



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 12:42 PM EST

PDB ID : 6WDA
EMDB ID : EMD-21629
Title : Cryo-EM of elongating ribosome with EF-Tu*GTP elucidates tRNA proof-reading (Cognate Structure III-C)
Authors : Loveland, A.B.; Demo, G.; Korostelev, A.A.
Deposited on : 2020-03-31
Resolution : 3.80 Å(reported)

This is a Full wwPDB EM Validation 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

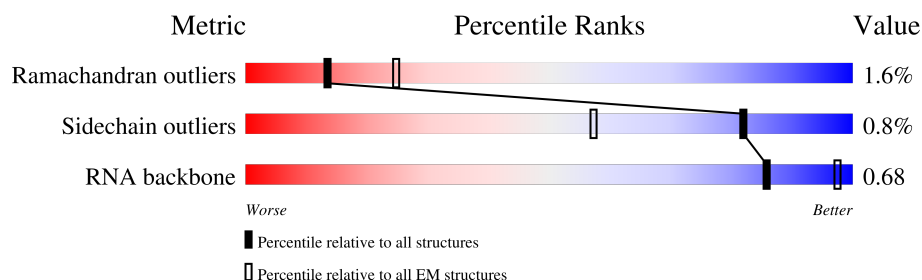
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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.



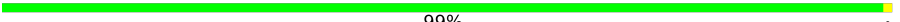
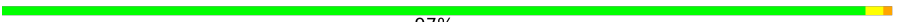
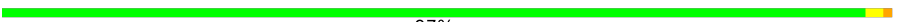












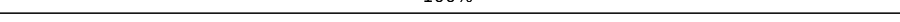
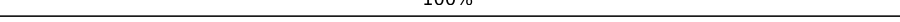
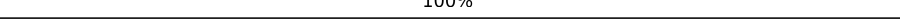
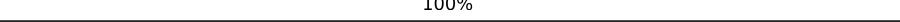
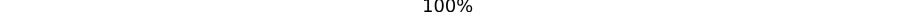
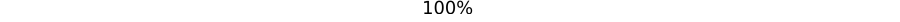
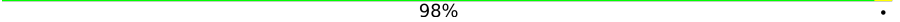
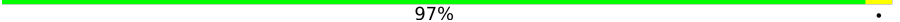
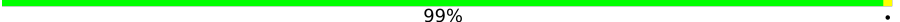
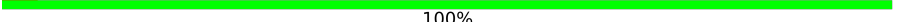
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	b	271	
2	c	209	
3	d	201	
4	e	177	
5	f	176	
6	g	149	
7	h	131	
8	i	141	

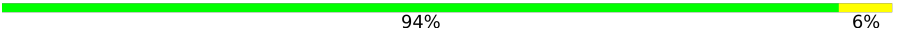
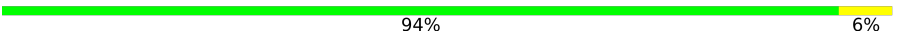
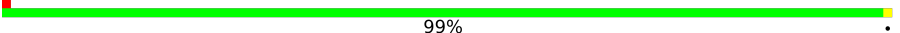
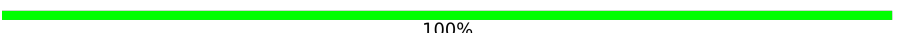
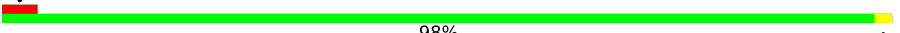

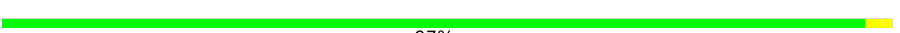








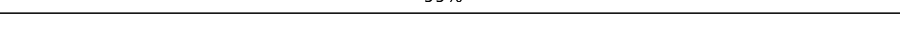
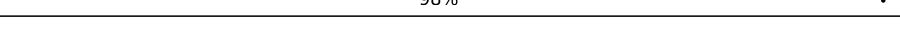








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Mol	Chain	Length	Quality of chain
9	j	142	 99% .
10	k	122	 97% ..
11	l	143	 97% ..
12	m	136	 99% .
13	n	120	 98% .
14	o	116	 99% .
15	p	114	 98% .
16	q	117	 100%
17	r	103	 95% 5%
18	s	110	 98% .
19	t	93	 99% .
20	u	102	 95% 5%
21	v	94	 99% .
22	w	75	 99% .
23	x	77	 100%
24	y	63	 100%
25	z	58	 100%
26	B	56	 100%
27	C	50	 100%
28	D	46	 100%
29	E	64	 98% .
30	F	38	 97% .
31	G	225	 99% .
32	H	206	 100%
33	I	205	 10% 97% .

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Mol	Chain	Length	Quality of chain
34	J	157	
35	K	100	
36	L	151	
37	M	129	
38	N	127	
39	O	98	
40	P	116	
41	Q	123	
42	R	114	
43	S	100	
44	T	88	
45	U	82	
46	V	80	
47	W	65	
48	X	79	
49	Y	85	
50	Z	65	
51	a	223	
52	3	1539	
53	1	2903	
54	2	120	
55	5	77	
55	6	77	
56	4	18	
57	7	76	

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Mol	Chain	Length	Quality of chain
58	8	400	<div> <div>20%</div> <div>86%</div> <div>13%</div> </div>

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 152933 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 protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	b	271	Total	C	N	O	S	0	0
			2083	1288	423	365	7		

- Molecule 2 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	c	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

- Molecule 3 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	d	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 4 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	177	Total	C	N	O	S	0	0
			1411	899	249	257	6		

- Molecule 5 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	f	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 6 is a protein called 50S ribosomal protein L9.

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

- Molecule 7 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	h	131	Total	C	N	O	S	0	0
			989	625	175	184	5		

- Molecule 8 is a protein called 50S ribosomal protein L11.

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

- Molecule 9 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	j	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 10 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	k	122	Total	C	N	O	S	0	0
			939	587	180	166	6		

- Molecule 11 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	l	143	Total	C	N	O	S	0	0
			1045	649	206	189	1		

- Molecule 12 is a protein called 50S ribosomal protein L16.

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

- Molecule 13 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	n	120	Total	C	N	O	S	0	0
			961	593	196	167	5		

- Molecule 14 is a protein called 50S ribosomal protein L18.

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

- Molecule 15 is a protein called 50S ribosomal protein L19.

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

- Molecule 16 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	q	117	Total	C	N	O		0
			947	604	192	151		0

- Molecule 17 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	r	103	Total	C	N	O	S	0
			816	516	153	145	2	0

- Molecule 18 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	s	110	Total	C	N	O	S	0
			857	532	166	156	3	0

- Molecule 19 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	t	93	Total	C	N	O	S	0
			739	466	139	132	2	0

- Molecule 20 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	u	102	Total	C	N	O		0
			780	492	146	142		0

- Molecule 21 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	v	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 22 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	w	75	Total	C	N	O	S	0	0
			575	356	116	102	1		

- Molecule 23 is a protein called 50S ribosomal protein L28.

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

- Molecule 24 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	y	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	z	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 26 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 27 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	C	50	Total	C	N	O	0	0
			410	263	75	72		

- Molecule 28 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 29 is a protein called 50S ribosomal protein L35.

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

- Molecule 30 is a protein called 50S ribosomal protein L36.

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

- Molecule 31 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	G	225	Total	C	N	O	S	0	0
			1757	1111	315	323	8		

- Molecule 32 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	206	Total	C	N	O	S	0	0
			1625	1028	305	289	3		

- Molecule 33 is a protein called 30S ribosomal protein S4.

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

- Molecule 34 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	J	157	Total	C	N	O	S	0	0
			1157	719	218	214	6		

- Molecule 35 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	K	100	Total	C	N	O	S	0	0
			818	515	148	149	6		

- Molecule 36 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L	151	Total	C	N	O	S	0	0
			1182	735	227	216	4		

- Molecule 37 is a protein called 30S ribosomal protein S8.

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

- Molecule 38 is a protein called 30S ribosomal protein S9.

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

- Molecule 39 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	O	98	Total	C	N	O	S	0	0
			787	493	150	143	1		

- Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	P	116	Total	C	N	O	S	0	0
			870	535	173	159	3		

- Molecule 41 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	Q	123	Total	C	N	O	S	0	0
			955	590	196	165	4		

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	R	114	Total	C	N	O	S	0	0
			884	546	178	157	3		

- Molecule 43 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	S	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 44 is a protein called 30S ribosomal protein S15.

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

- Molecule 45 is a protein called 30S ribosomal protein S16.

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

- Molecule 46 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	V	80	Total	C	N	O	S	0	0
			649	411	121	114	3		

- Molecule 47 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	W	65	Total	C	N	O	S	0	0
			536	339	100	96	1		

- Molecule 48 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	X	79	Total	C	N	O	S	0	0
			638	408	120	108	2		

- Molecule 49 is a protein called 30S ribosomal protein S20.

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

- Molecule 50 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Z	65	Total	C	N	O	S	0	0
			545	335	117	92	1		

- Molecule 51 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	a	134	Total	C	N	O	S	0	0
			1027	645	186	194	2		

- Molecule 52 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	3	1539	Total	C	N	O	P	0	0
			33012	14725	6052	10697	1538		

- Molecule 53 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	2903	Total	C	N	O	P	0	0
			62317	27801	11468	20146	2902		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	747	C	U	conflict	GB 1036415628

- Molecule 54 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	2	120	Total	C	N	O	P	0	0
			2568	1145	471	833	119		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
2	120	A	-	insertion	GB 1370526515

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

Mol	Chain	Residues	Atoms					AltConf	Trace
55	5	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		
55	6	77	Total	C	N	O	P	0	0
			1640	732	297	535	76		

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	4	18	Total	C	N	O	P	0	0
			388	175	76	120	17		

- Molecule 57 is a RNA chain called tRNA^{Phe}.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	7	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

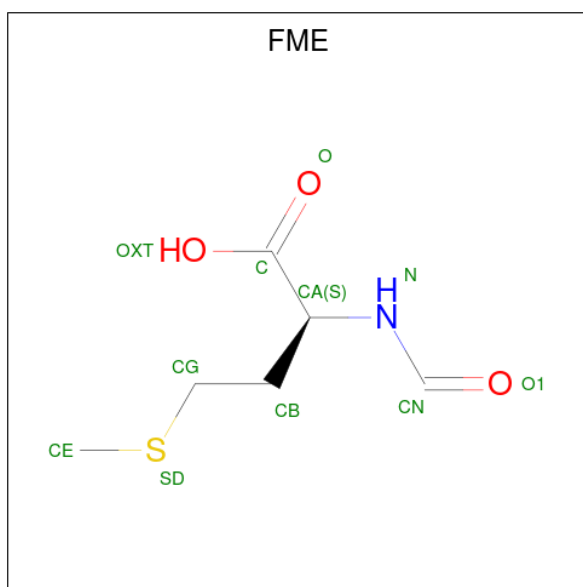
- Molecule 58 is a protein called Elongation factor Tu.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	8	348	Total	C	N	O	S	0	0
			2683	1702	459	509	13		

There are 7 discrepancies between the modelled and reference sequences:

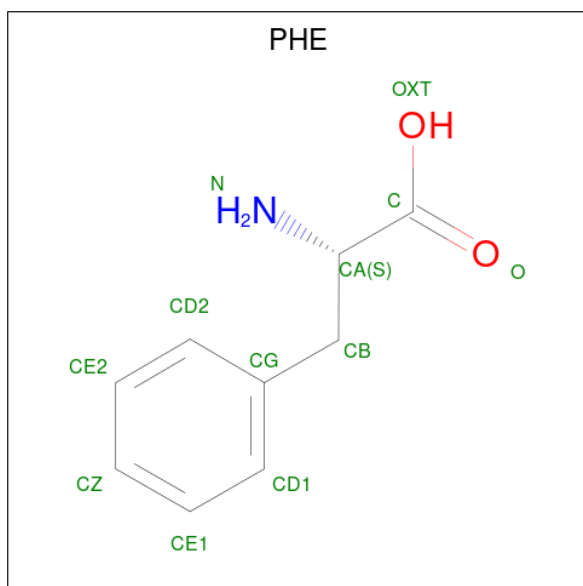
Chain	Residue	Modelled	Actual	Comment	Reference
8	395	SER	-	expression tag	UNP E2QFJ4
8	396	HIS	-	expression tag	UNP E2QFJ4
8	397	HIS	-	expression tag	UNP E2QFJ4
8	398	HIS	-	expression tag	UNP E2QFJ4
8	399	HIS	-	expression tag	UNP E2QFJ4
8	400	HIS	-	expression tag	UNP E2QFJ4
8	401	HIS	-	expression tag	UNP E2QFJ4

- Molecule 59 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



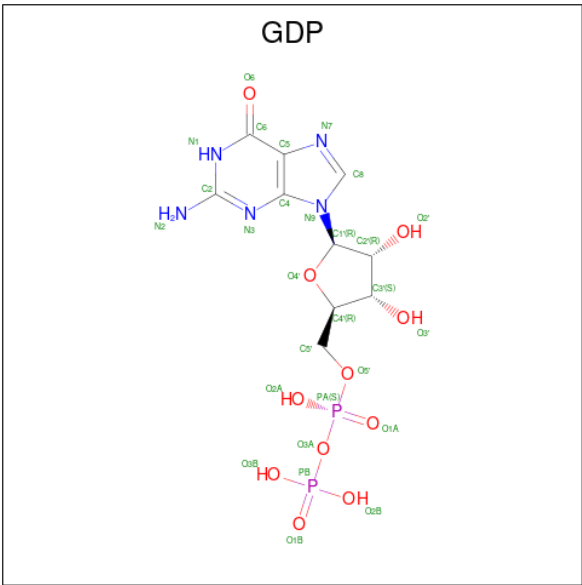
Mol	Chain	Residues	Atoms					AltConf
59	5	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 60 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



