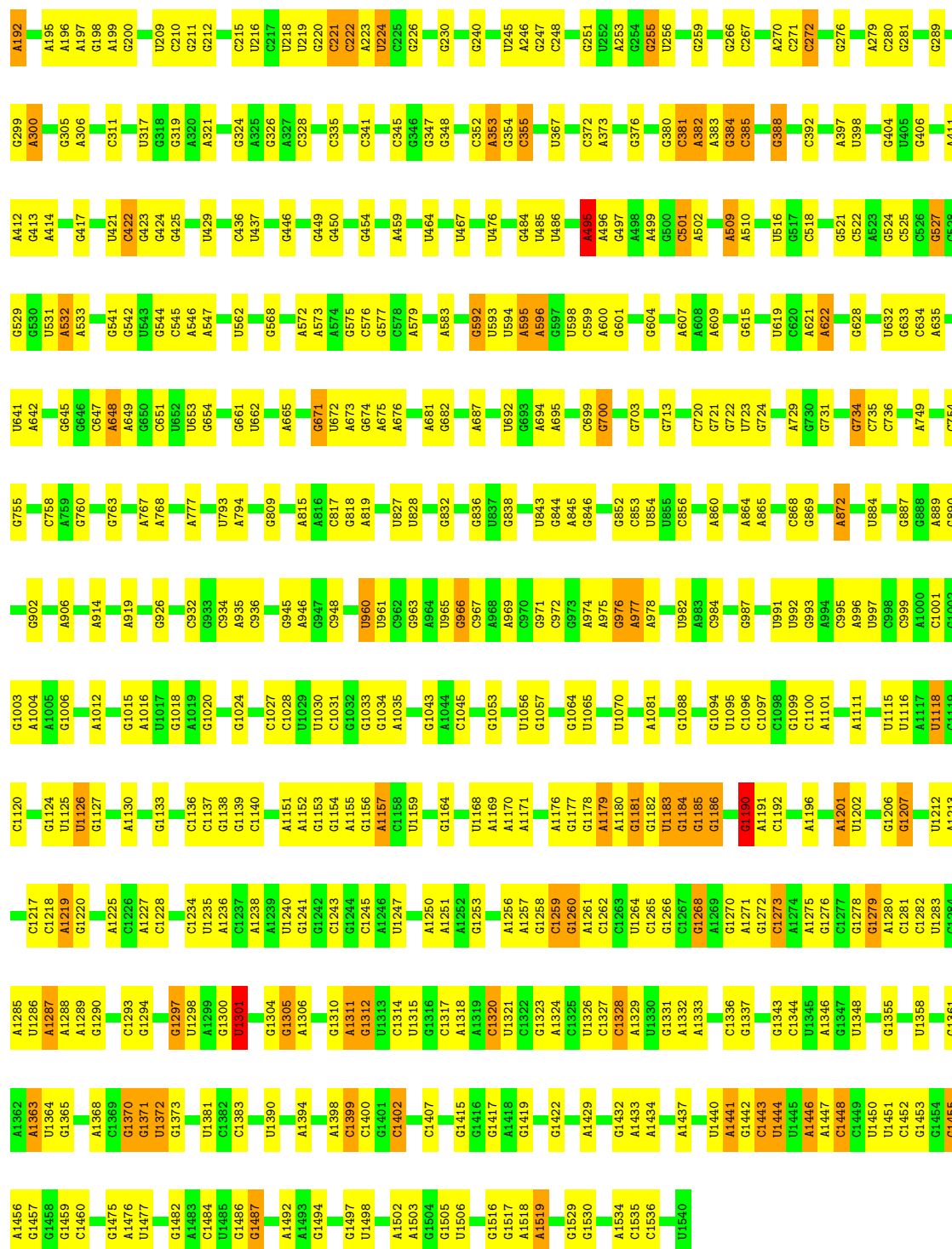
Chain 6:  9% 94% 6%



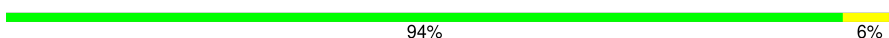
- Molecule 34: 16S rRNA

Chain a:  62% 32% 5%



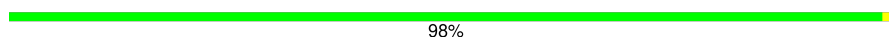


- Molecule 36: 30S ribosomal protein S3

Chain c:  94% 6%



- Molecule 37: 30S ribosomal protein S4

Chain d:  98% .



- Molecule 38: 30S ribosomal protein S5

Chain e:  94% 5% ..

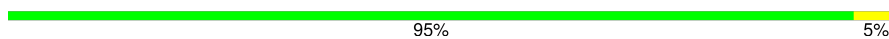


- Molecule 39: 30S ribosomal protein S6

Chain f:  85% 11% .

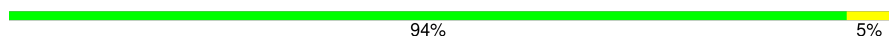


- Molecule 40: 30S ribosomal protein S7

Chain g:  95% 5%



- Molecule 41: 30S ribosomal protein S8

Chain h:  94% 5% .



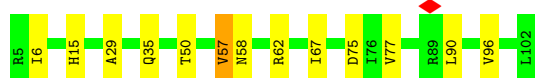
- Molecule 42: 30S ribosomal protein S9

Chain i:  91% 9%



• Molecule 43: 30S ribosomal protein S10

Chain j:  87% 12%



• Molecule 44: 30S ribosomal protein S11

Chain k:  91% 9%



• Molecule 45: 30S ribosomal protein S12

Chain l:  90% 10%

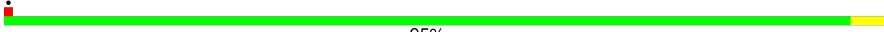


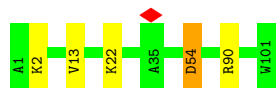
• Molecule 46: 30S ribosomal protein S13

Chain m:  93% 6%



• Molecule 47: 30S ribosomal protein S14

Chain n:  95%



• Molecule 48: 30S ribosomal protein S15

Chain o:  94% 6%



• Molecule 49: 30S ribosomal protein S16

Chain p:  90% 10%



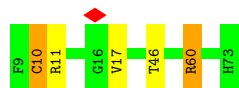
- Molecule 50: 30S ribosomal protein S17

Chain q: 94% 5% •



- Molecule 51: 30S ribosomal protein S18

Chain r: 92% 5% •



- Molecule 52: 30S ribosomal protein S19

Chain s: 91% 8% •



- Molecule 53: 30S ribosomal protein S20

Chain t: 94% 6% •



- Molecule 54: 30S ribosomal protein S21

Chain u: 91% 9% •



- Molecule 55: tRNA-fMet

Chain v: 73% 23% •



- Molecule 55: tRNA-fMet

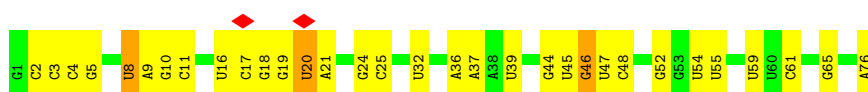
Chain w: 58% 35% 5% •



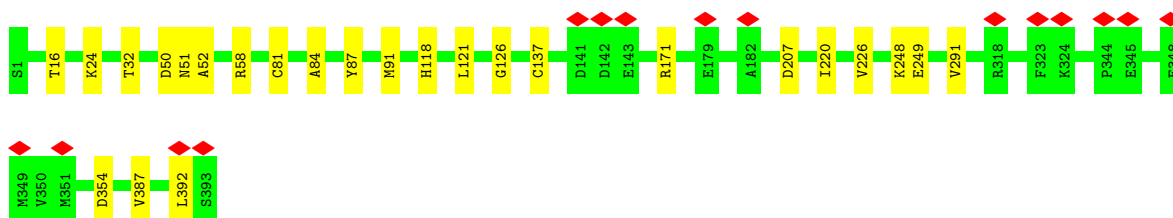
- Molecule 56: mRNA



- 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	82184	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5200	Depositor
Magnification	39683	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.339	Depositor
Minimum map value	-0.239	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	384.4, 384.4, 384.4	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0/69177	0.71	29/107915 (0.0%)
2	B	0.40	0/2876	0.72	0/4483
3	C	0.49	0/2121	0.74	0/2852
4	D	0.49	0/1578	0.74	0/2124
5	E	0.49	0/1563	0.80	0/2103
6	F	0.56	1/1434 (0.1%)	0.81	0/1926
7	G	0.53	0/1324	0.73	0/1794
8	H	0.57	0/1122	0.78	0/1515
9	I	0.67	0/1046	0.87	2/1410 (0.1%)
10	J	0.51	0/1143	0.82	2/1540 (0.1%)
11	K	0.51	0/947	0.77	1/1268 (0.1%)
12	L	0.49	0/1044	0.81	0/1391
13	M	0.48	0/1093	0.79	0/1460
14	N	0.53	0/964	0.83	0/1289
15	O	0.53	0/902	0.84	0/1209
16	P	0.51	0/929	0.74	0/1242
17	Q	0.51	0/946	0.85	0/1260
18	R	0.50	0/823	0.69	0/1100
19	S	0.49	0/852	0.83	0/1142
20	T	0.49	0/736	0.72	0/984
21	U	0.53	0/787	0.77	0/1051
22	V	0.50	0/752	0.76	0/1008
23	W	0.44	0/579	0.65	0/767
24	X	0.48	0/635	0.72	0/848
25	Y	0.51	0/495	0.84	0/658
26	Z	0.54	0/438	0.87	0/586
27	0	0.49	0/440	0.83	0/588
28	1	0.48	0/424	0.70	0/565
29	2	0.50	0/370	0.99	0/487
30	3	0.47	0/513	0.81	0/676
31	4	0.45	0/303	0.75	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.68	0/1001	0.88	0/1350
33	6	0.57	0/531	0.82	0/709
34	a	0.38	0/36700	0.72	19/57246 (0.0%)
35	b	0.56	0/1735	0.80	0/2338
36	c	0.54	0/1651	0.78	0/2225
37	d	0.56	0/1665	0.79	0/2227
38	e	0.54	0/1180	0.82	0/1587
39	f	0.57	1/835 (0.1%)	0.79	0/1128
40	g	0.54	0/1195	0.82	0/1602
41	h	0.51	0/989	0.81	0/1326
42	i	0.56	0/1034	0.79	0/1375
43	j	0.60	0/796	0.79	0/1077
44	k	0.52	0/885	0.78	0/1195
45	l	0.54	0/954	0.79	1/1282 (0.1%)
46	m	0.57	0/892	0.85	0/1193
47	n	0.55	0/822	0.78	0/1095
48	o	0.52	0/722	0.86	0/964
49	p	0.55	0/659	0.79	0/884
50	q	0.54	0/657	0.73	0/881
51	r	0.57	0/544	0.77	0/731
52	s	0.56	0/652	0.77	0/877
53	t	0.54	0/671	0.89	0/888
54	u	0.61	0/550	0.84	0/728
55	v	0.40	1/1747 (0.1%)	0.71	0/2721
55	w	0.67	1/1746 (0.1%)	0.90	5/2717 (0.2%)
56	x	0.39	0/280	0.72	0/433
57	y	0.39	0/1607	0.71	1/2501 (0.0%)
58	z	0.57	0/3086	0.77	0/4175
All	All	0.44	4/164142 (0.0%)	0.74	60/245093 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-22.64	1.27	1.61
39	f	18	VAL	CA-CB	5.99	1.57	1.54
6	F	107	VAL	CA-CB	5.73	1.56	1.54
55	v	7	4SU	O3'-P	5.16	1.61	1.56

