



wwPDB EM Validation Summary Report ⓘ

Nov 5, 2022 – 09:08 PM EDT

PDB ID : 5WE4
EMDB ID : EMD-8814
Title : 70S ribosome-EF-Tu wt complex with GppNHp
Authors : Fislage, M.; Brown, Z.; Frank, J.
Deposited on : 2017-07-07
Resolution : 3.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.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

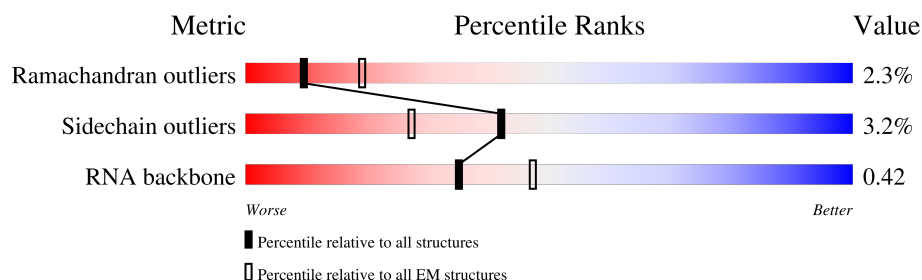
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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	A	2903	
2	B	120	
3	C	271	
4	D	208	
5	E	200	
6	F	177	
7	G	174	
8	H	149	


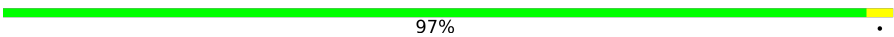
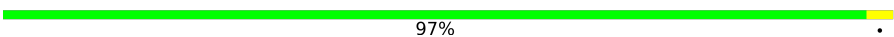
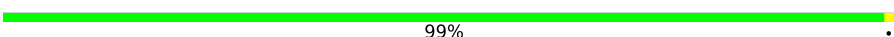






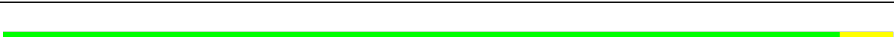


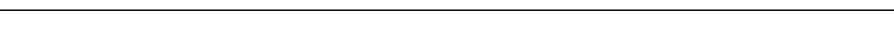
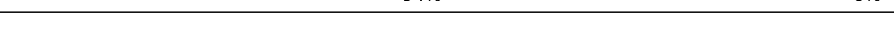
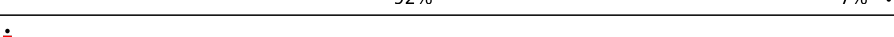
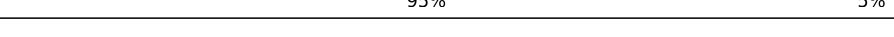
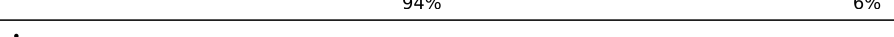

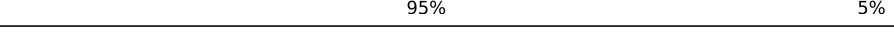
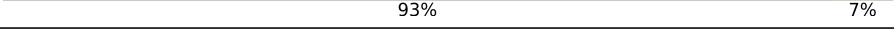




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Mol	Chain	Length	Quality of chain
9	I	141	 24% 92% 7%
10	J	141	 96%
11	K	122	 95% 5%
12	L	143	 90% 10%
13	M	136	 98% ..
14	N	119	 96% . .
15	O	116	 98% .
16	P	114	 99% .
17	Q	115	 98% .
18	R	102	 91% 9%
19	S	109	 94% 6%
20	T	92	 95% . .
21	U	102	 95% 5%
22	V	92	 98% .
23	W	75	 96% .
24	X	77	 97% .
25	Y	60	 98% .
26	Z	56	 98% .
27	0	55	 93% 7%
28	1	51	 94% 6%
29	2	45	 89% 11%
30	3	64	 97% .
31	4	38	 97% .
32	5	131	 76% 89% 11%
33	6	66	 97% .

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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	<div><div></div><div>95%</div><div>5%</div></div>

2 Entry composition

There are 64 unique types of molecules in this entry. The entry contains 155067 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2900	Total	C	N	O	P	0	0
			62277	27788	11459	20130	2900		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	747	5MC	U	conflict	GB 731469900
A	1723	G	A	conflict	GB 731469900
A	1847	G	A	conflict	GB 731469900

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	120	A	U	conflict	GB 1174070234

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	157	Total	C	N	O	S	1	0
			1164	724	221	213	6		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	35	ALA	-	insertion	UNP P0AG59

- Molecule 48 is a protein called 30S ribosomal protein S15.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 56 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	x	12	Total	C	N	O	P	0	0
			252	113	42	85	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
58	z	393	Total	C	N	O	S	0	0
			3036	1918	524	581	13		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
z	47	ASN	ASP	conflict	UNP P0CE48

- Molecule 59 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
59	A	1181	Total 1181	Mg 1181	0
59	B	31	Total 31	Mg 31	0
59	C	1	Total 1	Mg 1	0
59	K	1	Total 1	Mg 1	0
59	L	2	Total 2	Mg 2	0
59	M	1	Total 1	Mg 1	0
59	Q	1	Total 1	Mg 1	0
59	R	1	Total 1	Mg 1	0
59	S	1	Total 1	Mg 1	0
59	T	2	Total 2	Mg 2	0
59	0	2	Total 2	Mg 2	0
59	1	1	Total 1	Mg 1	0
59	3	1	Total 1	Mg 1	0
59	4	1	Total 1	Mg 1	0
59	a	373	Total 373	Mg 373	0
59	d	1	Total 1	Mg 1	0
59	h	1	Total 1	Mg 1	0
59	i	1	Total 1	Mg 1	0
59	s	1	Total 1	Mg 1	0
59	u	1	Total 1	Mg 1	0
59	v	7	Total 7	Mg 7	0
59	w	1	Total 1	Mg 1	0

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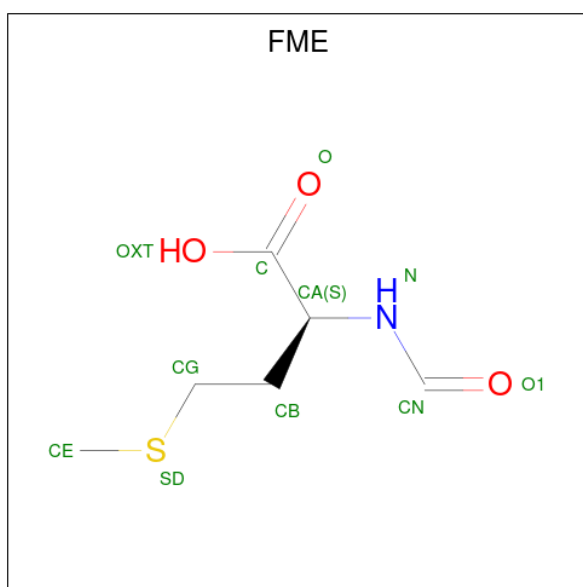
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Mol	Chain	Residues	Atoms		AltConf
59	y	4	Total	Mg	0
			4	4	
59	z	1	Total	Mg	0
			1	1	

- Molecule 60 is POTASSIUM ION (three-letter code: K) (formula: K).

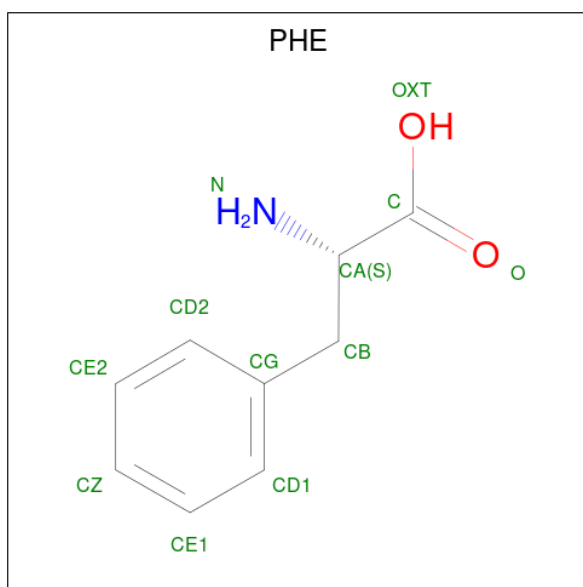
Mol	Chain	Residues	Atoms		AltConf
60	A	1	Total	K	0
			1	1	

- Molecule 61 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).



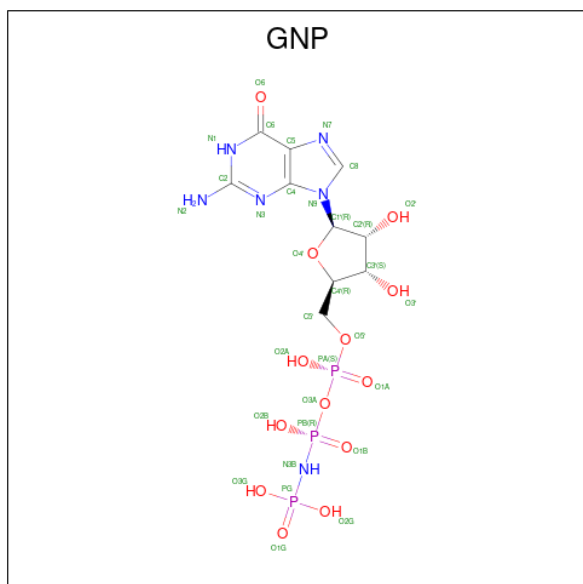
Mol	Chain	Residues	Atoms					AltConf
61	v	1	Total	C	N	O	S	0
			10	6	1	2	1	

- Molecule 62 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



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

- Molecule 63 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).



Mol	Chain	Residues	Atoms	AltConf
64	A	751	Total O 751 751	0
64	B	11	Total O 11 11	0
64	C	9	Total O 9 9	0
64	E	5	Total O 5 5	0
64	J	2	Total O 2 2	0
64	K	2	Total O 2 2	0
64	L	6	Total O 6 6	0
64	M	1	Total O 1 1	0
64	N	3	Total O 3 3	0
64	O	1	Total O 1 1	0
64	P	2	Total O 2 2	0
64	Q	3	Total O 3 3	0
64	R	1	Total O 1 1	0
64	S	2	Total O 2 2	0
64	T	3	Total O 3 3	0
64	U	2	Total O 2 2	0
64	W	1	Total O 1 1	0
64	X	1	Total O 1 1	0
64	Y	1	Total O 1 1	0
64	Z	3	Total O 3 3	0
64	2	5	Total O 5 5	0
64	3	4	Total O 4 4	0

Continued on next page...

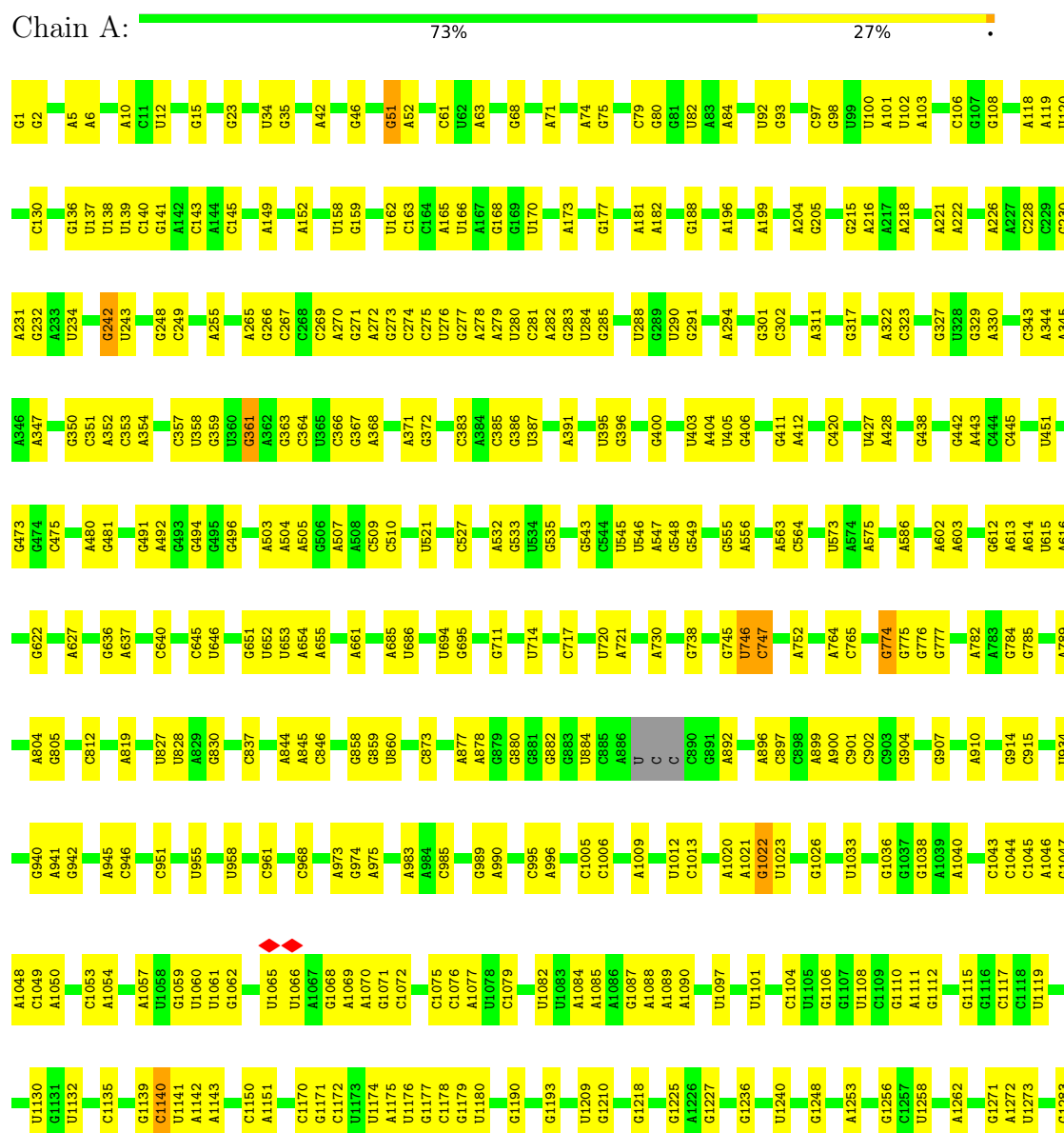
Continued from previous page...

