



## Full wwPDB EM Validation Report ⓘ

Apr 16, 2026 – 10:38 am BST

PDB ID : 9TZ5 / pdb\_00009tz5  
EMDB ID : EMD-56459  
Title : Triple Stack Doxycycline Bound 50S Subunit of the Coxiella burnetii Ribosome  
Authors : Stuart, W.S.; Isupov, M.N.; Harmer, N.J.  
Deposited on : 2026-01-22  
Resolution : 2.22 Å(reported)  
Based on initial model : .

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:

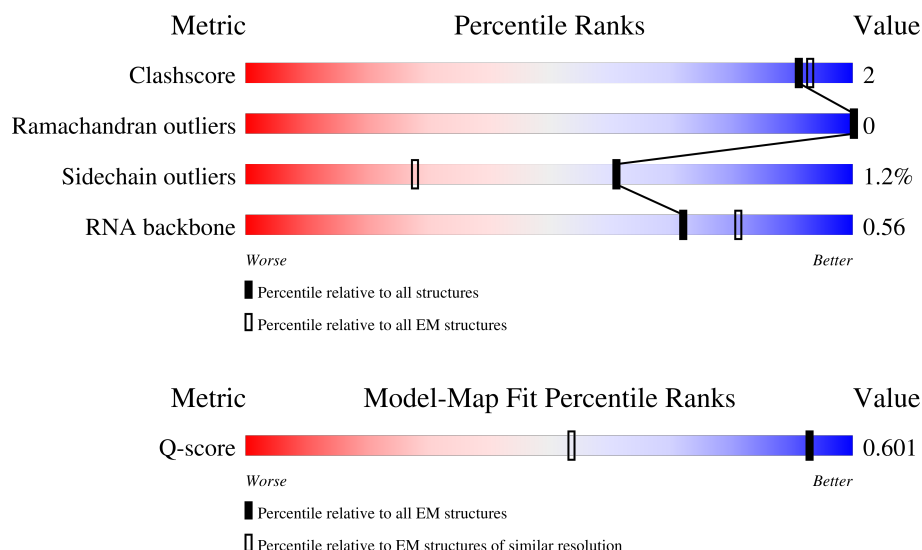
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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 2.22 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.








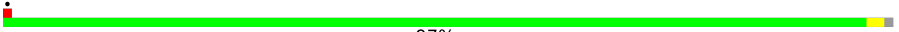






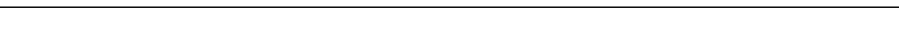

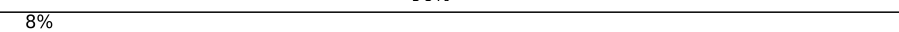

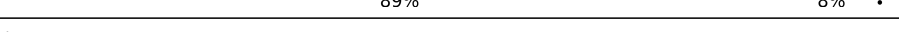
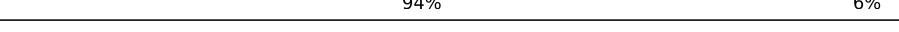



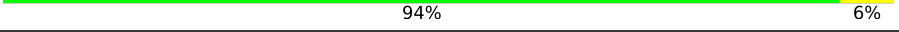
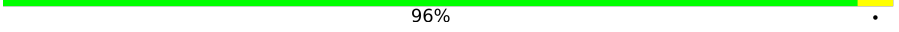
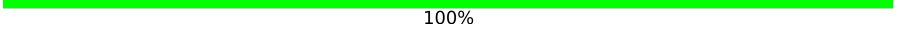
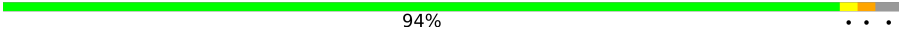
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3277 ( 1.73 - 2.72 )

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	Z	21	
2	0	70	
3	1	107	



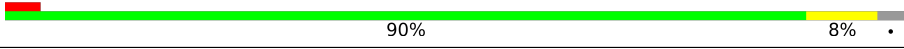
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Mol	Chain	Length	Quality of chain
4	2	117	 92% 6% ..
5	3	40	 92% 5%
6	b	117	 87% 12% .
7	c	115	 10% 90% 8% ..
8	d	217	 92% 5% .
9	e	119	 97% ..
10	f	182	 67% 93% 5% .
11	g	178	 20% 89% 9% .
12	h	115	 90% 10%
13	i	142	 95% ..
14	j	115	 88% 8% .
15	k	143	 93% 7%
16	m	126	 90% 6%
17	o	275	 96% .
18	q	152	 8% 28% 70%
19	r	65	 6% 89% 8% .
20	s	137	 94% 6%
21	t	63	 86% 11%
22	u	244	 22% 72% 6% 22%
23	v	64	 75% 9% 16%
24	w	205	 94% 6%
25	x	122	 96% .
26	y	44	 100%
27	z	64	 94% ..
28	a	2925	 6% 79% 17% ..

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Mol	Chain	Length	Quality of chain
29	8	90	 <div>79%7%14%</div>
30	7	95	 <div>88%7%</div>
31	9	79	 <div>90%8%</div>

## 2 Entry composition [i](#)

There are 36 unique types of molecules in this entry. The entry contains 90136 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 Coxiellacae Large Subunit Peptide (CLaSP).

Mol	Chain	Residues	Atoms				AltConf	Trace
1	Z	16	Total	C	N	O	0	0
			133	82	34	17		

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	0	68	Total	C	N	O	S	0	0
			550	349	99	99	3		

- Molecule 3 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	1	105	Total	C	N	O	0	0
			813	512	153	148		

- Molecule 4 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	116	Total	C	N	O	S	0	0
			913	566	188	157	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	38	Total	C	N	O	S	0	0
			307	183	73	46	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	b	117	Total	C	N	O	P	0	0
			2488	1112	445	815	116		

- Molecule 7 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	c	113	Total	C	N	O	0	0
			919	573	184	162		

- Molecule 8 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	d	211	Total	C	N	O	S	0	0
			1596	995	298	298	5		

- Molecule 9 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	e	118	Total	C	N	O	S	0	0
			941	595	194	151	1		

- Molecule 10 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	f	182	Total	C	N	O	S	0	0
			1457	930	258	261	8		

- Molecule 11 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	g	174	Total	C	N	O	S	0	0
			1310	818	245	243	4		

- Molecule 12 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	h	104	Total	C	N	O	S	0	0
			813	511	150	148	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	i	141	Total	C	N	O	S	0	0
			1108	707	206	193	2		

- Molecule 14 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	j	110	Total	C	N	O	S	0	0
			839	516	165	154	4		

- Molecule 15 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	k	143	Total	C	N	O	S	0	0
			1076	672	217	185	2		

- Molecule 16 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	m	119	Total	C	N	O	S	0	0
			967	605	195	162	5		

- Molecule 17 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	o	274	Total	C	N	O	S	0	0
			2131	1314	443	368	6		

- Molecule 18 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	q	45	Total	C	N	O	S	0	0
			339	221	59	58	1		

- Molecule 19 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	r	63	Total	C	N	O	S	0	0
			522	324	106	91	1		

- Molecule 20 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	s	137	Total	C	N	O	S	0	0
			1090	688	215	182	5		

- Molecule 21 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	t	56	Total	C	N	O	S	0	0
			449	281	86	78	4		

- Molecule 22 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	u	191	Total	C	N	O	S	0	0
			1486	940	260	281	5		

- Molecule 23 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	v	54	Total	C	N	O	S	0	0
			436	263	95	76	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	w	205	Total	C	N	O	S	0	0
			1571	974	296	296	5		

- Molecule 25 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	x	122	Total	C	N	O	S	0	0
			948	594	184	165	5		

- Molecule 26 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	y	44	Total	C	N	O	S	0	0
			374	224	91	57	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	z	62	Total	C	N	O	S	0	0
			500	308	110	80	2		

- Molecule 28 is a RNA chain called 23S ribosomal RNA.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	a	2873	Total	C	N	O	P	3	0
			61677	27530	11292	19979	2876		

- Molecule 29 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	8	77	Total	C	N	O	S	0	0
			613	381	124	105	3		

- Molecule 30 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	7	91	Total	C	N	O	S	0	0
			732	464	135	130	3		

- Molecule 31 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	77	Total	C	N	O	S	0	0
			631	395	128	106	2		

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
32	3	1	Total	Zn	0
			1	1	

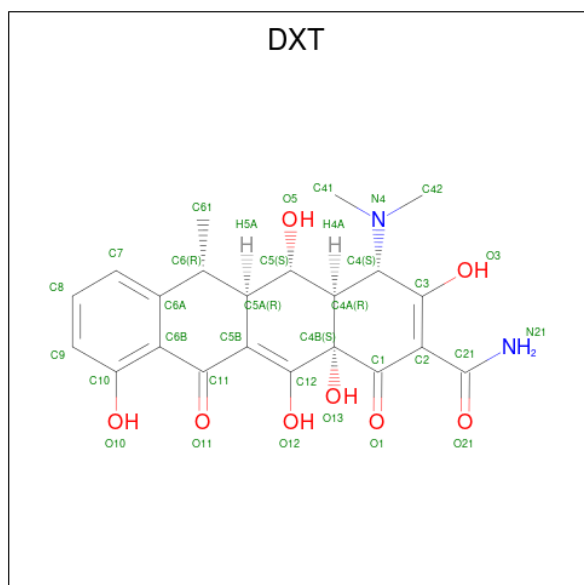
- Molecule 33 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
33	b	1	Total	Mg	0
			1	1	
33	d	1	Total	Mg	0
			1	1	
33	o	1	Total	Mg	0
			1	1	
33	a	164	Total	Mg	0
			164	164	

- Molecule 34 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
34	b	1	Total	K	0
			1	1	
34	d	1	Total	K	0
			1	1	
34	o	1	Total	K	0
			1	1	
34	s	1	Total	K	0
			1	1	
34	v	2	Total	K	0
			2	2	
34	w	1	Total	K	0
			1	1	
34	a	126	Total	K	0
			126	126	
34	8	1	Total	K	0
			1	1	

- Molecule 35 is (4S,4AR,5S,5AR,6R,12AS)-4-(DIMETHYLAMINO)-3,5,10,12,12A-PENTAHYDROXY-6-METHYL-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: DXT) (formula: C<sub>22</sub>H<sub>24</sub>N<sub>2</sub>O<sub>8</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
35	a	1	Total	C	N	O	0
			32	22	2	8	
35	a	1	Total	C	N	O	0
			32	22	2	8	

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Mol	Chain	Residues	Atoms				AltConf
35	a	1	Total	C	N	O	0
			32	22	2	8	


- Molecule 36 is water.

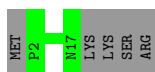
Mol	Chain	Residues	Atoms		AltConf
36	a	8	Total	O	0
			8	8	
36	9	1	Total	O	0
			1	1	

### 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.

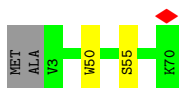
- Molecule 1: Coxiellaceae Large Subunit Peptide (CLaSP)

Chain Z: 



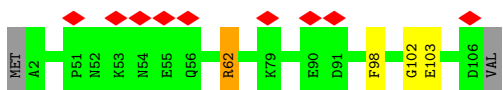
- Molecule 2: Large ribosomal subunit protein bL33

Chain 0: 



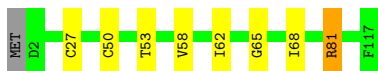
- Molecule 3: Large ribosomal subunit protein uL24

Chain 1: 



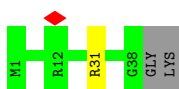
- Molecule 4: Large ribosomal subunit protein uL18

Chain 2: 




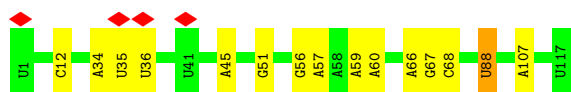
- Molecule 5: Large ribosomal subunit protein bL36

Chain 3: 

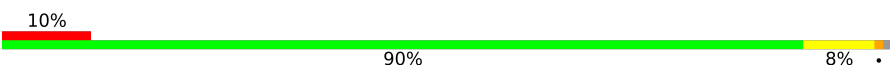


- Molecule 6: 5S ribosomal RNA

Chain b:  87% 12%



- Molecule 7: Large ribosomal subunit protein bL19

Chain c:  10% 90% 8%



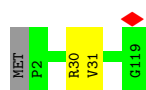
- Molecule 8: Large ribosomal subunit protein uL3

Chain d:  92% 5%

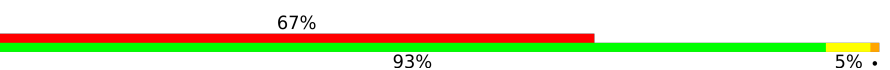


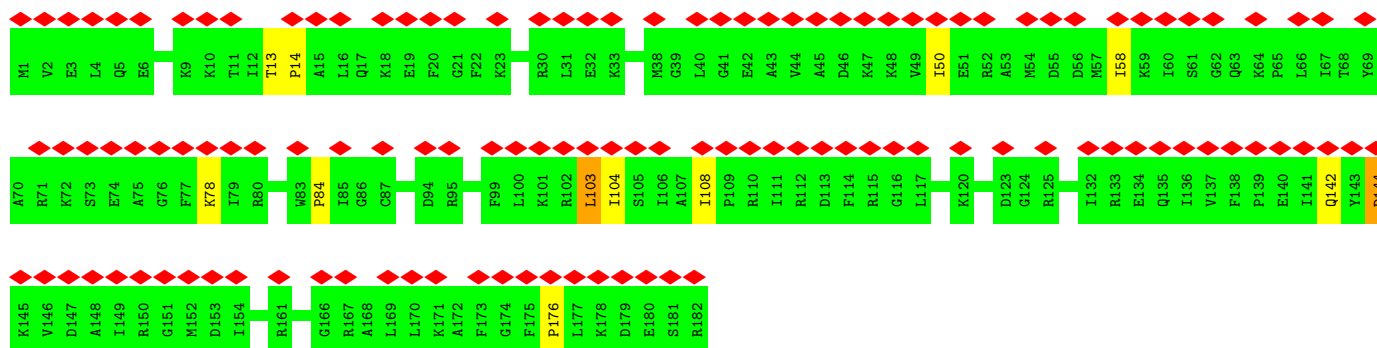
- Molecule 9: Large ribosomal subunit protein bL20

Chain e:  97%

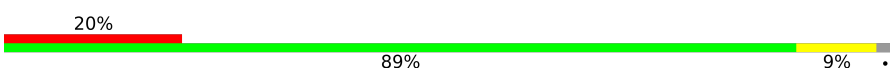


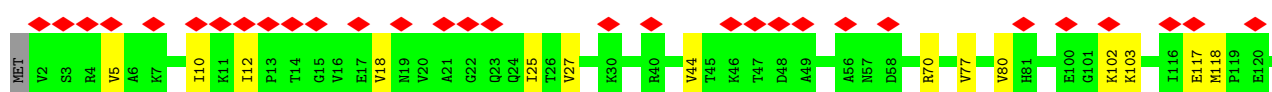
- Molecule 10: Large ribosomal subunit protein uL5

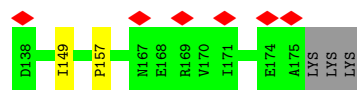
Chain f:  67% 93% 5%



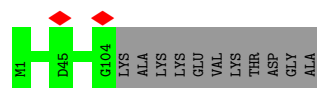
- Molecule 11: Large ribosomal subunit protein uL6

Chain g:  20% 89% 9%

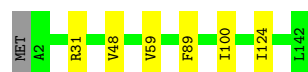




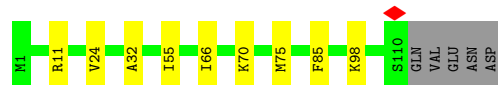
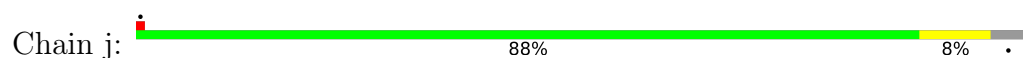
- Molecule 12: Large ribosomal subunit protein bL21



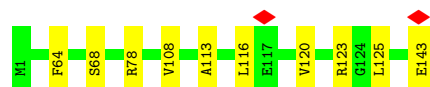
- Molecule 13: Large ribosomal subunit protein uL13



- Molecule 14: Large ribosomal subunit protein uL22



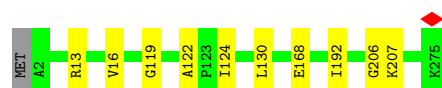
- Molecule 15: Large ribosomal subunit protein uL15