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	117	U	P-O3'-C3'	21.78	152.87	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	117	U	O3'-P-O5'	14.89	126.33	104.00
1	A	1022	G	C2'-C3'-O3'	11.13	126.20	109.50
1	A	1378	A	C4'-C3'-O3'	10.12	124.58	109.40
55	w	117	U	OP2-P-O3'	-9.56	79.33	108.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	62278	0	31344	162	0
2	B	2572	0	1302	21	0
3	C	2082	0	2157	4	0
4	D	1557	0	1604	4	0
5	E	1544	0	1607	2	0
6	F	1410	0	1447	0	0
7	G	1304	0	1348	2	0
8	H	1111	0	1148	2	0
9	I	1032	0	1088	1	0
10	J	1120	0	1151	3	0
11	K	938	0	1012	6	0
12	L	1035	0	1111	4	0
13	M	1074	0	1157	0	0
14	N	951	0	994	3	0
15	O	892	0	923	5	0
16	P	917	0	965	1	0
17	Q	933	0	1006	2	0
18	R	810	0	834	1	0
19	S	845	0	909	0	0
20	T	730	0	795	0	0
21	U	779	0	834	0	0
22	V	739	0	763	0	0
23	W	572	0	593	1	0
24	X	625	0	655	2	0
25	Y	494	0	530	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	Z	434	0	477	1	0
27	0	434	0	448	1	0
28	1	417	0	451	0	0
29	2	367	0	405	1	0
30	3	504	0	574	0	0
31	4	302	0	343	1	0
32	5	988	0	1025	2	0
33	6	522	0	524	1	0
34	a	33028	0	16644	205	0
35	b	1704	0	1732	3	0
36	c	1624	0	1699	3	0
37	d	1643	0	1710	0	0
38	e	1164	0	1212	3	0
39	f	817	0	808	11	0
40	g	1181	0	1240	1	0
41	h	979	0	1034	3	0
42	i	1022	0	1070	2	0
43	j	786	0	828	3	0
44	k	869	0	878	1	0
45	l	940	0	1001	3	0
46	m	883	0	944	1	0
47	n	810	0	852	0	0
48	o	714	0	737	0	0
49	p	649	0	666	3	0
50	q	648	0	691	2	0
51	r	535	0	552	2	0
52	s	637	0	665	2	0
53	t	665	0	714	0	0
54	u	544	0	579	1	0
55	v	1644	0	840	1	0
55	w	1644	0	841	2	0
56	x	252	0	129	0	0
57	y	1632	0	843	1	0
58	z	3031	0	3050	5	0
59	A	10	0	10	0	0
60	0	3	0	0	0	0
60	3	2	0	0	0	0
60	4	1	0	0	0	0
60	A	404	0	0	0	0
60	B	6	0	0	0	0
60	C	2	0	0	0	0
60	D	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
60	E	1	0	0	0	0
60	J	1	0	0	0	0
60	L	1	0	0	0	0
60	N	3	0	0	0	0
60	O	1	0	0	0	0
60	S	1	0	0	0	0
60	T	2	0	0	0	0
60	a	221	0	0	0	0
60	e	1	0	0	0	0
60	i	1	0	0	0	0
60	t	1	0	0	0	0
60	u	1	0	0	0	0
60	v	2	0	0	0	0
60	y	4	0	0	0	0
60	z	2	0	0	0	0
61	A	7	0	0	0	0
61	v	1	0	0	0	0
62	y	11	0	8	0	0
63	z	32	0	12	0	0
64	0	1	0	0	0	0
64	2	1	0	0	0	0
64	A	83	0	0	0	0
64	B	3	0	0	0	0
64	C	3	0	0	0	0
64	E	1	0	0	0	0
64	L	1	0	0	0	0
64	Q	1	0	0	0	0
64	U	1	0	0	0	0
64	W	3	0	0	0	0
64	X	2	0	0	0	0
64	Z	2	0	0	0	0
64	a	46	0	0	0	0
64	k	1	0	0	0	0
64	q	2	0	0	0	0
64	s	2	0	0	0	0
All	All	153233	0	103513	462	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 2.

The worst 5 of 462 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:827:U:O4	34:a:872:A:N1	1.68	1.25
1:A:1021:A:N1	1:A:1141:U:O4	1.73	1.20
1:A:2013:A:N1	1:A:2613:U:O4	1.75	1.18
1:A:2030:6MZ:O3'	1:A:2031:A:P	2.02	1.17
34:a:101:A:N1	34:a:152:A:H4'	1.58	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%)	235 (87%)	31 (12%)	3 (1%)	11	38
4	D	206/208 (99%)	189 (92%)	14 (7%)	3 (2%)	8	30
5	E	198/200 (99%)	170 (86%)	20 (10%)	8 (4%)	2	15
6	F	175/177 (99%)	159 (91%)	15 (9%)	1 (1%)	21	50
7	G	172/174 (99%)	161 (94%)	10 (6%)	1 (1%)	21	50
8	H	147/149 (99%)	130 (88%)	12 (8%)	5 (3%)	3	17
9	I	139/141 (99%)	112 (81%)	22 (16%)	5 (4%)	2	16
10	J	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
11	K	120/122 (98%)	105 (88%)	12 (10%)	3 (2%)	4	21
12	L	140/142 (99%)	116 (83%)	19 (14%)	5 (4%)	2	16
13	M	134/136 (98%)	122 (91%)	11 (8%)	1 (1%)	18	47
14	N	117/119 (98%)	102 (87%)	14 (12%)	1 (1%)	14	42
15	O	114/116 (98%)	105 (92%)	7 (6%)	2 (2%)	6	26
16	P	112/114 (98%)	97 (87%)	15 (13%)	0	100	100
17	Q	113/115 (98%)	109 (96%)	3 (3%)	1 (1%)	14	42
18	R	100/102 (98%)	86 (86%)	11 (11%)	3 (3%)	3	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	S	107/109 (98%)	99 (92%)	6 (6%)	2 (2%)	6	26
20	T	90/92 (98%)	78 (87%)	9 (10%)	3 (3%)	3	17
21	U	100/102 (98%)	86 (86%)	12 (12%)	2 (2%)	6	25
22	V	90/92 (98%)	82 (91%)	7 (8%)	1 (1%)	11	38
23	W	73/75 (97%)	67 (92%)	5 (7%)	1 (1%)	9	31
24	X	75/77 (97%)	67 (89%)	8 (11%)	0	100	100
25	Y	58/60 (97%)	51 (88%)	6 (10%)	1 (2%)	7	28
26	Z	54/56 (96%)	53 (98%)	1 (2%)	0	100	100
27	0	53/55 (96%)	46 (87%)	5 (9%)	2 (4%)	2	15
28	1	49/51 (96%)	43 (88%)	5 (10%)	1 (2%)	6	25
29	2	43/45 (96%)	39 (91%)	4 (9%)	0	100	100
30	3	62/64 (97%)	57 (92%)	5 (8%)	0	100	100
31	4	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	4	19
32	5	129/131 (98%)	102 (79%)	17 (13%)	10 (8%)	1	4
33	6	64/66 (97%)	55 (86%)	7 (11%)	2 (3%)	3	18
35	b	216/218 (99%)	184 (85%)	28 (13%)	4 (2%)	6	26
36	c	204/206 (99%)	181 (89%)	17 (8%)	6 (3%)	3	19
37	d	203/205 (99%)	177 (87%)	23 (11%)	3 (2%)	8	30
38	e	156/157 (99%)	128 (82%)	24 (15%)	4 (3%)	4	21
39	f	98/100 (98%)	84 (86%)	11 (11%)	3 (3%)	3	18
40	g	149/151 (99%)	125 (84%)	19 (13%)	5 (3%)	3	17
41	h	127/129 (98%)	112 (88%)	13 (10%)	2 (2%)	7	29
42	i	125/127 (98%)	98 (78%)	21 (17%)	6 (5%)	2	11
43	j	96/98 (98%)	73 (76%)	18 (19%)	5 (5%)	1	10
44	k	114/116 (98%)	94 (82%)	15 (13%)	5 (4%)	2	13
45	l	119/121 (98%)	96 (81%)	19 (16%)	4 (3%)	3	17
46	m	112/114 (98%)	100 (89%)	9 (8%)	3 (3%)	4	20
47	n	99/101 (98%)	85 (86%)	10 (10%)	4 (4%)	2	15
48	o	86/88 (98%)	79 (92%)	3 (4%)	4 (5%)	2	12
49	p	80/82 (98%)	69 (86%)	9 (11%)	2 (2%)	4	21
50	q	78/80 (98%)	67 (86%)	10 (13%)	1 (1%)	9	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	r	63/65 (97%)	54 (86%)	6 (10%)	3 (5%)	2	11
52	s	77/79 (98%)	67 (87%)	8 (10%)	2 (3%)	4	21
53	t	83/85 (98%)	78 (94%)	2 (2%)	3 (4%)	2	16
54	u	63/65 (97%)	43 (68%)	16 (25%)	4 (6%)	1	7
58	z	391/393 (100%)	351 (90%)	34 (9%)	6 (2%)	8	30
All	All	6217/6320 (98%)	5428 (87%)	642 (10%)	147 (2%)	7	22