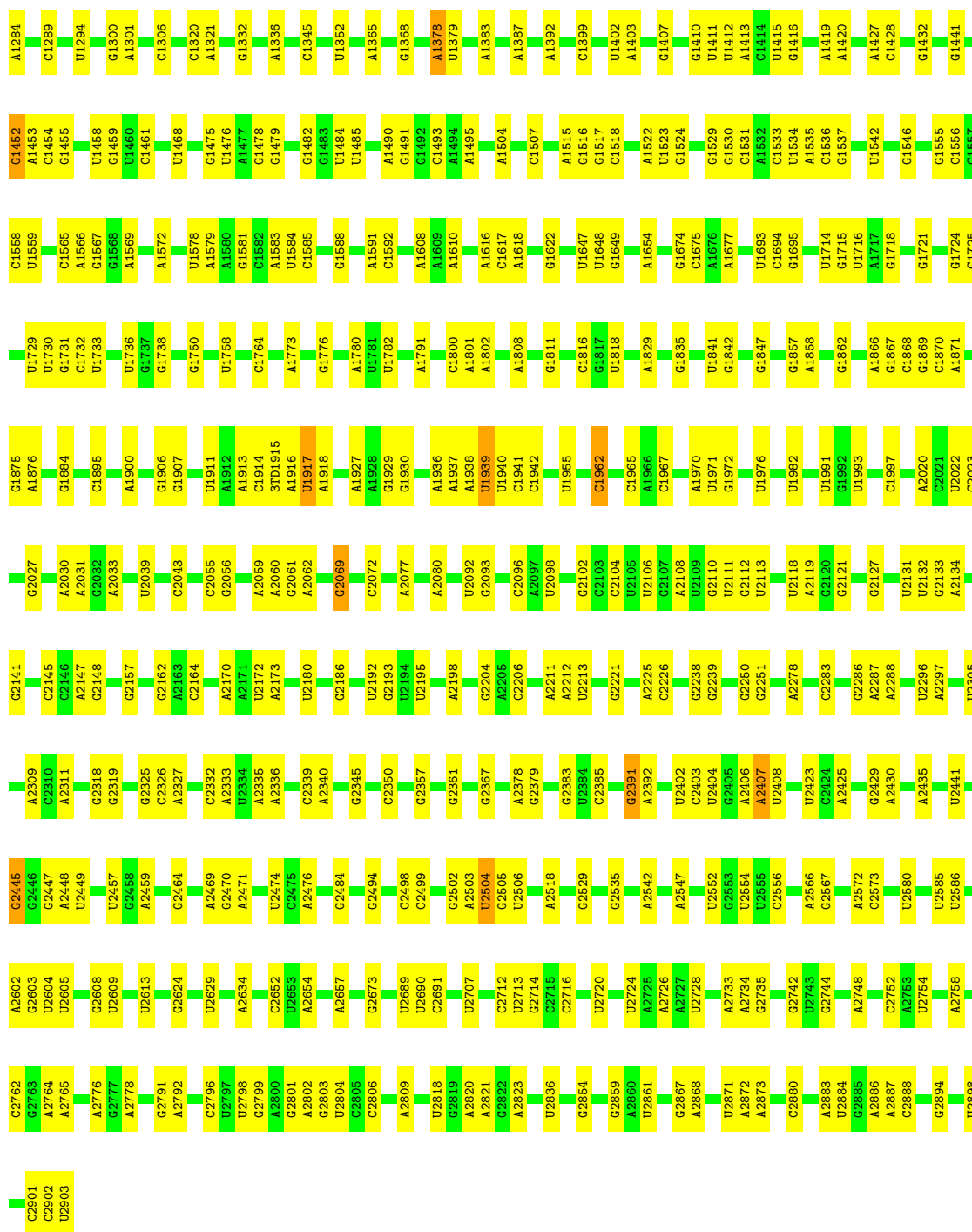
Mol	Chain	Residues	Atoms		AltConf
64	4	1	Total 1	O 1	0
64	a	160	Total 160	O 160	0
64	i	2	Total 2	O 2	0
64	j	1	Total 1	O 1	0
64	o	1	Total 1	O 1	0
64	p	1	Total 1	O 1	0
64	s	2	Total 2	O 2	0
64	t	1	Total 1	O 1	0
64	u	1	Total 1	O 1	0
64	v	3	Total 3	O 3	0
64	w	1	Total 1	O 1	0
64	y	3	Total 3	O 3	0

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.

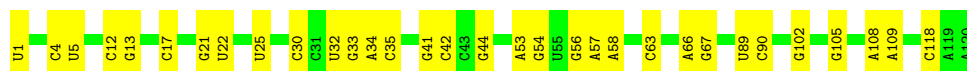
• Molecule 1: 23S rRNA





- Molecule 2: 5S rRNA

Chain B: 73% 27%



- Molecule 3: 50S ribosomal protein L2

Chain C:  97%



- Molecule 4: 50S ribosomal protein L3

Chain D:  96%



- Molecule 5: 50S ribosomal protein L4

Chain E:  98%



- Molecule 6: 50S ribosomal protein L5

Chain F:  98%



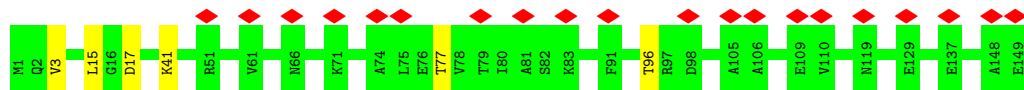
- Molecule 7: 50S ribosomal protein L6

Chain G:  98%

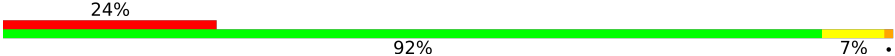


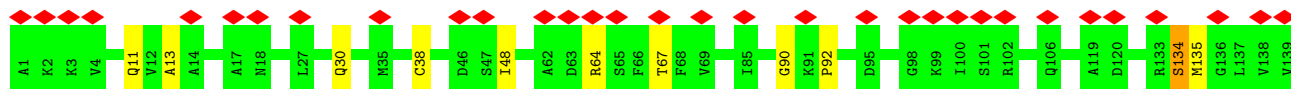
- Molecule 8: 50S ribosomal protein L9

Chain H:  13% 96%



- Molecule 9: 50S ribosomal protein L11

Chain I:  24% 92% 7%





- Molecule 10: 50S ribosomal protein L13

Chain J: 96%



- Molecule 11: 50S ribosomal protein L14

Chain K: 95%



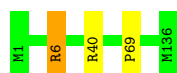
- Molecule 12: 50S ribosomal protein L15

Chain L: 90%



- Molecule 13: 50S ribosomal protein L16

Chain M: 98%



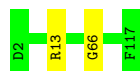
- Molecule 14: 50S ribosomal protein L17

Chain N: 96%



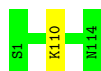
- Molecule 15: 50S ribosomal protein L18

Chain O: 98%



- Molecule 16: 50S ribosomal protein L19

Chain P: 99%



- Molecule 17: 50S ribosomal protein L20

Chain Q: 98%



- Molecule 18: 50S ribosomal protein L21

Chain R: 91%



- Molecule 19: 50S ribosomal protein L22

Chain S: 94%



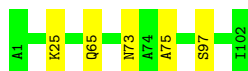
- Molecule 20: 50S ribosomal protein L23

Chain T: 95%



- Molecule 21: 50S ribosomal protein L24

Chain U: 95%



- Molecule 22: 50S ribosomal protein L25

Chain V: 98%



- Molecule 23: 50S ribosomal protein L27

Chain W: 96%



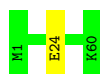
- Molecule 24: 50S ribosomal protein L28

Chain X:  97%



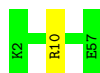
- Molecule 25: 50S ribosomal protein L29

Chain Y:  98%



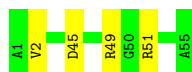
- Molecule 26: 50S ribosomal protein L30

Chain Z:  98%



- Molecule 27: 50S ribosomal protein L32

Chain 0:  93% 7%




- Molecule 28: 50S ribosomal protein L33

Chain 1:  94% 6%



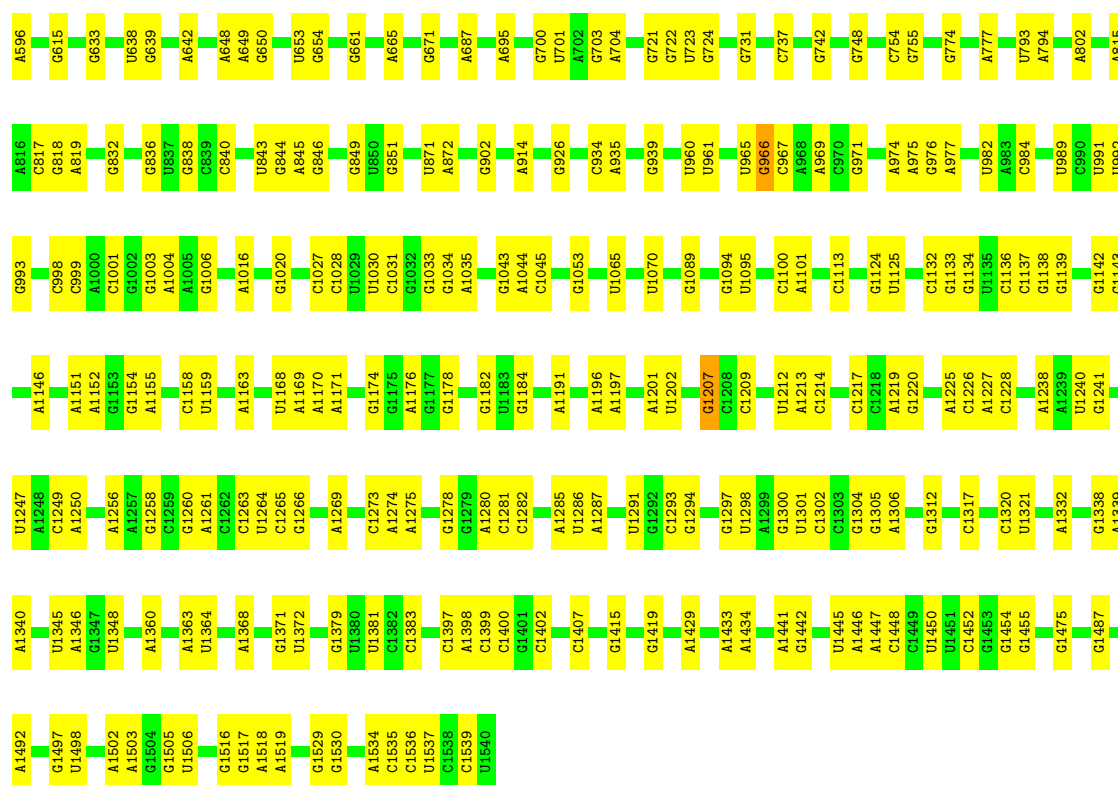
- Molecule 29: 50S ribosomal protein L34

Chain 2:  89% 11%



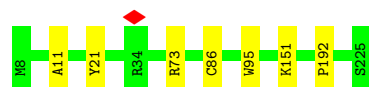
- Molecule 30: 50S ribosomal protein L35

