



Full wwPDB EM Validation Report ⓘ

May 21, 2026 – 11:03 am BST

PDB ID : 30QZ / pdb_000030qz
EMDB ID : EMD-57973
Title : E. coli 50S ribosome with peptidyl-tRNA and Hsp15
Authors : Larsson, D.S.D.; Akbar, S.; Selmer, M.
Deposited on : 2026-05-10
Resolution : 2.23 Å(reported)
Based on initial models : ., 7K00

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

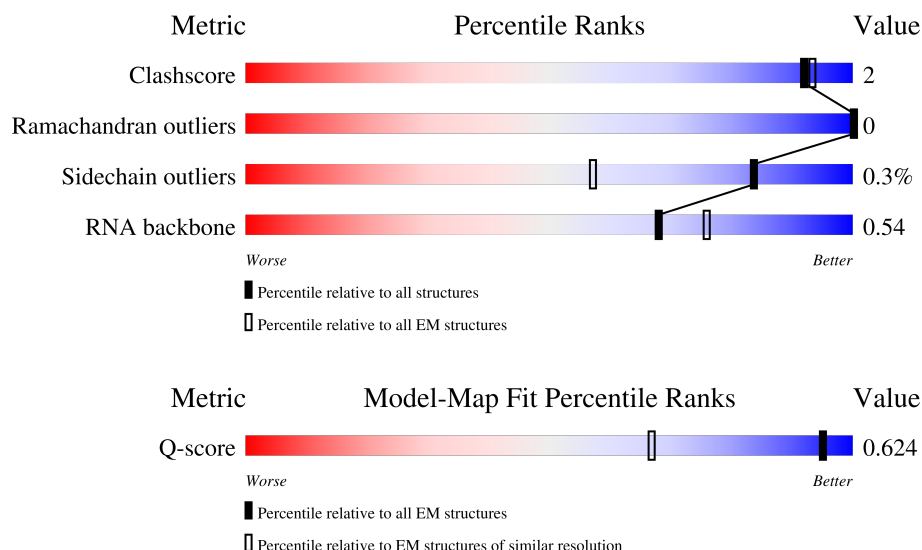
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal 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 2.23 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.




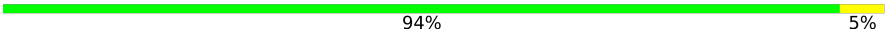





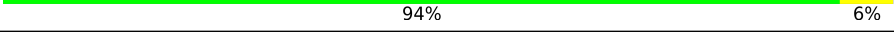


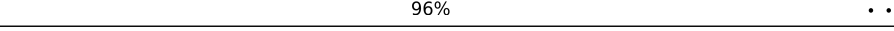
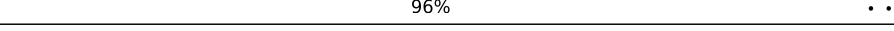

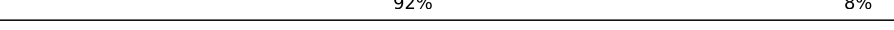
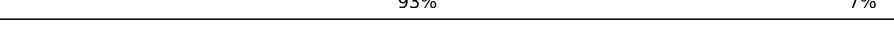


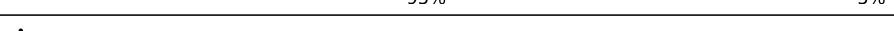

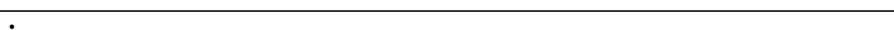

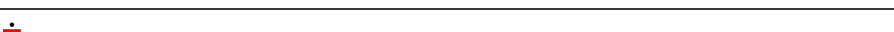
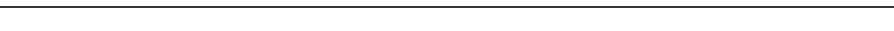


Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	3335 (1.73 - 2.73)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	a	2904	
2	b	120	
3	c	273	

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Mol	Chain	Length	Quality of chain
4	d	209	 90% 10%
5	e	201	 94% 5%
6	f	179	 89% 9% ..
7	g	177	 91% 8% .
8	h	149	 24% . 72%
9	i	142	 88% 11% .
10	j	123	 92% 7% .
11	k	144	 94% 6%
12	l	136	 90% 9% .
13	m	127	 80% 13% 7%
14	n	117	 96% ..
15	o	115	 96% ..
16	p	118	 88% 11% .
17	q	103	 92% 8%
18	r	110	 93% 7%
19	s	100	 88% 5% 7%
20	t	104	 85% 11% ..
21	u	94	 95% 5%
22	v	85	 87% 5% 8%
23	w	78	 88% 9% ..
24	x	63	 92% 6% .
25	y	59	 93% 5% .
26	z	57	 77% 21% .
27	0	55	 91% . 7%
28	1	46	 91% 9%

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Mol	Chain	Length	Quality of chain
29	2	65	<div><div></div><div>89%</div><div>9%</div><div>.</div></div>
30	3	38	<div><div></div><div>92%</div><div>8%</div><div></div></div>
31	6	105	<div><div></div><div>99%</div><div></div><div></div></div> <div><div></div><div>90%</div><div>10%</div><div></div></div>
32	V	142	<div><div></div><div>21%</div><div></div><div></div></div> <div><div></div><div>65%</div><div>.</div><div>33%</div></div>
33	Z	77	<div><div></div><div>16%</div><div></div><div></div></div> <div><div></div><div>71%</div><div>26%</div><div>..</div></div>

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 144501 atoms, of which 55465 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	a	2737	Total	C	H	N	O	P	0	0
			85621	26232	26827	10839	18986	2737		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	b	119	Total	C	H	N	O	P	0	0
			3720	1135	1171	466	829	119		

- Molecule 3 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	c	271	Total	C	H	N	O	S	0	0
			4196	1288	2114	423	364	7		

- Molecule 4 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	d	209	Total	C	H	N	O	S	0	0
			3152	980	1586	288	294	4		

- Molecule 5 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	e	201	Total	C	H	N	O	S	0	0
			3142	974	1590	283	290	5		

- Molecule 6 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	f	177	Total	C	H	N	O	S	0	0
			2831	899	1421	249	256	6		

- Molecule 7 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	g	176	Total	C	H	N	O	S	0	0
			2670	832	1347	243	246	2		

- Molecule 8 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	h	41	Total	C	H	N	O	S	0	0
			627	194	324	54	54	1		

- Molecule 9 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	i	142	Total	C	H	N	O	S	0	0
			2266	714	1137	212	199	4		

- Molecule 10 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	j	123	Total	C	H	N	O	S	0	0
			1946	591	1004	181	164	6		

- Molecule 11 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	k	144	Total	C	H	N	O	S	0	0
			2164	654	1111	207	190	2		

- Molecule 12 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	l	136	Total	C	H	N	O	S	0	0
			2217	686	1142	205	177	7		

- Molecule 13 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	m	118	Total	C	H	N	O	S	0	0
			1916	585	971	194	161	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	116	Total	C	H	N	O	0	0
			1800	552	908	178	162		

- Molecule 15 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	o	114	Total	C	H	N	O	S	0	0
			1864	574	947	179	163	1		

- Molecule 16 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	117	Total	C	H	N	O	0	0
			1955	604	1008	192	151		

- Molecule 17 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	q	103	Total	C	H	N	O	S	0	0
			1641	516	825	153	145	2		

- Molecule 18 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	r	110	Total	C	H	N	O	S	0	0
			1761	532	904	166	156	3		

- Molecule 19 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace	
19	s	93	Total	C	H	N	O	S	0	0
			1533	466	795	139	131	2		

- Molecule 20 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	102	Total	C	H	N	O	0	0
			1602	492	823	146	141		

- Molecule 21 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms						AltConf	Trace
21	u	94	Total	C	H	N	O	S	0	0
			1523	479	770	137	134	3		

- Molecule 22 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	v	78	Total	C	H	N	O	S	0	0
			1172	362	586	116	107	1		

- Molecule 23 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	w	77	Total	C	H	N	O	S	0	0
			1263	388	638	129	106	2		

- Molecule 24 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	x	62	Total	C	H	N	O	S	0	0
			1027	308	526	98	94	1		

- Molecule 25 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms						AltConf	Trace
25	y	58	Total	C	H	N	O	S	0	0
			928	281	479	87	79	2		

- Molecule 26 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	z	56	Total	C	H	N	O	S	0	0
			887	269	443	94	80	1		

- Molecule 27 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	51	Total	C	H	N	O	0	0
			858	269	441	76	72		

- Molecule 28 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms						AltConf	Trace
28	1	46	Total	C	H	N	O	S	0	0
			788	228	411	90	57	2		

- Molecule 29 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms						AltConf	Trace
29	2	64	Total	C	H	N	O	S	0	0
			1065	323	561	105	74	2		

- Molecule 30 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	3	38	Total	C	H	N	O	S	0	0
			639	185	337	65	48	4		

- Molecule 31 is a protein called Ribosomal silencing factor RsfS.