5 of 147 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	5	123	ILE
33	6	4	ASP
36	c	96	VAL
36	c	156	LEU
38	e	93	VAL

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%)	212 (98%)	4 (2%)	50	66
4	D	163/163 (100%)	160 (98%)	3 (2%)	51	67
5	E	164/164 (100%)	157 (96%)	7 (4%)	26	51
6	F	148/148 (100%)	145 (98%)	3 (2%)	48	65
7	G	135/135 (100%)	134 (99%)	1 (1%)	76	78
8	H	114/114 (100%)	113 (99%)	1 (1%)	70	76
9	I	109/109 (100%)	108 (99%)	1 (1%)	70	76
10	J	115/115 (100%)	110 (96%)	5 (4%)	26	51
11	K	103/103 (100%)	98 (95%)	5 (5%)	22	49
12	L	101/101 (100%)	98 (97%)	3 (3%)	36	59
13	M	109/109 (100%)	105 (96%)	4 (4%)	30	55

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	99/99 (100%)	96 (97%)	3 (3%)	36	59
15	O	86/86 (100%)	84 (98%)	2 (2%)	44	63
16	P	99/99 (100%)	96 (97%)	3 (3%)	36	59
17	Q	88/88 (100%)	85 (97%)	3 (3%)	32	57
18	R	84/84 (100%)	82 (98%)	2 (2%)	43	62
19	S	92/92 (100%)	88 (96%)	4 (4%)	26	51
20	T	79/79 (100%)	77 (98%)	2 (2%)	42	62
21	U	83/83 (100%)	82 (99%)	1 (1%)	63	72
22	V	77/77 (100%)	76 (99%)	1 (1%)	61	71
23	W	57/57 (100%)	56 (98%)	1 (2%)	51	67
24	X	67/67 (100%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	45 (96%)	2 (4%)	26	51
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	45 (98%)	1 (2%)	45	63
29	2	37/37 (100%)	37 (100%)	0	100	100
30	3	51/51 (100%)	50 (98%)	1 (2%)	48	65
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	98 (98%)	2 (2%)	48	65
33	6	59/59 (100%)	58 (98%)	1 (2%)	53	67
35	b	180/180 (100%)	174 (97%)	6 (3%)	33	57
36	c	170/170 (100%)	167 (98%)	3 (2%)	51	67
37	d	172/172 (100%)	171 (99%)	1 (1%)	78	80
38	e	120/119 (101%)	116 (97%)	4 (3%)	33	57
39	f	87/87 (100%)	83 (95%)	4 (5%)	24	50
40	g	124/124 (100%)	123 (99%)	1 (1%)	73	77
41	h	104/104 (100%)	102 (98%)	2 (2%)	50	66
42	i	105/105 (100%)	103 (98%)	2 (2%)	50	66
43	j	86/86 (100%)	82 (95%)	4 (5%)	23	50
44	k	89/89 (100%)	84 (94%)	5 (6%)	19	46
45	l	102/102 (100%)	99 (97%)	3 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	m	92/92 (100%)	88 (96%)	4 (4%)	26	51
47	n	83/83 (100%)	81 (98%)	2 (2%)	43	62
48	o	76/76 (100%)	75 (99%)	1 (1%)	61	71
49	p	65/65 (100%)	64 (98%)	1 (2%)	57	69
50	q	74/74 (100%)	72 (97%)	2 (3%)	39	60
51	r	56/56 (100%)	55 (98%)	1 (2%)	51	67
52	s	70/70 (100%)	67 (96%)	3 (4%)	26	51
53	t	65/65 (100%)	63 (97%)	2 (3%)	35	59
54	u	55/55 (100%)	55 (100%)	0	100	100
58	z	325/325 (100%)	314 (97%)	11 (3%)	32	57
All	All	5163/5162 (100%)	5035 (98%)	128 (2%)	42	62

5 of 128 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
53	t	24	ARG
58	z	50	ASP
18	R	66	HIS
17	Q	88	GLU
58	z	81	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
25	Y	31	GLN
58	z	124	GLN
33	6	61	ASN
58	z	22	HIS
49	p	79	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2898/2903 (99%)	757 (26%)	50 (1%)
2	B	119/120 (99%)	34 (28%)	3 (2%)
34	a	1538/1539 (99%)	455 (29%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
55	v	76/77 (98%)	18 (23%)	0
55	w	76/77 (98%)	29 (38%)	0
56	x	11/12 (91%)	4 (36%)	0
57	y	75/76 (98%)	23 (30%)	0
All	All	4793/4804 (99%)	1320 (27%)	53 (1%)

5 of 1320 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	4	U
1	A	10	A
1	A	12	U
1	A	13	A

5 of 53 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1314	C
1	A	1555	G
1	A	2873	A
1	A	1331	G
1	A	1432	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
57	PSU	y	55	57	18,21,22	1.38	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	A	2457	1	18,21,22	1.48	3 (16%)	21,30,33	2.05	4 (19%)
34	2MG	a	1207	34	23,26,27	1.27	3 (13%)	33,38,41	2.79	10 (30%)
1	5MC	A	747	1	19,22,23	1.98	2 (10%)	26,32,35	1.58	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
57	MIA	y	37	60,57	28,31,32	2.39	7 (25%)	38,44,47	2.87	14 (36%)
1	PSU	A	1917	1	18,21,22	1.42	2 (11%)	21,30,33	2.13	5 (23%)
34	MA6	a	1519	34	23,26,27	1.68	5 (21%)	33,38,41	2.35	10 (30%)
1	1MG	A	745	1	23,26,27	1.28	3 (13%)	33,39,42	2.03	7 (21%)
1	H2U	A	2449	1	18,21,22	0.97	2 (11%)	19,30,33	1.40	3 (15%)
1	OMG	A	2251	1,55	23,26,27	1.29	3 (13%)	32,38,41	1.98	6 (18%)
55	H2U	w	20	55	18,21,22	0.80	0	19,30,33	1.58	3 (15%)
1	2MG	A	1835	1	23,26,27	1.34	4 (17%)	33,38,41	2.25	8 (24%)
1	6MZ	A	2030	1	22,25,26	1.53	4 (18%)	29,36,39	2.28	10 (34%)
55	5MU	v	54	55	19,22,23	1.46	4 (21%)	27,32,35	2.01	7 (25%)
1	PSU	A	2580	1	18,21,22	1.50	3 (16%)	21,30,33	2.08	5 (23%)
34	4OC	a	1402	34	20,23,24	0.82	0	25,32,35	1.40	5 (20%)
34	5MC	a	967	34	19,22,23	2.01	2 (10%)	26,32,35	1.42	4 (15%)
34	2MG	a	966	34,60	23,26,27	1.29	3 (13%)	33,38,41	2.68	10 (30%)
1	5MC	A	1962	1	19,22,23	1.70	2 (10%)	26,32,35	1.42	4 (15%)
34	PSU	a	516	34	18,21,22	1.39	2 (11%)	21,30,33	2.12	5 (23%)
1	OMU	A	2552	1	19,22,23	1.31	4 (21%)	25,31,34	2.01	8 (32%)
1	6MZ	A	1618	1	22,25,26	1.53	4 (18%)	29,36,39	2.29	10 (34%)
57	PSU	y	32	57	18,21,22	1.32	2 (11%)	21,30,33	2.06	5 (23%)
57	7MG	y	46	57	23,26,27	1.44	4 (17%)	27,39,42	2.52	7 (25%)
1	PSU	A	746	1	18,21,22	1.40	2 (11%)	21,30,33	1.97	4 (19%)
34	5MC	a	1407	34	19,22,23	1.72	2 (10%)	26,32,35	1.52	5 (19%)
57	4SU	y	8	57	18,21,22	1.81	4 (22%)	25,30,33	2.33	6 (24%)
1	2MG	A	2445	1	23,26,27	1.26	3 (13%)	33,38,41	2.37	10 (30%)
1	7MG	A	2069	1	23,26,27	1.45	3 (13%)	27,39,42	2.52	10 (37%)
1	2MA	A	2503	1,60	22,25,26	1.59	5 (22%)	32,37,40	2.14	8 (25%)
34	7MG	a	527	34	23,26,27	1.45	3 (13%)	27,39,42	2.58	7 (25%)
34	UR3	a	1498	34	19,22,23	1.09	1 (5%)	26,32,35	1.97	5 (19%)
57	H2U	y	20	57	18,21,22	0.84	1 (5%)	19,30,33	1.62	3 (15%)
1	5MU	A	1939	1	19,22,23	1.44	4 (21%)	27,32,35	2.07	8 (29%)
1	3TD	A	1915	1	19,22,23	7.09	13 (68%)	23,32,35	2.04	5 (21%)
55	4SU	v	7	55	18,21,22	1.78	4 (22%)	25,30,33	2.39	5 (20%)
55	4SU	w	8	55	18,21,22	1.81	5 (27%)	25,30,33	2.26	6 (24%)
55	PSU	v	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.01	4 (19%)
1	PSU	A	2604	1	18,21,22	1.42	2 (11%)	21,30,33	1.96	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	1911	1	18,21,22	1.40	2 (11%)	21,30,33	2.13	4 (19%)
1	PSU	A	2504	1	18,21,22	1.40	2 (11%)	21,30,33	2.06	4 (19%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.35	3 (15%)
57	PSU	y	39	57	18,21,22	1.44	2 (11%)	21,30,33	2.03	4 (19%)
57	5MU	y	54	57	19,22,23	1.48	4 (21%)	27,32,35	2.05	7 (25%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.07	10 (37%)
55	H2U	v	20	55	18,21,22	0.80	1 (5%)	19,30,33	1.57	3 (15%)
55	PSU	w	55	55	18,21,22	1.36	2 (11%)	21,30,33	2.09	5 (23%)
1	OMC	A	2498	1,60	19,22,23	0.84	0	25,31,34	1.30	2 (8%)
1	PSU	A	955	1	18,21,22	1.39	4 (22%)	21,30,33	2.10	4 (19%)
34	MA6	a	1518	34	23,26,27	1.74	6 (26%)	33,38,41	2.26	11 (33%)
1	PSU	A	2605	1	18,21,22	1.35	2 (11%)	21,30,33	2.15	4 (19%)
34	2MG	a	1516	34	23,26,27	1.28	4 (17%)	33,38,41	2.26	9 (27%)