Chain 3:  97%



• Molecule 35: 30S ribosomal protein S2

Chain b: 97%



• Molecule 36: 30S ribosomal protein S3

Chain c: 97%



• Molecule 37: 30S ribosomal protein S4

Chain d: 99%



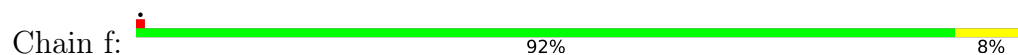
• Molecule 38: 30S ribosomal protein S5

Chain e: 94%

Chain e: 6%



- Molecule 39: 30S ribosomal protein S6



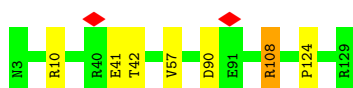
- Molecule 40: 30S ribosomal protein S7



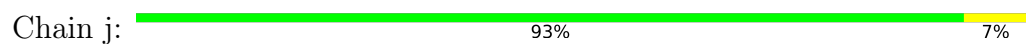
- Molecule 41: 30S ribosomal protein S8



- Molecule 42: 30S ribosomal protein S9



- Molecule 43: 30S ribosomal protein S10

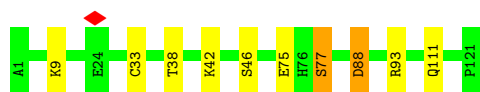


- Molecule 44: 30S ribosomal protein S11



- Molecule 45: 30S ribosomal protein S12





- Molecule 46: 30S ribosomal protein S13

Chain m: 96%



- Molecule 47: 30S ribosomal protein S14

Chain n: 94%



- Molecule 48: 30S ribosomal protein S15

Chain o: 92%



- Molecule 49: 30S ribosomal protein S16

Chain p: 95%



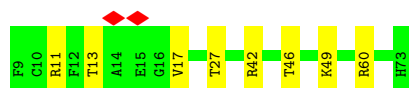
- Molecule 50: 30S ribosomal protein S17

Chain q: 94%



- Molecule 51: 30S ribosomal protein S18

Chain r: 88%



- Molecule 52: 30S ribosomal protein S19

Chain s: 95%



- Molecule 53: 30S ribosomal protein S20

Chain t: 93% 7%



- Molecule 54: 30S ribosomal protein S21

Chain u: 82% 18%



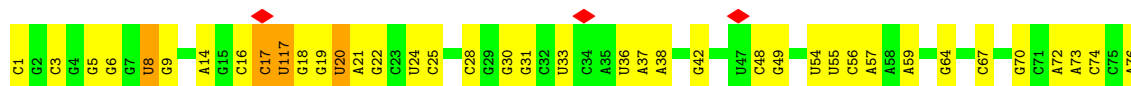
- Molecule 55: tRNA-fMet

Chain v: 69% 29%



- Molecule 55: tRNA-fMet

Chain w: 49% 45% 5%



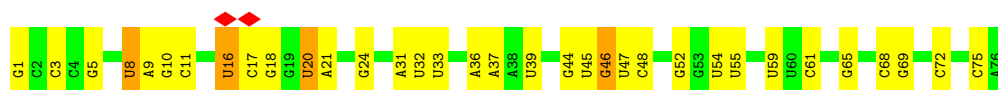
- Molecule 56: mRNA

Chain x: 92% 8%



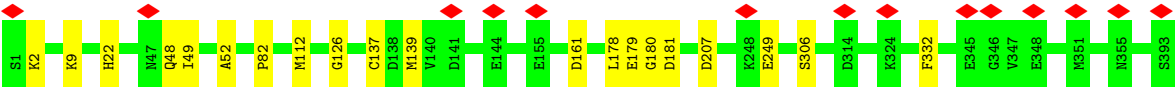
- Molecule 57: Phe-tRNA-Phe

Chain y: 55% 39% 5%



- Molecule 58: Elongation factor Tu 2

Chain z: 95% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	56963	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	67	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	51020	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.307	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.00677	Depositor
Map size (\AA)	390.04, 390.04, 390.04	wwPDB
Map dimensions	398, 398, 398	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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: 7MG, 1MG, MG, 5MU, GNP, 6MZ, OMG, PSU, MIA, 5MC, 4OC, FME, 3TD, OMC, MA6, 2MG, K, UR3, 4SU, 2MA, H2U, OMU

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.26	1/69174 (0.0%)	0.70	10/107907 (0.0%)
2	B	0.30	1/2876 (0.0%)	0.69	0/4483
3	C	0.34	0/2121	0.68	0/2852
4	D	0.35	0/1578	0.61	0/2124
5	E	0.36	0/1563	0.63	0/2103
6	F	0.37	0/1434	0.60	0/1926
7	G	0.35	0/1324	0.54	0/1794
8	H	0.38	0/1122	0.51	0/1515
9	I	0.42	0/1046	0.61	0/1410
10	J	0.35	0/1143	0.61	0/1540
11	K	0.36	0/947	0.69	0/1268
12	L	0.36	0/1052	0.70	0/1401
13	M	0.37	0/1093	0.62	0/1460
14	N	0.38	0/964	0.66	0/1289
15	O	0.37	0/902	0.63	0/1209
16	P	0.36	0/929	0.64	0/1242
17	Q	0.36	0/946	0.70	0/1260
18	R	0.35	0/823	0.61	0/1100
19	S	0.35	0/852	0.68	0/1142
20	T	0.35	0/736	0.63	0/984
21	U	0.35	0/787	0.60	0/1051
22	V	0.34	0/752	0.55	0/1008
23	W	0.35	0/579	0.66	0/767
24	X	0.37	0/635	0.66	0/848
25	Y	0.37	0/495	0.60	0/658
26	Z	0.36	0/438	0.60	0/586
27	0	0.35	0/440	0.75	0/588
28	1	0.35	0/424	0.55	0/565
29	2	0.38	0/370	0.81	0/487
30	3	0.34	0/513	0.64	0/676
31	4	0.32	0/303	0.66	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	5	0.45	0/1001	0.65	0/1350
33	6	0.40	0/531	0.54	0/709
34	a	0.24	0/36725	0.70	2/57285 (0.0%)
35	b	0.38	0/1735	0.53	0/2338
36	c	0.36	0/1651	0.59	0/2225
37	d	0.38	0/1665	0.59	0/2227
38	e	0.35	0/1180	0.62	0/1587
39	f	0.36	0/835	0.63	0/1128
40	g	0.36	0/1195	0.60	0/1602
41	h	0.33	0/989	0.60	0/1326
42	i	0.39	0/1034	0.69	0/1375
43	j	0.37	0/796	0.65	0/1077
44	k	0.35	0/885	0.62	0/1195
45	l	0.37	0/954	0.69	0/1282
46	m	0.36	0/900	0.65	0/1204
47	n	0.37	0/822	0.65	0/1095
48	o	0.37	0/722	0.67	1/964 (0.1%)
49	p	0.37	0/659	0.58	0/884
50	q	0.37	0/657	0.64	0/881
51	r	0.39	0/544	0.65	0/731
52	s	0.37	0/652	0.62	0/877
53	t	0.37	0/671	0.63	0/888
54	u	0.45	0/550	0.75	0/728
55	v	0.34	1/1747 (0.1%)	0.69	0/2721
55	w	0.61	2/1747 (0.1%)	0.80	2/2721 (0.1%)
56	x	0.21	0/280	0.65	0/433
57	y	0.33	1/1607 (0.1%)	0.67	0/2501
58	z	0.37	0/3092	0.58	0/4183
All	All	0.30	6/164187 (0.0%)	0.68	15/245157 (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
9	I	0	1
32	5	0	1
All	All	0	2

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	w	117	U	O3'-P	-21.55	1.35	1.61
55	v	0	C	OP3-P	-10.20	1.49	1.61
57	y	1	G	OP3-P	-10.19	1.49	1.61
2	B	1	U	OP3-P	-10.15	1.49	1.61
1	A	1	G	OP3-P	-10.14	1.49	1.61

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	w	17	C	O3'-P-O5'	17.11	136.50	104.00
55	w	17	C	OP1-P-O3'	-9.94	83.33	105.20
1	A	2407	A	C2'-C3'-O3'	7.86	126.78	109.50
1	A	1140	C	C2'-C3'-O3'	7.76	126.56	109.50
1	A	242	G	C2'-C3'-O3'	7.72	126.49	109.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	5	30	SER	Peptide
9	I	134	SER	Peptide

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%)	240 (89%)	27 (10%)	2 (1%)	22	57
4	D	206/208 (99%)	190 (92%)	15 (7%)	1 (0%)	29	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	198/200 (99%)	181 (91%)	15 (8%)	2 (1%)	15	49
6	F	175/177 (99%)	156 (89%)	19 (11%)	0	100	100
7	G	172/174 (99%)	159 (92%)	13 (8%)	0	100	100
8	H	147/149 (99%)	125 (85%)	19 (13%)	3 (2%)	7	31
9	I	139/141 (99%)	104 (75%)	29 (21%)	6 (4%)	2	16
10	J	139/141 (99%)	130 (94%)	7 (5%)	2 (1%)	11	40
11	K	120/122 (98%)	109 (91%)	7 (6%)	4 (3%)	4	21
12	L	141/143 (99%)	117 (83%)	19 (14%)	5 (4%)	3	20
13	M	134/136 (98%)	127 (95%)	5 (4%)	2 (2%)	10	39
14	N	117/119 (98%)	102 (87%)	12 (10%)	3 (3%)	5	26
15	O	114/116 (98%)	107 (94%)	6 (5%)	1 (1%)	17	52
16	P	112/114 (98%)	98 (88%)	14 (12%)	0	100	100
17	Q	113/115 (98%)	112 (99%)	1 (1%)	0	100	100
18	R	100/102 (98%)	84 (84%)	13 (13%)	3 (3%)	4	23
19	S	107/109 (98%)	99 (92%)	7 (6%)	1 (1%)	17	52
20	T	90/92 (98%)	79 (88%)	9 (10%)	2 (2%)	6	29
21	U	100/102 (98%)	87 (87%)	11 (11%)	2 (2%)	7	31
22	V	90/92 (98%)	86 (96%)	3 (3%)	1 (1%)	14	46
23	W	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	11	40
24	X	75/77 (97%)	71 (95%)	4 (5%)	0	100	100
25	Y	58/60 (97%)	54 (93%)	3 (5%)	1 (2%)	9	36
26	Z	54/56 (96%)	51 (94%)	3 (6%)	0	100	100
27	0	53/55 (96%)	45 (85%)	7 (13%)	1 (2%)	8	33
28	1	49/51 (96%)	44 (90%)	5 (10%)	0	100	100
29	2	43/45 (96%)	40 (93%)	3 (7%)	0	100	100
30	3	62/64 (97%)	59 (95%)	3 (5%)	0	100	100
31	4	36/38 (95%)	31 (86%)	5 (14%)	0	100	100
32	5	129/131 (98%)	96 (74%)	24 (19%)	9 (7%)	1	7
33	6	64/66 (97%)	56 (88%)	7 (11%)	1 (2%)	9	37
35	b	216/218 (99%)	187 (87%)	24 (11%)	5 (2%)	6	28
36	c	204/206 (99%)	180 (88%)	18 (9%)	6 (3%)	4	24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	d	203/205 (99%)	182 (90%)	19 (9%)	2 (1%)	15	49
38	e	156/157 (99%)	136 (87%)	16 (10%)	4 (3%)	5	26
39	f	98/100 (98%)	85 (87%)	9 (9%)	4 (4%)	3	16
40	g	149/151 (99%)	131 (88%)	13 (9%)	5 (3%)	3	21
41	h	127/129 (98%)	116 (91%)	11 (9%)	0	100	100
42	i	125/127 (98%)	94 (75%)	27 (22%)	4 (3%)	4	22
43	j	96/98 (98%)	70 (73%)	20 (21%)	6 (6%)	1	8
44	k	114/116 (98%)	101 (89%)	8 (7%)	5 (4%)	2	15
45	l	119/121 (98%)	94 (79%)	19 (16%)	6 (5%)	2	13
46	m	113/115 (98%)	104 (92%)	7 (6%)	2 (2%)	8	34
47	n	99/101 (98%)	84 (85%)	10 (10%)	5 (5%)	2	13
48	o	86/88 (98%)	77 (90%)	6 (7%)	3 (4%)	3	20
49	p	80/82 (98%)	70 (88%)	8 (10%)	2 (2%)	5	27
50	q	78/80 (98%)	67 (86%)	8 (10%)	3 (4%)	3	19
51	r	63/65 (97%)	51 (81%)	10 (16%)	2 (3%)	4	22
52	s	77/79 (98%)	67 (87%)	10 (13%)	0	100	100
53	t	83/85 (98%)	77 (93%)	4 (5%)	2 (2%)	6	27
54	u	63/65 (97%)	39 (62%)	14 (22%)	10 (16%)	0	0
58	z	391/393 (100%)	350 (90%)	29 (7%)	12 (3%)	4	23
All	All	6219/6322 (98%)	5469 (88%)	609 (10%)	141 (2%)	9	28

