



wwPDB EM Validation Summary Report ⓘ

Nov 4, 2023 – 05:11 PM EDT

PDB ID : 8G6X
EMDB ID : EMD-29787
Title : Structure of WT E.coli ribosome 50S subunit with complexed with mRNA, P-site fMet-NH-tRNA^{fMet} and A-site meta-aminobenzoic acid charged NH-tRNA^{Phe}
Authors : Majumdar, C.; Cate, J.H.D.
Deposited on : 2023-02-16
Resolution : 2.31 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:

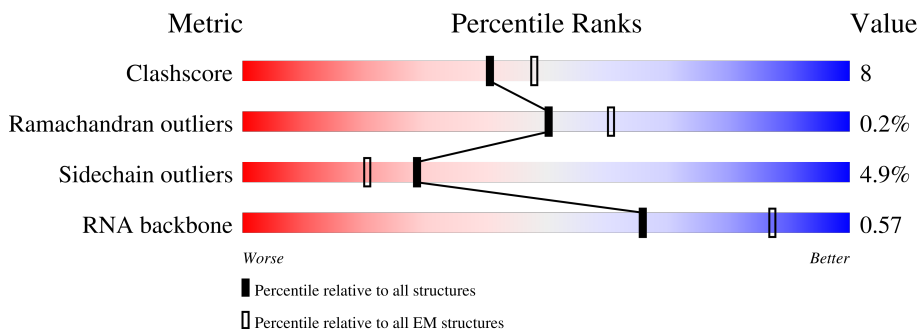
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 2.31 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 ≥ 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	2904	
2	b	120	
3	c	273	
4	d	209	
5	e	201	
6	f	179	
7	g	177	

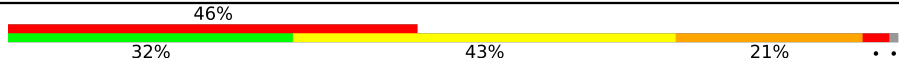
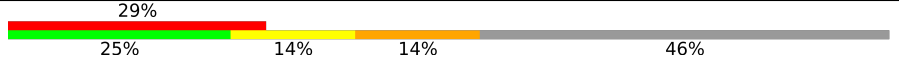
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Mol	Chain	Length	Quality of chain
8	h	149	9% 23% 72%
9	i	142	99%
10	j	123	98%
11	k	144	98%
12	l	136	96%
13	m	127	92% 7%
14	n	117	9% 93% 6%
15	o	115	5% 95%
16	p	118	97%
17	q	103	5% 92% 8%
18	r	110	97%
19	s	100	8% 93% 7%
20	t	104	12% 93% 5%
21	u	94	10% 96%
22	v	85	91% 8%
23	w	78	92% 6%
24	x	63	10% 95%
25	y	59	5% 93% 5%
26	z	57	98%
27	0	55	76% 16% 7%
28	1	46	93% 7%
29	2	65	85% 12%
30	3	38	82% 18%
31	4	70	70% 56% 27% 14%
32	Y	76	53% 16% 55% 25%

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Mol	Chain	Length	Quality of chain
33	Z	76	
34	X	28	

2 Entry composition [i](#)

There are 43 unique types of molecules in this entry. The entry contains 93873 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	a	2753	59130	26384	10897	19096	2753	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	b	119	2549	1135	466	829	119	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	209	1566	980	288	294	4	0	0

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	h	41	303	194	54	54	1	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	j	123	946	593	181	166	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	144	1053	654	207	190	2	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	l	136	1075	686	205	177	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	m	118	945	585	194	161	5	0	0

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

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

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

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

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

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

- Molecule 17 is a protein called Ribosomal protein L21.

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	93	Total	C	N	O	S	0	0
			738	466	139	131	2		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	v	78	Total	C	N	O	S	0	0
			586	362	116	107	1		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	x	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
27	0	51	Total	C	N	O	0	0
			417	269	76	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 31 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	60	Total	C	N	O	S	0	0
			480	299	90	85	6		

- Molecule 32 is a RNA chain called A-site tRNA Phe.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	74	Total	C	N	O	P	0	0
			1578	705	285	515	73		

- Molecule 33 is a RNA chain called P-site tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	Z	75	Total	C	N	O	P	0	0
			1601	713	289	524	75		

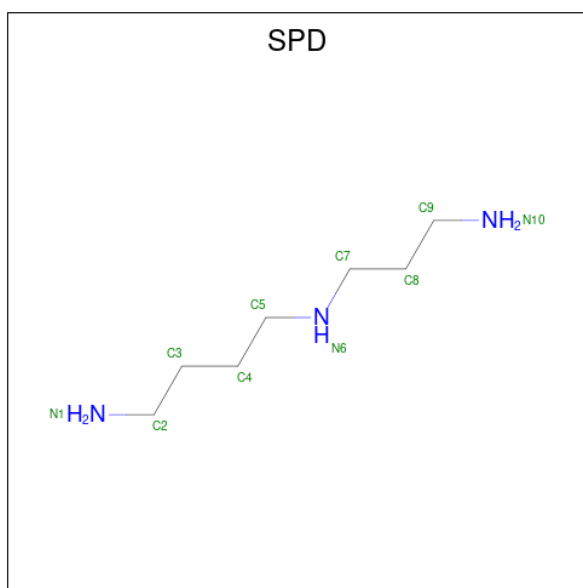
- Molecule 34 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	X	15	Total	C	N	O	P	0	0
			317	143	56	103	15		

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	a	211	Total	Mg	0
			211	211	
35	b	5	Total	Mg	0
			5	5	
35	c	2	Total	Mg	0
			2	2	
35	d	1	Total	Mg	0
			1	1	
35	m	1	Total	Mg	0
			1	1	
35	z	1	Total	Mg	0
			1	1	
35	Y	1	Total	Mg	0
			1	1	
35	Z	1	Total	Mg	0
			1	1	

- Molecule 36 is SPERMIDINE (three-letter code: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
36	a	1	Total	C	N	0
			10	7	3	
36	a	1	Total	C	N	0
			10	7	3	
36	a	1	Total	C	N	0
			10	7	3	
36	a	1	Total	C	N	0
			10	7	3	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0
36	a	1	10	7	3	0

- Molecule 37 is SPERMINE (three-letter code: SPM) (formula: C₁₀H₂₆N₄).

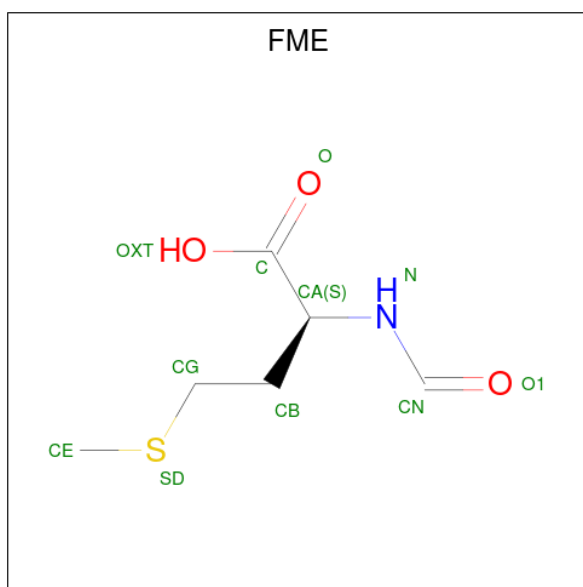


Mol	Chain	Residues	Atoms		AltConf
37	a	1	Total	C N	0
			14	10 4	

- Molecule 38 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
38	a	5	Total	K	0
			5	5	
38	c	1	Total	K	0
			1	1	
38	e	1	Total	K	0
			1	1	

- Molecule 39 is N-FORMYLMETHIONINE (three-letter code: FME) (formula: C₆H₁₁NO₃S).

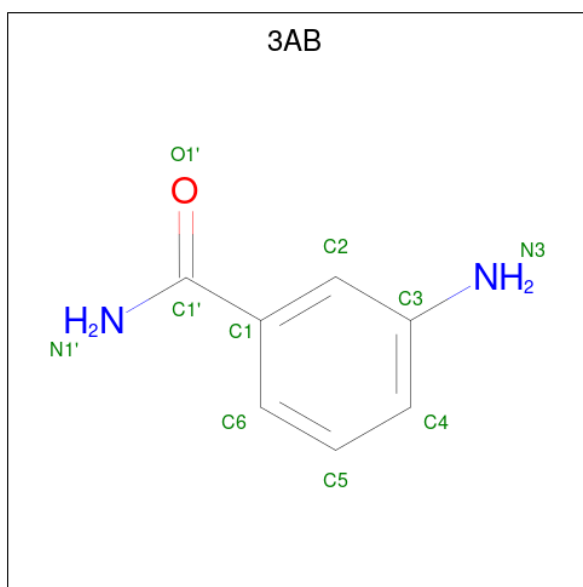


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
39	a	1	10	6	1	2	1	0

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula: Zn).

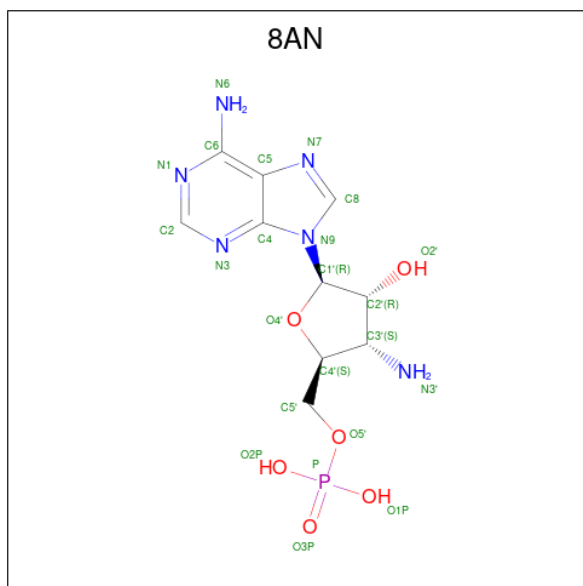
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
40	3	1	1	1	0
40	4	1	1	1	0

- Molecule 41 is 3-aminobenzamide (three-letter code: 3AB) (formula: C₇H₈N₂O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
41	Y	1	20	14	4	2	1

- Molecule 42 is 3'-amino-3'-deoxyadenosine 5'-(dihydrogen phosphate) (three-letter code: 8AN) (formula: $C_{10}H_{15}N_6O_6P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
42	Z	1	22	10	6	5	1	0

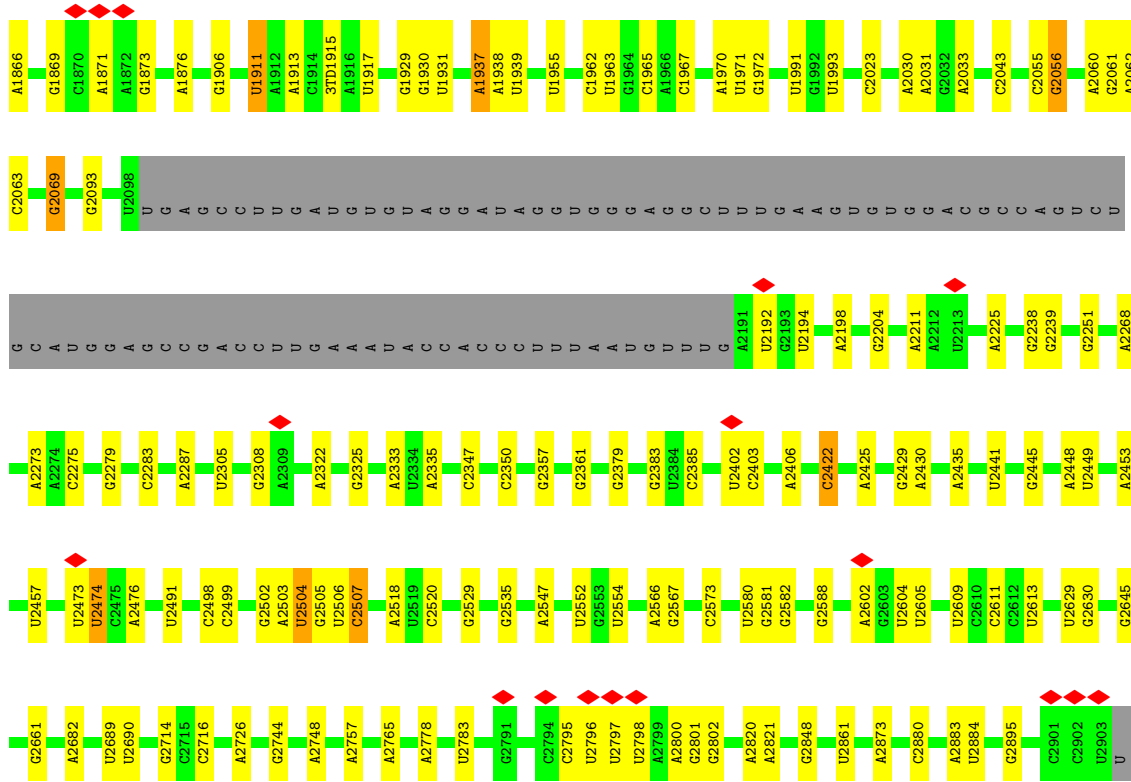
- Molecule 43 is water.