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	PSU	y	55	57	-	2/7/25/26	0/2/2/2
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	3/9/27/28	0/3/3/3
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
57	MIA	y	37	60,57	-	3/15/33/34	0/3/3/3
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	2/11/29/30	0/3/3/3
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
1	OMG	A	2251	1,55	-	1/9/27/28	0/3/3/3
55	H2U	w	20	55	-	1/7/38/39	0/2/2/2
1	2MG	A	1835	1	-	0/9/27/28	0/3/3/3
1	6MZ	A	2030	1	-	3/9/27/28	0/3/3/3
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	1/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34,60	-	3/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
34	PSU	a	516	34	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	2/9/27/28	0/2/2/2
1	6MZ	A	1618	1	-	5/9/27/28	0/3/3/3
57	PSU	y	32	57	-	3/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	PSU	A	746	1	-	1/7/25/26	0/2/2/2
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	3/9/27/28	0/3/3/3
1	7MG	A	2069	1	-	2/7/37/38	0/3/3/3
1	2MA	A	2503	1,60	-	2/7/25/26	0/3/3/3
34	7MG	a	527	34	-	3/7/37/38	0/3/3/3
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
1	5MU	A	1939	1	-	2/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
55	4SU	v	7	55	-	1/7/25/26	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	1/7/25/26	0/2/2/2
57	H2U	y	16	57	-	0/7/38/39	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	OMC	A	2498	1,60	-	0/9/27/28	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	4/11/29/30	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
34	2MG	a	1516	34	-	0/9/27/28	0/3/3/3

The worst 5 of 158 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.58	1.66	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	C6-C5	15.69	1.52	1.35
1	A	1915	3TD	C2'-C1'	-14.48	1.34	1.53
1	A	1915	3TD	C2-N1	8.50	1.47	1.37
1	A	747	5MC	C5-C4	7.60	1.49	1.44

The worst 5 of 318 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	a	527	7MG	N9-C4-N3	8.56	138.01	125.46
34	a	966	2MG	C2-N3-C4	8.50	122.63	112.00
34	a	1207	2MG	C2-N3-C4	8.47	122.59	112.00
57	y	46	7MG	N9-C4-N3	8.29	137.61	125.46
57	y	37	MIA	C5-C4-N3	-8.22	118.52	127.18

There are no chirality outliers.

5 of 78 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.

4 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	2030	6MZ	13	0
1	A	1618	6MZ	9	0
1	A	1915	3TD	1	0
1	A	2504	PSU	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 673 ligands modelled in this entry, 670 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	$\# Z > 2$
62	PHE	y	101	-	10,11,12	0.51	0	8,13,15	0.16	0
63	GTP	z	401	60	33,34,34	1.21	4 (12%)	50,54,54	1.79	8 (16%)
59	FME	A	3001	-	8,9,10	0.49	0	8,9,11	1.02	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
62	PHE	y	101	-	-	2/5/6/8	0/1/1/1
63	GTP	z	401	60	-	3/22/38/38	0/3/3/3
59	FME	A	3001	-	-	0/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	401	GTP	C5-C4	3.24	1.47	1.38
63	z	401	GTP	C5-N7	-2.18	1.34	1.39
63	z	401	GTP	PA-O3A	2.14	1.61	1.59
63	z	401	GTP	C6-N1	-2.10	1.34	1.38

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	401	GTP	C5-C4-N3	-6.15	118.60	128.39
63	z	401	GTP	C2-N3-C4	5.21	121.27	112.30
63	z	401	GTP	N9-C4-N3	4.59	135.13	125.95
63	z	401	GTP	C6-C5-N7	3.33	136.35	130.29
63	z	401	GTP	C3'-C2'-C1'	2.60	106.38	101.46

There are no chirality outliers.

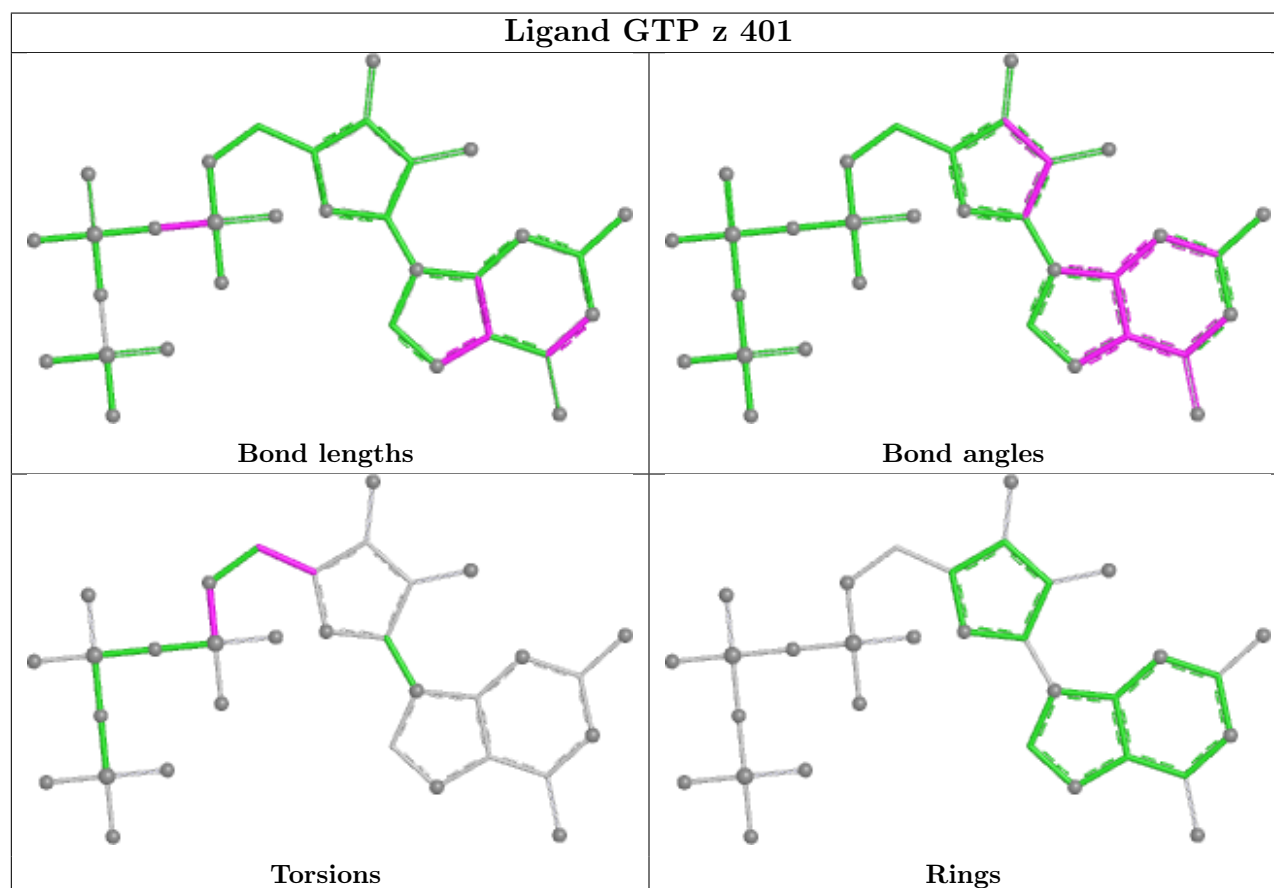
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
63	z	401	GTP	C5'-O5'-PA-O3A
63	z	401	GTP	C5'-O5'-PA-O1A
63	z	401	GTP	C3'-C4'-C5'-O5'
62	y	101	PHE	N-CA-CB-CG
62	y	101	PHE	C-CA-CB-CG

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
55	w	2
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	w	17:C	O3'	117:U	P	2.27
1	A	2030:6MZ	O3'	2031:A	P	2.02
1	A	1618:6MZ	O3'	1619:G	P	1.90
1	w	117:U	O3'	18:G	P	1.27

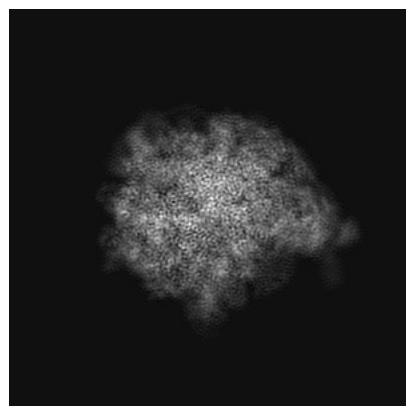
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8815. These allow visual inspection of the internal detail of the map and identification of artifacts.