Mol	Chain	Residues	Atoms						AltConf	Trace
31	6	105	Total	C	H	N	O	S	0	0
			1593	502	788	137	160	6		

- Molecule 32 is a protein called Heat shock protein 15.

Mol	Chain	Residues	Atoms						AltConf	Trace
32	V	95	Total	C	H	N	O	S	0	0
			1552	481	781	146	142	2		

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
V	-8	MET	-	initiating methionine	UNP P0ACG8
V	-7	HIS	-	expression tag	UNP P0ACG8
V	-6	HIS	-	expression tag	UNP P0ACG8
V	-5	HIS	-	expression tag	UNP P0ACG8
V	-4	HIS	-	expression tag	UNP P0ACG8
V	-3	HIS	-	expression tag	UNP P0ACG8
V	-2	HIS	-	expression tag	UNP P0ACG8
V	-1	GLY	-	expression tag	UNP P0ACG8
V	0	SER	-	expression tag	UNP P0ACG8
V	1	GLY	-	expression tag	UNP P0ACG8

- Molecule 33 is a RNA chain called tRNA Asp.

Mol	Chain	Residues	Atoms						AltConf	Trace
33	Z	76	Total	C	H	N	O	P	0	0
			2363	721	743	285	538	76		

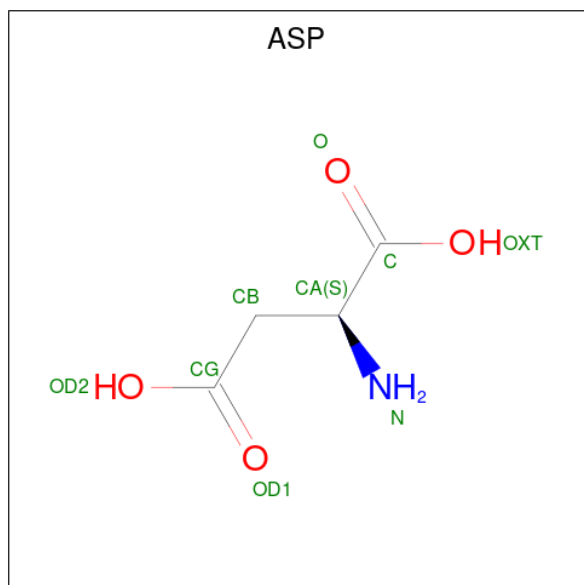
- Molecule 34 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
34	a	195	Total	Mg	0
			195	195	
34	b	5	Total	Mg	0
			5	5	
34	d	1	Total	Mg	0
			1	1	
34	k	1	Total	Mg	0
			1	1	
34	p	1	Total	Mg	0
			1	1	
34	z	1	Total	Mg	0
			1	1	

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

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

- Molecule 36 is ASPARTIC ACID (CCD ID: ASP) (formula: C₄H₇NO₄).

