



## Full wwPDB EM Validation Report ⓘ

Jun 18, 2026 – 09:28 am BST

PDB ID : 9TEZ / pdb\_00009tez  
EMDB ID : EMD-55849  
Title : DalDroS bound to the Escherichia coli 50S ribosomal subunit  
Authors : Berger, M.J.; Safdari, H.A.; Wilson, D.N.  
Deposited on : 2025-11-26  
Resolution : 2.88 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](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:

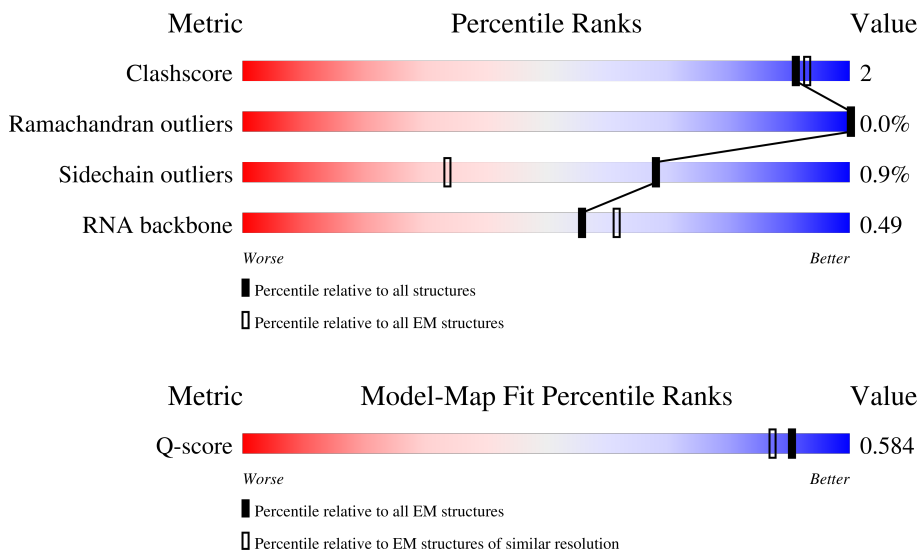
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 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 2.88 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12111 ( 2.38 - 3.38 )

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	3	38	100%
2	d	209	96% (with 70% upper red bar)
3	4	70	84% (with 16% grey segment)

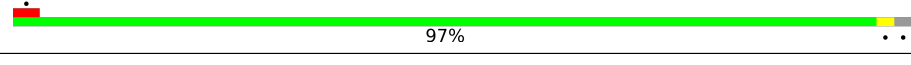
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Mol	Chain	Length	Quality of chain
4	V	2904	69% 22% 5%
5	8	20	65% 10% 25%
6	0	55	89% 7%
7	1	46	91% 9%
8	2	65	89% 8%
9	W	360	14% 69% 29%
10	b	120	88% 10%
11	c	273	90% 7%
12	e	201	98%
13	f	179	18% 98%
14	g	177	28% 96%
15	h	149	6% 28% 72%
16	i	142	93% 7%
17	j	123	95% 5%
18	k	144	95% 5%
19	m	127	86% 6% 7%
20	n	117	97%
21	o	115	95%
22	p	118	92% 8%
23	q	103	5% 95% 5%
24	r	110	97%
25	s	100	93% 7%
26	t	104	94%
27	u	94	91% 9%
28	v	85	80% 11% 9%

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Mol	Chain	Length	Quality of chain
29	w	78	 90% 9%
30	x	63	 90% 8%
31	y	59	 97%
32	z	57	 86% 11%
33	l	136	 94%
34	Z	76	 70% 25%

## 2 Entry composition [i](#)

There are 37 unique types of molecules in this entry. The entry contains 90140 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 Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	3	38	302	185	65	48	4	0	0

- Molecule 2 is a protein called Large ribosomal subunit protein uL3.

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

- Molecule 3 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	4	59	472	294	89	84	5	0	0

- Molecule 4 is a RNA chain called 23S rRNA.

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

- Molecule 5 is a protein called DalDroS.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	8	15	124	79	26	19	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	0	51	417	269	76	72	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	1	46	377	228	90	57	2	0	0

- Molecule 8 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	2	64	504	323	105	74	2	0	0

- Molecule 9 is a protein called Peptide chain release factor RF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	W	254	1977	1207	376	386	8	0	0

- Molecule 10 is a RNA chain called 5S rRNA.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	c	270	2076	1285	422	362	7	0	0

- Molecule 12 is a protein called Large ribosomal subunit protein uL4.

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

- Molecule 13 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 14 is a protein called Large ribosomal subunit protein uL6.

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

- Molecule 15 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 16 is a protein called Large ribosomal subunit protein uL13.

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

- Molecule 17 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 18 is a protein called 50S ribosomal protein L15.

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

- Molecule 19 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 20 is a protein called Large ribosomal subunit protein uL18.

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

- Molecule 21 is a protein called Large ribosomal subunit protein bL19.

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

- Molecule 22 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 23 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 25 is a protein called Large ribosomal subunit protein uL23.

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

- Molecule 26 is a protein called Large ribosomal subunit protein uL24.

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

- Molecule 27 is a protein called 50S ribosomal protein L25.

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

- Molecule 28 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	v	77	Total	C	N	O	S	0	0
			582	360	115	106	1		

- Molecule 29 is a protein called Large ribosomal subunit protein bL28.

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

- Molecule 30 is a protein called Large ribosomal subunit protein uL29.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 32 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 33 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	l	134	Total	C	N	O	S	0	0
			1055	675	200	175	5		

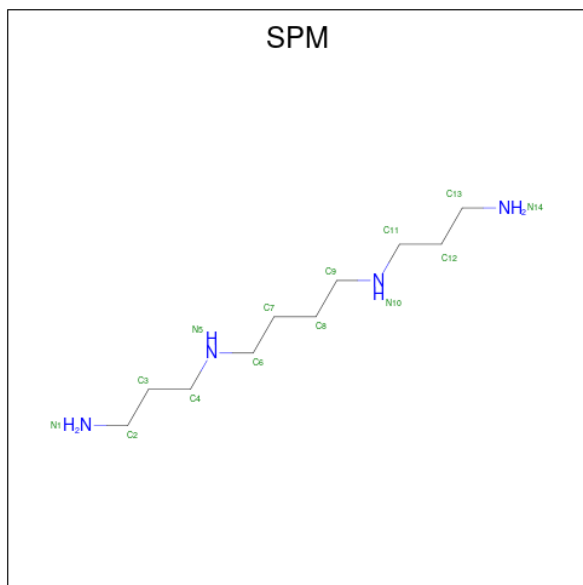
- Molecule 34 is a RNA chain called P-site Phe-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	76	Total	C	N	O	P	0	0
			1623	723	290	534	76		

- Molecule 35 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
35	3	1	Total	Zn	0
			1	1	
35	4	1	Total	Zn	0
			1	1	

- Molecule 36 is SPERMINE (CCD ID: SPM) (formula:  $C_{10}H_{26}N_4$ ).



Mol	Chain	Residues	Atoms			AltConf
36	V	1	Total	C	N	0
			14	10	4	

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	V	1	Total	Mg	0
			1	1	

### 3 Residue-property plots [i](#)

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

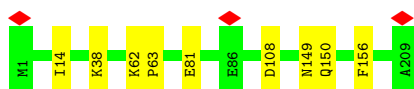
- Molecule 1: Large ribosomal subunit protein bL36A

Chain 3:  100%

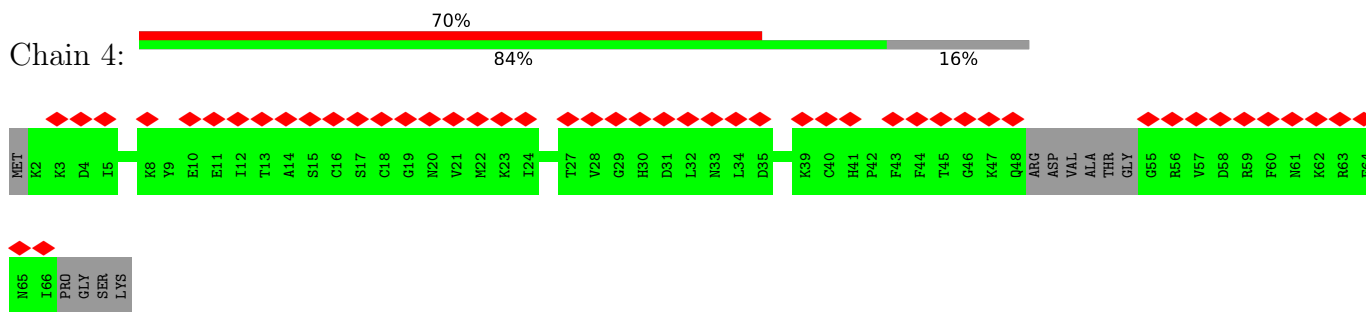
There are no outlier residues recorded for this chain.

- Molecule 2: Large ribosomal subunit protein uL3

Chain d:  96%

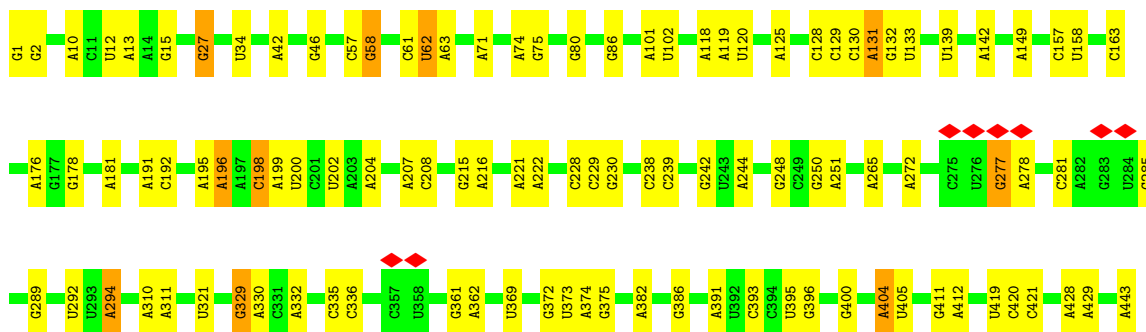


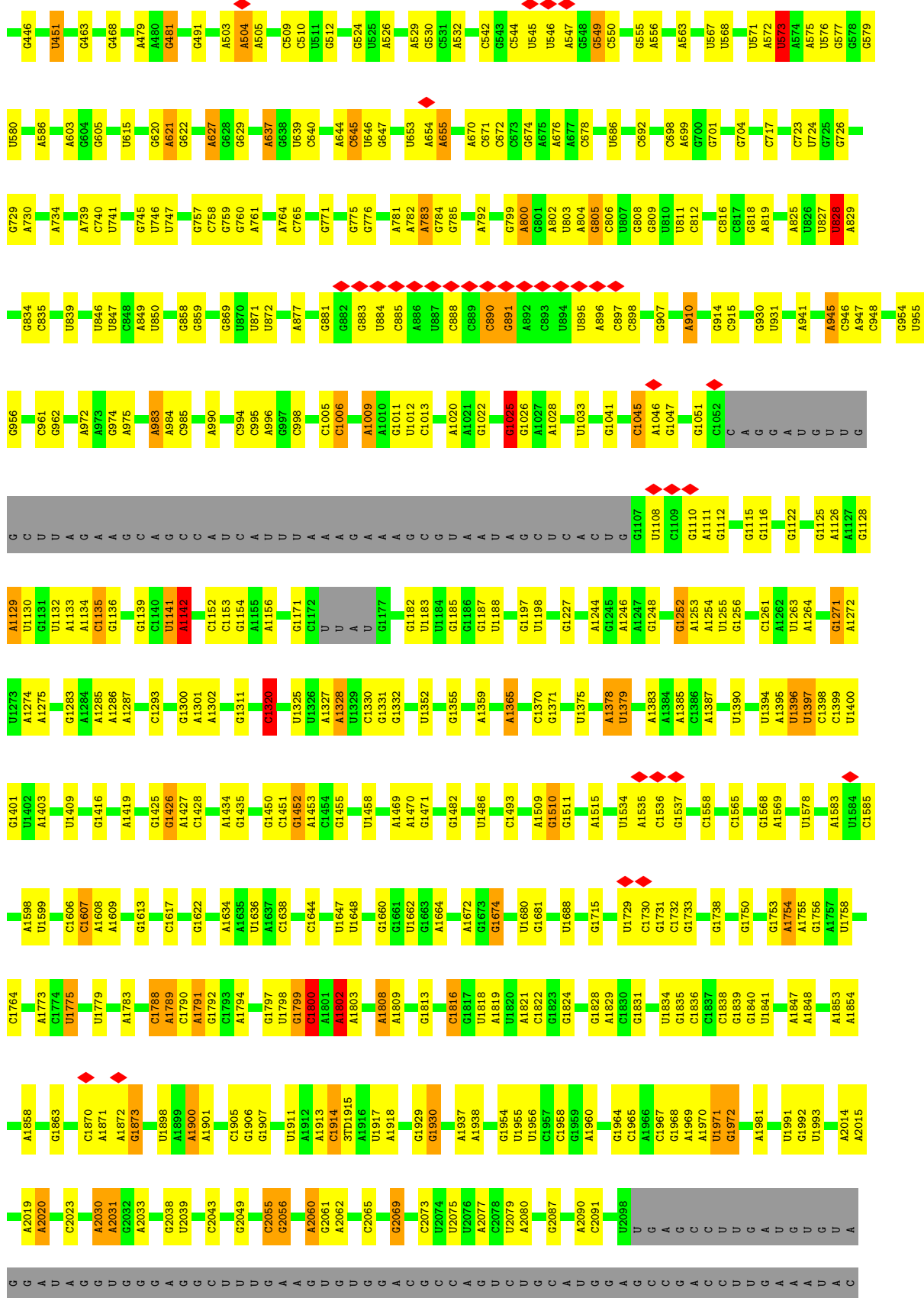
- Molecule 3: Large ribosomal subunit protein bL31A

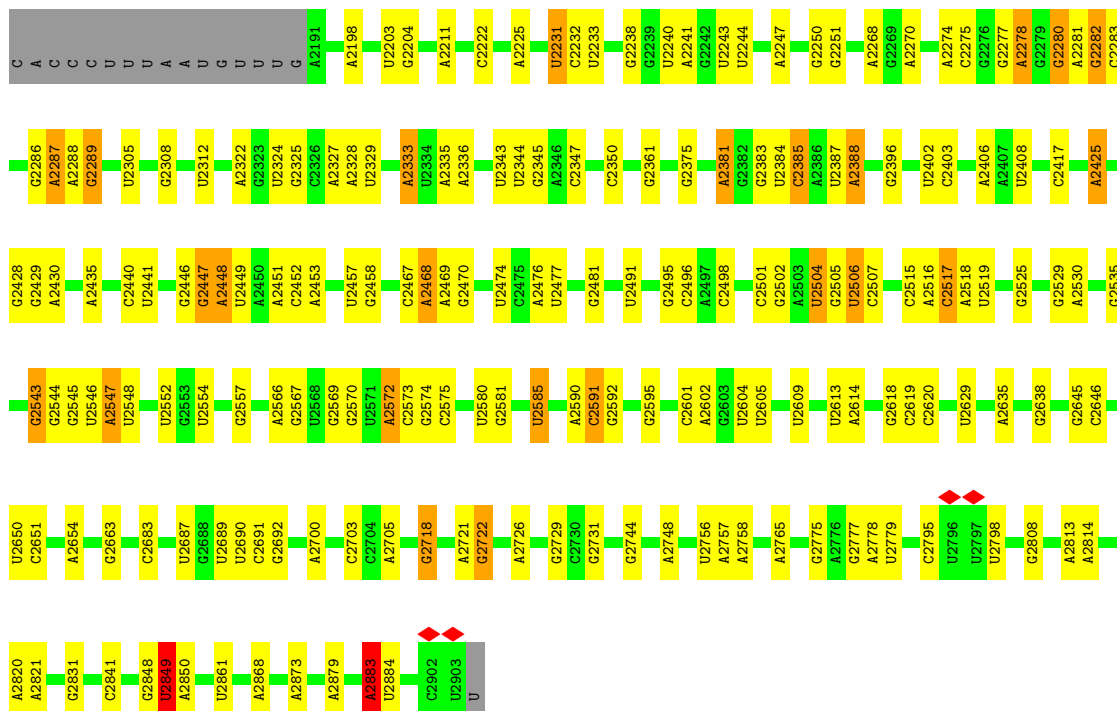


- Molecule 4: 23S rRNA

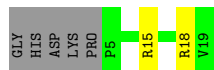
Chain V:  69% 22% 5%



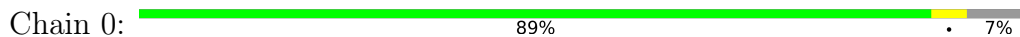




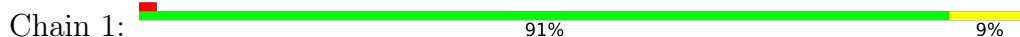
• Molecule 5: DalDroS



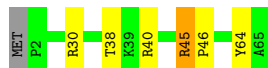
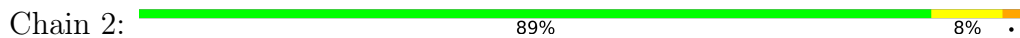
• Molecule 6: Large ribosomal subunit protein bL33



