wwPDB EM Validation Summary Report ⓘ

Oct 5, 2024 – 08:21 PM EDT

PDB ID	:	5WF0
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)

The following versions of software and data (see references ⓘ) were used in the production of this report:

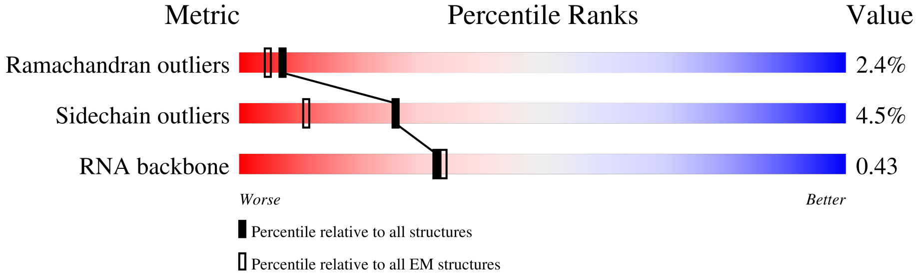
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance

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

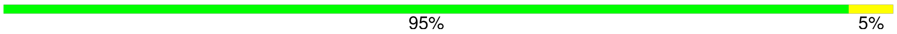
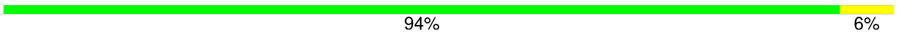
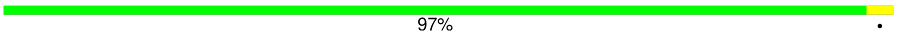
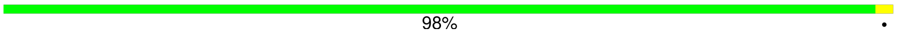
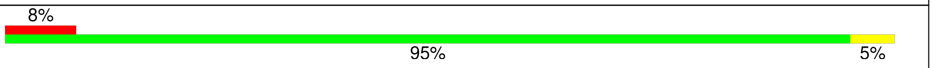
The reported resolution of this entry is 3.60 Å.

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	2903	
2	B	120	
3	C	271	
4	D	208	
5	E	200	
6	F	177	
7	G	174	
8	H	149	

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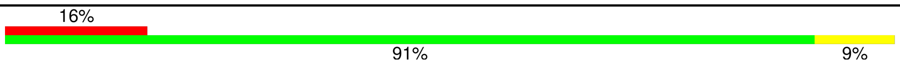
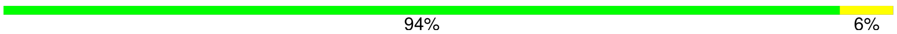
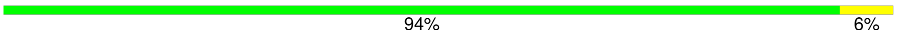
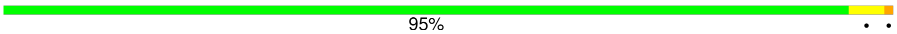
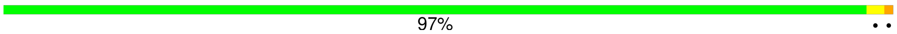
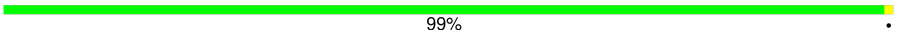
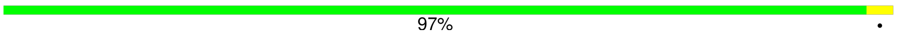
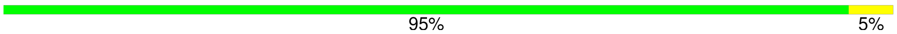
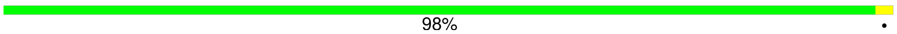
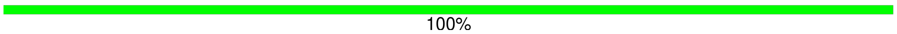
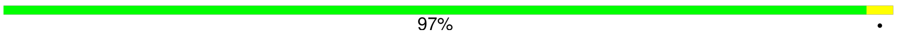
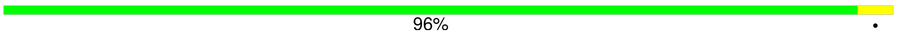
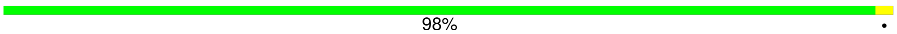
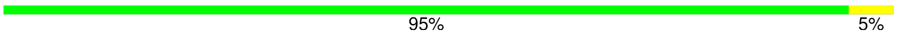
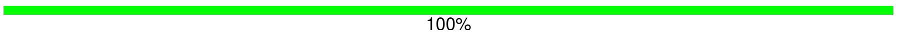
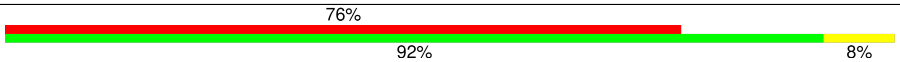
Mol	Chain	Length	Quality of chain
9	I	141	 16% 91% 9%
10	J	141	 94% 6%
11	K	122	 92% 7% •
12	L	143	 92% 8% •
13	M	136	 94% 6%
14	N	119	 95% • •
15	O	116	 97% • •
16	P	114	 99% •
17	Q	115	 97% •
18	R	102	 92% 7% •
19	S	109	 95% 5%
20	T	92	 92% 8%
21	U	102	 91% 9%
22	V	92	 98% •
23	W	75	 92% 8%
24	X	77	 100%
25	Y	60	 97% •
26	Z	56	 96% •
27	0	55	 98% •
28	1	51	 92% 8%
29	2	45	 91% 9%
30	3	64	 95% 5%
31	4	38	 100%
32	5	131	 76% 92% 8%
33	6	66	 • 89% 11%

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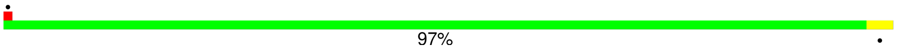
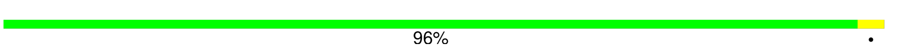
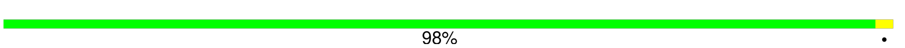
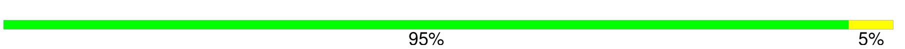
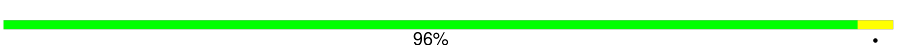
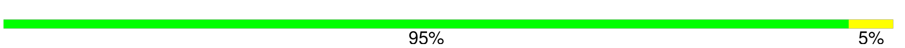
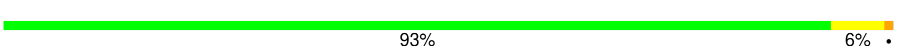
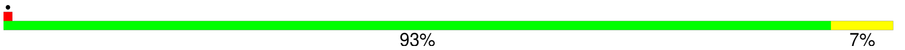
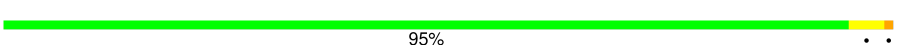
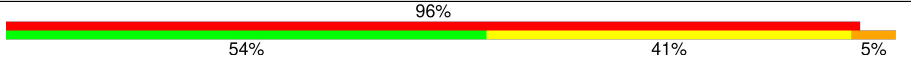
Mol	Chain	Length	Quality of chain
34	a	1540	
35	b	218	
36	c	206	
37	d	205	
38	e	157	
39	f	100	
40	g	151	
41	h	129	
42	i	127	
43	j	98	
44	k	116	
45	l	121	
46	m	115	
47	n	101	
48	o	88	
49	p	82	
50	q	80	
51	r	65	
52	s	79	
53	t	85	
54	u	65	
55	v	77	
55	w	77	
56	x	12	
57	y	76	

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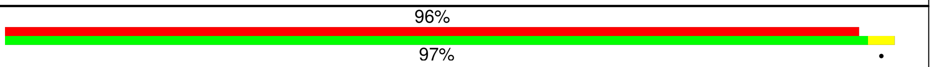
Mol	Chain	Length	Quality of chain
58	z	393	

2 Entry composition (i)

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

There are 3 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	e	157	1156	719	218	213	6	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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
			Total	C	N	O	S		
48	o	88	714	439	144	130	1	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called mRNA.

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

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

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

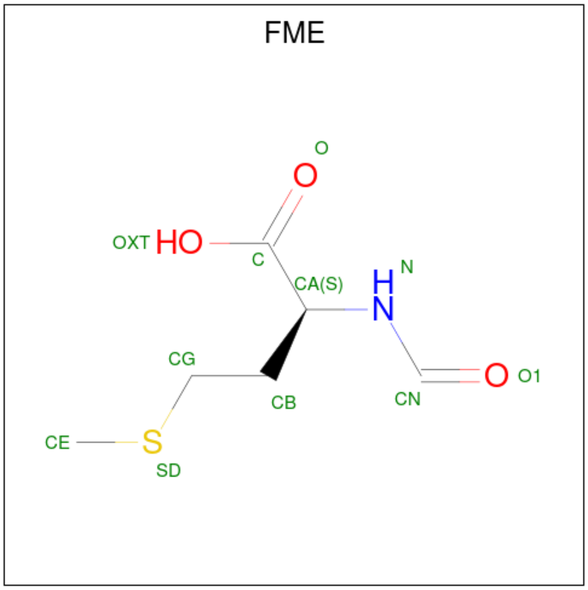
- Molecule 58 is a protein called Elongation factor Tu 2.

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

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 (three-letter code: FME) (formula: $C_6H_{11}NO_3S$).



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

- Molecule 60 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
60	A	1001	Total Mg 1001 1001	0
60	B	34	Total Mg 34 34	0
60	D	2	Total Mg 2 2	0
60	E	2	Total Mg 2 2	0
60	L	3	Total Mg 3 3	0
60	M	1	Total Mg 1 1	0
60	N	2	Total Mg 2 2	0
60	Q	2	Total Mg 2 2	0
60	T	1	Total Mg 1 1	0
60	W	2	Total Mg 2 2	0
60	X	2	Total Mg 2 2	0

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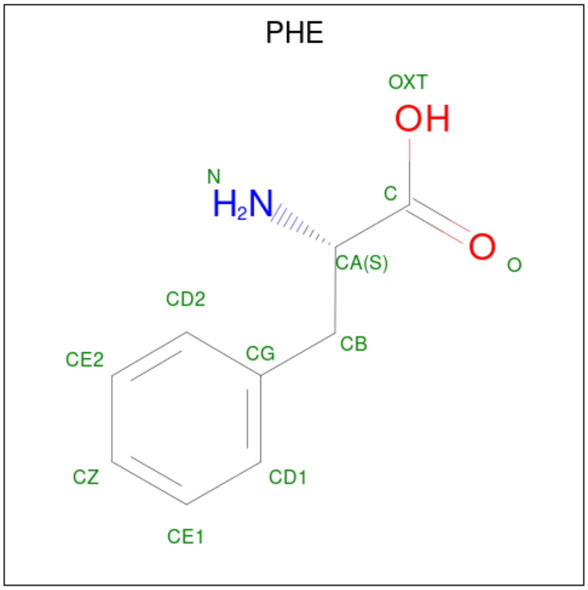
Mol	Chain	Residues	Atoms		AltConf
60	0	1	Total 1	Mg 1	0
60	4	1	Total 1	Mg 1	0
60	a	402	Total 402	Mg 402	0
60	d	3	Total 3	Mg 3	0
60	g	1	Total 1	Mg 1	0
60	i	2	Total 2	Mg 2	0
60	k	1	Total 1	Mg 1	0
60	m	1	Total 1	Mg 1	0
60	n	1	Total 1	Mg 1	0
60	o	2	Total 2	Mg 2	0
60	t	3	Total 3	Mg 3	0
60	v	8	Total 8	Mg 8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

- Molecule 61 is POTASSIUM ION (three-letter code: K) (formula: K).

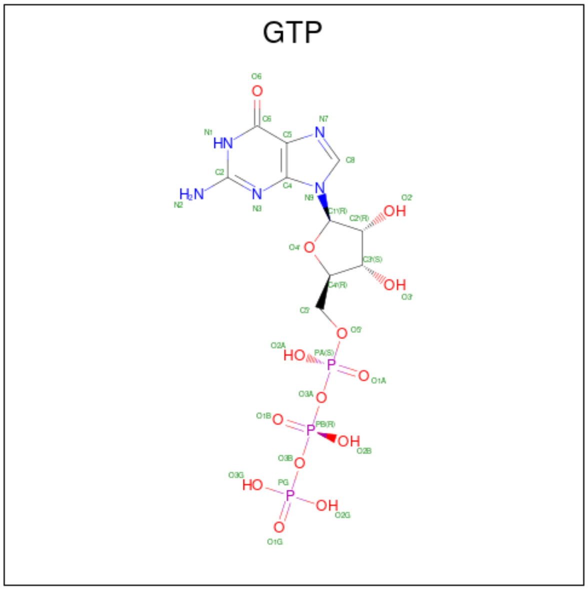
Mol	Chain	Residues	Atoms		AltConf
61	A	4	Total 4	K 4	0
61	a	1	Total 1	K 1	0

- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



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

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



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

- Molecule 64 is water.