5 of 141 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	J	81	ILE
11	K	89	ASN
32	5	55	VAL
32	5	123	ILE
33	6	4	ASP

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%)	210 (97%)	6 (3%)	43	73
4	D	163/163 (100%)	154 (94%)	9 (6%)	21	53
5	E	164/164 (100%)	162 (99%)	2 (1%)	71	88
6	F	148/148 (100%)	144 (97%)	4 (3%)	44	74
7	G	135/135 (100%)	132 (98%)	3 (2%)	52	78
8	H	114/114 (100%)	111 (97%)	3 (3%)	46	74
9	I	109/109 (100%)	104 (95%)	5 (5%)	27	59
10	J	115/115 (100%)	112 (97%)	3 (3%)	46	74
11	K	103/103 (100%)	101 (98%)	2 (2%)	57	81
12	L	102/102 (100%)	93 (91%)	9 (9%)	10	36
13	M	109/109 (100%)	107 (98%)	2 (2%)	59	82
14	N	99/99 (100%)	96 (97%)	3 (3%)	41	71
15	O	86/86 (100%)	85 (99%)	1 (1%)	71	88
16	P	99/99 (100%)	98 (99%)	1 (1%)	76	90
17	Q	88/88 (100%)	86 (98%)	2 (2%)	50	77
18	R	84/84 (100%)	78 (93%)	6 (7%)	14	44
19	S	92/92 (100%)	87 (95%)	5 (5%)	22	53
20	T	79/79 (100%)	75 (95%)	4 (5%)	24	56
21	U	83/83 (100%)	80 (96%)	3 (4%)	35	67
22	V	77/77 (100%)	76 (99%)	1 (1%)	69	87
23	W	57/57 (100%)	55 (96%)	2 (4%)	36	68
24	X	67/67 (100%)	65 (97%)	2 (3%)	41	71
25	Y	55/55 (100%)	55 (100%)	0	100	100
26	Z	47/47 (100%)	46 (98%)	1 (2%)	53	79
27	0	46/46 (100%)	43 (94%)	3 (6%)	17	47
28	1	46/46 (100%)	43 (94%)	3 (6%)	17	47
29	2	37/37 (100%)	32 (86%)	5 (14%)	4	16
30	3	51/51 (100%)	49 (96%)	2 (4%)	32	65
31	4	34/34 (100%)	33 (97%)	1 (3%)	42	72
32	5	100/100 (100%)	96 (96%)	4 (4%)	31	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
33	6	59/59 (100%)	58 (98%)	1 (2%)	60	83
35	b	180/180 (100%)	178 (99%)	2 (1%)	73	89
36	c	170/170 (100%)	168 (99%)	2 (1%)	71	88
37	d	172/172 (100%)	171 (99%)	1 (1%)	86	94
38	e	120/119 (101%)	115 (96%)	5 (4%)	30	62
39	f	87/87 (100%)	83 (95%)	4 (5%)	27	59
40	g	124/124 (100%)	122 (98%)	2 (2%)	62	84
41	h	104/104 (100%)	101 (97%)	3 (3%)	42	72
42	i	105/105 (100%)	101 (96%)	4 (4%)	33	66
43	j	86/86 (100%)	85 (99%)	1 (1%)	71	88
44	k	89/89 (100%)	87 (98%)	2 (2%)	52	78
45	l	102/102 (100%)	96 (94%)	6 (6%)	19	50
46	m	93/93 (100%)	90 (97%)	3 (3%)	39	69
47	n	83/83 (100%)	82 (99%)	1 (1%)	71	88
48	o	76/76 (100%)	72 (95%)	4 (5%)	22	54
49	p	65/65 (100%)	63 (97%)	2 (3%)	40	70
50	q	74/74 (100%)	72 (97%)	2 (3%)	44	74
51	r	56/56 (100%)	50 (89%)	6 (11%)	6	26
52	s	70/70 (100%)	66 (94%)	4 (6%)	20	52
53	t	65/65 (100%)	61 (94%)	4 (6%)	18	49
54	u	55/55 (100%)	53 (96%)	2 (4%)	35	67
58	z	326/326 (100%)	318 (98%)	8 (2%)	47	75
All	All	5166/5165 (100%)	5000 (97%)	166 (3%)	42	69

5 of 166 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	h	111	THR
51	r	13	THR
42	i	42	THR
46	m	28	ARG
52	s	12	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
16	P	114	ASN
45	l	111	GLN
58	z	51	ASN
53	t	69	ASN
14	N	62	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2892/2903 (99%)	744 (25%)	78 (2%)
2	B	119/120 (99%)	29 (24%)	3 (2%)
34	a	1536/1540 (99%)	426 (27%)	0
55	v	76/77 (98%)	21 (27%)	0
55	w	76/77 (98%)	36 (47%)	0
56	x	11/12 (91%)	1 (9%)	0
57	y	74/76 (97%)	28 (37%)	0
All	All	4784/4805 (99%)	1285 (26%)	81 (1%)

5 of 1285 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	G
1	A	5	A
1	A	6	A
1	A	10	A
1	A	12	U

5 of 81 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1558	C
1	A	2391	G
1	A	1647	U
1	A	1918	A
1	A	2712	C

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	$\# Z > 2$
55	PSU	v	55	55	18,21,22	1.30	3 (16%)	22,30,33	1.87	5 (22%)
55	H2U	w	20	55	18,21,22	0.81	0	21,30,33	1.75	3 (14%)
34	MA6	a	1518	34	19,26,27	1.29	2 (10%)	18,38,41	1.81	4 (22%)
1	PSU	A	1917	1	18,21,22	1.42	2 (11%)	22,30,33	1.85	5 (22%)
1	PSU	A	2605	1	18,21,22	1.39	2 (11%)	22,30,33	1.88	4 (18%)
34	2MG	a	1207	34	18,26,27	0.94	0	16,38,41	1.27	3 (18%)
34	5MC	a	967	34	18,22,23	1.02	1 (5%)	26,32,35	1.38	4 (15%)
34	MA6	a	1519	34,59	19,26,27	1.17	2 (10%)	18,38,41	1.78	3 (16%)
1	H2U	A	2449	1	18,21,22	1.10	2 (11%)	21,30,33	1.67	5 (23%)
1	2MA	A	2503	1,59	17,25,26	1.01	1 (5%)	17,37,40	1.27	3 (17%)
1	OMC	A	2498	1,59	19,22,23	0.86	1 (5%)	26,31,34	1.33	4 (15%)
1	OMU	A	2552	1,59	19,22,23	1.31	3 (15%)	26,31,34	2.07	8 (30%)
1	6MZ	A	1618	1	18,25,26	0.92	1 (5%)	16,36,39	2.58	6 (37%)
34	5MC	a	1407	34	18,22,23	0.97	1 (5%)	26,32,35	1.53	4 (15%)
57	PSU	y	32	57	18,21,22	1.32	2 (11%)	22,30,33	2.04	5 (22%)
55	H2U	v	20	55	18,21,22	0.81	1 (5%)	21,30,33	1.70	3 (14%)
1	PSU	A	746	1,59	18,21,22	1.35	2 (11%)	22,30,33	1.84	3 (13%)
1	PSU	A	2604	1	18,21,22	1.34	2 (11%)	22,30,33	1.73	4 (18%)
34	2MG	a	966	34	18,26,27	1.04	2 (11%)	16,38,41	1.35	3 (18%)
57	PSU	y	55	57	18,21,22	1.37	2 (11%)	22,30,33	1.93	5 (22%)
34	7MG	a	527	34	22,26,27	1.46	4 (18%)	29,39,42	2.45	8 (27%)
55	4SU	w	8	55	18,21,22	1.73	5 (27%)	26,30,33	2.16	6 (23%)
34	4OC	a	1402	34	20,23,24	0.80	0	26,32,35	1.31	4 (15%)
57	7MG	y	46	57	22,26,27	1.42	4 (18%)	29,39,42	2.39	7 (24%)
1	PSU	A	2580	1	18,21,22	1.45	3 (16%)	22,30,33	1.88	5 (22%)
57	MIA	y	37	57	24,31,32	2.23	4 (16%)	26,44,47	2.55	11 (42%)
1	2MG	A	1835	1	18,26,27	1.03	2 (11%)	16,38,41	1.22	2 (12%)
1	7MG	A	2069	1,59	22,26,27	1.51	4 (18%)	29,39,42	2.42	9 (31%)
1	1MG	A	745	1	18,26,27	0.95	0	19,39,42	1.46	3 (15%)
57	H2U	y	16	57	18,21,22	0.81	1 (5%)	21,30,33	1.50	4 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	2MG	a	1516	34	18,26,27	0.95	0	16,38,41	1.13	2 (12%)
1	5MC	A	747	1	18,22,23	0.99	2 (11%)	26,32,35	1.50	4 (15%)
57	PSU	y	39	57	18,21,22	1.42	2 (11%)	22,30,33	1.80	4 (18%)
57	4SU	y	8	57	18,21,22	1.75	5 (27%)	26,30,33	2.28	7 (26%)
34	UR3	a	1498	34	19,22,23	1.10	2 (10%)	26,32,35	1.66	4 (15%)
55	PSU	w	55	55	18,21,22	1.30	2 (11%)	22,30,33	1.90	5 (22%)
1	PSU	A	2457	1,59	18,21,22	1.51	3 (16%)	22,30,33	1.94	5 (22%)
1	5MU	A	1939	1	19,22,23	1.35	4 (21%)	28,32,35	2.00	8 (28%)
1	2MG	A	2445	1,59	18,26,27	1.05	1 (5%)	16,38,41	1.13	1 (6%)
55	4SU	v	7	55	18,21,22	1.71	5 (27%)	26,30,33	2.38	7 (26%)
1	OMG	A	2251	55,1,59	18,26,27	1.05	1 (5%)	19,38,41	1.00	1 (5%)
57	H2U	y	20	57	18,21,22	0.84	1 (5%)	21,30,33	1.56	4 (19%)
1	5MC	A	1962	1	18,22,23	1.00	1 (5%)	26,32,35	1.45	3 (11%)
1	PSU	A	955	1	18,21,22	1.41	3 (16%)	22,30,33	1.93	4 (18%)
1	PSU	A	2504	1	18,21,22	1.41	2 (11%)	22,30,33	1.92	4 (18%)
1	6MZ	A	2030	1,59	18,25,26	1.02	1 (5%)	16,36,39	2.29	5 (31%)
1	PSU	A	1911	1	18,21,22	1.39	2 (11%)	22,30,33	1.98	4 (18%)
34	PSU	a	516	34	18,21,22	1.34	2 (11%)	22,30,33	1.98	5 (22%)
57	5MU	y	54	57	19,22,23	1.41	4 (21%)	28,32,35	2.03	8 (28%)
55	5MU	w	54	55	19,22,23	1.49	4 (21%)	28,32,35	2.04	10 (35%)
55	5MU	v	54	55	19,22,23	1.45	5 (26%)	28,32,35	1.94	8 (28%)
1	3TD	A	1915	1	18,22,23	7.23	14 (77%)	22,32,35	1.78	4 (18%)