• Molecule 7: Large ribosomal subunit protein bL34



• Molecule 8: Large ribosomal subunit protein bL35





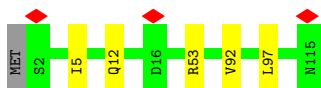


Chain n:  97%




- Molecule 21: Large ribosomal subunit protein bL19

Chain o:  95%



- Molecule 22: Large ribosomal subunit protein bL20

Chain p:  92% 8%



- Molecule 23: Large ribosomal subunit protein bL21

Chain q:  5% 95% 5%



- Molecule 24: Large ribosomal subunit protein uL22

Chain r:  97%



- Molecule 25: Large ribosomal subunit protein uL23

Chain s:  93% 7%

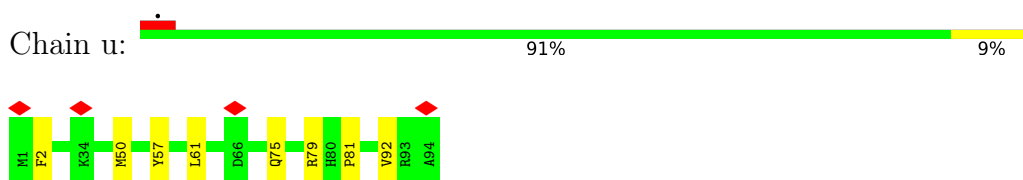


- Molecule 26: Large ribosomal subunit protein uL24

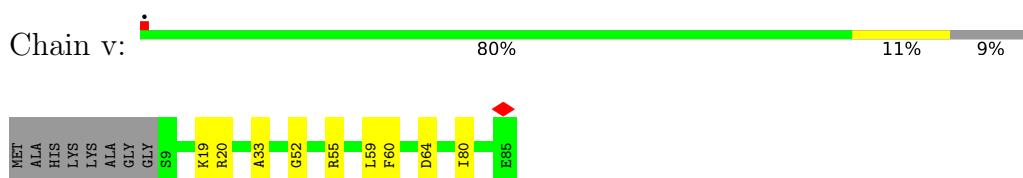
Chain t:  94%



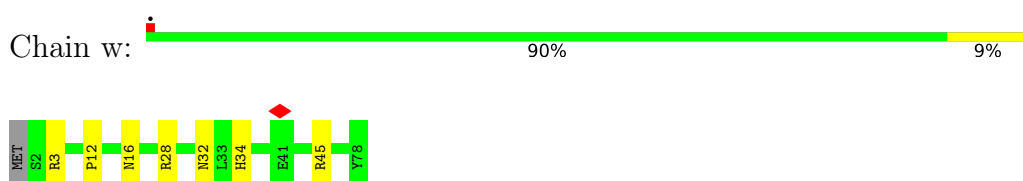
- Molecule 27: 50S ribosomal protein L25



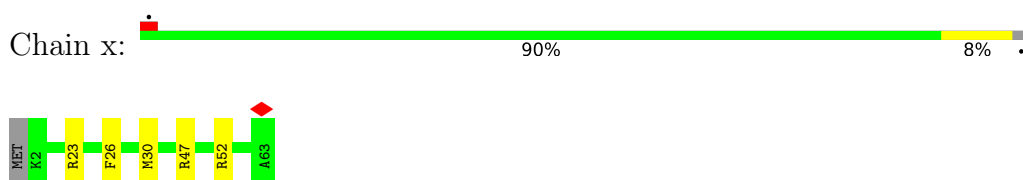
- Molecule 28: Large ribosomal subunit protein bL27



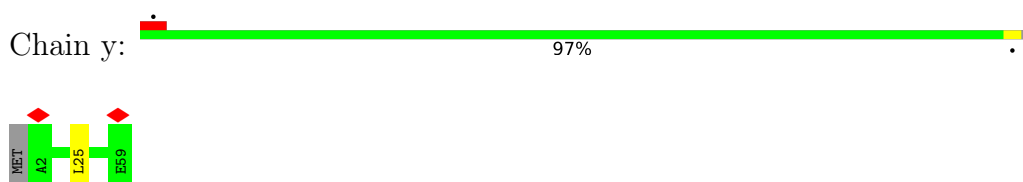
- Molecule 29: Large ribosomal subunit protein bL28



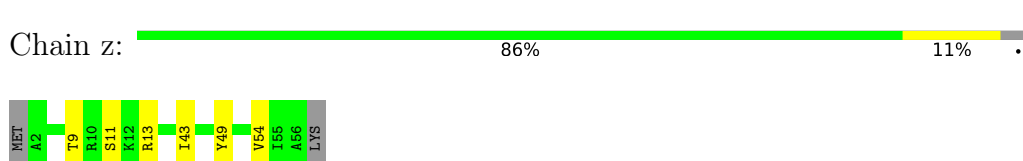
- Molecule 30: Large ribosomal subunit protein uL29



- Molecule 31: Large ribosomal subunit protein uL30

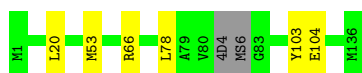


- Molecule 32: Large ribosomal subunit protein bL32

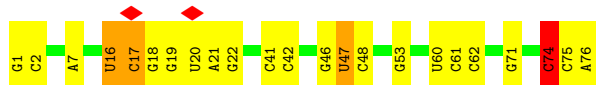


- Molecule 33: Large ribosomal subunit protein uL16





- Molecule 34: P-site Phe-tRNA



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	202610	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	1.14	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.054	Depositor
Minimum map value	-0.021	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size ( $\text{\AA}$ )	345.28, 345.28, 345.28	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.83, 0.83, 0.83	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: G7M, ZN, 5MC, 1MG, OMU, PSU, 6MZ, MEQ, 2MG, OMC, 5MU, SPM, MG, OMG, 3TD, H2U, 2MA

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	3	0.61	0/303	0.81	0/397
2	d	0.67	0/1576	0.93	1/2119 (0.0%)
3	4	0.61	0/480	0.87	0/639
4	V	0.63	1/65651 (0.0%)	1.01	171/102413 (0.2%)
5	8	0.76	0/130	0.93	0/178
6	0	0.64	0/424	0.90	0/565
7	1	0.79	0/380	1.04	0/498
8	2	0.74	0/513	0.97	1/676 (0.1%)
9	W	0.57	0/2007	0.85	0/2702
10	b	0.58	0/2850	0.88	1/4444 (0.0%)
11	c	0.70	1/2115 (0.0%)	0.95	0/2844
12	e	0.63	0/1571	0.93	0/2113
13	f	0.56	0/1434	0.93	0/1926
14	g	0.58	0/1343	0.89	0/1816
15	h	0.59	0/306	0.94	0/413
16	i	0.65	0/1152	0.92	0/1551
17	j	0.64	0/955	0.93	0/1279
18	k	0.66	0/1062	0.91	0/1413
19	m	0.72	0/958	0.97	0/1281
20	n	0.62	0/902	0.95	0/1209
21	o	0.66	0/929	0.88	0/1242
22	p	0.69	0/960	0.99	0/1278
23	q	0.59	0/829	0.82	0/1107
24	r	0.64	0/864	0.94	0/1156
25	s	0.60	0/744	0.88	0/994
26	t	0.58	0/787	0.88	0/1051
27	u	0.58	0/766	0.86	0/1025
28	v	0.68	0/589	0.84	0/780
29	w	0.66	0/635	0.92	0/848
30	x	0.52	0/502	0.95	0/667
31	y	0.61	0/453	0.94	0/605

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	z	0.72	0/440	0.94	0/588
33	l	0.65	0/1073	0.94	0/1433
34	Z	0.60	0/1813	0.88	3/2823 (0.1%)
All	All	0.63	2/97496 (0.0%)	0.98	177/146073 (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
4	V	0	9
5	8	0	2
7	1	0	1
8	2	0	3
9	W	0	1
11	c	0	6
12	e	0	1
16	i	0	1
18	k	0	3
19	m	0	2
21	o	0	1
22	p	0	4
29	w	0	2
30	x	0	2
All	All	0	38

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	2069	G7M	O3'-P	5.29	1.61	1.56
11	c	53	HIS	CG-CD2	-5.21	1.30	1.35

