



## wwPDB EM Validation Summary Report ⓘ

Nov 20, 2022 – 04:21 AM EST

PDB ID : 7M4V  
EMDB ID : EMD-23667  
Title : A. baumannii Ribosome-Eravacycline complex: 50S  
Authors : Morgan, C.E.; Yu, E.W.  
Deposited on : 2021-03-22  
Resolution : 2.54 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](mailto: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>.

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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

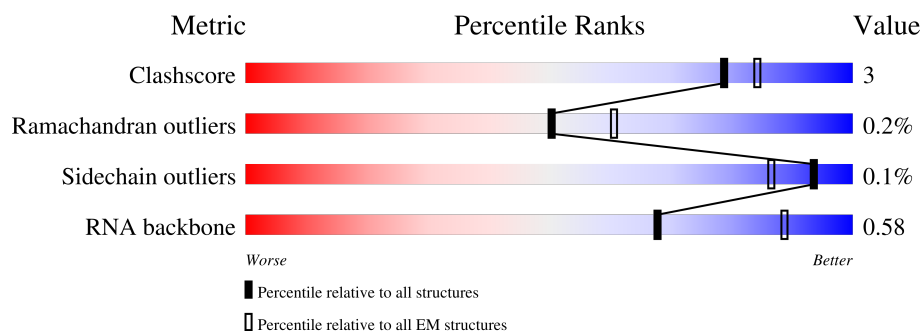
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.54 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.






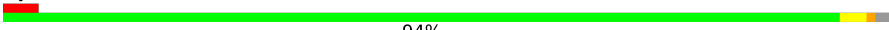






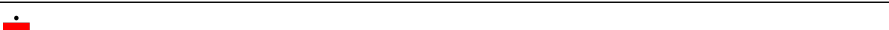

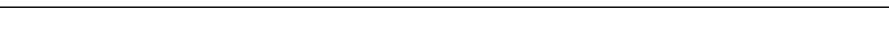
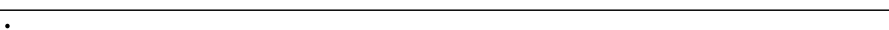
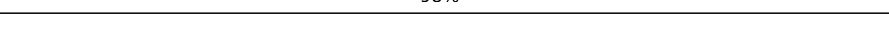



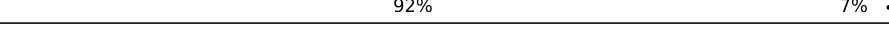

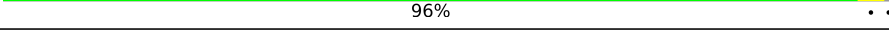

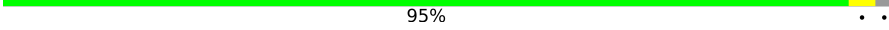
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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  $\geq 3$ , 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	0	51	
2	1	44	
3	2	64	
4	3	38	
5	A	2918	
6	B	115	
7	C	274	

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Mol	Chain	Length	Quality of chain
8	D	212	
9	E	200	
10	F	178	
11	G	177	
12	H	148	
13	I	142	
14	J	122	
15	K	146	
16	L	137	
17	M	125	
18	N	116	
19	O	122	
20	P	119	
21	Q	103	
22	R	109	
23	S	106	
24	T	105	
25	U	98	
26	V	85	
27	W	78	
28	X	65	
29	Y	58	
30	Z	61	

## 2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 86404 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 L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	0	51	Total	C	N	O	S	0	0
			427	274	77	73	3		

- Molecule 2 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	44	Total	C	N	O	S	0	0
			363	222	85	54	2		

- Molecule 3 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	63	Total	C	N	O	S	0	0
			509	319	110	76	4		

- Molecule 4 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			295	179	64	48	4		

- Molecule 5 is a RNA chain called 23s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	2732	Total	C	N	O	P	0	0
			58607	26163	10731	18982	2731		

- Molecule 6 is a RNA chain called 5s ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	B	115	Total	C	N	O	P	0	0
			2450	1095	440	800	115		

- Molecule 7 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	272	Total	C	N	O	S	0	0
			2111	1302	436	365	8		

- Molecule 8 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	211	Total	C	N	O	S	0	0
			1572	972	297	300	3		

- Molecule 9 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	200	Total	C	N	O	S	0	0
			1516	952	281	278	5		

- Molecule 10 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	174	Total	C	N	O	S	0	0
			1370	871	243	248	8		

- Molecule 11 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	174	Total	C	N	O	S	0	0
			1318	832	236	249	1		

- Molecule 12 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	60	Total	C	N	O	S	0	0
			458	287	84	86	1		

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	142	Total	C	N	O	S	0	0
			1125	718	200	203	4		

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	122	Total	C	N	O	S	0	0
			946	592	180	169	5		

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	144	Total	C	N	O	S	0	0
			1071	663	213	195			

- Molecule 16 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	137	Total	C	N	O	S	0	0
			1087	687	210	185	5		

- Molecule 17 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	119	Total	C	N	O	S	0	0
			942	590	186	163	3		

- Molecule 18 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	114	Total	C	N	O	S	0	0
			857	528	173	155	1		

- Molecule 19 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	116	Total	C	N	O	S	0	0
			913	575	176	162			

- Molecule 20 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	118	Total	C	N	O	S	0	0
			942	594	198	147	3		

- Molecule 21 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	103	Total	C	N	O	S	0	0
			807	506	155	143	3		

- Molecule 22 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	109	Total	C	N	O	S	0	0
			826	514	158	150	4		

- Molecule 23 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	91	Total	C	N	O	S	0	0
			710	452	128	129	1		

- Molecule 24 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	103	Total	C	N	O		0	0
			766	476	142	148			

- Molecule 25 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	97	Total	C	N	O	S	0	0
			760	477	143	139	1		

- Molecule 26 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	V	77	Total	C	N	O	S	0	0
			585	363	112	108	2		

- Molecule 27 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	W	77	Total	C	N	O	S	0	0
			632	395	130	105	2		

- Molecule 28 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	60	Total	C	N	O	S	0	0
			486	302	93	90	1		

- Molecule 29 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	57	Total	C	N	O	S	0	0
			455	281	87	84	3		

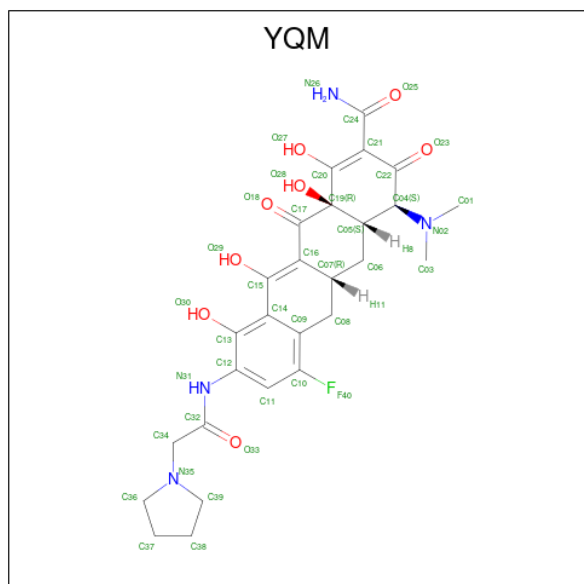
- Molecule 30 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	55	Total	C	N	O	S	0	0
			456	271	102	82	1		

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
31	3	1	Total Zn 1 1	0

- Molecule 32 is Eravacycline (three-letter code: YQM) (formula: C<sub>27</sub>H<sub>31</sub>FN<sub>4</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	F	N	O	0
			80	54	2	8	16	

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Mol	Chain	Residues	Atoms					AltConf
32	A	1	Total	C	F	N	O	0
			80	54	2	8	16	

- Molecule 33 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	A	157	Total	Mg	0
			157	157	
33	B	1	Total	Mg	0
			1	1	
33	K	1	Total	Mg	0
			1	1	

- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	1	1	Total	O	0
			1	1	
34	2	3	Total	O	0
			3	3	
34	A	759	Total	O	0
			759	759	
34	B	5	Total	O	0
			5	5	
34	C	9	Total	O	0
			9	9	
34	D	4	Total	O	0
			4	4	
34	E	4	Total	O	0
			4	4	
34	K	5	Total	O	0
			5	5	
34	P	3	Total	O	0
			3	3	
34	R	2	Total	O	0
			2	2	
34	S	3	Total	O	0
			3	3	
34	U	1	Total	O	0
			1	1	
34	W	1	Total	O	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
34	Z	2	Total	O	0
			2	2	

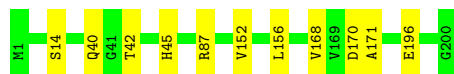






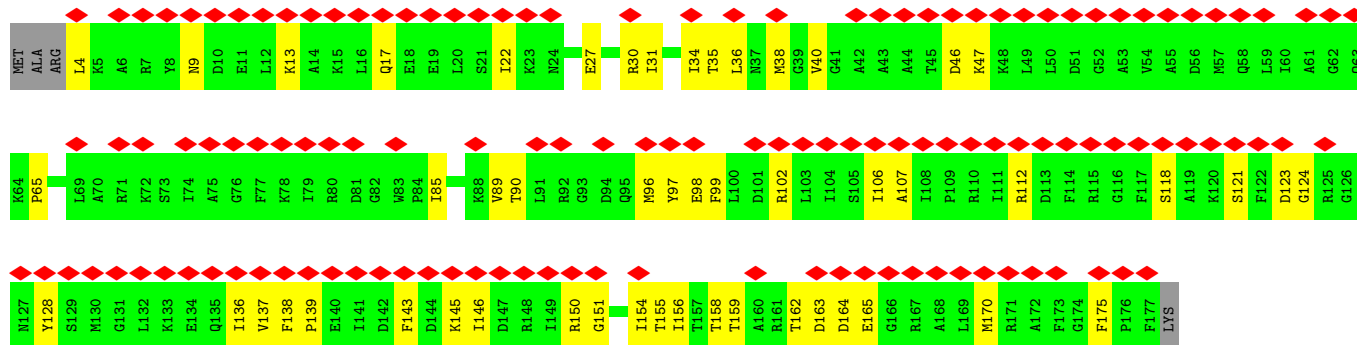
- Molecule 9: 50S ribosomal protein L4

Chain E:  94% 6%



- Molecule 10: 50S ribosomal protein L5

Chain F:  72% 69% 29%



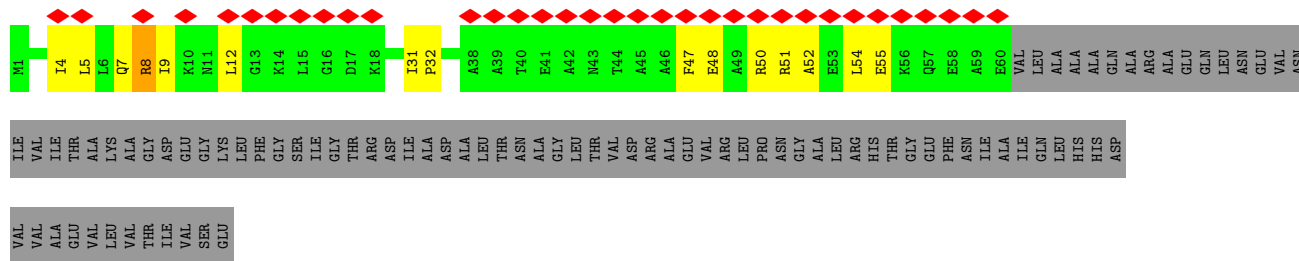
- Molecule 11: 50S ribosomal protein L6

Chain G:  94%



- Molecule 12: 50S ribosomal protein L9

Chain H:  23% 30% 9% 59%



- Molecule 13: 50S ribosomal protein L13

Chain I:  96%



- Molecule 14: 50S ribosomal protein L14

Chain J:  97% .




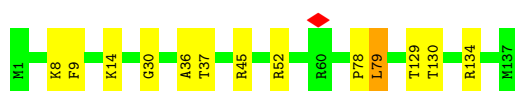
- Molecule 15: 50S ribosomal protein L15

Chain K:  97% ..



- Molecule 16: 50S ribosomal protein L16

Chain L:  91% 9% .




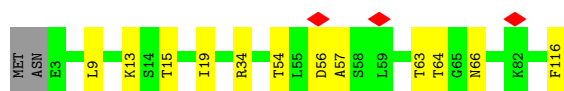
- Molecule 17: 50S ribosomal protein L17

Chain M:  91% . 5%




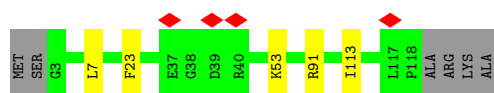
- Molecule 18: 50S ribosomal protein L18

Chain N:  88% 10% .



- Molecule 19: 50S ribosomal protein L19

Chain O:  91% . 5%

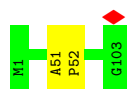


- Molecule 20: 50S ribosomal protein L20

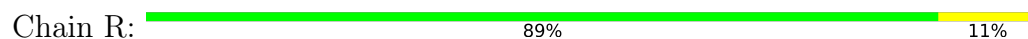
Chain P:  95% . .



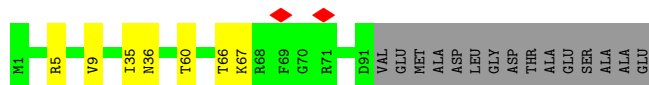
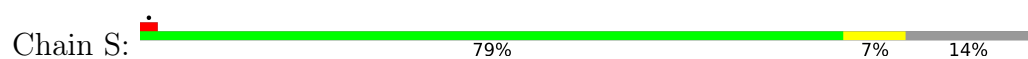
- Molecule 21: 50S ribosomal protein L21



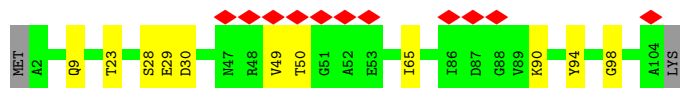
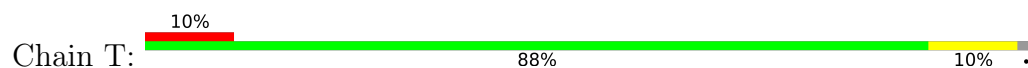
- Molecule 22: 50S ribosomal protein L22



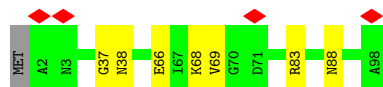
- Molecule 23: 50S ribosomal protein L23



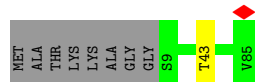
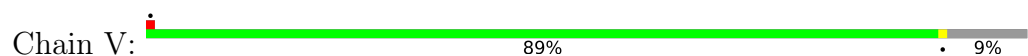
- Molecule 24: 50S ribosomal protein L24



- Molecule 25: 50S ribosomal protein L25



- Molecule 26: 50S ribosomal protein L27




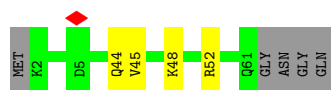
- Molecule 27: 50S ribosomal protein L28





- Molecule 28: 50S ribosomal protein L29

Chain X:  86% 6% 8%




- Molecule 29: 50S ribosomal protein L30

Chain Y:  95% . .