Mol	Chain	Residues	Atoms	AltConf
64	A	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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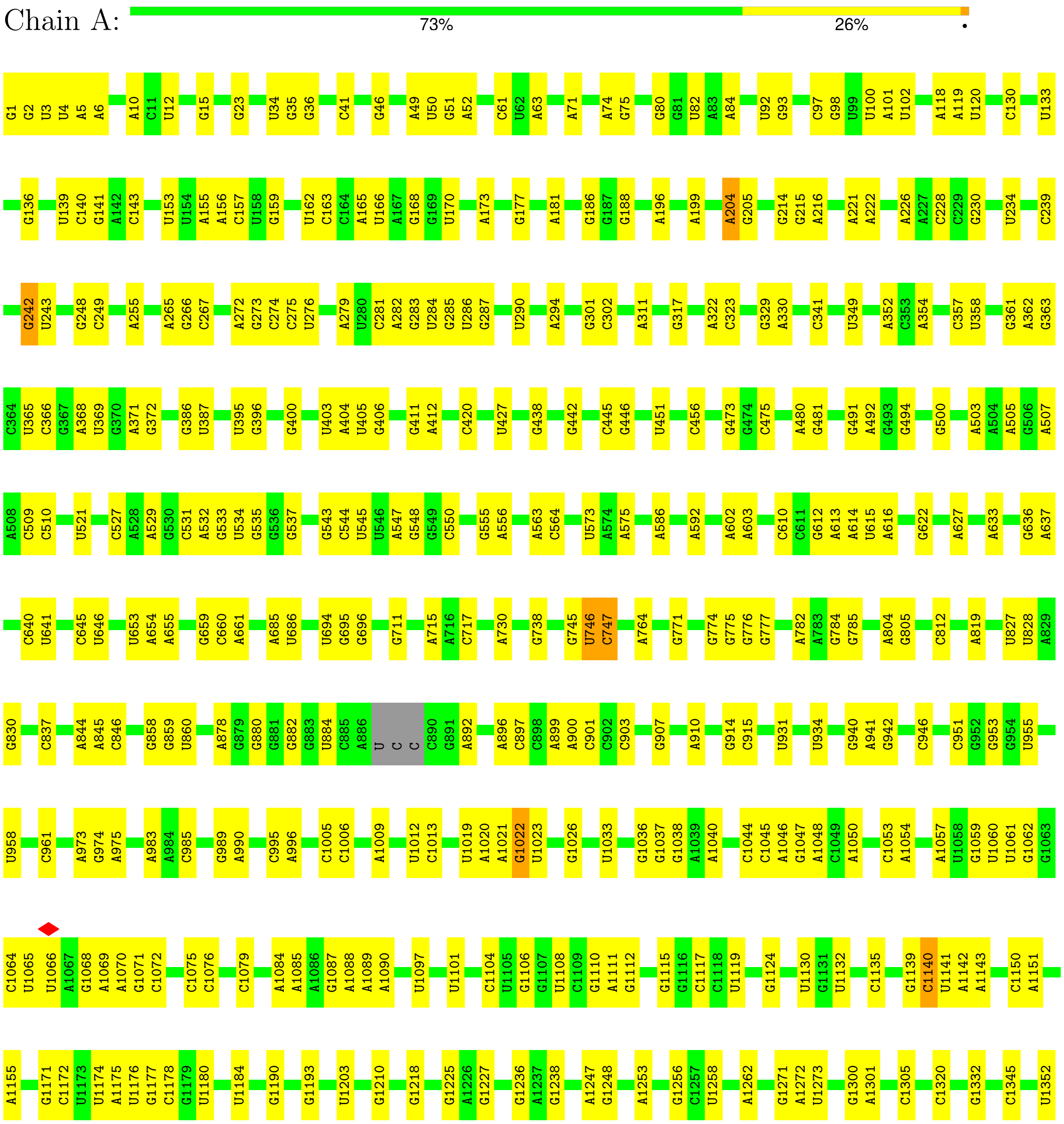
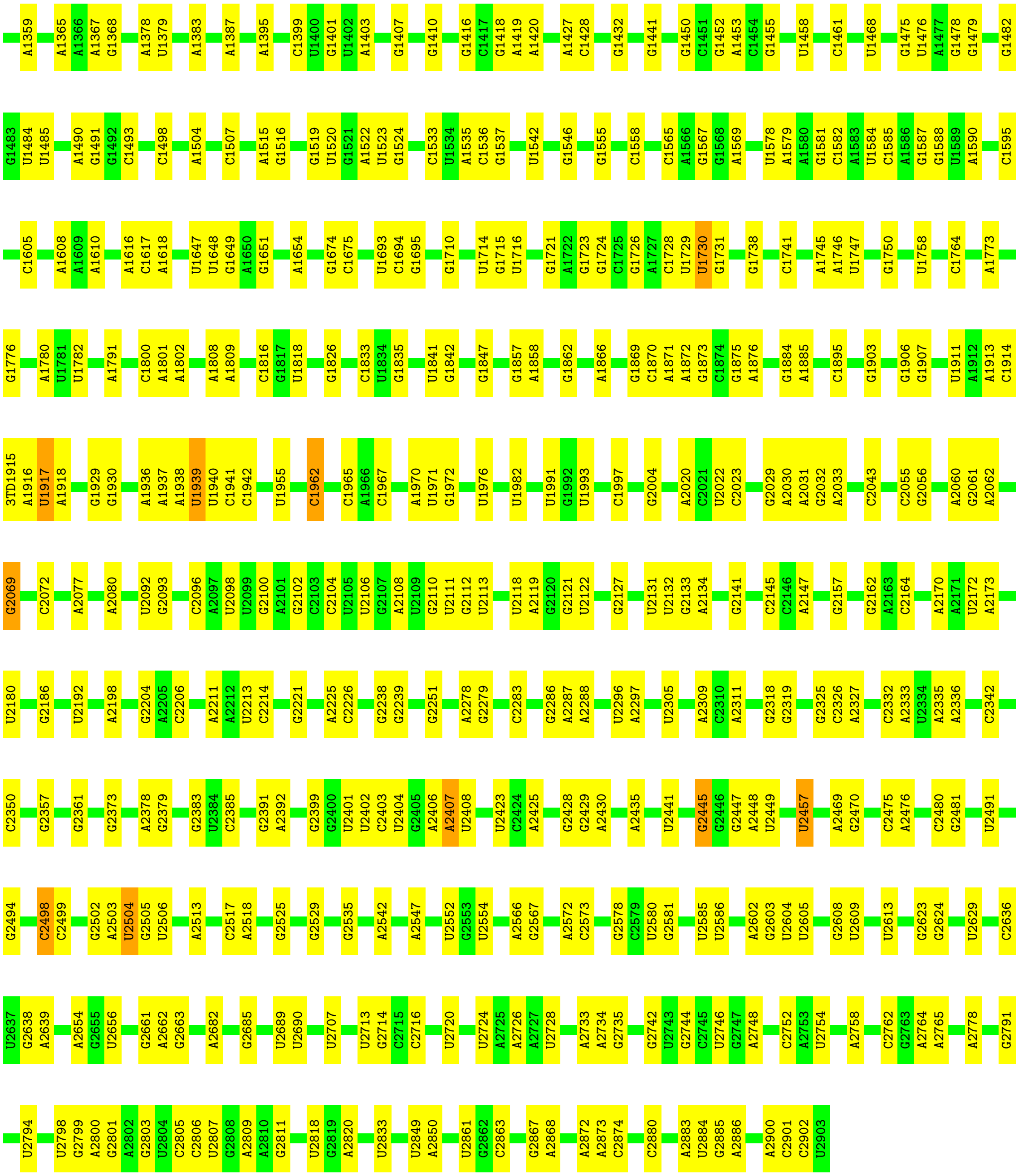
Mol	**Chain**	**Residues**	**Atoms**		**AltConf**
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	w	2	Total 2	O 2	0

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.

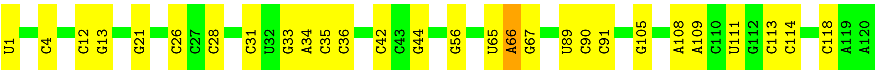
- Molecule 1: 23S rRNA





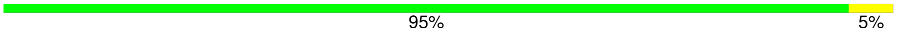
- Molecule 2: 5S rRNA

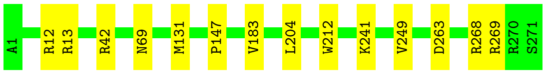
Chain B:



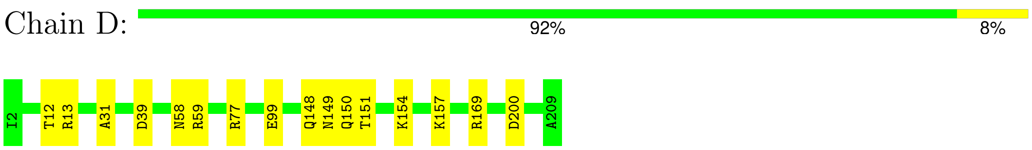
- Molecule 3: 50S ribosomal protein L2

Chain C:

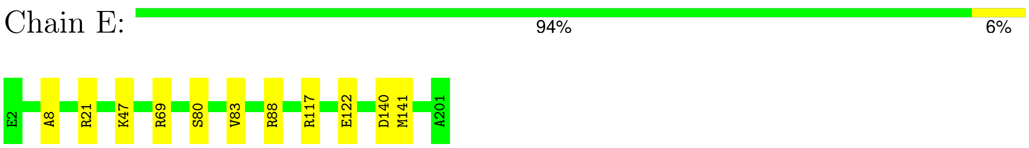




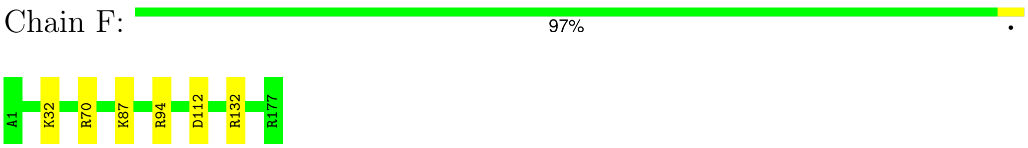
- Molecule 4: 50S ribosomal protein L3



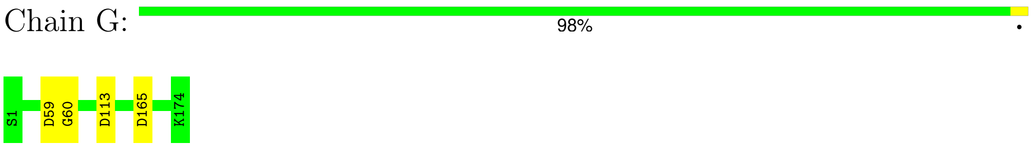
- Molecule 5: 50S ribosomal protein L4



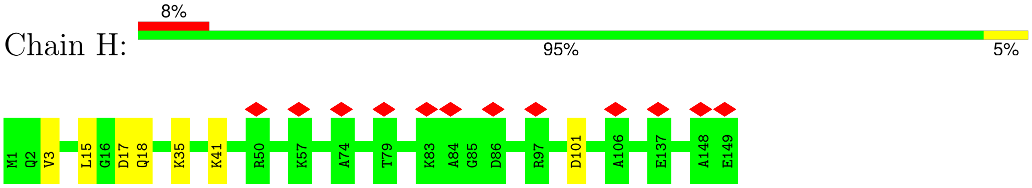
- Molecule 6: 50S ribosomal protein L5



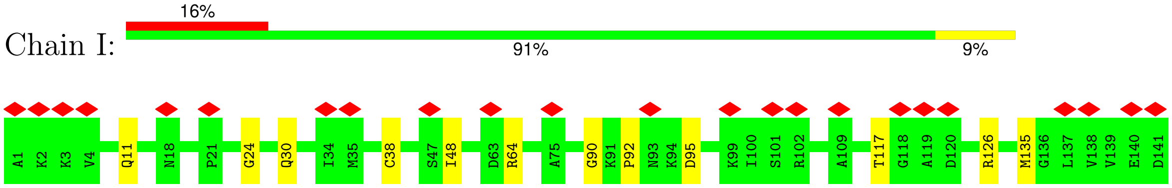
- Molecule 7: 50S ribosomal protein L6



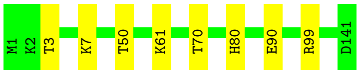
- Molecule 8: 50S ribosomal protein L9



- Molecule 9: 50S ribosomal protein L11

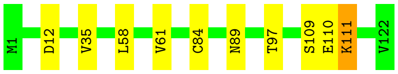


- Molecule 10: 50S ribosomal protein L13



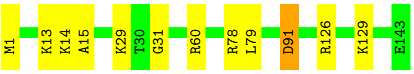
- Molecule 11: 50S ribosomal protein L14

Chain K:



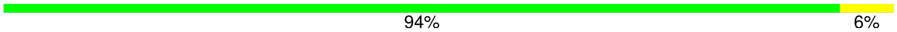
- Molecule 12: 50S ribosomal protein L15

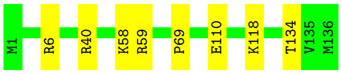
Chain L:



- Molecule 13: 50S ribosomal protein L16

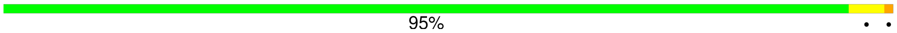
Chain M:

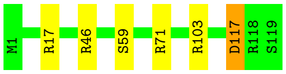




- Molecule 14: 50S ribosomal protein L17

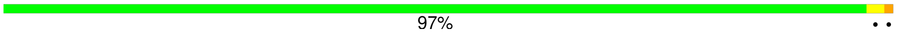
Chain N:

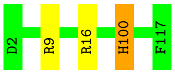




- Molecule 15: 50S ribosomal protein L18

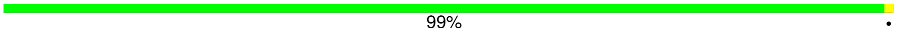
Chain O:

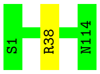




- Molecule 16: 50S ribosomal protein L19

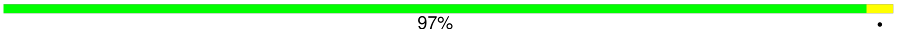
Chain P:

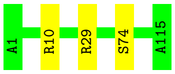




- Molecule 17: 50S ribosomal protein L20

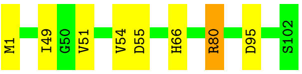
Chain Q:





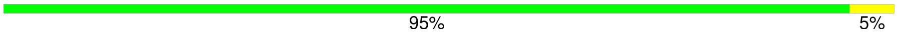
- Molecule 18: 50S ribosomal protein L21

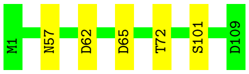
Chain R:



- Molecule 19: 50S ribosomal protein L22

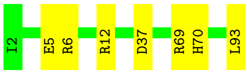
Chain S:





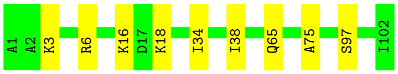
- Molecule 20: 50S ribosomal protein L23

Chain T:



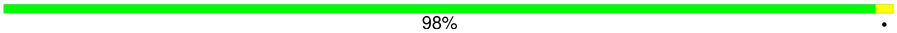
- Molecule 21: 50S ribosomal protein L24

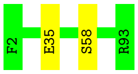
Chain U:



- Molecule 22: 50S ribosomal protein L25

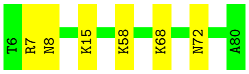
Chain V:





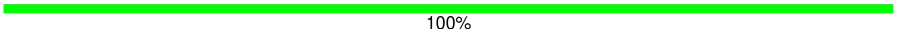
- Molecule 23: 50S ribosomal protein L27