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
55	PSU	v	55	55	-	2/7/25/26	0/2/2/2
55	H2U	w	20	55	-	2/7/38/39	0/2/2/2
34	MA6	a	1518	34	-	2/7/29/30	0/3/3/3
1	PSU	A	1917	1	-	2/7/25/26	0/2/2/2
1	PSU	A	2605	1	-	0/7/25/26	0/2/2/2
34	2MG	a	1207	34	-	1/5/27/28	0/3/3/3
34	5MC	a	967	34	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	MA6	a	1519	34,59	-	3/7/29/30	0/3/3/3
1	H2U	A	2449	1	-	0/7/38/39	0/2/2/2
1	2MA	A	2503	1,59	-	2/3/25/26	0/3/3/3
1	OMC	A	2498	1,59	-	0/9/27/28	0/2/2/2
1	OMU	A	2552	1,59	-	2/9/27/28	0/2/2/2
1	6MZ	A	1618	1	-	2/5/27/28	0/3/3/3
34	5MC	a	1407	34	-	0/7/25/26	0/2/2/2
57	PSU	y	32	57	-	0/7/25/26	0/2/2/2
55	H2U	v	20	55	-	0/7/38/39	0/2/2/2
1	PSU	A	746	1,59	-	1/7/25/26	0/2/2/2
1	PSU	A	2604	1	-	0/7/25/26	0/2/2/2
34	2MG	a	966	34	-	3/5/27/28	0/3/3/3
57	PSU	y	55	57	-	0/7/25/26	0/2/2/2
34	7MG	a	527	34	-	2/7/37/38	0/3/3/3
55	4SU	w	8	55	-	6/7/25/26	0/2/2/2
34	4OC	a	1402	34	-	2/9/29/30	0/2/2/2
57	7MG	y	46	57	-	4/7/37/38	0/3/3/3
1	PSU	A	2580	1	-	0/7/25/26	0/2/2/2
57	MIA	y	37	57	-	3/11/33/34	0/3/3/3
1	2MG	A	1835	1	-	0/5/27/28	0/3/3/3
1	7MG	A	2069	1,59	-	3/7/37/38	0/3/3/3
1	1MG	A	745	1	-	0/3/25/26	0/3/3/3
57	H2U	y	16	57	-	2/7/38/39	0/2/2/2
34	2MG	a	1516	34	-	0/5/27/28	0/3/3/3
1	5MC	A	747	1	-	0/7/25/26	0/2/2/2
57	PSU	y	39	57	-	0/7/25/26	0/2/2/2
57	4SU	y	8	57	-	2/7/25/26	0/2/2/2
34	UR3	a	1498	34	-	2/7/25/26	0/2/2/2
55	PSU	w	55	55	-	0/7/25/26	0/2/2/2
1	PSU	A	2457	1,59	-	2/7/25/26	0/2/2/2
1	5MU	A	1939	1	-	0/7/25/26	0/2/2/2
1	2MG	A	2445	1,59	-	2/5/27/28	0/3/3/3
55	4SU	v	7	55	-	2/7/25/26	0/2/2/2
1	OMG	A	2251	55,1,59	-	0/5/27/28	0/3/3/3
57	H2U	y	20	57	-	2/7/38/39	0/2/2/2
1	5MC	A	1962	1	-	2/7/25/26	0/2/2/2
1	PSU	A	955	1	-	0/7/25/26	0/2/2/2
1	PSU	A	2504	1	-	2/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	6MZ	A	2030	1,59	-	3/5/27/28	0/3/3/3
1	PSU	A	1911	1	-	0/7/25/26	0/2/2/2
34	PSU	a	516	34	-	2/7/25/26	0/2/2/2
57	5MU	y	54	57	-	0/7/25/26	0/2/2/2
55	5MU	w	54	55	-	0/7/25/26	0/2/2/2
55	5MU	v	54	55	-	0/7/25/26	0/2/2/2
1	3TD	A	1915	1	-	5/7/25/26	0/2/2/2

The worst 5 of 125 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1915	3TD	O4'-C1'	16.83	1.66	1.43
1	A	1915	3TD	C2'-C1'	-15.02	1.34	1.53
1	A	1915	3TD	C6-C5	14.81	1.52	1.35
1	A	1915	3TD	C2-N1	8.13	1.47	1.37
57	y	37	MIA	C13-C14	7.39	1.53	1.32

The worst 5 of 250 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	y	46	7MG	N9-C4-N3	7.98	137.40	125.47
34	a	527	7MG	N9-C4-N3	7.97	137.39	125.47
1	A	2069	7MG	N9-C4-N3	7.10	136.08	125.47
55	v	7	4SU	C4-N3-C2	-6.81	120.73	127.34
57	y	37	MIA	C12-C13-C14	-6.74	114.03	127.14

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1618	6MZ	O4'-C4'-C5'-O5'
1	A	1618	6MZ	C3'-C4'-C5'-O5'
1	A	1915	3TD	O4'-C1'-C5-C4
1	A	1915	3TD	C2'-C1'-C5-C6
1	A	1915	3TD	O4'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1622 ligands modelled in this entry, 1619 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	$\# Z > 2$
61	FME	v	101	-	8,9,10	0.62	0	7,9,11	1.92	2 (28%)
62	PHE	z	401	-	10,11,12	0.43	0	10,13,15	0.31	0
63	GNP	z	402	59	29,34,34	2.57	7 (24%)	33,54,54	2.05	9 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
61	FME	v	101	-	-	2/7/9/11	-
62	PHE	z	401	-	-	1/5/6/8	0/1/1/1
63	GNP	z	402	59	-	6/14/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
63	z	402	GNP	PG-O1G	9.60	1.61	1.46
63	z	402	GNP	C5-C6	4.49	1.49	1.41
63	z	402	GNP	PG-N3B	4.48	1.75	1.63
63	z	402	GNP	PB-N3B	4.47	1.75	1.63
63	z	402	GNP	PG-O3G	-3.12	1.48	1.56

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
63	z	402	GNP	C2-N3-C4	5.22	121.32	115.36
63	z	402	GNP	C4-C5-C6	-4.20	116.78	120.80
63	z	402	GNP	C2-N1-C6	3.81	121.98	115.93
61	v	101	FME	C-CA-N	3.77	116.53	109.73
63	z	402	GNP	N3-C2-N1	-3.58	122.44	127.22

There are no chirality outliers.

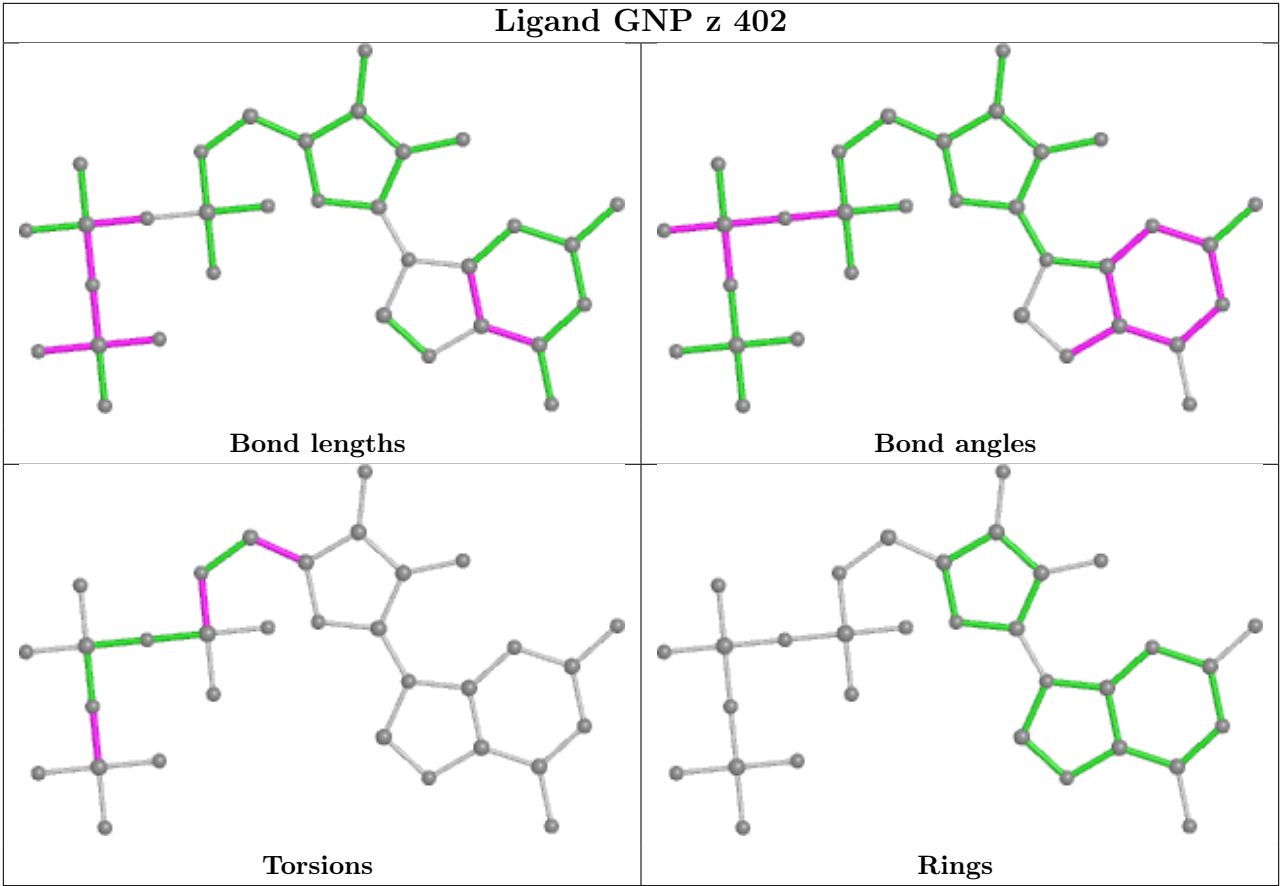
5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
61	v	101	FME	O1-CN-N-CA
62	z	401	PHE	O-C-CA-CB
63	z	402	GNP	PB-N3B-PG-O1G
63	z	402	GNP	C5'-O5'-PA-O3A
63	z	402	GNP	O4'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2
55	w	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1618:6MZ	O3'	1619:G	P	2.24
1	A	2030:6MZ	O3'	2031:A	P	1.77
1	w	117:U	O3'	18:G	P	1.35

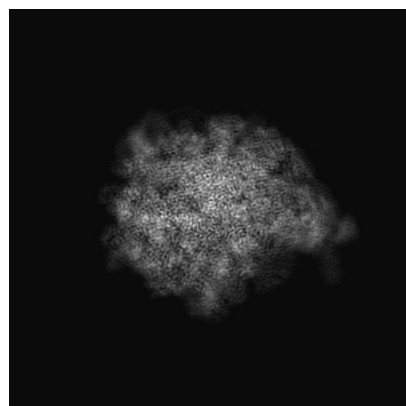
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8814. These allow visual inspection of the internal detail of the map and identification of artifacts.

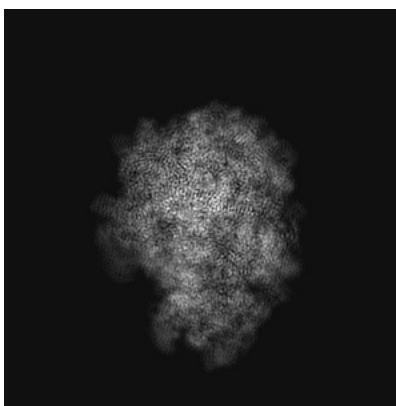
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

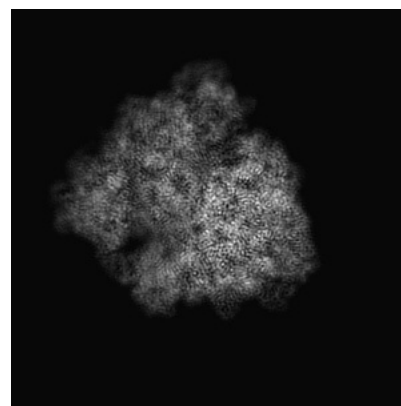
6.1.1 Primary map



X

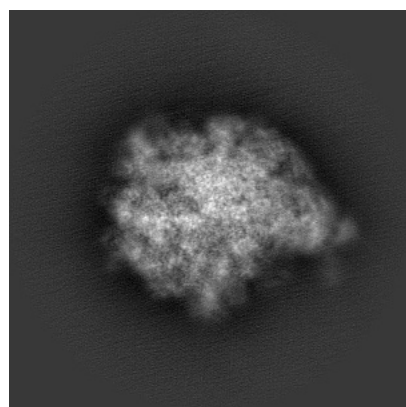


Y

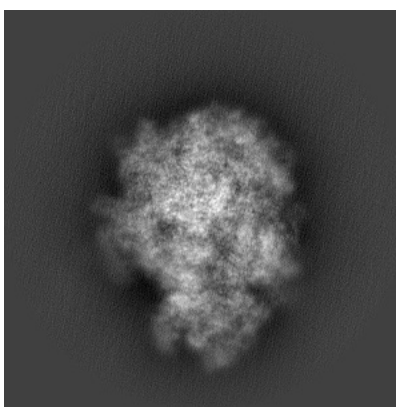


Z

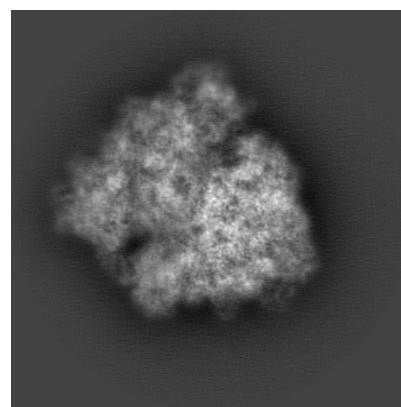
6.1.2 Raw map



X



Y

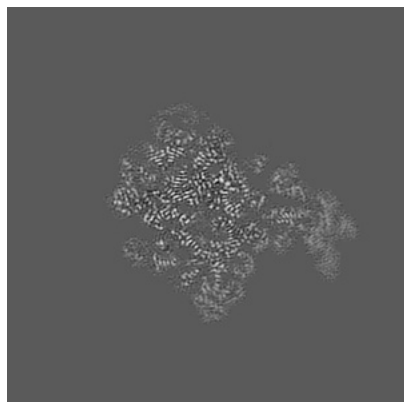


Z

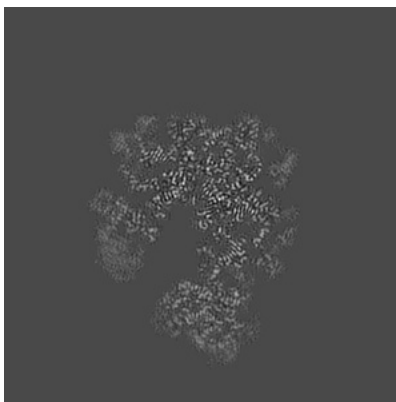
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