Mol	Chain	Residues	Atoms				AltConf
60	7	1	Total	C	N	O	0
			11	9	1	1	

- Molecule 61 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
61	8	1	Total	C	N	O	P	0
			28	10	5	11	2	

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 50S ribosomal protein L2

Chain b:  98%



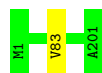
- Molecule 2: 50S ribosomal protein L3

Chain c:  99%



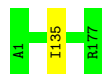
- Molecule 3: 50S ribosomal protein L4

Chain d:  100%



- Molecule 4: 50S ribosomal protein L5

Chain e:  99%

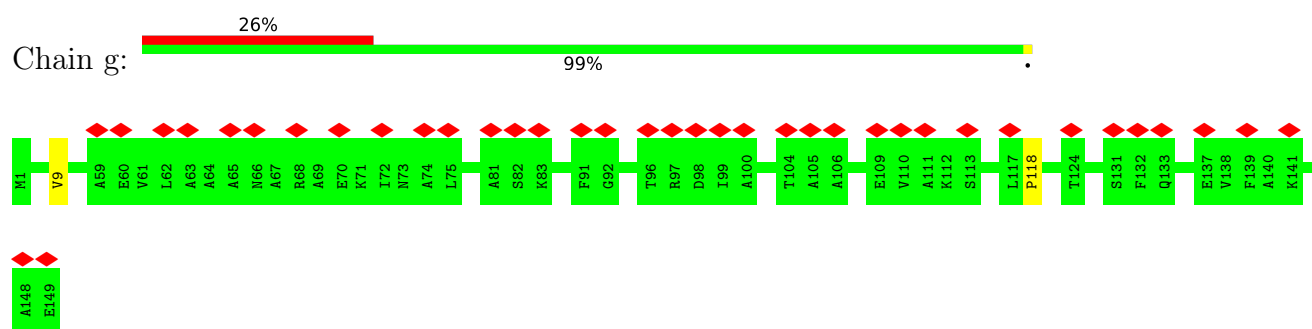


- Molecule 5: 50S ribosomal protein L6

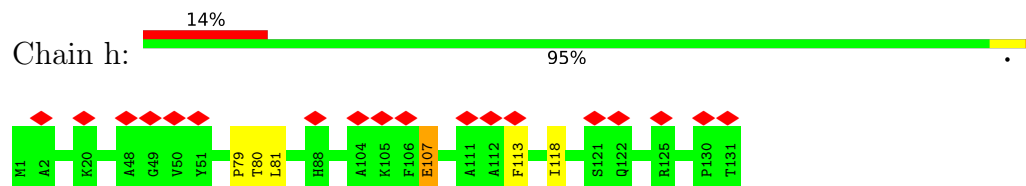
Chain f:  98%



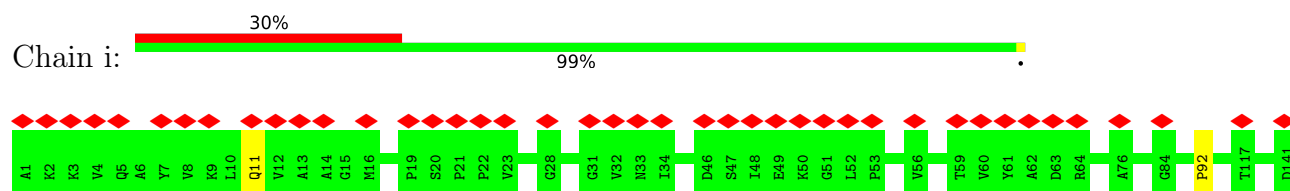
- Molecule 6: 50S ribosomal protein L9



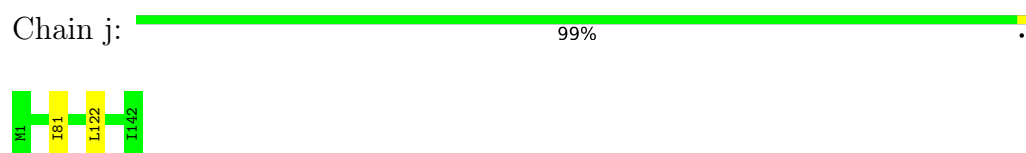
- Molecule 7: 50S ribosomal protein L10



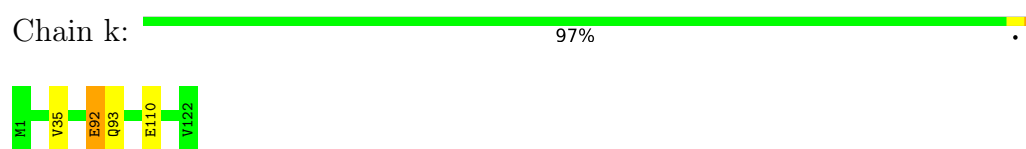
- Molecule 8: 50S ribosomal protein L11



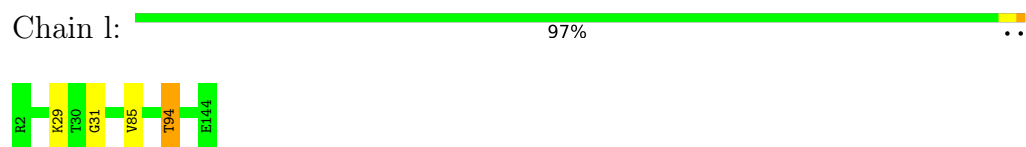
- Molecule 9: 50S ribosomal protein L13



- Molecule 10: 50S ribosomal protein L14

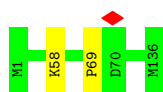


- Molecule 11: 50S ribosomal protein L15



- Molecule 12: 50S ribosomal protein L16





- Molecule 13: 50S ribosomal protein L17

Chain n:  98%



- Molecule 14: 50S ribosomal protein L18

Chain o:  99%



- Molecule 15: 50S ribosomal protein L19

Chain p:  98%



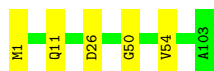
- Molecule 16: 50S ribosomal protein L20

Chain q:  100%

There are no outlier residues recorded for this chain.

- Molecule 17: 50S ribosomal protein L21

Chain r:  95% 5%



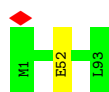
- Molecule 18: 50S ribosomal protein L22

Chain s:  98%



- Molecule 19: 50S ribosomal protein L23

Chain t:  99%



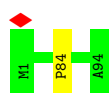
- Molecule 20: 50S ribosomal protein L24

Chain u:  95% 5%



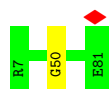
- Molecule 21: 50S ribosomal protein L25

Chain v:  99% .



- Molecule 22: 50S ribosomal protein L27

Chain w:  99% .



- Molecule 23: 50S ribosomal protein L28

Chain x:  100%

There are no outlier residues recorded for this chain.

- Molecule 24: 50S ribosomal protein L29

Chain y:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: 50S ribosomal protein L30

Chain z:  100%

There are no outlier residues recorded for this chain.

- Molecule 26: 50S ribosomal protein L32

Chain B:  100%

There are no outlier residues recorded for this chain.

- Molecule 27: 50S ribosomal protein L33

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 28: 50S ribosomal protein L34

Chain D:  100%



- Molecule 29: 50S ribosomal protein L35

Chain E:  98%



- Molecule 30: 50S ribosomal protein L36

Chain F:  97%



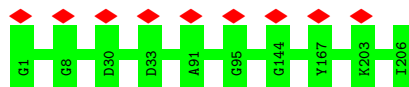
- Molecule 31: 30S ribosomal protein S2

Chain G:  99%



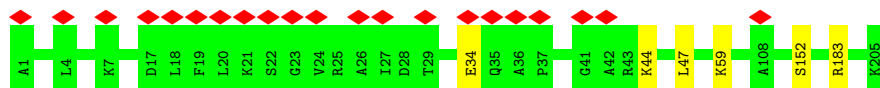
- Molecule 32: 30S ribosomal protein S3

Chain H:  100%



- Molecule 33: 30S ribosomal protein S4

Chain I:  97%



- Molecule 34: 30S ribosomal protein S5

Chain J:  94% 6%



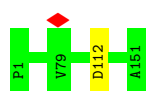
- Molecule 35: 30S ribosomal protein S6

Chain K:  94% 6%



- Molecule 36: 30S ribosomal protein S7

Chain L:  99% .



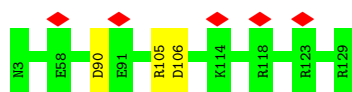
- Molecule 37: 30S ribosomal protein S8

Chain M:  100%

There are no outlier residues recorded for this chain.

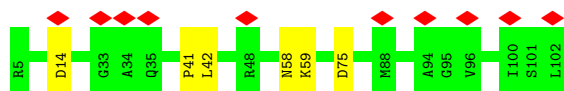
- Molecule 38: 30S ribosomal protein S9

Chain N:  98% .



- Molecule 39: 30S ribosomal protein S10

Chain O:  10% 94% 6%



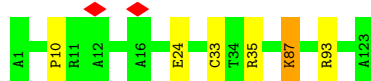
- Molecule 40: 30S ribosomal protein S11

Chain P:  97% .



- Molecule 41: 30S ribosomal protein S12

Chain Q:  95%



- Molecule 42: 30S ribosomal protein S13

Chain R:  96%



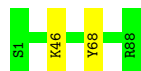
- Molecule 43: 30S ribosomal protein S14

Chain S:  8% 100%



- Molecule 44: 30S ribosomal protein S15

Chain T:  98%



- Molecule 45: 30S ribosomal protein S16

Chain U:  98%



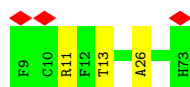
- Molecule 46: 30S ribosomal protein S17

Chain V:  96%



- Molecule 47: 30S ribosomal protein S18

Chain W:  5% 95% 5%



- Molecule 48: 30S ribosomal protein S19

Chain X:  99%



- Molecule 49: 30S ribosomal protein S20

Chain Y:  98%



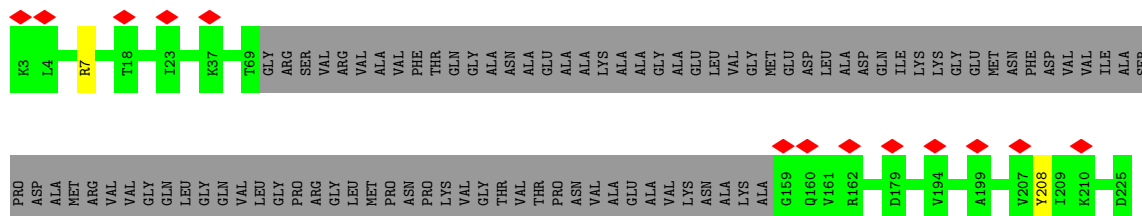
- Molecule 50: 30S ribosomal protein S21