- Molecule 30: 50S ribosomal protein L32

Chain Z:  5% 79% 11% 10%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	92112	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 ( $e^-/\text{\AA}^2$ )	46	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.051	Depositor
Minimum map value	-1.693	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.052	Depositor
Recommended contour level	0.12	Depositor
Map size ( $\text{\AA}$ )	434.176, 434.176, 434.176	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.848, 0.848, 0.848	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, 2MA, 6MZ, OMU, YQM, ZN, 3TD, MG, PSU, OMG, 7MG, 2MG

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	0	0.26	0/434	0.52	0/573
2	1	0.24	0/367	0.66	0/481
3	2	0.24	0/515	0.61	0/678
4	3	0.25	0/296	0.59	0/389
5	A	0.21	0/65276	0.76	7/101810 (0.0%)
6	B	0.20	0/2739	0.76	0/4266
7	C	0.24	0/2152	0.57	0/2891
8	D	0.24	0/1590	0.56	0/2142
9	E	0.25	0/1537	0.52	0/2073
10	F	0.27	0/1390	0.55	0/1863
11	G	0.25	0/1337	0.50	0/1807
12	H	0.26	0/461	0.55	0/616
13	I	0.25	0/1151	0.47	0/1551
14	J	0.25	0/956	0.58	0/1286
15	K	0.24	0/1079	0.57	0/1439
16	L	0.25	0/1104	0.57	0/1475
17	M	0.25	0/956	0.57	0/1282
18	N	0.24	0/865	0.56	0/1156
19	O	0.24	0/925	0.56	0/1241
20	P	0.26	0/955	0.58	0/1272
21	Q	0.24	0/818	0.54	0/1094
22	R	0.24	0/831	0.51	0/1113
23	S	0.26	0/716	0.51	0/957
24	T	0.23	0/770	0.50	0/1034
25	U	0.24	0/770	0.53	0/1036
26	V	0.24	0/593	0.55	0/793
27	W	0.22	0/642	0.54	0/856
28	X	0.24	0/487	0.48	0/646
29	Y	0.24	0/460	0.54	0/614
30	Z	0.23	0/462	0.63	0/615
All	All	0.22	0/92634	0.71	7/139049 (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
4	3	0	1

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1105	U	O4'-C1'-N1	11.66	117.53	108.20
5	A	727	G	O4'-C1'-N9	5.97	112.97	108.20
5	A	1105	U	N1-C1'-C2'	5.61	121.30	114.00
5	A	2470	U	C2-N1-C1'	5.50	124.29	117.70
5	A	788	U	C2-N1-C1'	5.45	124.24	117.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	3	36	ARG	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	0	427	0	462	4	0
2	1	363	0	401	0	0
3	2	509	0	566	3	0
4	3	295	0	326	7	0
5	A	58607	0	29474	228	0
6	B	2450	0	1241	17	0
7	C	2111	0	2176	12	0
8	D	1572	0	1610	13	0
9	E	1516	0	1569	6	0
10	F	1370	0	1420	38	0
11	G	1318	0	1373	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	H	458	0	480	17	0
13	I	1125	0	1148	5	0
14	J	946	0	1007	2	0
15	K	1071	0	1140	1	0
16	L	1087	0	1162	9	0
17	M	942	0	987	3	0
18	N	857	0	899	9	0
19	O	913	0	968	4	0
20	P	942	0	1009	6	0
21	Q	807	0	842	3	0
22	R	826	0	894	8	0
23	S	710	0	768	4	0
24	T	766	0	816	6	0
25	U	760	0	783	5	0
26	V	585	0	589	2	0
27	W	632	0	667	1	0
28	X	486	0	528	3	0
29	Y	455	0	476	2	0
30	Z	456	0	448	4	0
31	3	1	0	0	0	0
32	A	80	0	0	1	0
33	A	157	0	0	0	0
33	B	1	0	0	0	0
33	K	1	0	0	0	0
34	1	1	0	0	0	0
34	2	3	0	0	0	0
34	A	759	0	0	34	0
34	B	5	0	0	0	0
34	C	9	0	0	0	0
34	D	4	0	0	1	0
34	E	4	0	0	0	0
34	K	5	0	0	0	0
34	P	3	0	0	0	0
34	R	2	0	0	0	0
34	S	3	0	0	0	0
34	U	1	0	0	0	0
34	W	1	0	0	0	0
34	Z	2	0	0	0	0
All	All	86404	0	56229	396	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 396 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:799:G:O2'	5:A:800:A:OP1	1.81	0.97
19:O:91:ARG:NH2	19:O:113:ILE:O	2.01	0.93
10:F:9:ASN:OD1	10:F:13:LYS:NZ	2.02	0.92
5:A:84:U:OP1	28:X:52:ARG:NH1	2.03	0.90
5:A:1938:C:OP2	5:A:1939:U:O2'	1.91	0.88

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/51 (96%)	49 (100%)	0	0	100	100
2	1	42/44 (96%)	42 (100%)	0	0	100	100
3	2	61/64 (95%)	60 (98%)	1 (2%)	0	100	100
4	3	36/38 (95%)	35 (97%)	0	1 (3%)	5	4
7	C	270/274 (98%)	260 (96%)	10 (4%)	0	100	100
8	D	209/212 (99%)	198 (95%)	10 (5%)	1 (0%)	29	40
9	E	198/200 (99%)	198 (100%)	0	0	100	100
10	F	172/178 (97%)	153 (89%)	19 (11%)	0	100	100
11	G	172/177 (97%)	168 (98%)	2 (1%)	2 (1%)	13	17
12	H	58/148 (39%)	57 (98%)	1 (2%)	0	100	100
13	I	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
14	J	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
15	K	142/146 (97%)	139 (98%)	3 (2%)	0	100	100
16	L	135/137 (98%)	134 (99%)	0	1 (1%)	22	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	M	117/125 (94%)	113 (97%)	4 (3%)	0	100	100
18	N	112/116 (97%)	112 (100%)	0	0	100	100
19	O	114/122 (93%)	112 (98%)	2 (2%)	0	100	100
20	P	116/119 (98%)	116 (100%)	0	0	100	100
21	Q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
22	R	107/109 (98%)	105 (98%)	2 (2%)	0	100	100
23	S	89/106 (84%)	88 (99%)	1 (1%)	0	100	100
24	T	101/105 (96%)	99 (98%)	2 (2%)	0	100	100
25	U	95/98 (97%)	93 (98%)	2 (2%)	0	100	100
26	V	75/85 (88%)	74 (99%)	1 (1%)	0	100	100
27	W	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
28	X	58/65 (89%)	58 (100%)	0	0	100	100
29	Y	55/58 (95%)	55 (100%)	0	0	100	100
30	Z	53/61 (87%)	52 (98%)	1 (2%)	0	100	100
All	All	3072/3283 (94%)	2997 (98%)	70 (2%)	5 (0%)	50	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	D	101	VAL
11	G	81	GLU
16	L	79	LEU
11	G	13	ASN
4	3	37	GLN

### 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	0	47/47 (100%)	47 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	1	36/36 (100%)	36 (100%)	0	100	100
3	2	52/53 (98%)	52 (100%)	0	100	100
4	3	33/33 (100%)	33 (100%)	0	100	100
7	C	218/220 (99%)	218 (100%)	0	100	100
8	D	166/167 (99%)	166 (100%)	0	100	100
9	E	155/155 (100%)	155 (100%)	0	100	100
10	F	144/147 (98%)	143 (99%)	1 (1%)	84	90
11	G	139/142 (98%)	139 (100%)	0	100	100
12	H	45/112 (40%)	44 (98%)	1 (2%)	52	66
13	I	118/118 (100%)	118 (100%)	0	100	100
14	J	103/103 (100%)	103 (100%)	0	100	100
15	K	106/108 (98%)	106 (100%)	0	100	100
16	L	113/113 (100%)	113 (100%)	0	100	100
17	M	96/101 (95%)	96 (100%)	0	100	100
18	N	83/85 (98%)	83 (100%)	0	100	100
19	O	98/102 (96%)	98 (100%)	0	100	100
20	P	86/86 (100%)	86 (100%)	0	100	100
21	Q	84/84 (100%)	84 (100%)	0	100	100
22	R	88/88 (100%)	88 (100%)	0	100	100
23	S	77/87 (88%)	76 (99%)	1 (1%)	69	80
24	T	83/85 (98%)	83 (100%)	0	100	100
25	U	79/80 (99%)	79 (100%)	0	100	100
26	V	60/64 (94%)	60 (100%)	0	100	100
27	W	69/70 (99%)	69 (100%)	0	100	100
28	X	53/56 (95%)	53 (100%)	0	100	100
29	Y	53/54 (98%)	53 (100%)	0	100	100
30	Z	47/50 (94%)	47 (100%)	0	100	100
All	All	2531/2646 (96%)	2528 (100%)	3 (0%)	93	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	F	112	ARG

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Mol	Chain	Res	Type
12	H	8	ARG
23	S	67	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
8	D	137	HIS
13	I	13	HIS
30	Z	52	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	A	2725/2918 (93%)	431 (15%)	26 (0%)
6	B	114/115 (99%)	19 (16%)	2 (1%)
All	All	2839/3033 (93%)	450 (15%)	28 (0%)