Mol	Chain	Residues	Atoms		AltConf
43	a	3013	Total 3013	O 3013	0
43	b	40	Total 40	O 40	0
43	c	86	Total 86	O 86	0
43	d	33	Total 33	O 33	0
43	e	27	Total 27	O 27	0
43	h	1	Total 1	O 1	0
43	i	12	Total 12	O 12	0
43	j	12	Total 12	O 12	0
43	k	32	Total 32	O 32	0
43	l	20	Total 20	O 20	0
43	m	20	Total 20	O 20	0
43	o	10	Total 10	O 10	0
43	p	19	Total 19	O 19	0
43	q	14	Total 14	O 14	0
43	r	24	Total 24	O 24	0
43	s	5	Total 5	O 5	0
43	t	1	Total 1	O 1	0
43	u	3	Total 3	O 3	0
43	v	12	Total 12	O 12	0
43	w	9	Total 9	O 9	0
43	x	1	Total 1	O 1	0
43	y	1	Total 1	O 1	0

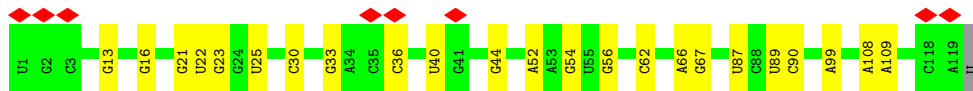
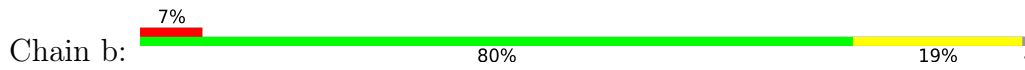
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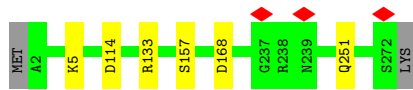
Mol	Chain	Residues	Atoms		AltConf
43	z	21	Total 21	O 21	0
43	1	17	Total 17	O 17	0
43	2	24	Total 24	O 24	0
43	3	3	Total 3	O 3	0
43	Z	2	Total 2	O 2	0



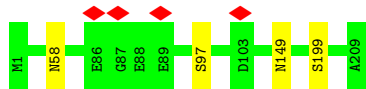
• Molecule 2: 5S rRNA



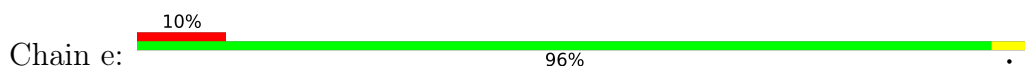
• Molecule 3: 50S ribosomal protein L2



• Molecule 4: 50S ribosomal protein L3

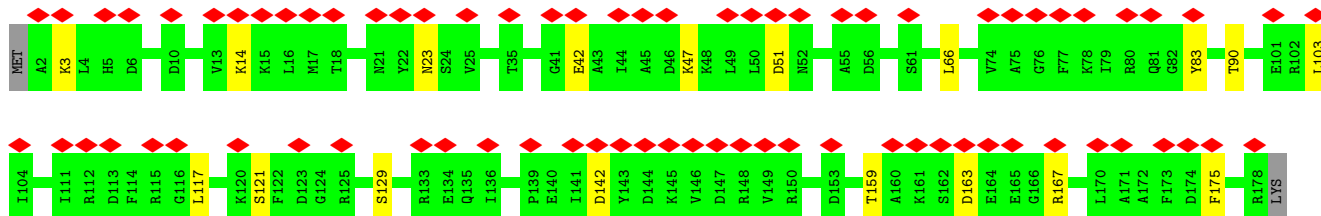
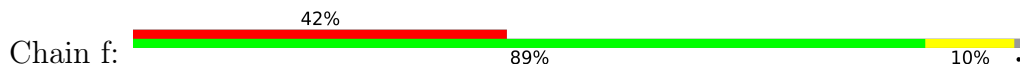


• Molecule 5: 50S ribosomal protein L4

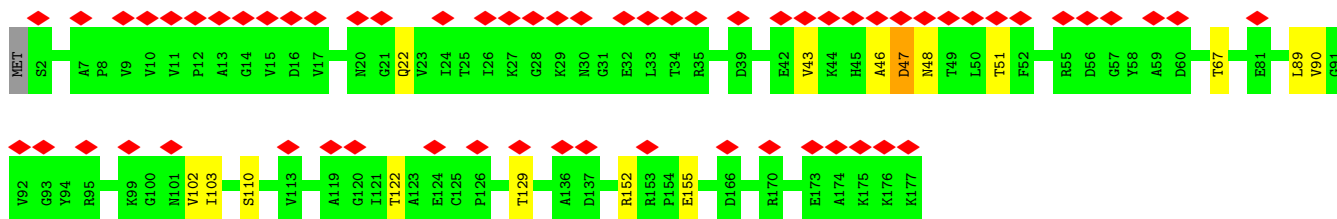
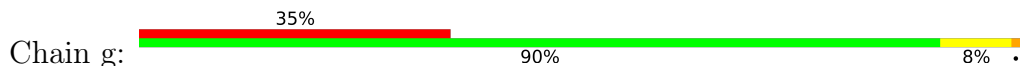




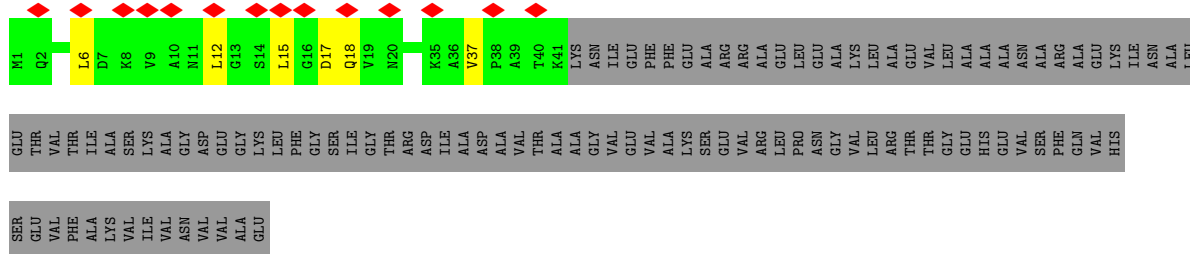
• Molecule 6: 50S ribosomal protein L5



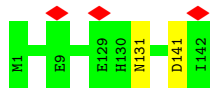
• Molecule 7: 50S ribosomal protein L6



• Molecule 8: 50S ribosomal protein L9

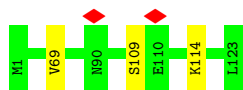


• Molecule 9: 50S ribosomal protein L13

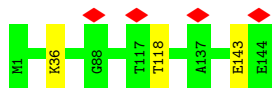


• Molecule 10: 50S ribosomal protein L14





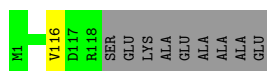
- Molecule 11: 50S ribosomal protein L15



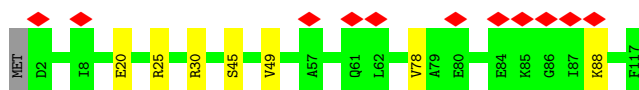
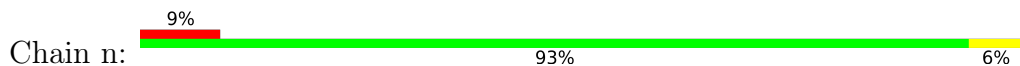
- Molecule 12: 50S ribosomal protein L16



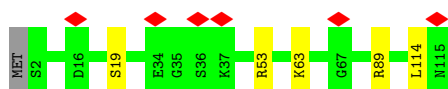
- Molecule 13: 50S ribosomal protein L17



- Molecule 14: 50S ribosomal protein L18



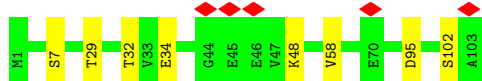
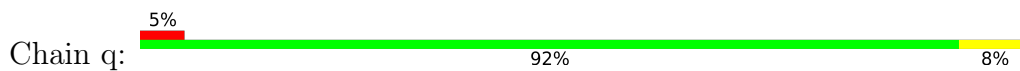
- Molecule 15: 50S ribosomal protein L19



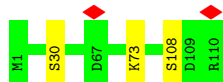
- Molecule 16: 50S ribosomal protein L20



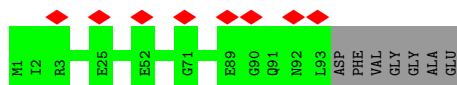
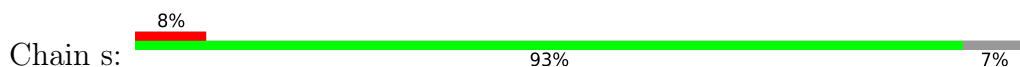
- Molecule 17: Ribosomal protein L21



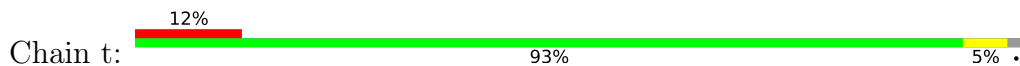
- Molecule 18: 50S ribosomal protein L22



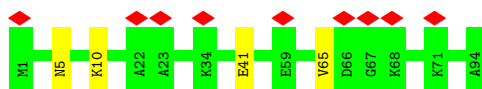
- Molecule 19: 50S ribosomal protein L23



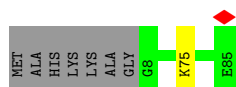
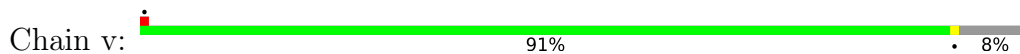
- Molecule 20: 50S ribosomal protein L24



- Molecule 21: 50S ribosomal protein L25



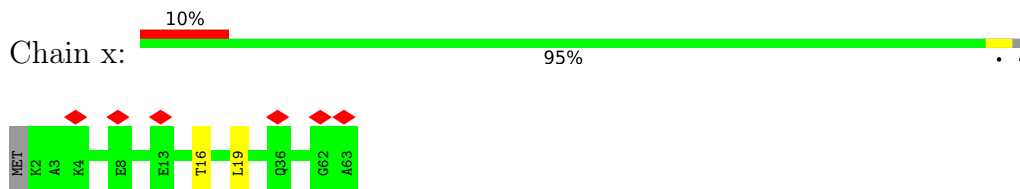
- Molecule 22: 50S ribosomal protein L27



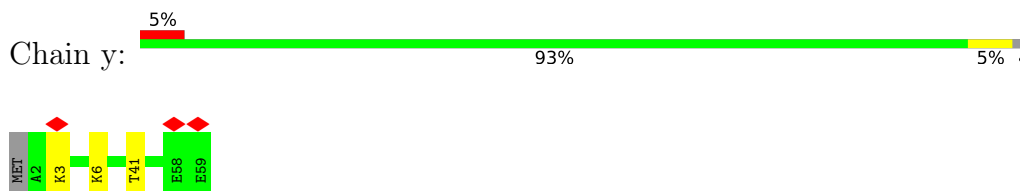
- Molecule 23: 50S ribosomal protein L28



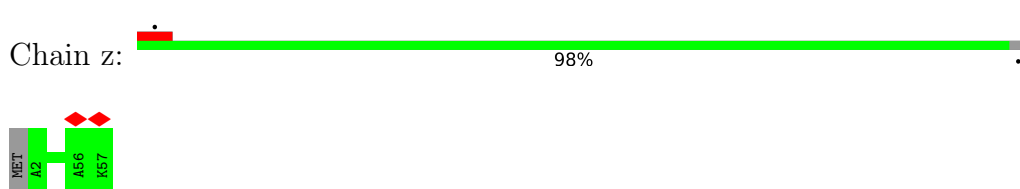
- Molecule 24: 50S ribosomal protein L29



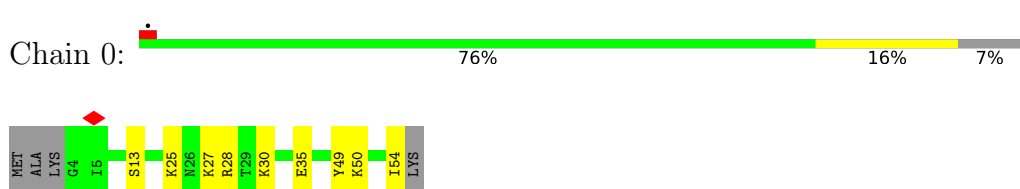
- Molecule 25: 50S ribosomal protein L30



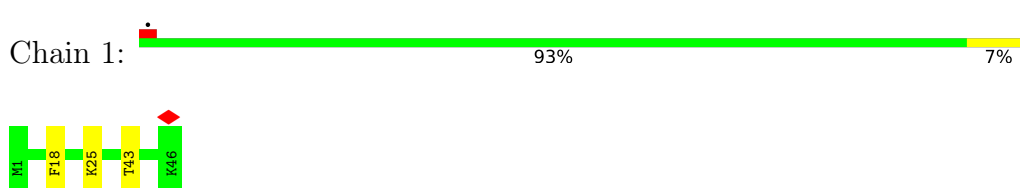
- Molecule 26: 50S ribosomal protein L32