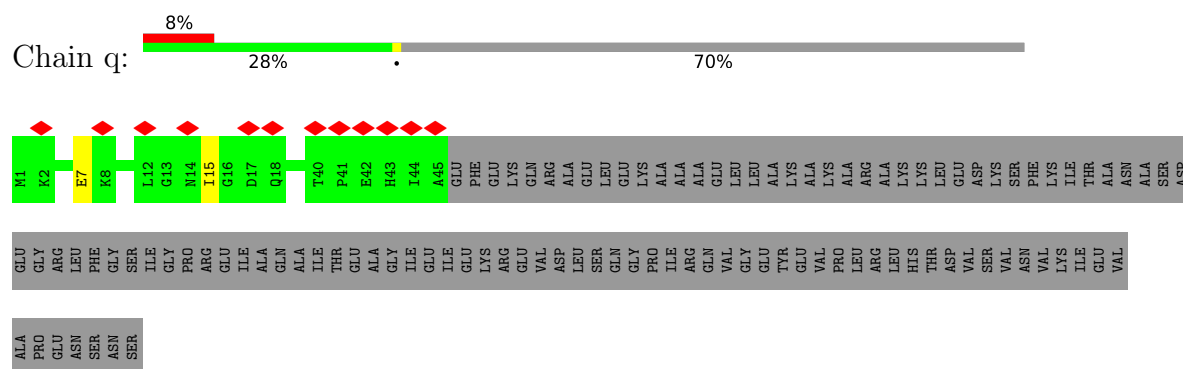
- Molecule 16: Large ribosomal subunit protein bL17



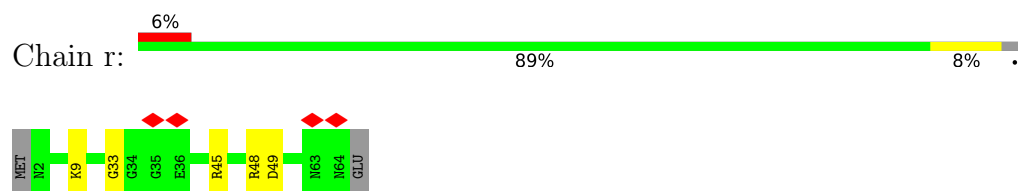
- Molecule 17: Large ribosomal subunit protein uL2



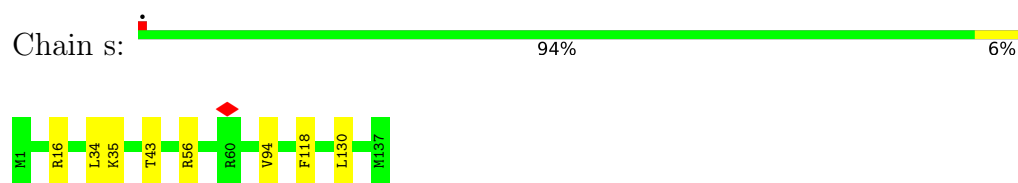
- Molecule 18: Large ribosomal subunit protein bL9



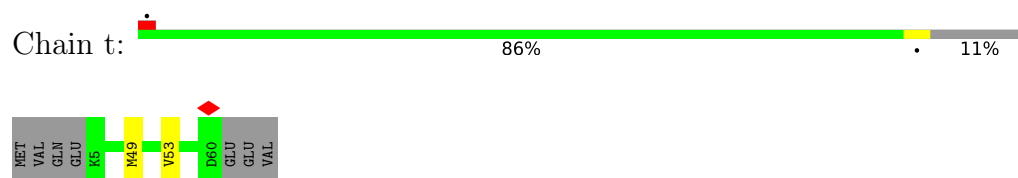
- Molecule 19: Large ribosomal subunit protein uL29



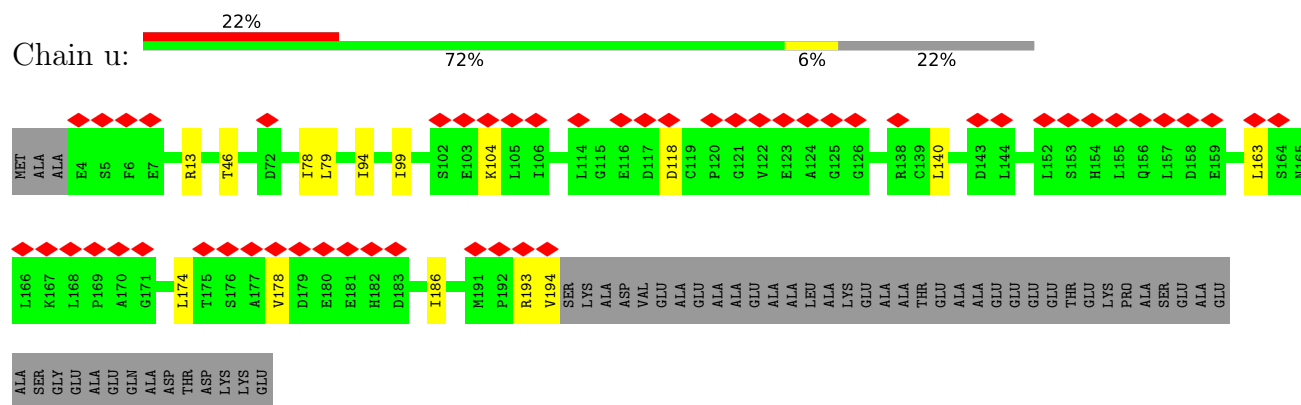
- Molecule 20: Large ribosomal subunit protein uL16



- Molecule 21: Large ribosomal subunit protein uL30



- Molecule 22: Large ribosomal subunit protein bL25



- Molecule 23: Large ribosomal subunit protein bL32





- Molecule 24: Large ribosomal subunit protein uL4



- Molecule 25: Large ribosomal subunit protein uL14



- Molecule 26: Large ribosomal subunit protein bL34

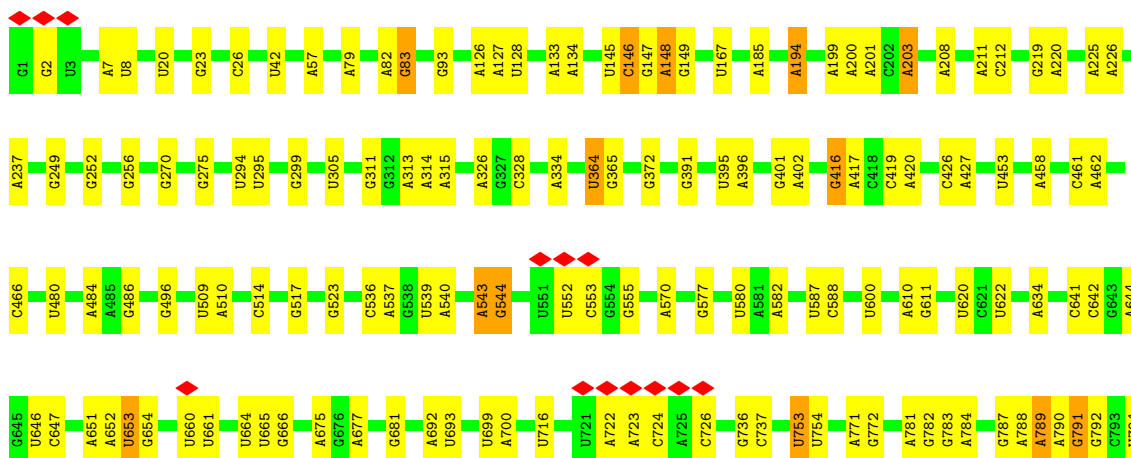
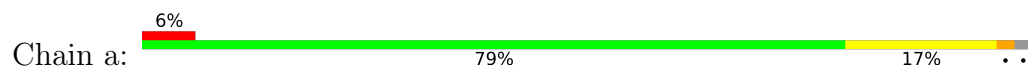


There are no outlier residues recorded for this chain.

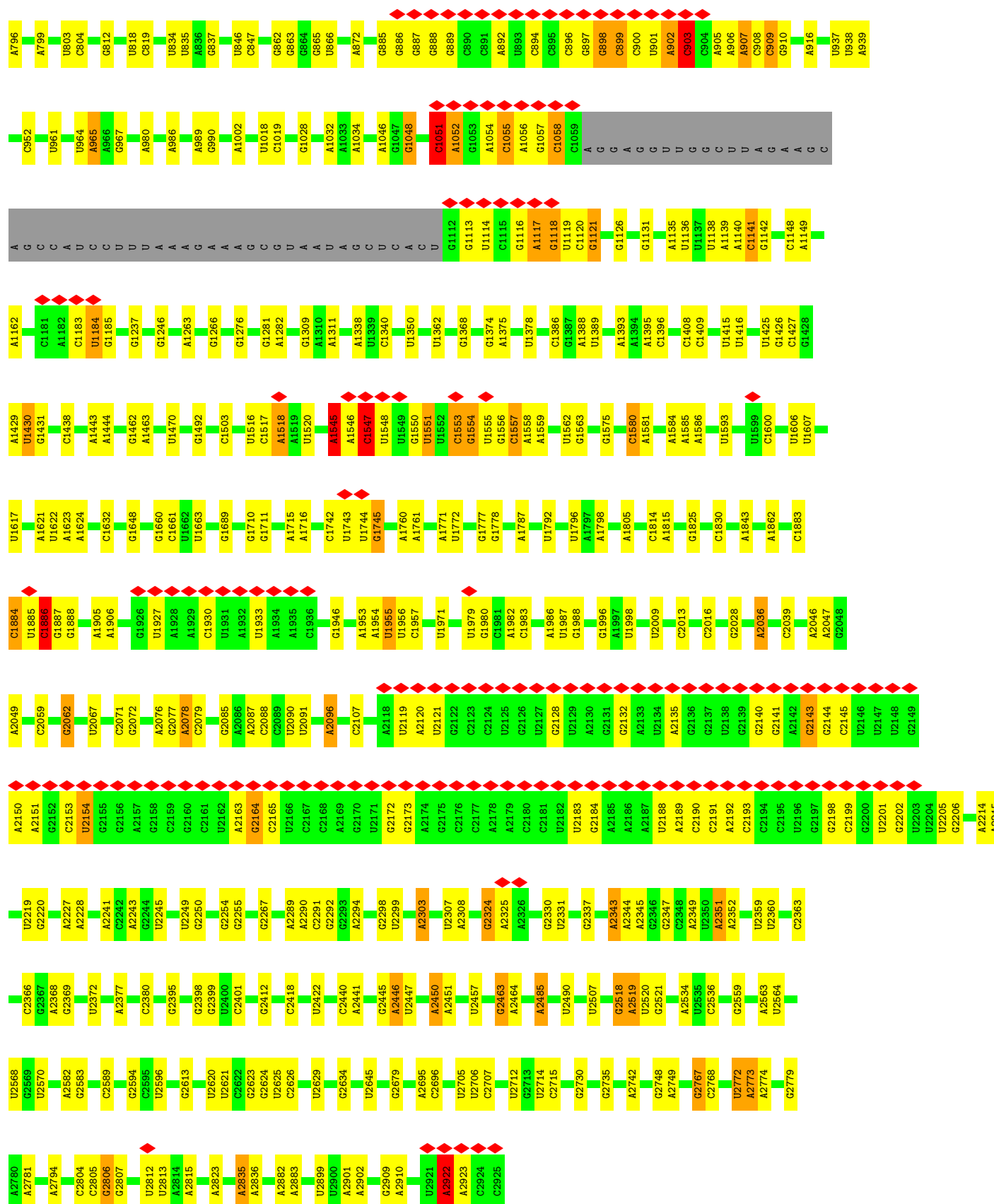
- Molecule 27: Large ribosomal subunit protein bL35

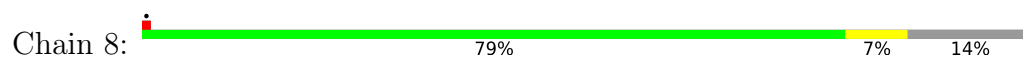


- Molecule 28: 23S ribosomal RNA





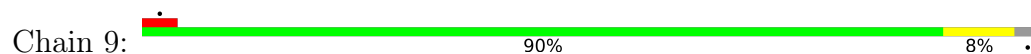




- Molecule 30: Large ribosomal subunit protein uL23



- Molecule 31: Large ribosomal subunit protein bL28



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91218	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.553	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: DXT, ZN, 2MA, OMG, OMU, PSU, MG, K

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	Z	0.46	0/137	0.94	0/178
2	0	0.43	0/561	0.86	0/747
3	1	0.44	0/820	0.90	0/1098
4	2	0.45	0/922	1.04	0/1227
5	3	0.44	0/307	0.89	0/402
6	b	0.38	0/2780	0.76	2/4331 (0.0%)
7	c	0.41	0/929	0.86	0/1241
8	d	0.45	0/1617	0.94	0/2173
9	e	0.42	0/954	1.06	0/1268
10	f	0.47	0/1480	1.01	0/1980
11	g	0.46	0/1325	0.96	1/1791 (0.1%)
12	h	0.42	0/822	0.84	0/1098
13	i	0.46	0/1132	0.95	0/1526
14	j	0.48	0/845	0.97	0/1131
15	k	0.47	0/1088	0.99	1/1443 (0.1%)
16	m	0.46	0/983	1.00	0/1316
17	o	0.49	0/2170	0.97	0/2909
18	q	0.47	0/345	0.93	0/468
19	r	0.39	0/526	1.16	0/697
20	s	0.44	0/1107	1.00	0/1475
21	t	0.45	0/454	0.94	0/605
22	u	0.46	0/1512	0.90	0/2041
23	v	0.47	0/443	1.01	0/589
24	w	0.47	1/1589 (0.1%)	0.99	0/2136
25	x	0.41	0/954	0.88	0/1277
26	y	0.41	0/377	1.11	0/493
27	z	0.44	0/505	1.02	0/665
28	a	0.37	1/68862 (0.0%)	0.79	80/107409 (0.1%)
29	8	0.45	0/623	0.90	0/829
30	7	0.44	0/744	0.98	0/999
31	9	0.43	0/640	1.00	0/853
All	All	0.39	2/97553 (0.0%)	0.83	84/146395 (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
28	a	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	w	1	MET	SD-CE	-6.44	1.63	1.79
28	a	2568	OMU	O3'-P	5.26	1.61	1.56