Chain Z:  89%  11%





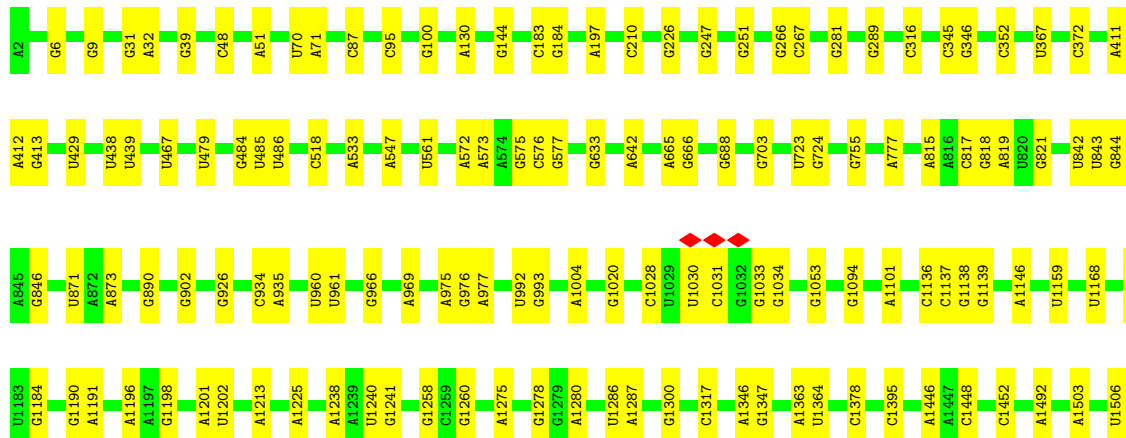
- Molecule 51: 50S ribosomal protein L1

Chain a:  6%  59%  40%

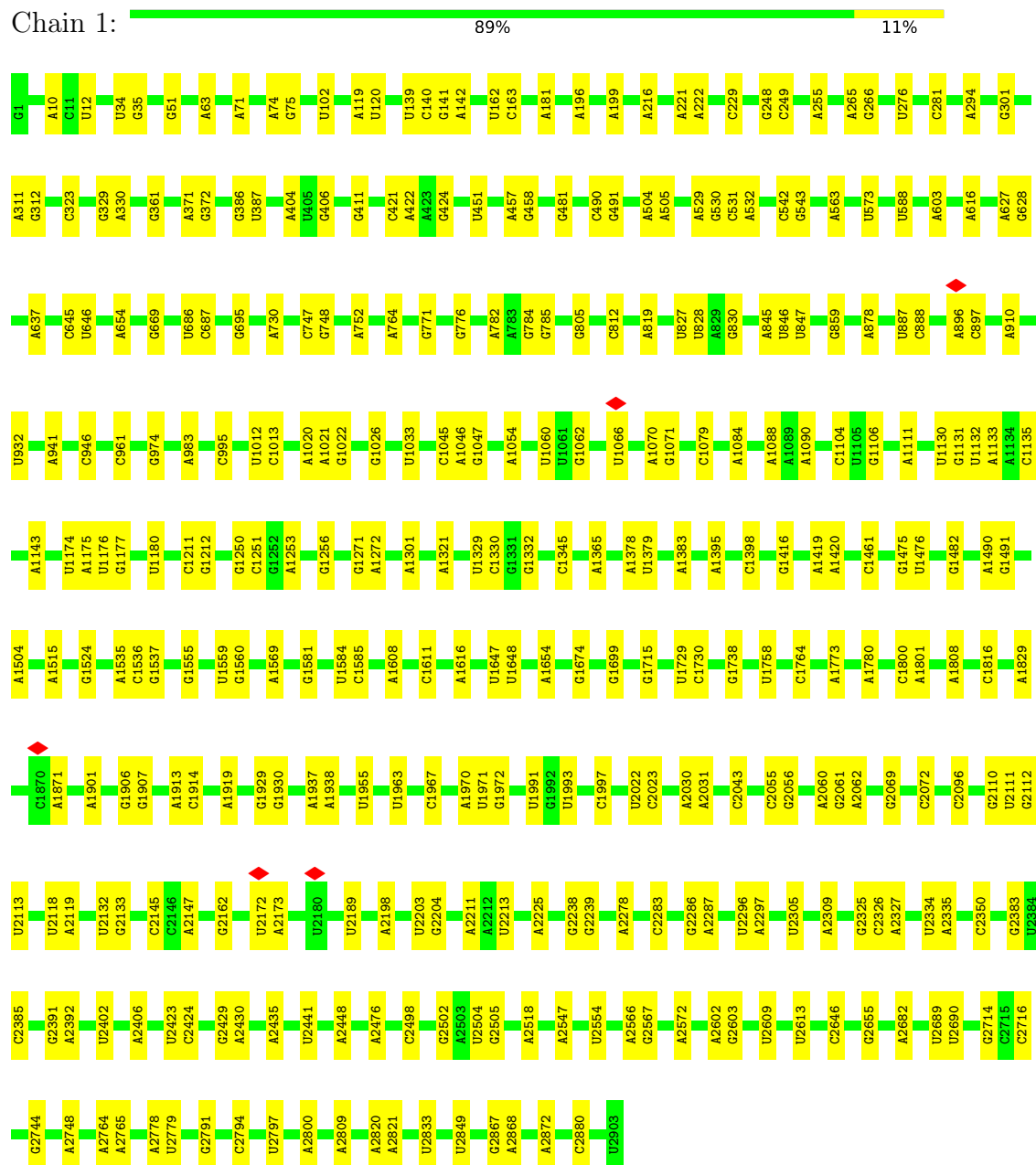


- Molecule 52: 16S ribosomal RNA

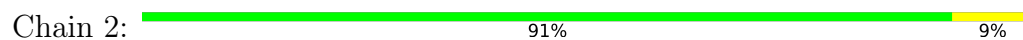
Chain 3:  91%  9%



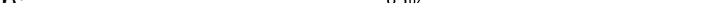
- Molecule 53: 23S ribosomal RNA



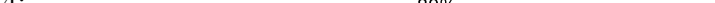
- Molecule 54: 5S ribosomal RNA



- Molecule 55: tRNA^{fMet}


Chain 6: 

A bar chart showing the distribution of 16 categories. The categories are C1, G2, C3, U8, G9, G10, A14, C17, G19, U20, A21, G22, C34, A35, U47, C61, G64, G70, and A76. The bars are colored green for categories C1, C3, C17, C34, A35, and U47, and yellow for the others. Red diamonds are placed above the bars for C17, C34, A35, and U47.

Chain 4:  6% 89% 11%

A5	A12	A22
A12	A13	A22
A5	A12	A22

Chain 7: 86% 14%

Chain 8:  20% 86% 13%

A187	A188	A189	A190	A191	A192	A193	A194	F195	I200	PRO	GLU	GLY	PRO	GLU	ARG	ALA	ILE	ASP	LYS	PRO	F211	I236	V239	K249	C256	K300	K325	R334	T335	T336	E346	G347	K353	M359	L393	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS										
T94	G95	A96	A97	A108	R124	Q125	V126	G127	L135	C138	D139	M140	V141	D142	D143	E144	E145	L146	L147	E148	L149	E150	E151	M152	E153	V154	R155	E156	L157	L158	S159	D162	F163	P164	G165	D166	I170	V171	R172	G173	S174	A175	L176	K177	A178	L179	E180	G181	D182	A183	E184	L185	F186
SER	LYS	GLU	LYS	PHE	GLU	ARG	THR	K10	D22	T26	T34	V36	L36	A37	K38	THR	TYR	GLY	GLY	ALA	ALA	ARG	ALA	PHE	ASP	GLN	ILE	ASP	ASN	ALA	PRO	GLU	GLU	LYS	ALA	ARG	GLY	ILE	THR	ILE	ILE	ASN	T65	S66	H67	V68	E69	P73	T74	D81	G84	H85	A86

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	10215	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	17.183	Depositor
Minimum map value	-9.143	Depositor
Average map value	0.114	Depositor
Map value standard deviation	0.787	Depositor
Recommended contour level	1.0	Depositor
Map size (Å)	383.904, 383.904, 383.904	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.333, 1.333, 1.333	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FME, GDP

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	b	0.25	0/2122	0.59	0/2852
2	c	0.28	0/1586	0.56	0/2134
3	d	0.27	0/1571	0.54	0/2113
4	e	0.29	0/1435	0.52	0/1926
5	f	0.26	0/1343	0.55	0/1816
6	g	0.28	0/1122	0.57	0/1515
7	h	0.31	0/1002	0.61	0/1350
8	i	0.29	0/1046	0.54	0/1410
9	j	0.26	0/1152	0.56	0/1551
10	k	0.26	0/948	0.58	0/1268
11	l	0.27	0/1054	0.57	0/1403
12	m	0.29	0/1093	0.55	0/1460
13	n	0.28	0/974	0.54	0/1301
14	o	0.27	0/902	0.52	0/1209
15	p	0.28	0/929	0.54	0/1242
16	q	0.28	0/960	0.46	0/1278
17	r	0.29	0/829	0.61	1/1107 (0.1%)
18	s	0.24	0/864	0.57	0/1156
19	t	0.26	0/745	0.54	0/994
20	u	0.29	0/788	0.58	0/1051
21	v	0.28	0/766	0.51	0/1025
22	w	0.30	0/582	0.52	0/769
23	x	0.28	0/635	0.52	0/848
24	y	0.26	0/510	0.52	0/677
25	z	0.26	0/453	0.54	0/605
26	B	0.25	0/450	0.57	0/599
27	C	0.31	0/417	0.52	0/554
28	D	0.30	0/380	0.54	0/498
29	E	0.28	0/513	0.59	0/676
30	F	0.25	0/303	0.54	0/397
31	G	0.28	0/1788	0.52	0/2408
32	H	0.28	0/1652	0.52	0/2225

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	I	0.27	0/1665	0.54	0/2227
34	J	0.28	0/1170	0.56	0/1573
35	K	0.28	0/836	0.62	0/1128
36	L	0.26	0/1196	0.53	0/1602
37	M	0.26	0/989	0.53	0/1326
38	N	0.28	0/1034	0.59	0/1375
39	O	0.26	0/797	0.56	0/1077
40	P	0.28	0/886	0.52	0/1195
41	Q	0.26	0/969	0.62	0/1300
42	R	0.24	0/893	0.55	0/1193
43	S	0.28	0/817	0.50	0/1088
44	T	0.27	0/722	0.56	0/964
45	U	0.32	0/659	0.58	0/884
46	V	0.28	0/658	0.58	0/881
47	W	0.29	0/545	0.54	0/731
48	X	0.29	0/653	0.51	0/877
49	Y	0.27	0/671	0.48	0/888
50	Z	0.31	0/551	0.64	0/728
51	a	0.27	0/1034	0.51	0/1387
52	3	0.28	0/36963	0.66	0/57662
53	1	0.26	0/69796	0.65	0/108888
54	2	0.27	0/2872	0.65	0/4479
55	5	0.28	0/1832	0.65	0/2855
55	6	0.28	0/1832	0.65	0/2855
56	4	0.27	0/436	0.62	0/679
57	7	0.28	0/1809	0.65	0/2819
58	8	0.28	0/2730	0.56	0/3693
All	All	0.27	0/165929	0.63	1/247771 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	r	50	GLY	N-CA-C	-6.39	97.12	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	b	269/271 (99%)	233 (87%)	32 (12%)	4 (2%)	10	46
2	c	207/209 (99%)	186 (90%)	20 (10%)	1 (0%)	29	66
3	d	199/201 (99%)	184 (92%)	14 (7%)	1 (0%)	29	66
4	e	175/177 (99%)	155 (89%)	20 (11%)	0	100	100
5	f	174/176 (99%)	149 (86%)	23 (13%)	2 (1%)	14	51
6	g	147/149 (99%)	130 (88%)	15 (10%)	2 (1%)	11	46
7	h	129/131 (98%)	96 (74%)	27 (21%)	6 (5%)	2	24
8	i	139/141 (99%)	126 (91%)	11 (8%)	2 (1%)	11	46
9	j	140/142 (99%)	128 (91%)	11 (8%)	1 (1%)	22	60
10	k	120/122 (98%)	93 (78%)	23 (19%)	4 (3%)	4	32
11	l	141/143 (99%)	109 (77%)	28 (20%)	4 (3%)	5	35
12	m	134/136 (98%)	117 (87%)	15 (11%)	2 (2%)	10	46
13	n	118/120 (98%)	103 (87%)	12 (10%)	3 (2%)	5	36
14	o	114/116 (98%)	104 (91%)	10 (9%)	0	100	100
15	p	112/114 (98%)	98 (88%)	12 (11%)	2 (2%)	8	42
16	q	115/117 (98%)	113 (98%)	2 (2%)	0	100	100
17	r	101/103 (98%)	83 (82%)	16 (16%)	2 (2%)	7	41
18	s	108/110 (98%)	100 (93%)	7 (6%)	1 (1%)	17	54
19	t	91/93 (98%)	82 (90%)	8 (9%)	1 (1%)	14	51
20	u	100/102 (98%)	82 (82%)	13 (13%)	5 (5%)	2	23
21	v	92/94 (98%)	83 (90%)	8 (9%)	1 (1%)	14	51
22	w	73/75 (97%)	66 (90%)	6 (8%)	1 (1%)	11	46
23	x	75/77 (97%)	70 (93%)	5 (7%)	0	100	100
24	y	61/63 (97%)	59 (97%)	2 (3%)	0	100	100
25	z	56/58 (97%)	54 (96%)	2 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	B	54/56 (96%)	49 (91%)	5 (9%)	0	100	100
27	C	48/50 (96%)	44 (92%)	4 (8%)	0	100	100
28	D	44/46 (96%)	39 (89%)	5 (11%)	0	100	100
29	E	62/64 (97%)	54 (87%)	7 (11%)	1 (2%)	9	44
30	F	36/38 (95%)	32 (89%)	3 (8%)	1 (3%)	5	35
31	G	223/225 (99%)	208 (93%)	14 (6%)	1 (0%)	34	70
32	H	204/206 (99%)	192 (94%)	12 (6%)	0	100	100
33	I	203/205 (99%)	180 (89%)	20 (10%)	3 (2%)	10	46
34	J	155/157 (99%)	126 (81%)	21 (14%)	8 (5%)	2	23
35	K	98/100 (98%)	77 (79%)	16 (16%)	5 (5%)	2	23
36	L	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
37	M	127/129 (98%)	114 (90%)	13 (10%)	0	100	100
38	N	125/127 (98%)	101 (81%)	22 (18%)	2 (2%)	9	44
39	O	96/98 (98%)	80 (83%)	12 (12%)	4 (4%)	3	26
40	P	114/116 (98%)	95 (83%)	16 (14%)	3 (3%)	5	36
41	Q	121/123 (98%)	91 (75%)	25 (21%)	5 (4%)	3	27
42	R	112/114 (98%)	97 (87%)	10 (9%)	5 (4%)	2	25
43	S	98/100 (98%)	81 (83%)	17 (17%)	0	100	100
44	T	86/88 (98%)	79 (92%)	6 (7%)	1 (1%)	13	50
45	U	80/82 (98%)	70 (88%)	9 (11%)	1 (1%)	12	48
46	V	78/80 (98%)	62 (80%)	15 (19%)	1 (1%)	12	48
47	W	63/65 (97%)	55 (87%)	6 (10%)	2 (3%)	4	32
48	X	77/79 (98%)	72 (94%)	4 (5%)	1 (1%)	12	48
49	Y	83/85 (98%)	78 (94%)	4 (5%)	1 (1%)	13	50
50	Z	63/65 (97%)	42 (67%)	15 (24%)	6 (10%)	0	11
51	a	130/223 (58%)	122 (94%)	7 (5%)	1 (1%)	19	57
58	8	342/400 (86%)	321 (94%)	20 (6%)	1 (0%)	41	74
All	All	6261/6512 (96%)	5500 (88%)	663 (11%)	98 (2%)	13	44