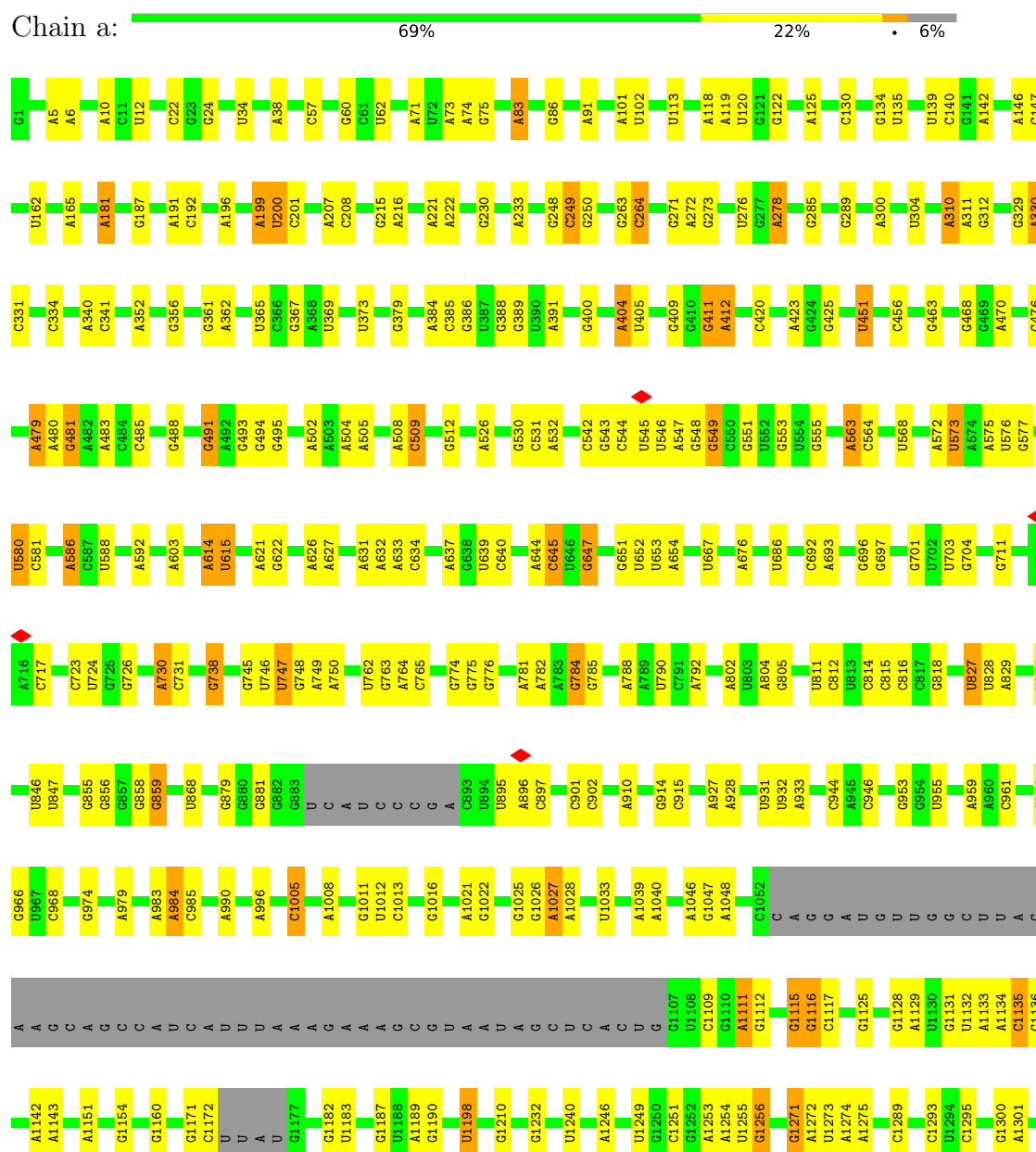


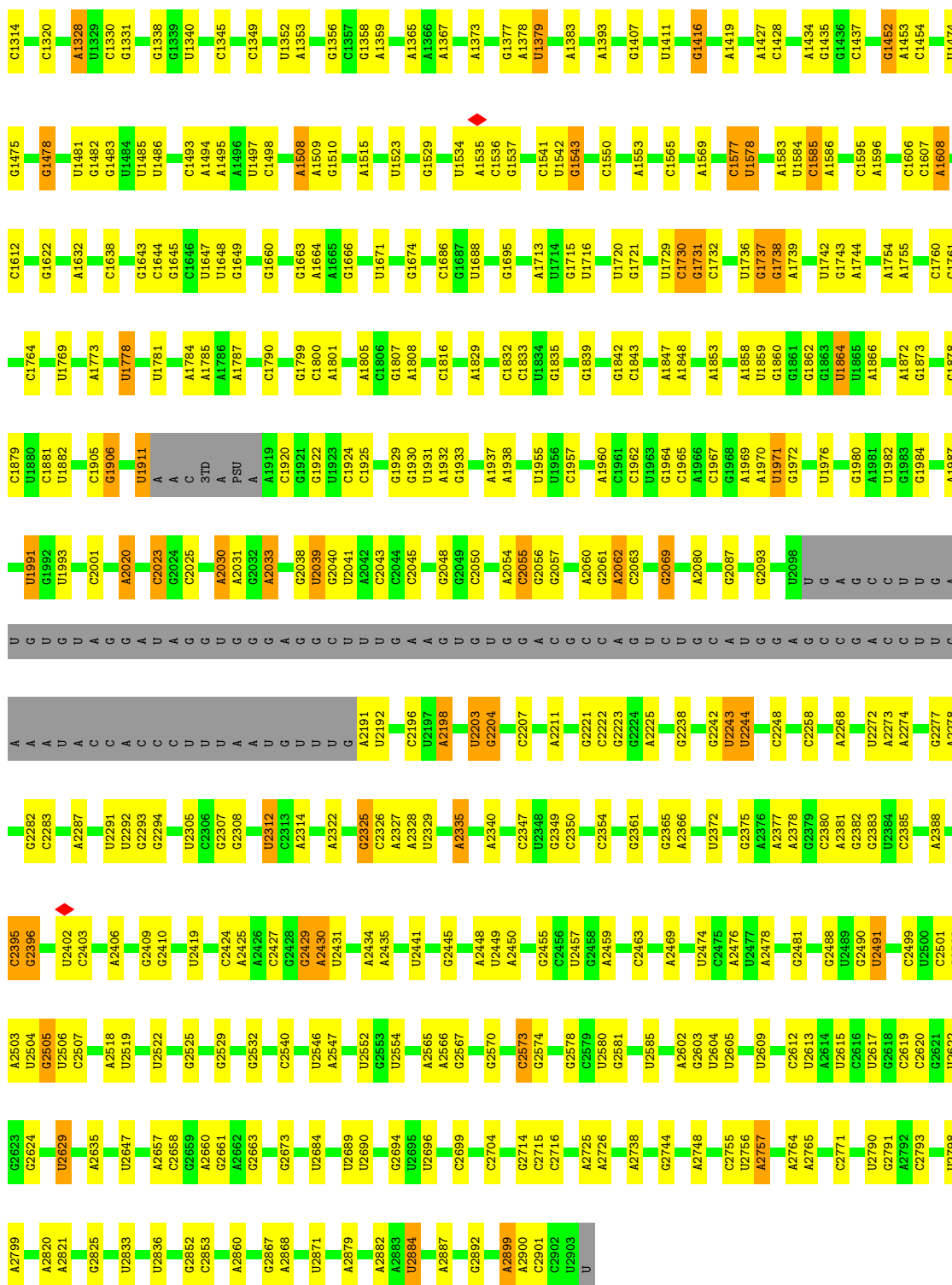
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
36	Z	1	14	4	6	1	3	0

3 Residue-property plots [i](#)

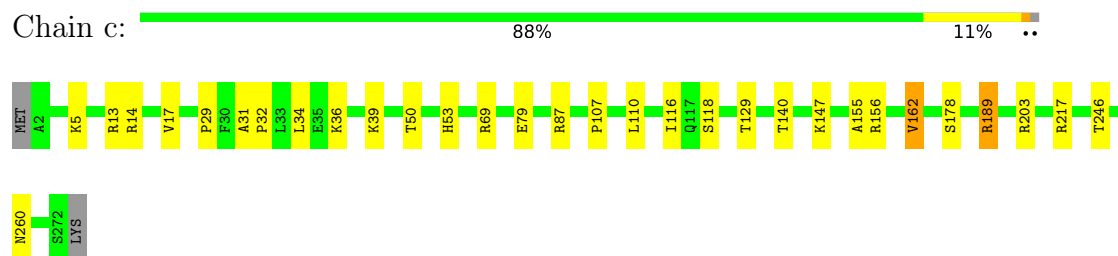
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 23S rRNA

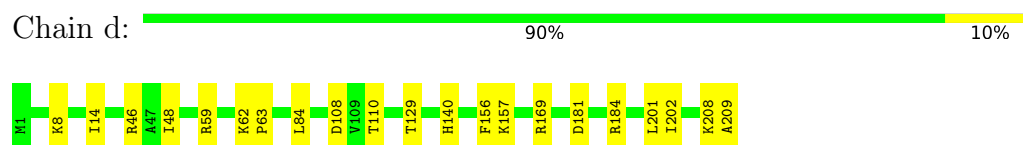




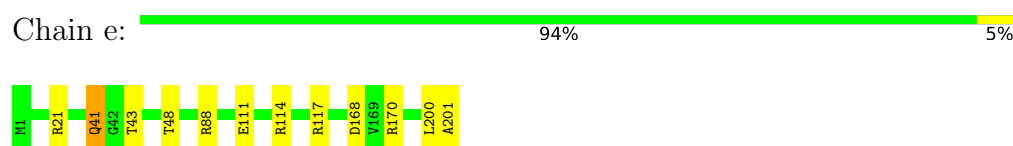
- Molecule 3: Large ribosomal subunit protein uL2



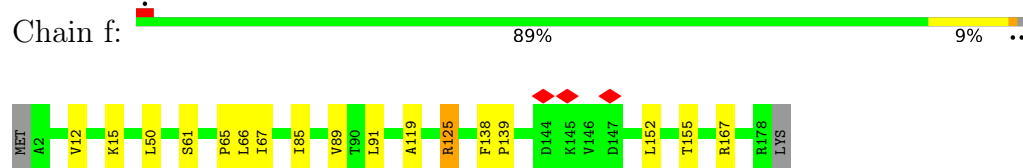
- Molecule 4: Large ribosomal subunit protein uL3



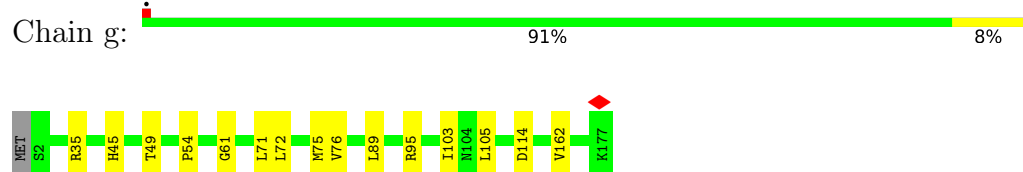
- Molecule 5: Large ribosomal subunit protein uL4



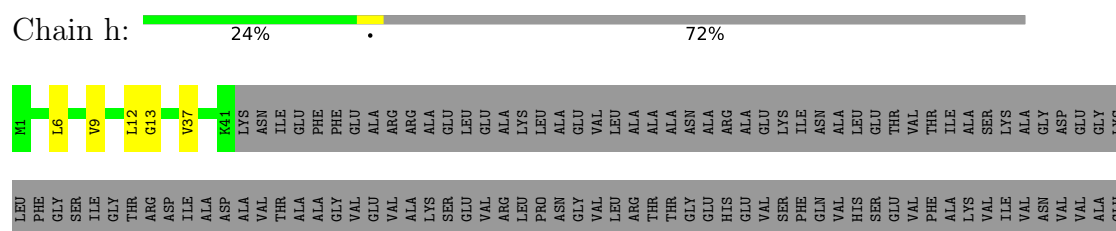
- Molecule 6: Large ribosomal subunit protein uL5




- Molecule 7: Large ribosomal subunit protein uL6



- Molecule 8: Large ribosomal subunit protein bL9



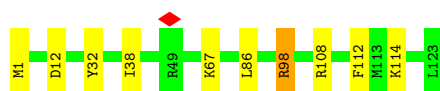
- Molecule 9: Large ribosomal subunit protein uL13

Chain i:  88% 11% .



- Molecule 10: Large ribosomal subunit protein uL14

Chain j:  92% 7% .




- Molecule 11: Large ribosomal subunit protein uL15

Chain k:  94% 6% .




- Molecule 12: Large ribosomal subunit protein uL16

Chain l:  90% 9% .



- Molecule 13: Large ribosomal subunit protein bL17

Chain m:  80% 13% 7% .



- Molecule 14: Large ribosomal subunit protein uL18

Chain n:  96% . .




- Molecule 15: Large ribosomal subunit protein bL19

Chain o:  96% . .