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	395	U	C4'-C3'-O3'	13.37	129.46	109.40
28	a	1184	U	C2'-C3'-O3'	11.72	127.08	109.50
28	a	426	C	C2'-C3'-O3'	11.36	126.53	109.50
6	b	34	A	C2'-C3'-O3'	-10.24	98.34	113.70
28	a	2835	A	C4'-C3'-O3'	-9.16	99.26	113.00
28	a	1051	C	C2'-C3'-O3'	8.96	122.95	109.50
28	a	1430	U	C2'-C3'-O3'	8.37	122.05	109.50
28	a	903	C	N1-C1'-C2'	8.19	124.29	112.00
28	a	1388	A	C2'-C3'-O3'	7.87	121.30	109.50
28	a	1771	A	C4'-C3'-O3'	-7.76	101.36	113.00
28	a	1744	U	C2'-C3'-O3'	7.62	120.93	109.50
28	a	1562	U	C2'-C3'-O3'	7.59	120.89	109.50
28	a	1956	U	C2'-C3'-O3'	7.55	120.83	109.50
28	a	1955	U	C1'-C2'-O2'	-7.47	100.60	111.80
28	a	2806	G	C2'-C3'-O3'	7.42	120.63	109.50
28	a	909	C	C2'-C3'-O3'	7.10	124.34	113.70
28	a	964	U	C2'-C3'-O3'	-7.00	103.20	113.70
28	a	1580	C	C2'-C3'-O3'	6.97	119.95	109.50
28	a	834	U	C2'-C3'-O3'	-6.95	103.28	113.70
28	a	1884	C	C4'-C3'-O3'	6.95	123.42	113.00
28	a	791	G	C2'-C3'-O3'	-6.87	103.39	113.70
28	a	2172	G	C4'-C3'-O3'	6.80	119.60	109.40
28	a	2779	G	C4'-C3'-O3'	-6.79	102.81	113.00
28	a	906	A	C2'-C3'-O3'	6.68	119.52	109.50
28	a	1617	U	C4'-C3'-O3'	6.55	119.23	109.40
28	a	938	U	C4'-C3'-O3'	6.42	119.03	109.40
28	a	653	U	C2'-C3'-O3'	6.33	119.00	109.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	364	U	C2'-C3'-O3'	6.31	118.96	109.50
28	a	753	U	C2'-C3'-O3'	6.25	118.88	109.50
28	a	2337	G	C2'-C3'-O3'	-6.20	104.41	113.70
28	a	395	U	C2'-C3'-O3'	-6.14	100.29	109.50
28	a	788	A	C4'-C3'-O3'	-6.13	103.80	113.00
28	a	1141	C	C4'-C3'-O3'	-6.11	103.84	113.00
28	a	208	A	C2'-C3'-O3'	-6.01	100.48	109.50
28	a	1886	C	C2'-C3'-O3'	-6.01	100.49	109.50
28	a	2303	A	C2'-C3'-O3'	-5.92	100.62	109.50
28	a	2518	G	C4'-C3'-O3'	5.92	121.88	113.00
28	a	2324	G	C2'-C3'-O3'	5.90	118.35	109.50
28	a	552	U	C4'-C3'-O3'	5.85	118.17	109.40
28	a	2735	G	C4'-C3'-O3'	-5.81	104.29	113.00
28	a	203	A	C2'-C3'-O3'	5.80	118.20	109.50
28	a	1982	A	C4'-C3'-O3'	5.78	118.07	109.40
28	a	2463	G	C4'-C3'-O3'	5.74	118.02	109.40
28	a	1710	G	C2'-C3'-O3'	-5.73	105.10	113.70
28	a	818	U	C2'-C3'-O3'	5.66	117.98	109.50
28	a	1116	G	C2'-C3'-O3'	5.65	122.17	113.70
28	a	1617	U	C3'-C2'-O2'	-5.59	106.21	114.60
6	b	88	U	C4'-C3'-O3'	-5.58	104.64	113.00
28	a	2767	G	C2'-C3'-O3'	5.56	117.84	109.50
28	a	458	A	C4'-C3'-O3'	-5.55	104.68	113.00
28	a	2450	A	C4'-C3'-O3'	-5.53	104.70	113.00
28	a	909	C	C4'-C3'-O3'	5.50	121.25	113.00
28	a	1982	A	C3'-C2'-O2'	-5.50	106.35	114.60
28	a	2351	A	C4'-C3'-O3'	-5.50	104.75	113.00
28	a	2806	G	C4'-C3'-O3'	5.48	117.62	109.40
28	a	2772	U	C4'-C3'-O3'	5.46	117.60	109.40
28	a	1374	G	P-O3'-C3'	-5.46	112.01	120.20
28	a	1368	G	C2'-C3'-O3'	5.45	121.87	113.70
28	a	1621	A	C4'-C3'-O3'	-5.45	104.83	113.00
28	a	986	A	N9-C1'-C2'	5.44	120.16	112.00
28	a	2368	A	P-O3'-C3'	-5.44	112.04	120.20
28	a	1744	U	C3'-C2'-O2'	5.41	122.71	114.60
28	a	1518	A	C4'-C3'-O3'	-5.39	104.91	113.00
28	a	2748	G	C4'-C3'-O3'	5.37	117.46	109.40
28	a	600	U	C4'-C3'-O3'	-5.32	105.03	113.00
28	a	199	A	C4'-C3'-O3'	-5.29	105.07	113.00
28	a	484	A	C2'-C3'-O3'	-5.27	101.60	109.50
11	g	157	PRO	N-CA-C	5.23	120.47	114.03
28	a	1148	C	C2'-C3'-O3'	-5.18	105.94	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2036	A	C4'-C3'-O3'	-5.16	105.27	113.00
28	a	1580	C	C4'-C3'-O3'	-5.15	101.67	109.40
28	a	1051	C	C4'-C3'-O3'	5.13	117.09	109.40
28	a	1648	G	C4'-C3'-O3'	-5.11	105.34	113.00
28	a	2922	A	N9-C1'-C2'	5.09	119.64	112.00
28	a	1388	A	C1'-C2'-O2'	5.09	119.44	111.80
28	a	2243	A	C3'-C2'-O2'	5.08	118.32	110.70
15	k	64	PHE	CA-CB-CG	5.08	118.88	113.80
28	a	1309	G	C2'-C3'-O3'	-5.07	106.09	113.70
28	a	1547	C	N1-C1'-C2'	5.07	119.60	112.00
28	a	1745	G	N9-C1'-C2'	5.07	119.60	112.00
28	a	1545	A	C2'-C3'-O3'	-5.06	106.11	113.70
28	a	2613	G	C4'-C3'-O3'	-5.04	105.44	113.00
28	a	965	A	N9-C1'-C2'	5.01	119.52	112.00
28	a	600	U	C2'-C3'-O3'	5.00	121.21	113.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	a	1246	G	Sidechain
28	a	1996	G	Sidechain
28	a	2559	G	Sidechain
28	a	2922	A	Sidechain
28	a	517	G	Sidechain
28	a	990	G	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	Z	133	0	143	0	0
2	0	550	0	580	1	0
3	1	813	0	884	3	0
4	2	913	0	974	4	0
5	3	307	0	342	0	0
6	b	2488	0	1265	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	c	919	0	966	7	0
8	d	1596	0	1647	9	0
9	e	941	0	1015	2	0
10	f	1457	0	1530	6	0
11	g	1310	0	1389	10	0
12	h	813	0	849	0	0
13	i	1108	0	1150	2	0
14	j	839	0	881	4	0
15	k	1076	0	1162	4	0
16	m	967	0	1018	4	0
17	o	2131	0	2231	8	0
18	q	339	0	367	1	0
19	r	522	0	559	3	0
20	s	1090	0	1163	5	0
21	t	449	0	481	1	0
22	u	1486	0	1523	7	0
23	v	436	0	446	7	0
24	w	1571	0	1631	6	0
25	x	948	0	1033	4	0
26	y	374	0	412	0	0
27	z	500	0	557	1	0
28	a	61677	0	30997	158	0
29	8	613	0	635	5	0
30	7	732	0	764	9	0
31	9	631	0	677	7	0
32	3	1	0	0	0	0
33	a	164	0	0	0	0
33	b	1	0	0	0	0
33	d	1	0	0	0	0
33	o	1	0	0	0	0
34	8	1	0	0	0	0
34	a	126	0	0	0	0
34	b	1	0	0	0	0
34	d	1	0	0	0	0
34	o	1	0	0	0	0
34	s	1	0	0	0	0
34	v	2	0	0	0	0
34	w	1	0	0	0	0
35	a	96	0	65	5	0
36	9	1	0	0	0	0
36	a	8	0	0	0	0
All	All	90136	0	59336	234	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 (234) 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)
13:i:59:VAL:HG21	13:i:124:ILE:HG23	1.50	0.91
6:b:12:C:O2'	29:8:74:PRO:HA	1.72	0.88
28:a:1048:G:H1	28:a:1119:U:H3	1.22	0.86
7:c:4:ILE:HD11	8:d:27:VAL:HG11	1.59	0.84
7:c:92:ASP:HB2	7:c:114:LYS:HB3	1.59	0.83
22:u:78:ILE:HG23	22:u:99:ILE:HD11	1.66	0.77
17:o:119:GLY:O	17:o:130:LEU:HD23	1.86	0.74
4:2:53:THR:HG21	4:2:65:GLY:HA3	1.69	0.74
28:a:466:C:P	30:7:70:ARG:HH12	2.09	0.74
23:v:16:ARG:HA	28:a:2062:G:H5'	1.70	0.73
28:a:790:A:H2'	28:a:791:G:C5'	2.20	0.72
28:a:20:U:H2'	28:a:20:U:O2	1.91	0.71
11:g:27:VAL:HG12	11:g:80:VAL:HG21	1.71	0.71
28:a:2245:U:O2	31:9:34:LYS:NZ	2.29	0.66
17:o:130:LEU:HD12	17:o:192:ILE:HD11	1.77	0.66
28:a:1547:C:O2	28:a:1547:C:H2'	1.96	0.65
25:x:64:ARG:NH1	25:x:99:PHE:O	2.29	0.65
28:a:790:A:H2'	28:a:791:G:H5''	1.78	0.65
11:g:25:ILE:HD11	11:g:44:VAL:HG21	1.80	0.63
15:k:116:LEU:HD21	15:k:120:VAL:HG22	1.81	0.62
28:a:2096:A:OP1	31:9:19:SER:HB2	2.00	0.61
24:w:113:LEU:HD12	24:w:204:LEU:HD11	1.83	0.61
28:a:194:A:OP1	31:9:26:ASN:ND2	2.22	0.61
28:a:790:A:H2'	28:a:791:G:H5'	1.83	0.61
28:a:466:C:P	30:7:70:ARG:NH1	2.73	0.61
19:r:45:ARG:NH2	19:r:49:ASP:OD2	2.35	0.60
7:c:4:ILE:CD1	8:d:27:VAL:HG11	2.30	0.60
28:a:2380:C:H4'	29:8:56:ASP:OD1	2.03	0.59
28:a:1046:A:H2	28:a:1121:G:H22	1.49	0.59
7:c:73:ARG:HD2	25:x:77:ILE:CD1	2.33	0.59
25:x:119:LEU:HD23	25:x:119:LEU:H	1.68	0.58
28:a:790:A:C2'	28:a:791:G:H5''	2.34	0.58
16:m:112:ILE:HD11	23:v:54:LEU:HD11	1.85	0.58
28:a:2625[B]:U:O2'	35:a:3302:DXT:H8	2.03	0.58
28:a:784:A:N1	28:a:794:U:H5	2.02	0.57
23:v:9:THR:CG2	28:a:2036:A:H5'	2.36	0.56
28:a:148:A:N3	28:a:148:A:C5'	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1350:U:OP2	30:7:78:LYS:NZ	2.38	0.56
28:a:2623:G:H2'	28:a:2624[B]:G:C8	2.41	0.56
4:2:53:THR:HG21	4:2:65:GLY:CA	2.36	0.56
28:a:2307:U:H2'	28:a:2308:A:C8	2.41	0.56
3:1:62:ARG:HH21	3:1:62:ARG:HB2	1.71	0.55
11:g:27:VAL:CG1	11:g:80:VAL:HG21	2.35	0.55
15:k:108:VAL:HB	15:k:125:LEU:HD22	1.87	0.55
28:a:148:A:N3	28:a:148:A:H5'	2.22	0.55
28:a:2201:U:H2'	28:a:2202:G:C8	2.41	0.55
11:g:118:MET:HE1	11:g:149:ILE:HD11	1.88	0.55
24:w:116:LEU:HD13	24:w:190:ILE:HD12	1.88	0.54
28:a:1034:A:N6	28:a:1131:G:H2'	2.22	0.54
11:g:103:LYS:NZ	11:g:117:GLU:OE1	2.41	0.54
28:a:1120:C:H2'	28:a:1121:G:C8	2.43	0.54
28:a:543:A:C2'	28:a:544:G:H5'	2.37	0.54
28:a:1052:A:C2	28:a:1119:U:H1'	2.43	0.54
28:a:2369:G:O2'	29:8:35:ASN:ND2	2.42	0.54
8:d:184:ASP:HB3	8:d:189:LEU:HB2	1.90	0.53
14:j:24:VAL:HG23	14:j:32:ALA:HB1	1.89	0.53
17:o:16:VAL:HG22	17:o:206:GLY:HA3	1.90	0.53
21:t:49:MET:O	21:t:53:VAL:HG22	2.08	0.53
28:a:466:C:OP1	30:7:70:ARG:NH1	2.42	0.53
3:1:103:GLU:OE1	3:1:103:GLU:N	2.42	0.53
17:o:207:LYS:HB2	28:a:736:G:C6	2.43	0.53
28:a:2107:C:H1'	31:9:34:LYS:HE3	1.91	0.53
10:f:103:LEU:HD23	10:f:104:ILE:HG13	1.90	0.53
28:a:396:A:H1'	28:a:416:G:O4'	2.09	0.53
28:a:2625[B]:U:H5'	35:a:3301:DXT:H9	1.90	0.53
28:a:2922:A:N6	28:a:2923:A:C6	2.76	0.53
24:w:161:ILE:HG22	24:w:173:VAL:HG21	1.90	0.52
28:a:148:A:H2'	28:a:149:G:O4'	2.09	0.52
28:a:641:C:H2'	28:a:642:C:C6	2.44	0.52
28:a:2143:G:H2'	28:a:2144:G:C8	2.44	0.52
28:a:1350:U:OP1	30:7:18:LYS:NZ	2.41	0.52
4:2:50:CYS:O	4:2:81:ARG:NH1	2.43	0.52
4:2:58:VAL:O	4:2:62:ILE:HG22	2.09	0.52
23:v:52:GLN:NE2	23:v:54:LEU:O	2.43	0.52
28:a:1052:A:N1	28:a:1119:U:H1'	2.25	0.52
28:a:2191:C:N4	28:a:2192:A:C2	2.78	0.52
8:d:32:LEU:HB3	8:d:34:ARG:HH21	1.73	0.52
24:w:73:ARG:HD3	28:a:681:G:H1'	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2164:G:H2'	28:a:2165:C:C6	2.46	0.51
15:k:123:ARG:NH2	15:k:143:GLU:OE2	2.44	0.51
20:s:35:LYS:HE2	20:s:130:LEU:HD23	1.93	0.51
20:s:56:ARG:CD	28:a:2485:A:H4'	2.41	0.51
28:a:7:A:H2'	28:a:8:U:C6	2.46	0.51
14:j:11:ARG:HH11	14:j:98:LYS:HE3	1.76	0.50
28:a:311:G:H22	28:a:314:A:H5'	1.77	0.50
28:a:2625[A]:U:H1'	28:a:2626[A]:C:C5	2.46	0.50
16:m:112:ILE:CD1	23:v:54:LEU:HD11	2.41	0.50
28:a:2626[B]:C:O3'	35:a:3303:DXT:H8	2.10	0.50
2:0:50:TRP:CZ2	2:0:55:SER:HA	2.47	0.49
20:s:34:LEU:HD13	20:s:118:PHE:HB3	1.94	0.49
28:a:2344:A:H2'	28:a:2345:A:C8	2.47	0.49
28:a:1117:A:H1'	28:a:1118:G:H4'	1.95	0.49
28:a:2215:A:O2'	31:9:36:ARG:NH2	2.45	0.49
28:a:646:U:H2'	28:a:647:C:C6	2.48	0.49
6:b:59:A:H2'	6:b:60:A:C8	2.48	0.49
17:o:124:ILE:HA	17:o:192:ILE:HD13	1.93	0.49
28:a:790:A:C2'	28:a:791:G:C5'	2.88	0.49
28:a:2625[A]:U:H2'	28:a:2625[A]:U:O2	2.12	0.49
28:a:587:U:H2'	28:a:588:C:C6	2.48	0.49
28:a:2191:C:H2'	28:a:2192:A:O4'	2.13	0.49
28:a:2289:A:H2'	28:a:2290:A:C8	2.48	0.49
11:g:10:ILE:CG2	11:g:77:VAL:HG21	2.43	0.48
22:u:163:LEU:HD23	22:u:186:ILE:HD11	1.94	0.48
27:z:63:ARG:HG2	27:z:63:ARG:HH21	1.78	0.48
28:a:1547:C:O2	28:a:1547:C:C2'	2.58	0.48
28:a:2372:U:O3'	29:8:20:MET:SD	2.71	0.48
28:a:1117:A:H1'	28:a:1118:G:C4'	2.43	0.48
28:a:1760:A:H2'	28:a:1761:A:C8	2.49	0.48
28:a:1883:C:H2'	28:a:1884:C:O4'	2.14	0.48
17:o:119:GLY:O	17:o:130:LEU:CD2	2.60	0.48
28:a:803:U:H2'	28:a:804:C:C6	2.49	0.48
28:a:2626[A]:C:O3'	35:a:3303:DXT:H8	2.13	0.48
10:f:13:THR:HB	10:f:14:PRO:HD3	1.95	0.47
28:a:902:A:C8	28:a:903:C:C6	3.02	0.47
28:a:1051:C:H1'	28:a:1052:A:OP2	2.13	0.47
28:a:2190:C:H2'	28:a:2191:C:C6	2.49	0.47
16:m:5:LYS:NZ	28:a:2016:C:OP1	2.42	0.47
28:a:907:A:H2'	28:a:908:C:O4'	2.14	0.47
8:d:149:ILE:HG12	28:a:2067:U:H4'	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:539:U:H2'	28:a:540:A:C8	2.50	0.47
28:a:2144:G:H2'	28:a:2145:C:C6	2.50	0.47
23:v:9:THR:HG21	28:a:2036:A:H5'	1.97	0.47
28:a:1545:A:N6	28:a:1551:U:C4	2.83	0.47
28:a:651:A:H2'	28:a:652:A:C8	2.50	0.47
28:a:675:A:H2'	28:a:677:A:H62	1.80	0.47
28:a:20:U:O2	28:a:20:U:C2'	2.62	0.46
7:c:73:ARG:HD2	25:x:77:ILE:HD13	1.98	0.46
23:v:26:MET:HE3	23:v:27:LEU:H	1.80	0.46
8:d:28:VAL:HG11	8:d:206:ILE:HD11	1.97	0.46
10:f:142:GLN:OE1	10:f:142:GLN:N	2.49	0.46
28:a:402:A:H5''	31:9:32:ASN:HB2	1.97	0.46
28:a:664:U:H2'	28:a:665:U:C6	2.50	0.46
28:a:2183:U:H2'	28:a:2184:G:O4'	2.16	0.46
11:g:102:LYS:HB3	11:g:117:GLU:OE1	2.16	0.46
28:a:898:G:H3'	28:a:899:C:H5''	1.98	0.46
28:a:201:A:N6	28:a:2446:A:H2'	2.31	0.46
28:a:781:A:H2	28:a:794:U:O2'	1.98	0.46
28:a:866:U:O2	28:a:866:U:O4'	2.33	0.46
28:a:2563:A:H2'	28:a:2564:U:C6	2.51	0.46
19:r:33:GLY:HA3	30:7:13:PRO:HG2	1.97	0.46
28:a:2623:G:H2'	28:a:2624[A]:G:C8	2.51	0.45
28:a:790:A:N3	28:a:791:G:H5'	2.31	0.45
28:a:2090:U:H2'	28:a:2091:U:C6	2.52	0.45
28:a:211:A:H2'	28:a:212:C:O4'	2.17	0.45
28:a:2205:U:H2'	28:a:2206:G:C8	2.52	0.45
28:a:148:A:H2'	28:a:149:G:C8	2.52	0.44
28:a:2153:C:H2'	28:a:2154:U:C1'	2.46	0.44
28:a:1338:A:H2'	28:a:1340:C:C4	2.53	0.44
17:o:122:ALA:HB3	17:o:130:LEU:HD21	1.98	0.44
24:w:99:LYS:HG2	28:a:666:G:H4'	1.98	0.44
28:a:699:U:H2'	28:a:700:A:C8	2.52	0.44
28:a:1905:A:H2'	28:a:1906:A:C8	2.53	0.44
28:a:543:A:H2'	28:a:544:G:H5'	2.00	0.44
28:a:1660:G:H5''	28:a:1661:C:H5'	1.99	0.44
28:a:2078:A:C2	35:a:3301:DXT:C21	3.01	0.44
3:1:98:PHE:O	3:1:102:GLY:N	2.50	0.44
28:a:1516:U:H2'	28:a:1517:C:C6	2.53	0.44
10:f:144:ASP:N	10:f:144:ASP:OD1	2.51	0.43
28:a:2087:A:H2'	28:a:2088:C:C6	2.53	0.43
7:c:18:ILE:CD1	7:c:77:LEU:HD21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:1742:C:H2'	28:a:1743:U:O4'	2.18	0.43
28:a:2695:A:H2'	28:a:2696:C:O4'	2.18	0.43
10:f:108:ILE:HG21	10:f:176:PRO:HG3	2.00	0.43
28:a:1051:C:C6	28:a:1117:A:N1	2.87	0.43
28:a:1350:U:OP1	30:7:80:TYR:OH	2.25	0.43
8:d:158:VAL:HG21	28:a:2634:G:H21	1.84	0.43
14:j:75:MET:HE3	28:a:523:G:H21	1.84	0.43
17:o:207:LYS:HB2	28:a:736:G:C5	2.54	0.43
10:f:50:ILE:HD13	10:f:84:PRO:HB2	2.01	0.43
28:a:1276:G:O2'	28:a:2028:G:O6	2.36	0.43
28:a:1408:C:OP1	30:7:55:ARG:NH2	2.43	0.43
22:u:174:LEU:HD13	22:u:178:VAL:HG21	2.00	0.43
28:a:1585:A:H2'	28:a:1586:A:C8	2.54	0.43
28:a:2714:U:H2'	28:a:2715:C:C6	2.54	0.43
18:q:7:GLU:HA	18:q:15:ILE:HG12	2.01	0.42
16:m:103:ARG:O	16:m:107:SER:HA	2.20	0.42
22:u:193:ARG:HH12	28:a:903:C:H5''	1.84	0.42
28:a:2804:C:H2'	28:a:2805:C:C6	2.54	0.42
11:g:12:ILE:HG12	11:g:18:VAL:HG21	2.02	0.42
28:a:2192:A:C2	28:a:2193:C:C5	3.07	0.42
28:a:787:G:H2'	28:a:789:A:N7	2.35	0.42
14:j:55:ILE:HG21	14:j:66:ILE:HD12	2.02	0.42
8:d:109:VAL:CG1	8:d:177:SER:HA	2.50	0.42
28:a:294:U:H2'	28:a:295:U:C6	2.54	0.42
28:a:784:A:N1	28:a:794:U:C5	2.85	0.42
28:a:1955:U:OP1	28:a:2620:U:O2'	2.38	0.42
7:c:80:PRO:HG2	8:d:20:GLY:HA2	2.02	0.42
20:s:43:THR:HG22	20:s:94:VAL:HG12	2.02	0.42
28:a:1443:A:H2'	28:a:1444:A:C8	2.54	0.42
20:s:56:ARG:HD2	28:a:2485:A:H4'	2.01	0.42
24:w:167:ASN:HB2	28:a:326:A:OP2	2.19	0.42
28:a:313:A:H2'	28:a:314:A:H5''	2.02	0.42
28:a:846:U:H2'	28:a:847:C:C6	2.55	0.42
28:a:862:G:H2'	28:a:863:G:C8	2.55	0.42
28:a:1557:C:N4	28:a:1558:A:C6	2.88	0.41
9:e:31:VAL:HG13	28:a:587:U:O3'	2.20	0.41
11:g:5:VAL:O	11:g:70:ARG:HD2	2.20	0.41
13:i:89:PHE:CE2	13:i:100:ILE:HD13	2.55	0.41
28:a:577:G:H2'	28:a:2046:A:N7	2.36	0.41
28:a:1772:U:C5	28:a:2712:U:H5'	2.55	0.41
28:a:1792:U:H2'	28:a:1798:A:N6	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:2330:G:H2'	28:a:2331:U:C6	2.55	0.41
15:k:78:ARG:HG2	15:k:113:ALA:HB3	2.02	0.41
28:a:2144:G:H2'	28:a:2145:C:H6	1.85	0.41
28:a:1409:C:OP1	30:7:82:MET:HE3	2.21	0.41
28:a:2249:U:H2'	28:a:2250:G:C8	2.55	0.41
28:a:2623:G:C6	28:a:2624[B]:G:C6	3.08	0.41
28:a:1553:C:O4'	28:a:1554:G:C8	2.73	0.41
28:a:1606:U:H2'	28:a:1607:U:C6	2.55	0.41
28:a:2120:A:H2'	28:a:2121:U:O4'	2.20	0.41
28:a:1055:C:N3	28:a:1056:A:C6	2.88	0.41
28:a:419:C:H2'	28:a:420:A:C8	2.56	0.41
22:u:13:ARG:HB2	22:u:46:THR:HG23	2.02	0.41
22:u:104:LYS:HG2	22:u:140:LEU:HD22	2.02	0.41
28:a:1058:C:O2	28:a:1058:C:H2'	2.20	0.41
28:a:2119:U:H2'	28:a:2120:A:O4'	2.21	0.41
28:a:2120:A:H1'	28:a:2202:G:N2	2.35	0.41
28:a:2343:A:H2'	28:a:2344:A:C8	2.55	0.41
28:a:146:C:O2	28:a:146:C:O4'	2.38	0.41
28:a:1052:A:N7	28:a:1117:A:N1	2.69	0.41
28:a:2359:U:H2'	28:a:2360:U:C6	2.56	0.41
28:a:2347:G:OP1	29:8:44:HIS:HD2	2.04	0.40
28:a:2772:U:H1'	28:a:2773:A:H5''	2.03	0.40
11:g:25:ILE:HD11	11:g:44:VAL:CG2	2.49	0.40
22:u:79:LEU:HD13	22:u:94:ILE:HD11	2.03	0.40
28:a:1886:C:O2	28:a:1886:C:H2'	2.21	0.40
28:a:2623:G:C6	28:a:2624[A]:G:C6	3.09	0.40
28:a:2901:A:H2'	28:a:2902:A:C8	2.56	0.40
28:a:401:G:H1'	31:9:29:PHE:HB3	2.03	0.40
28:a:543:A:H2'	28:a:544:G:O4'	2.20	0.40
28:a:1415:U:H2'	28:a:1416:U:C6	2.56	0.40
28:a:2198:G:H2'	28:a:2199:C:O4'	2.20	0.40
9:e:30:ARG:NH1	28:a:26:C:OP1	2.55	0.40
19:r:48:ARG:NH1	28:a:83:G:H4'	2.37	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Z	14/21 (67%)	14 (100%)	0	0	100	100
2	0	66/70 (94%)	66 (100%)	0	0	100	100
3	1	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
4	2	114/117 (97%)	112 (98%)	2 (2%)	0	100	100
5	3	36/40 (90%)	36 (100%)	0	0	100	100
7	c	111/115 (96%)	108 (97%)	3 (3%)	0	100	100
8	d	209/217 (96%)	203 (97%)	6 (3%)	0	100	100
9	e	116/119 (98%)	116 (100%)	0	0	100	100
10	f	180/182 (99%)	174 (97%)	6 (3%)	0	100	100
11	g	172/178 (97%)	167 (97%)	5 (3%)	0	100	100
12	h	102/115 (89%)	102 (100%)	0	0	100	100
13	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
14	j	108/115 (94%)	107 (99%)	1 (1%)	0	100	100
15	k	141/143 (99%)	135 (96%)	6 (4%)	0	100	100
16	m	117/126 (93%)	111 (95%)	6 (5%)	0	100	100
17	o	272/275 (99%)	265 (97%)	7 (3%)	0	100	100
18	q	43/152 (28%)	41 (95%)	2 (5%)	0	100	100
19	r	61/65 (94%)	60 (98%)	1 (2%)	0	100	100
20	s	135/137 (98%)	131 (97%)	4 (3%)	0	100	100
21	t	54/63 (86%)	52 (96%)	2 (4%)	0	100	100
22	u	189/244 (78%)	182 (96%)	7 (4%)	0	100	100
23	v	52/64 (81%)	51 (98%)	1 (2%)	0	100	100
24	w	203/205 (99%)	200 (98%)	3 (2%)	0	100	100
25	x	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
26	y	42/44 (96%)	42 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	z	60/64 (94%)	59 (98%)	1 (2%)	0	100	100
29	8	75/90 (83%)	73 (97%)	2 (3%)	0	100	100
30	7	89/95 (94%)	88 (99%)	1 (1%)	0	100	100
31	9	75/79 (95%)	75 (100%)	0	0	100	100
All	All	3198/3506 (91%)	3124 (98%)	74 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	13/18 (72%)	13 (100%)	0	100	100
2	0	62/63 (98%)	62 (100%)	0	100	100
3	1	91/93 (98%)	90 (99%)	1 (1%)	65	78
4	2	92/93 (99%)	89 (97%)	3 (3%)	33	44
5	3	34/35 (97%)	33 (97%)	1 (3%)	37	49
7	c	98/100 (98%)	94 (96%)	4 (4%)	27	35
8	d	169/175 (97%)	168 (99%)	1 (1%)	78	88
9	e	88/89 (99%)	88 (100%)	0	100	100
10	f	155/155 (100%)	151 (97%)	4 (3%)	40	53
11	g	142/146 (97%)	142 (100%)	0	100	100
12	h	85/93 (91%)	85 (100%)	0	100	100
13	i	115/116 (99%)	113 (98%)	2 (2%)	53	68
14	j	86/91 (94%)	84 (98%)	2 (2%)	44	58
15	k	107/107 (100%)	106 (99%)	1 (1%)	70	82
16	m	102/109 (94%)	101 (99%)	1 (1%)	68	80
17	o	223/224 (100%)	221 (99%)	2 (1%)	70	82
18	q	36/123 (29%)	36 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	r	56/58 (97%)	55 (98%)	1 (2%)	51	66
20	s	111/111 (100%)	110 (99%)	1 (1%)	70	82
21	t	50/57 (88%)	50 (100%)	0	100	100
22	u	167/201 (83%)	165 (99%)	2 (1%)	63	76
23	v	46/56 (82%)	46 (100%)	0	100	100
24	w	169/169 (100%)	166 (98%)	3 (2%)	51	66
25	x	105/105 (100%)	104 (99%)	1 (1%)	68	80
26	y	38/38 (100%)	38 (100%)	0	100	100
27	z	54/56 (96%)	52 (96%)	2 (4%)	30	39
29	8	64/73 (88%)	63 (98%)	1 (2%)	55	70
30	7	79/81 (98%)	79 (100%)	0	100	100
31	9	70/72 (97%)	70 (100%)	0	100	100
All	All	2707/2907 (93%)	2674 (99%)	33 (1%)	61	76