All (177) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	2572	A	O3'-P-O5'	-11.51	86.74	104.00
4	V	818	G	O3'-P-O5'	-9.71	89.44	104.00
4	V	2601	C	O3'-P-O5'	-9.55	89.67	104.00
4	V	1818	U	O3'-P-O5'	-9.13	90.30	104.00
4	V	2449	H2U	O3'-P-O5'	-8.93	90.60	104.00
4	V	2683	C	O3'-P-O5'	-8.76	90.86	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	808	G	O3'-P-O5'	-8.71	90.94	104.00
4	V	1606	C	O3'-P-O5'	-8.44	91.34	104.00
4	V	479	A	O3'-P-O5'	-8.41	91.39	104.00
4	V	446	G	O3'-P-O5'	-8.38	91.44	104.00
4	V	1968	G	O3'-P-O5'	-8.37	91.45	104.00
4	V	1378	A	O3'-P-O5'	-8.36	91.46	104.00
4	V	524	G	O3'-P-O5'	-8.27	91.59	104.00
4	V	1672	A	O3'-P-O5'	-8.21	91.68	104.00
4	V	2498	OMC	O3'-P-O5'	-8.21	91.69	104.00
4	V	1185	G	O3'-P-O5'	-8.18	91.73	104.00
4	V	825	A	O3'-P-O5'	-8.17	91.75	104.00
4	V	1800	C	O3'-P-O5'	-8.13	91.80	104.00
4	V	2731	G	O3'-P-O5'	-8.12	91.82	104.00
4	V	760	G	O3'-P-O5'	-8.02	91.98	104.00
4	V	1142	A	O3'-P-O5'	-8.01	91.98	104.00
4	V	125	A	O3'-P-O5'	-7.98	92.03	104.00
4	V	2883	A	O3'-P-O5'	-7.77	92.34	104.00
4	V	1025	G	O3'-P-O5'	7.65	115.47	104.00
4	V	62	U	O3'-P-O5'	-7.59	92.61	104.00
4	V	1816	C	O3'-P-O5'	-7.50	92.75	104.00
4	V	1568	G	O3'-P-O5'	-7.47	92.80	104.00
4	V	504	A	O3'-P-O5'	-7.41	92.89	104.00
4	V	1359	A	O3'-P-O5'	-7.38	92.93	104.00
4	V	2519	U	O3'-P-O5'	-7.33	93.00	104.00
4	V	640	C	O3'-P-O5'	-7.32	93.02	104.00
4	V	2722	G	O3'-P-O5'	-7.26	93.11	104.00
4	V	2635	A	O3'-P-O5'	-7.15	93.27	104.00
4	V	1824	G	O3'-P-O5'	-7.13	93.31	104.00
4	V	1930	G	O3'-P-O5'	-7.12	93.31	104.00
4	V	27	G	O3'-P-O5'	-7.00	93.50	104.00
4	V	396	G	O3'-P-O5'	-6.88	93.68	104.00
4	V	1664	A	O3'-P-O5'	-6.76	93.86	104.00
4	V	2388	A	C1'-C2'-O2'	6.72	118.48	108.40
4	V	2020	A	O3'-P-O5'	-6.61	94.08	104.00
4	V	2581	G	O3'-P-O5'	-6.57	94.14	104.00
4	V	2620	C	O3'-P-O5'	-6.56	94.16	104.00
4	V	655	A	O3'-P-O5'	-6.53	94.21	104.00
4	V	577	G	O3'-P-O5'	-6.50	94.25	104.00
4	V	1606	C	C2'-C3'-O3'	-6.46	104.00	113.70
4	V	244	A	O3'-P-O5'	-6.45	94.33	104.00
4	V	1992	G	O3'-P-O5'	-6.44	94.35	104.00
4	V	1964	G	O3'-P-O5'	6.43	113.65	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	1252	G	O3'-P-O5'	-6.40	94.40	104.00
4	V	2477	U	O3'-P-O5'	-6.40	94.41	104.00
4	V	2819	G	O3'-P-O5'	-6.38	94.44	104.00
10	b	90	C	O3'-P-O5'	-6.30	94.55	104.00
4	V	1831	G	O3'-P-O5'	-6.28	94.59	104.00
4	V	1674	G	O3'-P-O5'	-6.26	94.60	104.00
4	V	1607	C	C2'-C3'-O3'	6.21	118.81	109.50
4	V	176	A	O3'-P-O5'	-6.18	94.73	104.00
4	V	1375	U	O3'-P-O5'	-6.18	94.73	104.00
4	V	2467	C	O3'-P-O5'	-6.17	94.75	104.00
4	V	1788	C	OP1-P-O3'	6.15	126.45	108.00
4	V	481	G	O3'-P-O5'	-6.12	94.81	104.00
4	V	404	A	C2'-C3'-O3'	6.12	118.68	109.50
4	V	1328	A	O3'-P-O5'	-6.12	94.82	104.00
4	V	2721	A	O3'-P-O5'	-6.12	94.82	104.00
4	V	2222	C	O3'-P-O5'	-6.10	94.85	104.00
4	V	621	A	O3'-P-O5'	-6.10	94.85	104.00
4	V	1328	A	C4'-C3'-O3'	-6.02	103.97	113.00
4	V	2231	U	O3'-P-O5'	-6.02	94.97	104.00
4	V	2879	A	O3'-P-O5'	-5.96	95.07	104.00
4	V	998	C	O3'-P-O5'	-5.95	95.08	104.00
4	V	2557	G	O3'-P-O5'	-5.95	95.08	104.00
4	V	828	U	O3'-P-O5'	-5.93	95.10	104.00
4	V	2387	U	C2'-C3'-O3'	-5.93	104.80	113.70
4	V	1790	C	C2'-C3'-O3'	-5.92	104.81	113.70
4	V	2848	G	O3'-P-O5'	-5.91	95.13	104.00
4	V	2777	G	O3'-P-O5'	-5.91	95.14	104.00
4	V	576	U	O3'-P-O5'	-5.91	95.14	104.00
4	V	941	A	O3'-P-O5'	-5.91	95.14	104.00
4	V	2447	G	O3'-P-O5'	-5.90	95.15	104.00
4	V	2458	G	O3'-P-O5'	-5.87	95.20	104.00
4	V	2619	C	O3'-P-O5'	-5.83	95.25	104.00
4	V	1246	A	O3'-P-O5'	-5.83	95.26	104.00
4	V	375	G	O3'-P-O5'	-5.82	95.27	104.00
4	V	2381	A	C1'-C2'-O2'	5.80	117.10	108.40
4	V	2614	A	O3'-P-O5'	-5.79	95.32	104.00
4	V	1792	G	O3'-P-O5'	-5.78	95.33	104.00
4	V	1293	C	O3'-P-O5'	-5.77	95.34	104.00
4	V	781	A	O3'-P-O5'	-5.76	95.36	104.00
4	V	2703	C	O3'-P-O5'	-5.75	95.38	104.00
4	V	761	A	C4'-C3'-O3'	-5.75	104.38	113.00
4	V	1863	G	O3'-P-O5'	-5.71	95.44	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	2278	A	O3'-P-O5'	-5.68	95.48	104.00
4	V	391	A	O3'-P-O5'	-5.67	95.49	104.00
4	V	204	A	O3'-P-O5'	-5.67	95.50	104.00
4	V	2808	G	O3'-P-O5'	-5.61	95.58	104.00
34	Z	47	U	C2'-C3'-O3'	5.59	117.88	109.50
4	V	994	C	O3'-P-O5'	-5.58	95.63	104.00
4	V	605	G	C4'-C3'-C2'	-5.57	97.03	102.60
4	V	1129	A	C1'-C2'-O2'	5.56	116.74	108.40
4	V	692	C	O3'-P-O5'	-5.56	95.66	104.00
4	V	676	A	C4'-C3'-O3'	-5.55	104.68	113.00
4	V	1992	G	C1'-C2'-O2'	-5.55	103.48	111.80
4	V	1688	U	O3'-P-O5'	-5.53	95.71	104.00
4	V	1397	U	O3'-P-O5'	-5.51	95.73	104.00
4	V	1426	G	C2'-C3'-O3'	-5.49	105.46	113.70
4	V	526	A	C4'-C3'-O3'	-5.49	104.77	113.00
4	V	2575	C	C2'-C3'-O3'	-5.48	105.47	113.70
4	V	2408	U	O3'-P-O5'	-5.46	95.81	104.00
4	V	2250	G	C2'-C3'-O3'	5.45	117.68	109.50
4	V	1254	A	C4'-C3'-O3'	-5.45	104.83	113.00
4	V	2075	U	O3'-P-O5'	-5.44	95.84	104.00
4	V	46	G	O3'-P-O5'	-5.41	95.88	104.00
4	V	2073	C	O3'-P-O5'	-5.41	95.89	104.00
4	V	202	U	O3'-P-O5'	-5.39	95.91	104.00
4	V	428	A	C4'-C3'-O3'	-5.39	104.92	113.00
4	V	2618	G	O3'-P-O5'	-5.36	95.95	104.00
4	V	2240	U	C4'-C3'-C2'	-5.36	97.24	102.60
4	V	395	U	O3'-P-O5'	-5.36	95.97	104.00
4	V	369	U	O3'-P-O5'	-5.34	95.99	104.00
4	V	1565	C	O3'-P-O5'	-5.34	95.99	104.00
4	V	1025	G	C2'-C3'-O3'	5.32	117.48	109.50
4	V	1565	C	C2'-C3'-O3'	5.30	117.45	109.50
4	V	2729	G	O3'-P-O5'	-5.30	96.06	104.00
4	V	2849	U	O3'-P-O5'	-5.27	96.09	104.00
4	V	1971	U	C4'-C3'-O3'	-5.27	105.10	113.00
34	Z	41	C	O3'-P-O5'	-5.27	96.10	104.00
4	V	1960	A	O3'-P-O5'	-5.26	96.10	104.00
4	V	1311	G	O3'-P-O5'	-5.26	96.11	104.00
4	V	178	G	C1'-C2'-O2'	5.24	116.26	108.40
4	V	277	G	C2'-C3'-O3'	-5.24	105.84	113.70
4	V	542	C	O3'-P-O5'	-5.23	96.15	104.00
4	V	1320	C	O3'-P-O5'	-5.23	96.15	104.00
4	V	421	C	O3'-P-O5'	-5.22	96.16	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	2517	C	C2'-C3'-O3'	5.21	117.31	109.50
4	V	2700	A	O3'-P-O5'	-5.21	96.19	104.00
4	V	2343	U	O3'-P-O5'	-5.20	96.20	104.00
4	V	1452	G	C2'-C3'-O3'	5.20	117.29	109.50
4	V	2417	C	O3'-P-O5'	-5.20	96.21	104.00
4	V	573	U	O3'-P-O5'	-5.19	96.22	104.00
4	V	329	G	O3'-P-O5'	-5.18	96.23	104.00
4	V	783	A	O3'-P-O5'	-5.16	96.25	104.00
4	V	2280	G	O3'-P-O5'	-5.16	96.26	104.00
4	V	2385	C	O3'-P-O5'	-5.16	96.26	104.00
4	V	1394	U	O3'-P-O5'	-5.16	96.26	104.00
4	V	321	U	O3'-P-O5'	-5.15	96.28	104.00
4	V	2543	G	O3'-P-O5'	-5.15	96.28	104.00
4	V	198	C	O5'-P-OP1	-5.14	92.57	108.00
4	V	1379	U	O3'-P-O5'	-5.13	96.30	104.00
4	V	701	G	O3'-P-O5'	-5.13	96.31	104.00
8	2	38	THR	CA-CB-OG1	-5.13	101.91	109.60
4	V	1775	U	O3'-P-O5'	-5.12	96.31	104.00
4	V	238	C	O3'-P-O5'	-5.11	96.34	104.00
4	V	1390	U	O3'-P-O5'	-5.10	96.34	104.00
4	V	819	A	O3'-P-O5'	-5.09	96.36	104.00
4	V	972	A	O3'-P-O5'	-5.09	96.36	104.00
2	d	108	ASP	CA-CB-CG	5.09	117.69	112.60
4	V	567	U	O3'-P-O5'	-5.09	96.36	104.00
4	V	1958	C	O3'-P-O5'	-5.08	96.37	104.00
4	V	2591	C	O3'-P-O5'	-5.08	96.38	104.00
4	V	2841	C	O3'-P-O5'	-5.08	96.38	104.00
34	Z	74	C	C2'-C3'-O3'	5.08	121.32	113.70
4	V	451	U	C1'-O4'-C4'	-5.08	104.82	109.90
4	V	1261	C	O3'-P-O5'	-5.07	96.39	104.00
4	V	1638	C	O3'-P-O5'	-5.07	96.40	104.00
4	V	1802	A	C1'-C2'-O2'	5.05	115.98	108.40
4	V	336	C	O3'-P-O5'	-5.04	96.43	104.00
4	V	2375	G	O3'-P-O5'	-5.04	96.44	104.00
4	V	2451	A	O3'-P-O5'	-5.04	96.44	104.00
4	V	699	A	O3'-P-O5'	-5.04	96.45	104.00
4	V	674	G	O3'-P-O5'	-5.03	96.45	104.00
4	V	816	C	O3'-P-O5'	-5.03	96.45	104.00
4	V	2333	A	O3'-P-O5'	-5.03	96.45	104.00
4	V	1244	A	C3'-C2'-O2'	5.03	118.24	110.70
4	V	2329	U	O3'-P-O5'	-5.03	96.46	104.00
4	V	2060	A	C2'-C3'-O3'	5.03	117.04	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	149	A	O3'-P-O5'	-5.00	96.50	104.00
4	V	2718	G	O3'-P-O5'	-5.00	96.50	104.00
4	V	839	U	O3'-P-O5'	-5.00	96.50	104.00

There are no chirality outliers.

All (38) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	1	21	ARG	Sidechain
8	2	30	ARG	Sidechain
8	2	40	ARG	Sidechain
8	2	45	ARG	Sidechain
5	8	15	ARG	Sidechain
5	8	18	ARG	Sidechain
4	V	1188	U	Sidechain
4	V	1789	A	Sidechain
4	V	2595	G	Sidechain
4	V	2645	G	Sidechain
4	V	27	G	Sidechain
4	V	463	G	Sidechain
4	V	512	G	Sidechain
4	V	956	G	Sidechain
4	V	983	A	Sidechain
9	W	116	ARG	Sidechain
11	c	14	ARG	Sidechain
11	c	156	ARG	Sidechain
11	c	238	ARG	Sidechain
11	c	271	ARG	Sidechain
11	c	48	ARG	Sidechain
11	c	52	ARG	Sidechain
12	e	88	ARG	Sidechain
16	i	27	ARG	Sidechain
18	k	33	ARG	Sidechain
18	k	59	ARG	Sidechain
18	k	60	ARG	Sidechain
19	m	17	ARG	Sidechain
19	m	2	ARG	Sidechain
21	o	53	ARG	Sidechain
22	p	11	ARG	Sidechain
22	p	13	ARG	Sidechain
22	p	28	ARG	Sidechain
22	p	51	ARG	Sidechain

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Mol	Chain	Res	Type	Group
29	w	16	ASN	Peptide
29	w	45	ARG	Sidechain
30	x	23	ARG	Sidechain
30	x	52	ARG	Sidechain

## 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	3	302	0	340	0	0
2	d	1566	0	1618	5	0
3	4	472	0	466	0	0
4	V	59130	0	29770	181	0
5	8	124	0	127	0	0
6	0	417	0	451	1	0
7	1	377	0	418	2	0
8	2	504	0	572	3	0
9	W	1977	0	1932	3	0
10	b	2549	0	1291	1	0
11	c	2076	0	2149	11	0
12	e	1552	0	1619	1	0
13	f	1410	0	1444	0	0
14	g	1323	0	1371	1	0
15	h	303	0	327	0	0
16	i	1129	0	1162	6	0
17	j	946	0	1023	2	0
18	k	1053	0	1129	2	0
19	m	945	0	989	5	0
20	n	892	0	923	1	0
21	o	917	0	962	2	0
22	p	947	0	1019	3	0
23	q	816	0	839	2	0
24	r	857	0	922	1	0
25	s	738	0	807	0	0
26	t	779	0	831	1	0
27	u	753	0	780	4	0
28	v	582	0	593	5	0
29	w	625	0	652	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
30	x	501	0	531	3	0
31	y	449	0	488	1	0
32	z	434	0	445	4	0
33	l	1055	0	1134	3	0
34	Z	1623	0	821	4	0
35	3	1	0	0	0	0
35	4	1	0	0	0	0
36	V	14	0	26	0	0
37	V	1	0	0	0	0
All	All	90140	0	59971	236	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 2.