- Molecule 16: Large ribosomal subunit protein bL20

Chain p:  88% 11%



- Molecule 17: Large ribosomal subunit protein bL21

Chain q:  92% 8%




- Molecule 18: Large ribosomal subunit protein uL22

Chain r:  93% 7%




- Molecule 19: Large ribosomal subunit protein uL23

Chain s:  88% 5% 7%



- Molecule 20: Large ribosomal subunit protein uL24

Chain t:  85% 11%



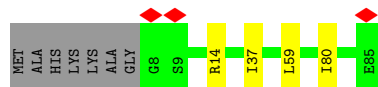
- Molecule 21: Large ribosomal subunit protein bL25

Chain u:  95% 5%




- Molecule 22: Large ribosomal subunit protein bL27

Chain v:  87% 5% 8%




- Molecule 23: Large ribosomal subunit protein bL28

Chain w:  88% 9% ..



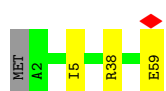
- Molecule 24: Large ribosomal subunit protein uL29

Chain x:  92% 6% .




- Molecule 25: Large ribosomal subunit protein uL30

Chain y:  93% 5% .




- Molecule 26: Large ribosomal subunit protein bL32

Chain z:  77% 21% .



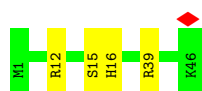
- Molecule 27: Large ribosomal subunit protein bL33

Chain 0:  91% 7% .




- Molecule 28: Large ribosomal subunit protein bL34

Chain 1:  91% 9% .



- Molecule 29: Large ribosomal subunit protein bL35

Chain 2:  89% 9% .

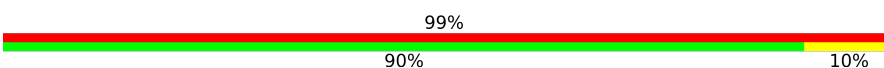


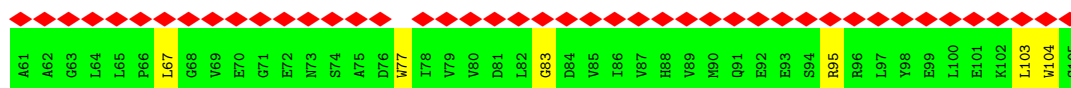
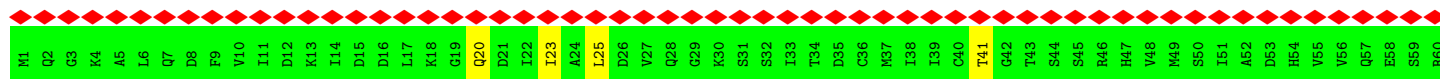
- Molecule 30: Large ribosomal subunit protein bL36A

Chain 3:  92% 8%



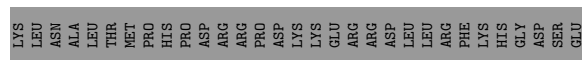
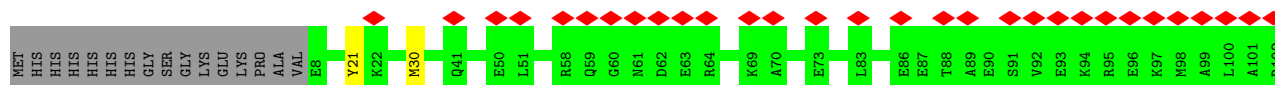
- Molecule 31: Ribosomal silencing factor RsfS

Chain 6:  99% 90% 10%



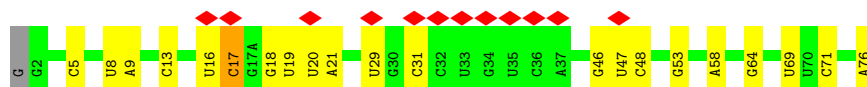
- Molecule 32: Heat shock protein 15

Chain V:  21% 65% 33%



- Molecule 33: tRNA Asp

Chain Z:  16% 71% 26%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	514726	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32.3	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	165000	Depositor
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.407	Depositor
Minimum map value	-0.083	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	411.36, 411.36, 411.36	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.8034375, 0.8034375, 0.8034375	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	a	0.61	1/65320 (0.0%)	1.14	288/101896 (0.3%)
2	b	0.55	0/2850	1.05	12/4444 (0.3%)
3	c	0.74	1/2121 (0.0%)	1.19	7/2852 (0.2%)
4	d	0.74	0/1576	1.09	4/2119 (0.2%)
5	e	0.70	0/1571	1.10	3/2113 (0.1%)
6	f	0.50	0/1434	1.04	1/1926 (0.1%)
7	g	0.55	0/1343	1.06	1/1816 (0.1%)
8	h	0.61	0/306	1.05	0/413
9	i	0.71	0/1152	1.09	1/1551 (0.1%)
10	j	0.63	0/951	1.10	1/1274 (0.1%)
11	k	0.75	0/1062	1.13	1/1413 (0.1%)
12	l	0.62	0/1073	1.12	1/1433 (0.1%)
13	m	0.80	0/958	1.26	6/1281 (0.5%)
14	n	0.55	0/902	1.03	1/1209 (0.1%)
15	o	0.65	0/929	1.07	0/1242
16	p	0.84	0/960	1.19	3/1278 (0.2%)
17	q	0.65	0/829	1.10	2/1107 (0.2%)
18	r	0.78	0/864	1.13	1/1156 (0.1%)
19	s	0.64	0/744	1.06	0/994
20	t	0.64	0/787	1.12	1/1051 (0.1%)
21	u	0.57	0/766	1.07	2/1025 (0.2%)
22	v	0.74	0/593	1.06	0/785
23	w	0.73	0/635	1.16	2/848 (0.2%)
24	x	0.55	0/502	1.11	1/667 (0.1%)
25	y	0.69	0/453	1.12	0/605
26	z	0.75	0/450	1.19	2/599 (0.3%)
27	0	0.59	0/424	1.05	0/565
28	1	0.86	0/380	1.35	2/498 (0.4%)
29	2	0.86	0/513	1.15	0/676
30	3	0.64	0/303	1.18	0/397
31	6	0.51	0/814	0.95	0/1098

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	V	0.48	0/781	0.93	0/1048
33	Z	0.60	0/1808	0.80	0/2817
All	All	0.62	2/96154 (0.0%)	1.13	343/144196 (0.2%)

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
1	a	0	4
3	c	0	6
4	d	0	3
5	e	0	4
6	f	0	1
7	g	0	1
9	i	0	5
10	j	0	2
11	k	0	2
12	l	0	7
13	m	0	4
14	n	0	1
15	o	0	2
16	p	0	3
17	q	0	1
18	r	0	3
20	t	0	4
21	u	0	1
22	v	0	1
23	w	0	2
24	x	0	1
25	y	0	1
26	z	0	2
29	2	0	2
31	6	0	1
All	All	0	64

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	53	HIS	CG-CD2	-6.61	1.28	1.35
1	a	2069	G7M	O3'-P	5.84	1.62	1.56