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1	62	ARG
4	2	27	CYS
4	2	68	ILE
4	2	81	ARG
5	3	31	ARG
7	c	4	ILE
7	c	5	ILE
7	c	54	ARG
7	c	101	LEU
8	d	34	ARG
10	f	58	ILE
10	f	78	LYS
10	f	103	LEU
10	f	144	ASP
13	i	31	ARG
13	i	48	VAL
14	j	70	LYS
14	j	85	PHE
15	k	68	SER
16	m	35	LYS
17	o	13	ARG

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Mol	Chain	Res	Type
17	o	168	GLU
19	r	9	LYS
20	s	16	ARG
22	u	118	ASP
22	u	194	VAL
24	w	92	LYS
24	w	179	VAL
24	w	199	ARG
25	x	80	ASP
27	z	6	THR
27	z	63	ARG
29	8	80	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
4	2	64	HIS
7	c	67	HIS
7	c	88	ASN
8	d	128	HIS
10	f	5	GLN
13	i	133	GLN
14	j	94	ASN
16	m	2	HIS
16	m	9	HIS
17	o	111	HIS
17	o	143	ASN
22	u	97	GLN
22	u	190	HIS
24	w	98	GLN
24	w	149	ASN
24	w	162	ASN
24	w	167	ASN
25	x	3	GLN
25	x	92	GLN
27	z	28	ASN
27	z	48	HIS
29	8	35	ASN
29	8	44	HIS
29	8	78	ASN
31	9	22	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	a	2868/2925 (98%)	348 (12%)	0
6	b	116/117 (99%)	11 (9%)	0
All	All	2984/3042 (98%)	359 (12%)	0

All (359) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	b	35	U
6	b	36	U
6	b	45	A
6	b	51	G
6	b	56	G
6	b	57	A
6	b	66	A
6	b	67	G
6	b	68	C
6	b	88	U
6	b	107	A
28	a	2	G
28	a	23	G
28	a	42	U
28	a	57	A
28	a	79	A
28	a	82	A
28	a	83	G
28	a	93	G
28	a	126	A
28	a	127	A
28	a	128	U
28	a	133	A
28	a	134	A
28	a	145	U
28	a	146	C
28	a	147	G
28	a	148	A
28	a	167	U
28	a	185	A
28	a	194	A
28	a	200	A
28	a	203	A
28	a	219	G

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Mol	Chain	Res	Type
28	a	220	A
28	a	225	A
28	a	226	A
28	a	237	A
28	a	249	G
28	a	252	G
28	a	256	G
28	a	270	G
28	a	275	G
28	a	299	G
28	a	305	U
28	a	315	A
28	a	328	C
28	a	334	A
28	a	364	U
28	a	365	G
28	a	372	G
28	a	391	G
28	a	416	G
28	a	417	A
28	a	427	A
28	a	453	U
28	a	461	C
28	a	462	A
28	a	480	U
28	a	486	G
28	a	496	G
28	a	509	U
28	a	510	A
28	a	514	C
28	a	536	C
28	a	537	A
28	a	543	A
28	a	544	G
28	a	553	C
28	a	555	G
28	a	570	A
28	a	580	U
28	a	582	A
28	a	610	A
28	a	611	G
28	a	620	U

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Mol	Chain	Res	Type
28	a	622	U
28	a	634	A
28	a	644	A
28	a	653	U
28	a	654	G
28	a	660	U
28	a	661	U
28	a	692	A
28	a	693	U
28	a	716	U
28	a	722	A
28	a	723	A
28	a	724	C
28	a	726	C
28	a	737	C
28	a	753	U
28	a	754	U
28	a	771	A
28	a	772	G
28	a	782	G
28	a	783	G
28	a	789	A
28	a	792	G
28	a	796	A
28	a	799	A
28	a	812	G
28	a	819	C
28	a	835	U
28	a	837	G
28	a	865	G
28	a	872	A
28	a	885	G
28	a	886	G
28	a	887	G
28	a	888	G
28	a	889	G
28	a	892	A
28	a	894	C
28	a	896	C
28	a	897	G
28	a	898	G
28	a	899	C

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Mol	Chain	Res	Type
28	a	900	C
28	a	901	U
28	a	902	A
28	a	903	C
28	a	905	A
28	a	907	A
28	a	909	C
28	a	910	G
28	a	916	A
28	a	937	U
28	a	939	A
28	a	952	C
28	a	965	A
28	a	967	G
28	a	980	A
28	a	989	A
28	a	1002	A
28	a	1018	U
28	a	1019	C
28	a	1028	G
28	a	1032	A
28	a	1048	G
28	a	1051	C
28	a	1052	A
28	a	1054	A
28	a	1055	C
28	a	1057	G
28	a	1058	C
28	a	1113	G
28	a	1114	U
28	a	1117	A
28	a	1118	G
28	a	1121	G
28	a	1126	G
28	a	1135	A
28	a	1136	U
28	a	1138	U
28	a	1139	A
28	a	1140	A
28	a	1141	C
28	a	1142	G
28	a	1149	A