5 of 450 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	10	U
5	A	41	U
5	A	53	G
5	A	56	A
5	A	57	U

5 of 28 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	1296	A
6	B	87	A
5	A	1448	U
5	A	2419	U
5	A	1337	A

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

15 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
5	5MU	A	1935	5	19,22,23	0.42	0	28,32,35	0.53	0
5	PSU	A	2453	5	18,21,22	1.10	1 (5%)	22,30,33	1.81	5 (22%)
5	PSU	A	1907	5	18,21,22	1.11	1 (5%)	22,30,33	1.79	5 (22%)
5	OMG	A	2247	5	18,26,27	1.10	2 (11%)	19,38,41	0.88	1 (5%)
5	PSU	A	2576	5	18,21,22	1.13	1 (5%)	22,30,33	1.82	5 (22%)
5	PSU	A	2601	5	18,21,22	1.06	1 (5%)	22,30,33	1.81	5 (22%)
5	2MG	A	2441	5	18,26,27	1.13	2 (11%)	16,38,41	0.86	1 (6%)
5	PSU	A	2500	5	18,21,22	1.10	1 (5%)	22,30,33	1.75	3 (13%)
5	3TD	A	1911	5	18,22,23	4.42	7 (38%)	22,32,35	1.70	2 (9%)
5	7MG	A	2065	5	22,26,27	1.22	1 (4%)	29,39,42	0.83	2 (6%)
5	2MA	A	2499	5,33	17,25,26	2.51	5 (29%)	17,37,40	1.40	3 (17%)
5	PSU	A	952	5	18,21,22	1.07	1 (5%)	22,30,33	1.74	3 (13%)
5	6MZ	A	2026	5	18,25,26	1.89	3 (16%)	16,36,39	3.30	4 (25%)
5	PSU	A	1913	5	18,21,22	1.07	1 (5%)	22,30,33	1.73	4 (18%)
5	OMU	A	2548	5	19,22,23	3.09	8 (42%)	26,31,34	1.67	4 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	5MU	A	1935	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2453	5	-	0/7/25/26	0/2/2/2
5	PSU	A	1907	5	-	0/7/25/26	0/2/2/2
5	OMG	A	2247	5	-	0/5/27/28	0/3/3/3
5	PSU	A	2576	5	-	0/7/25/26	0/2/2/2
5	PSU	A	2601	5	-	0/7/25/26	0/2/2/2
5	2MG	A	2441	5	-	2/5/27/28	0/3/3/3
5	PSU	A	2500	5	-	0/7/25/26	0/2/2/2
5	3TD	A	1911	5	-	4/7/25/26	0/2/2/2
5	7MG	A	2065	5	-	1/7/37/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	2MA	A	2499	5,33	-	3/3/25/26	0/3/3/3
5	PSU	A	952	5	-	0/7/25/26	0/2/2/2
5	6MZ	A	2026	5	-	1/5/27/28	0/3/3/3
5	PSU	A	1913	5	-	1/7/25/26	0/2/2/2
5	OMU	A	2548	5	-	2/9/27/28	0/2/2/2

The worst 5 of 35 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1911	3TD	C6-C5	12.92	1.50	1.35
5	A	1911	3TD	C2-N1	10.25	1.50	1.37
5	A	2548	OMU	C2-N1	7.34	1.50	1.38
5	A	2499	2MA	C2-N3	7.26	1.46	1.31
5	A	2548	OMU	C2-N3	6.90	1.50	1.38

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2026	6MZ	C1'-N9-C4	-11.30	106.80	126.64
5	A	2026	6MZ	N3-C2-N1	-5.32	120.37	128.68
5	A	1911	3TD	N1-C2-N3	5.20	120.25	116.14
5	A	2548	OMU	C4-N3-C2	-5.15	119.79	126.58
5	A	2601	PSU	C4-N3-C2	-4.70	119.57	126.34

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1911	3TD	C2'-C1'-C5-C4
5	A	1911	3TD	C2'-C1'-C5-C6
5	A	1913	PSU	O4'-C1'-C5-C6
5	A	2548	OMU	O4'-C4'-C5'-O5'
5	A	1911	3TD	O4'-C4'-C5'-O5'

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1911	3TD	2	0
5	A	2026	6MZ	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1913	PSU	1	0
5	A	2548	OMU	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 162 ligands modelled in this entry, 160 are monoatomic - leaving 2 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$
32	YQM	A	3202	33	42,44,44	3.44	22 (52%)	47,69,69	2.83	21 (44%)
32	YQM	A	3201	33	42,44,44	3.65	21 (50%)	47,69,69	2.91	21 (44%)

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
32	YQM	A	3202	33	-	5/16/81/81	0/5/5/5
32	YQM	A	3201	33	-	4/16/81/81	0/5/5/5

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	3201	YQM	C19-C20	14.37	1.64	1.52
32	A	3202	YQM	C19-C20	13.43	1.63	1.52
32	A	3201	YQM	C19-C17	8.29	1.66	1.55
32	A	3202	YQM	C19-C17	8.00	1.65	1.55
32	A	3201	YQM	C21-C24	5.76	1.59	1.47

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	3201	YQM	C34-C32-N31	7.24	127.74	114.12
32	A	3202	YQM	C34-C32-N31	7.19	127.64	114.12
32	A	3201	YQM	C34-N35-C39	-7.05	103.89	113.25
32	A	3202	YQM	C34-N35-C39	-6.17	105.06	113.25
32	A	3201	YQM	C11-C12-C13	-5.95	114.58	120.49