All (343) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	621	A	O3'-P-O5'	-8.27	91.60	104.00
1	a	551	G	O3'-P-O5'	-8.26	91.61	104.00
1	a	57	C	O3'-P-O5'	-8.23	91.66	104.00
1	a	2771	C	O3'-P-O5'	-8.20	91.70	104.00
1	a	1643	G	O3'-P-O5'	-8.10	91.85	104.00
1	a	2764	A	O3'-P-O5'	-8.04	91.95	104.00
1	a	577	G	O3'-P-O5'	-8.03	91.96	104.00
1	a	542	C	O3'-P-O5'	-7.87	92.20	104.00
1	a	2871	U	O3'-P-O5'	-7.78	92.34	104.00
1	a	400	G	O3'-P-O5'	-7.76	92.36	104.00
1	a	1969	A	O3'-P-O5'	-7.72	92.42	104.00
2	b	90	C	O3'-P-O5'	-7.64	92.54	104.00
1	a	2884	U	C2'-C3'-O3'	-7.64	102.24	113.70
1	a	62	U	O3'-P-O5'	-7.56	92.66	104.00
1	a	816	C	O3'-P-O5'	-7.55	92.68	104.00
1	a	1131	G	O3'-P-O5'	-7.47	92.79	104.00
1	a	310	A	O3'-P-O5'	-7.46	92.81	104.00
1	a	1632	A	O3'-P-O5'	-7.43	92.85	104.00
3	c	189	ARG	NE-CZ-NH1	-7.39	114.11	121.50
1	a	1565	C	O3'-P-O5'	-7.37	92.94	104.00
17	q	6	GLN	CB-CA-C	7.36	121.90	109.75
1	a	2062	A	O3'-P-O5'	-7.35	92.97	104.00
1	a	404	A	C2'-C3'-O3'	7.20	120.31	109.50
1	a	1606	C	C2'-C3'-O3'	-7.17	102.95	113.70
1	a	731	C	O3'-P-O5'	-7.16	93.26	104.00
1	a	1485	U	O3'-P-O5'	-7.15	93.27	104.00
1	a	1198	U	O3'-P-O5'	-7.14	93.29	104.00
1	a	1025	G	O3'-P-O5'	7.12	114.68	104.00
1	a	1011	G	O3'-P-O5'	-7.11	93.33	104.00
4	d	157	LYS	N-CA-CB	7.11	120.49	110.04
1	a	2378	A	O3'-P-O5'	-7.10	93.35	104.00
1	a	73	A	O3'-P-O5'	-7.05	93.42	104.00
4	d	129	THR	CA-CB-OG1	-7.05	99.03	109.60
1	a	2243	U	O3'-P-O5'	7.04	114.57	104.00
1	a	1358	G	O3'-P-O5'	-7.04	93.44	104.00
1	a	2023	C	C4'-C3'-O3'	-7.02	102.47	113.00
1	a	2025	C	C2'-C3'-O3'	-7.01	103.18	113.70
1	a	60	G	O3'-P-O5'	-7.01	93.48	104.00
1	a	134	G	O3'-P-O5'	-7.01	93.48	104.00
28	1	12	ARG	NE-CZ-NH2	7.00	125.50	119.20
1	a	1550	C	O3'-P-O5'	-6.99	93.51	104.00
1	a	1274	A	C4'-C3'-O3'	-6.97	102.54	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1359	A	O3'-P-O5'	-6.97	93.55	104.00
1	a	2198	A	O3'-P-O5'	-6.95	93.57	104.00
1	a	508	A	O3'-P-O5'	-6.92	93.63	104.00
1	a	1866	A	O3'-P-O5'	-6.91	93.64	104.00
3	c	246	THR	CA-CB-OG1	-6.90	99.24	109.60
1	a	2546	U	O3'-P-O5'	-6.89	93.66	104.00
1	a	763	G	O3'-P-O5'	-6.88	93.69	104.00
1	a	1452	G	O3'-P-O5'	-6.87	93.70	104.00
2	b	8	C	O3'-P-O5'	-6.86	93.71	104.00
1	a	1367	A	O3'-P-O5'	-6.84	93.74	104.00
4	d	108	ASP	CA-CB-CG	6.81	119.41	112.60
1	a	83	A	C2'-C3'-O3'	-6.77	103.54	113.70
1	a	2882	A	O3'-P-O5'	-6.77	93.84	104.00
1	a	2635	A	O3'-P-O5'	-6.76	93.85	104.00
1	a	2222	C	O3'-P-O5'	-6.75	93.87	104.00
1	a	2048	G	O3'-P-O5'	-6.68	93.97	104.00
1	a	2429	G	O3'-P-O5'	-6.67	94.00	104.00
1	a	2899	A	O3'-P-O5'	-6.66	94.01	104.00
1	a	1349	C	O3'-P-O5'	-6.65	94.03	104.00
23	w	45	ARG	NE-CZ-NH1	-6.62	114.88	121.50
1	a	631	A	C2'-C3'-O3'	-6.59	103.82	113.70
1	a	1454	C	O3'-P-O5'	-6.59	94.12	104.00
1	a	1743	G	O3'-P-O5'	-6.59	94.12	104.00
1	a	2001	C	O3'-P-O5'	-6.58	94.12	104.00
1	a	1254	A	C4'-C3'-O3'	-6.58	103.13	113.00
1	a	1660	G	C1'-C2'-O2'	6.58	118.27	108.40
1	a	1760	C	C2'-C3'-O3'	-6.58	103.83	113.70
1	a	855	G	O3'-P-O5'	-6.58	94.14	104.00
1	a	856	G	O3'-P-O5'	-6.56	94.16	104.00
1	a	1612	C	O3'-P-O5'	-6.56	94.16	104.00
1	a	634	C	O3'-P-O5'	-6.55	94.17	104.00
1	a	563	A	O3'-P-O5'	-6.55	94.18	104.00
1	a	1645	G	C4'-C3'-O3'	-6.55	103.17	113.00
1	a	586	A	C2'-C3'-O3'	-6.53	103.91	113.70
1	a	1293	C	O3'-P-O5'	-6.50	94.25	104.00
1	a	2278	A	O3'-P-O5'	-6.47	94.29	104.00
1	a	2434	A	O3'-P-O5'	-6.47	94.29	104.00
2	b	32	U	O3'-P-O5'	-6.46	94.32	104.00
1	a	932	U	O3'-P-O5'	-6.45	94.32	104.00
1	a	632	A	O3'-P-O5'	-6.42	94.38	104.00
1	a	676	A	O3'-P-O5'	-6.40	94.41	104.00
1	a	1785	A	O3'-P-O5'	-6.39	94.42	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	22	C	O3'-P-O5'	-6.37	94.45	104.00
1	a	1373	A	O3'-P-O5'	-6.34	94.49	104.00
1	a	495	G	O3'-P-O5'	-6.29	94.56	104.00
1	a	781	A	O3'-P-O5'	-6.29	94.56	104.00
1	a	2505	G	C2'-C3'-O3'	-6.29	104.27	113.70
18	r	72	THR	CA-CB-OG1	-6.29	100.17	109.60
1	a	1016	G	O3'-P-O5'	-6.28	94.57	104.00
1	a	2554	U	O3'-P-O5'	-6.28	94.57	104.00
1	a	1232	G	O3'-P-O5'	-6.26	94.61	104.00
1	a	2080	A	O3'-P-O5'	-6.26	94.61	104.00
1	a	2658	C	O3'-P-O5'	-6.25	94.63	104.00
13	m	21	PHE	CA-CB-CG	-6.24	107.56	113.80
1	a	2463	C	O3'-P-O5'	-6.23	94.65	104.00
1	a	388	G	O3'-P-O5'	-6.23	94.66	104.00
1	a	1843	C	O3'-P-O5'	-6.22	94.66	104.00
1	a	573	U	O3'-P-O5'	-6.22	94.67	104.00
1	a	162	U	O3'-P-O5'	-6.22	94.67	104.00
1	a	2684	U	O3'-P-O5'	-6.21	94.68	104.00
1	a	1964	G	O3'-P-O5'	6.20	113.30	104.00
13	m	17	ARG	CB-CA-C	-6.20	100.51	110.79
1	a	200	U	O3'-P-O5'	-6.18	94.73	104.00
13	m	96	ARG	N-CA-CB	-6.17	100.09	111.13
1	a	479	A	P-O5'-C5'	-6.13	111.70	120.90
1	a	1553	A	O3'-P-O5'	-6.13	94.80	104.00
1	a	2519	U	O3'-P-O5'	-6.12	94.82	104.00
13	m	17	ARG	N-CA-CB	6.10	119.09	110.12
1	a	622	G	C4'-C3'-O3'	-6.10	103.86	113.00
1	a	1135	C	C2'-C3'-O3'	-6.09	104.56	113.70
1	a	1991	U	C4'-C3'-O3'	-6.09	103.86	113.00
1	a	509	C	C4'-C3'-O3'	-6.07	103.90	113.00
1	a	2884	U	C1'-C2'-O2'	-6.06	99.31	108.40