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Mol	Chain	Res	Type
28	a	1162	A
28	a	1183	C
28	a	1184	U
28	a	1185	G
28	a	1237	G
28	a	1263	A
28	a	1266	G
28	a	1281	G
28	a	1282	A
28	a	1311	A
28	a	1362	U
28	a	1375	A
28	a	1378	U
28	a	1386	C
28	a	1389	U
28	a	1393	A
28	a	1395	A
28	a	1396	C
28	a	1425	U
28	a	1426	G
28	a	1427	C
28	a	1429	A
28	a	1430	U
28	a	1431	G
28	a	1438	C
28	a	1462	G
28	a	1463	A
28	a	1470	U
28	a	1492	G
28	a	1503	C
28	a	1518	A
28	a	1520	U
28	a	1545	A
28	a	1546	A
28	a	1547	C
28	a	1548	U
28	a	1550	G
28	a	1551	U
28	a	1553	C
28	a	1554	G
28	a	1555	U
28	a	1556	G

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Mol	Chain	Res	Type
28	a	1557	C
28	a	1559	A
28	a	1563	G
28	a	1575	G
28	a	1580	C
28	a	1581	A
28	a	1584	A
28	a	1593	U
28	a	1600	C
28	a	1622	U
28	a	1623	A
28	a	1624	A
28	a	1632	C
28	a	1663	U
28	a	1689	G
28	a	1711	G
28	a	1715	A
28	a	1716	A
28	a	1745	G
28	a	1777	G
28	a	1778	G
28	a	1787	A
28	a	1796	U
28	a	1805	A
28	a	1814	C
28	a	1815	A
28	a	1825	G
28	a	1830	C
28	a	1843	A
28	a	1862	A
28	a	1885	U
28	a	1886	C
28	a	1887	G
28	a	1888	G
28	a	1930	C
28	a	1946	G
28	a	1953	A
28	a	1954	A
28	a	1957	C
28	a	1971	U
28	a	1979	U
28	a	1980	G

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Mol	Chain	Res	Type
28	a	1983	C
28	a	1986	A
28	a	1987	U
28	a	1988	G
28	a	1998	U
28	a	2009	U
28	a	2013	C
28	a	2039	C
28	a	2047	A
28	a	2049	A
28	a	2059	C
28	a	2062	G
28	a	2071	C
28	a	2072	G
28	a	2076	A
28	a	2077	G
28	a	2078	A
28	a	2079	C
28	a	2085	G
28	a	2096	A
28	a	2128	G
28	a	2132	G
28	a	2135	A
28	a	2140	G
28	a	2141	G
28	a	2143	G
28	a	2150	A
28	a	2151	A
28	a	2154	U
28	a	2163	A
28	a	2164	G
28	a	2173	G
28	a	2188	U
28	a	2189	A
28	a	2214	A
28	a	2219	U
28	a	2220	G
28	a	2227	A
28	a	2228	A
28	a	2241	A
28	a	2254	G
28	a	2255	G

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Mol	Chain	Res	Type
28	a	2291	C
28	a	2292	G
28	a	2294	A
28	a	2298	G
28	a	2299	U
28	a	2303	A
28	a	2324	G
28	a	2325	A
28	a	2343	A
28	a	2349	A
28	a	2351	A
28	a	2352	A
28	a	2363	C
28	a	2366	C
28	a	2377	A
28	a	2395	G
28	a	2398	G
28	a	2399	G
28	a	2401	C
28	a	2412	G
28	a	2418	C
28	a	2422	U
28	a	2440	C
28	a	2441	A
28	a	2445	G
28	a	2446	A
28	a	2447	U
28	a	2450	A
28	a	2451	A
28	a	2457	U
28	a	2463	G
28	a	2464	A
28	a	2485	A
28	a	2490	U
28	a	2507	U
28	a	2518	G
28	a	2519	2MA
28	a	2521	G
28	a	2534	A
28	a	2536	C
28	a	2570	U
28	a	2582	A

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Mol	Chain	Res	Type
28	a	2583	G
28	a	2589	C
28	a	2594	G
28	a	2629	U
28	a	2645	U
28	a	2679	G
28	a	2705	U
28	a	2706	U
28	a	2707	C
28	a	2730	G
28	a	2742	A
28	a	2749	A
28	a	2767	G
28	a	2768	C
28	a	2773	A
28	a	2774	A
28	a	2781	A
28	a	2794	A
28	a	2806	G
28	a	2807	G
28	a	2812	U
28	a	2813	U
28	a	2815	A
28	a	2823	A
28	a	2835	A
28	a	2836	A
28	a	2882	A
28	a	2883	A
28	a	2899	U
28	a	2909	G
28	a	2910	A

There are no RNA pucker outliers to report.

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

9 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	$\# Z  > 2$
28	PSU	a	1933	28	18,21,22	1.44	3 (16%)	22,30,33	1.85	5 (22%)
28	PSU	a	2596	28,34	18,21,22	1.49	2 (11%)	22,30,33	1.81	5 (22%)
28	PSU	a	1927	28	18,21,22	1.44	3 (16%)	22,30,33	1.77	4 (18%)
28	PSU	a	2520	28,34	18,21,22	1.85	4 (22%)	22,30,33	3.29	6 (27%)
28	PSU	a	961	28	18,21,22	1.41	3 (16%)	22,30,33	1.87	4 (18%)
28	OMG	a	2267	28,34	23,26,27	1.21	3 (13%)	33,38,41	2.08	9 (27%)
28	2MA	a	2519	33,28	22,25,26	1.55	4 (18%)	33,37,40	2.13	8 (24%)
28	OMU	a	2568	33,28	19,22,23	1.20	2 (10%)	26,31,34	1.85	6 (23%)
28	PSU	a	2621	28	18,21,22	1.40	3 (16%)	22,30,33	1.87	5 (22%)

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
28	PSU	a	1933	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2596	28,34	-	0/7/25/26	0/2/2/2
28	PSU	a	1927	28	-	0/7/25/26	0/2/2/2
28	PSU	a	2520	28,34	-	0/7/25/26	0/2/2/2
28	PSU	a	961	28	-	0/7/25/26	0/2/2/2
28	OMG	a	2267	28,34	-	1/9/27/28	0/3/3/3
28	2MA	a	2519	33,28	-	2/7/25/26	0/3/3/3
28	OMU	a	2568	33,28	-	0/9/27/28	0/2/2/2
28	PSU	a	2621	28	-	2/7/25/26	0/2/2/2

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2520	PSU	O2-C2	5.33	1.34	1.23
28	a	1927	PSU	C6-C5	4.70	1.40	1.35
28	a	2519	2MA	C5-C4	4.52	1.47	1.39
28	a	1933	PSU	C6-C5	4.47	1.40	1.35
28	a	2596	PSU	C6-C5	4.44	1.40	1.35
28	a	961	PSU	C6-C5	4.16	1.40	1.35
28	a	2621	PSU	C6-C5	4.12	1.40	1.35
28	a	2520	PSU	C6-C5	3.44	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	a	2267	OMG	C5-C4	3.17	1.47	1.38
28	a	2519	2MA	C5-C6	2.91	1.49	1.41
28	a	2596	PSU	C4-N3	-2.77	1.33	1.38
28	a	2568	OMU	C2-N1	2.76	1.42	1.38
28	a	2519	2MA	C8-N7	2.41	1.36	1.31
28	a	961	PSU	C4-N3	-2.34	1.34	1.38
28	a	2621	PSU	C4-N3	-2.31	1.34	1.38
28	a	2520	PSU	C2-N1	-2.30	1.33	1.36
28	a	2520	PSU	C4-C5	2.27	1.50	1.44
28	a	2519	2MA	C5-N7	-2.21	1.34	1.39
28	a	2621	PSU	C4-C5	2.18	1.50	1.44
28	a	2568	OMU	C4-N3	-2.18	1.34	1.38
28	a	2267	OMG	C5-N7	-2.17	1.34	1.39
28	a	1933	PSU	C4-C5	2.15	1.50	1.44
28	a	1927	PSU	C4-C5	2.14	1.50	1.44
28	a	2267	OMG	C6-N1	-2.13	1.34	1.38
28	a	1933	PSU	C4-N3	-2.11	1.34	1.38
28	a	961	PSU	C4-C5	2.05	1.50	1.44
28	a	1927	PSU	C4-N3	-2.02	1.35	1.38

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	2520	PSU	O2-C2-N1	-12.04	109.53	122.79
28	a	2519	2MA	C5-C4-N3	-7.19	119.11	127.19
28	a	2520	PSU	O2-C2-N3	6.60	134.25	121.82
28	a	2267	OMG	C5-C4-N3	-6.11	118.54	128.46
28	a	961	PSU	N1-C2-N3	5.80	121.71	115.13
28	a	1933	PSU	N1-C2-N3	5.64	121.52	115.13
28	a	2621	PSU	N1-C2-N3	5.58	121.45	115.13
28	a	2519	2MA	N3-C4-N9	5.57	134.72	126.99
28	a	1927	PSU	N1-C2-N3	5.39	121.24	115.13
28	a	2267	OMG	C2-N3-C4	5.17	121.50	112.30
28	a	2596	PSU	N1-C2-N3	5.11	120.92	115.13
28	a	2520	PSU	C6-C5-C4	-4.76	114.87	118.20
28	a	2267	OMG	N9-C4-N3	4.53	135.03	125.94
28	a	2568	OMU	C4-N3-C2	-4.20	121.04	126.58
28	a	2568	OMU	N3-C2-N1	4.02	120.23	114.89
28	a	2568	OMU	C5-C4-N3	3.85	120.61	114.84
28	a	961	PSU	C4-N3-C2	-3.79	120.88	126.34
28	a	1933	PSU	C4-N3-C2	-3.63	121.11	126.34
28	a	2621	PSU	C4-N3-C2	-3.59	121.16	126.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	a	1927	PSU	C4-N3-C2	-3.51	121.28	126.34
28	a	2267	OMG	C6-C5-N7	3.42	136.61	130.25
28	a	2568	OMU	C2'-C1'-N1	-3.35	107.73	114.22
28	a	2519	2MA	C4-C5-N7	-3.29	106.61	110.62
28	a	961	PSU	O2-C2-N1	-3.20	119.27	122.79
28	a	2621	PSU	O2-C2-N1	-3.11	119.37	122.79
28	a	2596	PSU	C3'-C2'-C1'	3.06	105.20	101.64
28	a	2568	OMU	O4-C4-C5	-3.02	119.86	125.16
28	a	1933	PSU	O2-C2-N1	-2.99	119.50	122.79
28	a	1927	PSU	O2-C2-N1	-2.96	119.53	122.79
28	a	2596	PSU	C4-N3-C2	-2.94	122.11	126.34
28	a	2621	PSU	C6-C5-C4	-2.89	116.18	118.20
28	a	2519	2MA	C5-N7-C8	2.84	107.54	103.51
28	a	2519	2MA	C2-N1-C6	2.81	122.46	118.08
28	a	1927	PSU	C6-C5-C4	-2.76	116.27	118.20
28	a	2519	2MA	C6-C5-N7	2.73	137.12	132.02
28	a	2519	2MA	C4-N9-C8	2.73	108.69	105.73
28	a	2596	PSU	O2-C2-N3	-2.71	116.70	121.82
28	a	2520	PSU	C6-N1-C2	2.70	125.45	122.68
28	a	2568	OMU	O4'-C1'-N1	2.68	114.48	108.36
28	a	2267	OMG	C4-C5-N7	-2.64	106.55	110.72
28	a	2596	PSU	C6-C5-C4	-2.61	116.38	118.20
28	a	2267	OMG	O2'-C2'-C1'	2.50	113.95	109.08
28	a	2267	OMG	C2'-C1'-N9	-2.44	109.49	114.22
28	a	1933	PSU	C3'-C2'-C1'	2.35	104.37	101.64
28	a	961	PSU	C6-C5-C4	-2.28	116.61	118.20
28	a	1933	PSU	C6-C5-C4	-2.24	116.63	118.20
28	a	2520	PSU	C4-N3-C2	-2.23	123.12	126.34
28	a	2267	OMG	O6-C6-C5	-2.22	120.71	126.60
28	a	2621	PSU	C3'-C2'-C1'	2.15	104.14	101.64
28	a	2519	2MA	N9-C8-N7	-2.14	110.99	113.91
28	a	2267	OMG	C5-C6-N1	2.09	118.49	113.19
28	a	2520	PSU	C3'-C2'-C1'	2.04	104.02	101.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
28	a	2267	OMG	C1'-C2'-O2'-CM2
28	a	2621	PSU	O4'-C1'-C5-C4
28	a	2621	PSU	O4'-C1'-C5-C6
28	a	2519	2MA	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
28	a	2519	2MA	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 305 ligands modelled in this entry, 302 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
35	DXT	a	3302	33	33,35,35	1.00	2 (6%)	42,57,57	1.47	8 (19%)
35	DXT	a	3301	33	33,35,35	1.20	3 (9%)	42,57,57	1.49	9 (21%)
35	DXT	a	3303	33	33,35,35	1.30	3 (9%)	42,57,57	1.20	5 (11%)

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
35	DXT	a	3302	33	-	8/8/74/74	0/4/4/4
35	DXT	a	3301	33	-	6/8/74/74	0/4/4/4
35	DXT	a	3303	33	-	8/8/74/74	0/4/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	a	3303	DXT	C4B-C1	-3.62	1.50	1.55
35	a	3303	DXT	C4B-C12	-3.60	1.48	1.52
35	a	3302	DXT	C21-N21	3.32	1.42	1.33
35	a	3301	DXT	C4B-C1	-3.32	1.50	1.55
35	a	3301	DXT	C21-N21	3.31	1.42	1.33
35	a	3303	DXT	C21-N21	3.28	1.42	1.33
35	a	3302	DXT	C4B-C1	-2.29	1.52	1.55
35	a	3301	DXT	C4B-C12	-2.18	1.50	1.52

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	3303	DXT	C1-C4B-C12	-3.86	105.36	109.88
35	a	3301	DXT	C11-C5B-C12	-3.86	115.75	118.80
35	a	3302	DXT	C10-C6B-C6A	3.68	122.86	118.97
35	a	3302	DXT	O11-C11-C6B	-3.65	115.09	121.99
35	a	3301	DXT	C5A-C5-C4A	3.23	116.01	110.62
35	a	3301	DXT	O12-C12-C4B	3.15	117.93	113.37
35	a	3301	DXT	O21-C21-N21	-2.86	116.18	122.88
35	a	3301	DXT	C10-C6B-C6A	2.78	121.91	118.97
35	a	3303	DXT	C5A-C5-C4A	2.78	115.25	110.62
35	a	3302	DXT	O12-C12-C5B	-2.73	120.17	123.90
35	a	3302	DXT	O12-C12-C4B	2.71	117.29	113.37
35	a	3302	DXT	C21-C2-C1	-2.53	117.97	120.97
35	a	3301	DXT	O12-C12-C5B	-2.36	120.67	123.90
35	a	3303	DXT	C10-C6B-C6A	2.35	121.45	118.97
35	a	3301	DXT	C4B-C4A-C5	2.29	112.40	110.59
35	a	3302	DXT	O3-C3-C2	-2.22	119.06	122.96
35	a	3303	DXT	C4B-C4A-C5	2.16	112.29	110.59
35	a	3302	DXT	C10-C6B-C11	-2.13	118.35	121.47
35	a	3303	DXT	O3-C3-C2	-2.12	119.24	122.96
35	a	3301	DXT	C10-C6B-C11	-2.07	118.44	121.47
35	a	3302	DXT	C42-N4-C4	-2.02	109.35	114.09
35	a	3301	DXT	O3-C3-C2	-2.01	119.44	122.96

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
35	a	3301	DXT	C1-C2-C21-O21
35	a	3301	DXT	C1-C2-C21-N21
35	a	3301	DXT	C3-C2-C21-O21