Chain W:



- Molecule 24: 50S ribosomal protein L28

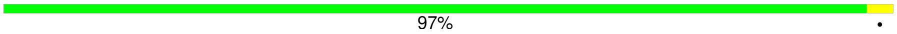
Chain X:

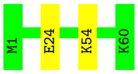


There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L29

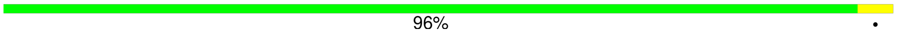
Chain Y:

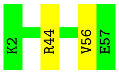




- Molecule 26: 50S ribosomal protein L30

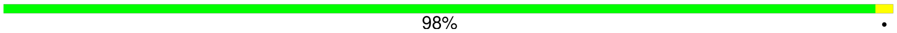
Chain Z:

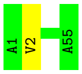




- Molecule 27: 50S ribosomal protein L32

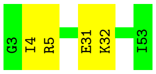
Chain 0:





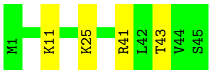
- Molecule 28: 50S ribosomal protein L33

Chain 1:



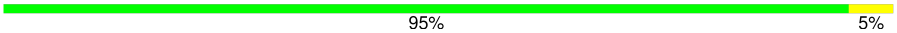
- Molecule 29: 50S ribosomal protein L34

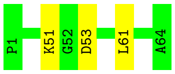
Chain 2:



- Molecule 30: 50S ribosomal protein L35

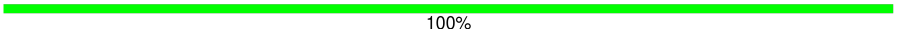
Chain 3:





- Molecule 31: 50S ribosomal protein L36 1

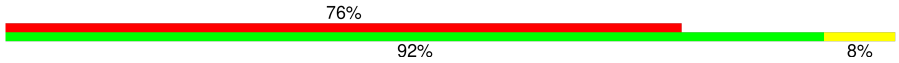
Chain 4:

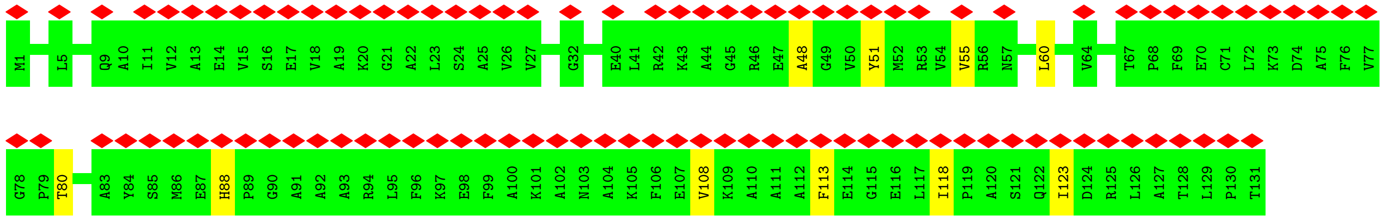


There are no outlier residues recorded for this chain.

- Molecule 32: 50S ribosomal protein L10

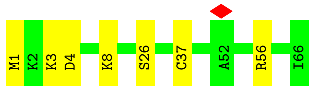
Chain 5:





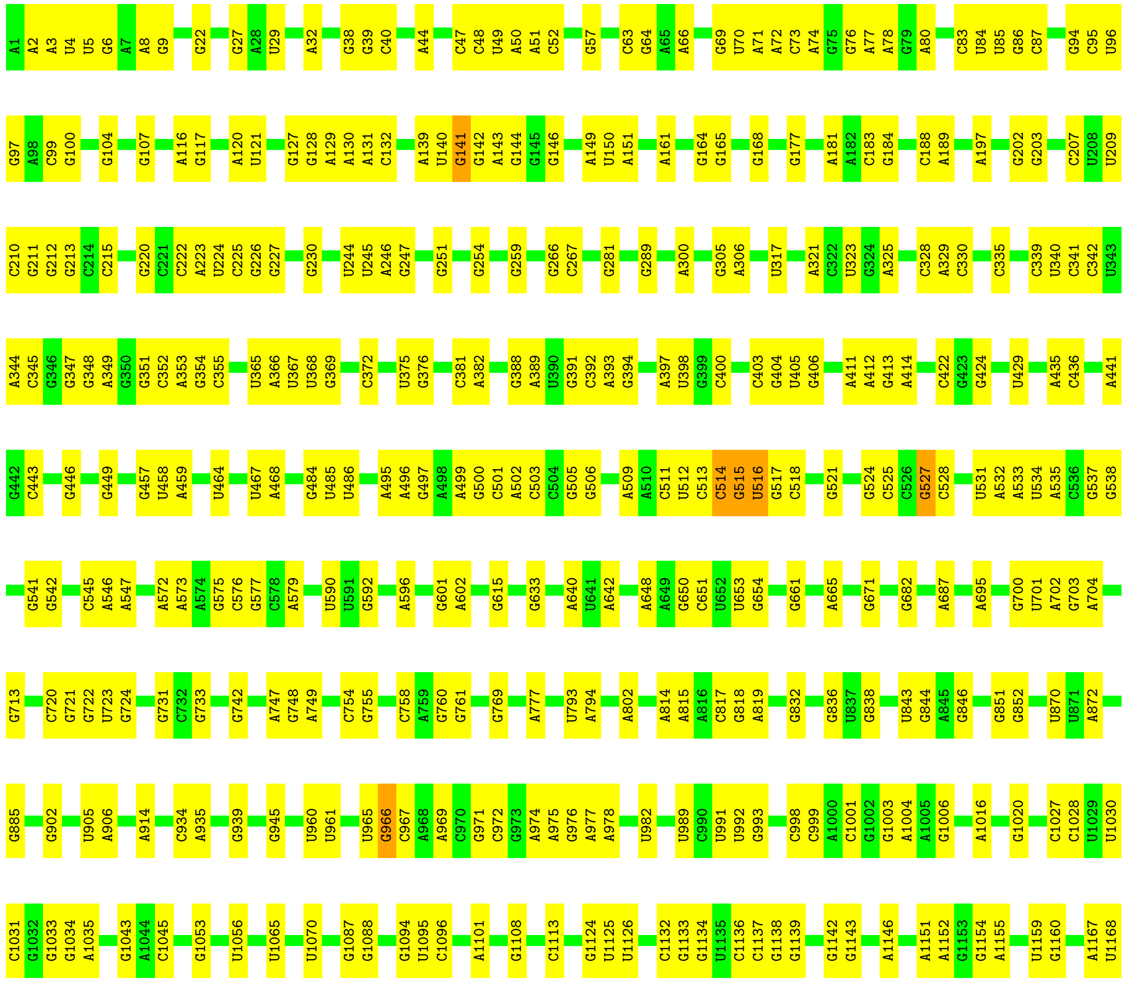
- Molecule 33: 50S ribosomal protein L31

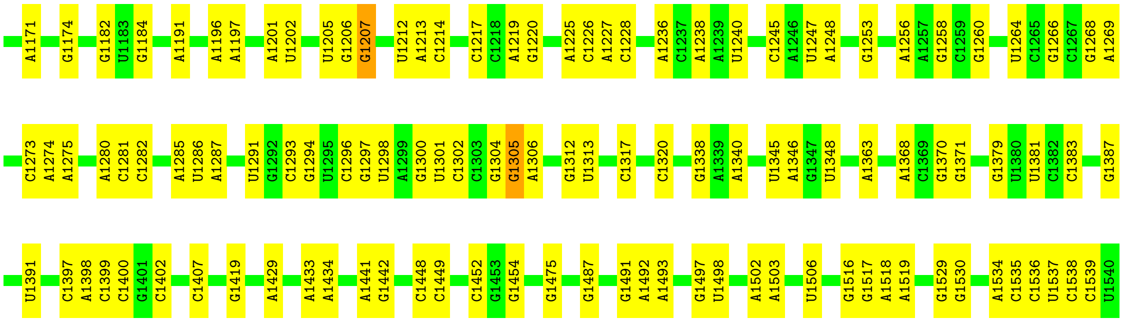
Chain 6:



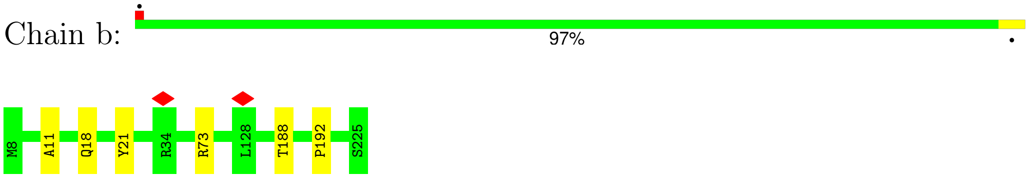
- Molecule 34: 16S rRNA

Chain a:

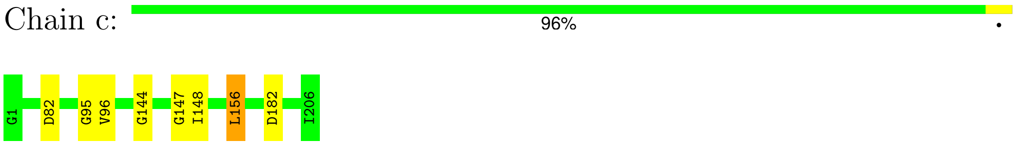




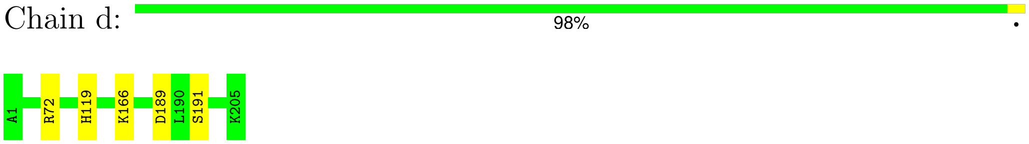
- Molecule 35: 30S ribosomal protein S2



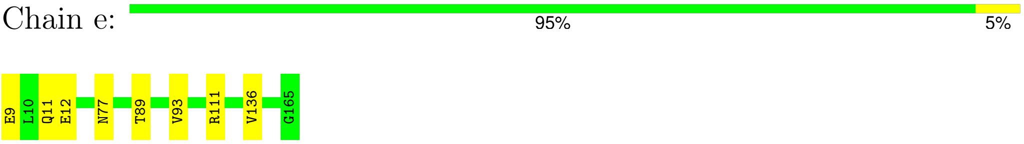
- Molecule 36: 30S ribosomal protein S3



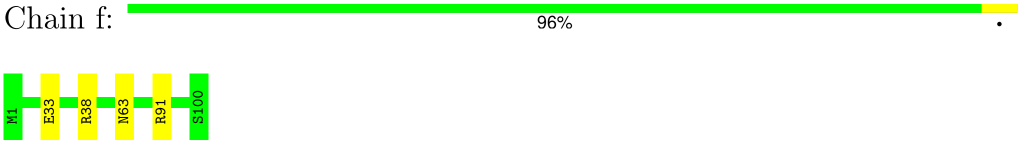
- Molecule 37: 30S ribosomal protein S4



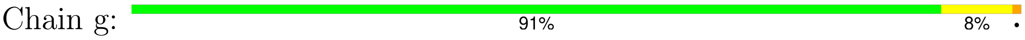
- Molecule 38: 30S ribosomal protein S5

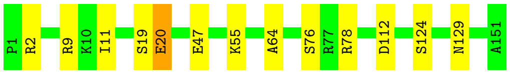


- Molecule 39: 30S ribosomal protein S6



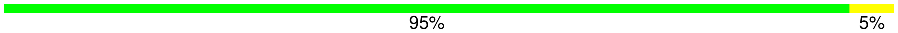
- Molecule 40: 30S ribosomal protein S7

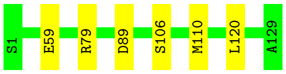




- Molecule 41: 30S ribosomal protein S8

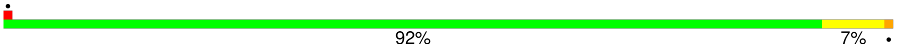
Chain h:

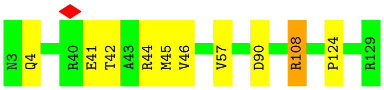




- Molecule 42: 30S ribosomal protein S9

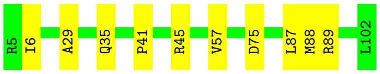
Chain i:





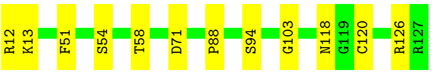
- Molecule 43: 30S ribosomal protein S10

Chain j:



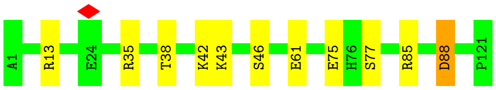
- Molecule 44: 30S ribosomal protein S11

Chain k:



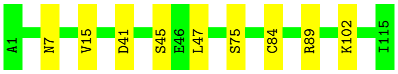
- Molecule 45: 30S ribosomal protein S12

Chain l:



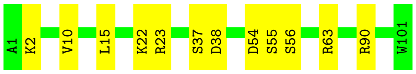
- Molecule 46: 30S ribosomal protein S13

Chain m:



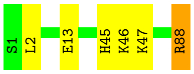
- Molecule 47: 30S ribosomal protein S14

Chain n:



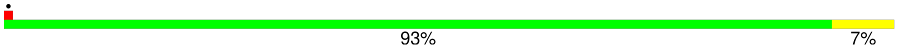
- Molecule 48: 30S ribosomal protein S15

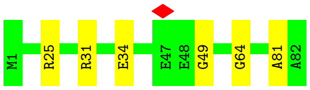
Chain o:



- Molecule 49: 30S ribosomal protein S16

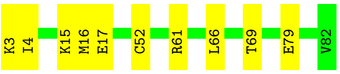
Chain p:





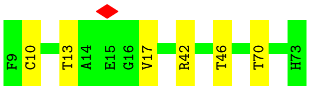
- Molecule 50: 30S ribosomal protein S17

Chain q:



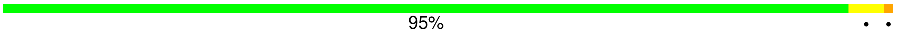
- Molecule 51: 30S ribosomal protein S18

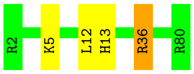
Chain r:



- Molecule 52: 30S ribosomal protein S19

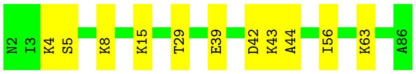
Chain s:





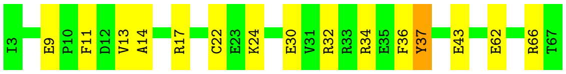
- Molecule 53: 30S ribosomal protein S20