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

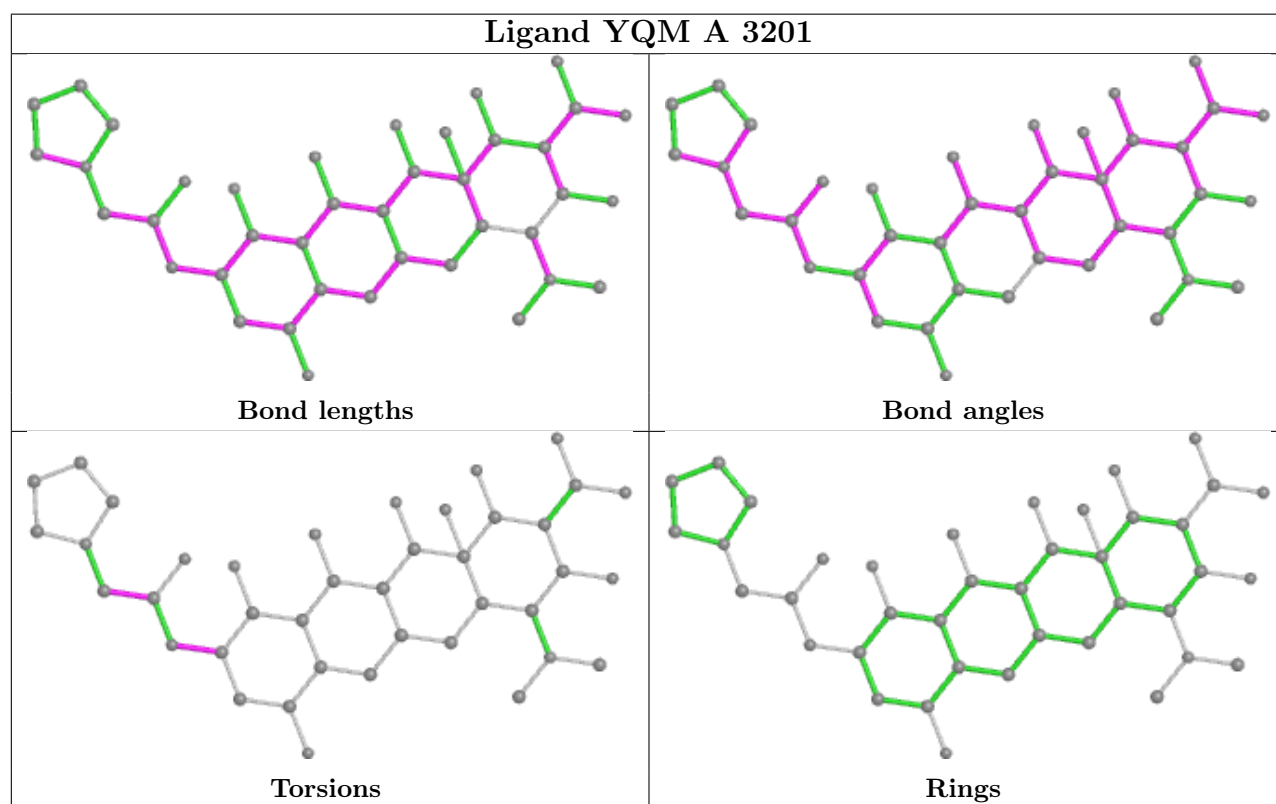
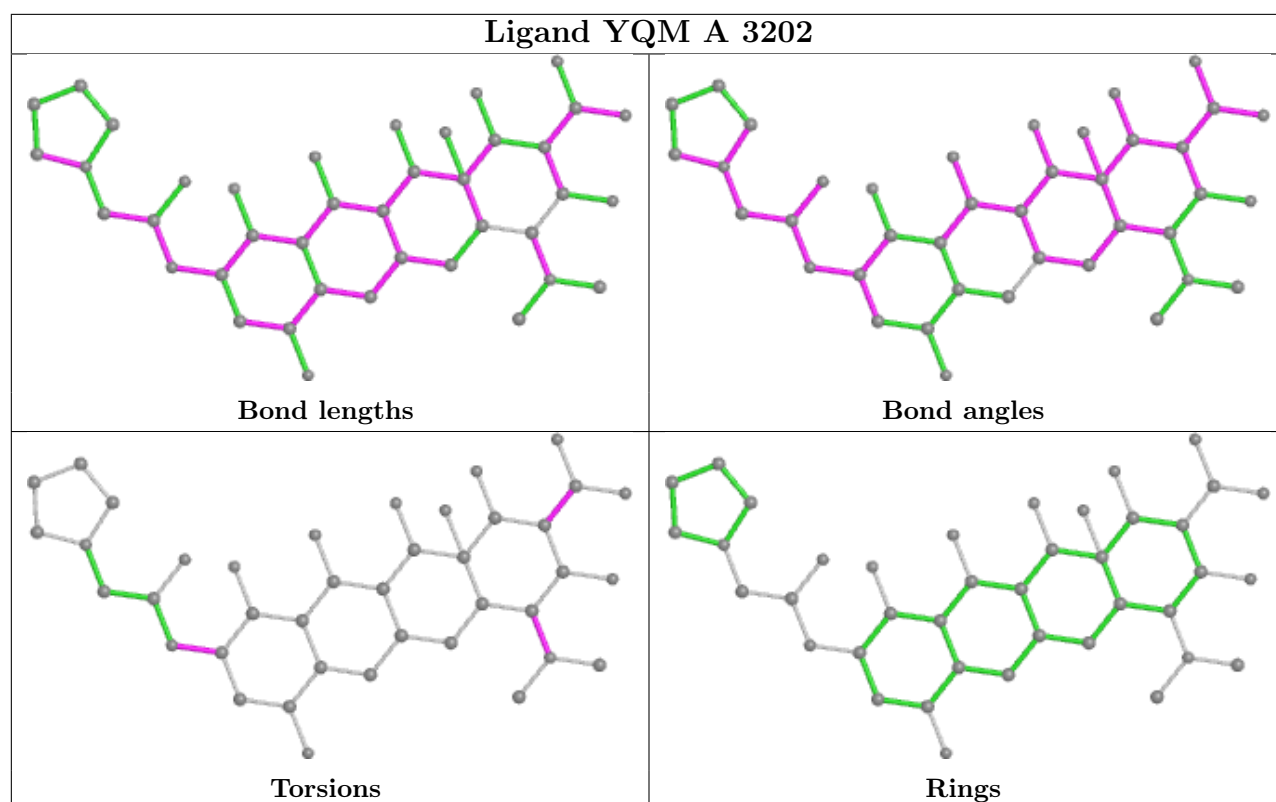
Mol	Chain	Res	Type	Atoms
32	A	3202	YQM	C20-C21-C24-N26
32	A	3202	YQM	C20-C21-C24-O25
32	A	3201	YQM	C11-C12-N31-C32
32	A	3201	YQM	C13-C12-N31-C32
32	A	3202	YQM	C13-C12-N31-C32

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
32	A	3201	YQM	1	0

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 ⓘ

There are no chain breaks in this entry.

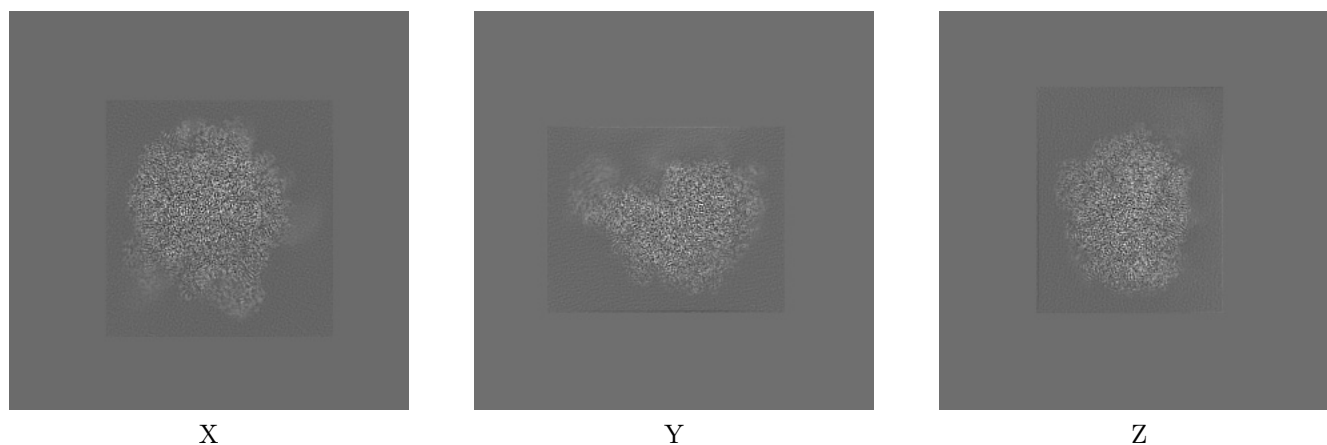
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23667. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

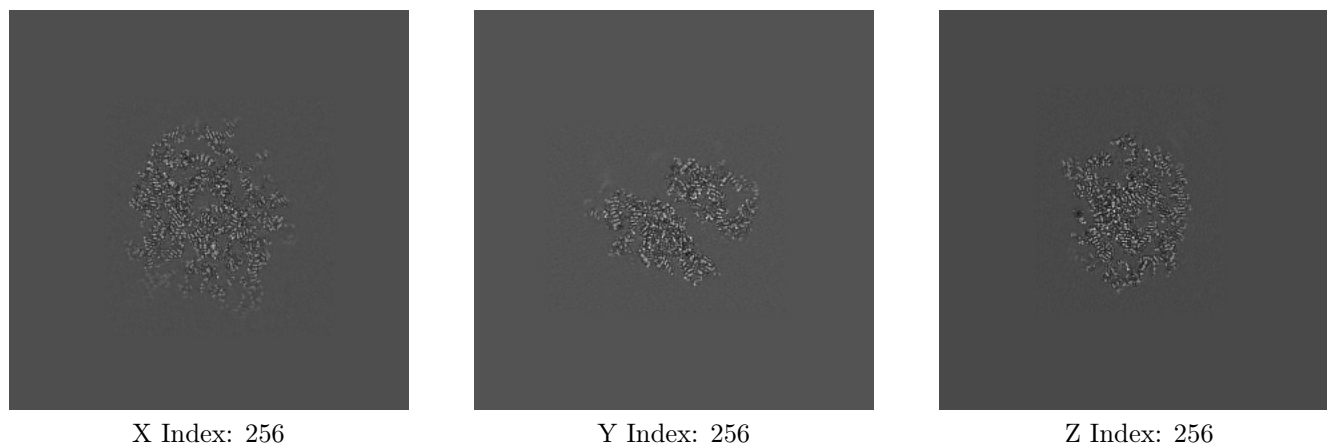
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map