1	a	409	G	O3'-P-O5'	-6.05	94.92	104.00
1	a	2892	G	O3'-P-O5'	-6.04	94.95	104.00
1	a	818	G	O3'-P-O5'	-6.03	94.95	104.00
1	a	2354	C	C4'-C3'-C2'	-6.03	96.57	102.60
1	a	1246	A	O3'-P-O5'	-6.02	94.97	104.00
1	a	701	G	O3'-P-O5'	-6.00	94.99	104.00
1	a	1151	A	O3'-P-O5'	-6.00	94.99	104.00
1	a	1416	G	O3'-P-O5'	-5.97	95.05	104.00
1	a	2629	U	O3'-P-O5'	-5.96	95.05	104.00
6	f	125	ARG	NE-CZ-NH1	-5.96	115.54	121.50
2	b	16	G	O3'-P-O5'	-5.96	95.06	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1543	G	C4'-C3'-O3'	-5.96	104.06	113.00
3	c	39	LYS	N-CA-CB	-5.96	100.93	110.46
1	a	1585	C	O3'-P-O5'	-5.96	95.07	104.00
2	b	65	U	O3'-P-O5'	-5.95	95.08	104.00
1	a	1778	U	C4'-C3'-O3'	-5.94	104.09	113.00
1	a	2565	A	C2'-C3'-O3'	-5.91	104.84	113.70
1	a	199	A	C1'-O4'-C4'	-5.91	103.79	109.70
1	a	1638	C	O3'-P-O5'	-5.90	95.14	104.00
26	z	44	THR	CA-CB-OG1	-5.90	100.75	109.60
1	a	1289	C	O3'-P-O5'	-5.89	95.16	104.00
1	a	696	G	C4'-C3'-C2'	-5.89	96.71	102.60
1	a	2377	A	O3'-P-O5'	-5.88	95.18	104.00
1	a	2054	A	C2'-C3'-O3'	-5.88	104.88	113.70
3	c	140	THR	CA-CB-OG1	-5.88	100.79	109.60
1	a	2673	G	O3'-P-O5'	-5.87	95.19	104.00
1	a	748	G	C1'-O4'-C4'	-5.87	104.03	109.90
1	a	334	C	O3'-P-O5'	-5.87	95.20	104.00
1	a	804	A	O3'-P-O5'	-5.86	95.20	104.00
4	d	140	HIS	CA-CB-CG	-5.86	107.94	113.80
1	a	990	A	C2'-C3'-O3'	-5.86	104.92	113.70
1	a	747	5MU	O3'-P-O5'	-5.86	95.22	104.00
1	a	1781	U	O3'-P-O5'	-5.85	95.23	104.00
1	a	2501	C	O3'-P-O5'	-5.83	95.26	104.00
1	a	1864	U	C4'-C3'-O3'	-5.82	104.28	113.00
1	a	1971	U	C4'-C3'-O3'	-5.80	104.29	113.00
1	a	1671	U	C3'-C2'-O2'	5.80	119.40	110.70
20	t	47	LYS	CB-CA-C	-5.79	99.94	109.27
1	a	1377	G	C4'-C3'-O3'	-5.78	104.33	113.00
1	a	1356	G	O3'-P-O5'	-5.77	95.34	104.00
2	b	81	G	O3'-P-O5'	-5.77	95.34	104.00
1	a	2427	C	O3'-P-O5'	-5.77	95.35	104.00
1	a	2738	A	O3'-P-O5'	-5.76	95.37	104.00
1	a	1437	C	O3'-P-O5'	-5.75	95.37	104.00
1	a	1008	A	O3'-P-O5'	-5.74	95.39	104.00
1	a	2624	G	C2'-C3'-O3'	-5.74	105.09	113.70
1	a	379	G	O3'-P-O5'	-5.74	95.39	104.00
3	c	189	ARG	NE-CZ-NH2	5.74	124.36	119.20
1	a	181	A	C4'-C3'-C2'	-5.73	96.87	102.60
11	k	35	HIS	CB-CG-CD2	-5.73	123.75	131.20
1	a	1481	U	O3'-P-O5'	-5.71	95.43	104.00
5	e	41	GLN	N-CA-CB	-5.71	101.75	110.26
1	a	2057	G	C4'-C3'-O3'	-5.71	104.44	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	2039	U	C2'-C3'-O3'	-5.70	105.15	113.70
1	a	839	U	C4'-C3'-O3'	-5.69	104.47	113.00
1	a	485	C	O3'-P-O5'	-5.69	95.47	104.00
1	a	543	G	O3'-P-O5'	-5.68	95.48	104.00
1	a	1761	C	C2'-C3'-O3'	-5.67	105.19	113.70
1	a	187	G	O3'-P-O5'	-5.67	95.50	104.00
1	a	2409	G	O3'-P-O5'	-5.67	95.50	104.00
24	x	36	GLN	N-CA-CB	-5.67	101.85	111.20
13	m	29	VAL	N-CA-CB	5.67	117.18	110.55
1	a	2836	U	C2'-C3'-O3'	-5.65	105.22	113.70
1	a	91	A	O3'-P-O5'	-5.65	95.53	104.00
1	a	814	C	C2'-C3'-O3'	-5.64	105.24	113.70
1	a	2381	A	C1'-C2'-O2'	5.63	116.84	108.40
16	p	101	PHE	CA-CB-CG	-5.63	108.17	113.80
1	a	1606	C	O3'-P-O5'	-5.61	95.59	104.00
1	a	2395	C	C2'-C3'-O3'	-5.61	105.29	113.70
1	a	667	U	O3'-P-O5'	-5.61	95.59	104.00
1	a	2050	C	O3'-P-O5'	-5.60	95.59	104.00
26	z	10	ARG	NE-CZ-NH1	-5.59	115.91	121.50
1	a	271	G	C2'-C3'-O3'	5.59	117.88	109.50
1	a	784	G	O3'-P-O5'	-5.58	95.62	104.00
1	a	300	A	O3'-P-O5'	5.58	112.37	104.00
1	a	815	C	O3'-P-O5'	-5.58	95.63	104.00
2	b	6	G	O3'-P-O5'	-5.58	95.64	104.00
1	a	470	A	C4'-C3'-O3'	-5.57	104.65	113.00
1	a	2525	G	C4'-C3'-C2'	-5.56	97.04	102.60
1	a	633	A	O3'-P-O5'	5.56	112.34	104.00
1	a	271	G	O3'-P-O5'	-5.55	95.68	104.00
1	a	1005	C	C4'-C3'-O3'	-5.54	104.68	113.00
1	a	2573	C	O3'-P-O5'	-5.54	95.68	104.00
1	a	1976	U	C3'-C2'-O2'	5.53	118.99	110.70
1	a	526	A	C3'-C2'-C1'	5.52	106.82	101.30
21	u	44	HIS	CA-CB-CG	-5.51	108.29	113.80
9	i	85	LYS	CB-CA-C	-5.50	100.20	109.50
1	a	2203	U	C4'-C3'-O3'	-5.50	104.75	113.00
1	a	588	U	C4'-C3'-O3'	-5.49	104.76	113.00
1	a	750	A	C4'-C3'-O3'	-5.48	104.77	113.00
1	a	697	G	O3'-P-O5'	-5.48	95.78	104.00
1	a	1251	C	O3'-P-O5'	-5.48	95.78	104.00
1	a	1039	A	O3'-P-O5'	-5.48	95.78	104.00
1	a	2620	C	C3'-C2'-O2'	5.48	118.91	110.70
1	a	1240	U	C4'-C3'-O3'	-5.47	104.79	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	12	ARG	NE-CZ-NH1	-5.47	116.03	121.50
1	a	1543	G	O3'-P-O5'	-5.46	95.80	104.00
1	a	330	A	O3'-P-O5'	-5.46	95.81	104.00
1	a	2272	U	O3'-P-O5'	-5.46	95.81	104.00
1	a	2325	G	O3'-P-O5'	-5.45	95.82	104.00
1	a	1787	A	C4'-C3'-O3'	-5.45	104.82	113.00
1	a	352	A	O3'-P-O5'	-5.44	95.84	104.00
1	a	2277	G	O3'-P-O5'	-5.44	95.84	104.00
1	a	389	G	O3'-P-O5'	-5.44	95.84	104.00
1	a	2612	C	C2'-C3'-O3'	-5.44	105.54	113.70
1	a	738	G	O5'-P-OP2	-5.44	91.69	108.00
1	a	2725	A	O3'-P-O5'	-5.44	95.85	104.00
1	a	966	G	O3'-P-O5'	-5.43	95.85	104.00
1	a	480	A	O3'-P-O5'	-5.43	95.86	104.00
1	a	2481	G	C4'-C3'-O3'	-5.42	104.87	113.00
1	a	2546	U	C4'-C3'-O3'	-5.41	104.88	113.00
1	a	2326	C	C2'-C3'-O3'	-5.41	105.58	113.70
1	a	2704	C	O3'-P-O5'	-5.41	95.88	104.00
1	a	2349	G	O3'-P-O5'	-5.40	95.89	104.00
1	a	2578	G	C4'-C3'-C2'	-5.40	97.20	102.60