Chain t:

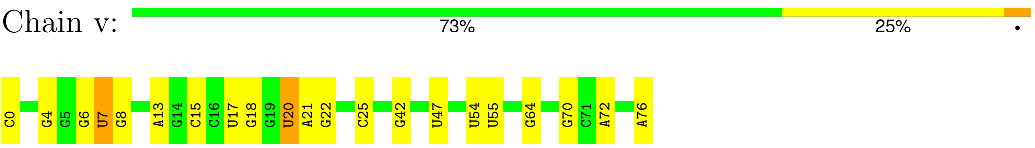


- Molecule 54: 30S ribosomal protein S21

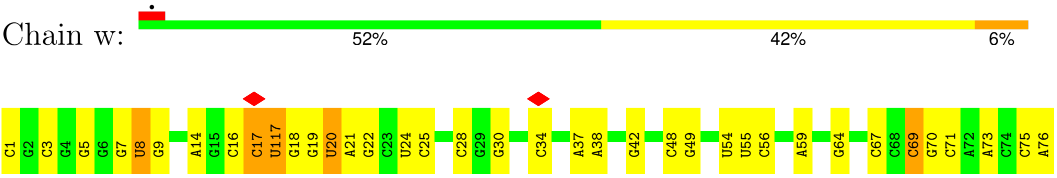
Chain u:



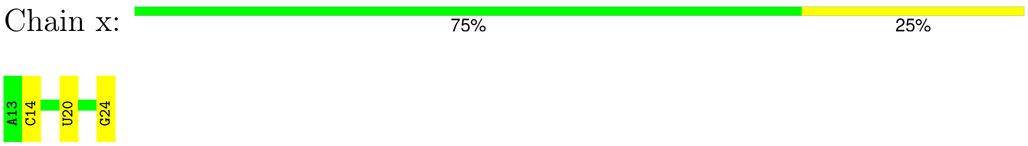
- Molecule 55: tRNA-fMet



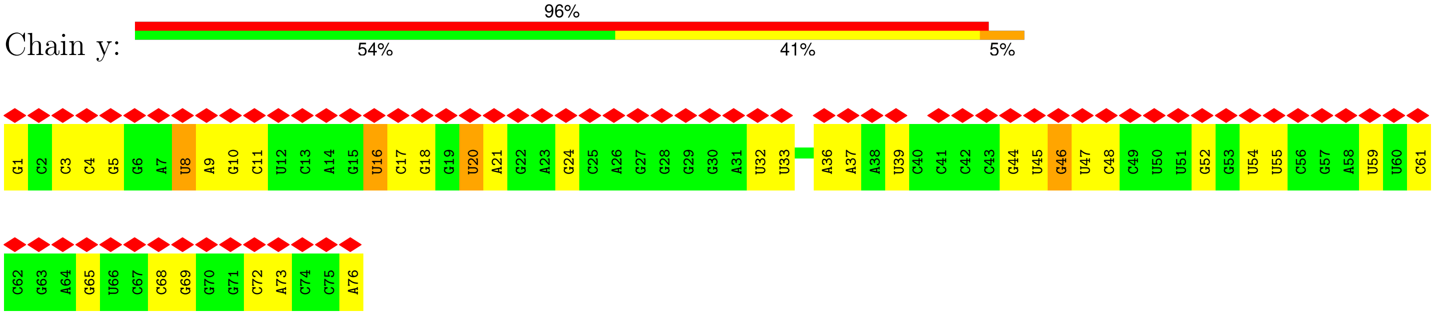
- Molecule 55: tRNA-fMet



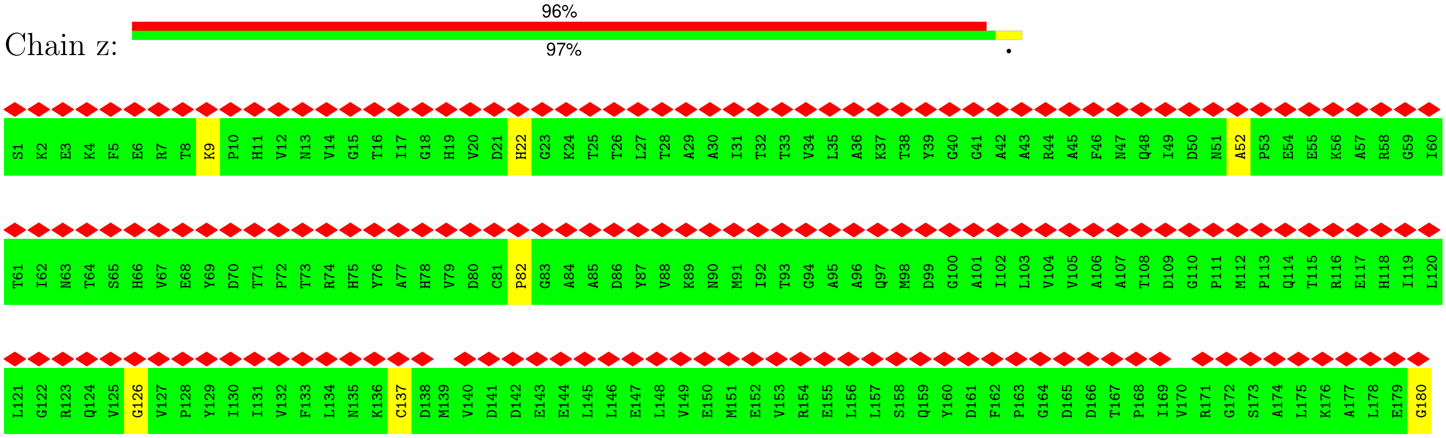
- Molecule 56: mRNA



- Molecule 57: Phe-tRNA-Phe



- Molecule 58: Elongation factor Tu 2




D181 A182 E183 W184 E185 A186 K187 I188 L189 E190 L191 A192 G193 F194 L195 D196 S197 Y198 I199 P200 E201 P202 E203 R204 A205 I206 D207 K208 P209 F210 L211 L212 P213 I214 E215 D216 V217 F218 S219 G222 T225 V226 V227 T228 G229 R230 V231 E232 R233 G234 I235 I236 K237 V238 G239 E240 E241 V242
E243 I244 V245 G246 I247 K248 E249 T250 Q251 K252 S253 T254 C255 T256 G257 V258 E259 M260 F261 R262 K263 L264 L265 D266 E267 G268 R269 A270 G271 E272 N273 V274 G275 V276 L277 L278 I281 K282 R283 E284 E285 I286 E287 R288 G289 Q290 V291 L292 A293 K294 P295 G296 T297 I298 K299 P300 H301 T302 K303
F304 E305 S306 E307 V308 Y309 I310 L311 S312 K313 D314 E315 G316 G317 R318 H319 T320 P321 F322 F323 K324 G325 Y326 R327 P328 Q329 F330 Y331 F332 R333 T334 T335 D336 V337 T338 G339 T340 I341 E342 L343 P344 E345 G346 V347 E348 M349 V350 M351 P352 G353 D354 N355 I356 K357 M358 V359 V360 T361 L362 I363
H364 P365 I366 A367 M368 D369 D370 G371 L372 R373 F374 A375 I376 R377 E378 G379 G380 R381 T382 V383 G384 A385 G386 V387 V388 A389 K390 V391 L392 S393

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 $(e^-/\text{Å}^2)$	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: MG, MIA, FME, OMU, UR3, 1MG, 4OC, 2MG, 5MC, H2U, 7MG, GTP, 3TD, K, OMG, 5MU, 6MZ, 2MA, OMC, 4SU, PSU, MA6

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	0.22	1/69174 (0.0%)	0.68	6/107907 (0.0%)
2	B	0.27	1/2876 (0.0%)	0.67	1/4483 (0.0%)
3	C	0.34	0/2121	0.65	0/2852
4	D	0.35	0/1578	0.59	0/2124
5	E	0.35	0/1563	0.59	0/2103
6	F	0.37	0/1434	0.62	0/1926
7	G	0.36	0/1324	0.55	0/1794
8	H	0.37	0/1122	0.51	0/1515
9	I	0.42	0/1046	0.63	0/1410
10	J	0.34	0/1143	0.58	0/1540
11	K	0.35	0/947	0.64	0/1268
12	L	0.36	0/1052	0.70	2/1401 (0.1%)
13	M	0.36	0/1093	0.64	0/1460
14	N	0.39	0/964	0.72	0/1289
15	O	0.37	0/902	0.64	0/1209
16	P	0.35	0/929	0.63	0/1242
17	Q	0.37	0/946	0.69	1/1260 (0.1%)
18	R	0.36	0/823	0.75	2/1100 (0.2%)
19	S	0.33	0/852	0.66	0/1142
20	T	0.36	0/736	0.67	0/984
21	U	0.35	0/787	0.60	0/1051
22	V	0.36	0/752	0.56	0/1008
23	W	0.34	0/579	0.64	0/767
24	X	0.36	0/635	0.60	0/848
25	Y	0.37	0/495	0.60	0/658
26	Z	0.37	0/438	0.62	0/586
27	0	0.33	0/440	0.64	0/588
28	1	0.34	0/424	0.57	0/565
29	2	0.40	0/370	0.75	0/487
30	3	0.33	0/513	0.57	0/676
31	4	0.33	0/303	0.64	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	5	0.42	0/1001	0.59	0/1350
33	6	0.40	0/531	0.58	0/709
34	a	0.23	0/36725	0.70	7/57285 (0.0%)
35	b	0.37	0/1735	0.53	0/2338
36	c	0.36	0/1651	0.57	0/2225
37	d	0.37	0/1665	0.60	0/2227
38	e	0.35	0/1169	0.60	0/1573
39	f	0.37	0/835	0.59	0/1128
40	g	0.36	0/1195	0.61	0/1602
41	h	0.35	0/989	0.61	0/1326
42	i	0.38	0/1034	0.67	0/1375
43	j	0.37	0/796	0.64	0/1077
44	k	0.37	0/885	0.64	0/1195
45	l	0.37	0/954	0.67	0/1282
46	m	0.38	0/900	0.66	0/1204
47	n	0.39	0/822	0.65	0/1095
48	o	0.36	0/722	0.63	1/964 (0.1%)
49	p	0.37	0/659	0.66	0/884
50	q	0.37	0/657	0.65	0/881
51	r	0.39	0/544	0.59	0/731
52	s	0.37	0/652	0.61	0/877
53	t	0.36	0/671	0.62	0/888
54	u	0.45	0/550	0.78	0/728
55	v	0.32	1/1747 (0.1%)	0.68	0/2721
55	w	0.38	2/1747 (0.1%)	0.80	6/2721 (0.2%)
56	x	0.27	0/280	0.68	0/433
57	y	0.33	1/1607 (0.1%)	0.66	0/2501
58	z	0.36	0/3086	0.55	0/4175
All	All	0.28	6/164170 (0.0%)	0.67	26/245135 (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

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	1	C	OP3-P	-10.20	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	v	0	C	OP3-P	-10.18	1.49	1.61
57	y	1	G	OP3-P	-10.18	1.49	1.61
2	B	1	U	OP3-P	-10.15	1.49	1.61
1	A	1	G	OP3-P	-10.10	1.49	1.61

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	w	117	U	P-O3'-C3'	14.22	136.76	119.70
55	w	17	C	O3'-P-O5'	12.87	128.46	104.00
18	R	80	ARG	NE-CZ-NH1	9.52	125.06	120.30
34	a	515	G	C2'-C3'-O3'	7.58	126.16	109.50
1	A	242	G	C2'-C3'-O3'	7.44	125.88	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)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	19	53
4	D	206/208 (99%)	187 (91%)	15 (7%)	4 (2%)	6	35
5	E	198/200 (99%)	181 (91%)	13 (7%)	4 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	175/177 (99%)	158 (90%)	17 (10%)	0	100	100
7	G	172/174 (99%)	156 (91%)	15 (9%)	1 (1%)	22	55
8	H	147/149 (99%)	126 (86%)	18 (12%)	3 (2%)	6	34
9	I	139/141 (99%)	110 (79%)	24 (17%)	5 (4%)	3	23
10	J	139/141 (99%)	132 (95%)	7 (5%)	0	100	100
11	K	120/122 (98%)	104 (87%)	12 (10%)	4 (3%)	3	25
12	L	141/143 (99%)	115 (82%)	22 (16%)	4 (3%)	4	27
13	M	134/136 (98%)	124 (92%)	7 (5%)	3 (2%)	5	32
14	N	117/119 (98%)	105 (90%)	10 (8%)	2 (2%)	7	37
15	O	114/116 (98%)	105 (92%)	8 (7%)	1 (1%)	14	48
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	21
19	S	107/109 (98%)	98 (92%)	8 (8%)	1 (1%)	14	48
20	T	90/92 (98%)	77 (86%)	11 (12%)	2 (2%)	5	32
21	U	100/102 (98%)	84 (84%)	12 (12%)	4 (4%)	2	21
22	V	90/92 (98%)	84 (93%)	5 (6%)	1 (1%)	12	45
23	W	73/75 (97%)	65 (89%)	7 (10%)	1 (1%)	9	40
24	X	75/77 (97%)	69 (92%)	6 (8%)	0	100	100
25	Y	58/60 (97%)	55 (95%)	2 (3%)	1 (2%)	7	37
26	Z	54/56 (96%)	52 (96%)	2 (4%)	0	100	100
27	0	53/55 (96%)	47 (89%)	5 (9%)	1 (2%)	6	35
28	1	49/51 (96%)	41 (84%)	6 (12%)	2 (4%)	2	20
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	9
33	6	64/66 (97%)	54 (84%)	9 (14%)	1 (2%)	8	38
35	b	216/218 (99%)	187 (87%)	25 (12%)	4 (2%)	6	35
36	c	204/206 (99%)	184 (90%)	14 (7%)	6 (3%)	3	27
37	d	203/205 (99%)	181 (89%)	20 (10%)	2 (1%)	13	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	e	155/157 (99%)	129 (83%)	23 (15%)	3 (2%)	6	35
39	f	98/100 (98%)	84 (86%)	12 (12%)	2 (2%)	6	34
40	g	149/151 (99%)	132 (89%)	12 (8%)	5 (3%)	3	25
41	h	127/129 (98%)	118 (93%)	9 (7%)	0	100	100
42	i	125/127 (98%)	96 (77%)	24 (19%)	5 (4%)	2	21
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	19
45	l	119/121 (98%)	98 (82%)	14 (12%)	7 (6%)	1	14
46	m	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	7	35
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	1	16
48	o	86/88 (98%)	79 (92%)	3 (4%)	4 (5%)	2	18
49	p	80/82 (98%)	69 (86%)	8 (10%)	3 (4%)	2	22
50	q	78/80 (98%)	71 (91%)	4 (5%)	3 (4%)	2	22
51	r	63/65 (97%)	52 (82%)	7 (11%)	4 (6%)	1	13
52	s	77/79 (98%)	68 (88%)	8 (10%)	1 (1%)	10	41
53	t	83/85 (98%)	73 (88%)	7 (8%)	3 (4%)	3	23
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	27
All	All	6218/6322 (98%)	5461 (88%)	605 (10%)	152 (2%)	7	30