All (236) 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)
4:V:2030:6MZ:O3'	4:V:2031:A:OP2	1.91	0.87
4:V:2030:6MZ:O3'	4:V:2031:A:P	2.41	0.78
4:V:2327:A:H2'	4:V:2328:A:C8	2.25	0.70
4:V:568:U:H1'	4:V:2030:6MZ:H9C1	1.75	0.68
20:n:27:VAL:HG21	20:n:40:ILE:HD12	1.79	0.65
2:d:156:PHE:CE1	16:i:81:ILE:HD13	2.33	0.64
4:V:192:C:O2'	4:V:802:A:N3	2.31	0.63
4:V:1434:A:H2'	4:V:1435:G:C8	2.33	0.63
19:m:55:ALA:HA	19:m:80:PHE:CE2	2.35	0.62
4:V:1853:A:N1	4:V:2087:G:H1'	2.16	0.60
4:V:1800:C:O2	4:V:1802:A:C8	2.55	0.60
4:V:1425:G:H2'	4:V:1426:G:C8	2.37	0.60
4:V:1853:A:H2'	4:V:1854:A:C8	2.37	0.60
4:V:251:A:OP1	18:k:58:TYR:OH	2.16	0.58
4:V:2849:U:H4'	4:V:2868:A:C2	2.39	0.56
4:V:419:U:H2'	4:V:420:C:C6	2.41	0.56
14:g:89:LEU:HD22	14:g:162:VAL:HG22	1.88	0.55
4:V:468:G:N7	7:l:39:ARG:NH2	2.50	0.55
4:V:2243:U:H2'	4:V:2244:U:C6	2.42	0.55
29:w:32:ASN:OD1	29:w:34:HIS:NE2	2.39	0.54
4:V:242:G:H5''	8:2:64:TYR:CE2	2.42	0.54
4:V:572:A:H5''	4:V:573:U:OP2	2.07	0.54
4:V:1834:U:O4'	4:V:1969:A:C2	2.62	0.53
4:V:2543:G:H2'	4:V:2544:G:C8	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:811:U:H2'	18:k:21:ARG:HA	1.91	0.53
4:V:1283:G:N2	4:V:1285:A:H3'	2.24	0.53
4:V:1802:A:H2'	4:V:1803:A:C8	2.44	0.53
24:r:29:VAL:HB	24:r:55:ILE:HD11	1.91	0.52
4:V:1197:G:H2'	4:V:1198:U:H6	1.75	0.52
4:V:704:G:N3	4:V:726:G:C2	2.77	0.52
4:V:1434:A:H2'	4:V:1435:G:H8	1.74	0.52
4:V:1797:G:C5	4:V:1798:U:C5	2.97	0.52
4:V:2515:C:O2	4:V:2570:G:C2	2.63	0.52
4:V:382:A:C2	4:V:393:C:C2	2.99	0.51
4:V:2289:G:N2	4:V:2344:U:O2	2.44	0.51
16:i:24:THR:O	16:i:25:LEU:C	2.53	0.51
4:V:2452:C:C4	4:V:2453:A:C6	2.98	0.51
4:V:1470:A:H2'	4:V:1471:G:O4'	2.10	0.51
16:i:36:LEU:O	16:i:51:GLY:HA3	2.09	0.51
4:V:196:A:O2'	4:V:805:G:O6	2.21	0.51
4:V:1141:U:H4'	4:V:1142:A:O4'	2.10	0.51
4:V:1753:G:C2	4:V:1756:G:C2	2.99	0.51
4:V:849:A:H2'	4:V:850:U:C6	2.46	0.51
4:V:1152:C:H2'	4:V:1153:C:H6	1.76	0.51
4:V:1969:A:O2'	4:V:1972:G:N3	2.43	0.51
4:V:759:G:O4'	4:V:1981:A:C2	2.65	0.50
4:V:373:U:H2'	4:V:374:A:H8	1.77	0.50
4:V:954:G:O2'	4:V:2274:A:N1	2.38	0.50
4:V:1252:G:H1	22:p:37:GLN:HE21	1.59	0.50
4:V:1779:U:C6	4:V:1783:A:N7	2.80	0.50
11:c:29:PRO:HG2	11:c:34:LEU:HD11	1.93	0.50
4:V:2638:G:O2'	4:V:2775:G:N2	2.37	0.50
4:V:1680:U:H2'	4:V:1681:G:O4'	2.11	0.49
4:V:945:A:C5	4:V:2448:A:C2	2.99	0.49
4:V:1799:G:O2'	11:c:182:ARG:NH2	2.45	0.49
4:V:2646:C:O5'	4:V:2646:C:H6	1.95	0.49
4:V:1263:U:OP1	32:z:13:ARG:NH1	2.39	0.49
4:V:1662:U:O2'	4:V:2687:U:OP1	2.29	0.49
4:V:627:A:C6	4:V:637:A:C8	3.01	0.49
4:V:1399:C:H2'	4:V:1400:U:H6	1.77	0.48
4:V:2547:A:H2'	4:V:2548:U:C6	2.48	0.48
4:V:1271:G:N7	4:V:1325:U:H5	2.11	0.48
4:V:1799:G:N7	11:c:178:SER:OG	2.40	0.48
4:V:741:U:C2	4:V:757:G:N2	2.82	0.48
10:b:24:G:N7	10:b:56:G:H2'	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:61:C:OP2	30:x:47:ARG:NH2	2.40	0.48
4:V:1125:G:C6	4:V:1126:A:N6	2.82	0.48
4:V:1450:G:C6	4:V:1451:C:N4	2.82	0.48
30:x:26:PHE:HE1	30:x:30:MET:HE3	1.79	0.48
19:m:98:LEU:HD13	32:z:54:VAL:HG11	1.96	0.48
4:V:12:U:H2'	4:V:12:U:O2	2.12	0.48
4:V:2020:A:H5'	32:z:9:THR:CG2	2.43	0.48
19:m:69:ARG:O	19:m:71:ARG:N	2.44	0.48
4:V:739:A:N3	4:V:740:C:N4	2.61	0.47
34:Z:17:C:C6	34:Z:60:U:O2	2.67	0.47
23:q:14:VAL:HG11	23:q:20:VAL:HG21	1.96	0.47
4:V:672:C:C2	4:V:809:G:N2	2.82	0.47
4:V:2516:A:O2'	4:V:2517:C:H5'	2.15	0.47
8:2:45:ARG:N	8:2:46:PRO:HD2	2.30	0.47
4:V:729:G:C4	4:V:1775:U:O2	2.68	0.47
4:V:945:A:C4	4:V:2448:A:C2	3.02	0.47
4:V:1395:A:C6	4:V:1398:C:C2	3.02	0.47
29:w:3:ARG:O	29:w:12:PRO:HD3	2.15	0.47
4:V:207:A:H2'	4:V:208:C:O4'	2.14	0.47
4:V:1135:C:N4	4:V:1139:G:C6	2.82	0.47
4:V:1385:A:O2'	4:V:1396:U:O2	2.29	0.47
4:V:132:G:C6	4:V:133:U:C4	3.03	0.47
4:V:1370:C:H2'	4:V:1371:G:O4'	2.15	0.47
4:V:1598:A:C5	4:V:1599:U:C5	3.03	0.47
4:V:332:A:C5	4:V:335:C:C4	3.03	0.47
4:V:1153:C:H2'	4:V:1154:G:O4'	2.14	0.46
4:V:1248:G:OP1	12:e:44:ARG:NH2	2.48	0.46
4:V:2038:G:H2'	4:V:2039:U:O4'	2.14	0.46
4:V:2079:U:C2	4:V:2080:A:C8	3.02	0.46
4:V:2506:U:O2	4:V:2506:U:C2'	2.64	0.46
4:V:800:A:C2	4:V:802:A:C8	3.03	0.46
27:u:81:PRO:HG2	33:l:20:LEU:HD13	1.97	0.46
28:v:55:ARG:HG3	28:v:55:ARG:HH11	1.80	0.46
4:V:372:G:O2'	4:V:400:G:O6	2.28	0.46
19:m:14:SER:HA	19:m:17:ARG:NH1	2.31	0.46
4:V:2065:C:H4'	4:V:2251:OMG:HM22	1.97	0.46
4:V:2345:G:N3	4:V:2381:A:H2'	2.31	0.46
11:c:260:ASN:ND2	11:c:263:THR:OG1	2.48	0.46
4:V:1365:A:O5'	29:w:28:ARG:NH2	2.36	0.46
4:V:723:C:H2'	4:V:724:U:O4'	2.16	0.46
4:V:930:G:H1'	31:y:25:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:1754:A:C6	4:V:1755:A:C6	3.04	0.46
11:c:40:SER:OG	11:c:42:GLY:N	2.41	0.46
4:V:792:A:C5	4:V:2440:C:C2	3.04	0.45
4:V:1835:2MG:HM23	4:V:1836:C:H1'	1.98	0.45
4:V:2231:U:H2'	4:V:2232:C:O5'	2.16	0.45
4:V:1009:A:N3	4:V:1153:C:O2'	2.49	0.45
4:V:2280:G:C6	4:V:2281:A:N7	2.85	0.45
4:V:2850:A:N7	4:V:2868:A:O2'	2.44	0.45
11:c:199:GLU:O	11:c:200:HIS:C	2.60	0.45
4:V:871:U:H2'	4:V:872:U:C6	2.52	0.45
4:V:1914:C:O3'	9:W:116:ARG:NH1	2.50	0.45
4:V:828:U:H2'	4:V:829:A:C8	2.51	0.45
2:d:14:ILE:HA	21:o:12:GLN:HE22	1.81	0.45
4:V:549:G:H2'	4:V:550:C:H6	1.81	0.45
4:V:1840:G:C5	4:V:1841:U:C5	3.03	0.45
4:V:698:C:O2'	4:V:734:A:N6	2.49	0.45
4:V:1332:G:H2'	4:V:1332:G:N3	2.31	0.45
4:V:1020:A:C2	4:V:1141:U:C2	3.04	0.45
11:c:67:PHE:CE1	11:c:156:ARG:HD2	2.52	0.45
17:j:1:MET:HE3	17:j:32:TYR:CZ	2.52	0.45
4:V:1327:A:H2'	4:V:1328:A:O4'	2.17	0.45
4:V:1182:G:H2'	4:V:1183:U:O4'	2.17	0.44
4:V:2286:G:H2'	4:V:2286:G:N3	2.31	0.44
6:0:37:LYS:HA	6:0:47:VAL:O	2.17	0.44
4:V:2055:C:H5'	4:V:2056:G:O5'	2.17	0.44
4:V:1006:C:O2'	16:i:108:MET:O	2.35	0.44
26:t:54:GLN:N	26:t:55:PRO:HD2	2.31	0.44
4:V:644:A:H2'	4:V:645:C:O4'	2.18	0.44
4:V:1613:G:C6	4:V:1617:C:C5	3.05	0.44
4:V:1794:A:O4'	4:V:1900:A:C2	2.70	0.44
11:c:31:ALA:N	11:c:32:PRO:CD	2.80	0.44
4:V:802:A:C5	4:V:803:U:C4	3.05	0.44
4:V:2090:A:C6	4:V:2091:C:C4	3.06	0.44
2:d:62:LYS:N	2:d:63:PRO:CD	2.80	0.44
4:V:191:A:H2'	4:V:192:C:C6	2.53	0.44
4:V:1197:G:H2'	4:V:1198:U:C6	2.52	0.44
28:v:59:LEU:HD12	28:v:80:ILE:HD12	2.00	0.44
4:V:1263:U:H2'	4:V:1264:A:C8	2.53	0.44
4:V:580:U:O3'	22:p:31:VAL:HG13	2.18	0.44
4:V:2516:A:C4	4:V:2569:G:N2	2.86	0.44
7:1:31:LEU:O	7:1:34:ARG:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:i:52:ASP:O	16:i:121:LYS:HE2	2.18	0.43
4:V:2469:A:N6	4:V:2481:G:O2'	2.51	0.43
4:V:799:G:N1	4:V:800:A:N6	2.66	0.43
4:V:1798:U:OP2	11:c:271:ARG:NH2	2.52	0.43
4:V:2345:G:C5	4:V:2381:A:C2	3.06	0.43
2:d:149:ASN:OD1	2:d:150:MEQ:N	2.51	0.43
4:V:2014:A:H2'	4:V:2015:A:C8	2.54	0.43
17:j:2:ILE:HG23	17:j:6:THR:HG21	1.99	0.43
4:V:802:A:C5	4:V:803:U:C5	3.06	0.43
4:V:1798:U:C4	4:V:1819:A:C2	3.06	0.43
23:q:74:ILE:N	23:q:74:ILE:HD12	2.34	0.43
28:v:19:LYS:O	28:v:20:ARG:C	2.62	0.43
33:l:53:MET:HE1	33:l:103:TYR:CD2	2.53	0.43
4:V:195:A:H61	4:V:198:C:H3'	1.84	0.43
4:V:1821:A:C6	4:V:1822:C:C4	3.07	0.43
4:V:2585:U:O2	4:V:2585:U:O4'	2.35	0.43
4:V:947:A:H2'	4:V:948:C:C6	2.53	0.43
4:V:2281:A:C2	4:V:2282:G:C5	3.07	0.43
4:V:1274:A:N1	4:V:1644:C:O2'	2.39	0.43
4:V:1275:A:C5	19:m:16:HIS:CD2	3.07	0.43
4:V:1808:A:H3'	4:V:1809:A:C8	2.54	0.43
4:V:1872:A:H3'	4:V:1873:G:O4'	2.19	0.43
21:o:92:VAL:HG11	21:o:97:LEU:HD11	2.01	0.43
4:V:128:C:H2'	4:V:129:C:H6	1.84	0.43
27:u:57:TYR:OH	27:u:79:ARG:NH2	2.52	0.43
4:V:671:C:H2'	4:V:672:C:H6	1.84	0.42
4:V:1025:G:H1'	4:V:1135:C:O5'	2.19	0.42
4:V:1797:G:C4	4:V:1798:U:C6	3.06	0.42
4:V:2495:G:C6	4:V:2496:C:N3	2.87	0.42
33:l:66:ARG:NH1	33:l:104:GLU:OE2	2.52	0.42
4:V:2231:U:C2'	4:V:2232:C:O5'	2.66	0.42
4:V:740:C:C4	4:V:758:C:O2	2.72	0.42
4:V:804:A:H5''	4:V:805:G:OP1	2.19	0.42
4:V:2692:G:C6	4:V:2718:G:C6	3.06	0.42
4:V:157:C:H2'	4:V:158:U:O4'	2.19	0.42
4:V:2030:6MZ:H3'	4:V:2031:A:OP1	2.20	0.42
4:V:579:G:O2'	4:V:2019:A:OP1	2.38	0.42
4:V:629:G:N3	4:V:639:U:O2'	2.50	0.42
4:V:1872:A:C5	4:V:1873:G:H1'	2.55	0.42
28:v:52:GLY:HA3	28:v:60:PHE:CZ	2.54	0.42
4:V:57:C:H2'	4:V:58:G:O4'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:1320:C:N3	4:V:1331:G:O6	2.53	0.42
4:V:1387:A:C2	4:V:1401:G:C2	3.08	0.42
11:c:203:ARG:NH2	11:c:205:LEU:HD21	2.35	0.42
27:u:2:PHE:HB3	27:u:50:MET:HE3	2.02	0.42
4:V:2282:G:N3	4:V:2425:A:N6	2.68	0.42
4:V:1469:A:H2'	4:V:1470:A:C8	2.54	0.41
8:2:45:ARG:N	8:2:46:PRO:CD	2.83	0.41
32:z:43:ILE:HG22	32:z:49:TYR:HB2	2.03	0.41
4:V:2286:G:H4'	4:V:2287:A:O4'	2.20	0.41
4:V:2543:G:H2'	4:V:2544:G:H8	1.85	0.41
4:V:80:G:O2'	4:V:294:A:N1	2.44	0.41
4:V:910:A:N1	4:V:2277:G:H1'	2.35	0.41
4:V:1385:A:C4	4:V:1403:A:C2	3.08	0.41
2:d:38:LYS:NZ	2:d:81:GLU:OE1	2.53	0.41
4:V:130:C:H2'	4:V:131:A:O5'	2.21	0.41
4:V:239:C:HO2'	4:V:622:G:HO2'	1.69	0.41
4:V:995:C:O2	16:i:3:THR:OG1	2.35	0.41
4:V:2447:G:C4	4:V:2501:C:C5	3.08	0.41
34:Z:1:G:H2'	34:Z:2:C:C6	2.55	0.41
4:V:771:G:O2'	4:V:1355:G:O2'	2.34	0.41
4:V:1399:C:H2'	4:V:1400:U:C6	2.56	0.41
4:V:2545:G:H2'	4:V:2546:U:O4'	2.20	0.41
9:W:217:ILE:HD11	9:W:275:GLY:HA2	2.01	0.41
9:W:261:ARG:NH2	34:Z:74:C:O3'	2.53	0.41
4:V:2452:C:N4	4:V:2453:A:C6	2.89	0.41
4:V:2813:A:H2'	4:V:2814:A:C8	2.55	0.41
27:u:75:GLN:HB2	27:u:92:VAL:HG23	2.02	0.41
4:V:890:C:H3'	4:V:891:G:O4'	2.20	0.41
4:V:1788:C:C2	4:V:1789:A:C8	3.09	0.41
4:V:1028:A:N6	4:V:1125:G:H2'	2.36	0.41
4:V:1954:G:O2'	4:V:1956:U:O4	2.26	0.41
4:V:2468:A:O2'	4:V:2481:G:N2	2.50	0.41
4:V:2831:G:H1'	4:V:2883:A:H2'	2.03	0.41
28:v:33:ALA:N	28:v:64:ASP:OD1	2.52	0.41
4:V:834:G:C5	4:V:835:C:C5	3.09	0.41
4:V:2650:U:H2'	4:V:2651:C:C6	2.56	0.41
22:p:76:TYR:CZ	22:p:80:ILE:HG13	2.56	0.41
34:Z:16:U:H2'	34:Z:17:C:C6	2.56	0.41
4:V:1510:G:H2'	4:V:1511:G:O4'	2.21	0.40
30:x:26:PHE:CE1	30:x:30:MET:HE3	2.56	0.40
4:V:1838:C:N4	4:V:1898:U:H2'	2.37	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:V:2591:C:H2'	4:V:2592:G:C8	2.56	0.40
4:V:1791:A:N6	4:V:1828:G:O2'	2.51	0.40
4:V:13:A:O2'	4:V:15:G:N7	2.44	0.40
4:V:1045:C:O2	4:V:1045:C:O4'	2.39	0.40
4:V:382:A:C2	4:V:393:C:N3	2.89	0.40
4:V:804:A:H2'	4:V:806:C:C4	2.57	0.40
4:V:2590:A:O3'	11:c:238:ARG:NH1	2.55	0.40

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	3	36/38 (95%)	36 (100%)	0	0	100	100
2	d	206/209 (99%)	197 (96%)	9 (4%)	0	100	100
3	4	55/70 (79%)	52 (94%)	3 (6%)	0	100	100
5	8	13/20 (65%)	13 (100%)	0	0	100	100
6	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
7	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
8	2	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
9	W	252/360 (70%)	241 (96%)	11 (4%)	0	100	100
11	c	268/273 (98%)	255 (95%)	13 (5%)	0	100	100
12	e	199/201 (99%)	191 (96%)	8 (4%)	0	100	100
13	f	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
14	g	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
15	h	39/149 (26%)	35 (90%)	4 (10%)	0	100	100
16	i	140/142 (99%)	136 (97%)	4 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	j	121/123 (98%)	114 (94%)	7 (6%)	0	100	100
18	k	142/144 (99%)	133 (94%)	8 (6%)	1 (1%)	18	44
19	m	116/127 (91%)	109 (94%)	7 (6%)	0	100	100
20	n	114/117 (97%)	107 (94%)	7 (6%)	0	100	100
21	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
22	p	115/118 (98%)	113 (98%)	2 (2%)	0	100	100
23	q	101/103 (98%)	97 (96%)	4 (4%)	0	100	100
24	r	108/110 (98%)	104 (96%)	4 (4%)	0	100	100
25	s	91/100 (91%)	89 (98%)	2 (2%)	0	100	100
26	t	100/104 (96%)	96 (96%)	4 (4%)	0	100	100
27	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
28	v	75/85 (88%)	72 (96%)	3 (4%)	0	100	100
29	w	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
30	x	60/63 (95%)	60 (100%)	0	0	100	100
31	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
32	z	53/57 (93%)	50 (94%)	3 (6%)	0	100	100
33	l	130/136 (96%)	121 (93%)	9 (7%)	0	100	100
All	All	3373/3717 (91%)	3222 (96%)	150 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
18	k	29	LYS

### 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	
1	3	34/34 (100%)	34 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	d	163/163 (100%)	163 (100%)	0	100	100
3	4	54/62 (87%)	54 (100%)	0	100	100
5	8	15/19 (79%)	15 (100%)	0	100	100
6	0	46/49 (94%)	46 (100%)	0	100	100
7	1	38/38 (100%)	38 (100%)	0	100	100
8	2	51/52 (98%)	51 (100%)	0	100	100
9	W	205/300 (68%)	203 (99%)	2 (1%)	68	87
11	c	215/218 (99%)	214 (100%)	1 (0%)	81	93
12	e	165/165 (100%)	163 (99%)	2 (1%)	63	84
13	f	148/150 (99%)	147 (99%)	1 (1%)	76	90
14	g	137/138 (99%)	133 (97%)	4 (3%)	37	68
15	h	32/114 (28%)	32 (100%)	0	100	100
16	i	116/116 (100%)	116 (100%)	0	100	100
17	j	104/104 (100%)	102 (98%)	2 (2%)	50	77
18	k	103/103 (100%)	102 (99%)	1 (1%)	68	87
19	m	98/103 (95%)	98 (100%)	0	100	100
20	n	86/87 (99%)	86 (100%)	0	100	100
21	o	99/100 (99%)	98 (99%)	1 (1%)	68	87
22	p	89/90 (99%)	88 (99%)	1 (1%)	65	86
23	q	84/84 (100%)	82 (98%)	2 (2%)	43	73
24	r	93/93 (100%)	92 (99%)	1 (1%)	65	86
25	s	80/84 (95%)	80 (100%)	0	100	100
26	t	83/85 (98%)	80 (96%)	3 (4%)	31	63
27	u	78/78 (100%)	77 (99%)	1 (1%)	61	84
28	v	58/63 (92%)	58 (100%)	0	100	100
29	w	67/68 (98%)	67 (100%)	0	100	100
30	x	54/55 (98%)	54 (100%)	0	100	100
31	y	48/49 (98%)	48 (100%)	0	100	100
32	z	46/48 (96%)	45 (98%)	1 (2%)	45	75
33	l	107/107 (100%)	106 (99%)	1 (1%)	70	88
All	All	2796/3019 (93%)	2772 (99%)	24 (1%)	68	88