*Continued on next page...*



*Continued from previous page...*

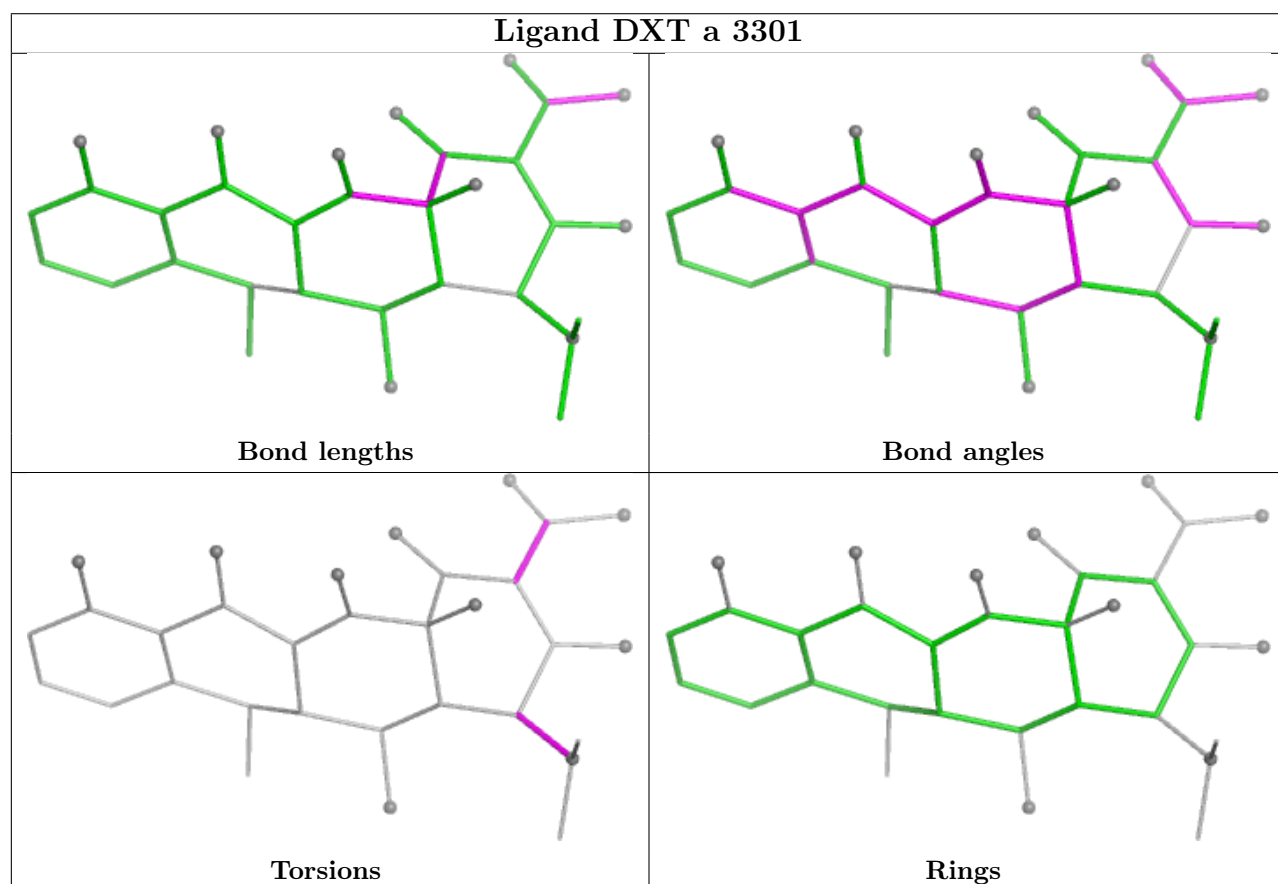
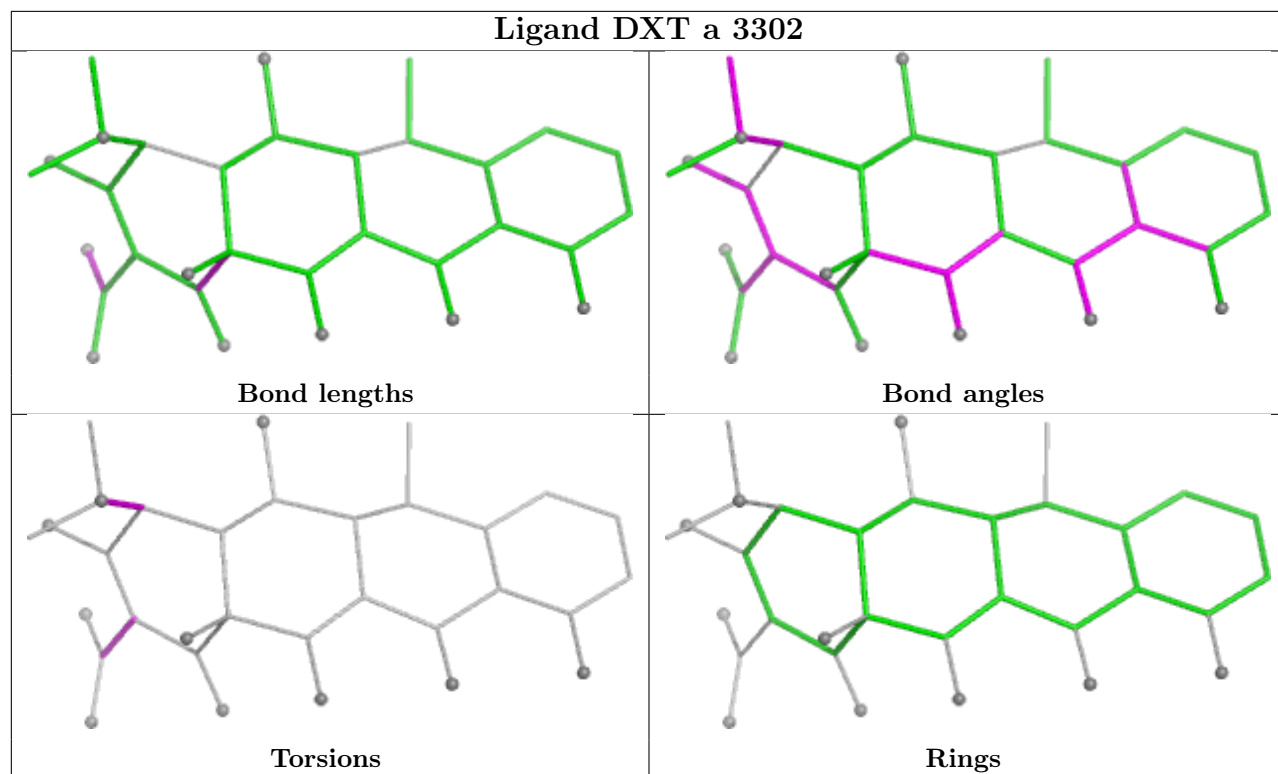
Mol	Chain	Res	Type	Atoms
35	a	3301	DXT	C3-C2-C21-N21
35	a	3301	DXT	C4A-C4-N4-C42
35	a	3302	DXT	C1-C2-C21-O21
35	a	3302	DXT	C1-C2-C21-N21
35	a	3302	DXT	C3-C2-C21-O21
35	a	3302	DXT	C3-C2-C21-N21
35	a	3302	DXT	C3-C4-N4-C41
35	a	3302	DXT	C3-C4-N4-C42
35	a	3303	DXT	C1-C2-C21-O21
35	a	3303	DXT	C1-C2-C21-N21
35	a	3303	DXT	C3-C4-N4-C42
35	a	3303	DXT	C4A-C4-N4-C41
35	a	3301	DXT	C3-C4-N4-C41
35	a	3302	DXT	C4A-C4-N4-C41
35	a	3302	DXT	C4A-C4-N4-C42
35	a	3303	DXT	C3-C4-N4-C41
35	a	3303	DXT	C4A-C4-N4-C42
35	a	3303	DXT	C3-C2-C21-N21
35	a	3303	DXT	C3-C2-C21-O21

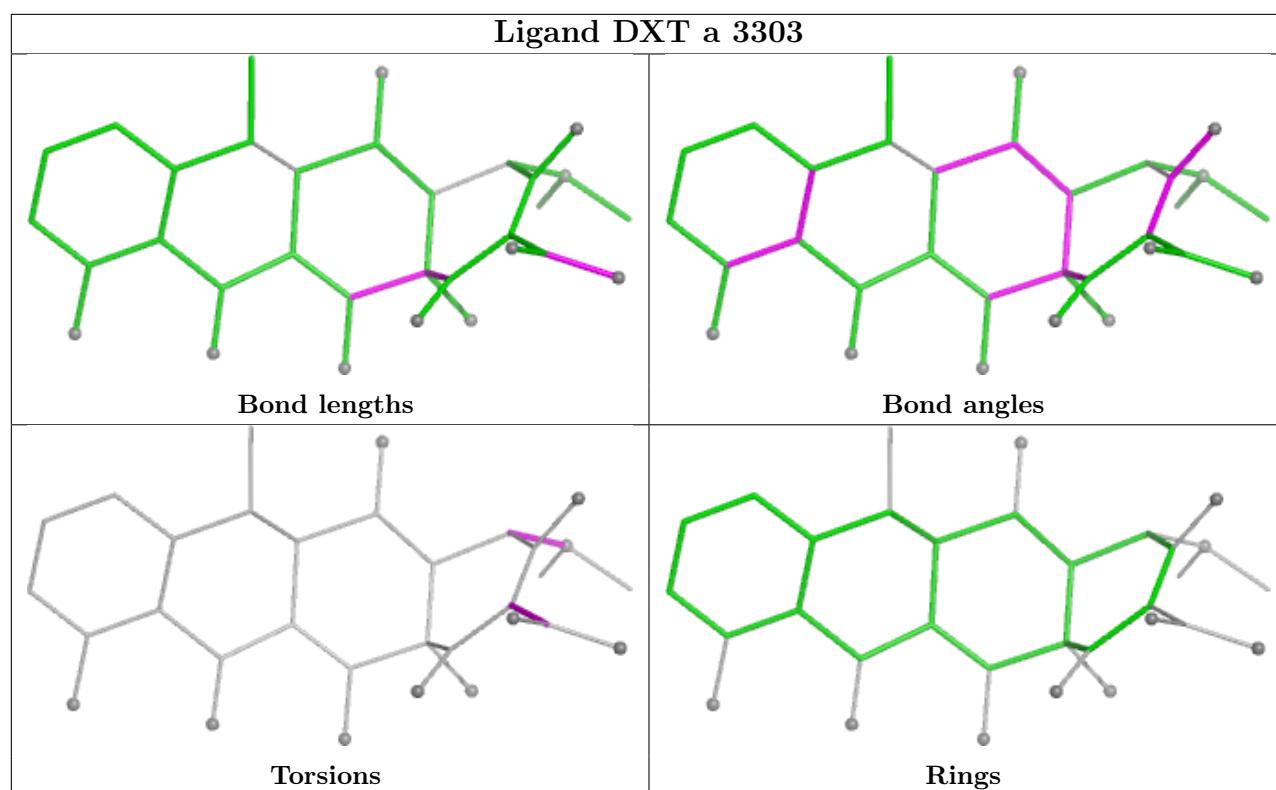
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	a	3302	DXT	1	0
35	a	3301	DXT	2	0
35	a	3303	DXT	2	0

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





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

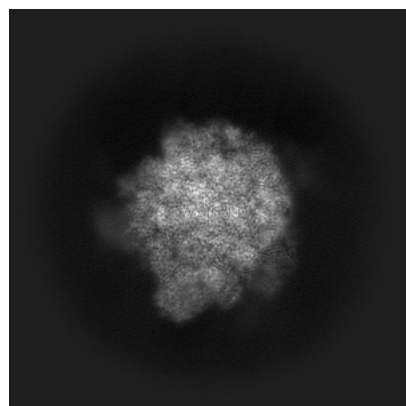
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-56459. These allow visual inspection of the internal detail of the map and identification of artifacts.

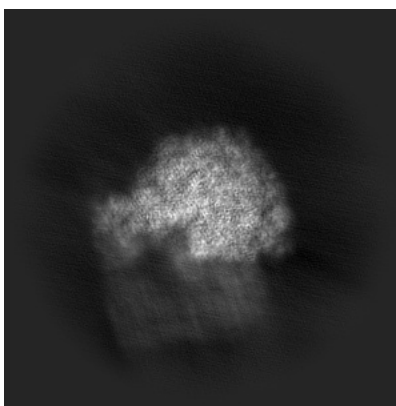
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

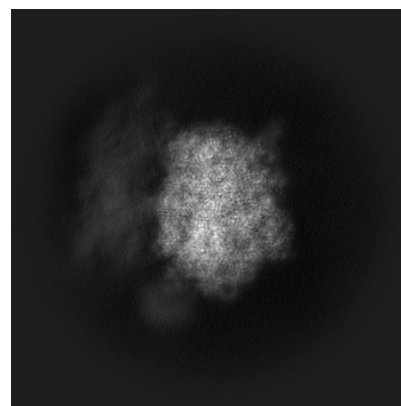
#### 6.1.1 Primary map



X

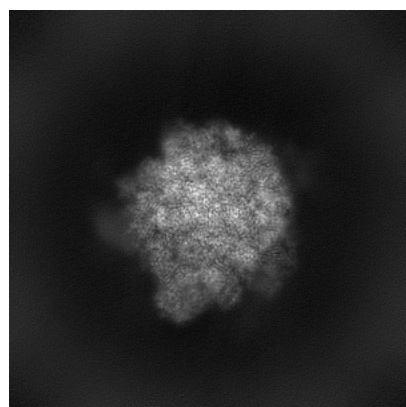


Y

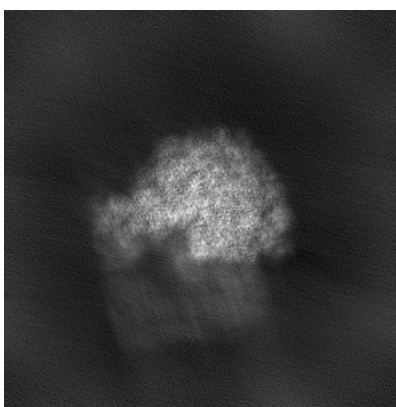


Z

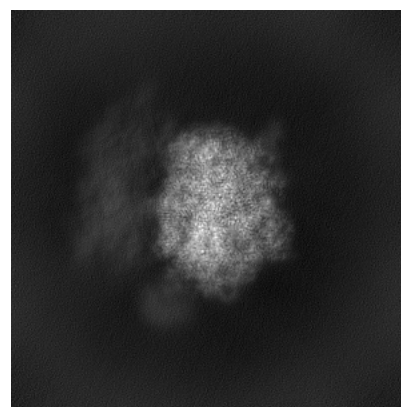
#### 6.1.2 Raw map



X



Y

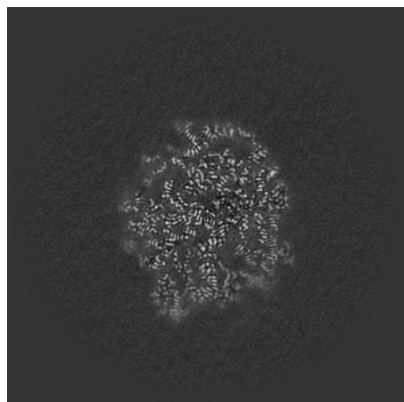


Z

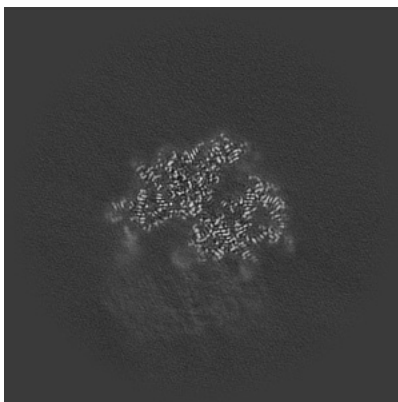
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

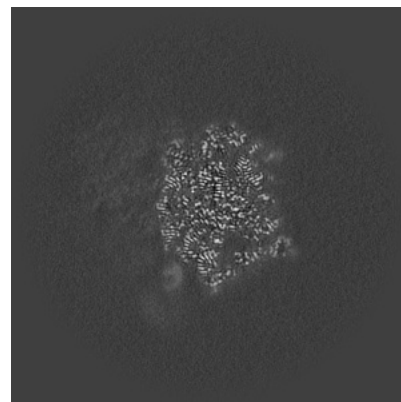
### 6.2.1 Primary map



X Index: 200

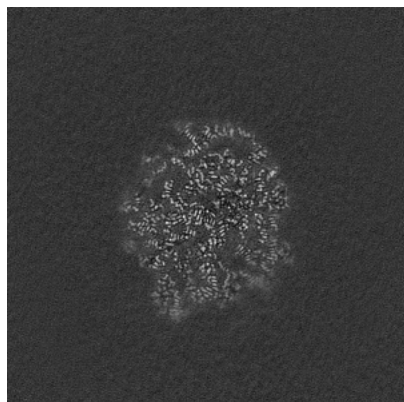


Y Index: 200

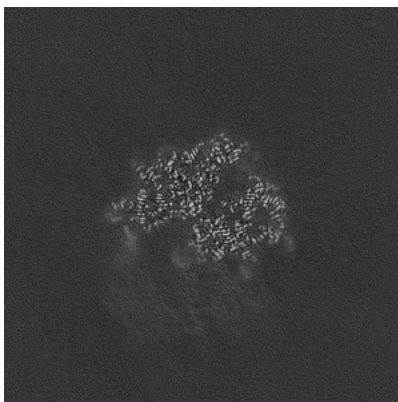


Z Index: 200

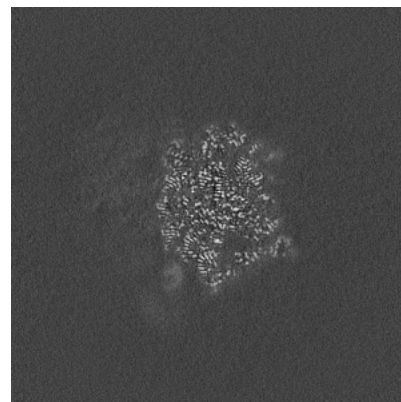
### 6.2.2 Raw map



X Index: 200



Y Index: 200

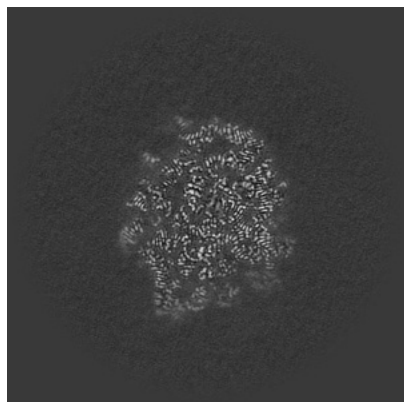


Z Index: 200

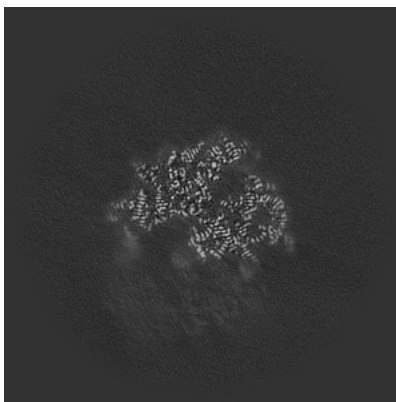
The images above show central slices of the map in three orthogonal directions.