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%)	204 (94%)	12 (6%)	17	47
4	D	163/163 (100%)	151 (93%)	12 (7%)	11	37
5	E	164/164 (100%)	157 (96%)	7 (4%)	25	54
6	F	148/148 (100%)	142 (96%)	6 (4%)	26	55
7	G	135/135 (100%)	132 (98%)	3 (2%)	47	69
8	H	114/114 (100%)	110 (96%)	4 (4%)	31	60
9	I	109/109 (100%)	102 (94%)	7 (6%)	14	43
10	J	115/115 (100%)	107 (93%)	8 (7%)	12	40
11	K	103/103 (100%)	96 (93%)	7 (7%)	13	41
12	L	102/102 (100%)	94 (92%)	8 (8%)	10	36
13	M	109/109 (100%)	104 (95%)	5 (5%)	23	52
14	N	99/99 (100%)	94 (95%)	5 (5%)	20	49
15	O	86/86 (100%)	83 (96%)	3 (4%)	31	60
16	P	99/99 (100%)	98 (99%)	1 (1%)	73	85
17	Q	88/88 (100%)	86 (98%)	2 (2%)	45	68
18	R	84/84 (100%)	80 (95%)	4 (5%)	21	51
19	S	92/92 (100%)	88 (96%)	4 (4%)	25	54
20	T	79/79 (100%)	74 (94%)	5 (6%)	15	44
21	U	83/83 (100%)	78 (94%)	5 (6%)	16	45
22	V	77/77 (100%)	76 (99%)	1 (1%)	65	81
23	W	57/57 (100%)	52 (91%)	5 (9%)	8	32
24	X	67/67 (100%)	67 (100%)	0	100	100
25	Y	55/55 (100%)	54 (98%)	1 (2%)	54	74
26	Z	47/47 (100%)	45 (96%)	2 (4%)	25	54
27	0	46/46 (100%)	46 (100%)	0	100	100
28	1	46/46 (100%)	44 (96%)	2 (4%)	25	54
29	2	37/37 (100%)	33 (89%)	4 (11%)	5	25
30	3	51/51 (100%)	48 (94%)	3 (6%)	16	45
31	4	34/34 (100%)	34 (100%)	0	100	100
32	5	100/100 (100%)	100 (100%)	0	100	100
33	6	59/59 (100%)	53 (90%)	6 (10%)	6	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	b	180/180 (100%)	178 (99%)	2 (1%)	70	83
36	c	170/170 (100%)	167 (98%)	3 (2%)	54	74
37	d	172/172 (100%)	169 (98%)	3 (2%)	56	75
38	e	119/119 (100%)	114 (96%)	5 (4%)	25	54
39	f	87/87 (100%)	85 (98%)	2 (2%)	45	68
40	g	124/124 (100%)	115 (93%)	9 (7%)	11	38
41	h	104/104 (100%)	98 (94%)	6 (6%)	17	46
42	i	105/105 (100%)	99 (94%)	6 (6%)	17	46
43	j	86/86 (100%)	83 (96%)	3 (4%)	31	60
44	k	89/89 (100%)	82 (92%)	7 (8%)	10	35
45	l	102/102 (100%)	97 (95%)	5 (5%)	21	50
46	m	93/93 (100%)	86 (92%)	7 (8%)	11	37
47	n	83/83 (100%)	76 (92%)	7 (8%)	9	34
48	o	76/76 (100%)	74 (97%)	2 (3%)	41	65
49	p	65/65 (100%)	62 (95%)	3 (5%)	23	52
50	q	74/74 (100%)	67 (90%)	7 (10%)	7	30
51	r	56/56 (100%)	54 (96%)	2 (4%)	30	59
52	s	70/70 (100%)	66 (94%)	4 (6%)	17	46
53	t	65/65 (100%)	57 (88%)	8 (12%)	4	20
54	u	55/55 (100%)	48 (87%)	7 (13%)	3	19
58	z	325/325 (100%)	324 (100%)	1 (0%)	91	96
All	All	5164/5164 (100%)	4933 (96%)	231 (4%)	26	53

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

Mol	Chain	Res	Type
26	Z	44	ARG
53	t	56	ILE
38	e	111	ARG
53	t	42	ASP
49	p	25	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
38	e	121	ASN
48	o	36	ASN
58	z	135	ASN
48	o	45	HIS
7	G	63	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2893/2903 (99%)	718 (24%)	74 (2%)
2	B	119/120 (99%)	25 (21%)	5 (4%)
34	a	1536/1540 (99%)	461 (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	74/76 (97%)	29 (39%)	0
All	All	4785/4805 (99%)	1288 (26%)	79 (1%)

5 of 1288 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	OMG	A	2251	55,1	19,26,27	1.04	2 (10%)	21,38,41	1.14	2 (9%)
1	PSU	A	2605	1	18,21,22	1.39	2 (11%)	21,30,33	2.07	4 (19%)
57	PSU	y	39	57	18,21,22	1.41	2 (11%)	21,30,33	2.00	4 (19%)
55	H2U	w	20	55	18,21,22	0.81	0	19,30,33	1.34	3 (15%)
34	PSU	a	516	34	18,21,22	1.36	2 (11%)	21,30,33	2.12	5 (23%)
34	MA6	a	1519	34	19,26,27	1.49	4 (21%)	18,38,41	2.54	6 (33%)
57	MIA	y	37	57	24,31,32	2.30	7 (29%)	22,44,47	2.58	8 (36%)
57	PSU	y	55	57	18,21,22	1.38	2 (11%)	21,30,33	2.03	4 (19%)
34	UR3	a	1498	34	19,22,23	1.13	2 (10%)	26,32,35	1.97	5 (19%)
55	4SU	w	8	55	18,21,22	1.82	5 (27%)	25,30,33	2.26	6 (24%)
57	H2U	y	16	57	18,21,22	0.82	1 (5%)	19,30,33	1.40	3 (15%)
1	PSU	A	1911	1	18,21,22	1.41	2 (11%)	21,30,33	2.15	5 (23%)
57	7MG	y	46	57	23,26,27	1.42	3 (13%)	27,39,42	2.48	7 (25%)
1	5MC	A	1962	1	19,22,23	2.00	2 (10%)	26,32,35	1.52	4 (15%)
1	PSU	A	2604	1,60	18,21,22	1.43	2 (11%)	21,30,33	1.95	4 (19%)
57	5MU	y	54	57	19,22,23	1.47	4 (21%)	27,32,35	2.04	8 (29%)
1	2MG	A	2445	1	18,26,27	0.97	1 (5%)	16,38,41	1.62	4 (25%)
1	H2U	A	2449	1	18,21,22	0.94	2 (11%)	19,30,33	1.61	4 (21%)
1	OMC	A	2498	1,60	19,22,23	0.86	0	25,31,34	1.25	2 (8%)
1	PSU	A	2457	1	18,21,22	1.44	2 (11%)	21,30,33	2.12	5 (23%)
34	2MG	a	966	34	18,26,27	1.01	1 (5%)	16,38,41	2.18	5 (31%)
57	PSU	y	32	57	18,21,22	1.35	2 (11%)	21,30,33	2.10	5 (23%)
1	PSU	A	1917	1	18,21,22	1.44	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%)
55	4SU	v	7	55	18,21,22	1.81	4 (22%)	25,30,33	2.34	6 (24%)
1	3TD	A	1915	1	19,22,23	7.09	13 (68%)	23,32,35	1.95	5 (21%)
1	2MG	A	1835	1	18,26,27	1.07	2 (11%)	16,38,41	1.20	2 (12%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	27,32,35	2.02	11 (40%)
1	PSU	A	2580	1	18,21,22	1.44	2 (11%)	21,30,33	2.03	5 (23%)
1	OMU	A	2552	1	19,22,23	1.30	3 (15%)	25,31,34	2.03	8 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	2MG	a	1207	34	18,26,27	0.93	1 (5%)	16,38,41	2.63	6 (37%)
34	5MC	a	1407	34	19,22,23	1.98	2 (10%)	26,32,35	1.60	5 (19%)
1	5MC	A	747	1	19,22,23	1.97	2 (10%)	26,32,35	1.59	4 (15%)
34	MA6	a	1518	34	19,26,27	1.51	4 (21%)	18,38,41	2.65	5 (27%)
34	2MG	a	1516	34	18,26,27	0.93	1 (5%)	16,38,41	1.66	5 (31%)
1	6MZ	A	1618	1	17,25,26	1.07	1 (5%)	15,36,39	2.39	5 (33%)
55	PSU	v	55	55	18,21,22	1.37	3 (16%)	21,30,33	2.00	4 (19%)
1	6MZ	A	2030	1,60	17,25,26	1.07	1 (5%)	15,36,39	2.39	5 (33%)
34	7MG	a	527	34,60	23,26,27	1.42	3 (13%)	27,39,42	2.55	7 (25%)
55	5MU	v	54	55	19,22,23	1.49	4 (21%)	27,32,35	1.97	7 (25%)
1	PSU	A	955	1	18,21,22	1.42	2 (11%)	21,30,33	2.08	4 (19%)
34	4OC	a	1402	34	20,23,24	0.84	0	25,32,35	1.33	5 (20%)
57	H2U	y	20	57	18,21,22	0.85	1 (5%)	19,30,33	1.50	2 (10%)
1	5MU	A	1939	1	19,22,23	1.47	4 (21%)	27,32,35	2.10	8 (29%)
55	PSU	w	55	55	18,21,22	1.33	2 (11%)	21,30,33	2.07	5 (23%)
1	1MG	A	745	1	19,26,27	1.32	2 (10%)	18,39,42	1.86	5 (27%)
55	H2U	v	20	55,60	18,21,22	0.83	1 (5%)	19,30,33	1.57	3 (15%)
1	PSU	A	746	1,60	18,21,22	1.40	2 (11%)	21,30,33	2.05	5 (23%)
1	PSU	A	2504	1	18,21,22	1.39	2 (11%)	21,30,33	2.04	4 (19%)
57	4SU	y	8	57	18,21,22	1.82	5 (27%)	25,30,33	2.37	7 (28%)
1	2MA	A	2503	1,60	17,25,26	1.13	3 (17%)	16,37,40	1.44	3 (18%)
1	7MG	A	2069	1	23,26,27	1.46	3 (13%)	27,39,42	2.52	11 (40%)

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	OMG	A	2251	55,1	-	0/5/27/28	0/3/3/3
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
55	H2U	w	20	55	-	2/7/38/39	0/2/2/2
34	PSU	a	516	34	-	3/7/25/26	0/2/2/2
34	MA6	a	1519	34	-	4/7/29/30	0/3/3/3
57	MIA	y	37	57	-	4/11/33/34	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PSU	y	55	57	-	2/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2604	1,60	-	0/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1	-	2/5/27/28	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	OMC	A	2498	1,60	-	1/9/27/28	0/2/2/2
1	PSU	A	2457	1	-	2/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
57	PSU	y	32	57	-	1/7/25/26	0/2/2/2
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	4/7/25/26	0/2/2/2
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
1	OMU	A	2552	1	-	2/9/27/28	0/2/2/2
34	2MG	a	1207	34	-	2/5/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
34	MA6	a	1518	34	-	2/7/29/30	0/3/3/3
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
1	6MZ	A	1618	1	-	3/5/27/28	0/3/3/3
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
1	6MZ	A	2030	1,60	-	3/5/27/28	0/3/3/3
34	7MG	a	527	34,60	-	2/7/37/38	0/3/3/3
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	PSU	w	55	55	-	1/7/25/26	0/2/2/2
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
55	H2U	v	20	55,60	-	0/7/38/39	0/2/2/2
1	PSU	A	746	1,60	-	1/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2
57	4SU	y	8	57	-	1/7/25/26	0/2/2/2
1	2MA	A	2503	1,60	-	2/3/25/26	0/3/3/3
1	7MG	A	2069	1	-	2/7/37/38	0/3/3/3

The worst 5 of 131 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 264 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	a	527	7MG	N9-C4-N3	8.41	137.79	125.46
57	y	46	7MG	N9-C4-N3	8.18	137.45	125.46
57	y	37	MIA	C12-C13-C14	-8.01	112.63	127.01
34	a	1207	2MG	N1-C2-N2	7.36	124.08	116.56
1	A	2069	7MG	N9-C4-N3	7.32	136.18	125.46

There are no chirality outliers.

5 of 79 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.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#\|Z\| > 2$
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
63	GTP	z	402	-	29,34,34	1.07	1 (3%)	35,54,54	1.16	3 (8%)

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	z	401	-	-	1/5/6/8	0/1/1/1
59	FME	A	3001	-	-	1/7/9/11	-
63	GTP	z	402	-	-	1/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GTP	O4'-C1'	2.13	1.43	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
63	z	402	GTP	C8-N7-C5	3.02	107.69	102.55
63	z	402	GTP	C5-C6-N1	2.26	118.39	114.07
63	z	402	GTP	C4'-O4'-C1'	2.16	111.90	109.92

There are no chirality outliers.