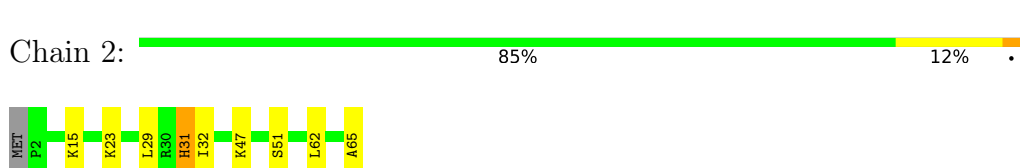
- Molecule 27: 50S ribosomal protein L33



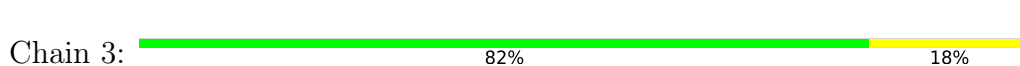
- Molecule 28: 50S ribosomal protein L34

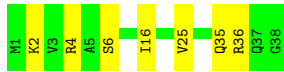


- Molecule 29: 50S ribosomal protein L35

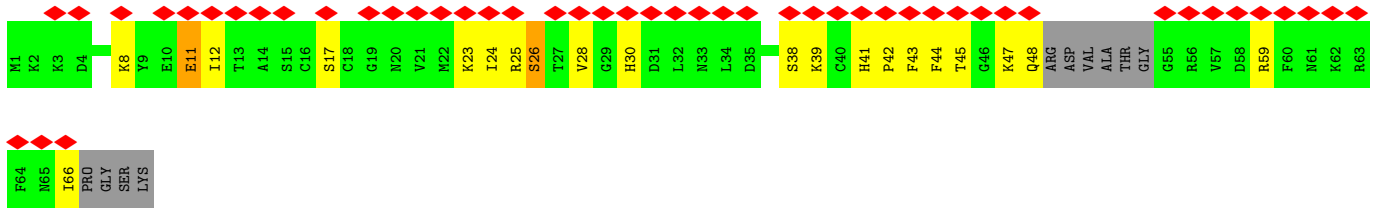


- Molecule 30: 50S ribosomal protein L36

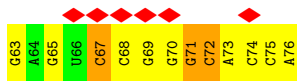
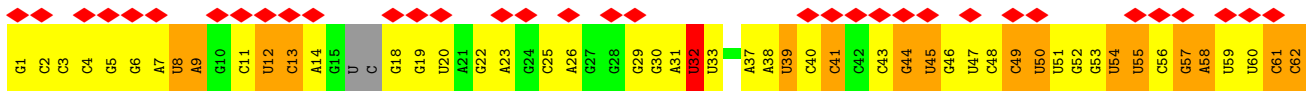
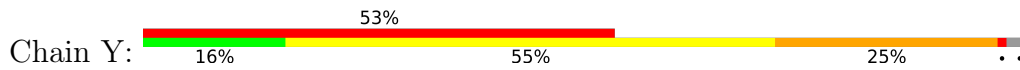




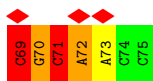
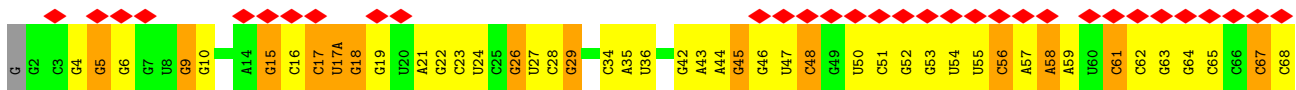
- Molecule 31: 50S ribosomal protein L31



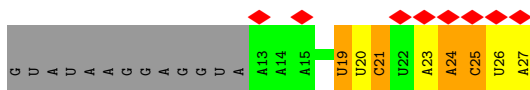
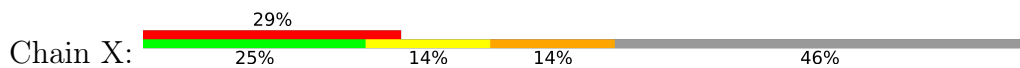
- Molecule 32: A-site tRNA Phe



- Molecule 33: P-site tRNA fMet



- Molecule 34: mRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	144049	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.238	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.0246	Depositor
Map size (\AA)	353.4, 353.4, 353.4	wwPDB
Map dimensions	496, 496, 496	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.7125, 0.7125, 0.7125	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MS6, OMG, 2MA, 4D4, OMC, 1MG, 8AN, 2MG, 3AB, SPD, MEQ, MG, PSU, 5MU, 6MZ, FME, G7M, H2U, SPM, 3TD, OMU, K, 5MC, ZN

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	0.68	2/65651 (0.0%)	0.95	52/102413 (0.1%)
2	b	0.57	0/2850	0.92	0/4444
3	c	0.34	0/2121	0.55	0/2852
4	d	0.35	0/1576	0.53	0/2119
5	e	0.33	0/1571	0.52	0/2113
6	f	0.33	0/1434	0.55	0/1926
7	g	0.34	0/1343	0.61	0/1816
8	h	0.32	0/306	0.69	0/413
9	i	0.34	0/1152	0.49	0/1551
10	j	0.37	0/955	0.58	0/1279
11	k	0.36	0/1062	0.57	0/1413
12	l	0.35	0/1073	0.54	0/1433
13	m	0.35	0/958	0.52	0/1281
14	n	0.33	0/902	0.52	0/1209
15	o	0.34	0/929	0.51	0/1242
16	p	0.36	0/960	0.52	1/1278 (0.1%)
17	q	0.38	0/829	0.58	0/1107
18	r	0.33	0/864	0.52	0/1156
19	s	0.33	0/744	0.50	0/994
20	t	0.35	0/787	0.55	0/1051
21	u	0.35	0/766	0.54	0/1025
22	v	0.36	0/593	0.50	0/785
23	w	0.39	1/635 (0.2%)	0.52	0/848
24	x	0.34	0/502	0.50	0/667
25	y	0.31	0/453	0.56	0/605
26	z	0.33	0/450	0.53	0/599
27	0	0.33	0/424	0.54	0/565
28	1	0.32	0/380	0.50	0/498
29	2	0.32	0/513	0.55	0/676
30	3	0.37	0/303	0.55	0/397
31	4	0.32	0/488	0.58	0/649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Y	3.78	15/1763 (0.9%)	2.15	44/2745 (1.6%)
33	Z	0.51	0/1788	1.14	5/2786 (0.2%)
34	X	0.63	2/354 (0.6%)	1.00	0/548
All	All	0.79	20/97479 (0.0%)	0.91	102/146483 (0.1%)

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
7	g	0	2
29	2	0	1
All	All	0	3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	Y	39	U	C1'-N1	147.25	3.69	1.48
32	Y	8	U	C4-O4	44.91	1.59	1.23
1	a	2605	PSU	O3'-P	-14.99	1.43	1.61
32	Y	55	U	N1-C2	12.04	1.49	1.38
32	Y	32	U	N1-C2	10.91	1.48	1.38

The worst 5 of 102 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Y	39	U	C6-N1-C1'	-72.71	19.41	121.20
32	Y	39	U	O4'-C1'-N1	-23.07	89.75	108.20
1	a	2453	A	P-O3'-C3'	15.93	138.81	119.70
1	a	2453	A	O3'-P-O5'	-14.89	75.72	104.00
32	Y	54	U	N1-C2-N3	13.34	122.90	114.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	2	31	HIS	Peptide
7	g	46	ALA	Peptide
7	g	47	ASP	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	59130	0	29767	0	0
2	b	2549	0	1291	0	0
3	c	2082	0	2154	0	0
4	d	1566	0	1618	0	0
5	e	1552	0	1619	0	0
6	f	1410	0	1444	0	0
7	g	1323	0	1371	0	0
8	h	303	0	327	0	0
9	i	1129	0	1162	0	0
10	j	946	0	1023	0	0
11	k	1053	0	1129	0	0
12	l	1075	0	1146	0	0
13	m	945	0	989	0	0
14	n	892	0	923	0	0
15	o	917	0	962	0	0
16	p	947	0	1019	0	0
17	q	816	0	839	0	0
18	r	857	0	922	0	0
19	s	738	0	807	0	0
20	t	779	0	831	0	0
21	u	753	0	780	0	0
22	v	586	0	596	0	0
23	w	625	0	652	0	0
24	x	501	0	531	0	0
25	y	449	0	488	0	0
26	z	444	0	458	0	0
27	0	417	0	451	4	0
28	1	377	0	418	1	0
29	2	504	0	572	3	0
30	3	302	0	340	2	0
31	4	480	0	478	14	0
32	Y	1578	0	800	39	0
33	Z	1601	0	813	31	0
34	X	317	0	161	5	0
35	Y	1	0	0	0	0
35	Z	1	0	0	0	0
35	a	211	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	b	5	0	0	0	0
35	c	2	0	0	0	0
35	d	1	0	0	0	0
35	m	1	0	0	0	0
35	z	1	0	0	0	0
36	a	170	0	322	0	0
37	a	14	0	26	0	0
38	a	5	0	0	0	0
38	c	1	0	0	0	0
38	e	1	0	0	0	0
39	a	10	0	10	0	0
40	3	1	0	0	0	0
40	4	1	0	0	0	0
41	Y	20	0	14	0	0
42	Z	22	0	12	0	0
43	1	17	0	0	0	0
43	2	24	0	0	0	0
43	3	3	0	0	0	0
43	Z	2	0	0	0	0
43	a	3013	0	0	0	0
43	b	40	0	0	0	0
43	c	86	0	0	0	0
43	d	33	0	0	0	0
43	e	27	0	0	0	0
43	h	1	0	0	0	0
43	i	12	0	0	0	0
43	j	12	0	0	0	0
43	k	32	0	0	0	0
43	l	20	0	0	0	0
43	m	20	0	0	0	0
43	o	10	0	0	0	0
43	p	19	0	0	0	0
43	q	14	0	0	0	0
43	r	24	0	0	0	0
43	s	5	0	0	0	0
43	t	1	0	0	0	0
43	u	3	0	0	0	0
43	v	12	0	0	0	0
43	w	9	0	0	0	0
43	x	1	0	0	0	0
43	y	1	0	0	0	0
43	z	21	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	93873	0	59265	99	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 8.

The worst 5 of 99 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)
32:Y:26:A:N6	32:Y:44:G:H1	1.49	1.10
33:Z:18:G:N2	33:Z:58:A:OP2	2.14	0.80
31:4:42:PRO:HB2	31:4:48:GLN:HG3	1.72	0.72
30:3:25:VAL:HB	30:3:35:GLN:HG2	1.72	0.71
32:Y:51:U:H3	32:Y:63:G:H22	1.37	0.71

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	c	269/273 (98%)	262 (97%)	7 (3%)	0	100	100
4	d	206/209 (99%)	199 (97%)	6 (3%)	1 (0%)	29	35
5	e	199/201 (99%)	196 (98%)	3 (2%)	0	100	100
6	f	175/179 (98%)	159 (91%)	16 (9%)	0	100	100
7	g	174/177 (98%)	154 (88%)	18 (10%)	2 (1%)	14	15
8	h	39/149 (26%)	32 (82%)	7 (18%)	0	100	100
9	i	140/142 (99%)	138 (99%)	2 (1%)	0	100	100
10	j	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
11	k	142/144 (99%)	137 (96%)	4 (3%)	1 (1%)	22	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
13	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
14	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
15	o	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
16	p	115/118 (98%)	115 (100%)	0	0	100	100
17	q	101/103 (98%)	96 (95%)	5 (5%)	0	100	100
18	r	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
19	s	91/100 (91%)	85 (93%)	6 (7%)	0	100	100
20	t	100/104 (96%)	95 (95%)	4 (4%)	1 (1%)	15	17
21	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
22	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
23	w	75/78 (96%)	73 (97%)	2 (3%)	0	100	100
24	x	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
25	y	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
26	z	54/57 (95%)	53 (98%)	1 (2%)	0	100	100
27	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
28	1	44/46 (96%)	44 (100%)	0	0	100	100
29	2	62/65 (95%)	59 (95%)	2 (3%)	1 (2%)	9	8
30	3	36/38 (95%)	36 (100%)	0	0	100	100
31	4	56/70 (80%)	49 (88%)	7 (12%)	0	100	100
All	All	3114/3337 (93%)	2981 (96%)	127 (4%)	6 (0%)	50	58

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	g	47	ASP
7	g	48	ASN
29	2	32	ILE
11	k	36	LYS
20	t	99	ASN