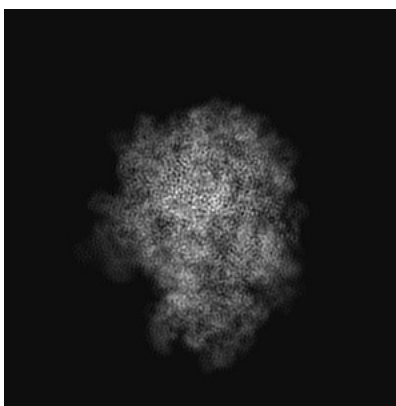
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

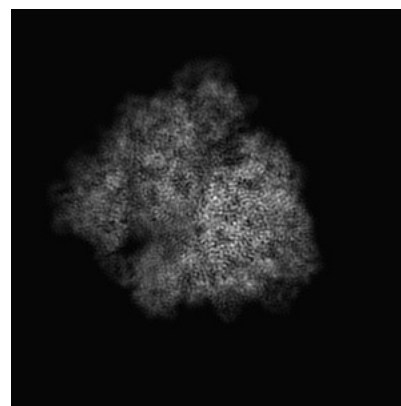
6.1.1 Primary map



X

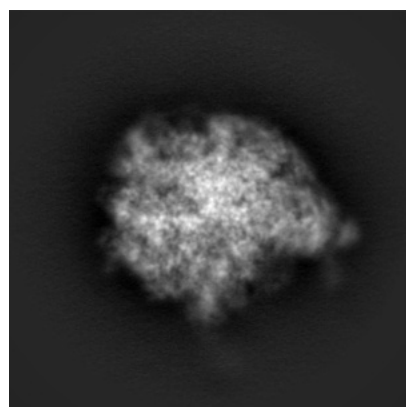


Y

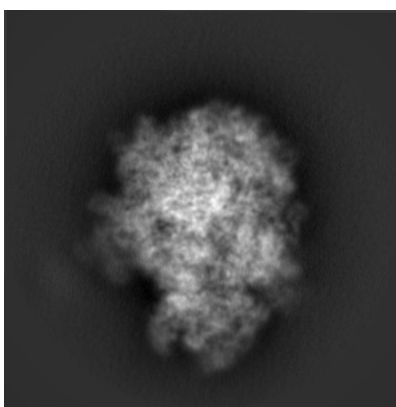


Z

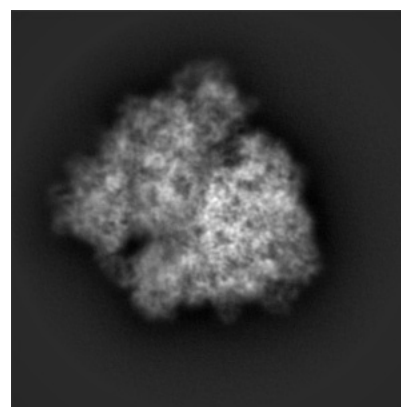
6.1.2 Raw map



X



Y

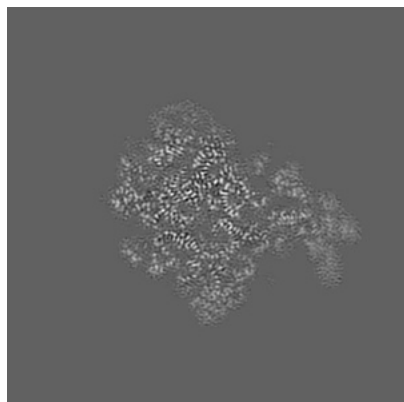


Z

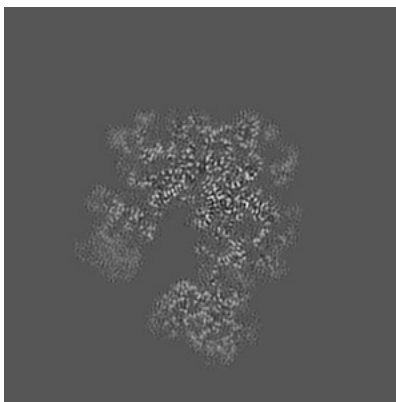
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

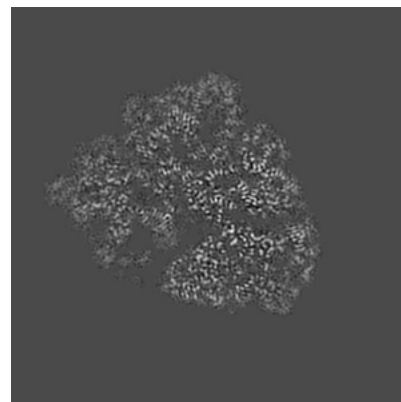
6.2.1 Primary map



X Index: 155

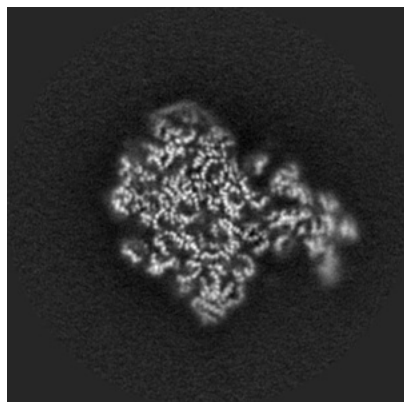


Y Index: 155

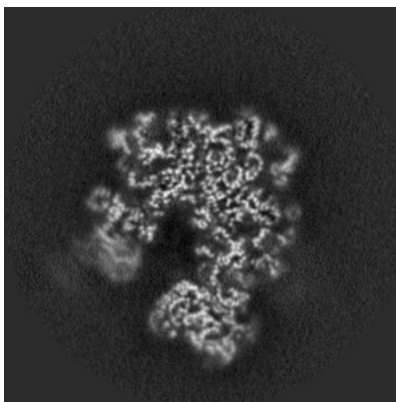


Z Index: 155

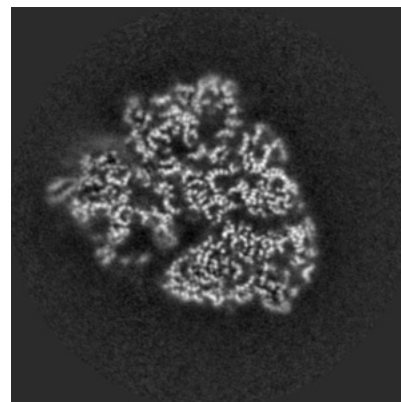
6.2.2 Raw map



X Index: 155



Y Index: 155

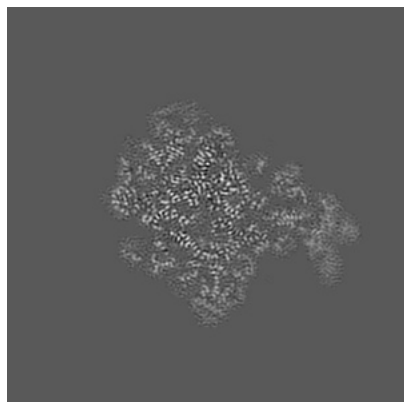


Z Index: 155

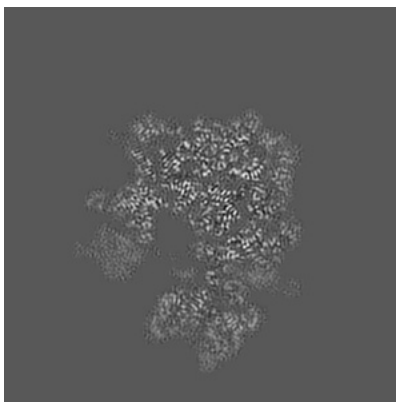
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

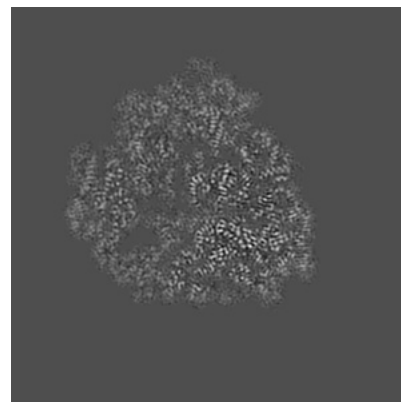
6.3.1 Primary map



X Index: 156

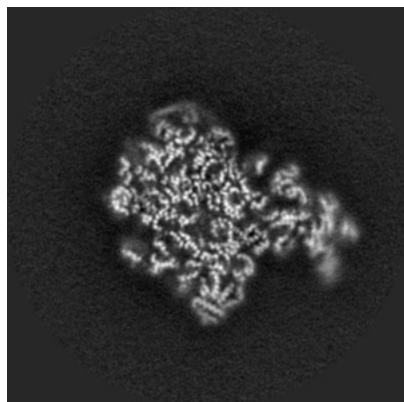


Y Index: 162

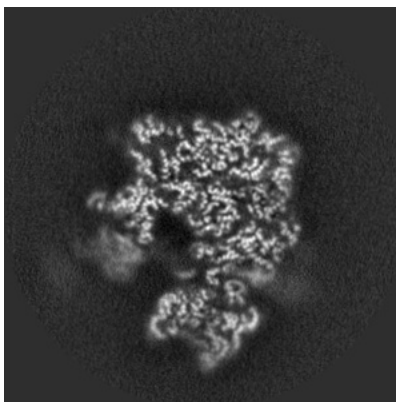


Z Index: 147

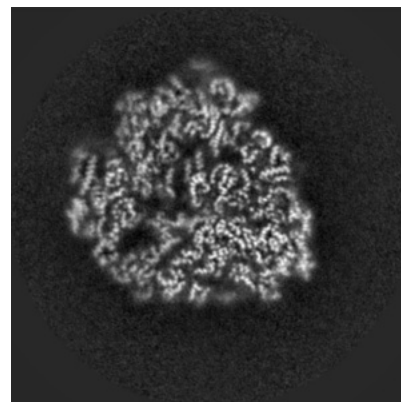
6.3.2 Raw map



X Index: 156



Y Index: 162

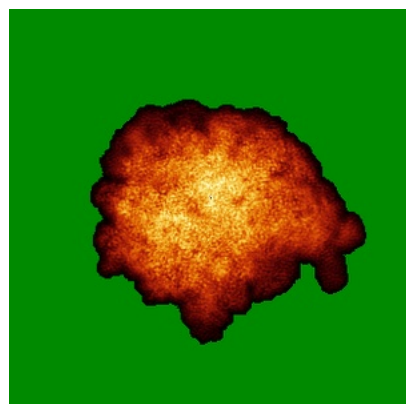


Z Index: 147

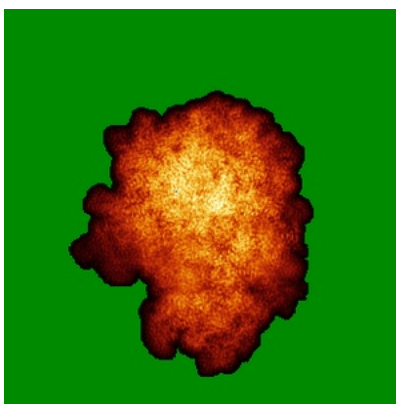
The images above show the largest variance slices of the map in three orthogonal directions.