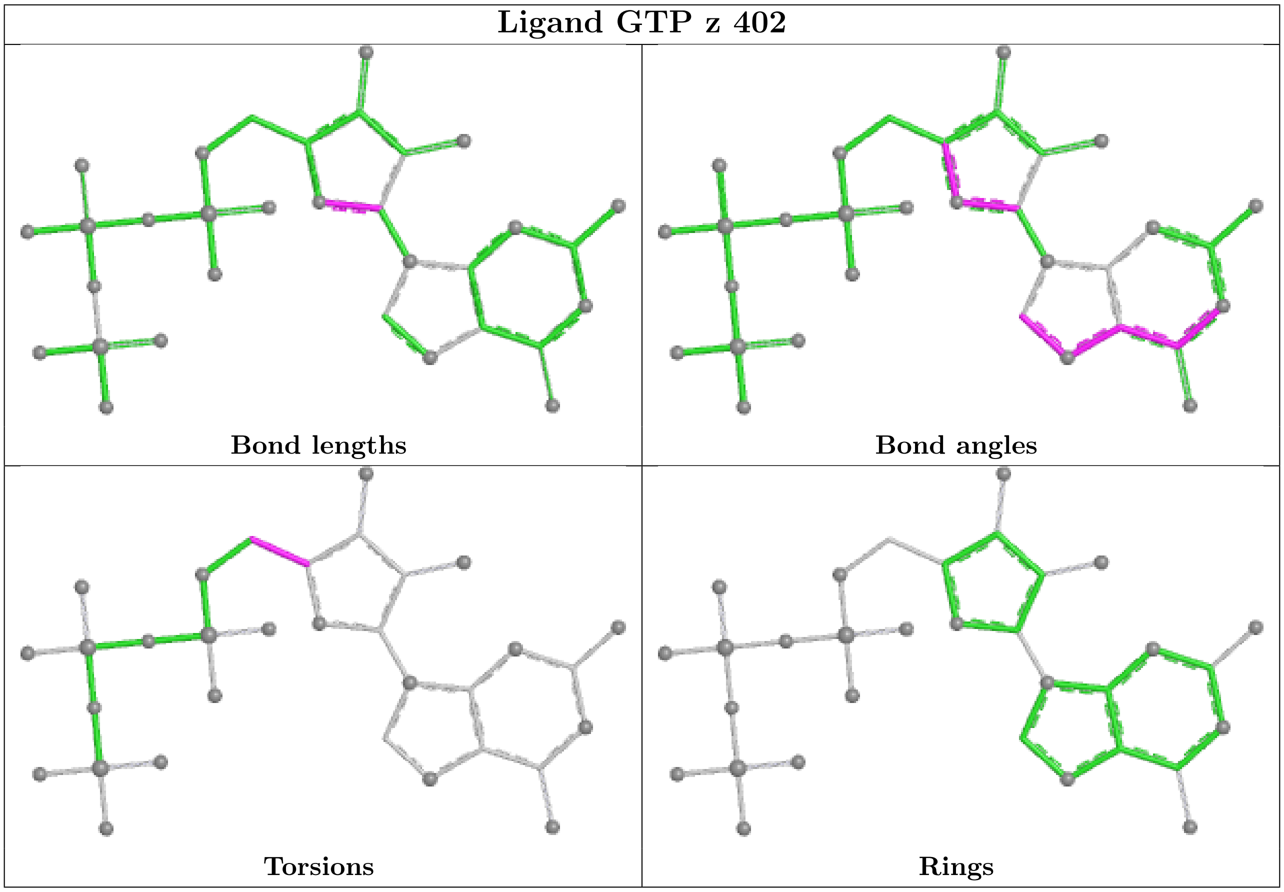
All (3) torsion outliers are listed below:

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand GTP z 402

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

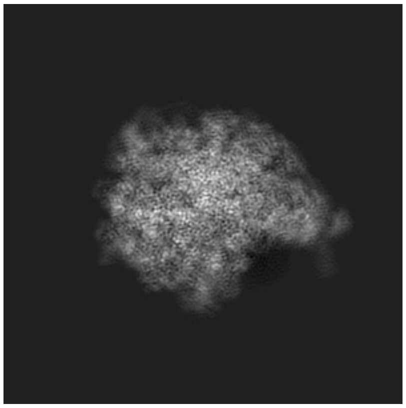
6 Map visualisation

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.

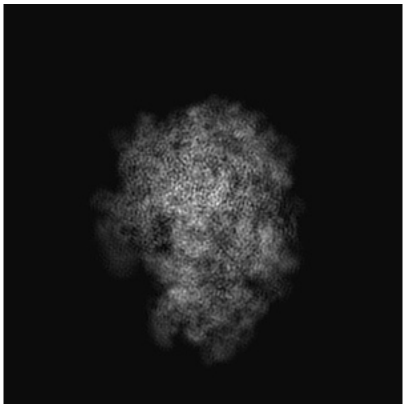
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

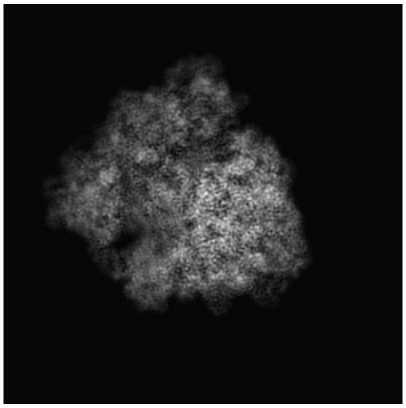
6.1.1 Primary map



X

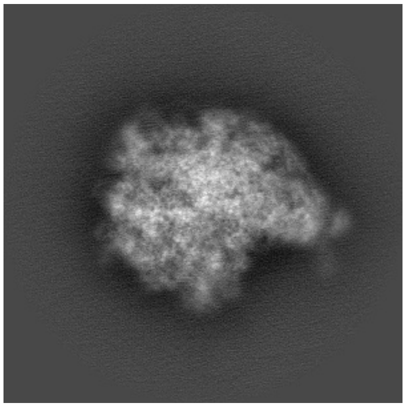


Y

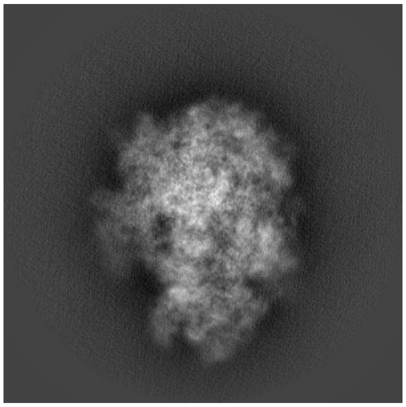


Z

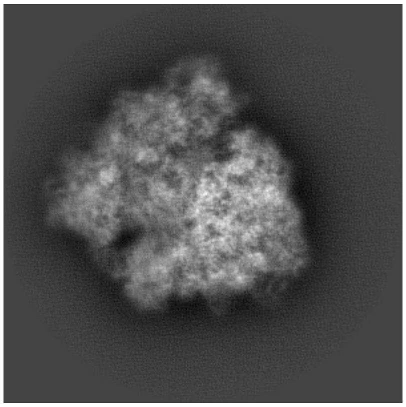
6.1.2 Raw map



X



Y

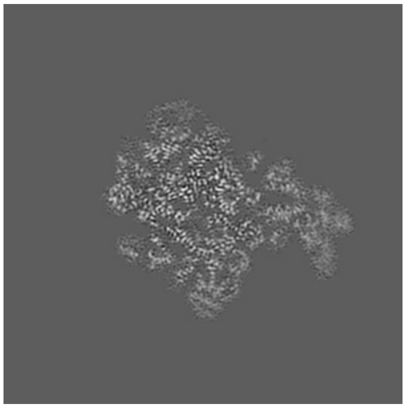


Z

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

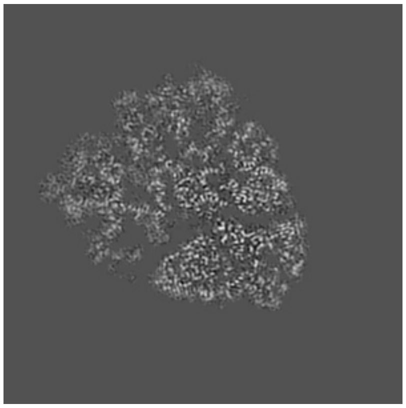
6.2 Central slices

6.2.1 Primary map



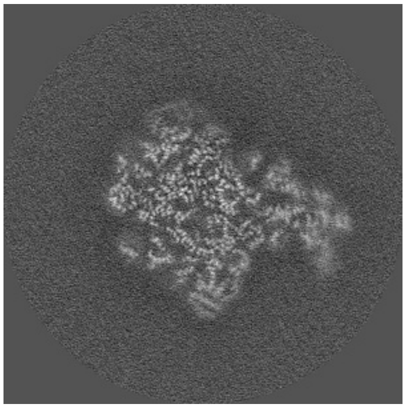
X Index: 199

Y Index: 199

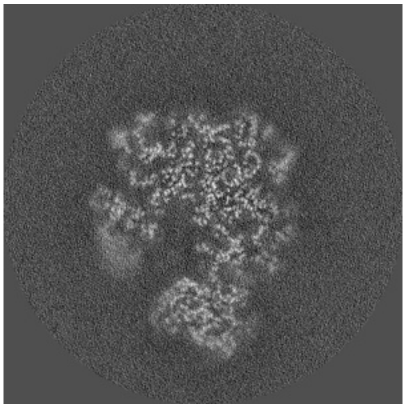


Z Index: 199

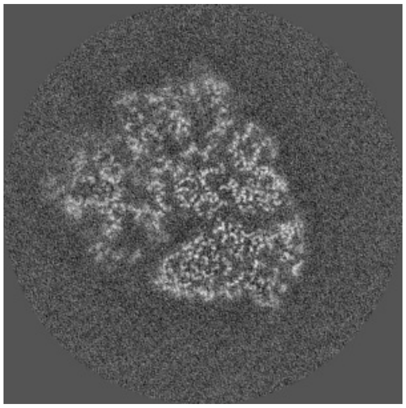
6.2.2 Raw map



X Index: 199



Y Index: 199

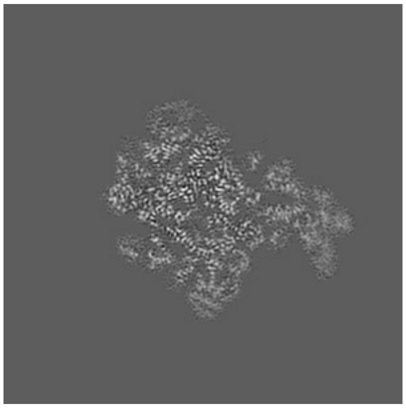


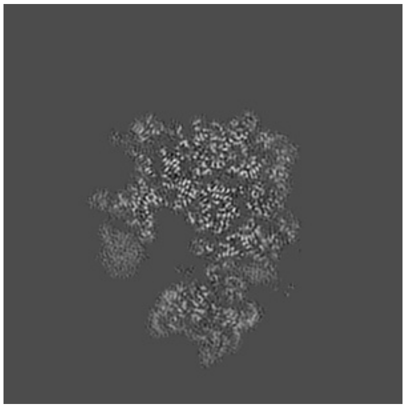
Z Index: 199

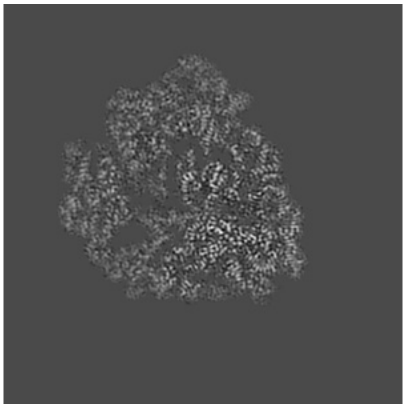
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

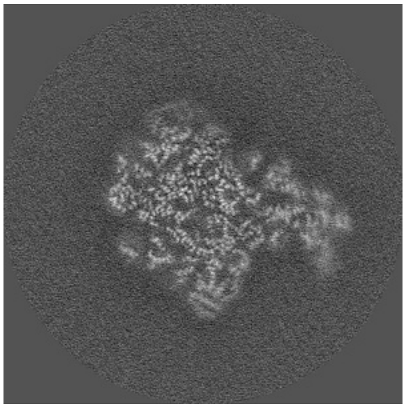
6.3.1 Primary map

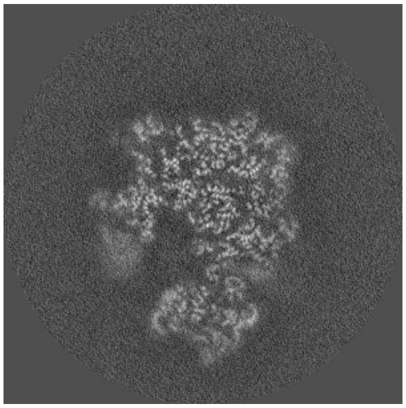

X Index: 199

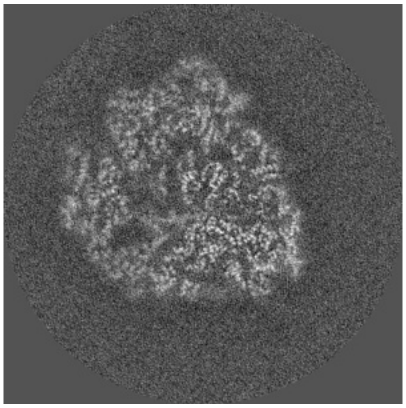

Y Index: 207


Z Index: 190

6.3.2 Raw map


X Index: 199

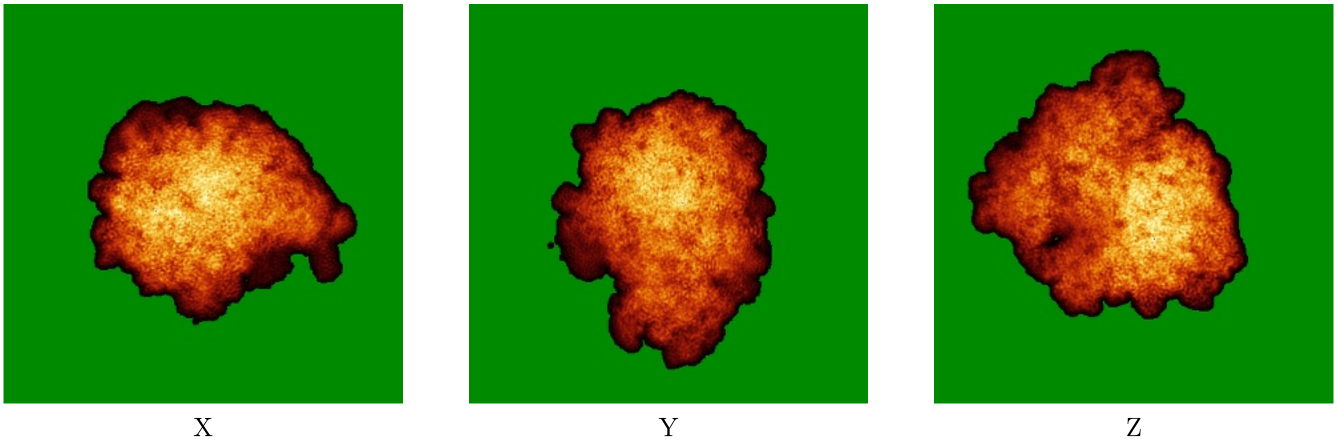

Y Index: 207


Z Index: 190

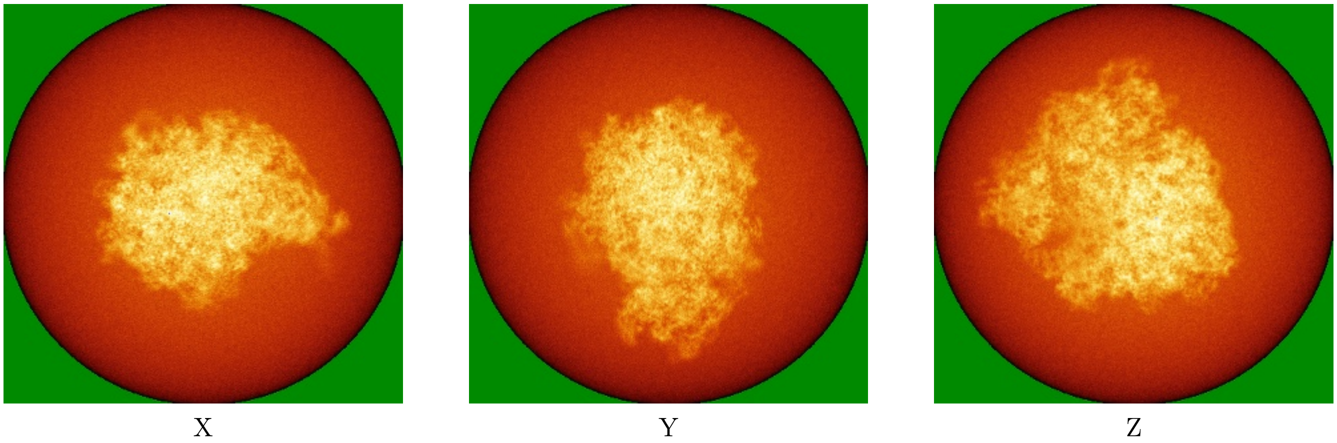
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