All (98) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	d	83	VAL

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Mol	Chain	Res	Type
5	f	45	ALA
5	f	174	LYS
7	h	80	THR
10	k	92	GLU
11	l	31	GLY
12	m	58	LYS
13	n	71	ARG
15	p	18	SER
17	r	54	VAL
30	F	37	GLN
34	J	25	LYS
34	J	93	VAL
34	J	122	VAL
35	K	53	LYS
35	K	54	LEU
38	N	90	ASP
41	Q	33	CYS
44	T	46	LYS
45	U	79	ASN
50	Z	8	ASN
50	Z	25	ALA
7	h	113	PHE
8	i	11	GLN
10	k	110	GLU
11	l	85	VAL
19	t	52	GLU
20	u	51	LEU
20	u	88	ASP
20	u	99	SER
29	E	31	ILE
34	J	121	ASN
38	N	106	ASP
40	P	125	LYS
41	Q	24	GLU
42	R	4	ALA
42	R	7	ASN
46	V	17	GLU
50	Z	24	LYS
50	Z	36	PHE
58	8	334	ARG
1	b	107	LYS
2	c	86	GLU

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Mol	Chain	Res	Type
7	h	81	LEU
7	h	107	GLU
7	h	118	ILE
10	k	35	VAL
11	l	29	LYS
12	m	69	PRO
13	n	2	ARG
17	r	26	ASP
18	s	65	ASP
33	I	34	GLU
33	I	47	LEU
34	J	23	THR
35	K	86	ARG
35	K	92	THR
40	P	92	ARG
41	Q	35	ARG
41	Q	87	LYS
47	W	13	THR
49	Y	5	SER
1	b	38	LYS
1	b	175	LEU
13	n	32	GLU
20	u	6	ARG
39	O	41	PRO
39	O	75	ASP
40	P	13	LYS
42	R	65	GLU
6	g	9	VAL
15	p	94	ALA
33	I	152	SER
34	J	11	GLN
34	J	49	TYR
34	J	99	SER
39	O	42	LEU
39	O	58	ASN
47	W	26	ALA
50	Z	14	ALA
51	a	208	TYR
6	g	118	PRO
9	j	81	ILE
10	k	93	GLN
11	l	94	THR

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Mol	Chain	Res	Type
31	G	19	THR
50	Z	66	ARG
20	u	56	GLY
21	v	84	PRO
41	Q	10	PRO
22	w	50	GLY
42	R	5	GLY
48	X	7	GLY
1	b	253	GLY
7	h	79	PRO
8	i	92	PRO
35	K	50	PRO
42	R	6	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	
1	b	216/216 (100%)	214 (99%)	2 (1%)	78	88
2	c	164/164 (100%)	162 (99%)	2 (1%)	71	84
3	d	165/165 (100%)	165 (100%)	0	100	100
4	e	148/148 (100%)	147 (99%)	1 (1%)	84	91
5	f	137/137 (100%)	135 (98%)	2 (2%)	65	81
6	g	114/114 (100%)	114 (100%)	0	100	100
7	h	100/100 (100%)	99 (99%)	1 (1%)	76	86
8	i	109/109 (100%)	109 (100%)	0	100	100
9	j	116/116 (100%)	115 (99%)	1 (1%)	78	88
10	k	103/103 (100%)	102 (99%)	1 (1%)	76	86
11	l	102/102 (100%)	101 (99%)	1 (1%)	76	86
12	m	109/109 (100%)	109 (100%)	0	100	100
13	n	100/100 (100%)	100 (100%)	0	100	100
14	o	86/86 (100%)	85 (99%)	1 (1%)	71	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	p	99/99 (100%)	99 (100%)	0	100	100
16	q	89/89 (100%)	89 (100%)	0	100	100
17	r	84/84 (100%)	82 (98%)	2 (2%)	49	71
18	s	93/93 (100%)	92 (99%)	1 (1%)	73	85
19	t	80/80 (100%)	80 (100%)	0	100	100
20	u	83/83 (100%)	83 (100%)	0	100	100
21	v	78/78 (100%)	78 (100%)	0	100	100
22	w	57/57 (100%)	57 (100%)	0	100	100
23	x	67/67 (100%)	67 (100%)	0	100	100
24	y	55/55 (100%)	55 (100%)	0	100	100
25	z	48/48 (100%)	48 (100%)	0	100	100
26	B	47/47 (100%)	47 (100%)	0	100	100
27	C	45/45 (100%)	45 (100%)	0	100	100
28	D	38/38 (100%)	38 (100%)	0	100	100
29	E	51/51 (100%)	51 (100%)	0	100	100
30	F	34/34 (100%)	34 (100%)	0	100	100
31	G	186/186 (100%)	185 (100%)	1 (0%)	88	94
32	H	170/170 (100%)	170 (100%)	0	100	100
33	I	172/172 (100%)	169 (98%)	3 (2%)	60	78
34	J	119/119 (100%)	118 (99%)	1 (1%)	81	89
35	K	87/87 (100%)	86 (99%)	1 (1%)	73	85
36	L	124/124 (100%)	123 (99%)	1 (1%)	81	89
37	M	104/104 (100%)	104 (100%)	0	100	100
38	N	105/105 (100%)	104 (99%)	1 (1%)	76	86
39	O	86/86 (100%)	84 (98%)	2 (2%)	50	72
40	P	89/89 (100%)	88 (99%)	1 (1%)	73	85
41	Q	103/103 (100%)	101 (98%)	2 (2%)	57	76
42	R	92/92 (100%)	92 (100%)	0	100	100
43	S	83/83 (100%)	83 (100%)	0	100	100
44	T	76/76 (100%)	75 (99%)	1 (1%)	69	82
45	U	65/65 (100%)	64 (98%)	1 (2%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	V	74/74 (100%)	72 (97%)	2 (3%)	44	69
47	W	56/56 (100%)	55 (98%)	1 (2%)	59	77
48	X	70/70 (100%)	70 (100%)	0	100	100
49	Y	65/65 (100%)	64 (98%)	1 (2%)	65	81
50	Z	55/55 (100%)	54 (98%)	1 (2%)	59	77
51	a	110/174 (63%)	109 (99%)	1 (1%)	78	88
58	8	290/332 (87%)	286 (99%)	4 (1%)	67	81
All	All	5198/5304 (98%)	5158 (99%)	40 (1%)	82	89

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	212	TRP
1	b	239	PHE
2	c	16	THR
2	c	142	VAL
4	e	135	ILE
5	f	48	THR
5	f	70	LEU
7	h	107	GLU
9	j	122	LEU
10	k	92	GLU
11	l	94	THR
14	o	56	LYS
17	r	1	MET
17	r	11	GLN
18	s	11	ARG
31	G	144	GLU
33	I	44	LYS
33	I	59	LYS
33	I	183	ARG
34	J	55	VAL
35	K	39	LEU
36	L	112	ASP
38	N	105	ARG
39	O	14	ASP
39	O	59	LYS
40	P	127	ARG
41	Q	87	LYS
41	Q	93	ARG

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Mol	Chain	Res	Type
44	T	68	TYR
45	U	77	GLU
46	V	27	PHE
46	V	38	LYS
47	W	11	ARG
49	Y	73	ARG
50	Z	13	VAL
51	a	7	ARG
58	8	300	LYS
58	8	336	THR
58	8	358	LYS
58	8	359	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (96) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	52	HIS
1	b	85	ASN
1	b	127	ASN
1	b	196	ASN
1	b	199	HIS
1	b	225	ASN
1	b	238	ASN
2	c	32	ASN
2	c	49	GLN
2	c	130	GLN
2	c	134	HIS
2	c	148	GLN
2	c	150	GLN
2	c	173	GLN
3	d	41	GLN
3	d	90	GLN
3	d	97	ASN
4	e	51	ASN
5	f	21	GLN
5	f	44	HIS
5	f	100	ASN
5	f	115	GLN
6	g	11	ASN
6	g	43	ASN
6	g	66	ASN
8	i	5	GLN

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Mol	Chain	Res	Type
8	i	18	ASN
9	j	58	ASN
9	j	135	GLN
10	k	3	GLN
11	l	38	GLN
12	m	22	GLN
12	m	88	ASN
13	n	3	HIS
13	n	13	ASN
13	n	62	ASN
14	o	38	GLN
15	p	40	GLN
16	q	36	GLN
18	s	7	HIS
20	u	39	ASN
20	u	44	HIS
20	u	52	ASN
20	u	65	GLN
20	u	73	ASN
21	v	12	GLN
21	v	49	ASN
22	w	8	ASN
22	w	53	HIS
23	x	16	ASN
24	y	20	ASN
25	z	8	GLN
25	z	19	HIS
26	B	4	GLN
31	G	38	HIS
31	G	50	ASN
31	G	177	ASN
32	H	7	ASN
32	H	18	ASN
32	H	139	ASN
32	H	184	ASN
33	I	35	GLN
33	I	53	GLN
33	I	70	GLN
33	I	88	ASN
33	I	115	GLN
33	I	195	ASN
34	J	77	ASN

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Mol	Chain	Res	Type
34	J	81	GLN
34	J	96	GLN
34	J	131	ASN
36	L	141	HIS
37	M	37	ASN
38	N	36	GLN
38	N	125	GLN
39	O	70	HIS
40	P	118	ASN
41	Q	4	ASN
42	R	11	HIS
43	S	42	ASN
43	S	65	GLN
44	T	36	ASN
44	T	41	HIS
44	T	61	GLN
46	V	8	GLN
46	V	30	HIS
47	W	30	ASN
47	W	51	GLN
49	Y	81	GLN
49	Y	83	ASN
51	a	160	GLN
51	a	188	ASN
58	8	14	ASN
58	8	98	GLN
58	8	115	GLN
58	8	160	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
52	3	1538/1539 (99%)	139 (9%)	4 (0%)
53	1	2902/2903 (99%)	323 (11%)	9 (0%)
54	2	119/120 (99%)	10 (8%)	1 (0%)
55	5	76/77 (98%)	7 (9%)	0
55	6	76/77 (98%)	14 (18%)	0
56	4	17/18 (94%)	2 (11%)	0
57	7	75/76 (98%)	10 (13%)	1 (1%)
All	All	4803/4810 (99%)	505 (10%)	15 (0%)

All (505) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
52	3	6	G
52	3	9	G
52	3	31	G
52	3	32	A
52	3	39	G
52	3	48	C
52	3	51	A
52	3	71	A
52	3	87	C
52	3	95	C
52	3	100	G
52	3	130	A
52	3	144	G
52	3	183	C
52	3	184	G
52	3	197	A
52	3	210	C
52	3	226	G
52	3	247	G
52	3	251	G
52	3	266	G
52	3	267	C
52	3	281	G
52	3	289	G
52	3	316	C
52	3	345	C
52	3	346	G
52	3	352	C
52	3	367	U
52	3	372	C
52	3	411	A
52	3	412	A
52	3	413	G
52	3	429	U
52	3	439	U
52	3	467	U
52	3	479	U
52	3	484	G
52	3	485	U
52	3	486	U
52	3	518	C
52	3	533	A
52	3	547	A

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Mol	Chain	Res	Type
52	3	561	U
52	3	572	A
52	3	573	A
52	3	575	G
52	3	576	C
52	3	577	G
52	3	633	G
52	3	642	A
52	3	665	A
52	3	666	G
52	3	688	G
52	3	703	G
52	3	723	U
52	3	724	G
52	3	755	G
52	3	777	A
52	3	815	A
52	3	817	C
52	3	818	G
52	3	819	A
52	3	821	G
52	3	842	U
52	3	843	U
52	3	844	G
52	3	846	G
52	3	871	U
52	3	873	A
52	3	890	G
52	3	902	G
52	3	926	G
52	3	934	C
52	3	935	A
52	3	960	U
52	3	961	U
52	3	966	G
52	3	969	A
52	3	975	A
52	3	976	G
52	3	977	A
52	3	992	U
52	3	993	G
52	3	1004	A

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Mol	Chain	Res	Type
52	3	1020	G
52	3	1028	C
52	3	1030	U
52	3	1031	C
52	3	1033	G
52	3	1034	G
52	3	1053	G
52	3	1094	G
52	3	1101	A
52	3	1136	C
52	3	1137	C
52	3	1138	G
52	3	1139	G
52	3	1146	A
52	3	1159	U
52	3	1168	U
52	3	1182	G
52	3	1184	G
52	3	1191	A
52	3	1196	A
52	3	1198	G
52	3	1201	A
52	3	1202	U
52	3	1213	A
52	3	1225	A
52	3	1238	A
52	3	1240	U
52	3	1241	G
52	3	1258	G
52	3	1260	G
52	3	1275	A
52	3	1278	G
52	3	1280	A
52	3	1286	U
52	3	1287	A
52	3	1300	G
52	3	1317	C
52	3	1346	A
52	3	1347	G
52	3	1363	A
52	3	1364	U
52	3	1378	C