5.3.2 Protein sidechains [i](#)

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	216/218 (99%)	210 (97%)	6 (3%)	43	59
4	d	163/163 (100%)	160 (98%)	3 (2%)	59	74
5	e	165/165 (100%)	157 (95%)	8 (5%)	25	35
6	f	148/150 (99%)	130 (88%)	18 (12%)	5	5
7	g	137/138 (99%)	124 (90%)	13 (10%)	8	9
8	h	32/114 (28%)	26 (81%)	6 (19%)	1	1
9	i	116/116 (100%)	114 (98%)	2 (2%)	60	75
10	j	104/104 (100%)	101 (97%)	3 (3%)	42	57
11	k	103/103 (100%)	101 (98%)	2 (2%)	57	73
12	l	107/107 (100%)	103 (96%)	4 (4%)	34	47
13	m	98/103 (95%)	97 (99%)	1 (1%)	76	87
14	n	86/87 (99%)	79 (92%)	7 (8%)	11	14
15	o	99/100 (99%)	94 (95%)	5 (5%)	24	33
16	p	89/90 (99%)	87 (98%)	2 (2%)	52	68
17	q	84/84 (100%)	76 (90%)	8 (10%)	8	9
18	r	93/93 (100%)	90 (97%)	3 (3%)	39	53
19	s	80/84 (95%)	80 (100%)	0	100	100
20	t	83/85 (98%)	79 (95%)	4 (5%)	25	35
21	u	78/78 (100%)	74 (95%)	4 (5%)	24	33
22	v	58/63 (92%)	57 (98%)	1 (2%)	60	75
23	w	67/68 (98%)	63 (94%)	4 (6%)	19	26
24	x	54/55 (98%)	52 (96%)	2 (4%)	34	47
25	y	48/49 (98%)	45 (94%)	3 (6%)	18	24
26	z	47/48 (98%)	47 (100%)	0	100	100
27	0	46/49 (94%)	44 (96%)	2 (4%)	29	40
28	1	38/38 (100%)	37 (97%)	1 (3%)	46	62
29	2	51/52 (98%)	48 (94%)	3 (6%)	19	26
30	3	34/34 (100%)	30 (88%)	4 (12%)	5	5
31	4	55/62 (89%)	48 (87%)	7 (13%)	4	4

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2579/2700 (96%)	2453 (95%)	126 (5%)	29 34

5 of 126 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	j	109	SER
27	0	54	ILE
14	n	78	VAL
27	0	28	ARG
30	3	36	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
7	g	104	ASN
31	4	6	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	2745/2904 (94%)	354 (12%)	0
2	b	118/120 (98%)	23 (19%)	0
32	Y	71/76 (93%)	29 (40%)	2 (2%)
33	Z	74/76 (97%)	26 (35%)	0
34	X	14/28 (50%)	5 (35%)	1 (7%)
All	All	3022/3204 (94%)	437 (14%)	3 (0%)

5 of 437 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	A
1	a	12	U
1	a	13	A
1	a	34	U
1	a	42	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
32	Y	13	C

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Mol	Chain	Res	Type
32	Y	57	G
34	X	24	A

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

26 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	PSU	a	2604	1	18,21,22	1.37	3 (16%)	22,30,33	2.01	4 (18%)
1	3TD	a	1915	1	18,22,23	1.57	5 (27%)	22,32,35	2.08	3 (13%)
1	H2U	a	2449	1	18,21,22	1.17	2 (11%)	21,30,33	1.24	1 (4%)
1	OMU	a	2552	35,1	19,22,23	1.24	3 (15%)	26,31,34	1.70	5 (19%)
1	PSU	a	2580	1	18,21,22	1.45	4 (22%)	22,30,33	2.01	5 (22%)
1	PSU	a	1911	1	18,21,22	1.44	3 (16%)	22,30,33	1.96	4 (18%)
1	5MU	a	747	1	19,22,23	1.41	5 (26%)	28,32,35	2.17	9 (32%)
1	PSU	a	1917	1	18,21,22	1.39	3 (16%)	22,30,33	1.88	3 (13%)
1	OMC	a	2498	35,1	19,22,23	0.84	0	26,31,34	0.93	1 (3%)
1	PSU	a	2605	1	18,21,22	1.36	3 (16%)	22,30,33	1.91	3 (13%)
1	5MU	a	1939	1	19,22,23	1.41	5 (26%)	28,32,35	2.20	6 (21%)
1	OMG	a	2251	38,1,33	18,26,27	0.89	1 (5%)	19,38,41	1.09	2 (10%)
1	5MC	a	1962	1	18,22,23	0.97	2 (11%)	26,32,35	1.11	3 (11%)
1	G7M	a	2069	1	20,26,27	1.10	2 (10%)	17,39,42	0.76	0
1	6MZ	a	2030	1	18,25,26	0.82	1 (5%)	16,36,39	2.73	5 (31%)
1	2MA	a	2503	38,35,1	17,25,26	1.02	2 (11%)	17,37,40	1.01	2 (11%)
1	6MZ	a	1618	1	18,25,26	0.78	1 (5%)	16,36,39	2.37	4 (25%)
1	2MG	a	2445	1	18,26,27	1.05	1 (5%)	16,38,41	1.19	3 (18%)
1	PSU	a	746	35,1	18,21,22	1.39	2 (11%)	22,30,33	2.00	3 (13%)
12	4D4	l	81	12	9,11,12	1.99	2 (22%)	8,13,15	0.77	0
1	PSU	a	2504	38,1	18,21,22	1.47	3 (16%)	22,30,33	2.01	4 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	a	2457	1	18,21,22	1.38	3 (16%)	22,30,33	1.95	4 (18%)
4	MEQ	d	150	4	8,9,10	0.41	0	5,10,12	0.46	0
1	PSU	a	955	1	18,21,22	1.51	3 (16%)	22,30,33	1.87	4 (18%)
1	2MG	a	1835	1	18,26,27	0.96	1 (5%)	16,38,41	1.00	2 (12%)
1	1MG	a	745	1	18,26,27	0.70	0	19,39,42	1.14	3 (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
1	PSU	a	2604	1	-	0/7/25/26	0/2/2/2
1	3TD	a	1915	1	-	2/7/25/26	0/2/2/2
1	H2U	a	2449	1	-	1/7/38/39	0/2/2/2
1	OMU	a	2552	35,1	-	1/9/27/28	0/2/2/2
1	PSU	a	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	a	1911	1	-	2/7/25/26	0/2/2/2
1	5MU	a	747	1	-	0/7/25/26	0/2/2/2
1	PSU	a	1917	1	-	0/7/25/26	0/2/2/2
1	OMC	a	2498	35,1	-	1/9/27/28	0/2/2/2
1	PSU	a	2605	1	-	0/7/25/26	0/2/2/2
1	5MU	a	1939	1	-	0/7/25/26	0/2/2/2
1	OMG	a	2251	38,1,33	-	1/5/27/28	0/3/3/3
1	5MC	a	1962	1	-	2/7/25/26	0/2/2/2
1	G7M	a	2069	1	-	1/3/25/26	0/3/3/3
1	6MZ	a	2030	1	-	2/5/27/28	0/3/3/3
1	2MA	a	2503	38,35,1	-	2/3/25/26	0/3/3/3
1	6MZ	a	1618	1	-	0/5/27/28	0/3/3/3
1	2MG	a	2445	1	-	0/5/27/28	0/3/3/3
1	PSU	a	746	35,1	-	2/7/25/26	0/2/2/2
12	4D4	l	81	12	-	2/11/12/14	-
1	PSU	a	2504	38,1	-	2/7/25/26	0/2/2/2
1	PSU	a	2457	1	-	0/7/25/26	0/2/2/2
4	MEQ	d	150	4	-	2/8/9/11	-
1	PSU	a	955	1	-	0/7/25/26	0/2/2/2
1	2MG	a	1835	1	-	0/5/27/28	0/3/3/3
1	1MG	a	745	1	-	0/3/25/26	0/3/3/3

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	81	4D4	CZ-NE	4.48	1.42	1.33
1	a	955	PSU	C6-C5	3.56	1.39	1.35
1	a	2504	PSU	C6-C5	3.47	1.39	1.35
1	a	1911	PSU	C6-C5	3.40	1.39	1.35
1	a	2580	PSU	C4-N3	-3.14	1.33	1.38

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1915	3TD	N1-C2-N3	7.81	122.30	116.14
1	a	1618	6MZ	C2-N1-C6	7.03	122.62	116.59
1	a	2504	PSU	N1-C2-N3	6.73	122.76	115.13
1	a	2030	6MZ	C9-N6-C6	-6.65	117.14	122.87
1	a	2030	6MZ	C2-N1-C6	6.61	122.26	116.59

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	746	PSU	C2'-C1'-C5-C4
1	a	1911	PSU	O4'-C4'-C5'-O5'
1	a	2030	6MZ	O4'-C4'-C5'-O5'
1	a	2251	OMG	C1'-C2'-O2'-CM2
1	a	2498	OMC	C1'-C2'-O2'-CM2

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 254 ligands modelled in this entry, 232 are monoatomic - leaving 22 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
39	FME	a	6222	42	8,9,10	0.97	0	7,9,11	0.88	0
41	3AB	Y	101[A]	32	10,10,10	2.50	1 (10%)	13,13,13	0.82	0
41	3AB	Y	101[B]	32	10,10,10	2.45	1 (10%)	13,13,13	0.64	0
36	SPD	a	6207	-	9,9,9	0.17	0	8,8,8	0.18	0
36	SPD	a	6202	-	9,9,9	0.18	0	8,8,8	0.20	0
36	SPD	a	6217	-	9,9,9	0.15	0	8,8,8	0.19	0
36	SPD	a	6200	-	9,9,9	0.17	0	8,8,8	0.28	0
36	SPD	a	6201	-	9,9,9	0.16	0	8,8,8	0.26	0
36	SPD	a	6199	-	9,9,9	0.17	0	8,8,8	0.40	0
36	SPD	a	6211	-	9,9,9	0.17	0	8,8,8	0.28	0
36	SPD	a	6204	-	9,9,9	0.16	0	8,8,8	0.29	0
36	SPD	a	6216	-	9,9,9	0.16	0	8,8,8	0.19	0
37	SPM	a	6213	-	13,13,13	0.34	0	12,12,12	0.76	0
36	SPD	a	6210	-	9,9,9	0.18	0	8,8,8	0.16	0
36	SPD	a	6212	-	9,9,9	0.15	0	8,8,8	0.26	0
36	SPD	a	6203	-	9,9,9	0.18	0	8,8,8	0.31	0
36	SPD	a	6205	-	9,9,9	0.17	0	8,8,8	0.21	0
42	8AN	Z	101	39,35,33	19,24,25	0.90	1 (5%)	13,35,38	1.05	1 (7%)
36	SPD	a	6214	-	9,9,9	0.14	0	8,8,8	0.19	0
36	SPD	a	6208	-	9,9,9	0.14	0	8,8,8	0.22	0
36	SPD	a	6209	-	9,9,9	0.17	0	8,8,8	0.39	0
36	SPD	a	6206	-	9,9,9	0.16	0	8,8,8	0.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	FME	a	6222	42	-	2/7/9/11	-
41	3AB	Y	101[A]	32	-	0/4/4/4	0/1/1/1
41	3AB	Y	101[B]	32	-	0/4/4/4	0/1/1/1
36	SPD	a	6207	-	-	2/7/7/7	-
36	SPD	a	6202	-	-	0/7/7/7	-
36	SPD	a	6217	-	-	6/7/7/7	-
36	SPD	a	6200	-	-	1/7/7/7	-
36	SPD	a	6201	-	-	1/7/7/7	-
36	SPD	a	6199	-	-	1/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	SPD	a	6211	-	-	0/7/7/7	-
36	SPD	a	6204	-	-	2/7/7/7	-
36	SPD	a	6216	-	-	5/7/7/7	-
37	SPM	a	6213	-	-	5/11/11/11	-
36	SPD	a	6210	-	-	0/7/7/7	-
36	SPD	a	6212	-	-	1/7/7/7	-
36	SPD	a	6203	-	-	2/7/7/7	-
36	SPD	a	6205	-	-	0/7/7/7	-
42	8AN	Z	101	39,35,33	-	1/3/25/26	0/3/3/3
36	SPD	a	6214	-	-	6/7/7/7	-
36	SPD	a	6208	-	-	0/7/7/7	-
36	SPD	a	6209	-	-	0/7/7/7	-
36	SPD	a	6206	-	-	0/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
41	Y	101[A]	3AB	C1-C1'	-7.73	1.38	1.50
41	Y	101[B]	3AB	C1-C1'	-7.56	1.39	1.50
42	Z	101	8AN	C3'-N3'	-2.49	1.43	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	Z	101	8AN	C5-C6-N6	2.47	124.10	120.35