2	b	7	G	O3'-P-O5'	-5.40	95.90	104.00
1	a	868	U	O3'-P-O5'	-5.39	95.91	104.00
1	a	1379	U	C4'-C3'-O3'	-5.39	104.92	113.00
1	a	1190	G	O4'-C4'-C3'	-5.39	98.61	104.00
1	a	827	U	C2'-C3'-O3'	-5.37	105.65	113.70
1	a	2033	A	C4'-C3'-O3'	5.35	117.43	109.40
5	e	48	THR	CA-CB-OG1	-5.35	101.58	109.60
1	a	1769	U	C4'-C3'-C2'	-5.34	97.26	102.60
1	a	2382	G	O3'-P-O5'	-5.34	96.00	104.00
1	a	555	G	N9-C1'-C2'	-5.33	106.00	114.00
1	a	1189	A	O4'-C4'-C3'	-5.32	98.68	104.00
1	a	652	U	O3'-P-O5'	-5.32	96.02	104.00
1	a	1249	U	C4'-C3'-O3'	-5.32	105.03	113.00
1	a	2833	U	O3'-P-O5'	-5.31	96.04	104.00
1	a	1256	G	O3'-P-O5'	-5.31	96.04	104.00
12	l	8	LYS	N-CA-CB	5.31	118.50	110.28
1	a	1378	A	O3'-P-O5'	-5.30	96.04	104.00
1	a	312	G	O3'-P-O5'	-5.30	96.05	104.00
1	a	2499	C	C4'-C3'-O3'	-5.29	105.06	113.00
1	a	412	A	C2'-C3'-O3'	-5.28	105.77	113.70
1	a	1663	G	C4'-C3'-C2'	-5.28	97.32	102.60
1	a	576	U	C4'-C3'-O3'	-5.28	105.08	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	774	G	O5'-C5'-C4'	-5.28	103.78	111.70
1	a	1255	U	C4'-C3'-O3'	-5.28	105.09	113.00
1	a	1695	G	O3'-P-O5'	-5.28	96.09	104.00
1	a	979	A	C4'-C3'-C2'	-5.26	97.34	102.60
10	j	12	ASP	CA-CB-CG	5.26	117.86	112.60
1	a	2396	G	C4'-C3'-C2'	-5.25	97.35	102.60
1	a	2716	C	C4'-C3'-O3'	-5.25	105.12	113.00
1	a	384	A	O3'-P-O5'	5.25	111.88	104.00
1	a	1666	G	C4'-C3'-C2'	-5.25	97.35	102.60
1	a	553	G	C4'-C3'-C2'	-5.25	97.35	102.60
1	a	2490	G	O3'-P-O5'	-5.25	96.13	104.00
1	a	2755	C	O3'-P-O5'	-5.25	96.13	104.00
1	a	784	G	C2'-C3'-O3'	-5.25	105.83	113.70
1	a	2242	G	O3'-P-O5'	-5.25	96.13	104.00
1	a	1117	C	O3'-P-O5'	-5.24	96.14	104.00
1	a	2335	A	C4'-C3'-O3'	-5.23	105.15	113.00
3	c	36	LYS	CB-CA-C	5.23	118.59	109.65
3	c	162	VAL	N-CA-CB	-5.23	103.69	112.47
23	w	51	VAL	N-CA-CB	-5.22	102.88	111.45
1	a	726	G	O3'-P-O5'	-5.22	96.17	104.00
1	a	1761	C	C1'-C2'-O2'	-5.22	100.57	108.40
1	a	1755	A	O3'-P-O5'	5.22	111.83	104.00
17	q	79	ARG	CD-NE-CZ	-5.22	117.09	124.40
1	a	451	U	C1'-O4'-C4'	-5.21	104.69	109.90
1	a	859	G	O3'-P-O5'	-5.21	96.19	104.00
1	a	2860	A	O3'-P-O5'	5.21	111.81	104.00
1	a	230	G	O3'-P-O5'	-5.20	96.20	104.00
1	a	1577	C	O3'-P-O5'	-5.20	96.21	104.00
1	a	369	U	O3'-P-O5'	-5.19	96.21	104.00
1	a	626	A	C4'-C3'-C2'	-5.19	97.41	102.60
1	a	2619	C	C3'-C2'-O2'	5.19	118.49	110.70
1	a	1027	A	O3'-P-O5'	-5.19	96.22	104.00
1	a	572	A	O3'-P-O5'	-5.17	96.24	104.00
1	a	2620	C	O3'-P-O5'	-5.17	96.25	104.00
1	a	2696	U	O3'-P-O5'	-5.17	96.25	104.00
1	a	200	U	C4'-C3'-O3'	-5.17	105.25	113.00
1	a	1160	G	O3'-P-O5'	-5.17	96.25	104.00
1	a	1688	U	O3'-P-O5'	-5.16	96.26	104.00
1	a	692	C	C1'-C2'-O2'	-5.16	100.66	108.40
1	a	2388	A	C4'-C3'-O3'	-5.16	105.26	113.00
1	a	2879	A	O3'-P-O5'	-5.16	96.26	104.00
1	a	130	C	O3'-P-O5'	-5.16	96.27	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	89	U	C3'-C2'-C1'	-5.16	96.34	101.50
1	a	2258	C	O3'-P-O5'	-5.15	96.27	104.00
21	u	90	ASP	CA-CB-CG	5.15	117.75	112.60
1	a	2617	U	C4'-C3'-O3'	-5.15	105.28	113.00
5	e	111	GLU	CB-CA-C	-5.15	102.25	110.79
16	p	3	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	a	1407	G	C4'-C3'-C2'	-5.14	97.46	102.60
1	a	1314	C	C4'-C3'-O3'	-5.14	105.29	113.00
1	a	2196	C	O3'-P-O5'	-5.13	96.30	104.00
1	a	331	C	O3'-P-O5'	-5.13	96.31	104.00
1	a	580	U	C3'-C2'-O2'	5.13	118.39	110.70
1	a	1695	G	C4'-C3'-O3'	-5.13	105.31	113.00
1	a	2055	C	C2'-C3'-O3'	-5.13	106.01	113.70
1	a	2715	C	C4'-C3'-O3'	-5.12	105.32	113.00
1	a	385	C	O3'-P-O5'	-5.11	96.34	104.00
1	a	1486	U	O3'-P-O5'	-5.11	96.34	104.00
1	a	2350	C	O5'-C5'-C4'	-5.10	103.85	111.50
1	a	2699	C	O3'-P-O5'	5.09	111.63	104.00
1	a	1328	A	O3'-P-O5'	-5.08	96.39	104.00
16	p	31	VAL	N-CA-CB	-5.07	105.05	111.64
1	a	1737	G	O3'-P-O5'	-5.07	96.40	104.00
1	a	2540	C	C4'-C3'-C2'	-5.06	97.54	102.60
1	a	944	C	C4'-C3'-C2'	-5.06	97.54	102.60
1	a	1790	C	C4'-C3'-O3'	-5.06	105.41	113.00
1	a	1478	G	C4'-C3'-C2'	-5.06	97.54	102.60
2	b	99	A	C2'-C3'-O3'	-5.06	106.11	113.70
1	a	730	A	C1'-C2'-O2'	5.05	115.98	108.40
1	a	1154	G	O3'-P-O5'	-5.05	96.42	104.00
2	b	24	G	O3'-P-O5'	-5.05	96.43	104.00
1	a	2694	G	C2'-C3'-O3'	-5.04	106.13	113.70
1	a	965	C	C4'-C3'-O3'	-5.04	105.44	113.00
1	a	953	G	C4'-C3'-C2'	-5.04	97.56	102.60
1	a	2430	A	P-O5'-C5'	-5.04	113.34	120.90
2	b	49	C	O3'-P-O5'	-5.04	96.44	104.00
1	a	113	U	C4'-C3'-O3'	-5.04	105.45	113.00
1	a	2445	2MG	O3'-P-O5'	-5.03	96.45	104.00
1	a	38	A	O3'-P-O5'	-5.03	96.45	104.00
1	a	762	U	C1'-C2'-O2'	-5.03	104.25	111.80
1	a	2349	G	C4'-C3'-O3'	-5.03	105.45	113.00
1	a	959	A	C4'-C3'-O3'	-5.03	105.46	113.00
1	a	2207	C	O3'-P-O5'	-5.03	96.46	104.00
13	m	29	VAL	N-CA-C	-5.03	105.59	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	1835	2MG	O3'-P-O5'	-5.02	96.47	104.00
1	a	2045	C	O3'-P-O5'	-5.02	96.47	104.00
14	n	10	ARG	N-CA-CB	-5.02	102.06	110.39
1	a	2455	G	C4'-C3'-O3'	-5.01	105.49	113.00
1	a	1378	A	C2'-C3'-O3'	5.00	117.01	109.50
7	g	114	ASP	CA-CB-CG	5.00	117.60	112.60
1	a	122	G	C1'-C2'-O2'	5.00	115.90	108.40