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

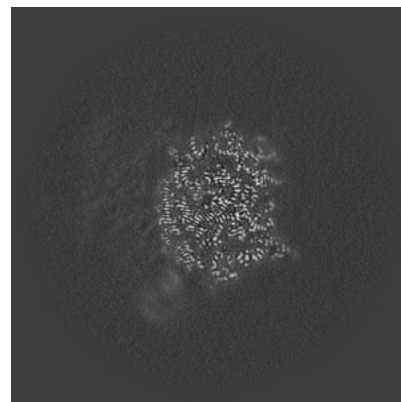
### 6.3.1 Primary map



X Index: 194

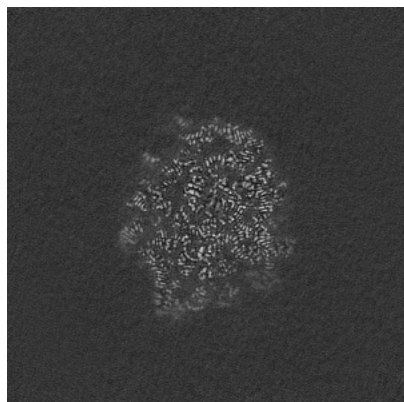


Y Index: 201

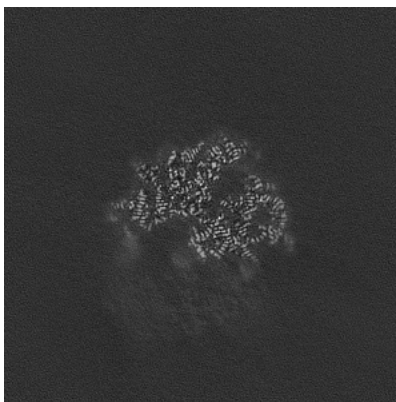


Z Index: 194

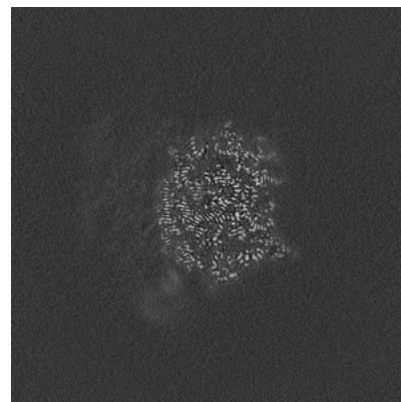
### 6.3.2 Raw map



X Index: 194



Y Index: 201



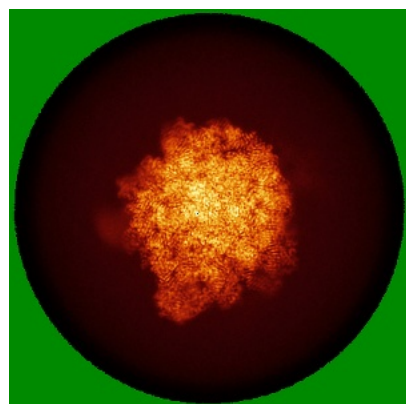
Z Index: 194

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

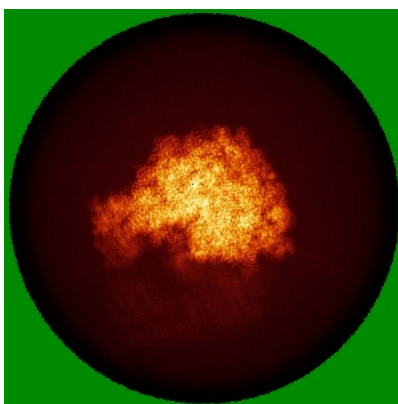


## 6.4 Orthogonal standard-deviation projections (False-color) ⓘ

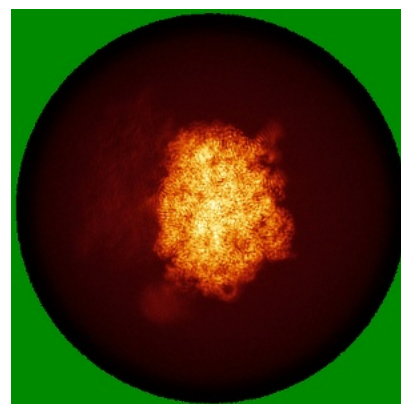
### 6.4.1 Primary map



X

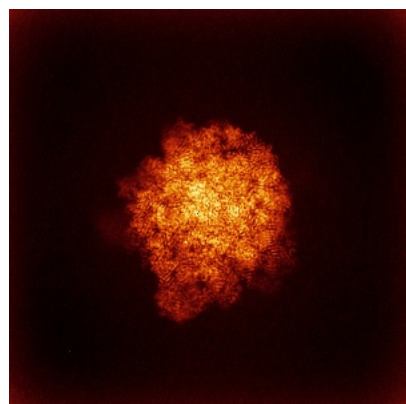


Y

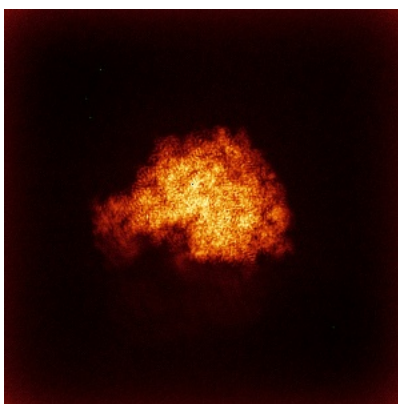


Z

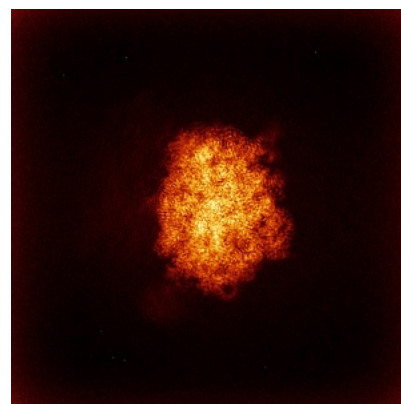
### 6.4.2 Raw map



X



Y



Z

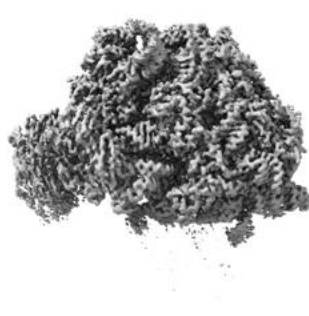
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

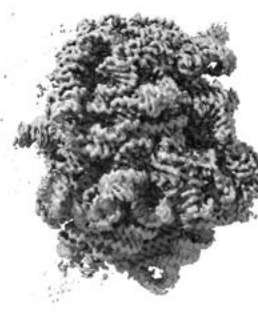
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. 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



X



Y



Z

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](#)

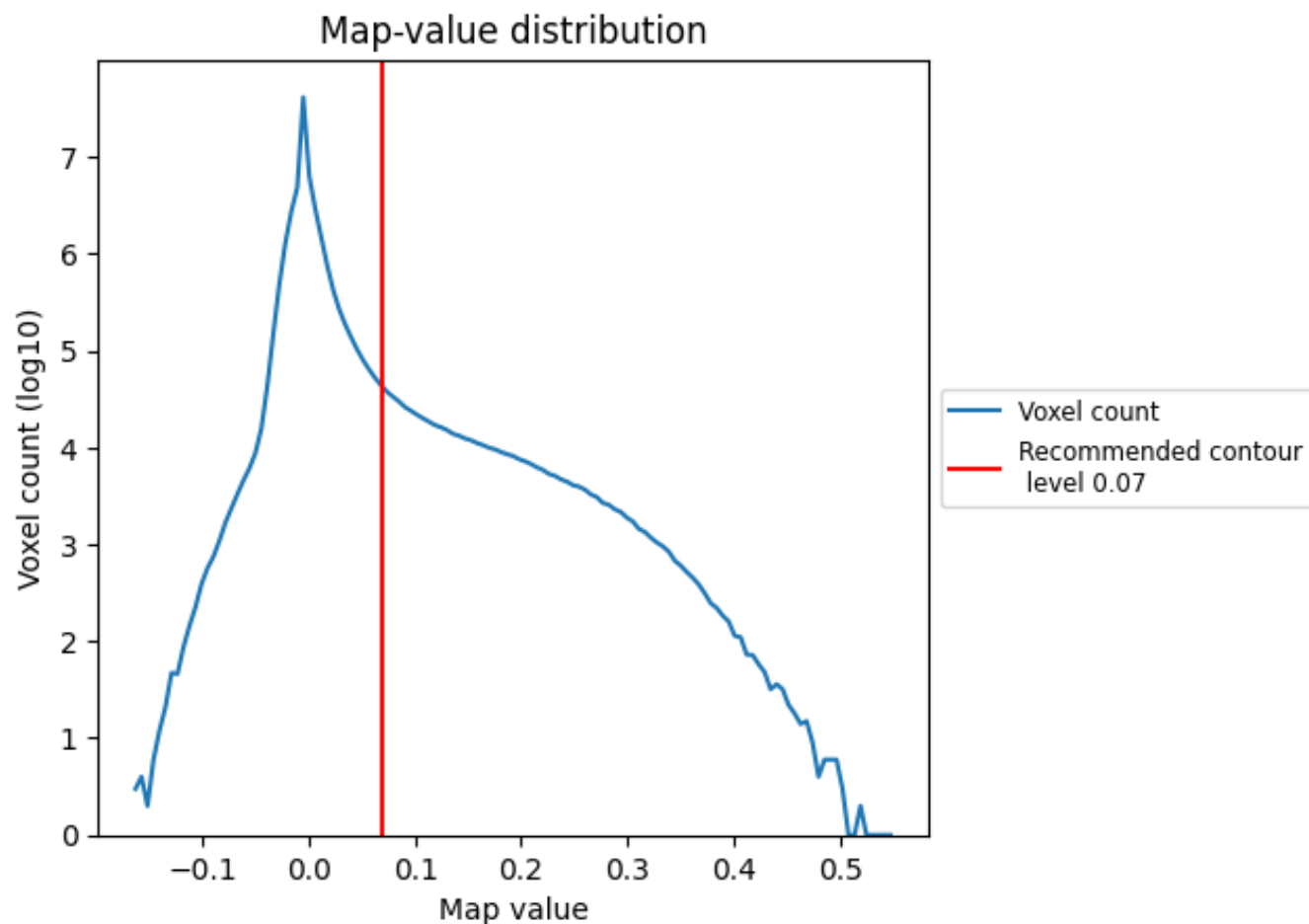
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

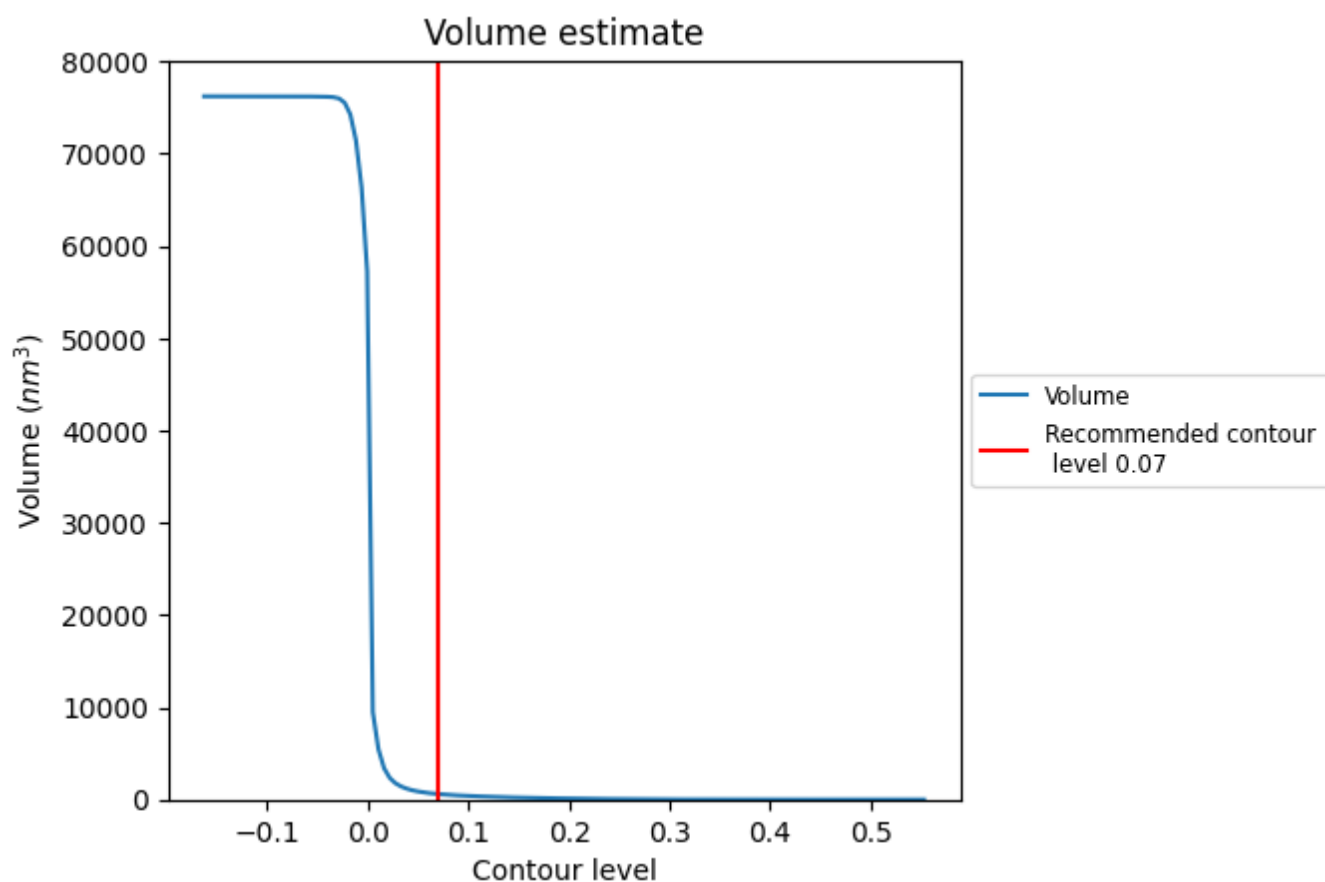
This section contains the results of statistical analysis of the map.