6.4.1 Primary map



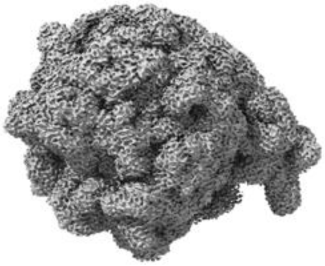
6.4.2 Raw map



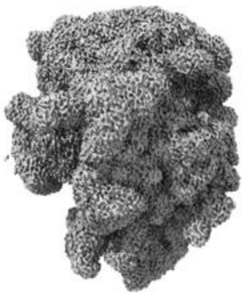
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views ⓘ

6.5.1 Primary map



X

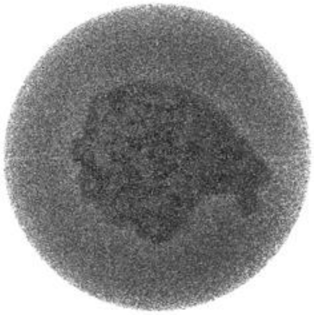


Y

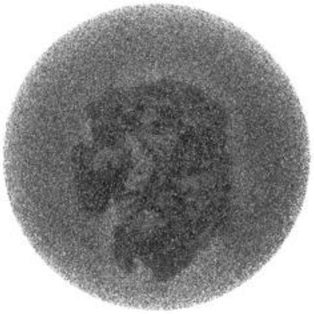
Z

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.

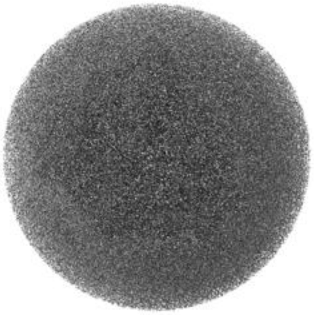
6.5.2 Raw map



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.

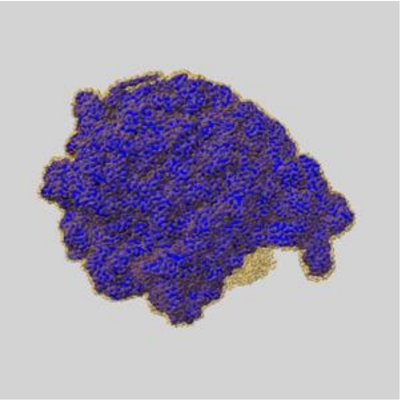
6.6 Mask visualisation ⓘ

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

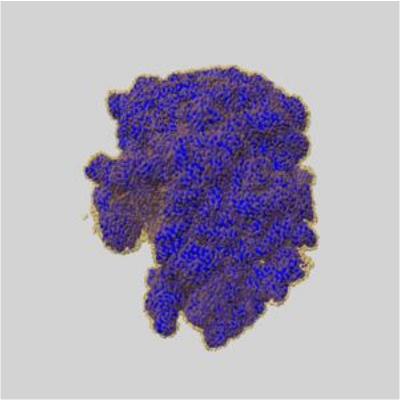
A mask typically either:

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

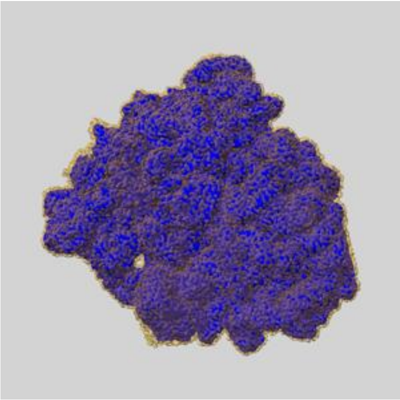
6.6.1 emd_8826_msk_1.map ⓘ



X



Y

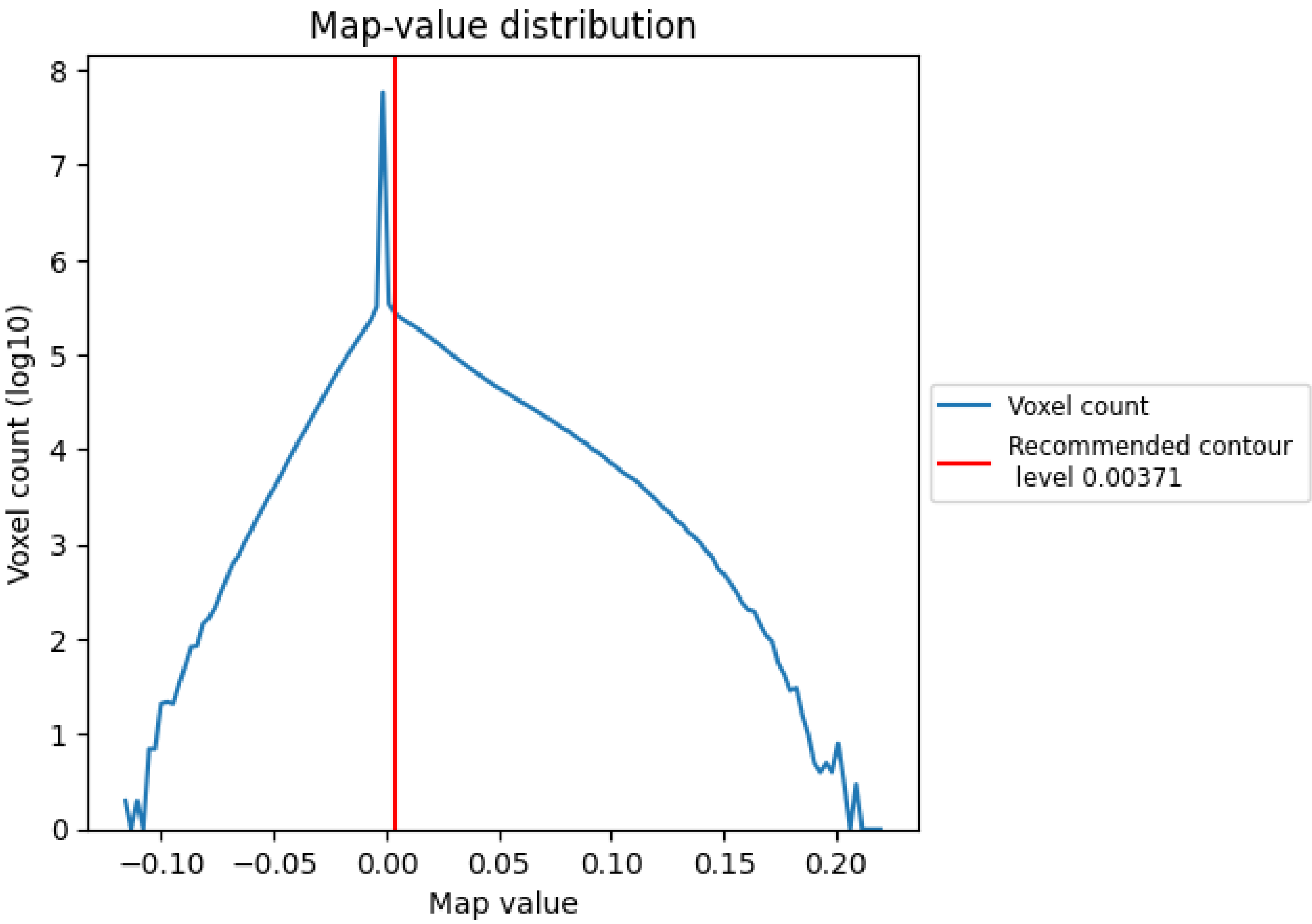


Z

7 Map analysis ⓘ

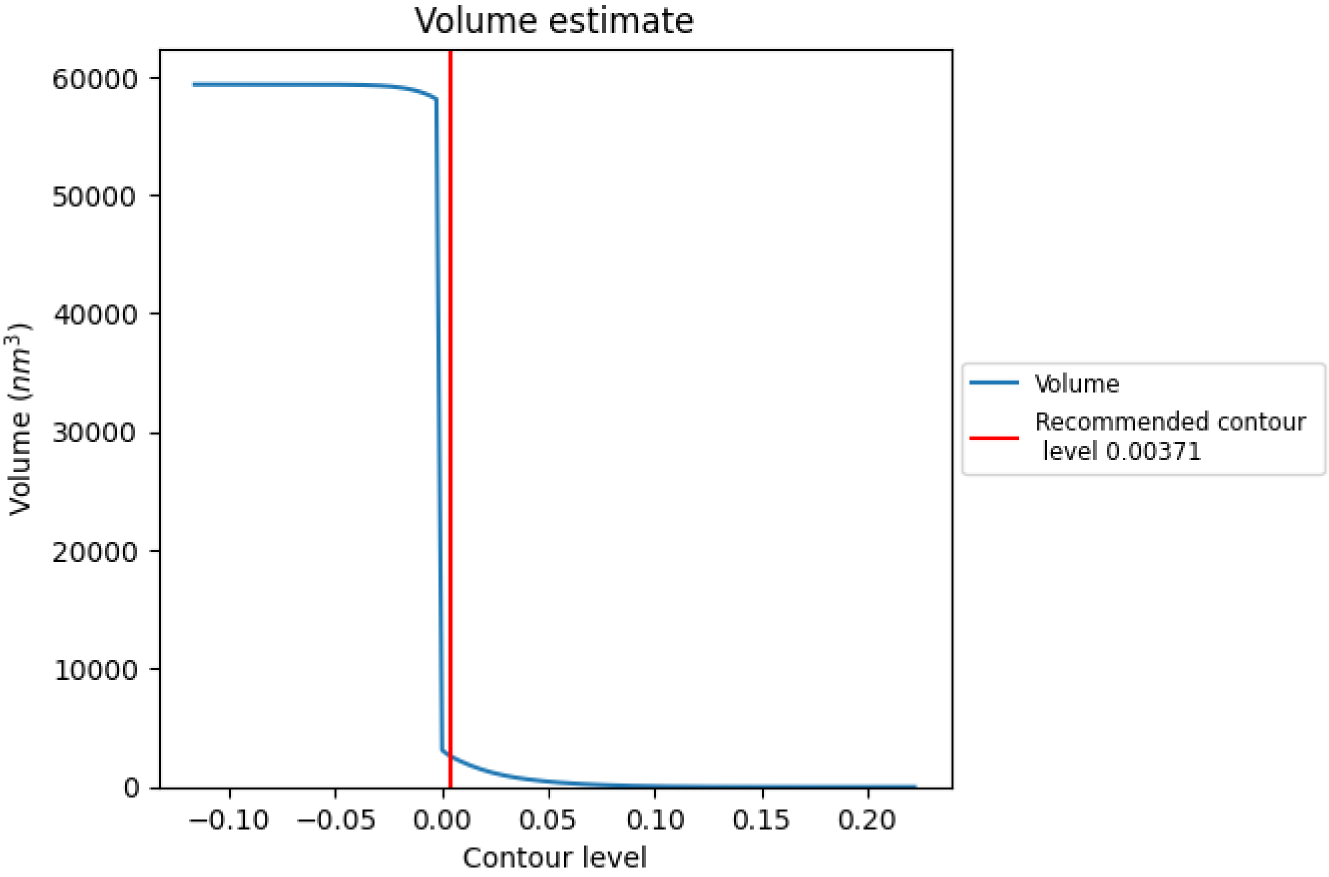
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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