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	W	242	SER
9	W	259	ASP
11	c	162	VAL
12	e	96	VAL
12	e	163	ASN
13	f	148	ARG
14	g	47	ASP
14	g	60	ASP
14	g	81	GLU
14	g	130	GLU
17	j	51	LYS
17	j	76	VAL
18	k	42	SER
21	o	5	ILE
22	p	41	LYS
23	q	46	GLU
23	q	102	SER
24	r	83	LYS
26	t	52	LEU
26	t	54	GLN
26	t	68	SER
27	u	61	LEU
32	z	11	SER
33	l	78	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
2	d	32	ASN
2	d	49	GLN
2	d	58	ASN
2	d	148	GLN
9	W	185	GLN
9	W	258	GLN
9	W	263	GLN
11	c	25	HIS
11	c	90	ASN
11	c	153	GLN
11	c	197	ASN
11	c	260	ASN
12	e	94	GLN

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Mol	Chain	Res	Type
13	f	21	ASN
13	f	27	GLN
14	g	22	GLN
14	g	30	ASN
14	g	88	GLN
14	g	104	ASN
16	i	76	HIS
17	j	9	ASN
19	m	9	GLN
20	n	29	HIS
21	o	12	GLN
22	p	37	GLN
24	r	9	HIS
24	r	31	GLN
25	s	92	ASN
26	t	53	ASN
26	t	54	GLN
27	u	49	ASN
29	w	6	GLN
30	x	27	ASN
32	z	6	ASN
33	l	13	HIS
33	l	60	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	b	118/120 (98%)	13 (11%)	0
34	Z	75/76 (98%)	16 (21%)	6 (8%)
4	V	2750/2904 (94%)	371 (13%)	59 (2%)
All	All	2943/3100 (94%)	400 (13%)	65 (2%)

All (400) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	V	2	G
4	V	10	A
4	V	34	U
4	V	42	A
4	V	58	G
4	V	62	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	63	A
4	V	71	A
4	V	74	A
4	V	75	G
4	V	86	G
4	V	101	A
4	V	102	U
4	V	118	A
4	V	119	A
4	V	120	U
4	V	131	A
4	V	139	U
4	V	142	A
4	V	163	C
4	V	181	A
4	V	196	A
4	V	199	A
4	V	200	U
4	V	215	G
4	V	216	A
4	V	221	A
4	V	222	A
4	V	229	C
4	V	230	G
4	V	248	G
4	V	250	G
4	V	265	A
4	V	272	A
4	V	277	G
4	V	278	A
4	V	281	C
4	V	285	G
4	V	289	G
4	V	292	U
4	V	294	A
4	V	310	A
4	V	311	A
4	V	329	G
4	V	330	A
4	V	361	G
4	V	362	A
4	V	386	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	405	U
4	V	411	G
4	V	412	A
4	V	429	A
4	V	443	A
4	V	451	U
4	V	481	G
4	V	491	G
4	V	503	A
4	V	504	A
4	V	505	A
4	V	509	C
4	V	510	C
4	V	529	A
4	V	530	G
4	V	532	A
4	V	544	C
4	V	545	U
4	V	546	U
4	V	547	A
4	V	549	G
4	V	555	G
4	V	556	A
4	V	563	A
4	V	573	U
4	V	575	A
4	V	586	A
4	V	603	A
4	V	615	U
4	V	620	G
4	V	621	A
4	V	627	A
4	V	637	A
4	V	645	C
4	V	646	U
4	V	647	G
4	V	653	U
4	V	654	A
4	V	655	A
4	V	670	A
4	V	678	C
4	V	686	U

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	717	C
4	V	730	A
4	V	747	5MU
4	V	764	A
4	V	765	C
4	V	775	G
4	V	776	G
4	V	782	A
4	V	783	A
4	V	784	G
4	V	785	G
4	V	805	G
4	V	812	C
4	V	827	U
4	V	828	U
4	V	846	U
4	V	847	U
4	V	858	G
4	V	859	G
4	V	869	G
4	V	877	A
4	V	881	G
4	V	883	G
4	V	884	U
4	V	885	C
4	V	888	C
4	V	890	C
4	V	891	G
4	V	895	U
4	V	896	A
4	V	897	C
4	V	898	C
4	V	907	G
4	V	910	A
4	V	914	G
4	V	915	C
4	V	931	U
4	V	945	A
4	V	946	C
4	V	961	C
4	V	962	G
4	V	974	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	975	A
4	V	983	A
4	V	984	A
4	V	985	C
4	V	990	A
4	V	996	A
4	V	1005	C
4	V	1006	C
4	V	1009	A
4	V	1012	U
4	V	1013	C
4	V	1022	G
4	V	1026	G
4	V	1033	U
4	V	1041	G
4	V	1045	C
4	V	1046	A
4	V	1047	G
4	V	1051	G
4	V	1108	U
4	V	1110	G
4	V	1111	A
4	V	1112	G
4	V	1115	G
4	V	1116	G
4	V	1122	G
4	V	1128	G
4	V	1129	A
4	V	1130	U
4	V	1132	U
4	V	1133	A
4	V	1134	A
4	V	1135	C
4	V	1136	G
4	V	1142	A
4	V	1156	A
4	V	1171	G
4	V	1187	G
4	V	1227	G
4	V	1253	A
4	V	1255	U
4	V	1256	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	1271	G
4	V	1272	A
4	V	1286	A
4	V	1287	A
4	V	1300	G
4	V	1301	A
4	V	1302	A
4	V	1330	C
4	V	1352	U
4	V	1365	A
4	V	1378	A
4	V	1379	U
4	V	1383	A
4	V	1396	U
4	V	1397	U
4	V	1409	U
4	V	1416	G
4	V	1419	A
4	V	1427	A
4	V	1428	C
4	V	1452	G
4	V	1453	A
4	V	1455	G
4	V	1458	U
4	V	1482	G
4	V	1486	U
4	V	1493	C
4	V	1509	A
4	V	1510	G
4	V	1515	A
4	V	1534	U
4	V	1535	A
4	V	1536	C
4	V	1537	G
4	V	1558	C
4	V	1569	A
4	V	1578	U
4	V	1583	A
4	V	1585	C
4	V	1607	C
4	V	1608	A
4	V	1609	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	1622	G
4	V	1634	A
4	V	1636	U
4	V	1647	U
4	V	1648	U
4	V	1660	G
4	V	1674	G
4	V	1715	G
4	V	1729	U
4	V	1730	C
4	V	1731	G
4	V	1732	C
4	V	1733	G
4	V	1738	G
4	V	1750	G
4	V	1754	A
4	V	1758	U
4	V	1764	C
4	V	1773	A
4	V	1791	A
4	V	1800	C
4	V	1802	A
4	V	1808	A
4	V	1813	G
4	V	1816	C
4	V	1829	A
4	V	1839	G
4	V	1847	A
4	V	1848	A
4	V	1858	A
4	V	1870	C
4	V	1871	A
4	V	1873	G
4	V	1900	A
4	V	1901	A
4	V	1905	C
4	V	1906	G
4	V	1907	G
4	V	1913	A
4	V	1914	C
4	V	1929	G
4	V	1930	G

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	1937	A
4	V	1938	A
4	V	1955	U
4	V	1965	C
4	V	1967	C
4	V	1970	A
4	V	1971	U
4	V	1972	G
4	V	1991	U
4	V	1993	U
4	V	2023	C
4	V	2031	A
4	V	2033	A
4	V	2043	C
4	V	2049	G
4	V	2055	C
4	V	2056	G
4	V	2060	A
4	V	2061	G
4	V	2062	A
4	V	2069	G7M
4	V	2077	A
4	V	2198	A
4	V	2203	U
4	V	2204	G
4	V	2211	A
4	V	2225	A
4	V	2233	U
4	V	2238	G
4	V	2241	A
4	V	2247	A
4	V	2268	A
4	V	2270	A
4	V	2278	A
4	V	2283	C
4	V	2287	A
4	V	2288	A
4	V	2289	G
4	V	2305	U
4	V	2308	G
4	V	2312	U
4	V	2322	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	2325	G
4	V	2333	A
4	V	2335	A
4	V	2336	A
4	V	2347	C
4	V	2350	C
4	V	2361	G
4	V	2383	G
4	V	2384	U
4	V	2385	C
4	V	2388	A
4	V	2396	G
4	V	2402	U
4	V	2403	C
4	V	2406	A
4	V	2425	A
4	V	2428	G
4	V	2429	G
4	V	2430	A
4	V	2435	A
4	V	2441	U
4	V	2446	G
4	V	2448	A
4	V	2470	G
4	V	2474	U
4	V	2476	A
4	V	2491	U
4	V	2502	G
4	V	2505	G
4	V	2506	U
4	V	2507	C
4	V	2518	A
4	V	2525	G
4	V	2529	G
4	V	2530	A
4	V	2535	G
4	V	2547	A
4	V	2552	OMU
4	V	2554	U
4	V	2566	A
4	V	2567	G
4	V	2572	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	2573	C
4	V	2574	G
4	V	2585	U
4	V	2602	A
4	V	2609	U
4	V	2613	U
4	V	2629	U
4	V	2654	A
4	V	2663	G
4	V	2689	U
4	V	2690	U
4	V	2691	C
4	V	2705	A
4	V	2722	G
4	V	2726	A
4	V	2744	G
4	V	2748	A
4	V	2757	A
4	V	2758	A
4	V	2765	A
4	V	2778	A
4	V	2795	C
4	V	2798	U
4	V	2820	A
4	V	2821	A
4	V	2849	U
4	V	2861	U
4	V	2883	A
4	V	2884	U
10	b	9	G
10	b	25	U
10	b	35	C
10	b	36	C
10	b	37	C
10	b	42	C
10	b	56	G
10	b	57	A
10	b	67	G
10	b	89	U
10	b	90	C
10	b	99	A
10	b	109	A

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Mol	Chain	Res	Type
34	Z	17	C
34	Z	18	G
34	Z	19	G
34	Z	20	U
34	Z	21	A
34	Z	22	G
34	Z	42	C
34	Z	46	G
34	Z	47	U
34	Z	48	C
34	Z	53	G
34	Z	61	C
34	Z	62	C
34	Z	71	G
34	Z	75	C
34	Z	76	A

All (65) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	V	1	G
4	V	62	U
4	V	102	U
4	V	199	A
4	V	221	A
4	V	228	C
4	V	277	G
4	V	310	A
4	V	404	A
4	V	503	A
4	V	545	U
4	V	555	G
4	V	571	U
4	V	620	G
4	V	654	A
4	V	764	A
4	V	776	G
4	V	784	G
4	V	800	A
4	V	846	U
4	V	858	G
4	V	961	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	V	974	G
4	V	984	A
4	V	1011	G
4	V	1025	G
4	V	1045	C
4	V	1128	G
4	V	1133	A
4	V	1141	U
4	V	1253	A
4	V	1286	A
4	V	1301	A
4	V	1320	C
4	V	1396	U
4	V	1397	U
4	V	1535	A
4	V	1608	A
4	V	1647	U
4	V	1799	G
4	V	1847	A
4	V	1900	A
4	V	1913	A
4	V	1918	A
4	V	2275	C
4	V	2282	G
4	V	2324	U
4	V	2335	A
4	V	2430	A
4	V	2468	A
4	V	2504	PSU
4	V	2529	G
4	V	2573	C
4	V	2602	A
4	V	2756	U
4	V	2778	A
4	V	2779	U
4	V	2820	A
4	V	2873	A
34	Z	7	A
34	Z	16	U
34	Z	18	G
34	Z	46	G
34	Z	53	G

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Mol	Chain	Res	Type
34	Z	74	C

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

25 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
4	5MC	V	1962	4	18,22,23	0.44	0	26,32,35	0.58	0
4	6MZ	V	2030	4	22,25,26	1.08	2 (9%)	30,36,39	0.86	0
4	1MG	V	745	4	22,26,27	0.82	1 (4%)	33,39,42	0.47	0
4	OMG	V	2251	34,4	23,26,27	0.48	0	33,38,41	0.56	0
4	3TD	V	1915	4	18,22,23	0.96	1 (5%)	22,32,35	0.64	0
4	G7M	V	2069	4	23,26,27	0.65	0	35,39,42	0.72	1 (2%)
2	MEQ	d	150	2	8,9,10	0.68	0	5,10,12	0.65	0
4	5MU	V	1939	4	19,22,23	0.57	0	28,32,35	0.65	0
4	PSU	V	746	4	18,21,22	0.89	1 (5%)	22,30,33	0.75	0
4	2MG	V	2445	4	23,26,27	0.62	0	32,38,41	0.52	0
4	PSU	V	2604	4	18,21,22	0.90	1 (5%)	22,30,33	0.82	0
4	H2U	V	2449	4	18,21,22	0.67	0	21,30,33	1.03	2 (9%)
4	6MZ	V	1618	4	22,25,26	0.64	0	30,36,39	0.68	0
4	PSU	V	1911	4	18,21,22	1.00	1 (5%)	22,30,33	0.63	0
4	PSU	V	955	4	18,21,22	0.88	1 (5%)	22,30,33	0.77	1 (4%)
4	PSU	V	2457	4	18,21,22	0.86	1 (5%)	22,30,33	0.66	0
4	OMU	V	2552	4	19,22,23	0.45	0	26,31,34	0.40	0
4	PSU	V	2504	4	18,21,22	0.99	1 (5%)	22,30,33	0.80	1 (4%)
4	PSU	V	2580	4	18,21,22	0.97	1 (5%)	22,30,33	0.81	1 (4%)
4	PSU	V	2605	4	18,21,22	1.28	2 (11%)	22,30,33	0.91	0
4	5MU	V	747	4	19,22,23	0.37	0	28,32,35	0.56	0
4	OMC	V	2498	4	19,22,23	0.58	0	26,31,34	0.48	0
4	PSU	V	1917	4	18,21,22	0.94	1 (5%)	22,30,33	0.54	0
4	2MA	V	2503	4	22,25,26	0.56	0	33,37,40	0.72	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	2MG	V	1835	4	23,26,27	0.43	0	32,38,41	0.47	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
4	5MC	V	1962	4	-	2/7/25/26	0/2/2/2
4	6MZ	V	2030	4	-	2/9/27/28	0/3/3/3
4	1MG	V	745	4	-	0/7/25/26	0/3/3/3
4	OMG	V	2251	34,4	-	0/9/27/28	0/3/3/3
4	3TD	V	1915	4	-	0/7/25/26	0/2/2/2
4	G7M	V	2069	4	-	1/7/25/26	0/3/3/3
2	MEQ	d	150	2	-	2/8/9/11	-
4	5MU	V	1939	4	-	0/7/25/26	0/2/2/2
4	PSU	V	746	4	-	4/7/25/26	0/2/2/2
4	2MG	V	2445	4	-	0/9/27/28	0/3/3/3
4	PSU	V	2604	4	-	0/7/25/26	0/2/2/2
4	H2U	V	2449	4	-	0/7/38/39	0/2/2/2
4	6MZ	V	1618	4	-	0/9/27/28	0/3/3/3
4	PSU	V	1911	4	-	0/7/25/26	0/2/2/2
4	PSU	V	955	4	-	0/7/25/26	0/2/2/2
4	PSU	V	2457	4	-	0/7/25/26	0/2/2/2
4	OMU	V	2552	4	-	2/9/27/28	0/2/2/2
4	PSU	V	2504	4	-	0/7/25/26	0/2/2/2
4	PSU	V	2580	4	-	1/7/25/26	0/2/2/2
4	PSU	V	2605	4	-	0/7/25/26	0/2/2/2
4	5MU	V	747	4	-	1/7/25/26	0/2/2/2
4	OMC	V	2498	4	-	0/9/27/28	0/2/2/2
4	PSU	V	1917	4	-	0/7/25/26	0/2/2/2
4	2MA	V	2503	4	-	2/7/25/26	0/3/3/3
4	2MG	V	1835	4	-	1/9/27/28	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	1911	PSU	C6-C5	3.97	1.39	1.35
4	V	1917	PSU	C6-C5	3.67	1.39	1.35
4	V	1915	3TD	C6-C5	3.54	1.39	1.35
4	V	2504	PSU	C6-C5	3.45	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	V	2604	PSU	C6-C5	3.39	1.39	1.35
4	V	2580	PSU	C6-C5	3.38	1.39	1.35
4	V	2605	PSU	C6-C5	3.27	1.39	1.35
4	V	2030	6MZ	C6-N6	-3.21	1.30	1.34
4	V	2605	PSU	C4-C5	-3.20	1.35	1.44
4	V	746	PSU	C6-C5	3.11	1.38	1.35
4	V	2457	PSU	C6-C5	2.84	1.38	1.35
4	V	2030	6MZ	C1'-N9	-2.69	1.38	1.46
4	V	745	1MG	C5-C6	-2.54	1.39	1.45
4	V	955	PSU	C6-C5	2.17	1.37	1.35