### 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.

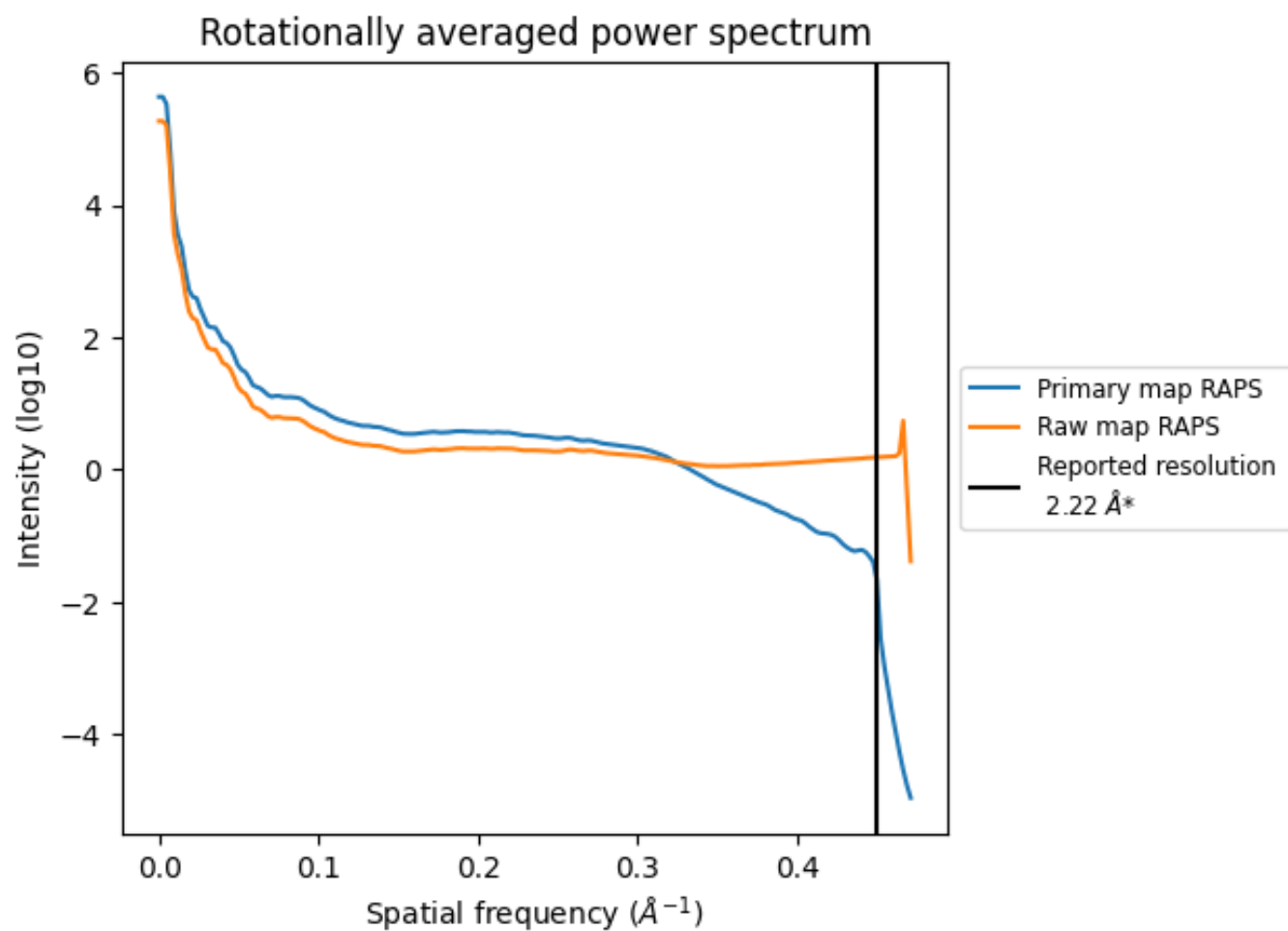
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 600  $\text{nm}^3$ ; this corresponds to an approximate mass of 542 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ

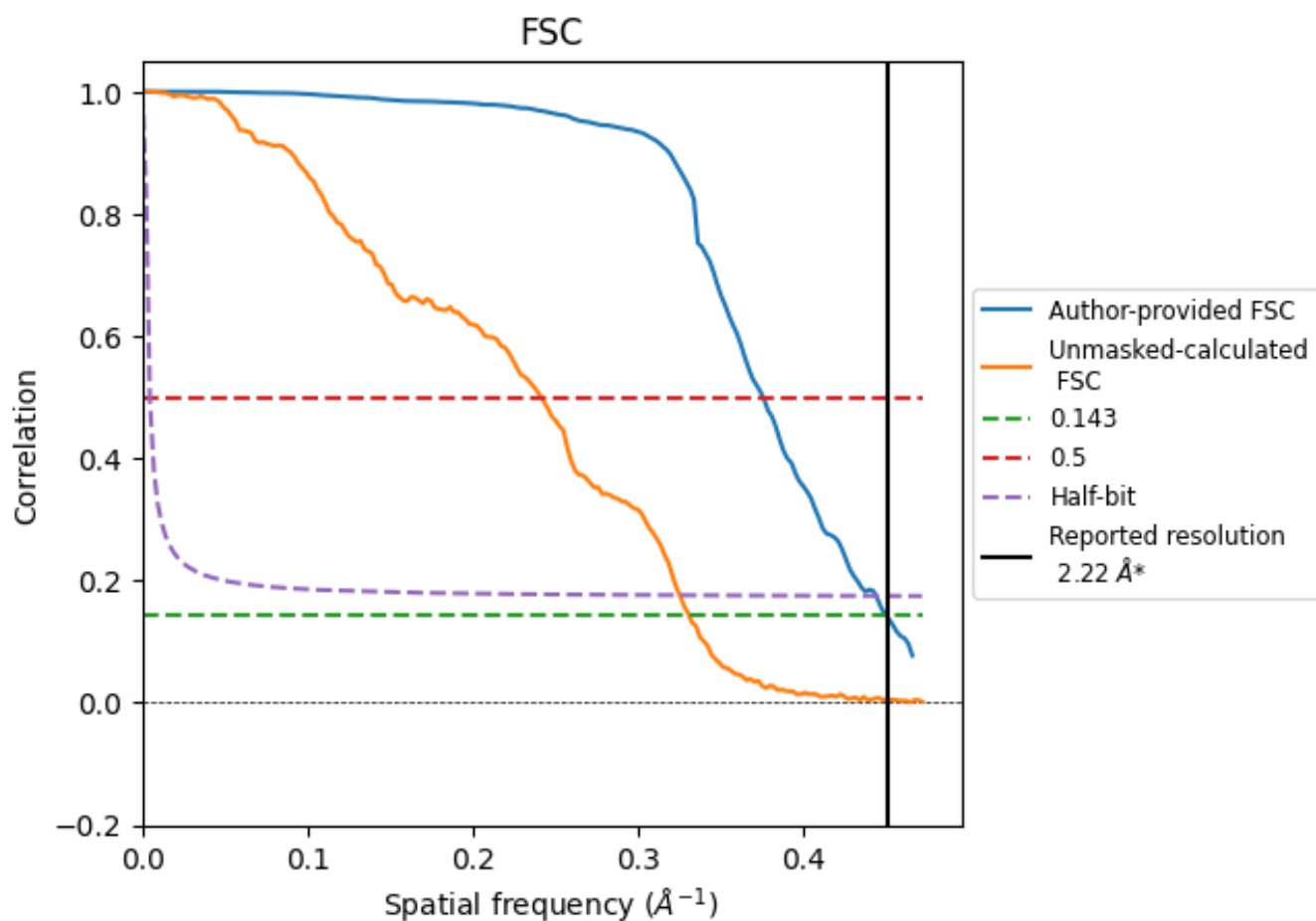


\*Reported resolution corresponds to spatial frequency of 0.450  $\text{\AA}^{-1}$

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.450 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

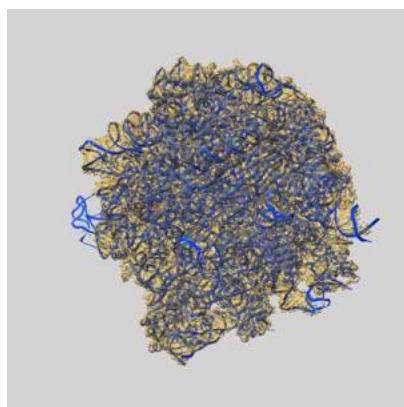
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.22	-	-
Author-provided FSC curve	2.22	2.66	2.25
Unmasked-calculated*	3.02	4.15	3.08

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.02 differs from the reported value 2.22 by more than 10 %

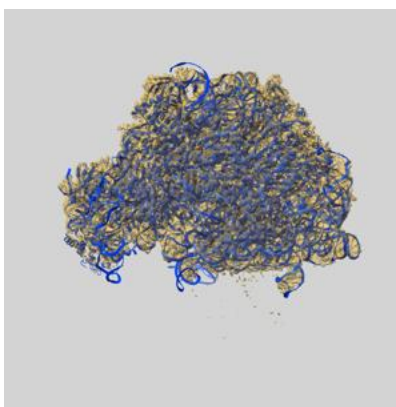
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-56459 and PDB model 9TZ5. Per-residue inclusion information can be found in section [3](#) on page [12](#).

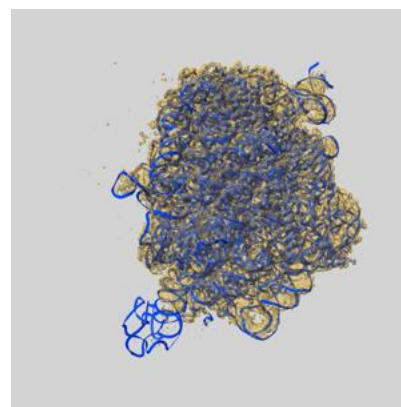
### 9.1 Map-model overlay [i](#)



X



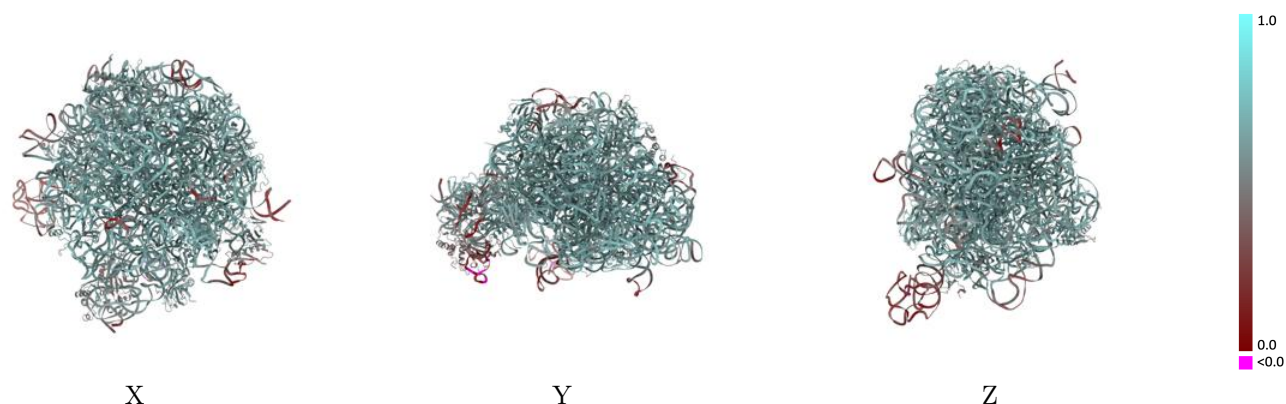
Y



Z

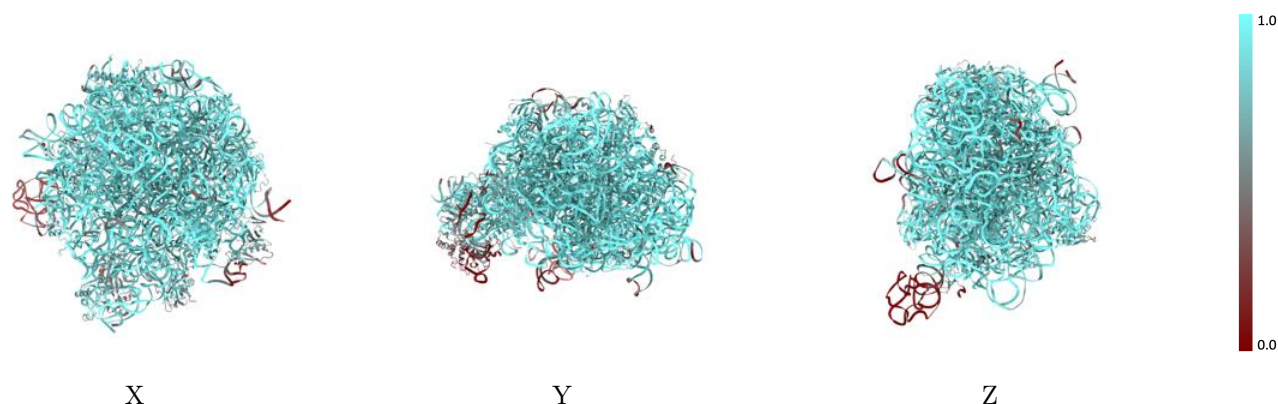
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



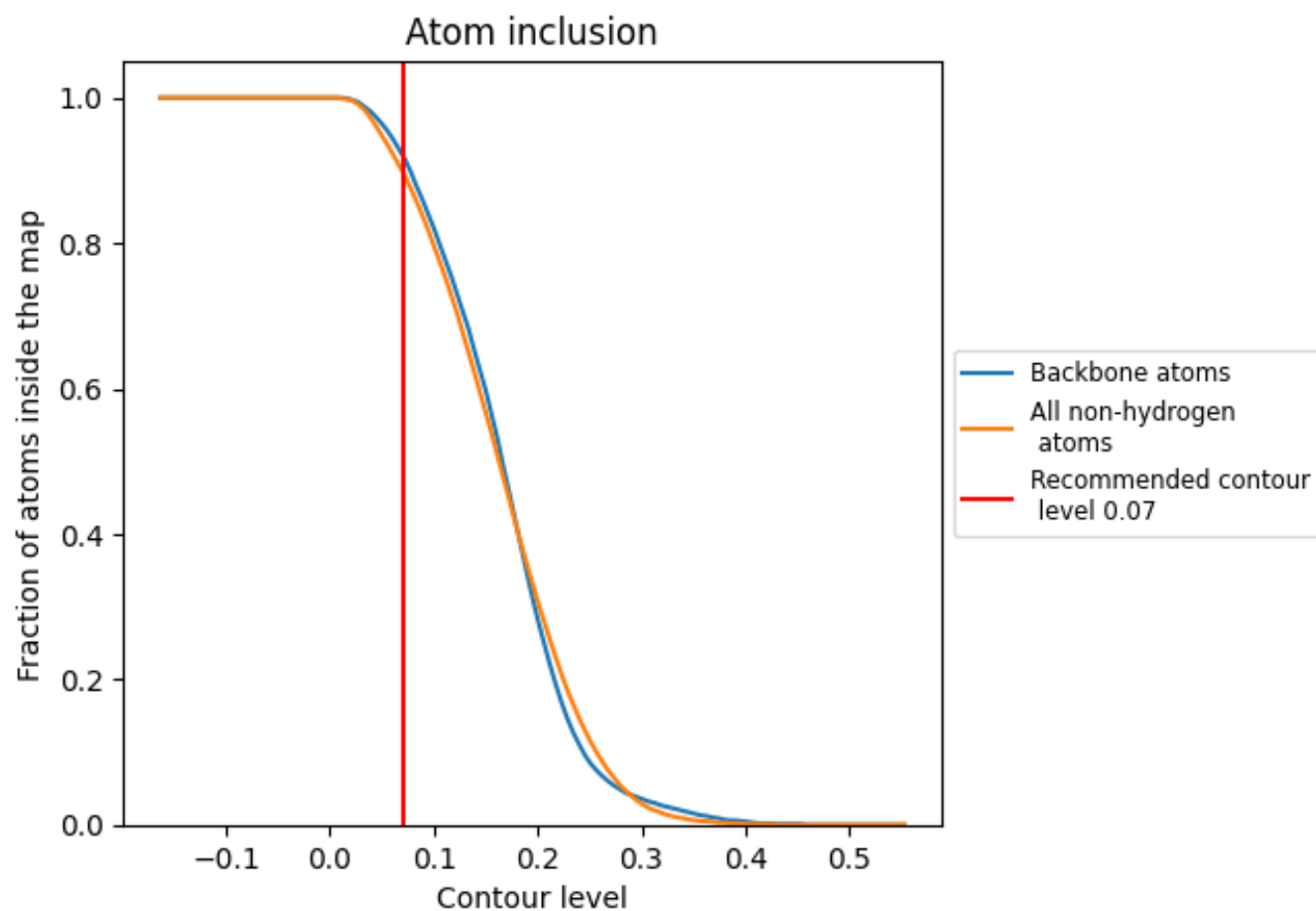
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

## 9.4 Atom inclusion ⓘ



































































At the recommended contour level, 92% of all backbone atoms, 90% of all non-hydrogen atoms, are inside the map.



## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8980	 0.6010
0	 0.8780	 0.6140
1	 0.7820	 0.5610
2	 0.8230	 0.5550
3	 0.9210	 0.6240
7	 0.8750	 0.6020
8	 0.9050	 0.6190
9	 0.8690	 0.6080
Z	 0.9200	 0.6270
a	 0.9250	 0.6040
b	 0.9280	 0.5590
c	 0.8320	 0.6010
d	 0.9360	 0.6410
e	 0.9580	 0.6590
f	 0.2830	 0.3460
g	 0.6160	 0.4990
h	 0.8910	 0.6300
i	 0.9490	 0.6440
j	 0.9180	 0.6350
k	 0.9090	 0.6270
m	 0.9540	 0.6440
o	 0.9290	 0.6450
q	 0.5950	 0.5350
r	 0.8080	 0.5650
s	 0.9100	 0.6210
t	 0.9190	 0.6370
u	 0.6090	 0.5400
v	 0.9450	 0.6340
w	 0.8790	 0.6170
x	 0.8880	 0.6180
y	 0.9660	 0.6630
z	 0.9630	 0.6540