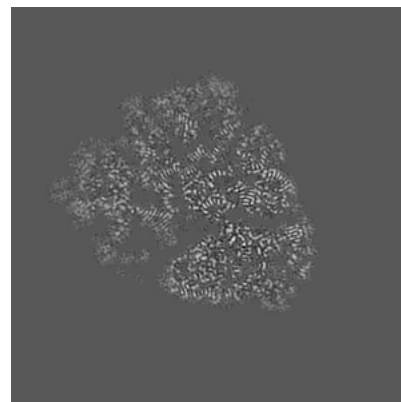
6.2.1 Primary map



X Index: 199

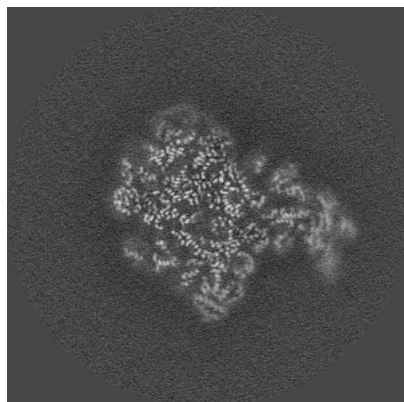


Y Index: 199

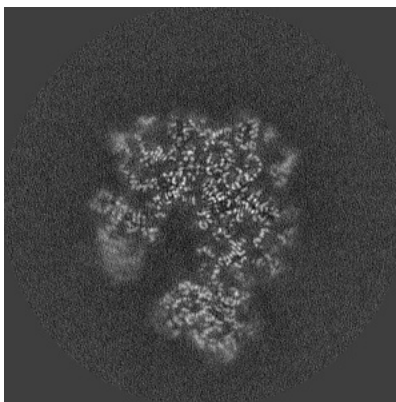


Z Index: 199

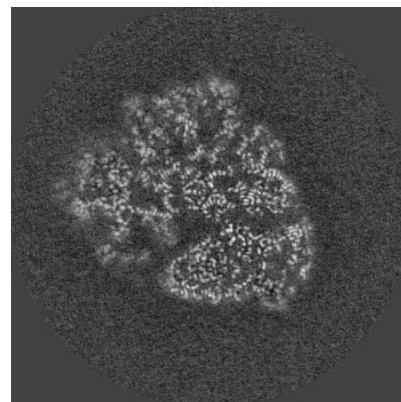
6.2.2 Raw map



X Index: 199



Y Index: 199

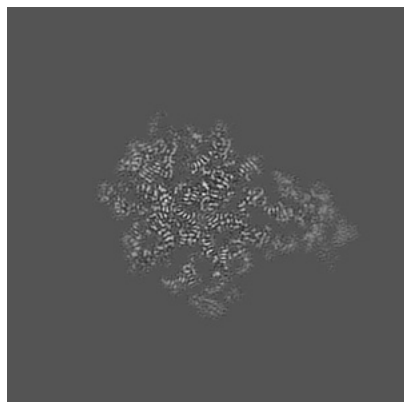


Z Index: 199

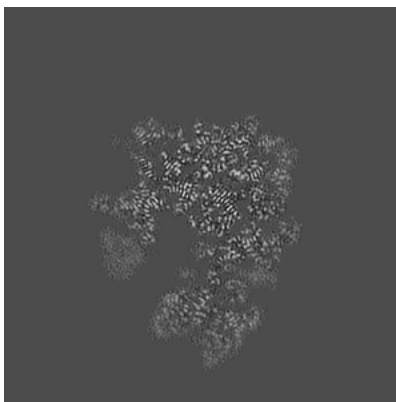
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

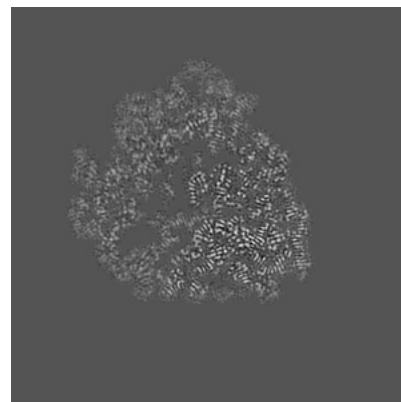
6.3.1 Primary map



X Index: 208

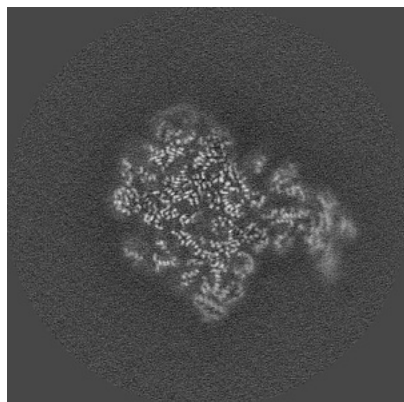


Y Index: 208

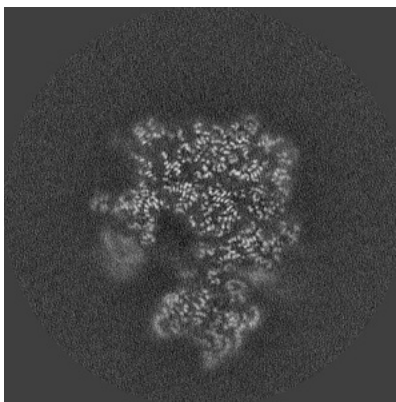


Z Index: 189

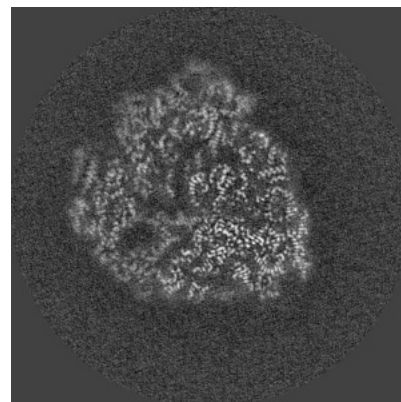
6.3.2 Raw map



X Index: 199



Y Index: 208

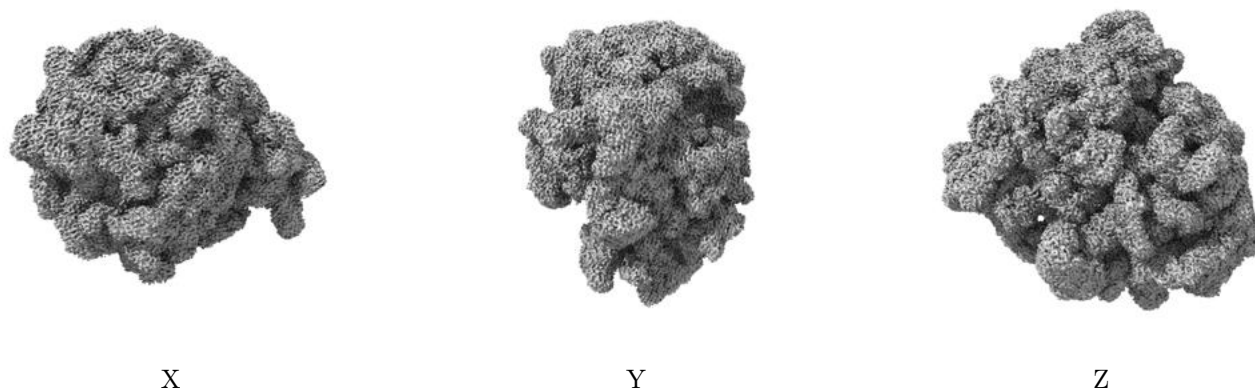


Z Index: 190

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

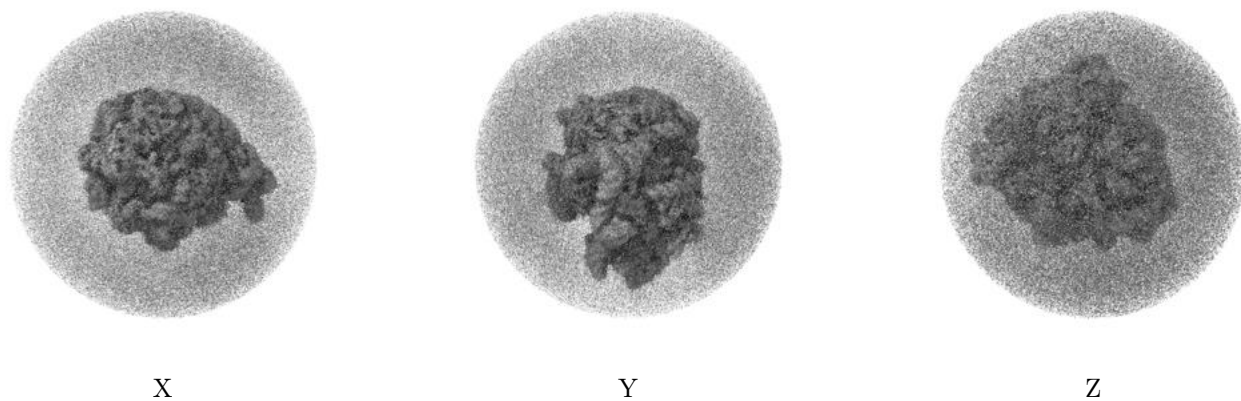
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00677. 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.

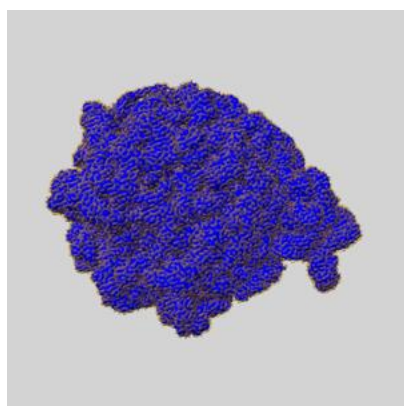
6.5 Mask visualisation [i](#)

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

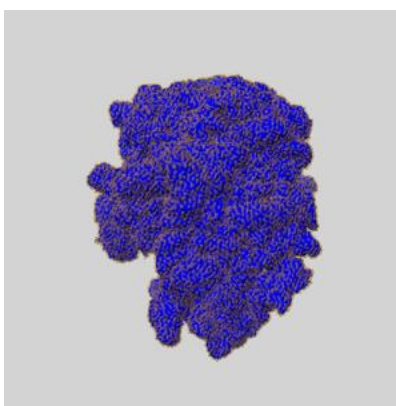
A mask typically either:

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

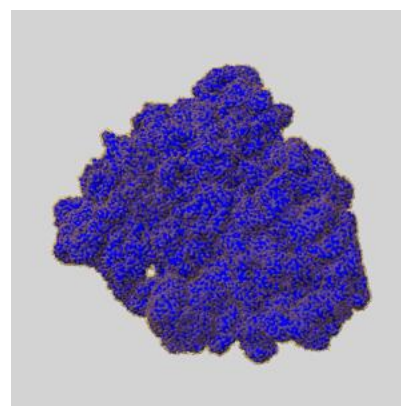
6.5.1 emd_8814_msk_1.map [i](#)