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

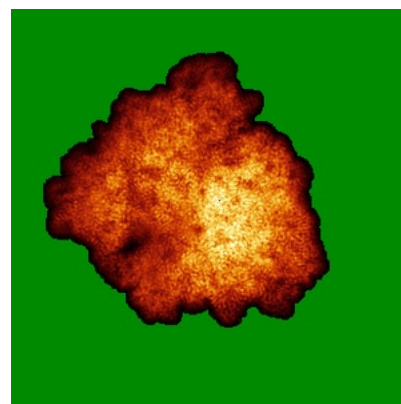
6.4.1 Primary map



X

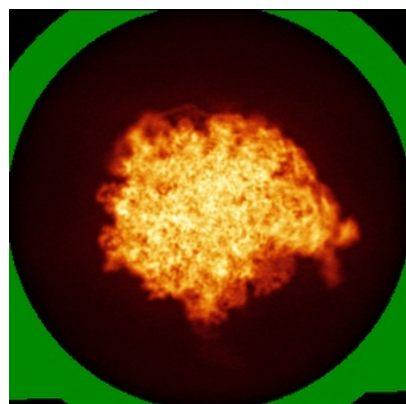


Y

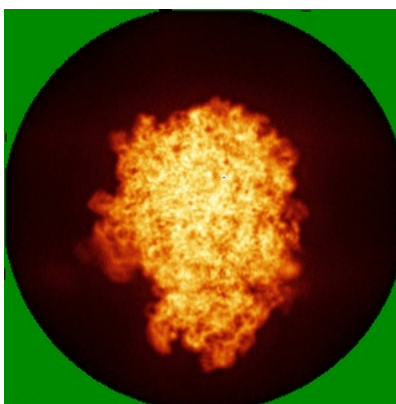


Z

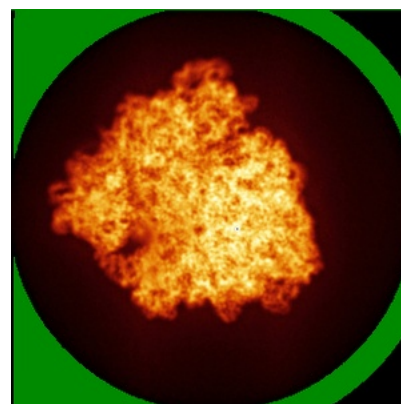
6.4.2 Raw map



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](#)

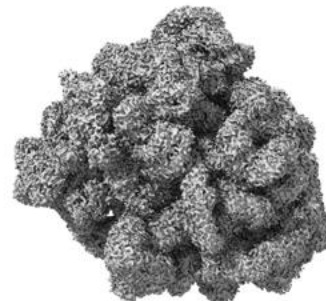
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. 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.

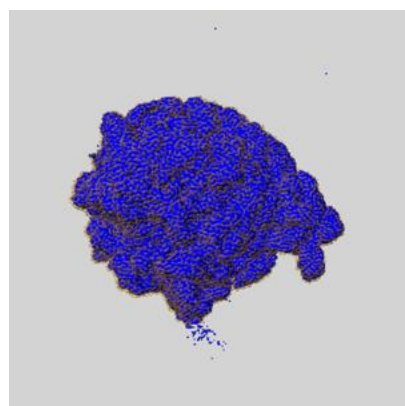
6.6 Mask visualisation [i](#)

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

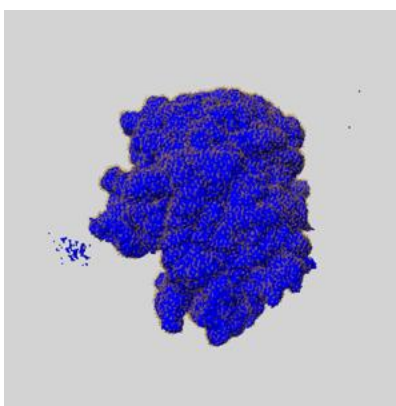
A mask typically either:

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

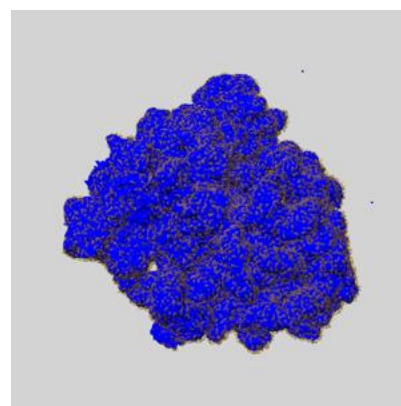
6.6.1 emd_8815_msk_1.map [i](#)



X



Y

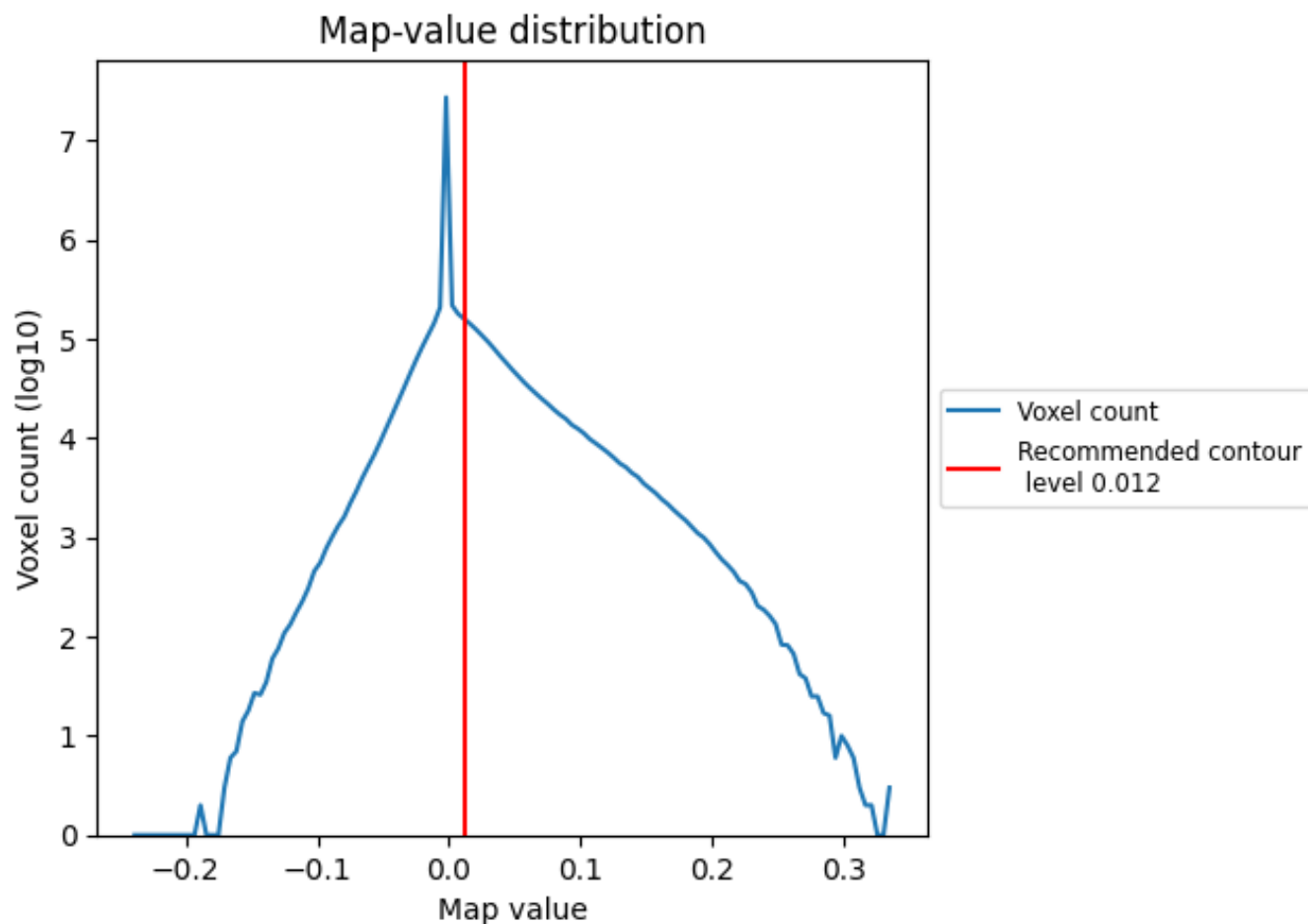


Z

7 Map analysis [i](#)

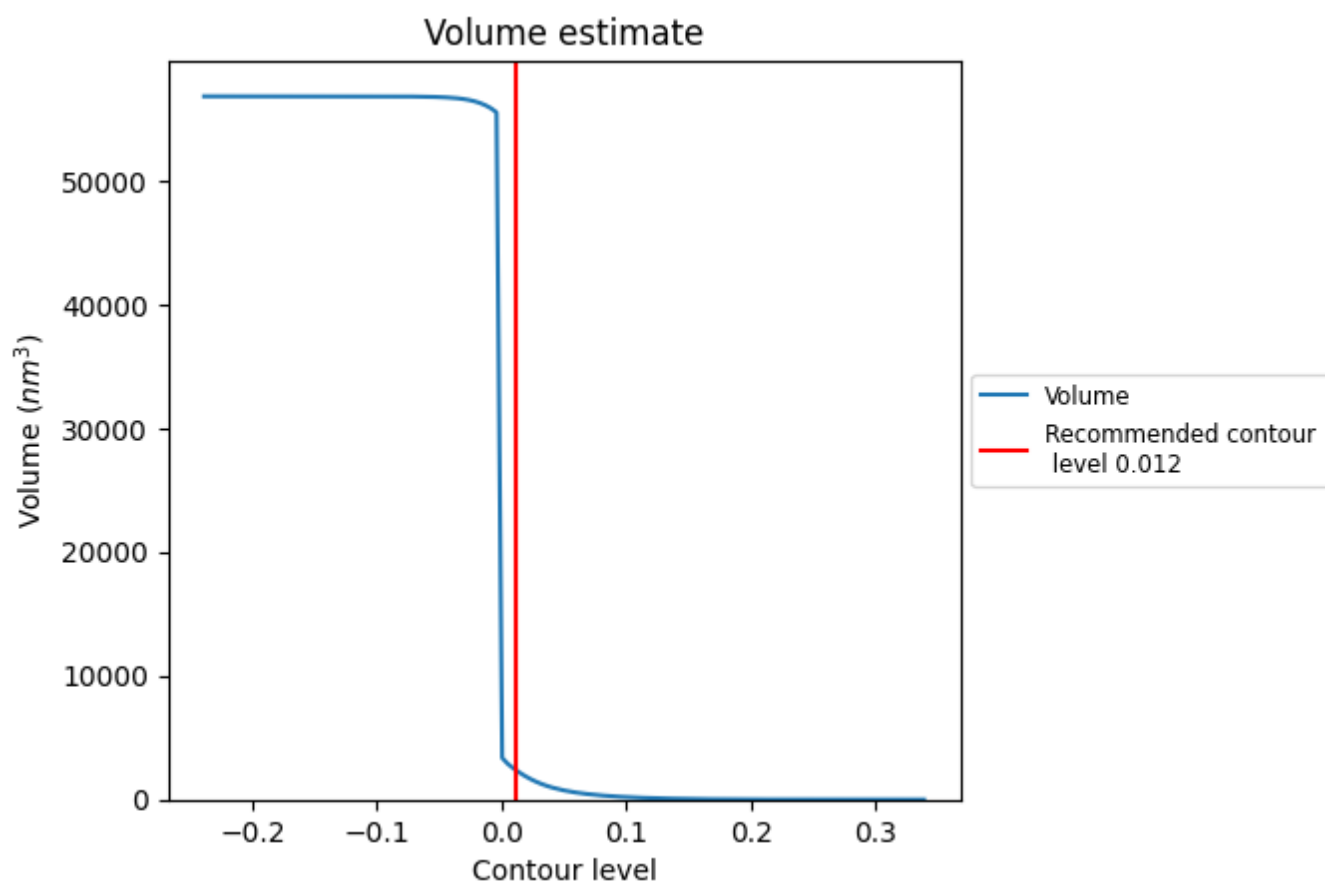
This section contains the results of statistical analysis of the map.