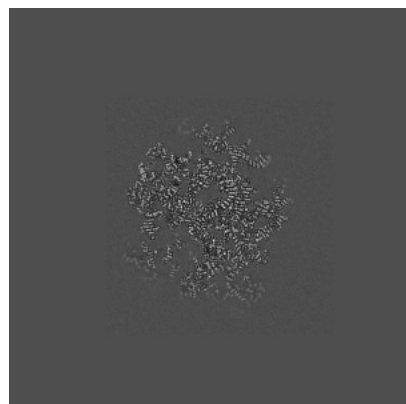




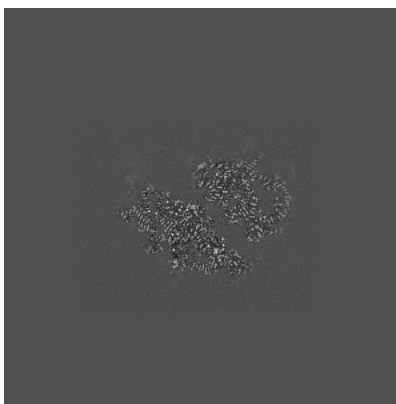
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

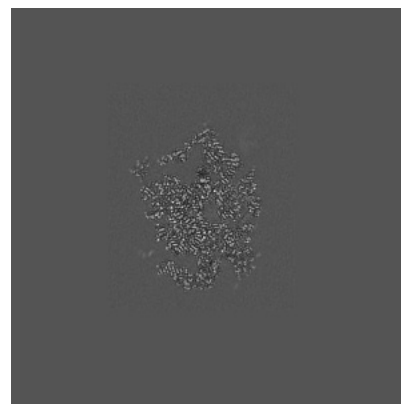
### 6.3.1 Primary map



X Index: 247



Y Index: 250

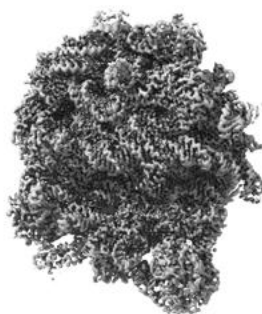


Z Index: 264

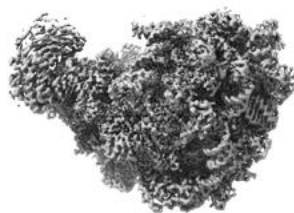
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

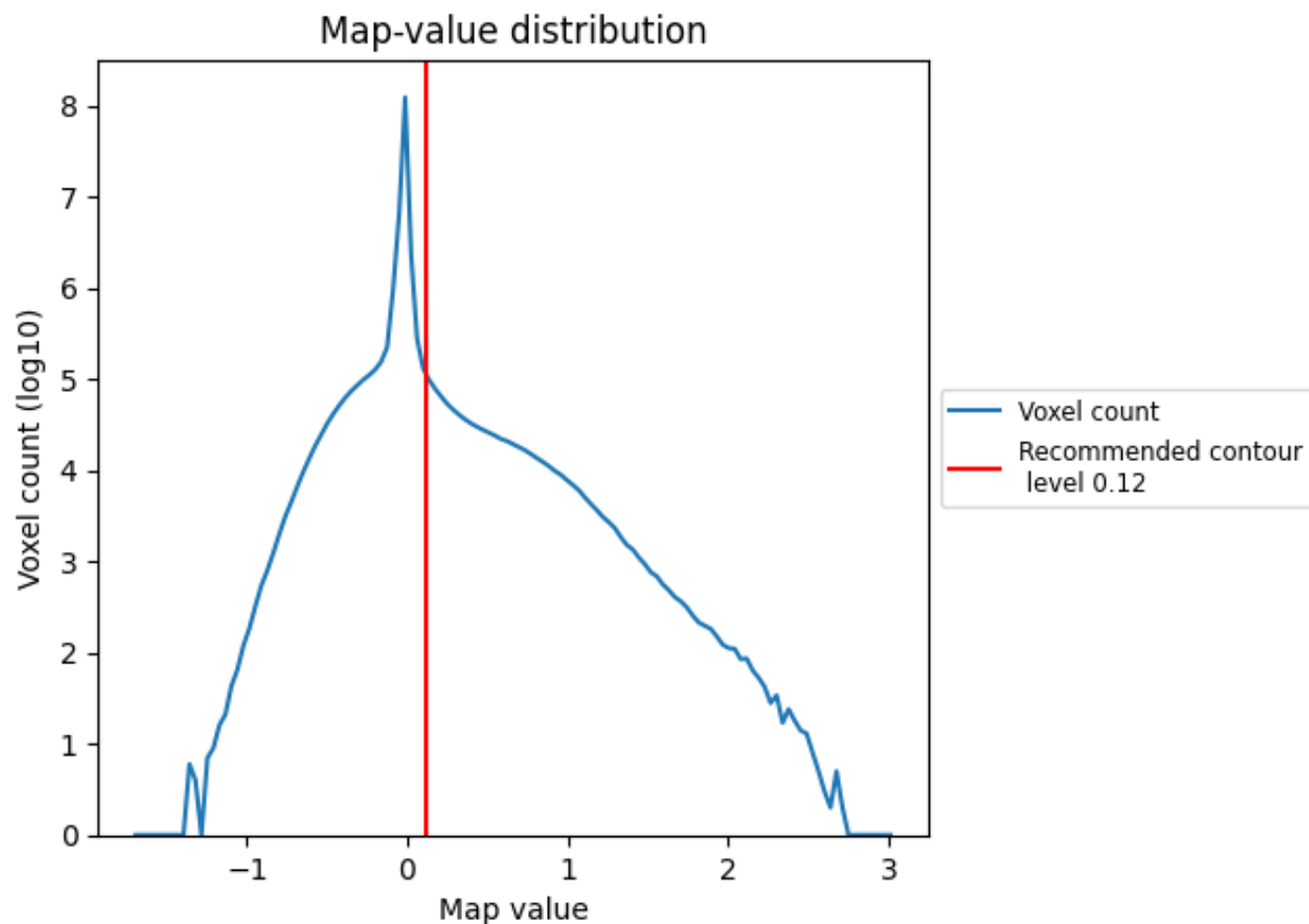
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