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

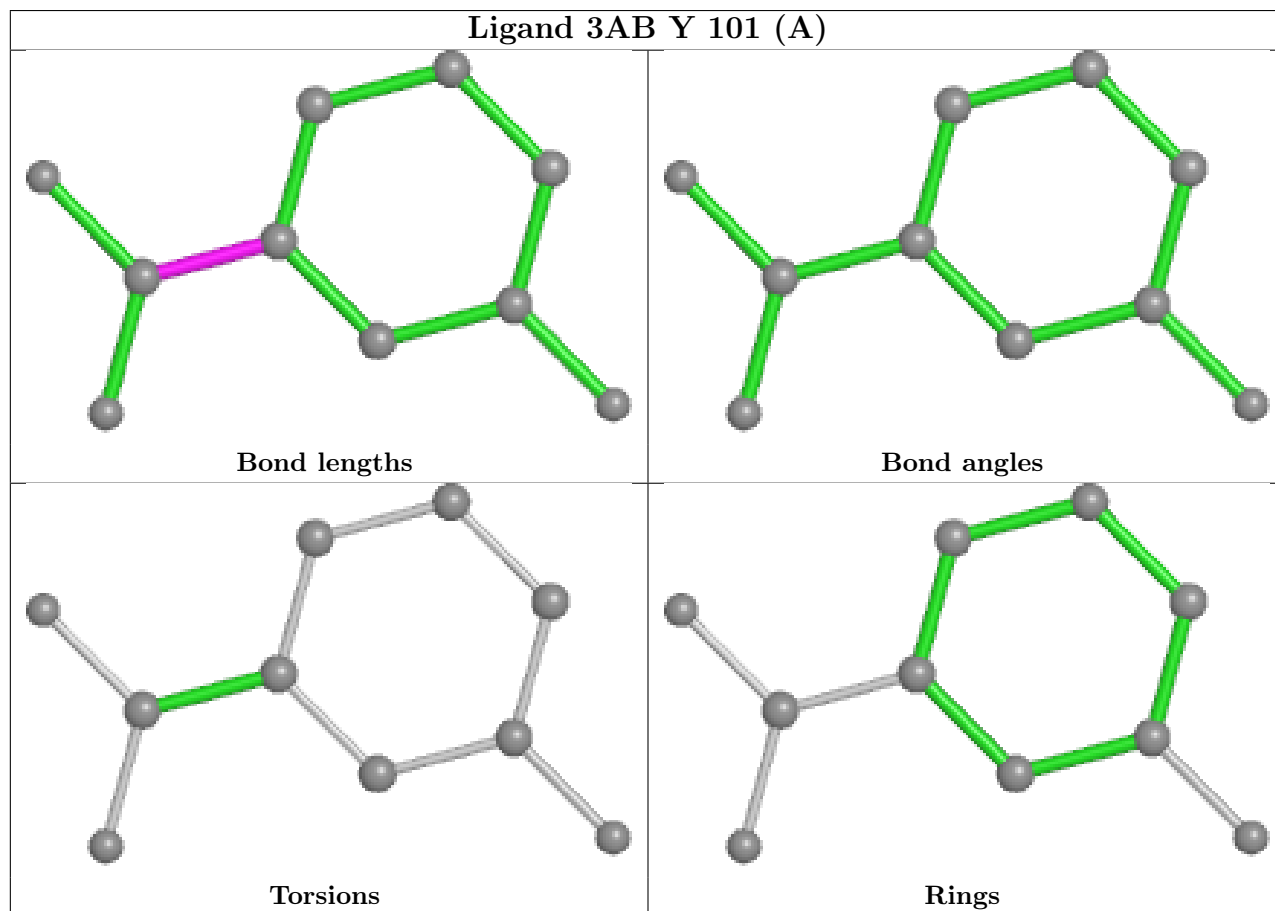
Mol	Chain	Res	Type	Atoms
36	a	6216	SPD	C4-C5-N6-C7
36	a	6217	SPD	C4-C5-N6-C7
39	a	6222	FME	N-CA-CB-CG
39	a	6222	FME	C-CA-CB-CG
42	Z	101	8AN	C4'-C5'-O5'-P

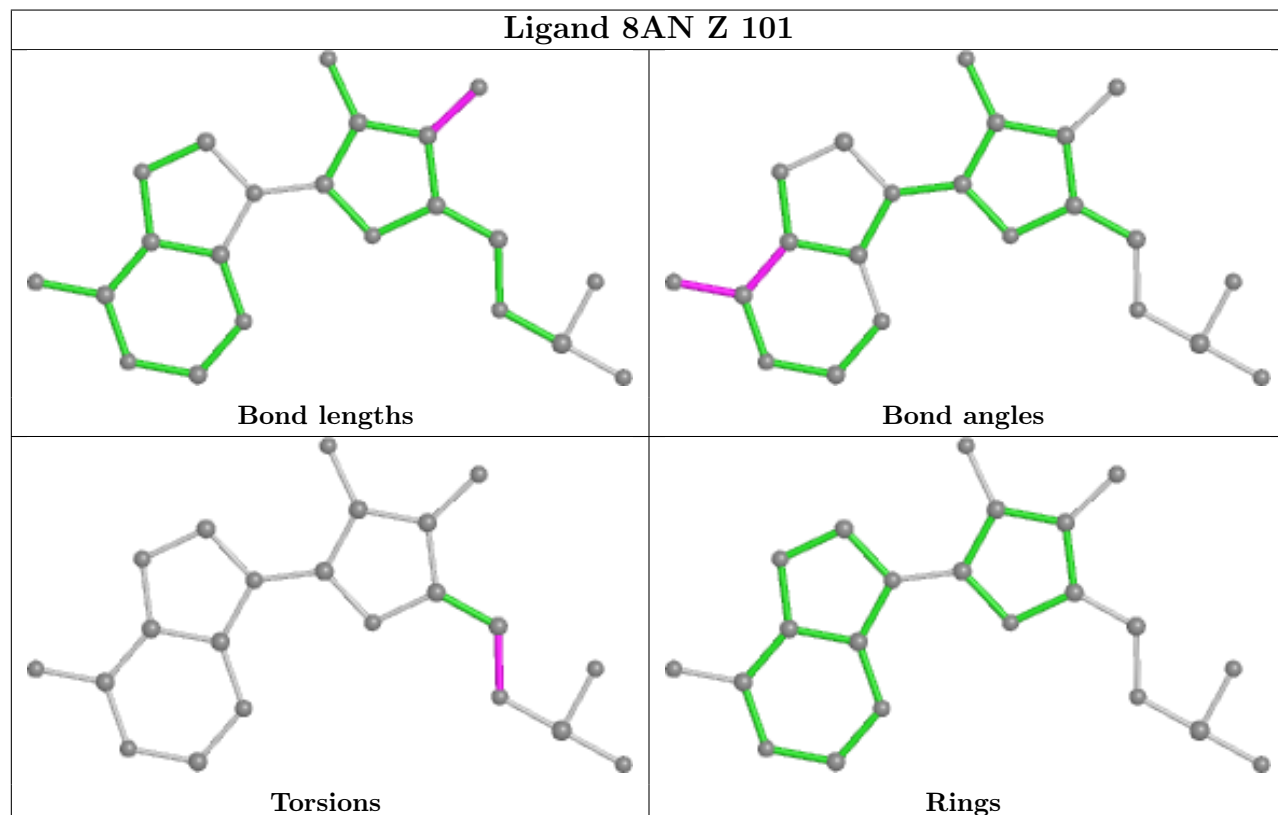
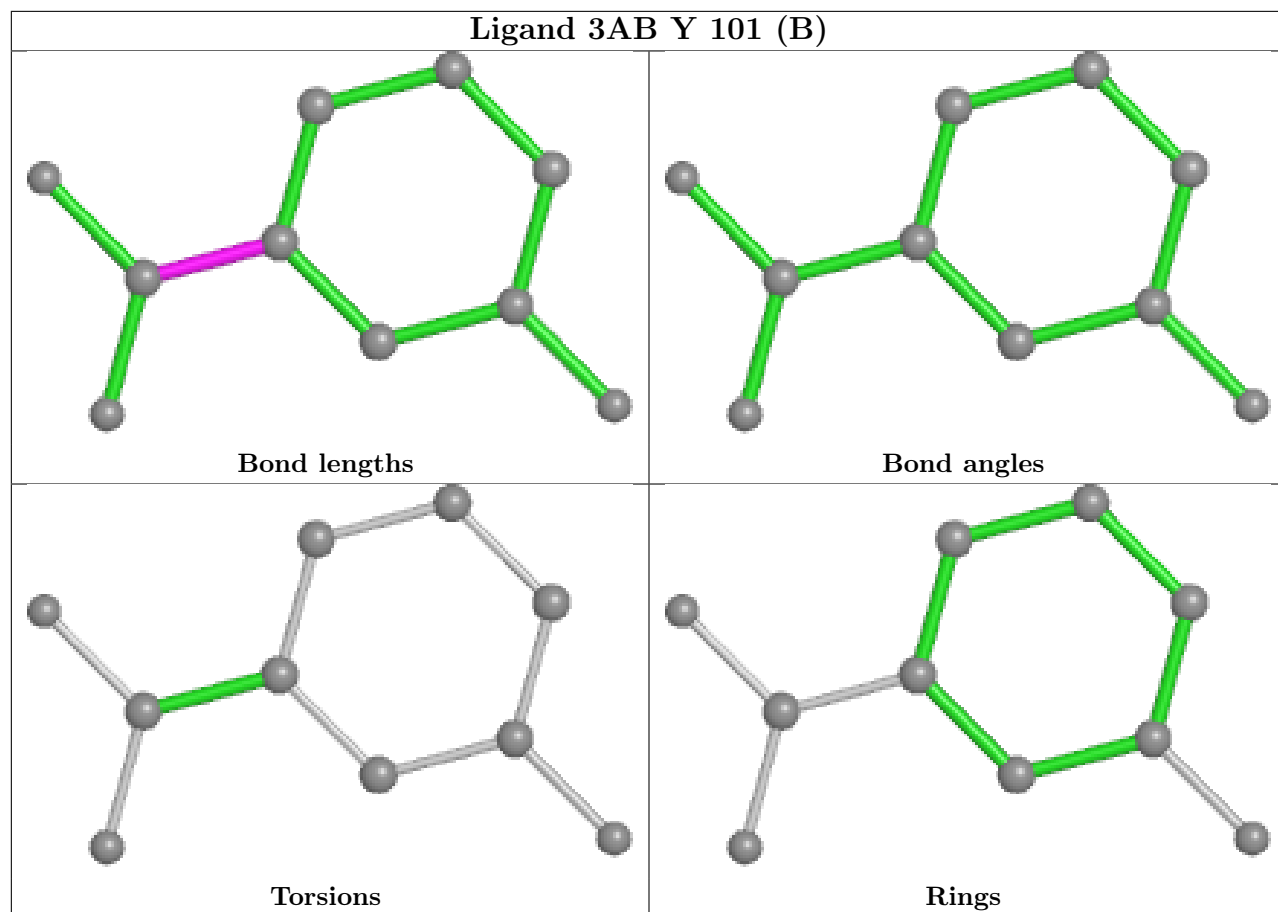
There are no ring outliers.

No monomer is involved in short contacts.

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

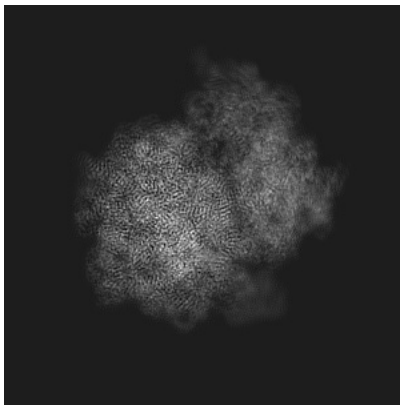
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29787. These allow visual inspection of the internal detail of the map and identification of artifacts.

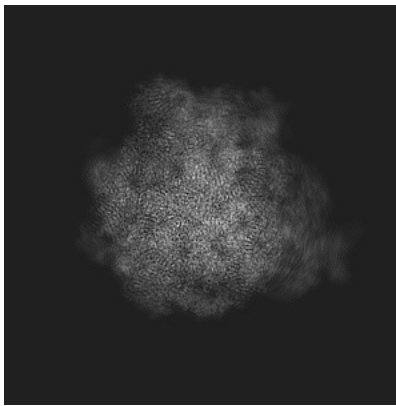
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

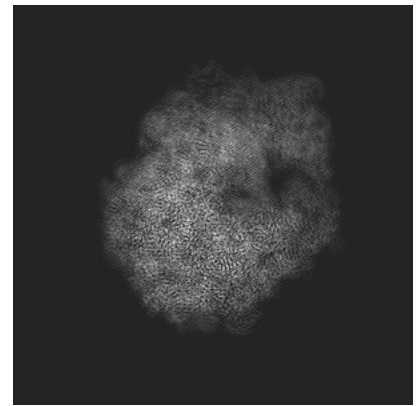
6.1.1 Primary map



X

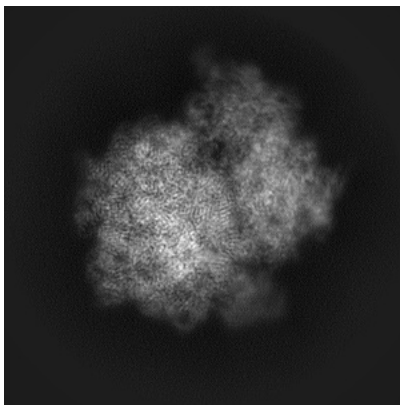


Y

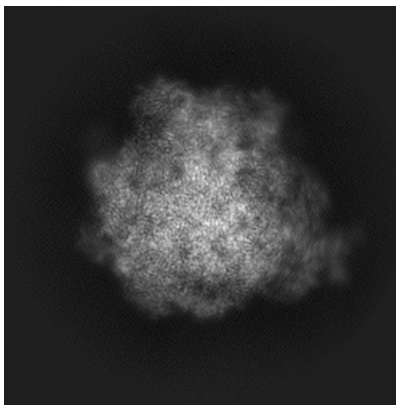


Z

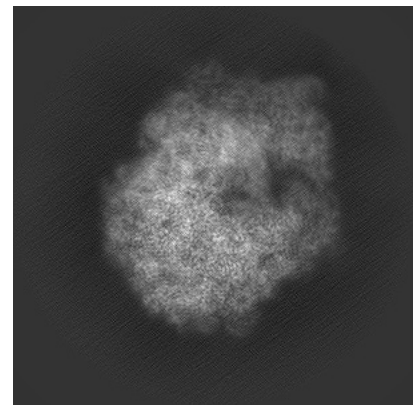
6.1.2 Raw map



X



Y

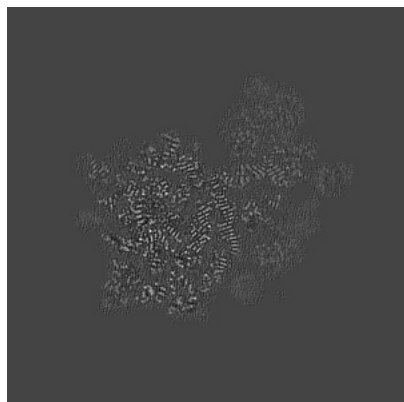


Z

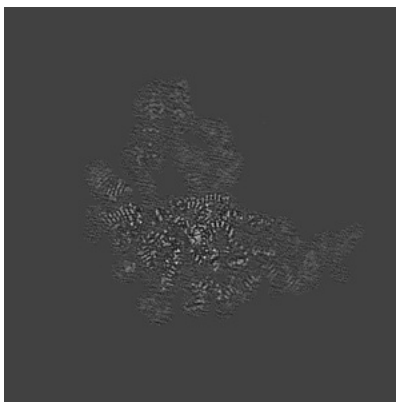
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