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.

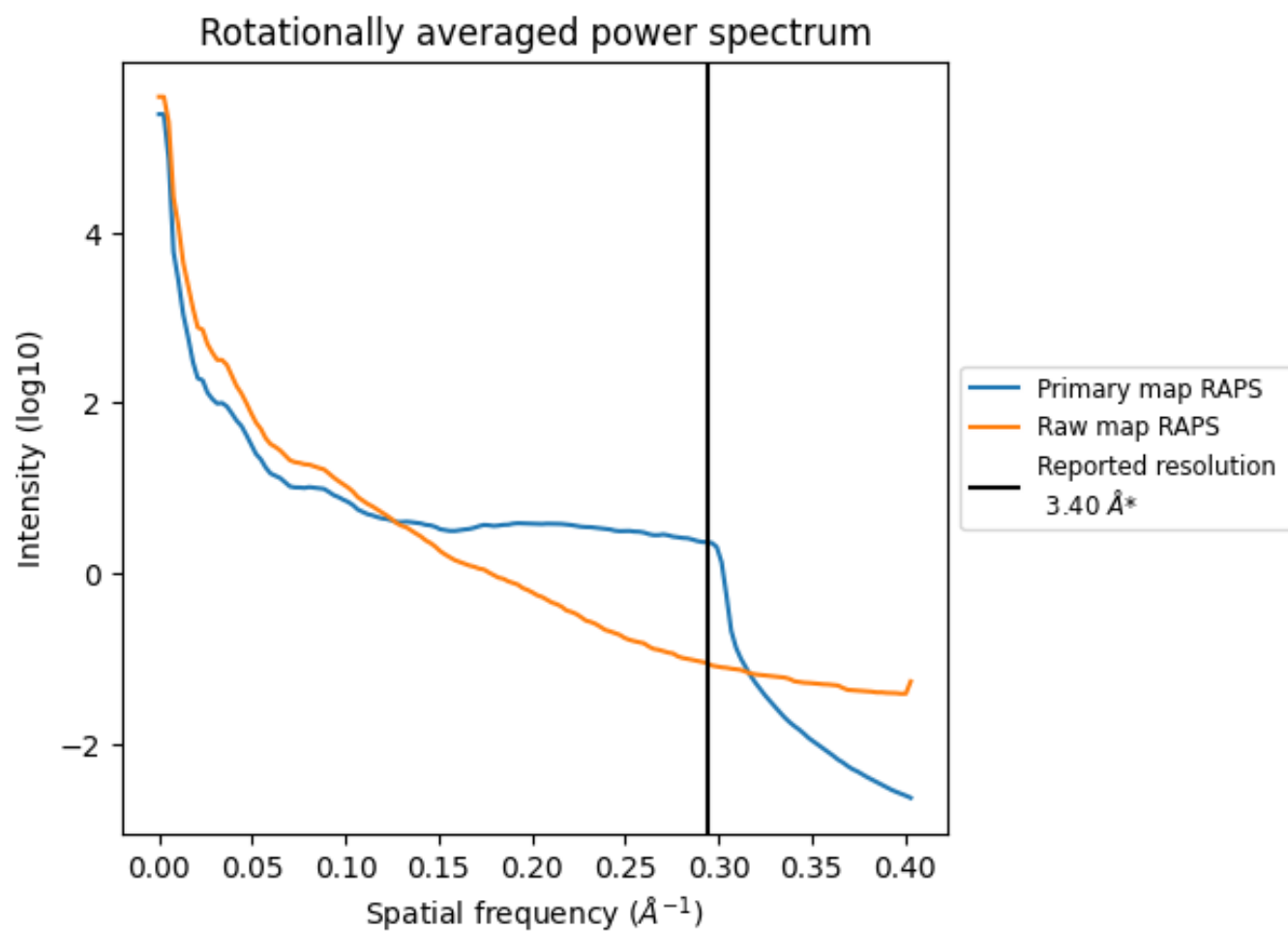
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2345 nm³; this corresponds to an approximate mass of 2119 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 ⓘ

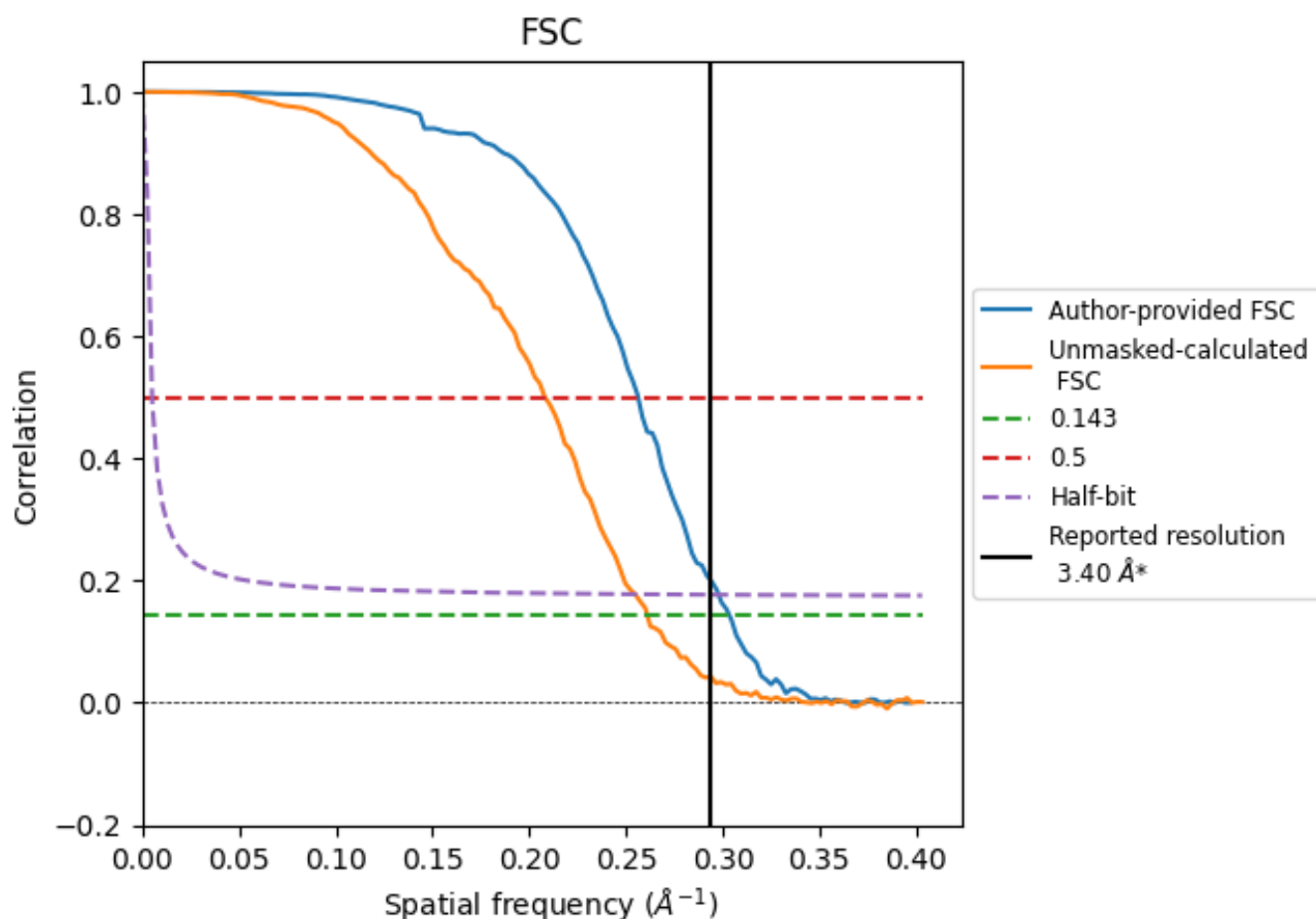


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 Å⁻¹

8.2 Resolution estimates [i](#)

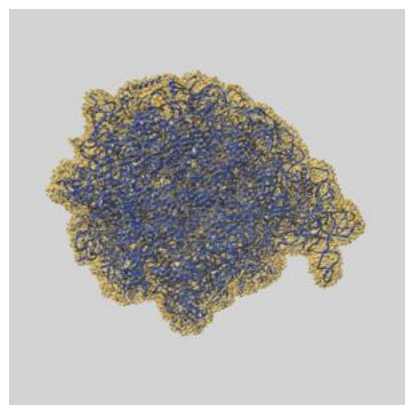
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.29	3.90	3.36
Unmasked-calculated*	3.83	4.80	3.92

*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 3.83 differs from the reported value 3.4 by more than 10 %

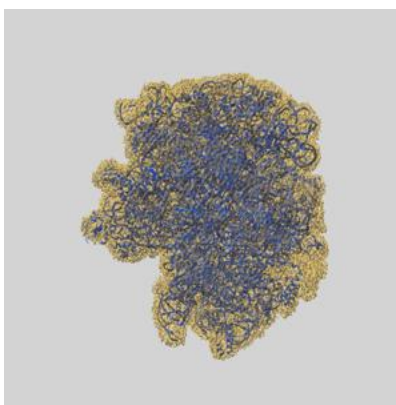
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8815 and PDB model 5WE6. Per-residue inclusion information can be found in section [3](#) on page [19](#).