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Mol	Chain	Res	Type
52	3	1395	C
52	3	1446	A
52	3	1448	C
52	3	1452	C
52	3	1492	A
52	3	1503	A
52	3	1506	U
52	3	1517	G
52	3	1529	G
52	3	1530	G
52	3	1533	C
52	3	1540	U
53	1	10	A
53	1	12	U
53	1	34	U
53	1	35	G
53	1	51	G
53	1	63	A
53	1	71	A
53	1	74	A
53	1	75	G
53	1	102	U
53	1	119	A
53	1	120	U
53	1	139	U
53	1	140	C
53	1	141	G
53	1	142	A
53	1	162	U
53	1	163	C
53	1	181	A
53	1	196	A
53	1	199	A
53	1	216	A
53	1	221	A
53	1	222	A
53	1	229	C
53	1	248	G
53	1	249	C
53	1	255	A
53	1	265	A
53	1	266	G

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Mol	Chain	Res	Type
53	1	276	U
53	1	281	C
53	1	294	A
53	1	301	G
53	1	311	A
53	1	312	G
53	1	323	C
53	1	329	G
53	1	330	A
53	1	361	G
53	1	371	A
53	1	372	G
53	1	386	G
53	1	387	U
53	1	404	A
53	1	406	G
53	1	411	G
53	1	422	A
53	1	424	G
53	1	451	U
53	1	457	A
53	1	458	G
53	1	481	G
53	1	491	G
53	1	504	A
53	1	505	A
53	1	529	A
53	1	530	G
53	1	531	C
53	1	532	A
53	1	542	C
53	1	543	G
53	1	563	A
53	1	573	U
53	1	588	U
53	1	603	A
53	1	616	A
53	1	627	A
53	1	628	G
53	1	637	A
53	1	645	C
53	1	646	U

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Mol	Chain	Res	Type
53	1	654	A
53	1	669	G
53	1	686	U
53	1	687	C
53	1	695	G
53	1	730	A
53	1	747	C
53	1	748	G
53	1	752	A
53	1	764	A
53	1	771	G
53	1	776	G
53	1	782	A
53	1	784	G
53	1	785	G
53	1	805	G
53	1	812	C
53	1	819	A
53	1	827	U
53	1	828	U
53	1	830	G
53	1	845	A
53	1	846	U
53	1	847	U
53	1	859	G
53	1	878	A
53	1	887	U
53	1	888	C
53	1	896	A
53	1	897	C
53	1	910	A
53	1	932	U
53	1	941	A
53	1	946	C
53	1	961	C
53	1	974	G
53	1	983	A
53	1	995	C
53	1	1012	U
53	1	1013	C
53	1	1021	A
53	1	1022	G

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Mol	Chain	Res	Type
53	1	1026	G
53	1	1033	U
53	1	1045	C
53	1	1046	A
53	1	1047	G
53	1	1054	A
53	1	1060	U
53	1	1062	G
53	1	1066	U
53	1	1070	A
53	1	1071	G
53	1	1079	C
53	1	1084	A
53	1	1088	A
53	1	1090	A
53	1	1104	C
53	1	1106	G
53	1	1111	A
53	1	1131	G
53	1	1132	U
53	1	1133	A
53	1	1135	C
53	1	1143	A
53	1	1174	U
53	1	1175	A
53	1	1176	U
53	1	1177	G
53	1	1180	U
53	1	1211	C
53	1	1212	G
53	1	1250	G
53	1	1251	C
53	1	1253	A
53	1	1256	G
53	1	1271	G
53	1	1272	A
53	1	1301	A
53	1	1321	A
53	1	1329	U
53	1	1330	C
53	1	1332	G
53	1	1345	C

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Mol	Chain	Res	Type
53	1	1365	A
53	1	1378	A
53	1	1379	U
53	1	1383	A
53	1	1395	A
53	1	1398	C
53	1	1416	G
53	1	1419	A
53	1	1420	A
53	1	1461	C
53	1	1476	U
53	1	1482	G
53	1	1490	A
53	1	1491	G
53	1	1504	A
53	1	1515	A
53	1	1524	G
53	1	1535	A
53	1	1536	C
53	1	1537	G
53	1	1555	G
53	1	1559	U
53	1	1560	G
53	1	1569	A
53	1	1581	G
53	1	1584	U
53	1	1585	C
53	1	1608	A
53	1	1611	C
53	1	1616	A
53	1	1647	U
53	1	1648	U
53	1	1654	A
53	1	1674	G
53	1	1699	G
53	1	1715	G
53	1	1729	U
53	1	1730	C
53	1	1738	G
53	1	1758	U
53	1	1764	C
53	1	1773	A

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Mol	Chain	Res	Type
53	1	1780	A
53	1	1800	C
53	1	1801	A
53	1	1808	A
53	1	1816	C
53	1	1829	A
53	1	1871	A
53	1	1901	A
53	1	1906	G
53	1	1907	G
53	1	1913	A
53	1	1914	C
53	1	1919	A
53	1	1929	G
53	1	1930	G
53	1	1937	A
53	1	1938	A
53	1	1955	U
53	1	1963	U
53	1	1967	C
53	1	1970	A
53	1	1971	U
53	1	1972	G
53	1	1991	U
53	1	1993	U
53	1	1997	C
53	1	2022	U
53	1	2023	C
53	1	2030	A
53	1	2031	A
53	1	2043	C
53	1	2055	C
53	1	2056	G
53	1	2060	A
53	1	2061	G
53	1	2062	A
53	1	2069	G
53	1	2072	C
53	1	2096	C
53	1	2110	G
53	1	2111	U
53	1	2112	G

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Mol	Chain	Res	Type
53	1	2113	U
53	1	2118	U
53	1	2119	A
53	1	2132	U
53	1	2133	G
53	1	2145	C
53	1	2147	A
53	1	2162	G
53	1	2172	U
53	1	2173	A
53	1	2189	U
53	1	2198	A
53	1	2203	U
53	1	2204	G
53	1	2211	A
53	1	2213	U
53	1	2225	A
53	1	2238	G
53	1	2239	G
53	1	2278	A
53	1	2283	C
53	1	2287	A
53	1	2297	A
53	1	2305	U
53	1	2309	A
53	1	2325	G
53	1	2327	A
53	1	2334	U
53	1	2335	A
53	1	2350	C
53	1	2383	G
53	1	2385	C
53	1	2392	A
53	1	2402	U
53	1	2406	A
53	1	2423	U
53	1	2424	C
53	1	2429	G
53	1	2430	A
53	1	2435	A
53	1	2441	U
53	1	2448	A

Continued on next page...

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Mol	Chain	Res	Type
53	1	2476	A
53	1	2498	C
53	1	2502	G
53	1	2504	U
53	1	2505	G
53	1	2518	A
53	1	2547	A
53	1	2554	U
53	1	2566	A
53	1	2567	G
53	1	2572	A
53	1	2602	A
53	1	2603	G
53	1	2609	U
53	1	2613	U
53	1	2646	C
53	1	2655	G
53	1	2682	A
53	1	2689	U
53	1	2690	U
53	1	2714	G
53	1	2716	C
53	1	2744	G
53	1	2748	A
53	1	2764	A
53	1	2765	A
53	1	2778	A
53	1	2779	U
53	1	2791	G
53	1	2794	C
53	1	2797	U
53	1	2800	A
53	1	2809	A
53	1	2820	A
53	1	2821	A
53	1	2833	U
53	1	2849	U
53	1	2867	G
53	1	2868	A
53	1	2872	A
53	1	2880	C
54	2	4	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
54	2	13	G
54	2	24	G
54	2	35	C
54	2	44	G
54	2	67	G
54	2	89	U
54	2	90	C
54	2	108	A
54	2	109	A
55	5	9	G
55	5	18	G
55	5	19	G
55	5	20	U
55	5	47	U
55	5	48	C
55	5	61	C
55	6	2	G
55	6	3	C
55	6	8	U
55	6	9	G
55	6	10	G
55	6	14	A
55	6	19	G
55	6	20	U
55	6	21	A
55	6	22	G
55	6	34	C
55	6	61	C
55	6	64	G
55	6	70	G
56	4	12	A
56	4	13	A
57	7	8	U
57	7	9	A
57	7	17	C
57	7	18	G
57	7	21	A
57	7	43	C
57	7	44	G
57	7	45	U
57	7	46	G
57	7	48	C

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
52	3	70	U
52	3	438	U
52	3	1190	G
52	3	1201	A
53	1	421	C
53	1	490	C
53	1	1020	A
53	1	1130	U
53	1	1475	G
53	1	2286	G
53	1	2296	U
53	1	2326	C
53	1	2391	G
54	2	88	C
57	7	42	C

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands 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	$\# Z > 2$
61	GDP	8	501	-	24,30,30	1.70	5 (20%)	30,47,47	1.58	7 (23%)
59	FME	5	101	55	8,9,10	0.54	0	7,9,11	0.91	0
60	PHE	7	101	57	10,11,12	0.65	0	10,13,15	0.39	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
61	GDP	8	501	-	-	4/12/32/32	0/3/3/3
59	FME	5	101	55	-	1/7/9/11	-
60	PHE	7	101	57	-	0/5/6/8	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
61	8	501	GDP	O4'-C1'	4.72	1.47	1.41
61	8	501	GDP	PB-O1B	2.92	1.60	1.50
61	8	501	GDP	PA-O1A	2.66	1.60	1.50
61	8	501	GDP	PB-O3B	-2.46	1.45	1.54
61	8	501	GDP	C8-N7	-2.12	1.31	1.35

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
61	8	501	GDP	O4'-C4'-C3'	3.27	111.58	105.11
61	8	501	GDP	C8-N7-C5	3.23	109.14	102.99
61	8	501	GDP	C3'-C2'-C1'	2.90	105.35	100.98
61	8	501	GDP	C5-C6-N1	2.84	118.96	113.95
61	8	501	GDP	C2-N1-C6	-2.21	121.03	125.10
61	8	501	GDP	O2A-PA-O1A	2.11	122.67	112.24
61	8	501	GDP	O4'-C4'-C5'	2.09	116.24	109.37

There are no chirality outliers.

All (5) torsion outliers are listed below:

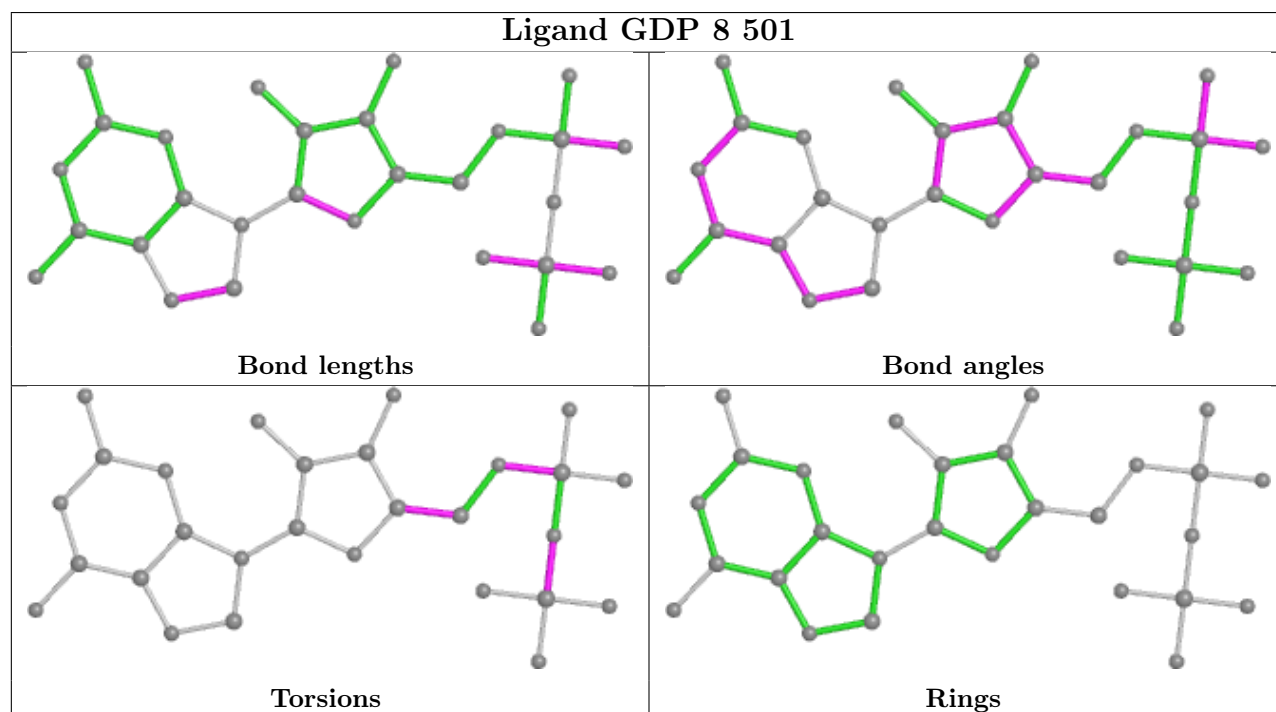
Mol	Chain	Res	Type	Atoms
59	5	101	FME	O1-CN-N-CA
61	8	501	GDP	PA-O3A-PB-O3B
61	8	501	GDP	O4'-C4'-C5'-O5'
61	8	501	GDP	C3'-C4'-C5'-O5'
61	8	501	GDP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

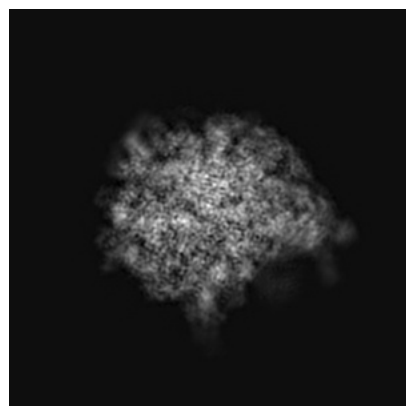
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21629. These allow visual inspection of the internal detail of the map and identification of artifacts.