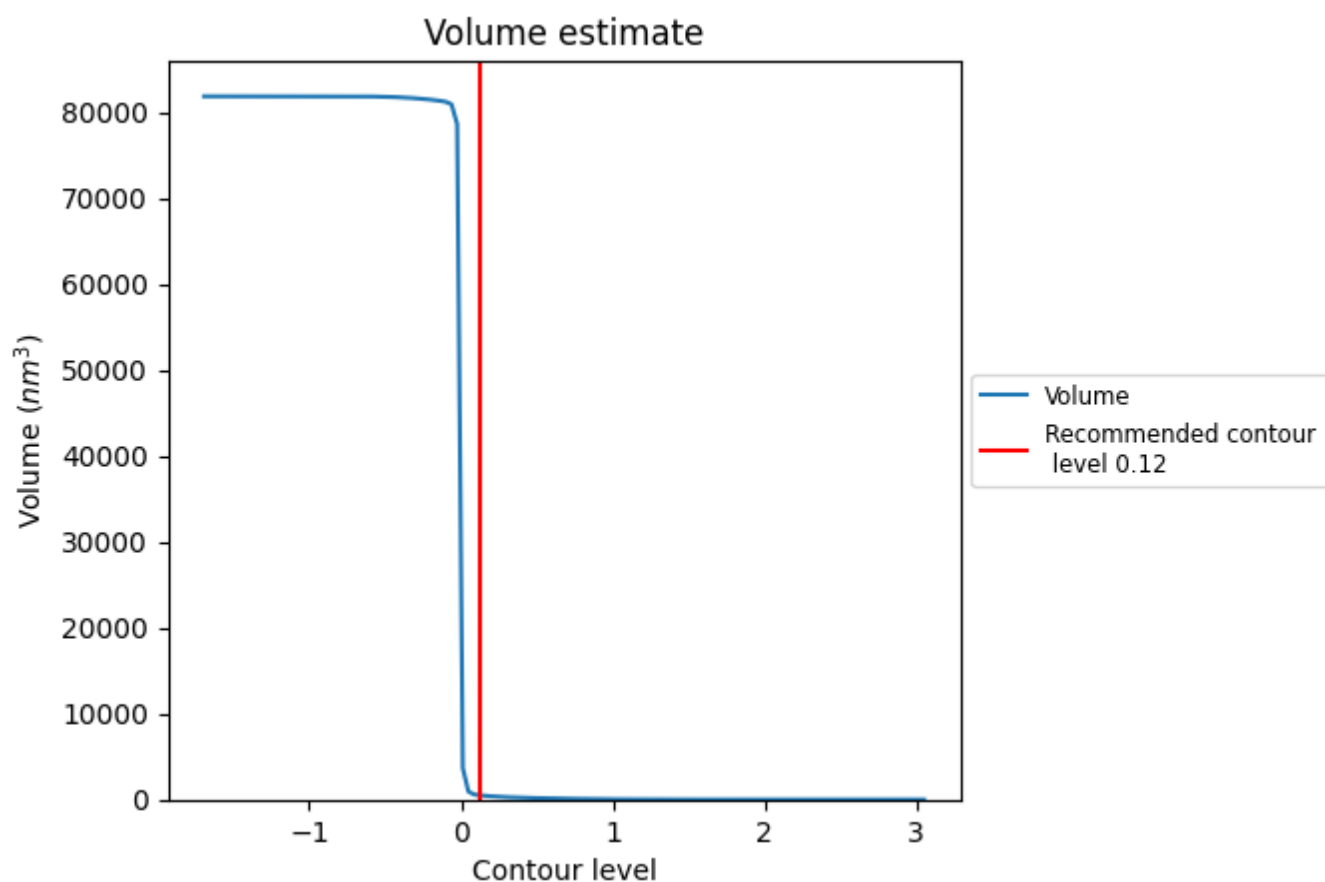
This section contains the results of statistical analysis of the map.

### 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.

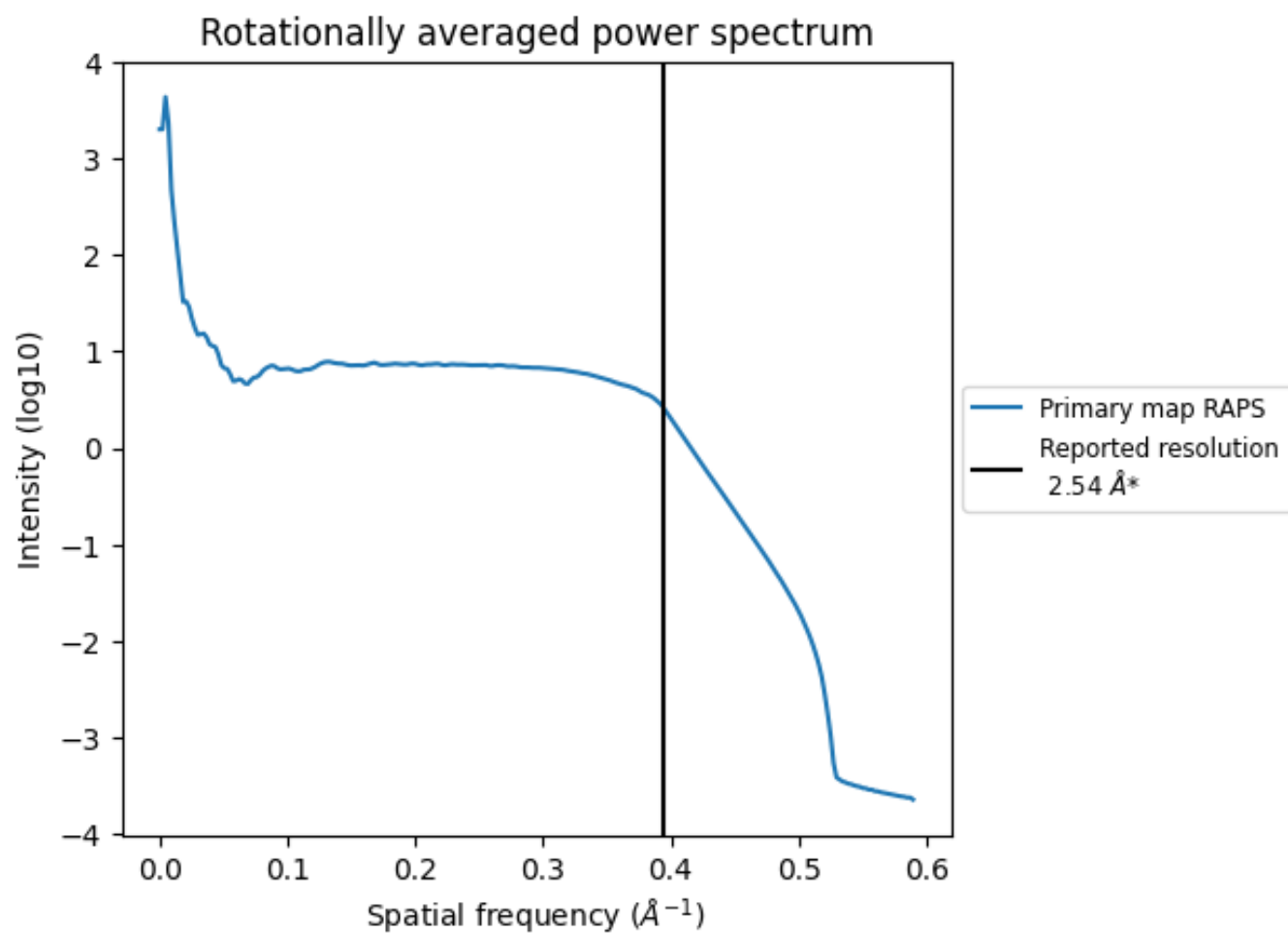
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 508  $\text{nm}^3$ ; this corresponds to an approximate mass of 459 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 0.394 Å<sup>-1</sup>

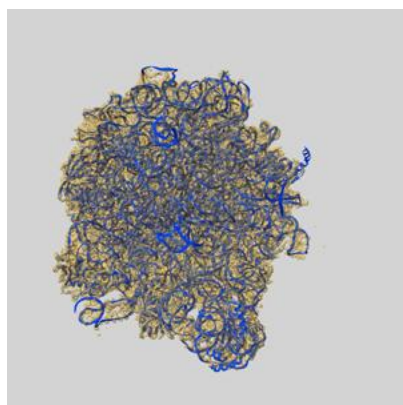
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

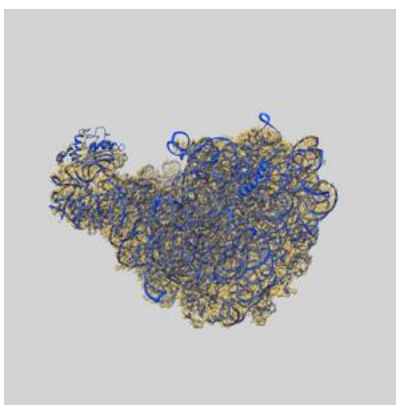
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-23667 and PDB model 7M4V. Per-residue inclusion information can be found in section 3 on page 11.