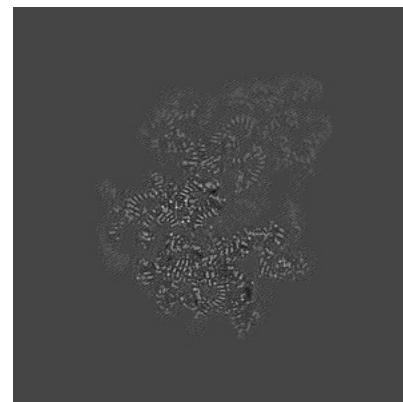
6.2.1 Primary map



X Index: 248

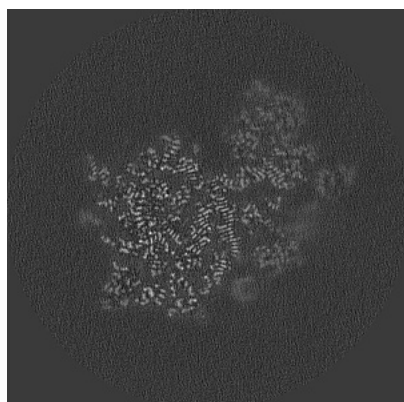


Y Index: 248

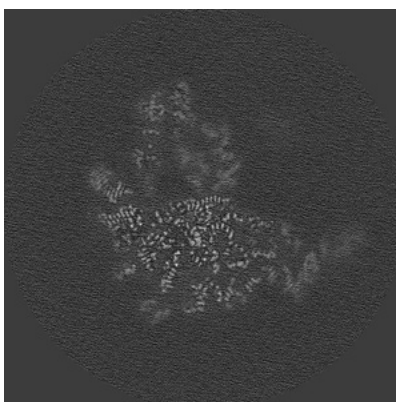


Z Index: 248

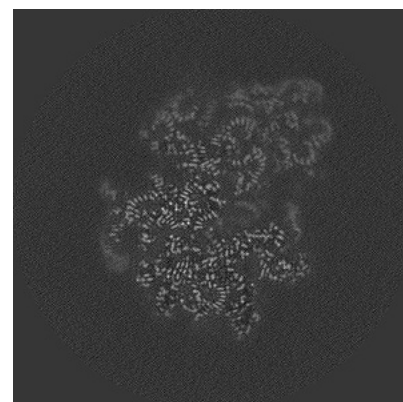
6.2.2 Raw map



X Index: 248



Y Index: 248

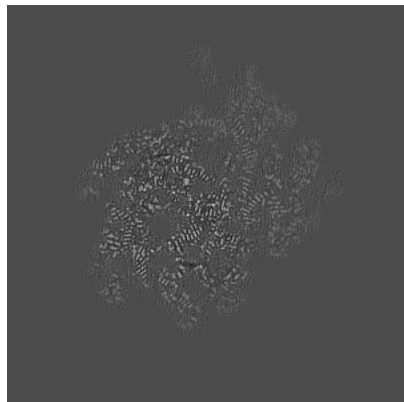


Z Index: 248

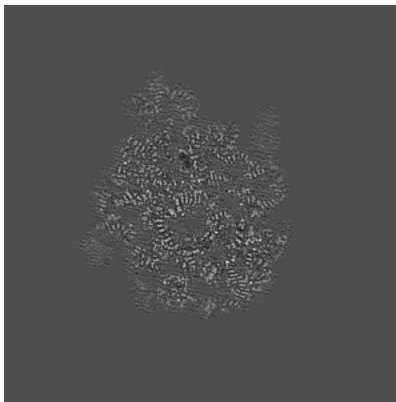
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

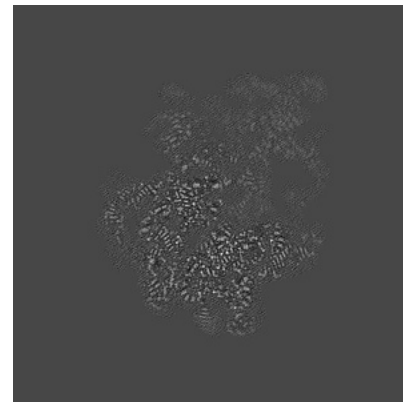
6.3.1 Primary map



X Index: 214

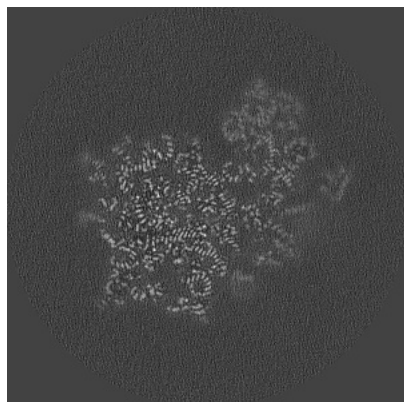


Y Index: 207

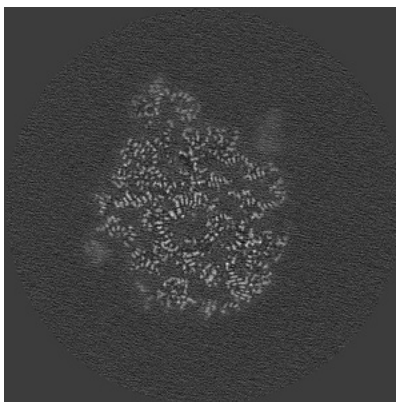


Z Index: 236

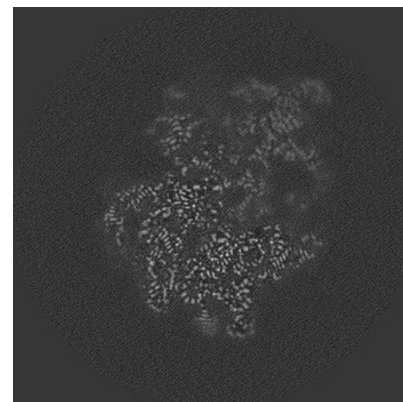
6.3.2 Raw map



X Index: 242



Y Index: 207

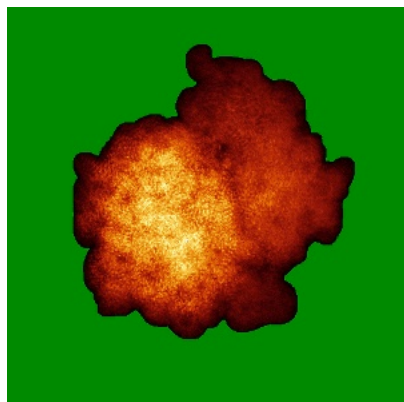


Z Index: 236

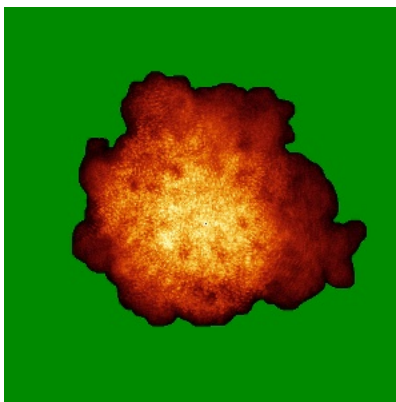
The images above show the largest variance slices of the map in three orthogonal directions.

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

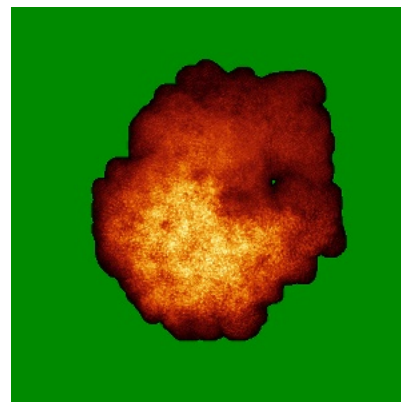
6.4.1 Primary map



X

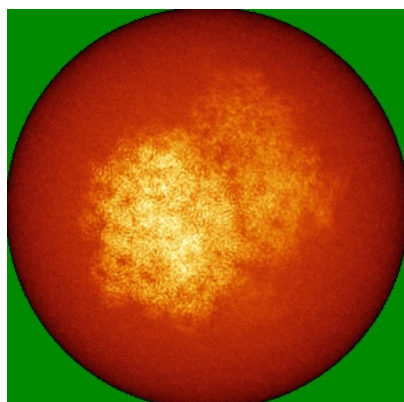


Y

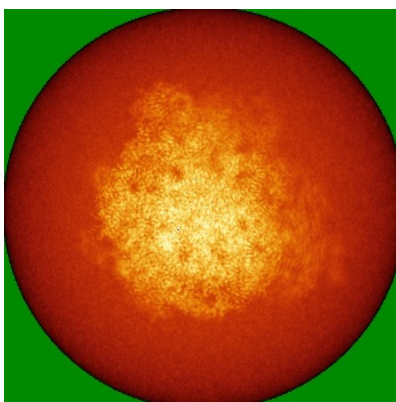


Z

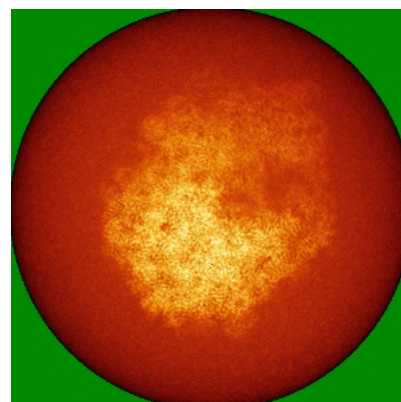
6.4.2 Raw map



X



Y

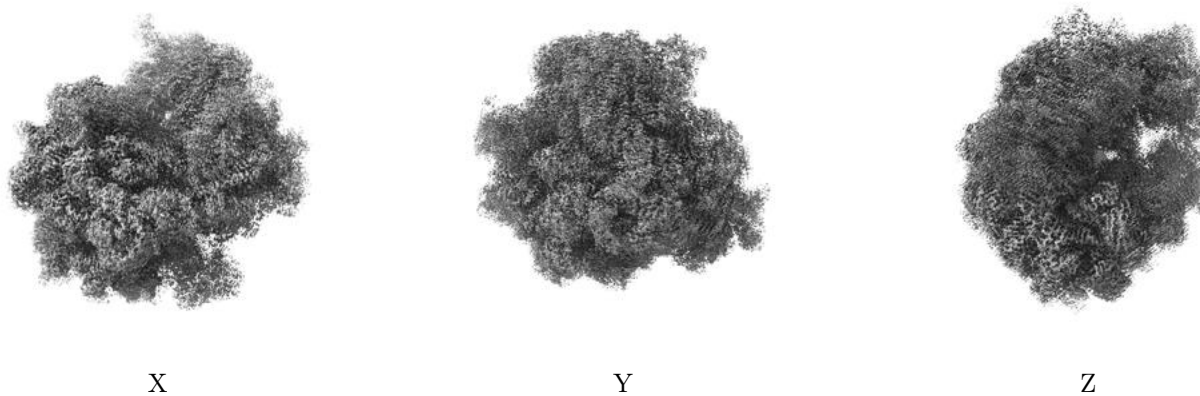


Z

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

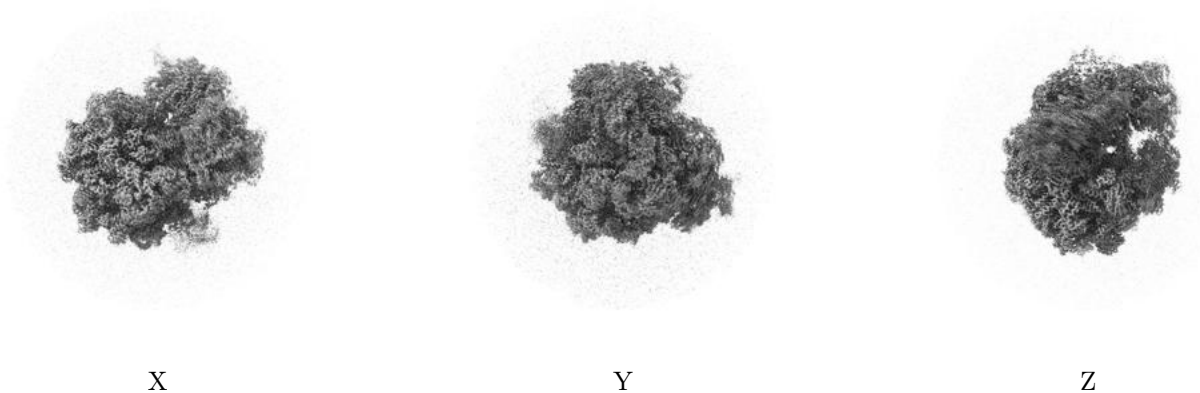
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0246. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