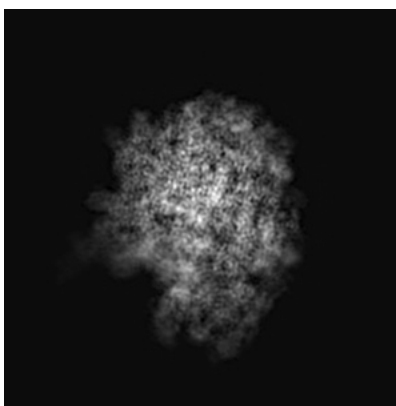
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

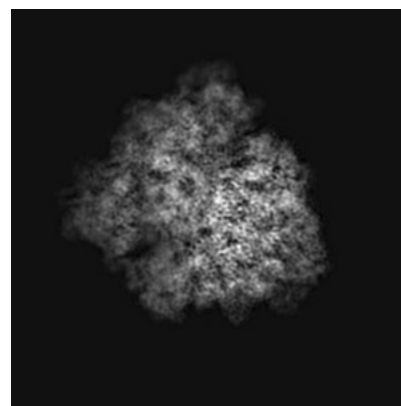
6.1.1 Primary map



X

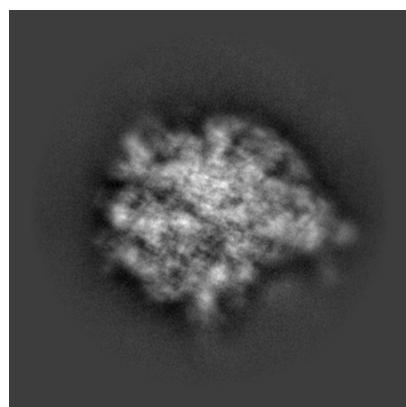


Y

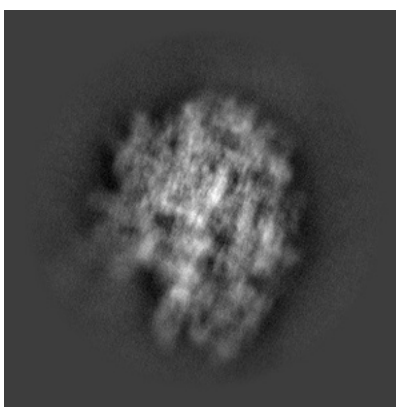


Z

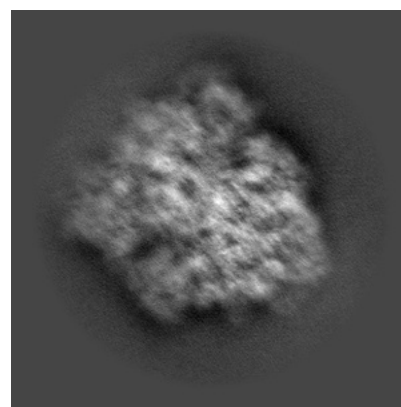
6.1.2 Raw map



X



Y

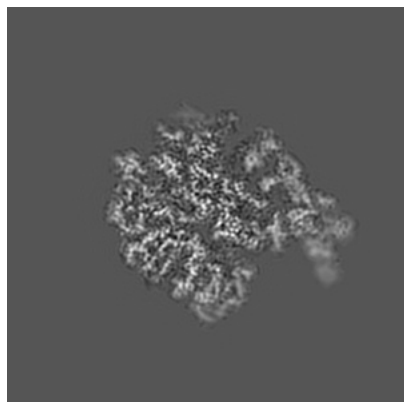


Z

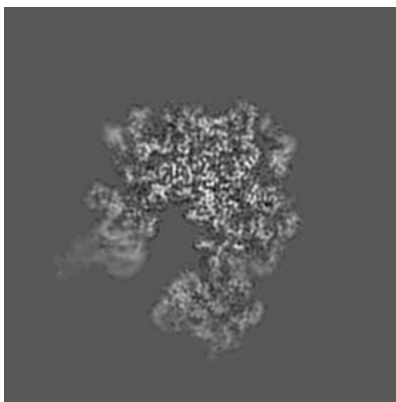
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

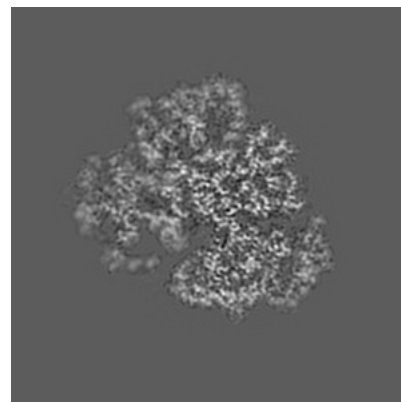
6.2.1 Primary map



X Index: 144

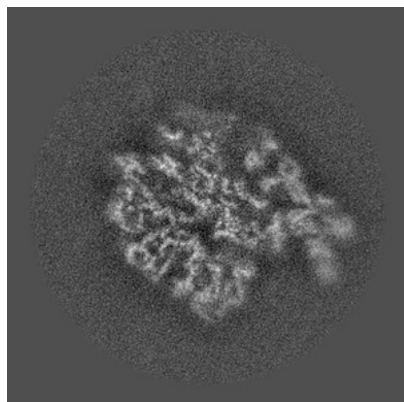


Y Index: 144

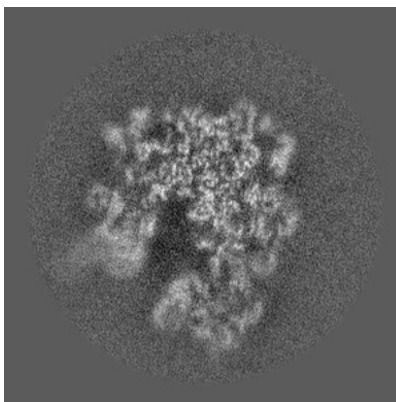


Z Index: 144

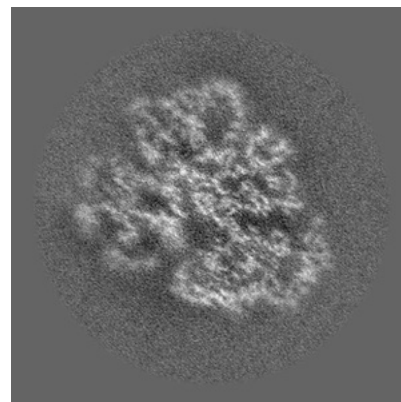
6.2.2 Raw map



X Index: 144



Y Index: 144

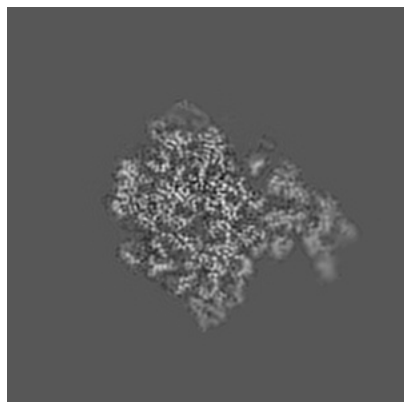


Z Index: 144

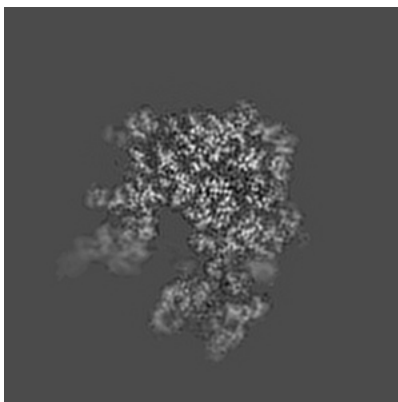
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

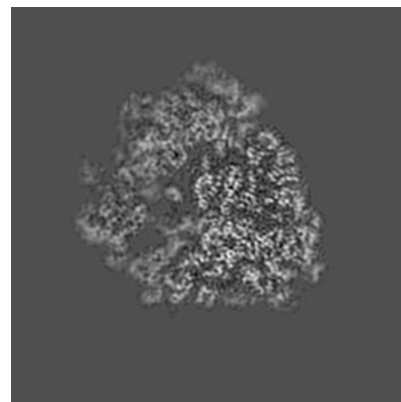
6.3.1 Primary map



X Index: 149

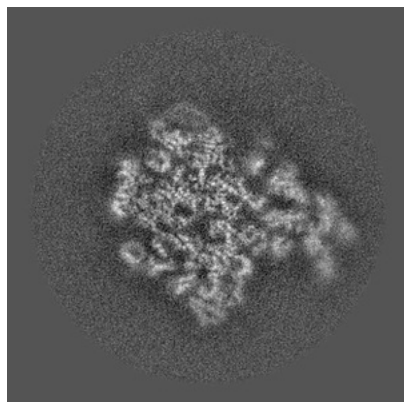


Y Index: 148

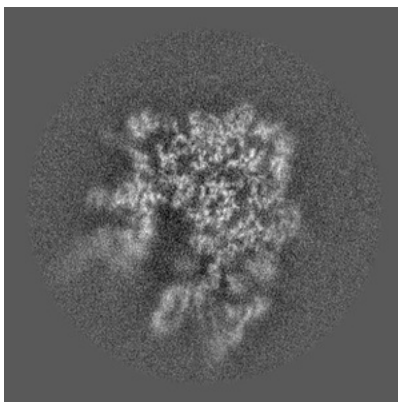


Z Index: 135

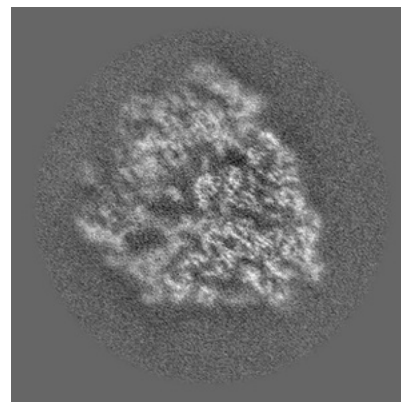
6.3.2 Raw map



X Index: 149



Y Index: 149

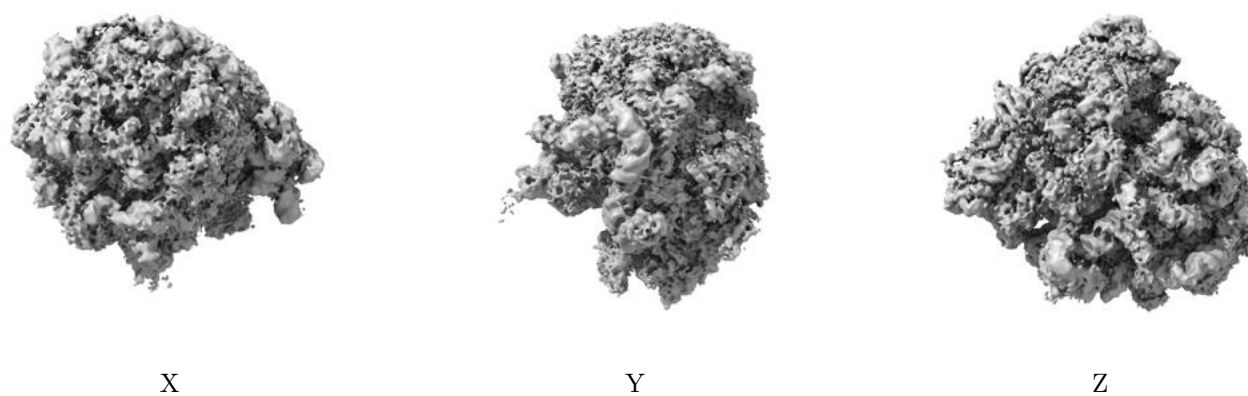


Z Index: 135

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

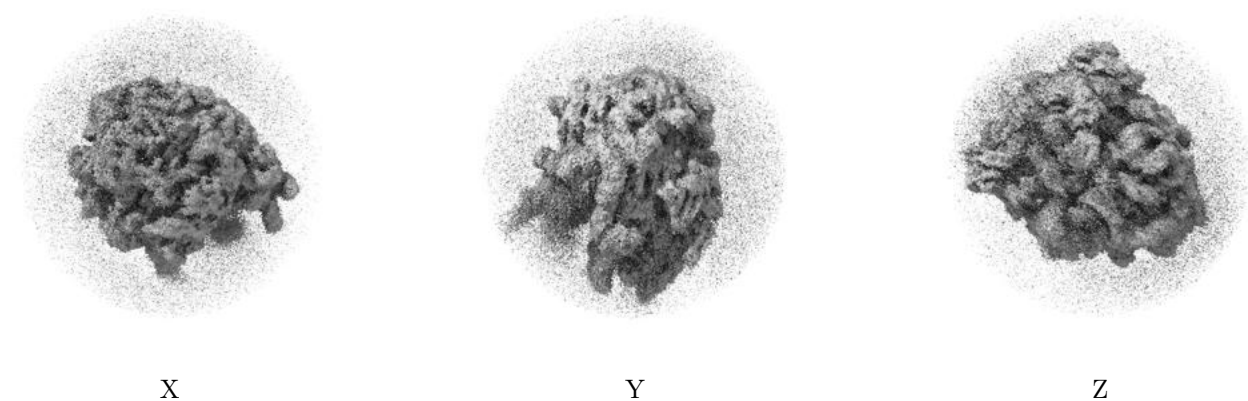
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



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.