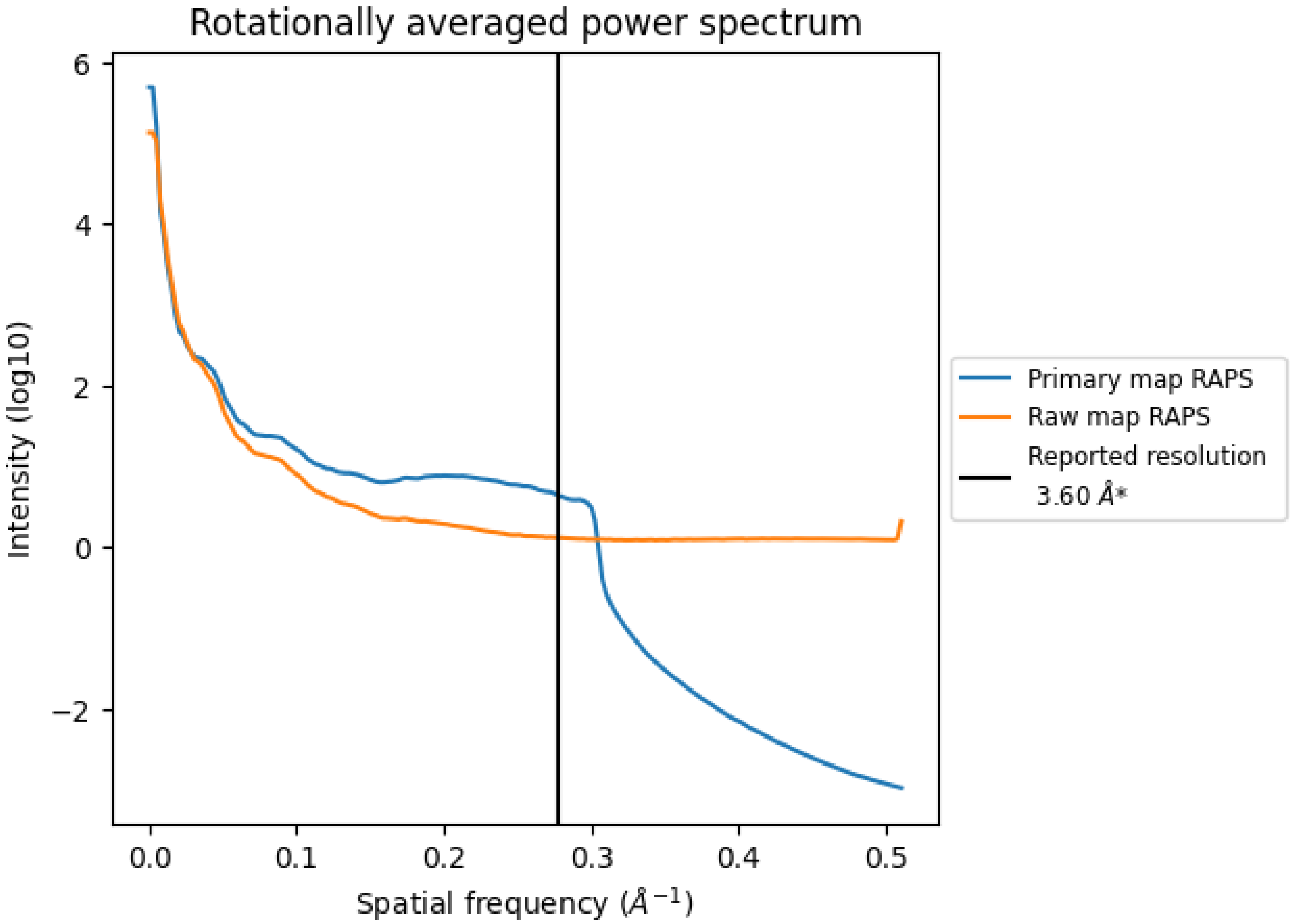
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 2650 nm^3; 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 ⓘ

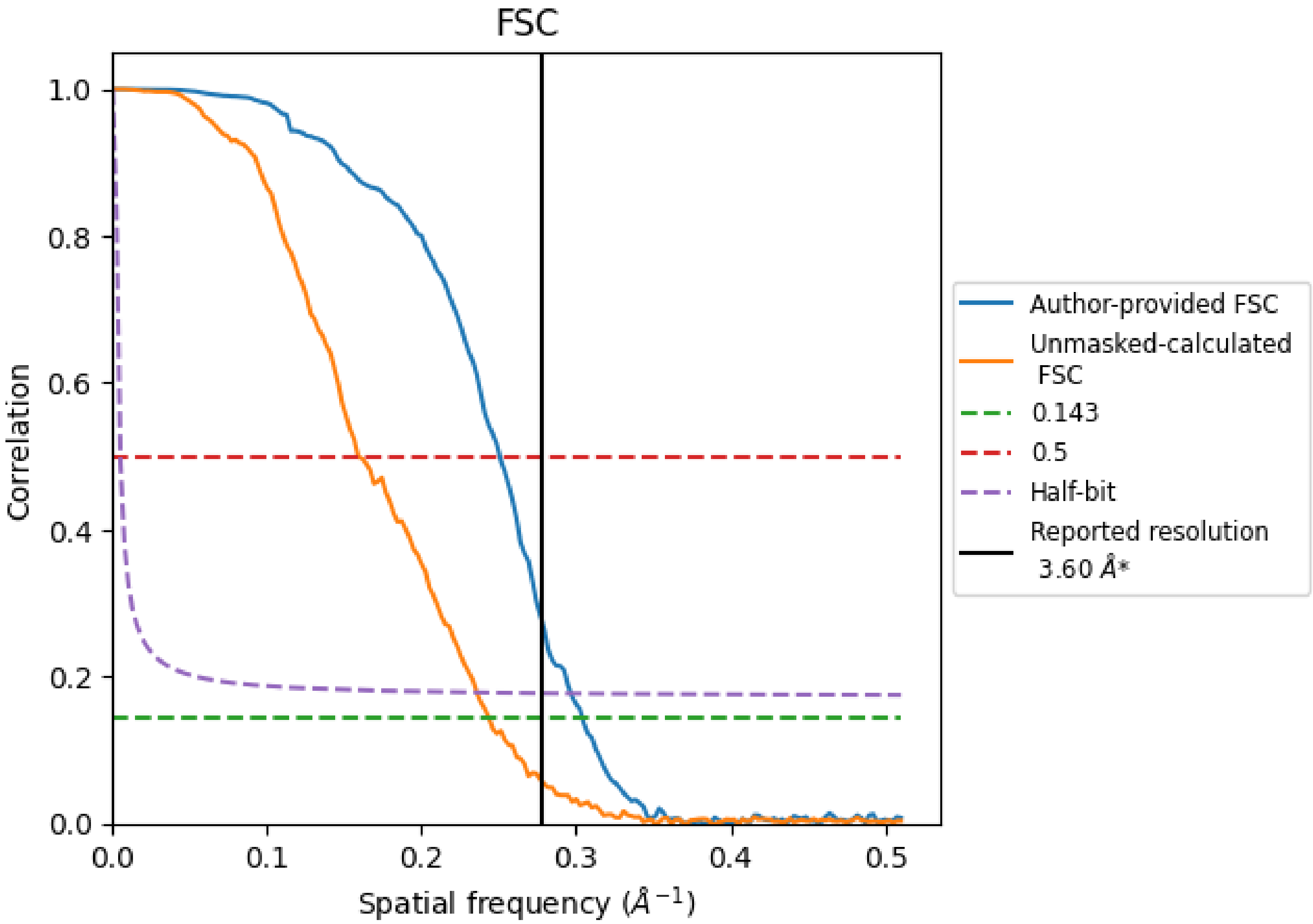


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

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 0.278 Å^{-1}

8.2 Resolution estimates ⓘ

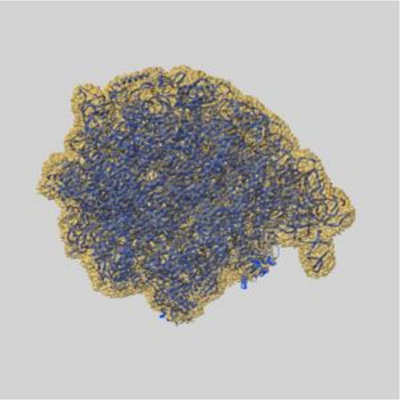
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.29	3.99	3.37
Unmasked-calculated*	4.10	6.29	4.24

*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 %

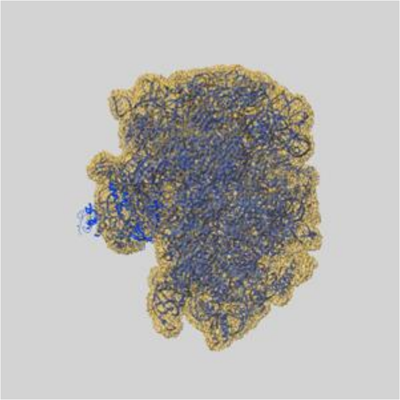
9 Map-model fit (i)

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.

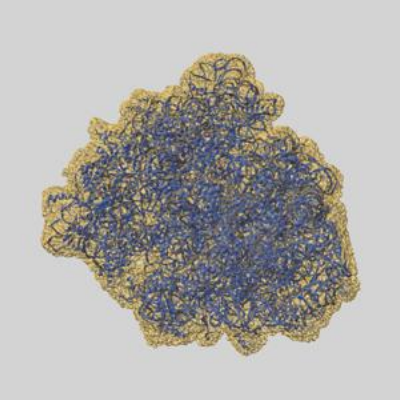
9.1 Map-model overlay (i)



X



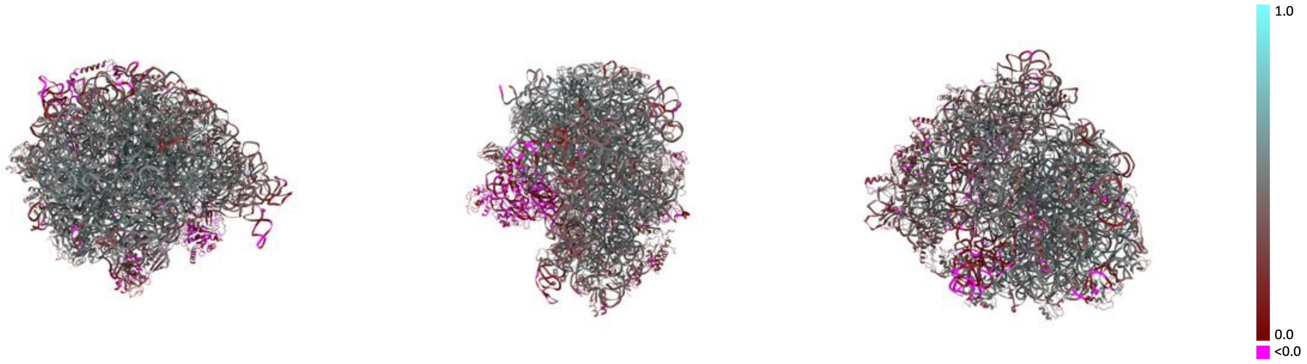
Y



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.

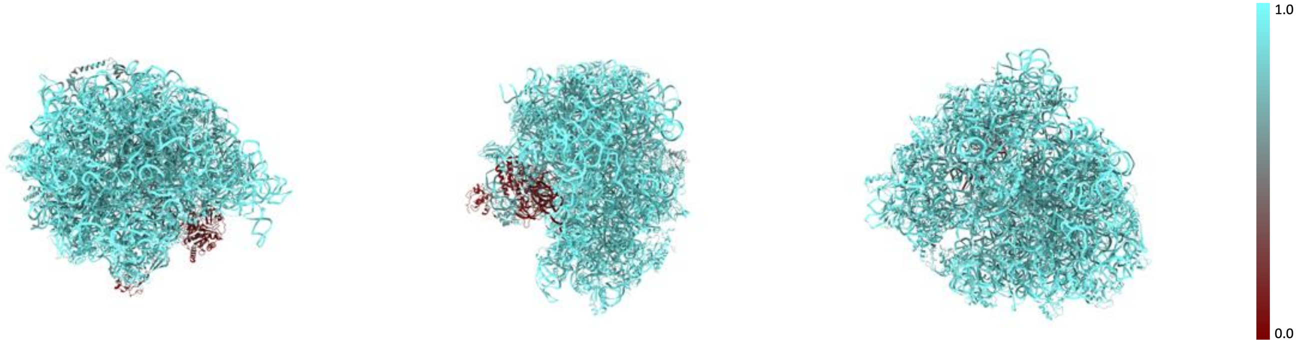
9.2 Q-score mapped to coordinate model



X Y Z

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

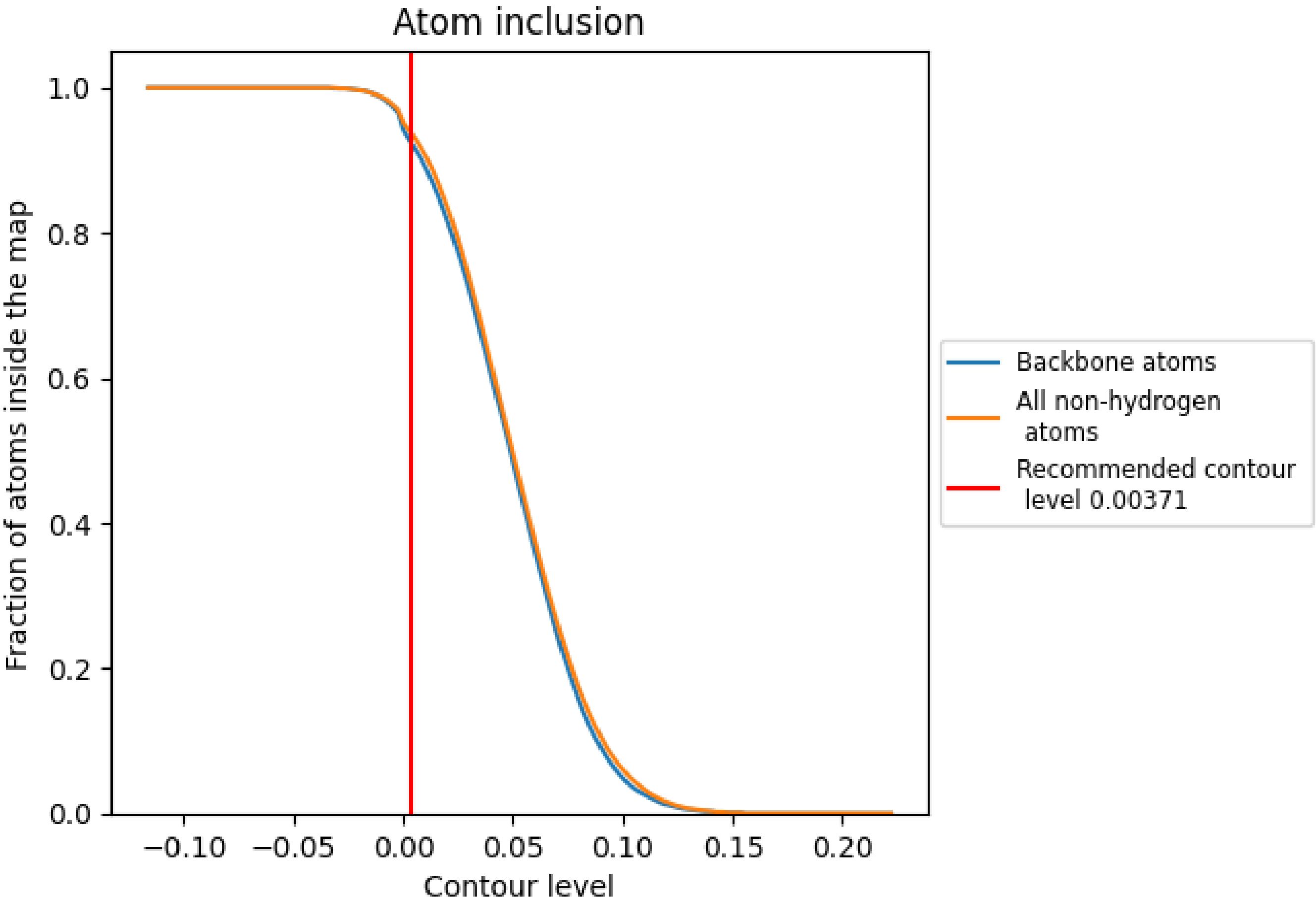
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00371).

9.4 Atom inclusion ⓘ



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