X



Y

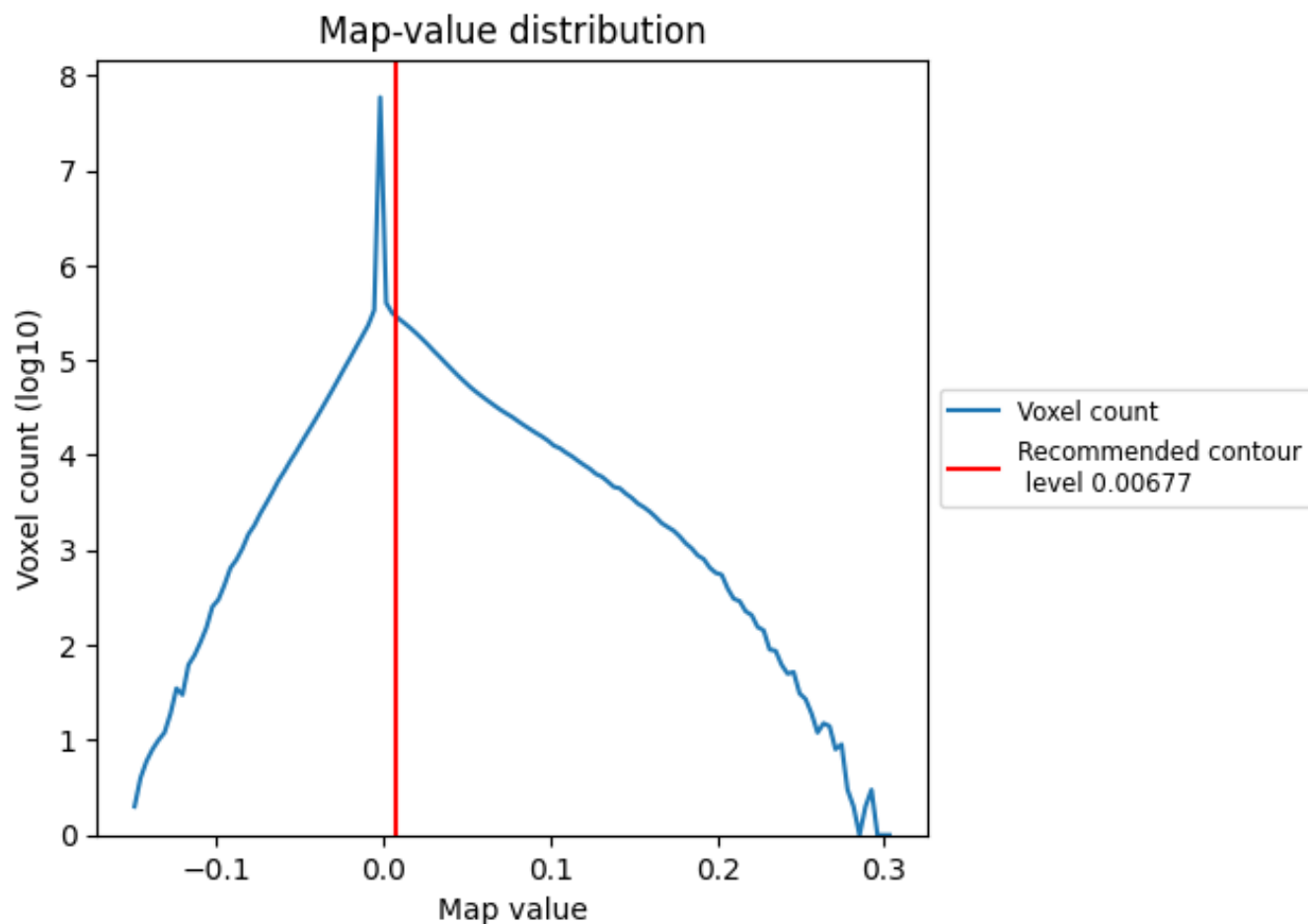


Z

7 Map analysis [i](#)

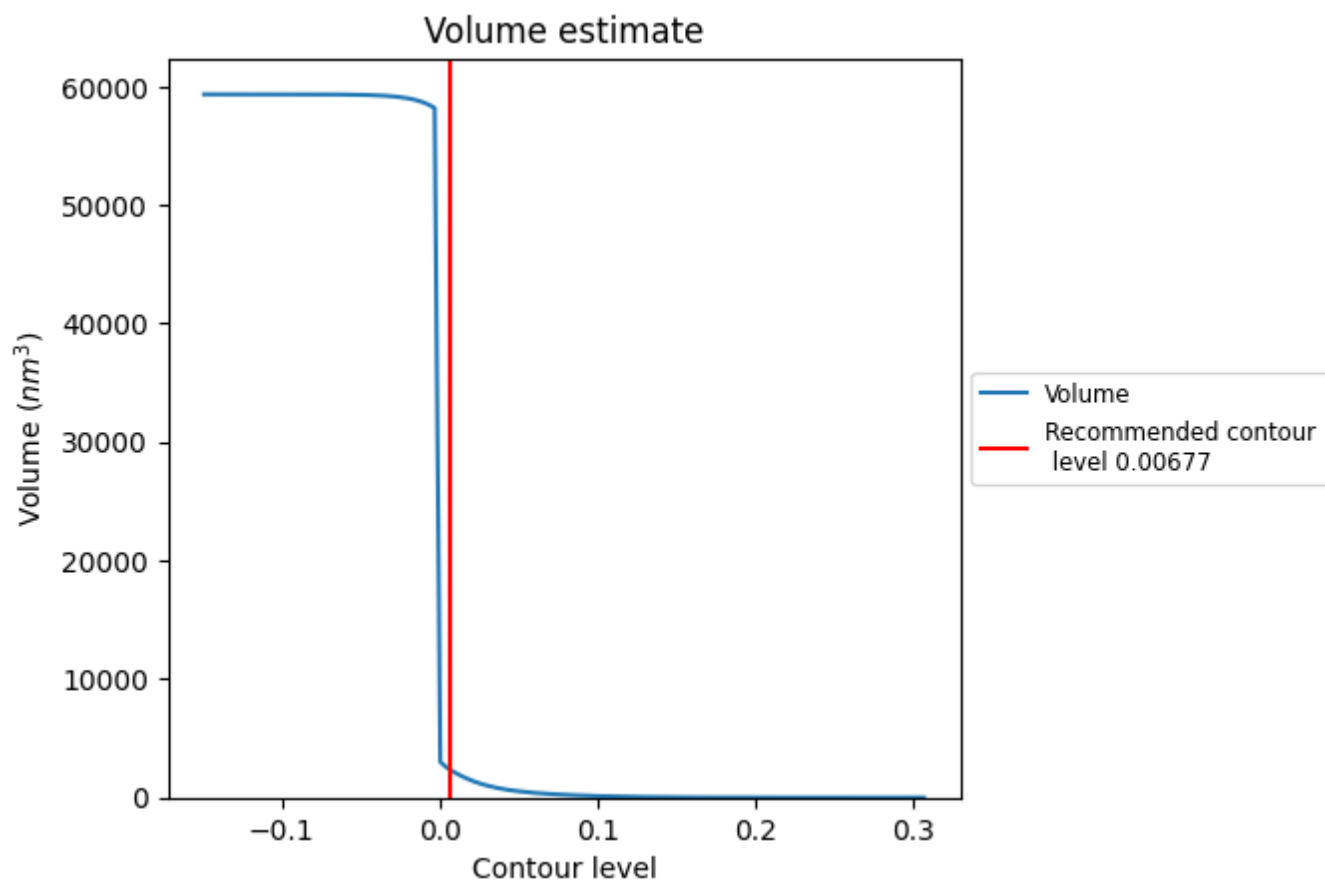
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

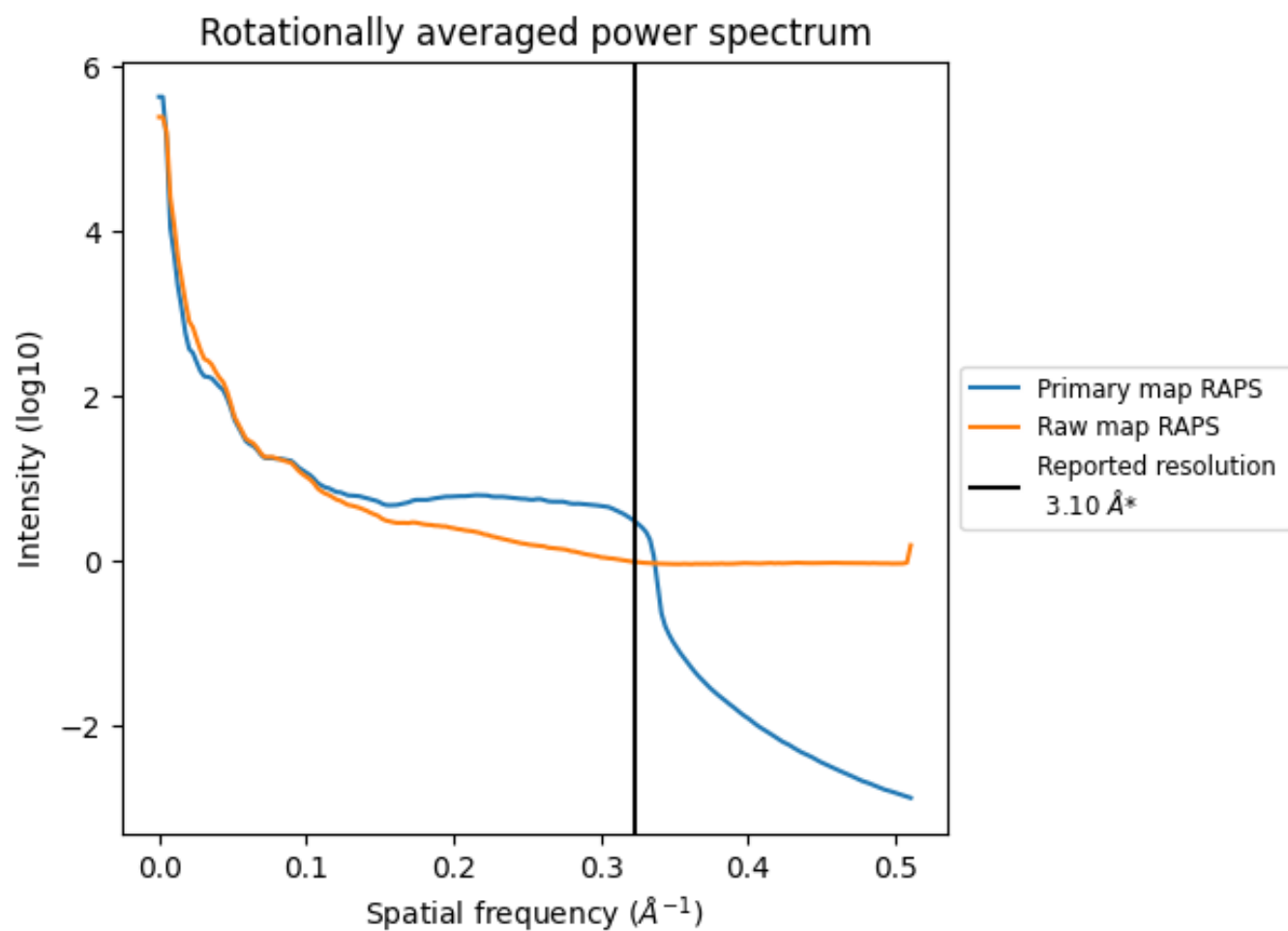
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2337 nm³; this corresponds to an approximate mass of 2111 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 ⓘ