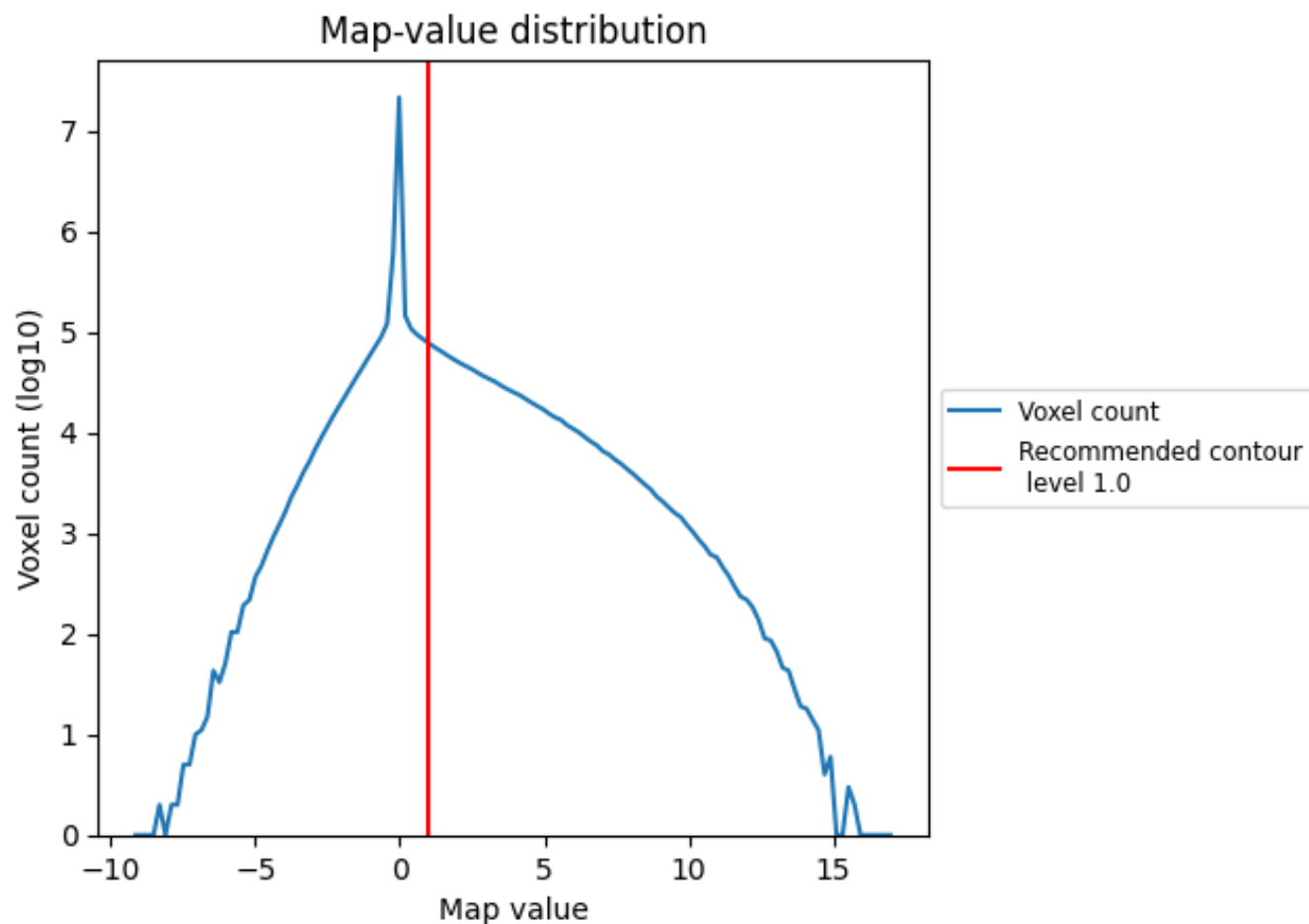
6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

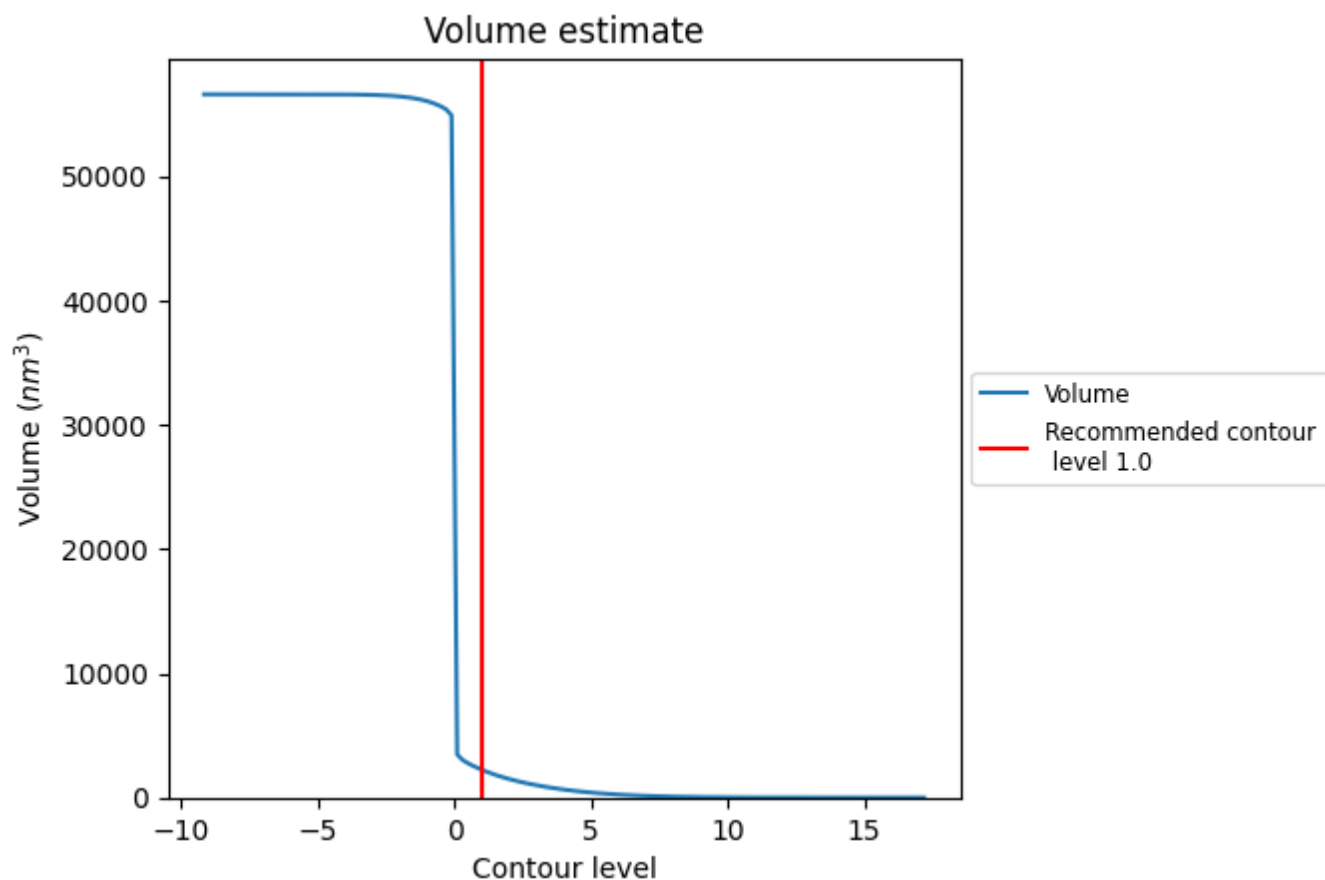
This section contains the results of statistical analysis of the map.

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.

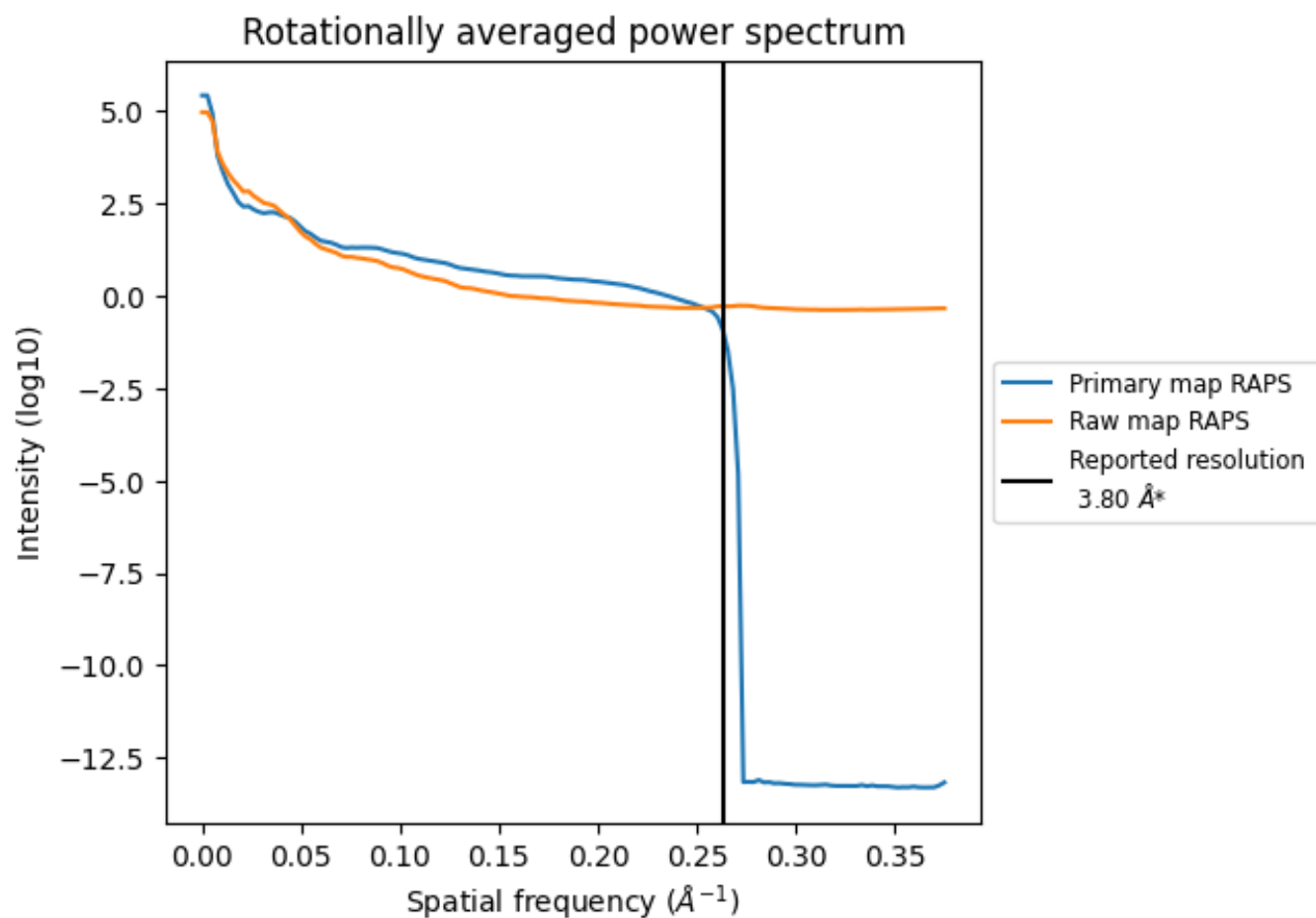
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2247 nm³; this corresponds to an approximate mass of 2030 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 ⓘ