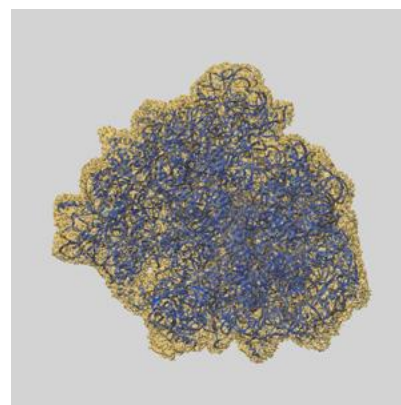
9.1 Map-model overlay [i](#)



X



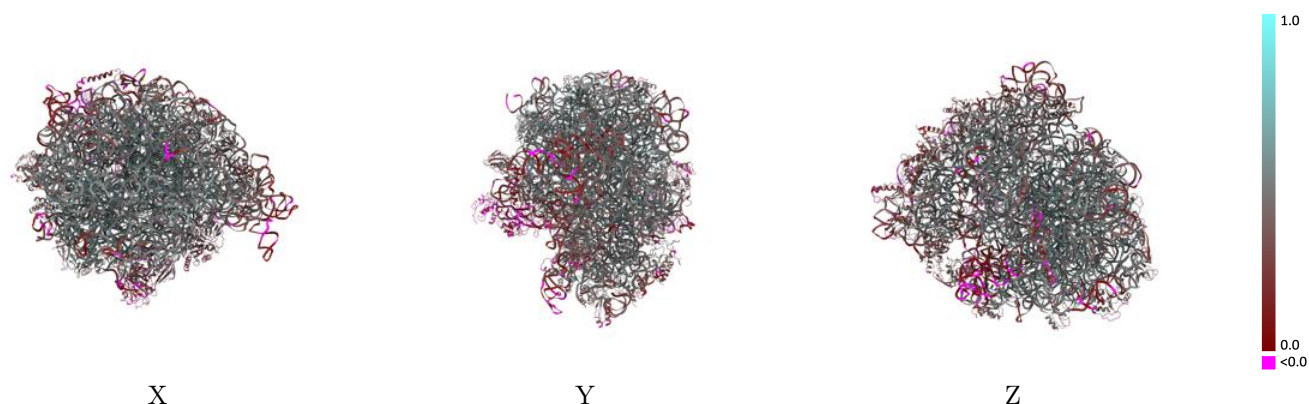
Y



Z

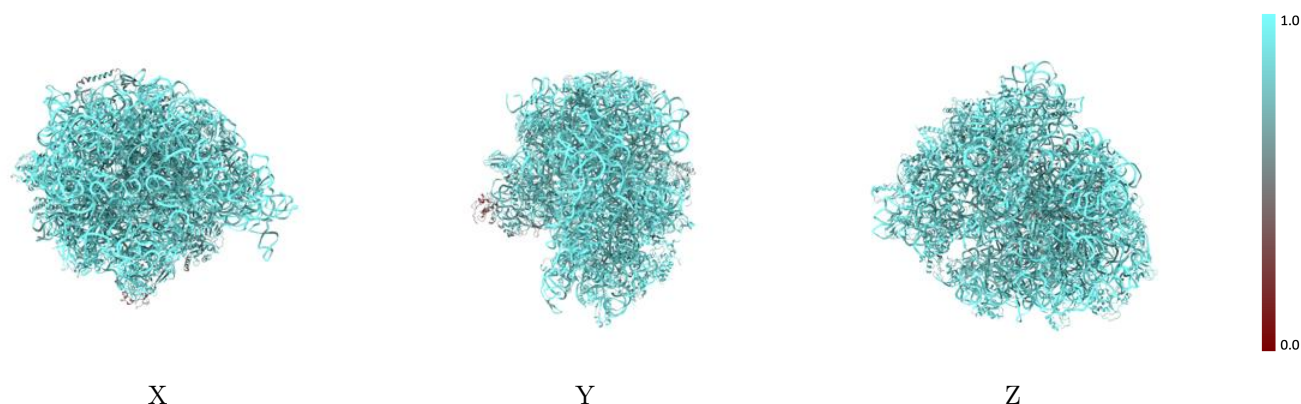
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



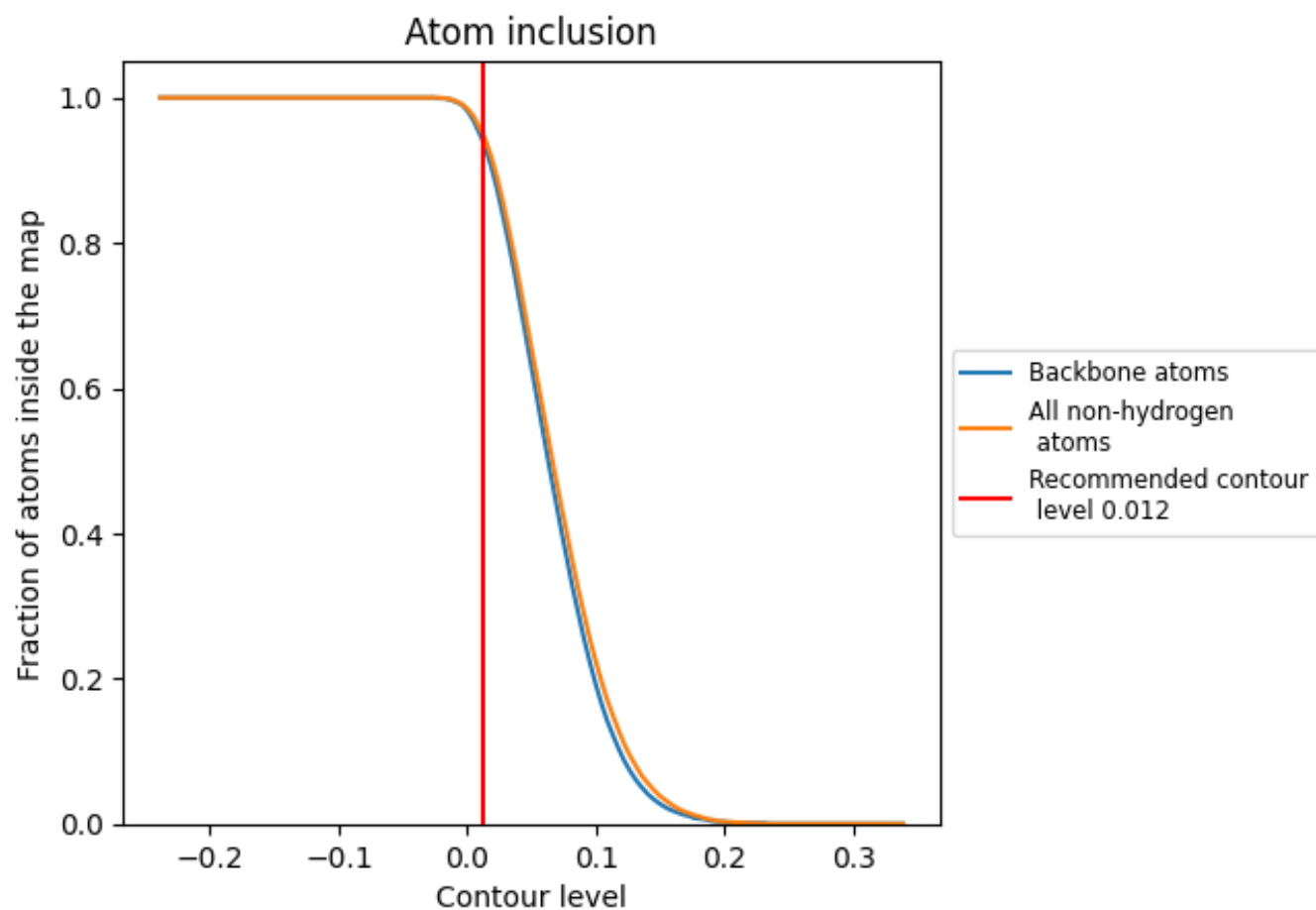
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 95% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.4300
0	 0.9550	 0.4670
1	 0.9360	 0.4560
2	 0.9680	 0.5380
3	 0.9660	 0.5360
4	 0.9520	 0.4900
5	 0.4510	 0.0600
6	 0.8160	 0.2270
A	 0.9770	 0.4660
B	 0.9880	 0.4460
C	 0.9540	 0.5210
D	 0.9510	 0.4850
E	 0.9300	 0.4370
F	 0.9180	 0.3760
G	 0.9260	 0.3680
H	 0.7450	 0.2170
I	 0.6590	 0.0620
J	 0.9540	 0.4880
K	 0.9330	 0.4840
L	 0.9440	 0.4660
M	 0.9590	 0.4920
N	 0.9710	 0.5000
O	 0.9410	 0.4150
P	 0.9300	 0.4700
Q	 0.9500	 0.5030
R	 0.9300	 0.4500
S	 0.9470	 0.4840
T	 0.9440	 0.4340
U	 0.9320	 0.3930
V	 0.9250	 0.4200
W	 0.9590	 0.5040
X	 0.9600	 0.4980
Y	 0.9150	 0.3980
Z	 0.9530	 0.4760
a	 0.9790	 0.4320



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Chain	Atom inclusion	Q-score
b	 0.8970	 0.3290
c	 0.9190	 0.4030
d	 0.9000	 0.3200
e	 0.9440	 0.4660
f	 0.9060	 0.3880
g	 0.9110	 0.3490
h	 0.9380	 0.4540
i	 0.8990	 0.3540
j	 0.8870	 0.3190
k	 0.9530	 0.4630
l	 0.9240	 0.4540
m	 0.9240	 0.3980
n	 0.9230	 0.4110
o	 0.9450	 0.4440
p	 0.9190	 0.3680
q	 0.9260	 0.4080
r	 0.9160	 0.4050
s	 0.9210	 0.3740
t	 0.9290	 0.3720
u	 0.8280	 0.3150
v	 0.9680	 0.4300
w	 0.8360	 0.1220
x	 0.9560	 0.4200
y	 0.8940	 0.2930
z	 0.8150	 0.2890