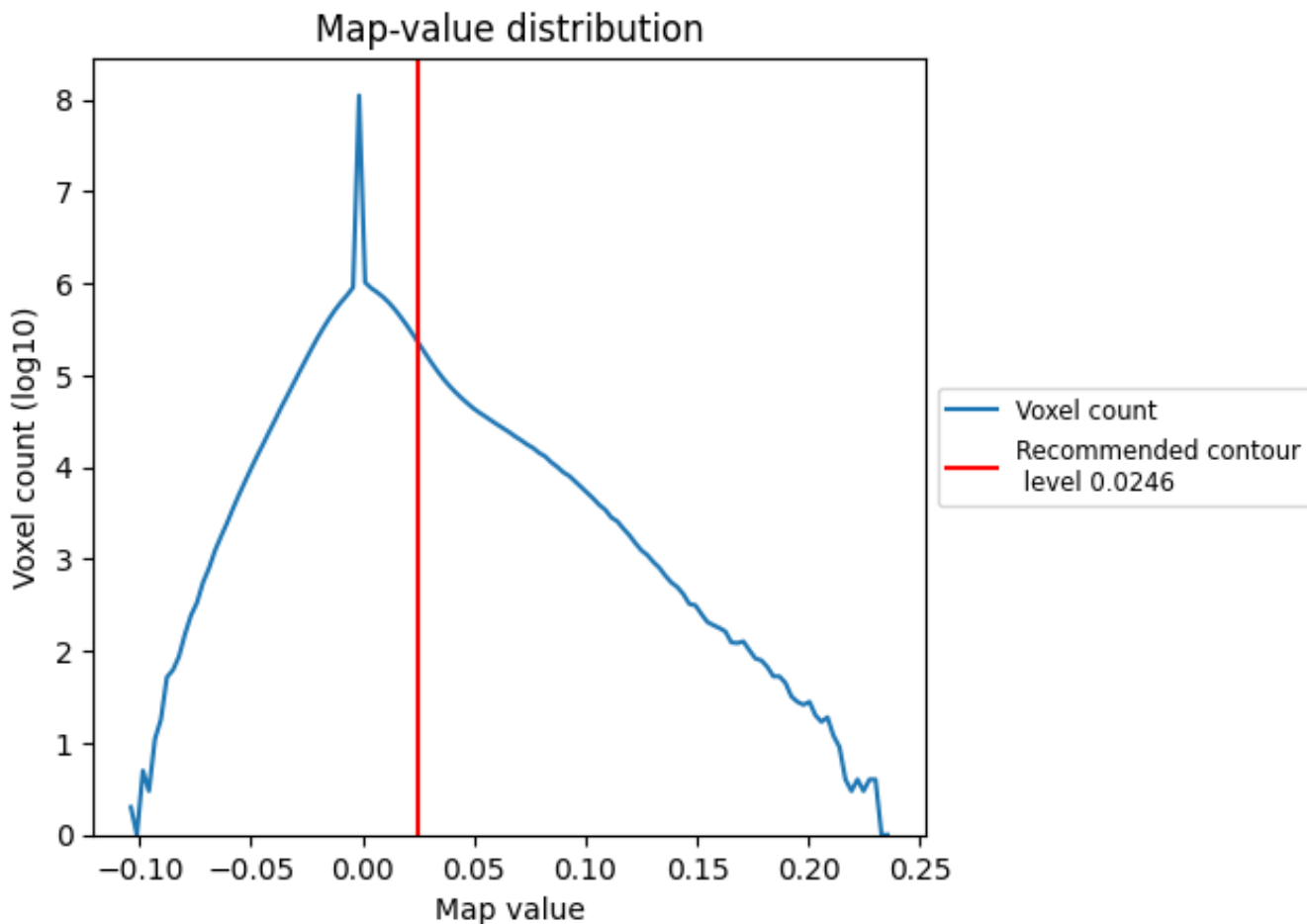
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

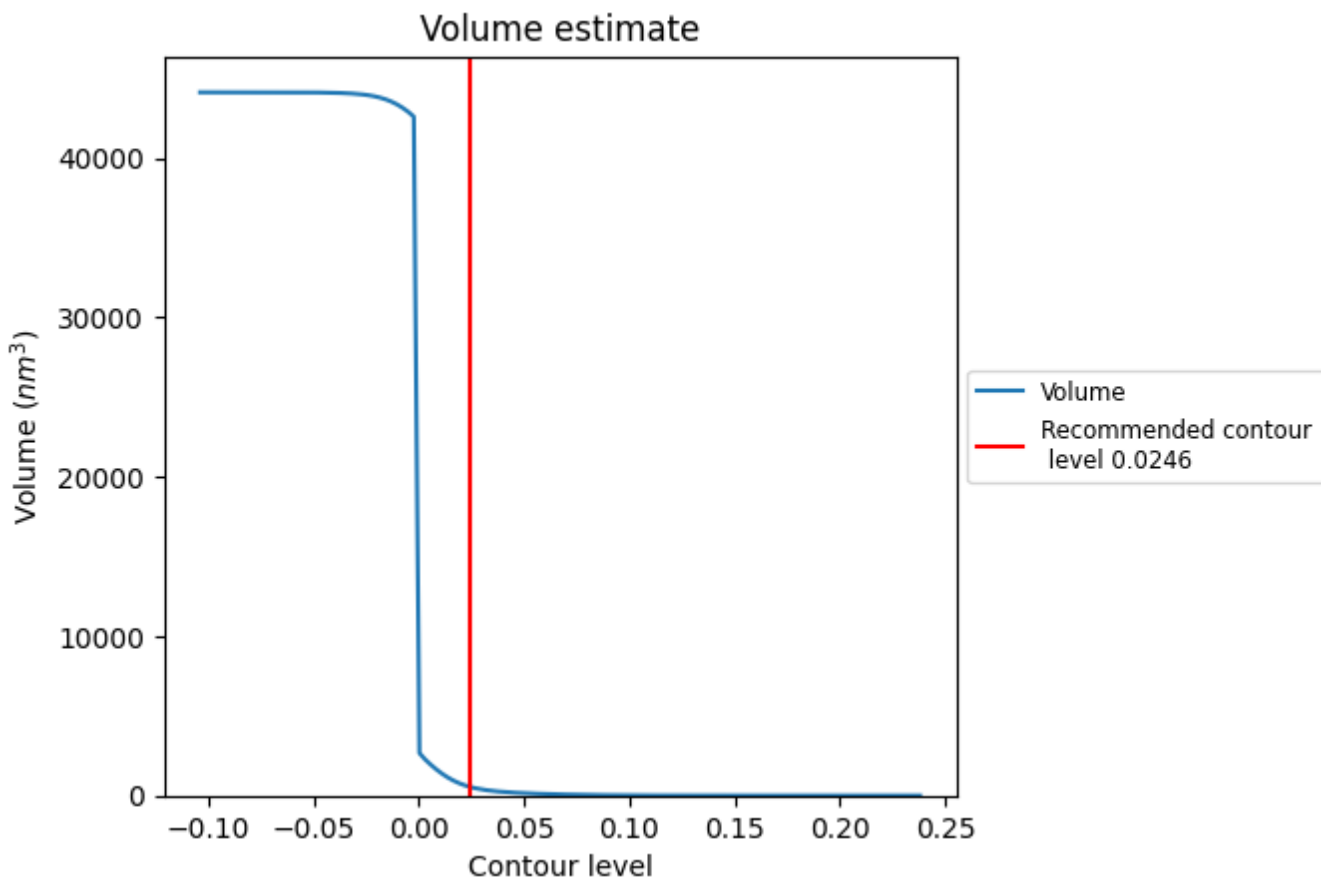
This section contains the results of statistical analysis of the map.

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.

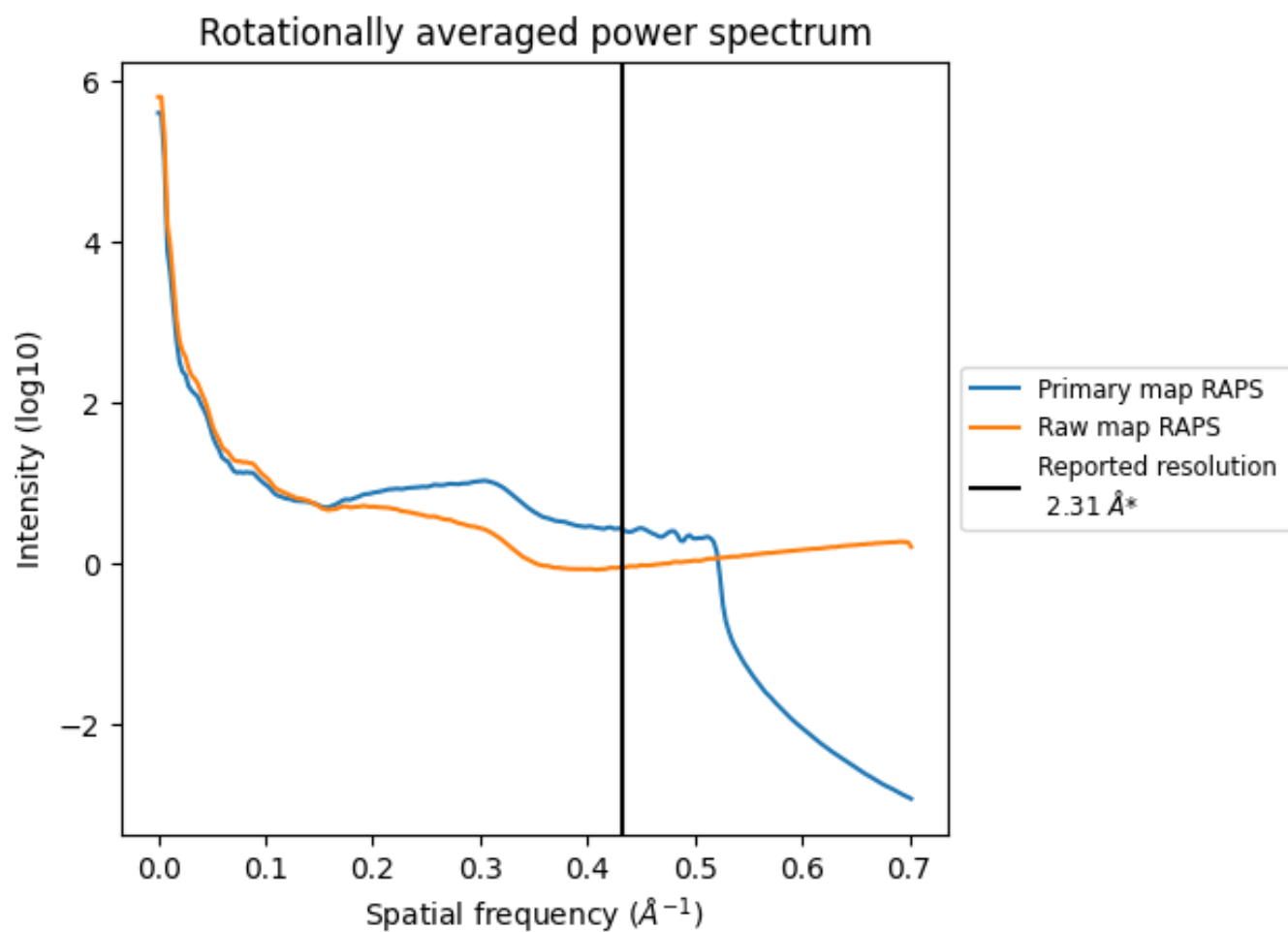
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 537 nm^3 ; this corresponds to an approximate mass of 485 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 i