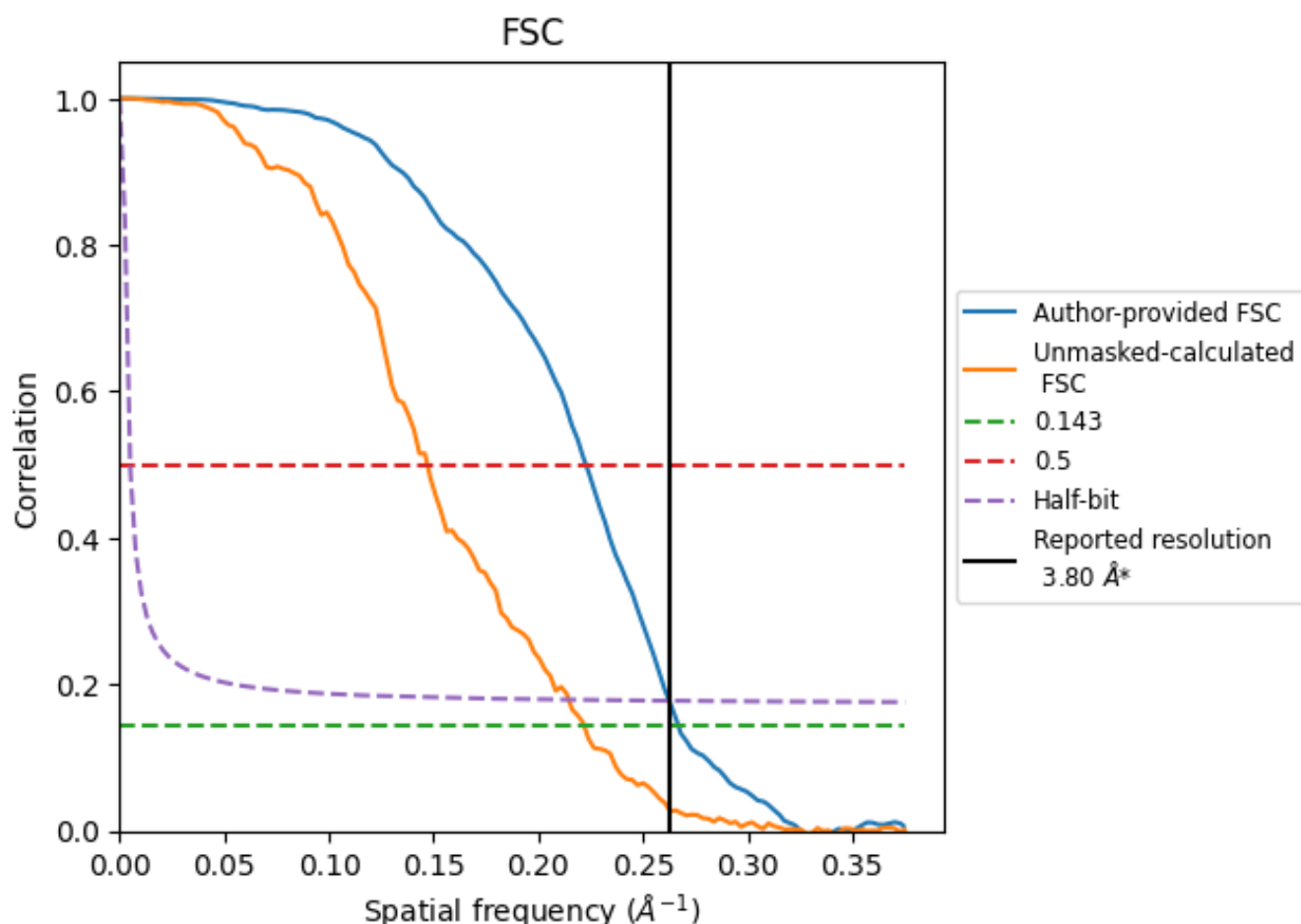


*Reported resolution corresponds to spatial frequency of 0.263 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

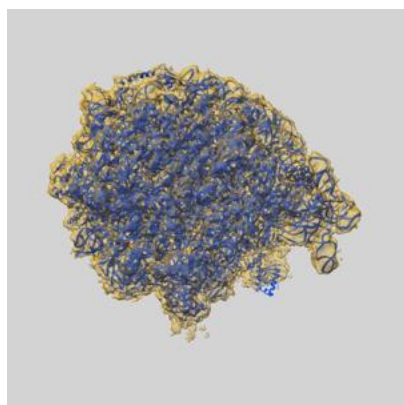
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.75	4.49	3.81
Unmasked-calculated*	4.50	6.80	4.66

*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 4.50 differs from the reported value 3.8 by more than 10 %

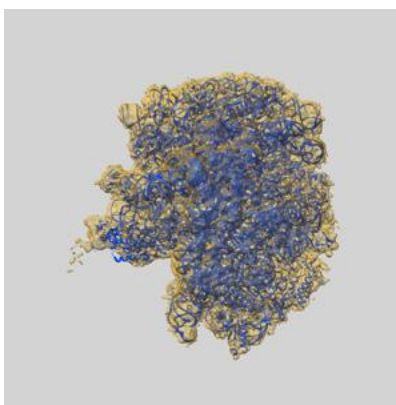
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-21629 and PDB model 6WDA. Per-residue inclusion information can be found in section [3](#) on page [17](#).

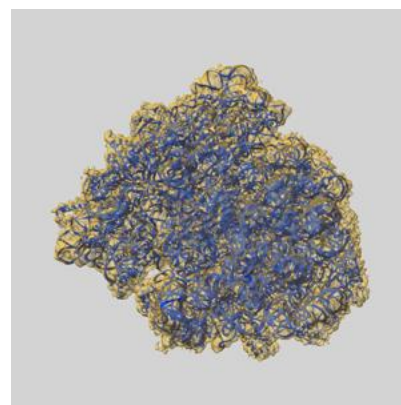
9.1 Map-model overlay [i](#)



X



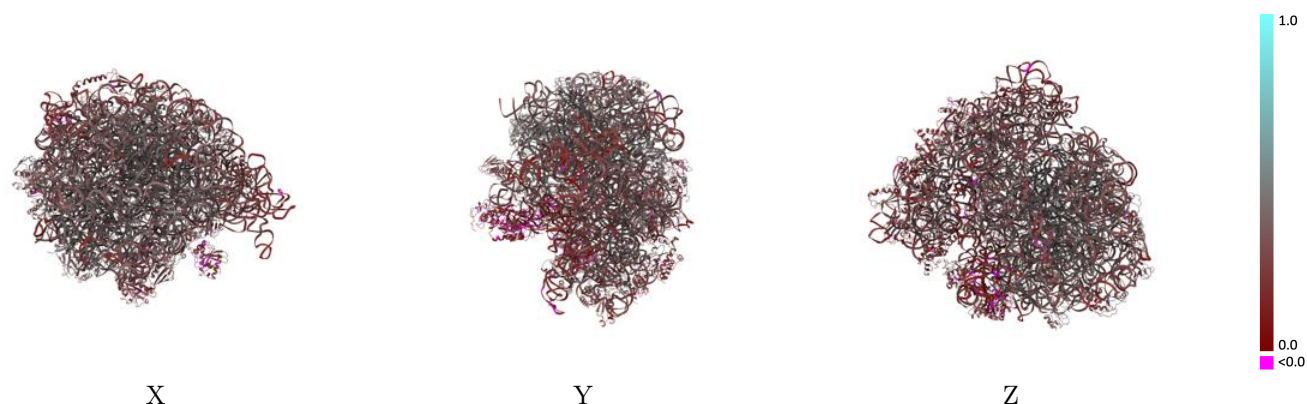
Y



Z

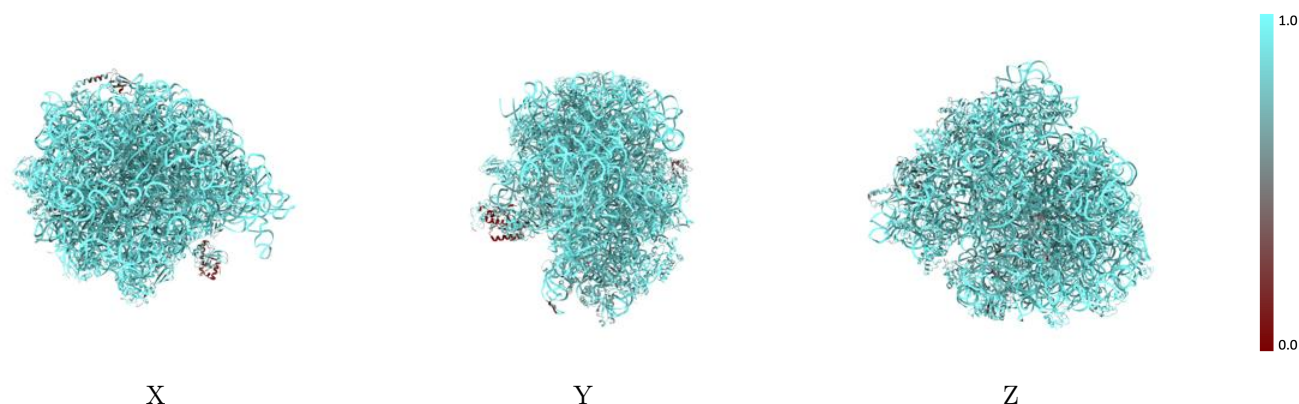
The images above show the 3D surface view of the map at the recommended contour level 1.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



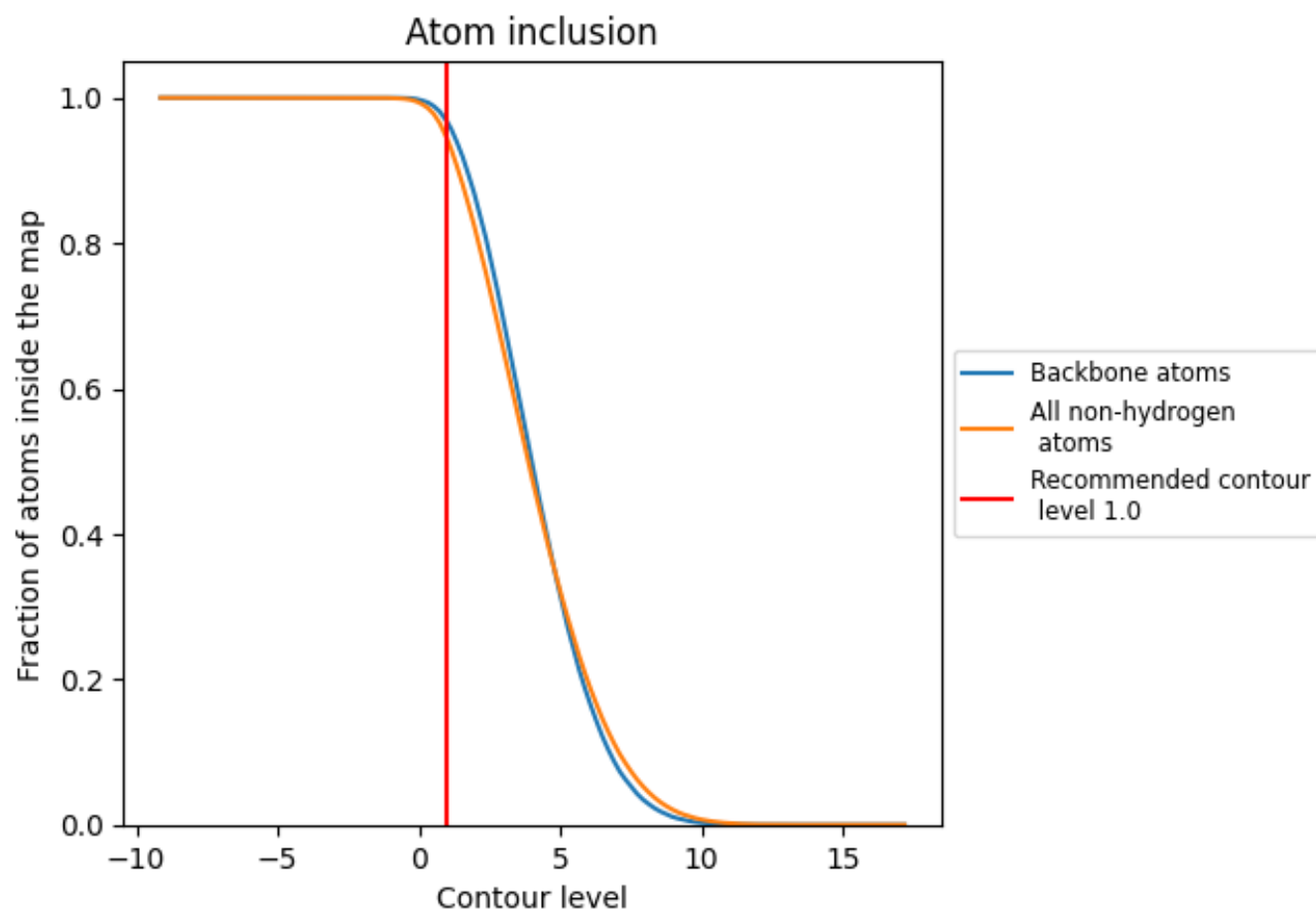
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (1.0).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 97% 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 (1.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9434	 0.3320
1	 0.9809	 0.3610
2	 0.9817	 0.3160
3	 0.9753	 0.3080
4	 0.8789	 0.2360
5	 0.9685	 0.2890
6	 0.8189	 0.1350
7	 0.9276	 0.1450
8	 0.6981	 0.1460
B	 0.9393	 0.4060
C	 0.8284	 0.3600
D	 0.9268	 0.4330
E	 0.9185	 0.4380
F	 0.8253	 0.3670
G	 0.8691	 0.2920
H	 0.7739	 0.3050
I	 0.7723	 0.2170
J	 0.9154	 0.3650
K	 0.9322	 0.3550
L	 0.8987	 0.2690
M	 0.9250	 0.3560
N	 0.8621	 0.2830
O	 0.7178	 0.2840
P	 0.9267	 0.3480
Q	 0.9218	 0.3460
R	 0.9143	 0.2810
S	 0.7545	 0.2790
T	 0.9449	 0.3520
U	 0.8915	 0.3040
V	 0.9084	 0.3280
W	 0.8951	 0.3250
X	 0.9486	 0.2800
Y	 0.9338	 0.2880
Z	 0.8571	 0.2900
a	 0.7851	 0.1230



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.9465	 0.4420
c	 0.9363	 0.4280
d	 0.9336	 0.3790
e	 0.9294	 0.2790
f	 0.9406	 0.3010
g	 0.6515	 0.2480
h	 0.7513	 0.1410
i	 0.6429	 0.1390
j	 0.9473	 0.4230
k	 0.9289	 0.4250
l	 0.9321	 0.4050
m	 0.9117	 0.4070
n	 0.9350	 0.4160
o	 0.9258	 0.3340
p	 0.9583	 0.4100
q	 0.9295	 0.4120
r	 0.9460	 0.3960
s	 0.9187	 0.4190
t	 0.9322	 0.4010
u	 0.9310	 0.3580
v	 0.9404	 0.3800
w	 0.9213	 0.4180
x	 0.9334	 0.4270
y	 0.9235	 0.3270
z	 0.9451	 0.4130