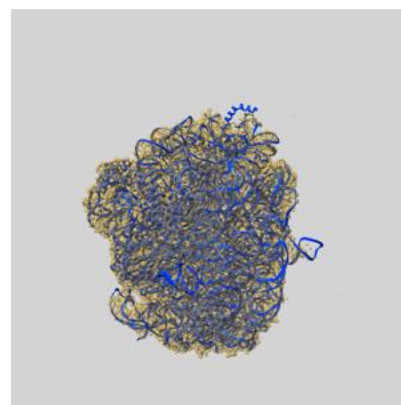
### 9.1 Map-model overlay [i](#)



X



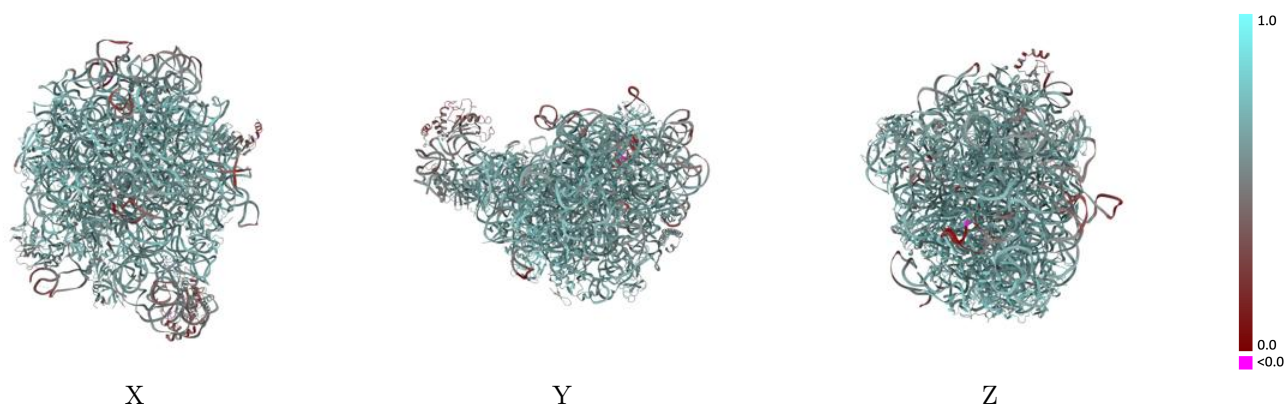
Y



Z

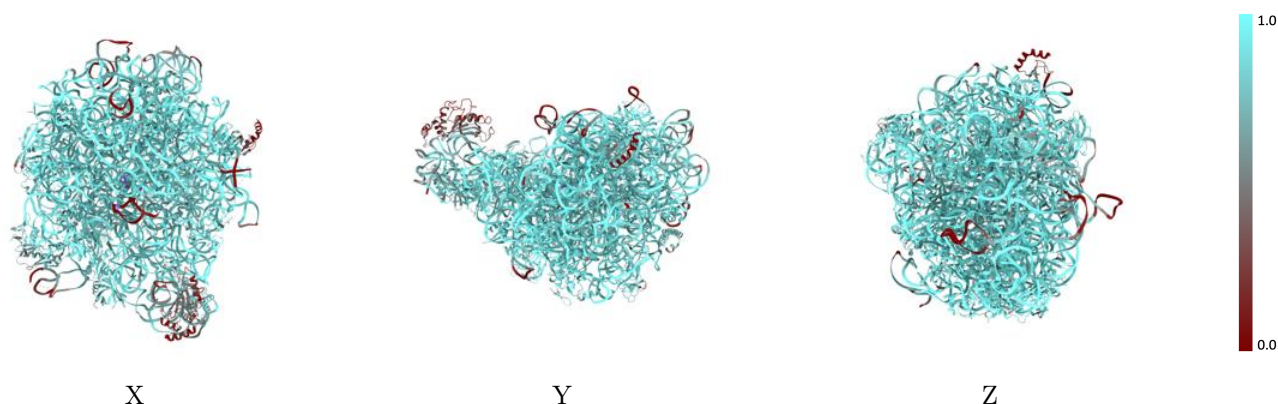
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

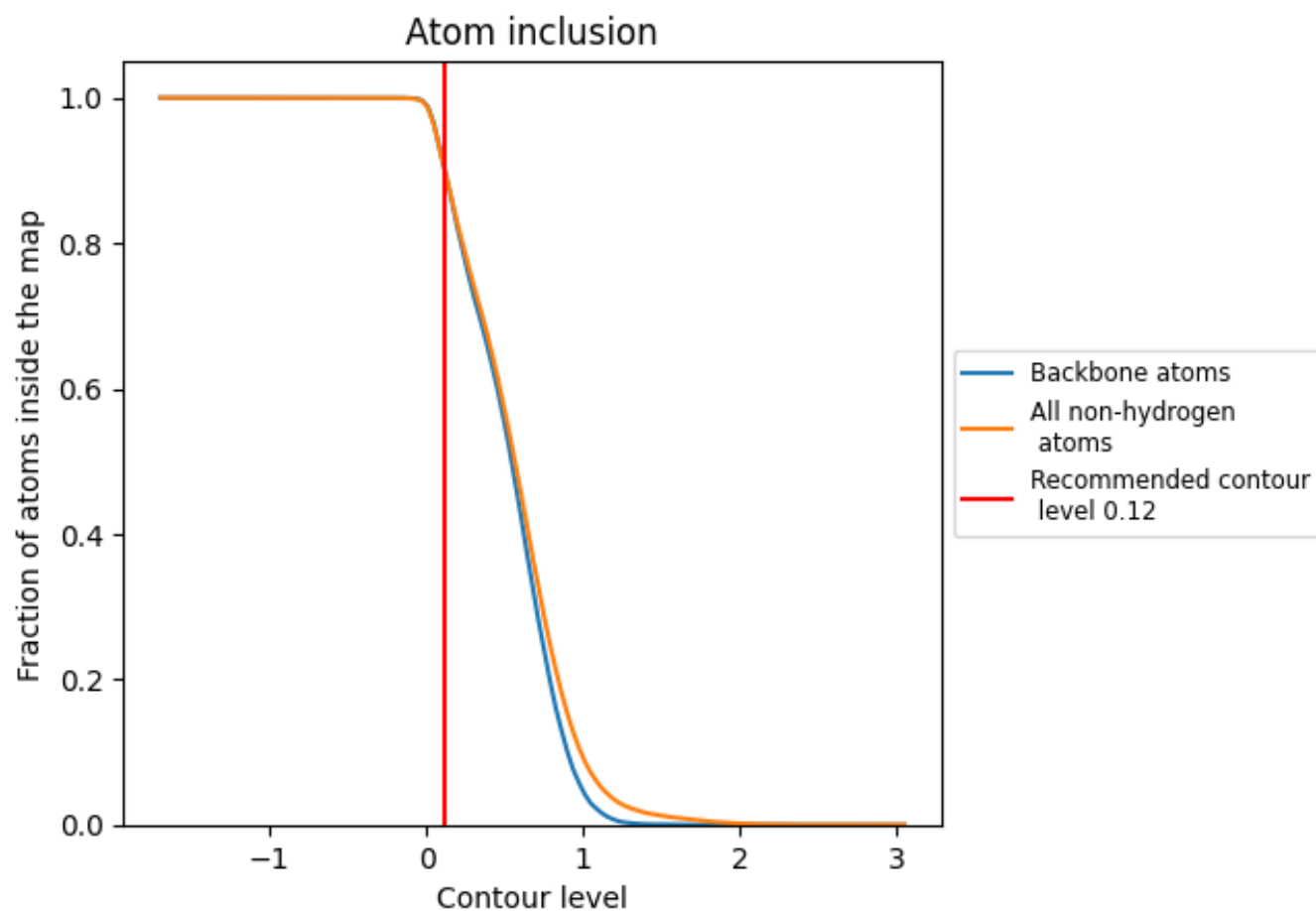
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.12).

































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 90% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9001	 0.6320
0	 0.8681	 0.6400
1	 0.9738	 0.7060
2	 0.9836	 0.7030
3	 0.9161	 0.6450
A	 0.9232	 0.6360
B	 0.8148	 0.5480
C	 0.9466	 0.6720
D	 0.9519	 0.6900
E	 0.9028	 0.6550
F	 0.2470	 0.3670
G	 0.7259	 0.5490
H	 0.3541	 0.3910
I	 0.9503	 0.6770
J	 0.9195	 0.6640
K	 0.9548	 0.6860
L	 0.9068	 0.6500
M	 0.9758	 0.6970
N	 0.7600	 0.5540
O	 0.8895	 0.6540
P	 0.9755	 0.6960
Q	 0.9315	 0.6670
R	 0.9543	 0.6870
S	 0.8567	 0.6180
T	 0.7817	 0.5910
U	 0.8358	 0.6090
V	 0.9475	 0.6850
W	 0.9152	 0.6630
X	 0.7647	 0.5490
Y	 0.9348	 0.6710
Z	 0.8874	 0.6620