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	V	2580	PSU	C3'-C2'-C1'	2.95	105.08	101.64
4	V	2449	H2U	N3-C2-N1	2.72	119.53	116.65
4	V	2449	H2U	O2-C2-N1	-2.43	120.06	123.11
4	V	2504	PSU	C2'-C3'-C4'	-2.35	98.08	102.64
4	V	955	PSU	C2'-C3'-C4'	-2.11	98.54	102.64
4	V	2069	G7M	N9-C8-N7	-2.04	107.17	112.21

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	V	746	PSU	C2'-C1'-C5-C4
4	V	746	PSU	C2'-C1'-C5-C6
4	V	1835	2MG	N3-C2-N2-CM2
4	V	2030	6MZ	O4'-C4'-C5'-O5'
4	V	2030	6MZ	C3'-C4'-C5'-O5'
2	d	150	MEQ	NE2-CD-CG-CB
2	d	150	MEQ	OE1-CD-CG-CB
4	V	2552	OMU	O4'-C4'-C5'-O5'
4	V	747	5MU	C3'-C4'-C5'-O5'
4	V	2552	OMU	C3'-C4'-C5'-O5'
4	V	746	PSU	O4'-C1'-C5-C4
4	V	2580	PSU	O4'-C1'-C5-C4
4	V	1962	5MC	O4'-C1'-N1-C6
4	V	746	PSU	O4'-C1'-C5-C6
4	V	2503	2MA	O4'-C1'-N9-C8
4	V	2069	G7M	O4'-C4'-C5'-O5'
4	V	2503	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
4	V	1962	5MC	C2'-C1'-N1-C6

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	V	2030	6MZ	4	0
4	V	2251	OMG	1	0
2	d	150	MEQ	1	0
4	V	1835	2MG	1	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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
36	SPM	V	3001	-	13,13,13	0.23	0	12,12,12	0.28	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
36	SPM	V	3001	-	-	2/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	V	3001	SPM	C7-C8-C9-N10
36	V	3001	SPM	C8-C9-N10-C11

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
4	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	2030:6MZ	O3'	2031:A	P	2.41

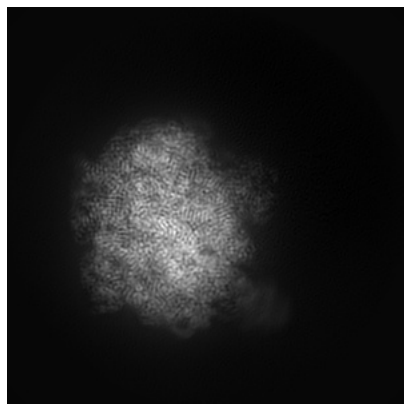
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55849. These allow visual inspection of the internal detail of the map and identification of artifacts.

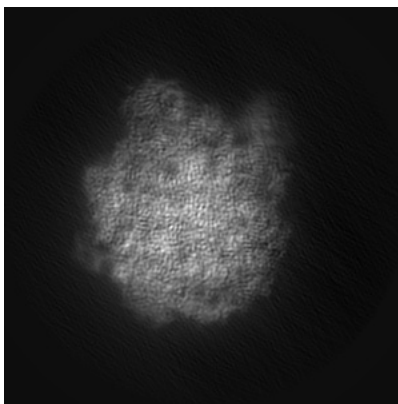
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

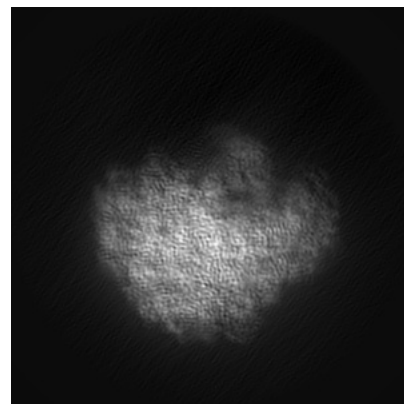
#### 6.1.1 Primary map



X

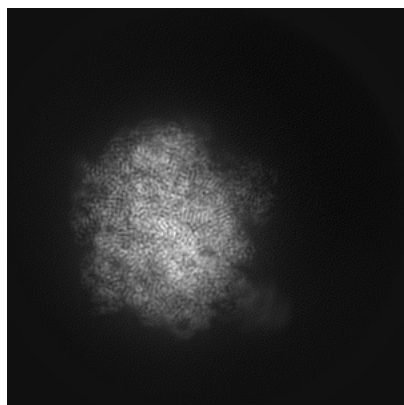


Y

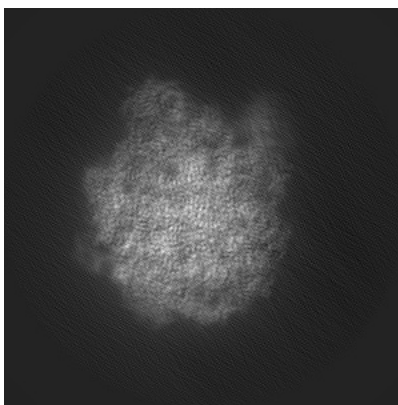


Z

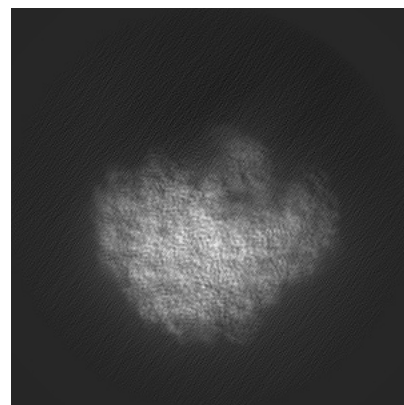
#### 6.1.2 Raw map



X



Y

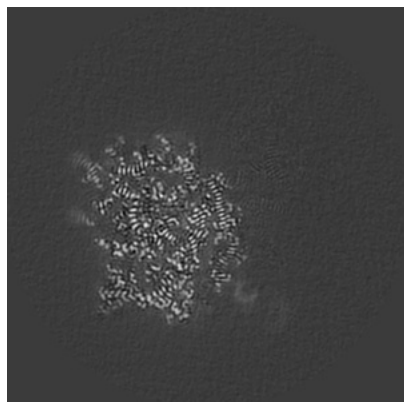


Z

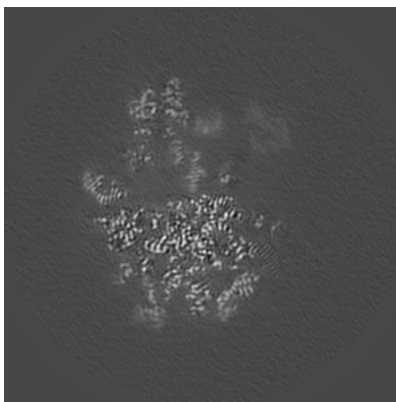
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

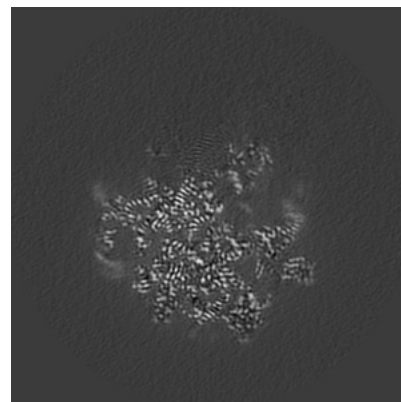
### 6.2.1 Primary map



X Index: 208

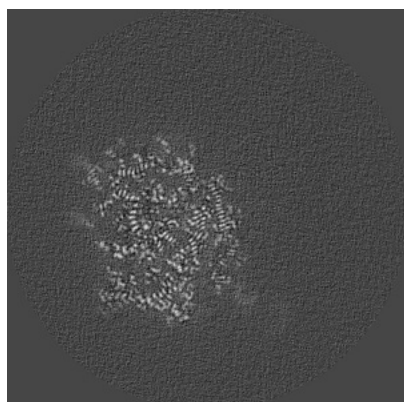


Y Index: 208

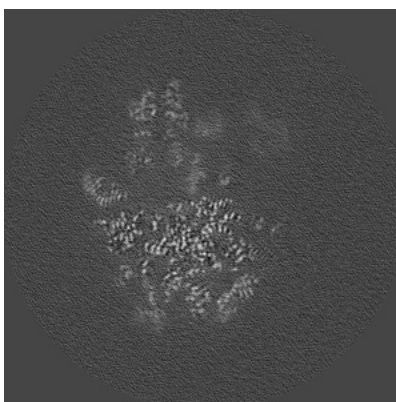


Z Index: 208

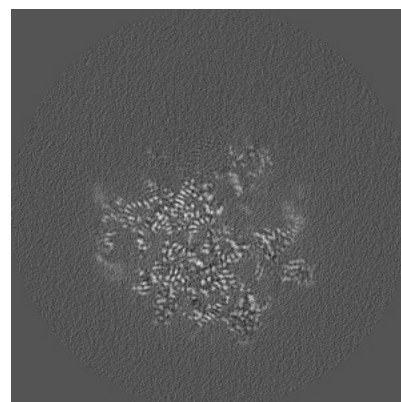
### 6.2.2 Raw map



X Index: 208



Y Index: 208

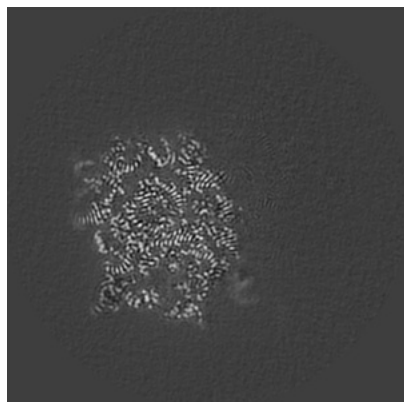


Z Index: 208

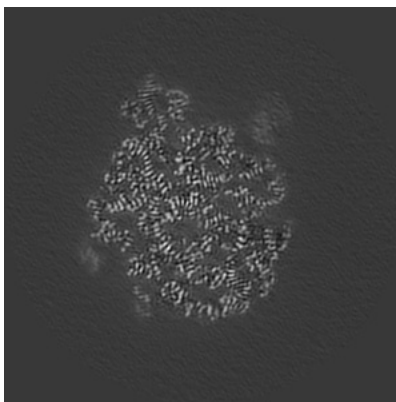
The images above show central slices of the map in three orthogonal directions.

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

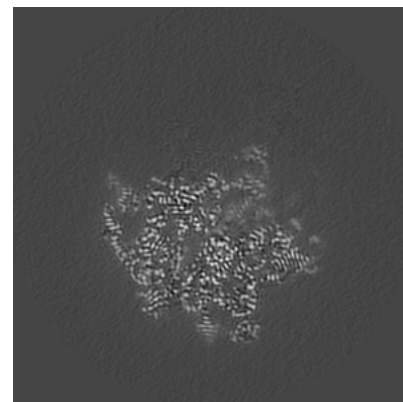
### 6.3.1 Primary map



X Index: 200

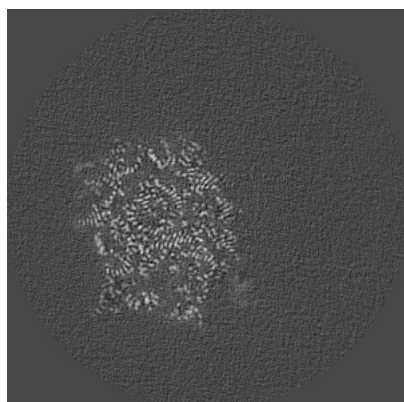


Y Index: 169

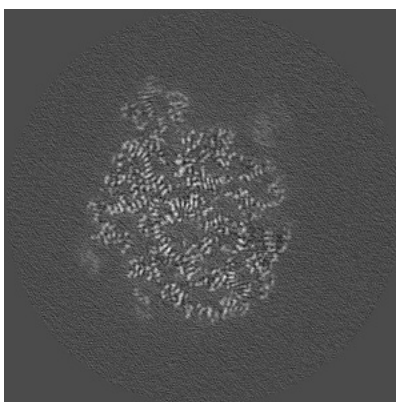


Z Index: 194

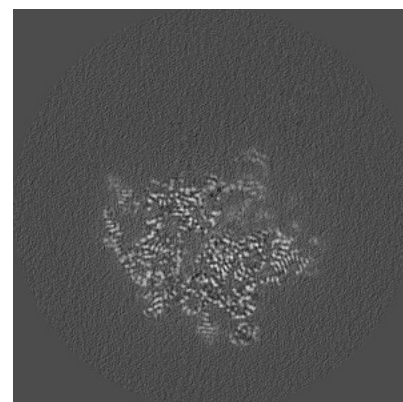
### 6.3.2 Raw map



X Index: 200



Y Index: 169

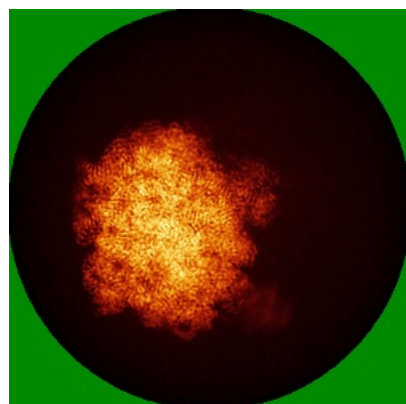


Z Index: 193

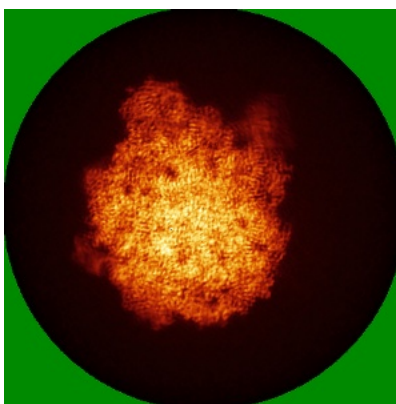
The images above show the largest variance slices of the map in three orthogonal directions.