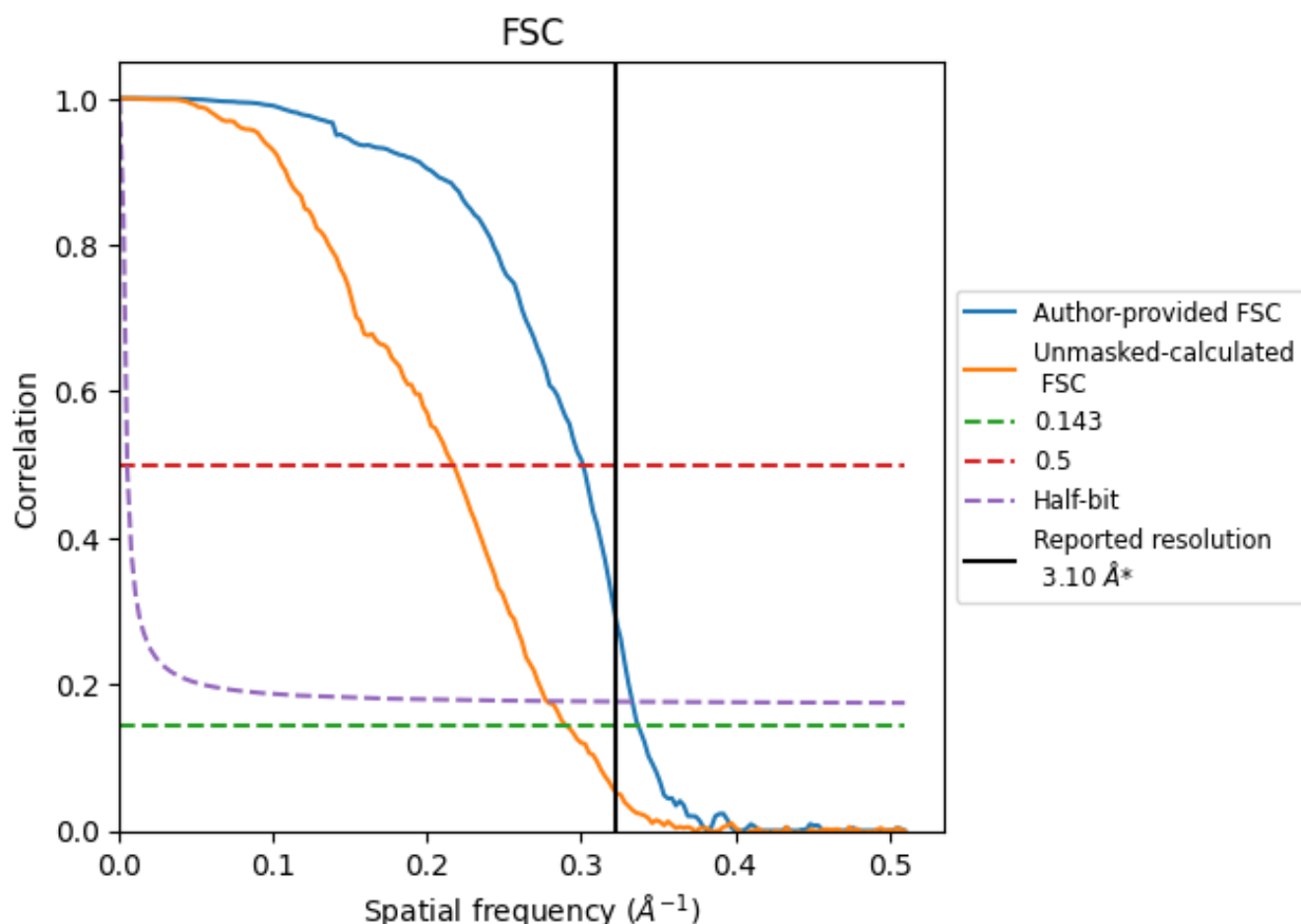


*Reported resolution corresponds to spatial frequency of 0.323 \AA^{-1}

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 0.323 \AA^{-1}

8.2 Resolution estimates [i](#)

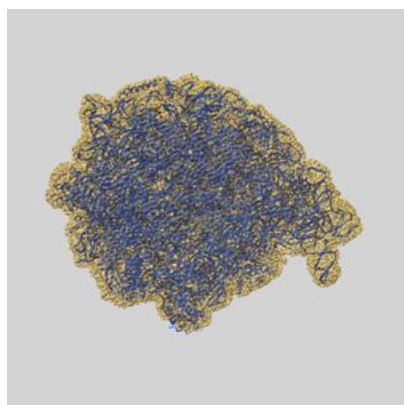
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	2.97	3.32	3.00
Unmasked-calculated*	3.44	4.61	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.44 differs from the reported value 3.1 by more than 10 %

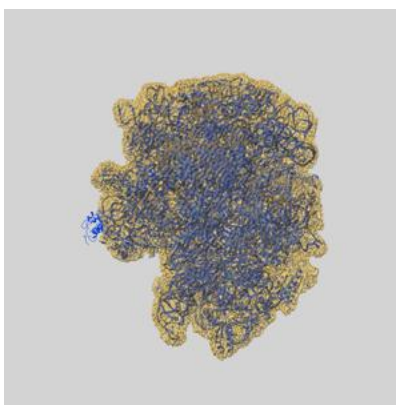
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8814 and PDB model 5WE4. Per-residue inclusion information can be found in section [3](#) on page [20](#).

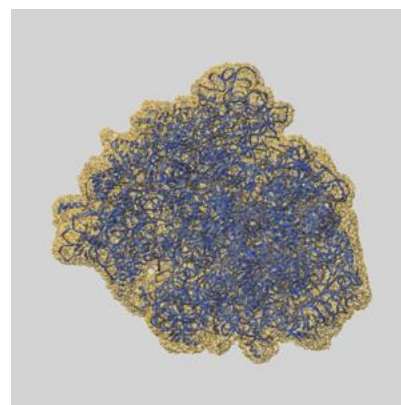
9.1 Map-model overlay [i](#)



X



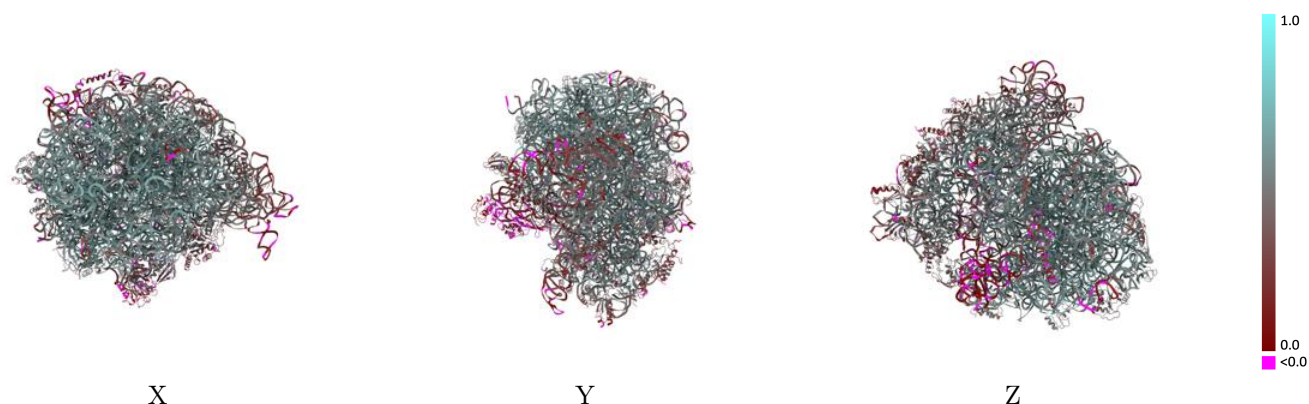
Y



Z

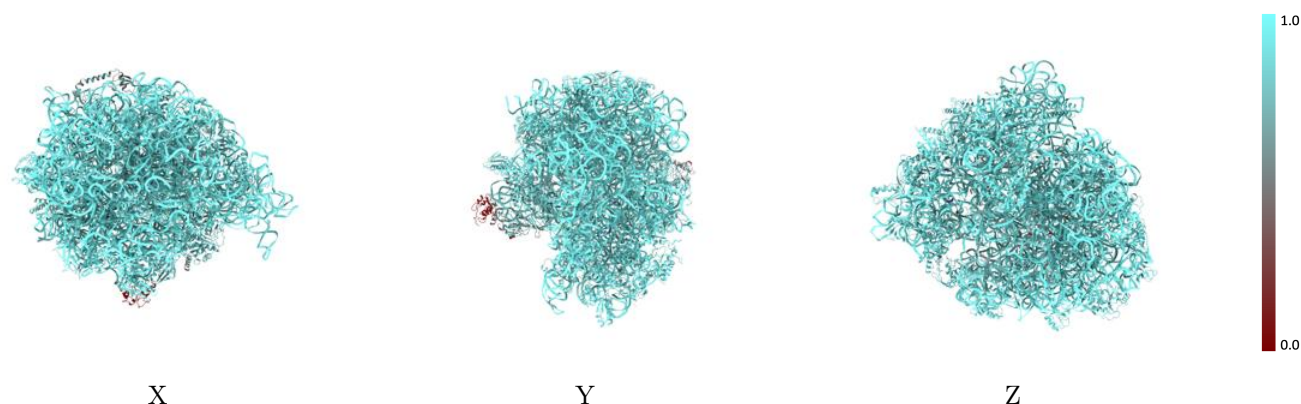
The images above show the 3D surface view of the map at the recommended contour level 0.00677 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



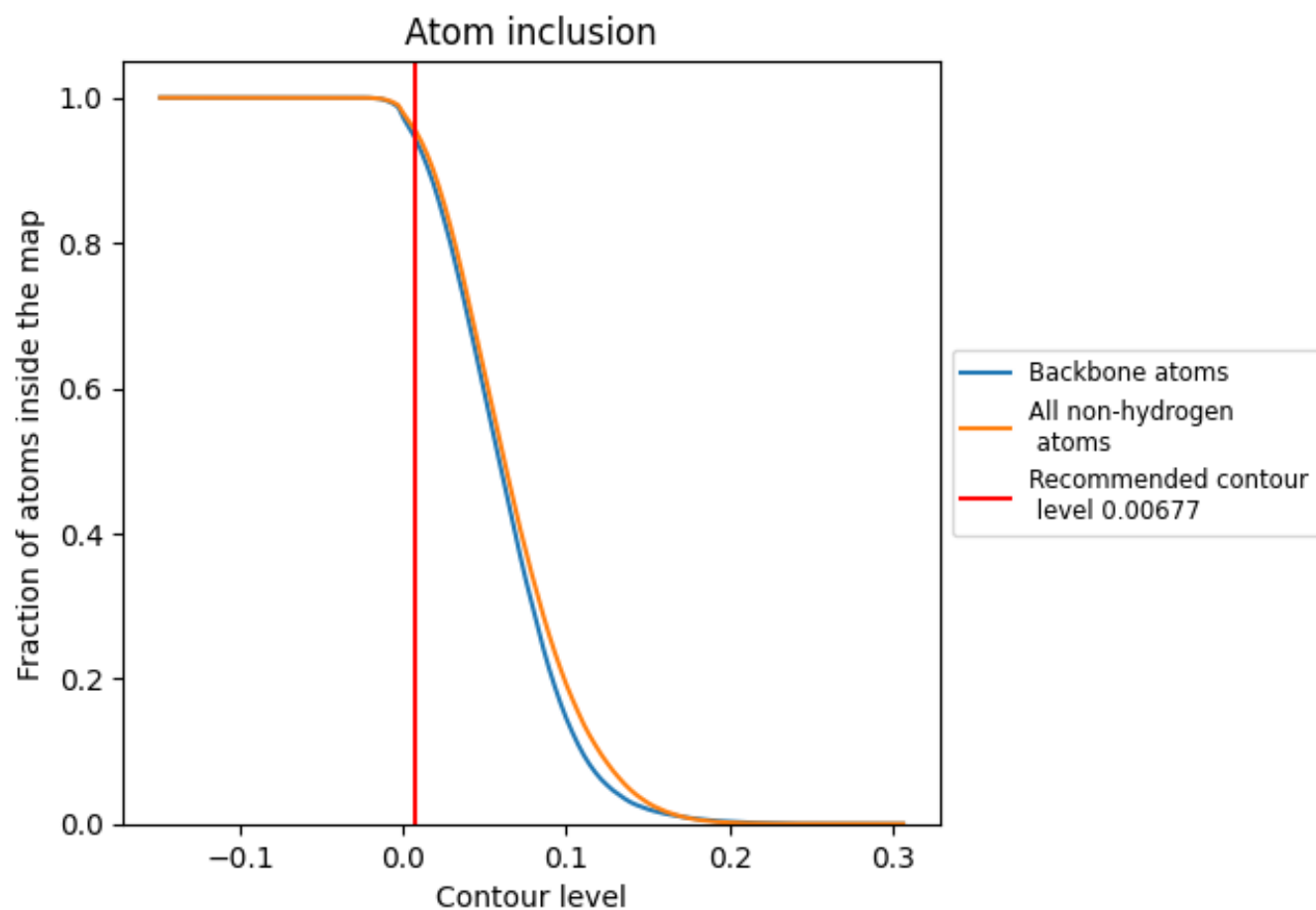
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00677).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 95% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



















































The table lists the average atom inclusion at the recommended contour level (0.00677) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9569	 0.4810
0	 0.9619	 0.5180
1	 0.9512	 0.4830
2	 0.9797	 0.5960
3	 0.9776	 0.5800
4	 0.9659	 0.5270
5	 0.1932	 -0.0150
6	 0.8591	 0.2790
A	 0.9861	 0.5370
B	 0.9927	 0.5010
C	 0.9688	 0.5610
D	 0.9673	 0.5420
E	 0.9577	 0.5050
F	 0.9476	 0.4040
G	 0.9241	 0.3720
H	 0.6807	 0.1800
I	 0.5861	 0.0360
J	 0.9624	 0.5340
K	 0.9508	 0.5220
L	 0.9685	 0.5240
M	 0.9578	 0.5320
N	 0.9825	 0.5580
O	 0.9641	 0.4620
P	 0.9572	 0.5190
Q	 0.9721	 0.5670
R	 0.9609	 0.5120
S	 0.9770	 0.5500
T	 0.9316	 0.4640
U	 0.9505	 0.4710
V	 0.9420	 0.4660
W	 0.9676	 0.5420
X	 0.9567	 0.5450
Y	 0.9232	 0.4250
Z	 0.9550	 0.5250
a	 0.9870	 0.4870



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Chain	Atom inclusion	Q-score
b	 0.9051	 0.3400
c	 0.9360	 0.4370
d	 0.9133	 0.3180
e	 0.9462	 0.4860
f	 0.9108	 0.4000
g	 0.9108	 0.3590
h	 0.9490	 0.4850
i	 0.9276	 0.3820
j	 0.9159	 0.3340
k	 0.9574	 0.4700
l	 0.9338	 0.4540
m	 0.9464	 0.4210
n	 0.9397	 0.4220
o	 0.9420	 0.4460
p	 0.9123	 0.3620
q	 0.9415	 0.4140
r	 0.9358	 0.4610
s	 0.9566	 0.4380
t	 0.9292	 0.3770
u	 0.8147	 0.2750
v	 0.9759	 0.4880
w	 0.7623	 0.0970
x	 0.9683	 0.4610
y	 0.8979	 0.2860
z	 0.8154	 0.2680