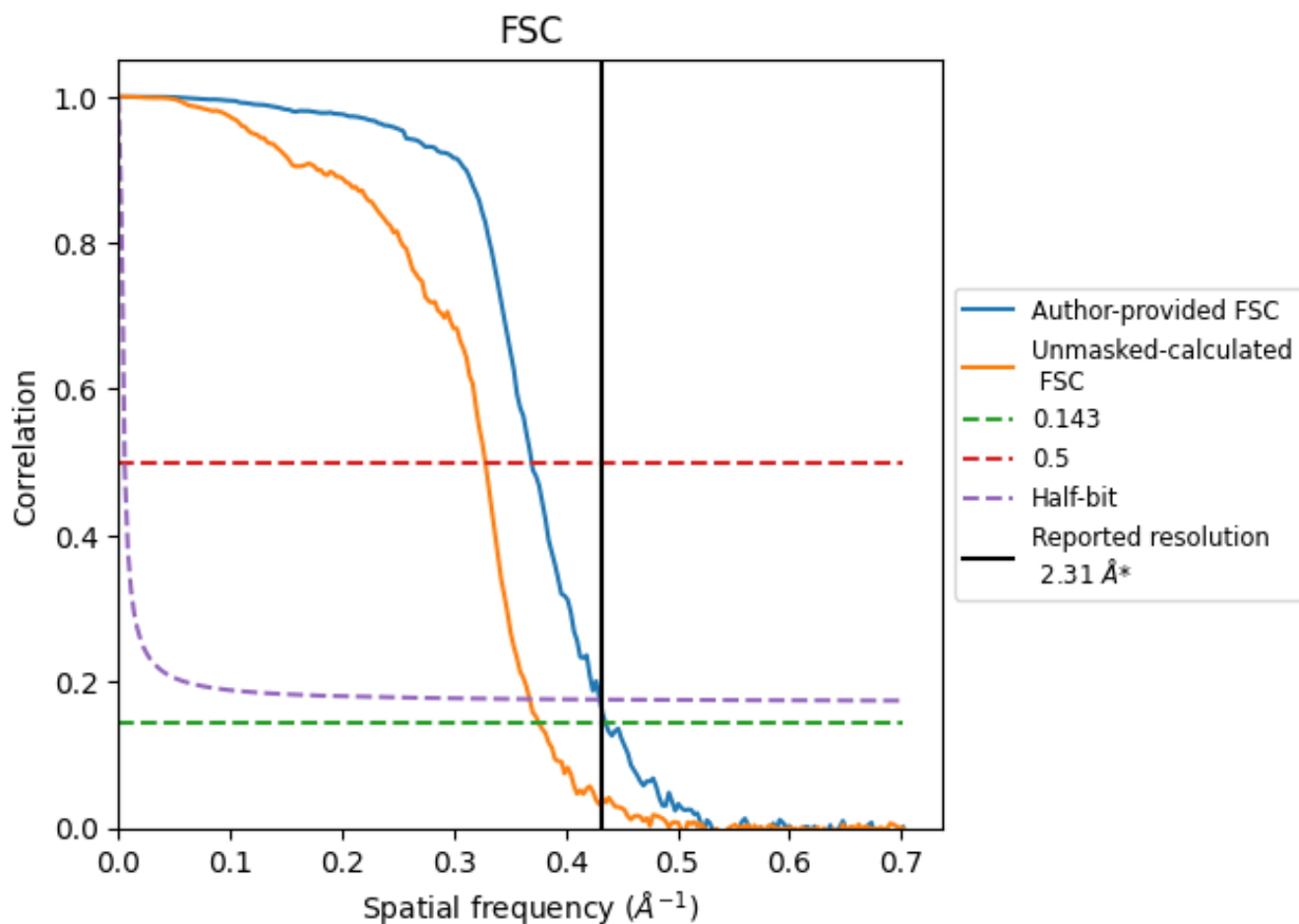


*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.433 Å⁻¹

8.2 Resolution estimates [i](#)

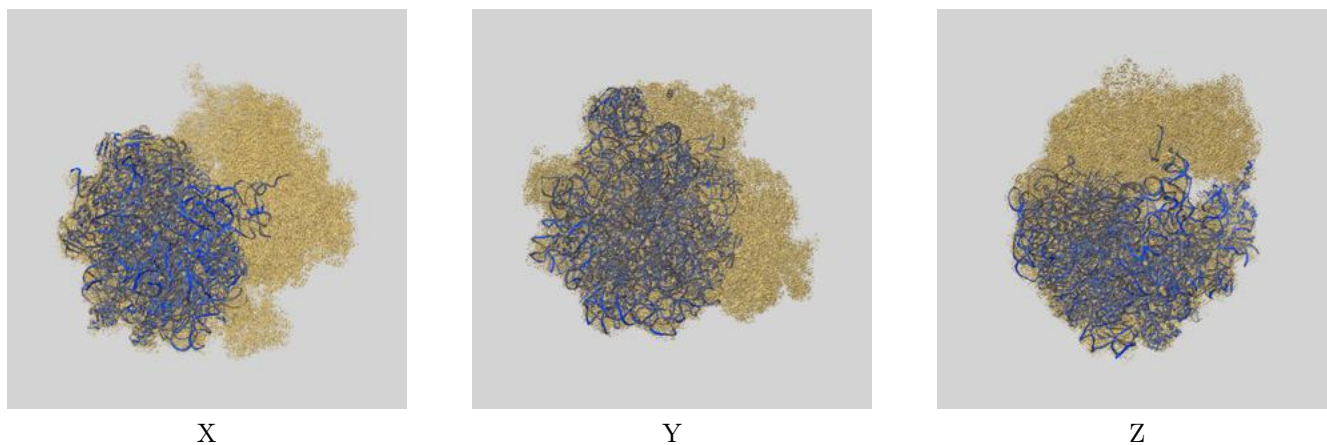
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.31	-	-
Author-provided FSC curve	2.30	2.71	2.32
Unmasked-calculated*	2.66	3.05	2.72

*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 2.66 differs from the reported value 2.31 by more than 10 %

9 Map-model fit [i](#)

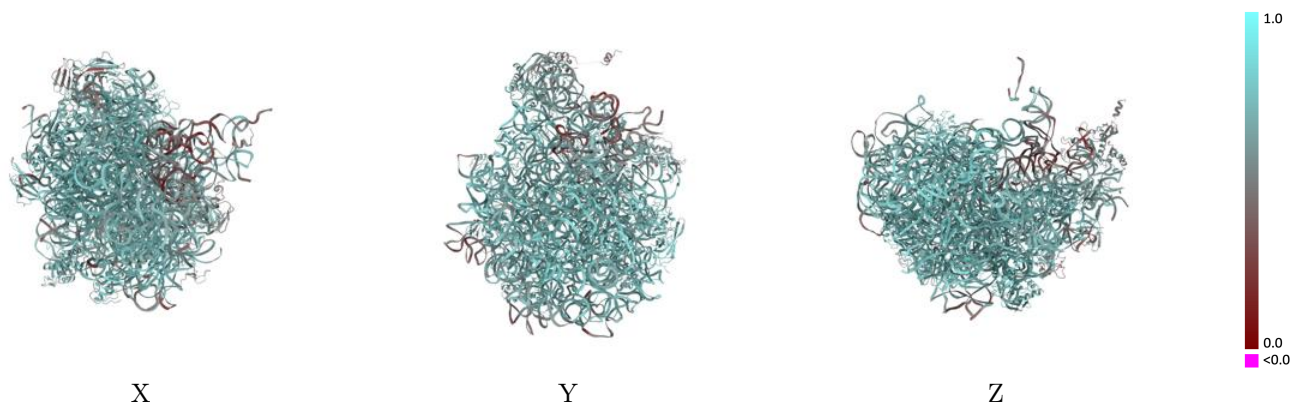
This section contains information regarding the fit between EMDB map EMD-29787 and PDB model 8G6X. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



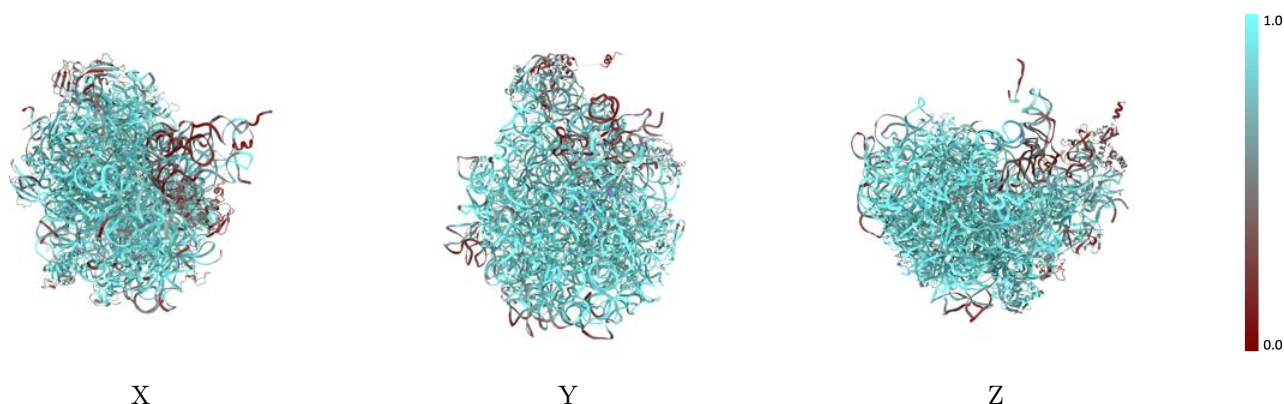
The images above show the 3D surface view of the map at the recommended contour level 0.0246 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



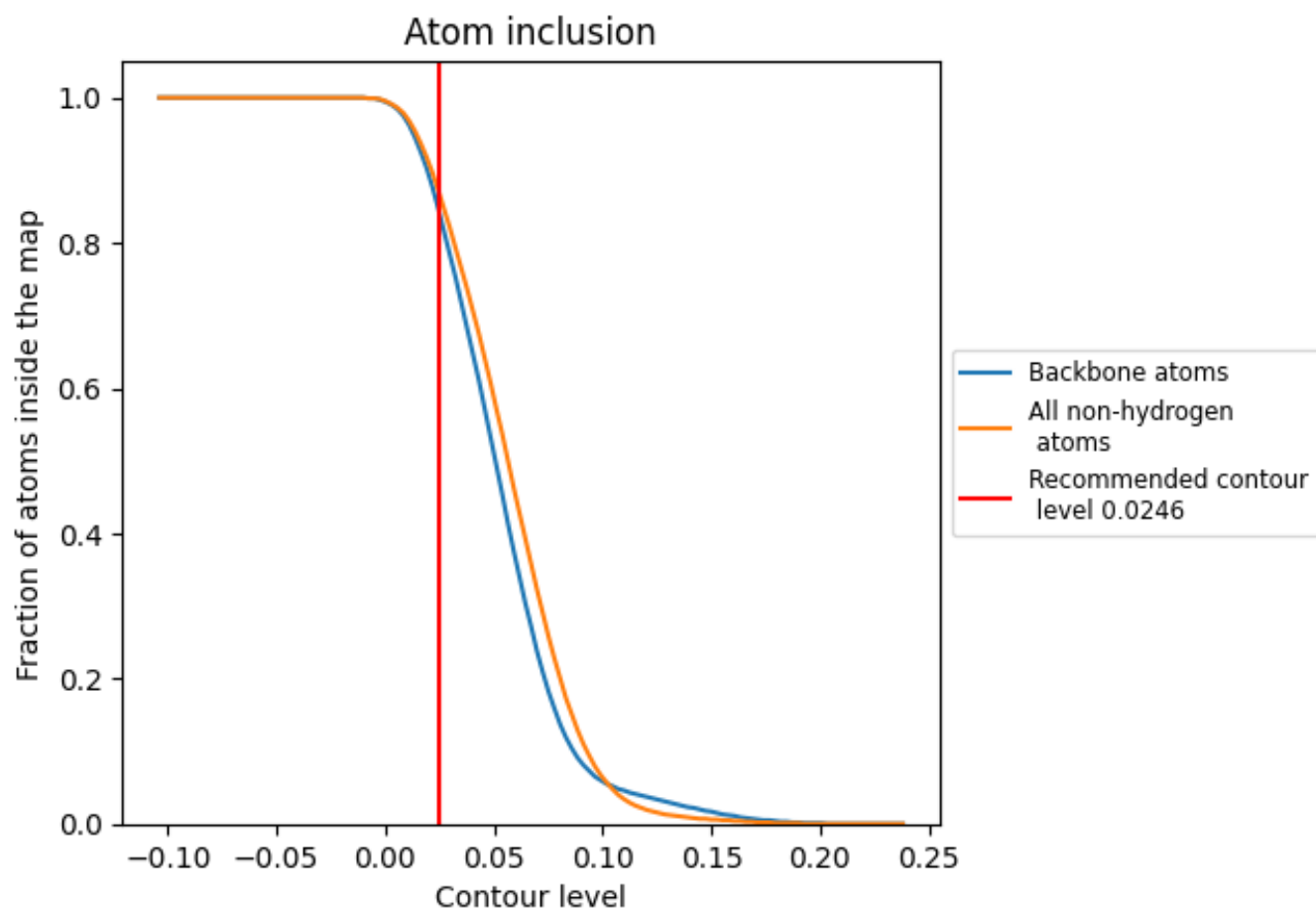
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0246).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 87% 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 (0.0246) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8710	 0.6930
0	 0.8750	 0.7110
1	 0.9610	 0.7710
2	 0.9630	 0.7710
3	 0.9110	 0.7190
4	 0.2460	 0.4640
X	 0.4610	 0.4910
Y	 0.4240	 0.4320
Z	 0.4760	 0.4560
a	 0.9150	 0.7070
b	 0.8240	 0.6450
c	 0.9460	 0.7560
d	 0.9300	 0.7460
e	 0.8350	 0.7050
f	 0.4600	 0.5490
g	 0.5200	 0.5570
h	 0.5600	 0.5970
i	 0.9250	 0.7350
j	 0.9120	 0.7450
k	 0.9060	 0.7310
l	 0.9260	 0.7400
m	 0.9750	 0.7620
n	 0.7600	 0.6570
o	 0.8720	 0.7260
p	 0.9420	 0.7520
q	 0.8420	 0.7010
r	 0.9150	 0.7360
s	 0.8350	 0.6920
t	 0.7520	 0.6550
u	 0.7720	 0.6710
v	 0.9390	 0.7440
w	 0.9070	 0.7350
x	 0.7380	 0.6570
y	 0.8900	 0.7070
z	 0.9040	 0.7260