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

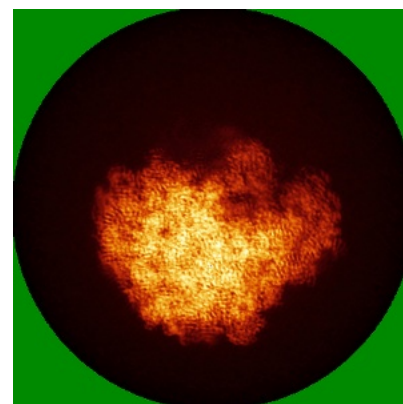
### 6.4.1 Primary map



X

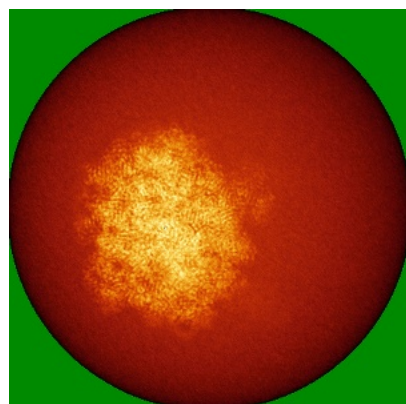


Y

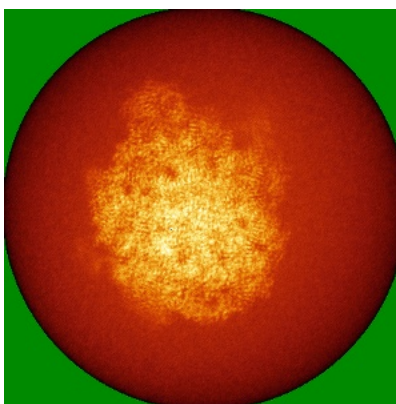


Z

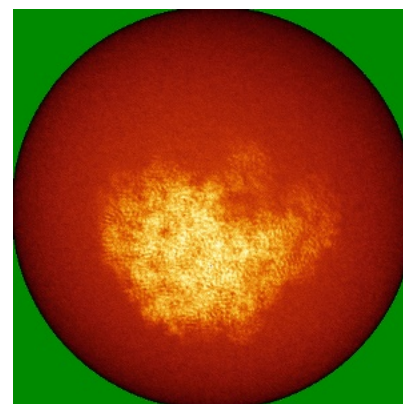
### 6.4.2 Raw map



X



Y

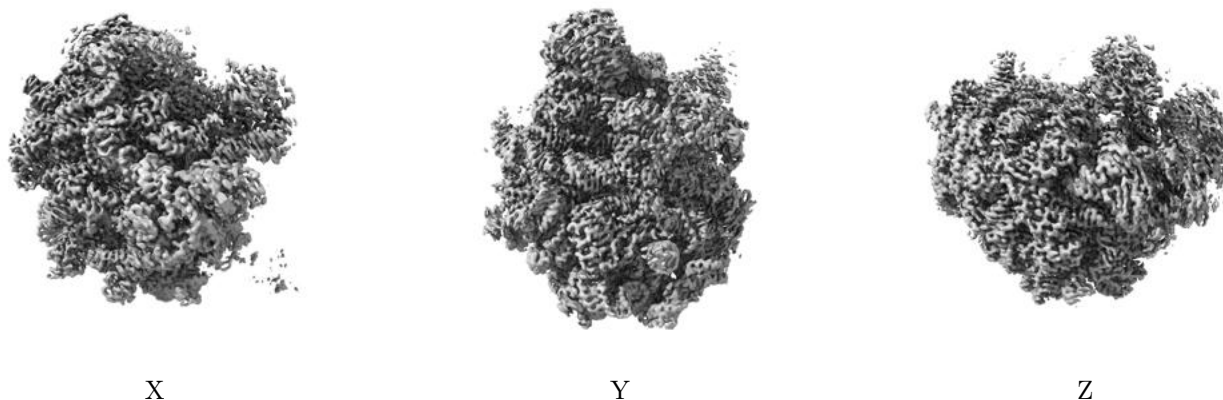


Z

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.

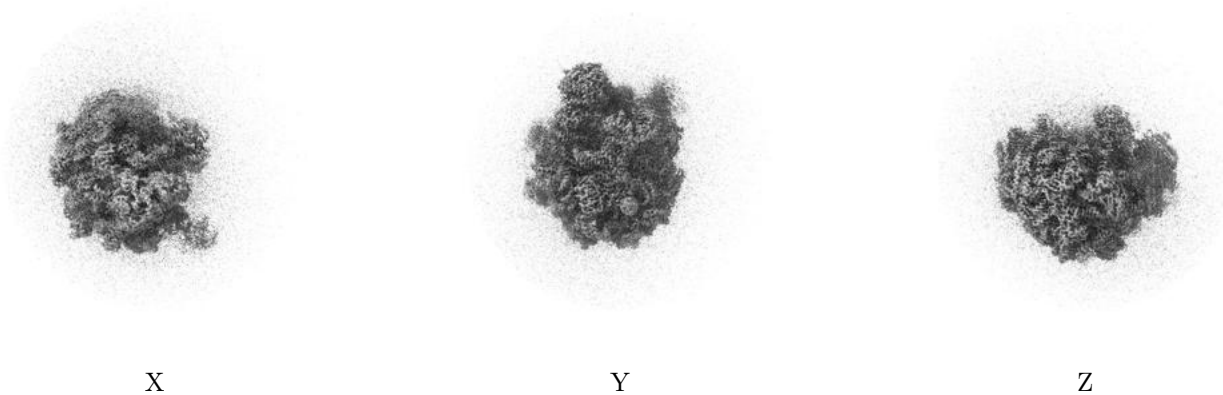
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

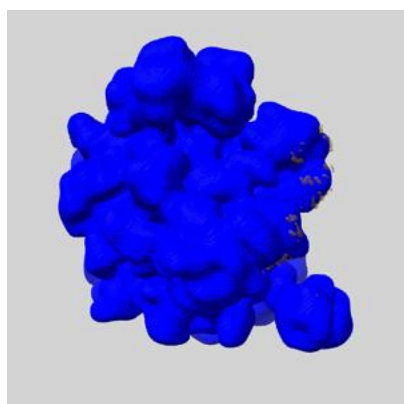
## 6.6 Mask visualisation [i](#)

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

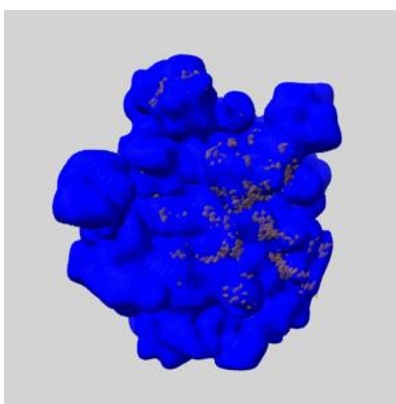
A mask typically either:

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

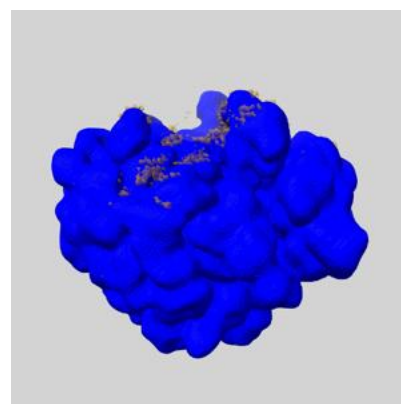
### 6.6.1 emd\_55849\_msk\_1.map [i](#)



X



Y

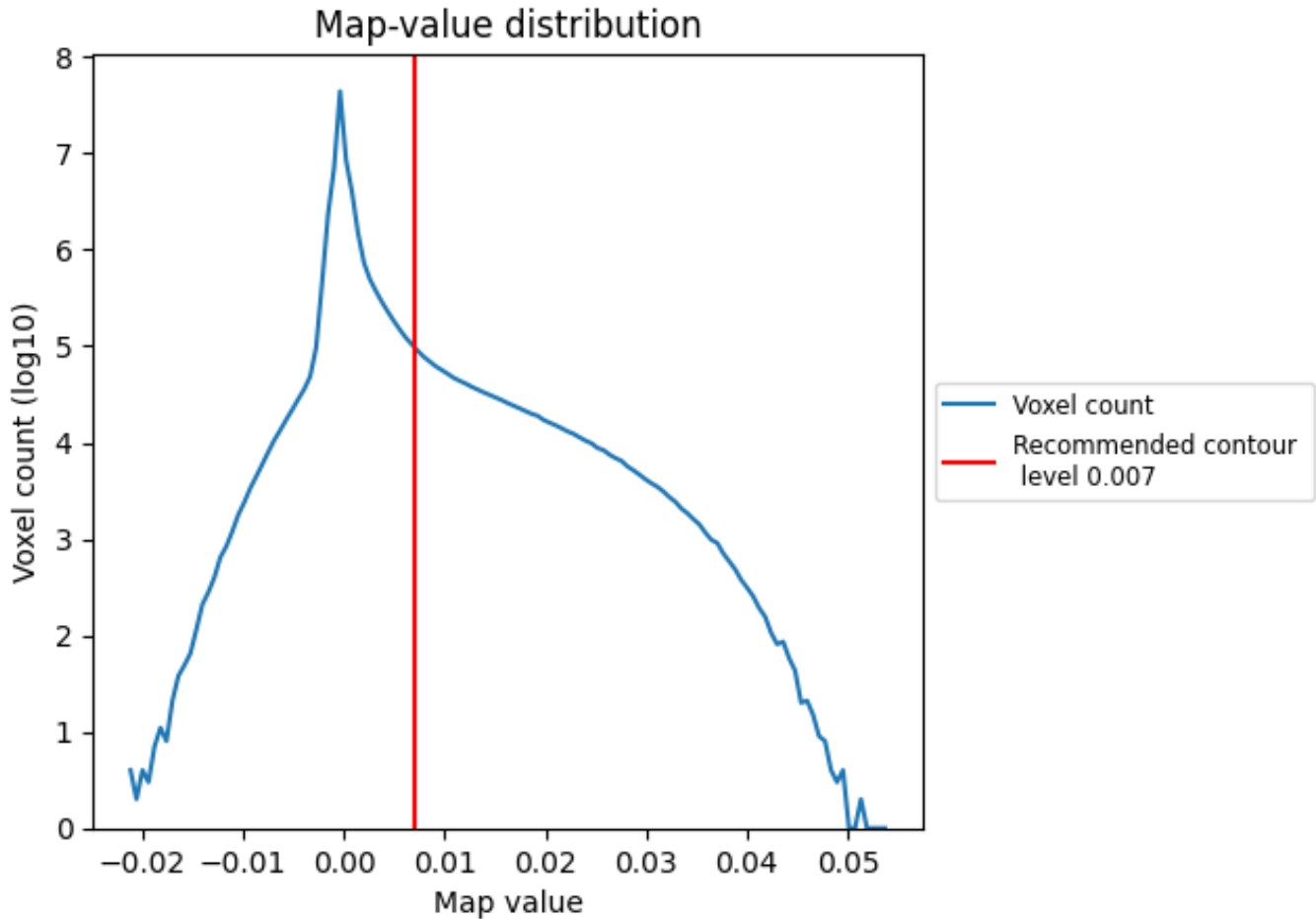


Z

## 7 Map analysis [i](#)

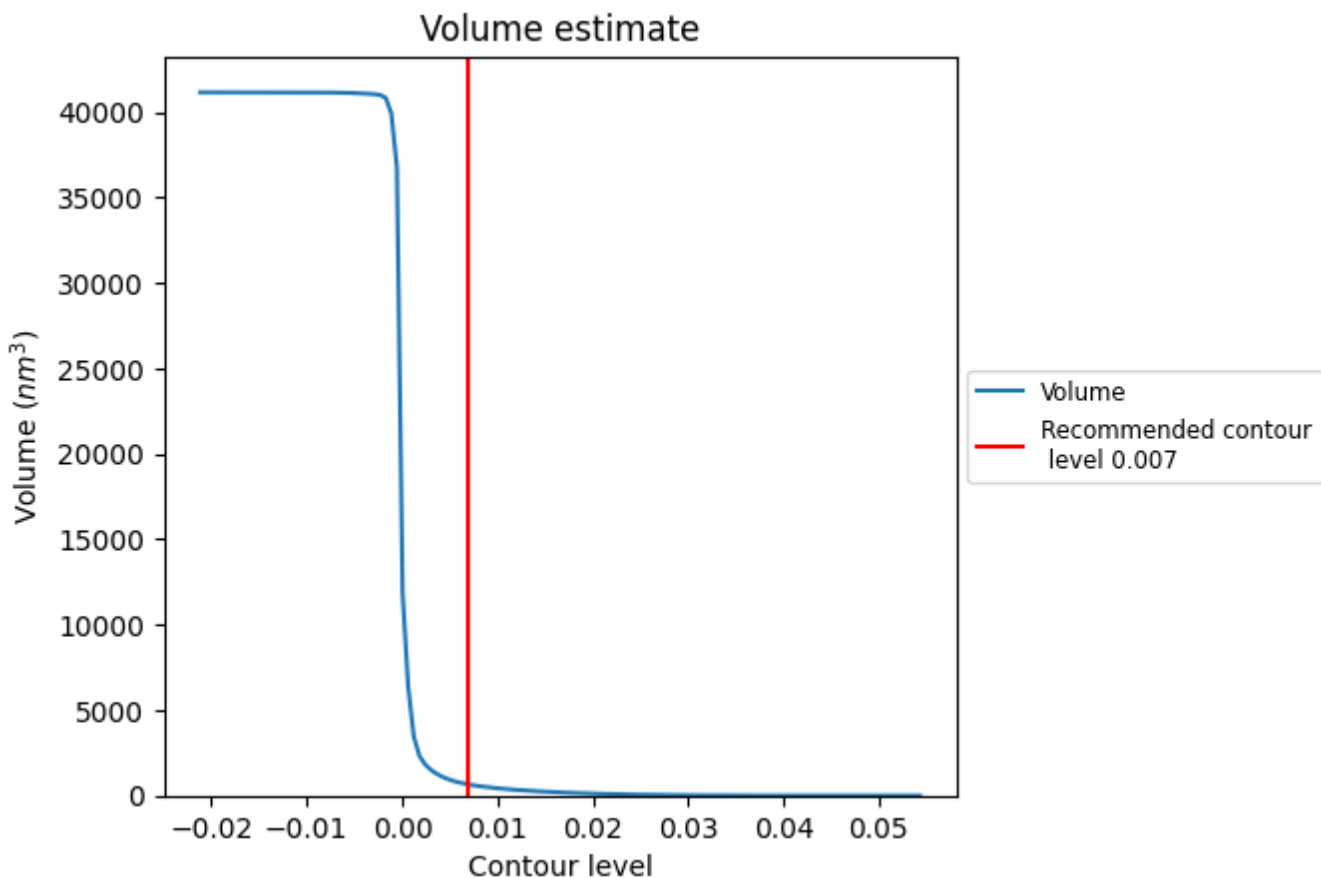
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

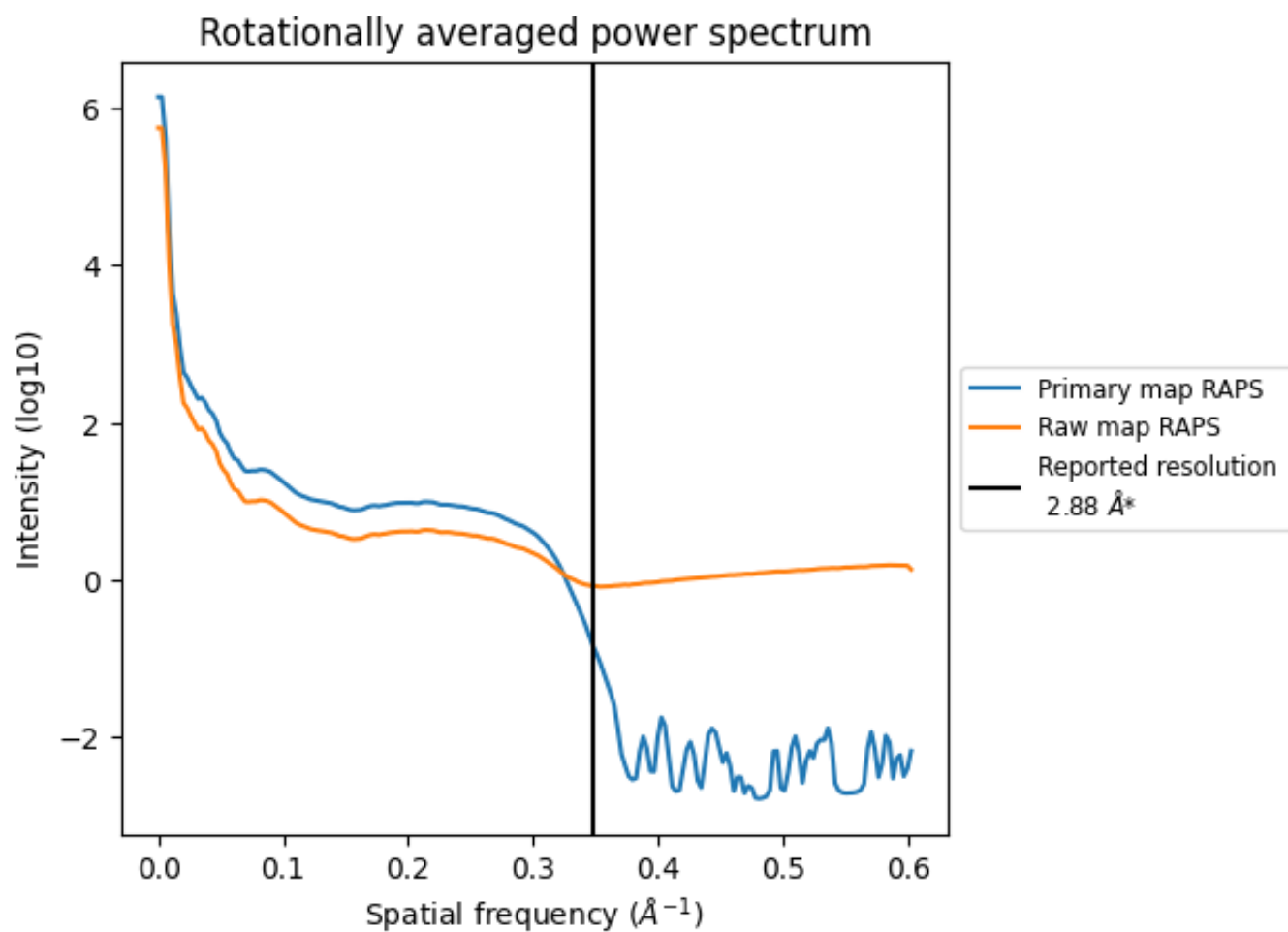
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 647 nm<sup>3</sup>; this corresponds to an approximate mass of 584 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

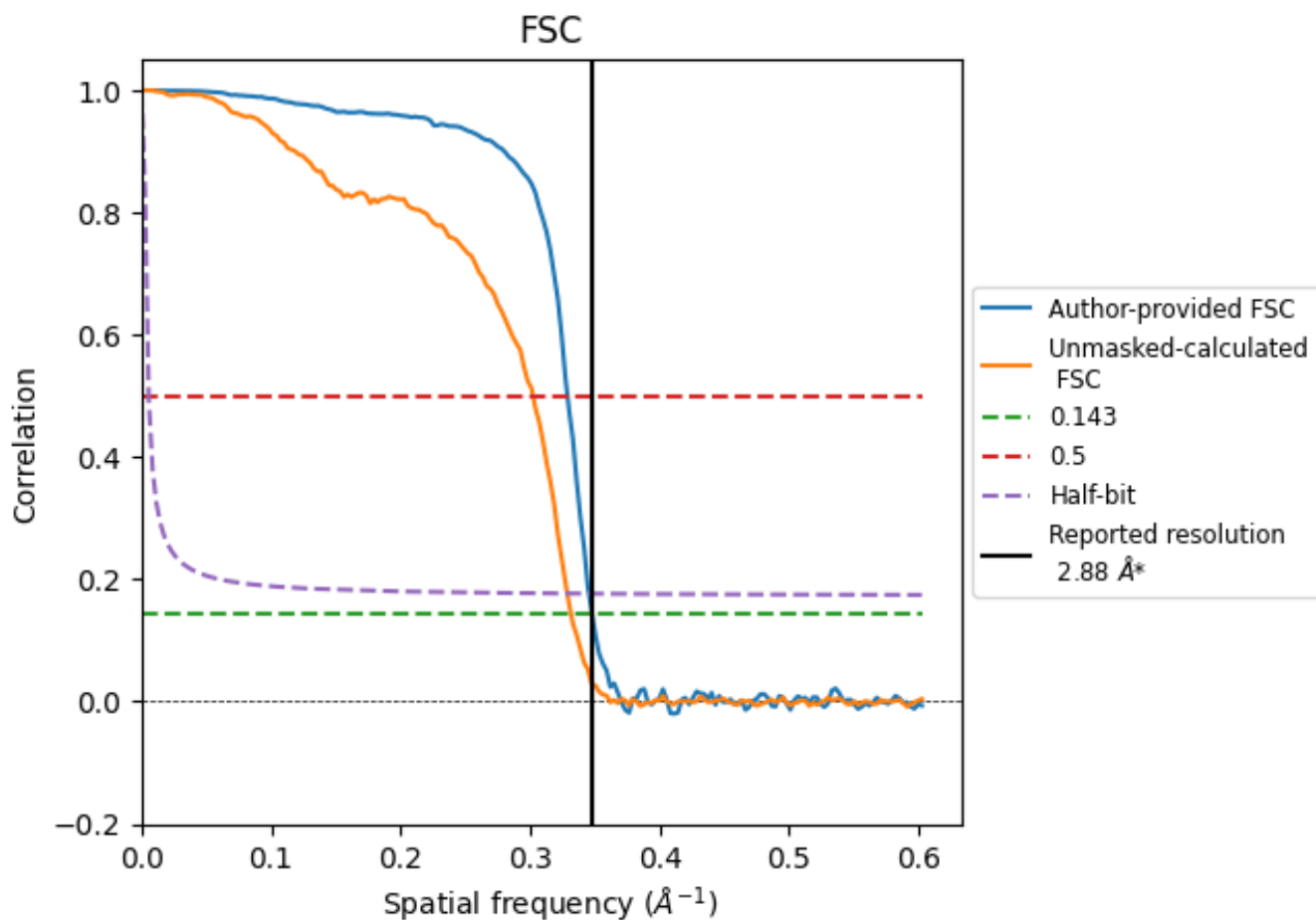


\*Reported resolution corresponds to spatial frequency of 0.347 Å<sup>-1</sup>

## 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 0.347 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

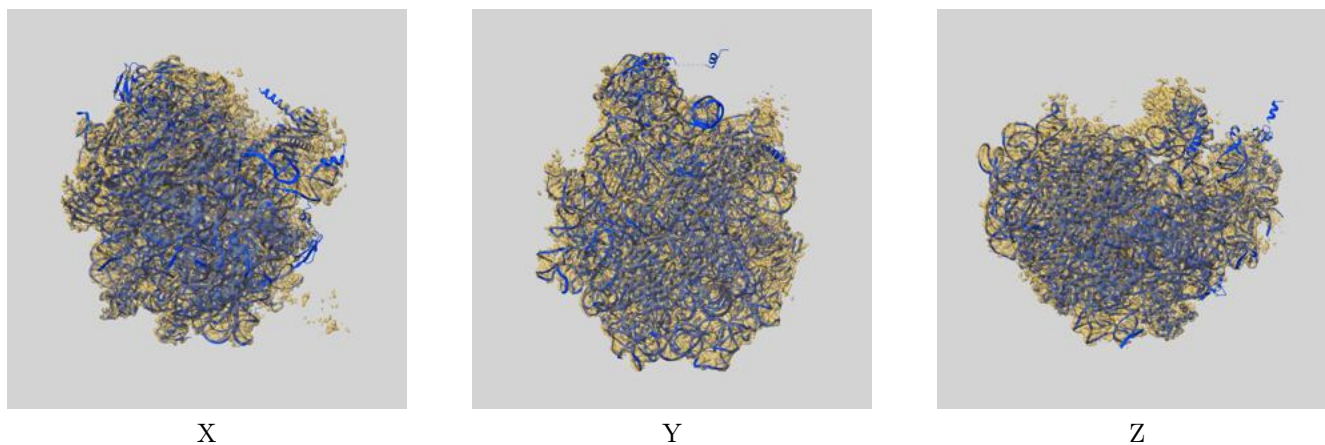
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.88	-	-
Author-provided FSC curve	2.87	3.04	2.89
Unmasked-calculated*	3.02	3.31	3.04

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

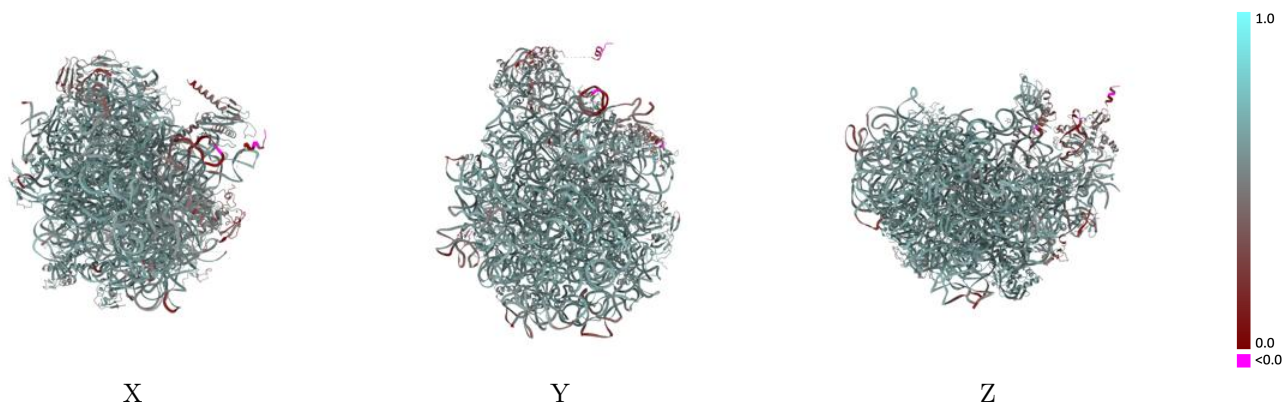
This section contains information regarding the fit between EMDB map EMD-55849 and PDB model 9TEZ. Per-residue inclusion information can be found in section 3 on page 11.

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



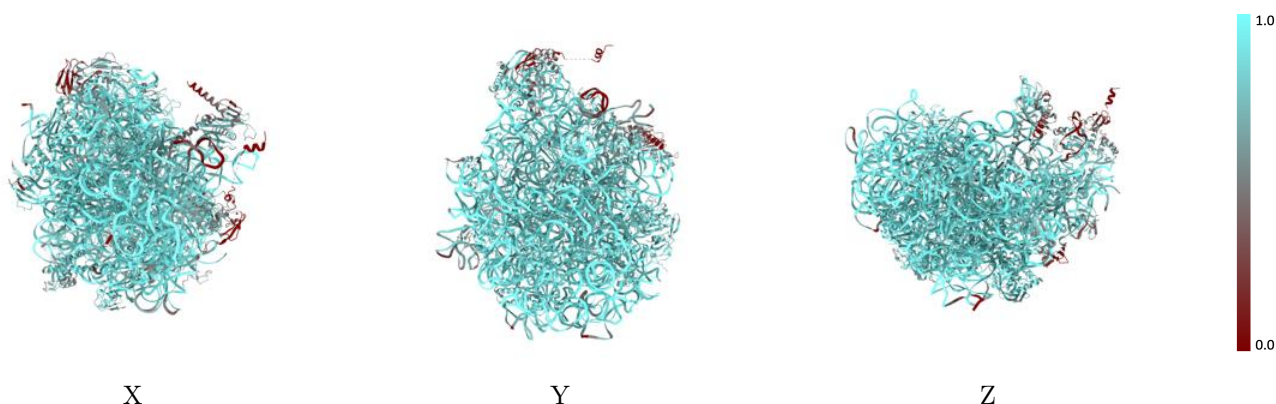
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



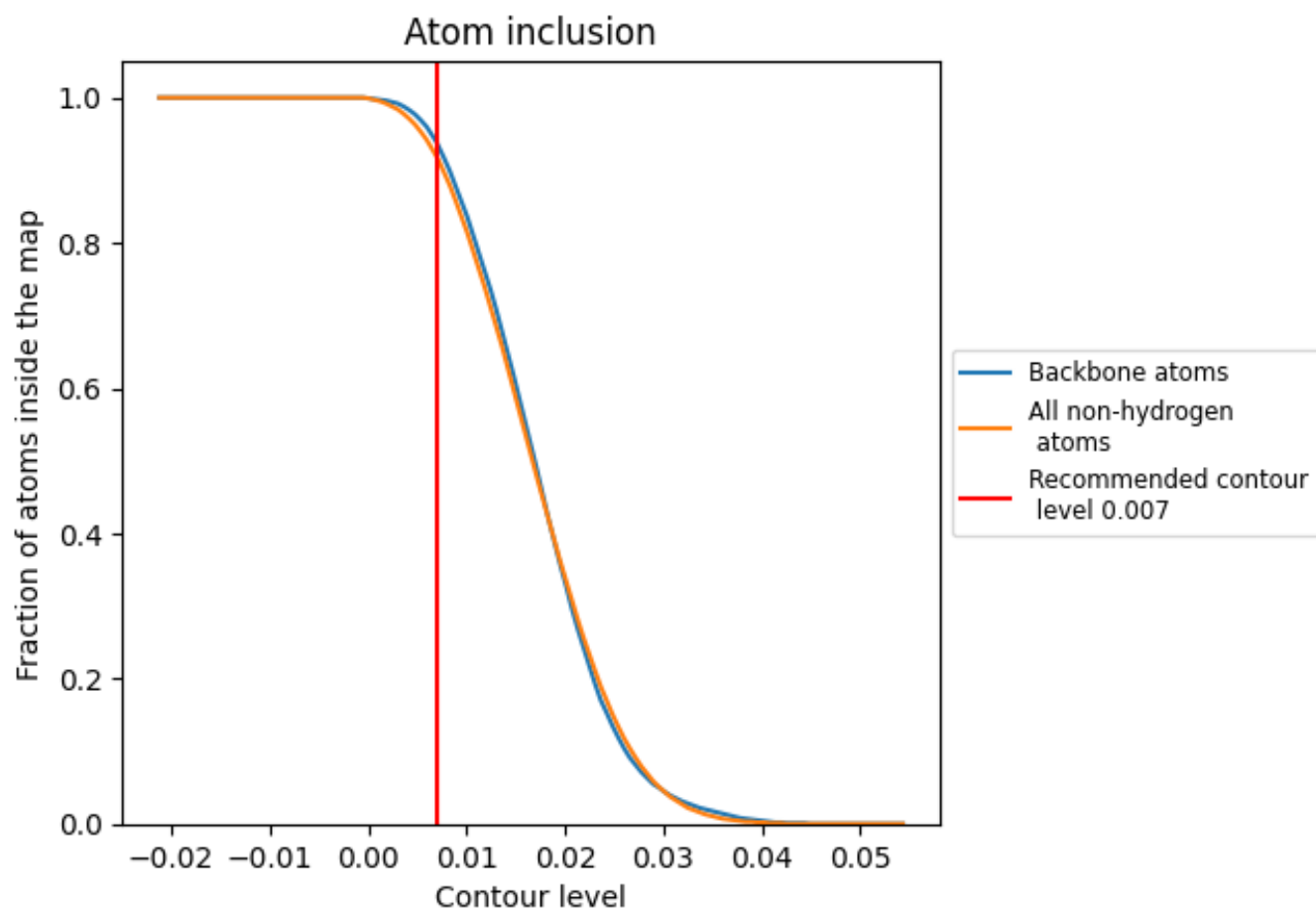
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9180	 0.5840
0	 0.8630	 0.5610
1	 0.9520	 0.6160
2	 0.9610	 0.6230
3	 0.9040	 0.5830
4	 0.1400	 0.2720
8	 0.9660	 0.5940
V	 0.9620	 0.5950
W	 0.6290	 0.4940
Z	 0.8740	 0.5330
b	 0.9310	 0.5740
c	 0.9230	 0.6060
d	 0.9120	 0.6020
e	 0.8330	 0.5840
f	 0.6130	 0.4680
g	 0.5480	 0.4720
h	 0.6370	 0.4780
i	 0.9160	 0.5990
j	 0.8780	 0.5880
k	 0.8970	 0.5960
l	 0.9090	 0.5920
m	 0.9560	 0.6140
n	 0.7980	 0.5470
o	 0.8410	 0.5850
p	 0.9530	 0.6170
q	 0.8620	 0.5930
r	 0.9080	 0.5950
s	 0.8630	 0.5780
t	 0.8270	 0.5570
u	 0.7910	 0.5540
v	 0.9080	 0.5950
w	 0.9200	 0.5990
x	 0.8160	 0.5550
y	 0.8670	 0.5790
z	 0.9020	 0.6000