There are no chirality outliers.

All (64) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	2	13	ARG	Sidechain
29	2	40	ARG	Sidechain
31	6	95	ARG	Sidechain
1	a	2375	G	Sidechain
1	a	249	C	Sidechain
1	a	463	G	Sidechain
1	a	512	G	Sidechain
3	c	156	ARG	Sidechain
3	c	189	ARG	Sidechain
3	c	203	ARG	Sidechain
3	c	217	ARG	Sidechain
3	c	69	ARG	Sidechain
3	c	87	ARG	Sidechain
4	d	169	ARG	Sidechain
4	d	46	ARG	Sidechain
4	d	59	ARG	Sidechain
5	e	114	ARG	Sidechain
5	e	117	ARG	Sidechain
5	e	21	ARG	Sidechain
5	e	88	ARG	Sidechain
6	f	125	ARG	Sidechain
7	g	95	ARG	Sidechain
9	i	120	ARG	Sidechain
9	i	35	ARG	Sidechain
9	i	37	ARG	Sidechain
9	i	95	ARG	Sidechain
9	i	96	ARG	Sidechain
10	j	108	ARG	Sidechain
10	j	98	ARG	Sidechain
11	k	41	ARG	Sidechain

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Mol	Chain	Res	Type	Group
11	k	59	ARG	Sidechain
12	l	10	ARG	Sidechain
12	l	114	ARG	Sidechain
12	l	44	ARG	Sidechain
12	l	50	ARG	Sidechain
12	l	51	ARG	Sidechain
12	l	55	ARG	Sidechain
12	l	66	ARG	Sidechain
13	m	2	ARG	Sidechain
13	m	22	ARG	Sidechain
13	m	63	ARG	Sidechain
13	m	64	ARG	Sidechain
14	n	81	ARG	Sidechain
15	o	51	ARG	Sidechain
15	o	53	ARG	Sidechain
16	p	11	ARG	Sidechain
16	p	28	ARG	Sidechain
16	p	51	ARG	Sidechain
17	q	68	ARG	Sidechain
18	r	110	ARG	Sidechain
18	r	8	ARG	Sidechain
18	r	84	ARG	Sidechain
20	t	22	ARG	Sidechain
20	t	7	ARG	Sidechain
20	t	86	ARG	Sidechain
20	t	94	ARG	Sidechain
21	u	79	ARG	Sidechain
22	v	14	ARG	Sidechain
23	w	45	ARG	Sidechain
23	w	74	ARG	Sidechain
24	x	7	ARG	Sidechain
25	y	38	ARG	Sidechain
26	z	13	ARG	Sidechain
26	z	17	ARG	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	a	58794	26827	29597	116	0
2	b	2549	1171	1291	2	0
3	c	2082	2114	2154	11	0
4	d	1566	1586	1618	9	0
5	e	1552	1590	1619	3	0
6	f	1410	1421	1444	10	0
7	g	1323	1347	1371	6	0
8	h	303	324	327	4	0
9	i	1129	1137	1162	8	0
10	j	942	1004	1019	5	0
11	k	1053	1111	1129	6	0
12	l	1075	1142	1145	3	0
13	m	945	971	989	5	0
14	n	892	908	923	1	0
15	o	917	947	962	2	0
16	p	947	1008	1019	5	0
17	q	816	825	839	3	0
18	r	857	904	922	3	0
19	s	738	795	807	4	0
20	t	779	823	831	7	0
21	u	753	770	780	1	0
22	v	586	586	596	2	0
23	w	625	638	652	2	0
24	x	501	526	531	1	0
25	y	449	479	488	1	0
26	z	444	443	458	6	0
27	0	417	441	451	1	0
28	1	377	411	418	2	0
29	2	504	561	572	3	0
30	3	302	337	340	2	0
31	6	805	788	806	6	0
32	V	771	781	794	1	0
33	Z	1620	743	819	2	0
34	a	195	0	0	0	0
34	b	5	0	0	0	0
34	d	1	0	0	0	0
34	k	1	0	0	0	0
34	p	1	0	0	0	0
34	z	1	0	0	0	0
35	3	1	0	0	0	0
36	Z	8	6	3	0	0
All	All	89036	55465	58876	215	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 (215) 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)
1:a:568:U:H1'	1:a:2030:6MZ:H9C1	1.78	0.65
8:h:9:VAL:HB	8:h:12:LEU:HD11	1.81	0.61
5:e:200:LEU:O	5:e:201:ALA:C	2.46	0.59
1:a:1182:G:H2'	1:a:1183:U:O4'	2.04	0.57
9:i:18:VAL:HG21	9:i:142:ILE:HD12	1.87	0.57
1:a:2478:A:OP2	30:3:2:LYS:NZ	2.36	0.56
5:e:41:GLN:HG2	5:e:43:THR:HG23	1.86	0.56
9:i:142:ILE:OXT	9:i:142:ILE:HG22	2.05	0.56
1:a:788:A:OP1	1:a:790:U:H5	1.88	0.56
21:u:75:GLN:HB2	21:u:92:VAL:HG23	1.88	0.55
8:h:12:LEU:HD12	8:h:13:GLY:N	2.21	0.55
1:a:2900:A:H2'	1:a:2901:C:O4'	2.07	0.54
1:a:1980:G:O2'	1:a:1982:U:OP2	2.26	0.54
11:k:77:ILE:HD13	11:k:108:ALA:HB1	1.90	0.54
1:a:1320:C:N3	1:a:1331:G:O6	2.42	0.53
9:i:141:ASP:O	9:i:142:ILE:C	2.52	0.53
19:s:61:LEU:HD12	19:s:61:LEU:C	2.33	0.53
1:a:1115:G:O2'	1:a:1116:G:O5'	2.27	0.52
1:a:1607:C:H42	1:a:1622:G:P	2.33	0.52
13:m:55:ALA:HB1	13:m:79:LEU:O	2.11	0.51
7:g:103:ILE:HG22	7:g:105:LEU:CD2	2.41	0.51
1:a:1778:U:H2'	1:a:1784:A:N6	2.25	0.51
2:b:42:C:C5	6:f:66:LEU:HD22	2.46	0.51
11:k:132:ARG:HG3	11:k:142:ILE:HD12	1.93	0.50
3:c:107:PRO:HD2	3:c:110:LEU:HD22	1.94	0.50
1:a:1338:G:O2'	1:a:1393:A:N1	2.39	0.50
1:a:1932:A:H2'	1:a:1933:G:O4'	2.12	0.49
1:a:1275:A:N1	1:a:1295:C:O2'	2.38	0.49
4:d:208:LYS:O	4:d:209:ALA:C	2.56	0.49
3:c:31:ALA:N	3:c:32:PRO:CD	2.76	0.49
1:a:2243:U:H2'	1:a:2244:U:C6	2.48	0.49
12:l:74:THR:HA	12:l:88:ASN:O	2.13	0.49
1:a:2756:U:H1'	1:a:2757:A:H5'	1.94	0.49
1:a:1508:A:O2'	1:a:1509:A:O4'	2.31	0.48
7:g:54:PRO:HB3	7:g:61:GLY:HA3	1.93	0.48
1:a:273:G:N2	1:a:365:U:C2	2.82	0.48
4:d:110:THR:HG23	4:d:202:ILE:HB	1.95	0.48
9:i:11:VAL:HG21	9:i:50:THR:HA	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:181:ASP:OD2	4:d:184:ARG:HD2	2.14	0.48
26:z:43:ILE:HG22	26:z:49:TYR:HB2	1.95	0.48
28:1:15:SER:OG	28:1:16:HIS:CD2	2.67	0.48
4:d:110:THR:CG2	4:d:202:ILE:HB	2.43	0.48
1:a:1720:U:H2'	1:a:1721:G:O4'	2.14	0.48
23:w:6:GLN:HE21	23:w:50:ARG:H	1.62	0.48
23:w:72:ARG:NH1	23:w:78:TYR:OH	2.44	0.48
1:a:1494:A:H2'	1:a:1495:A:C8	2.49	0.47
6:f:119:ALA:O	6:f:167:ARG:NH1	2.45	0.47
10:j:114:LYS:HE3	31:6:77:TRP:CE3	2.50	0.47
1:a:1738:G:HO2'	1:a:1739:A:H8	1.63	0.47
1:a:1864:U:OP1	1:a:2410:G:O2'	2.29	0.47
20:t:33:LYS:HB3	20:t:64:ALA:HB1	1.96	0.47
29:2:45:ARG:N	29:2:46:PRO:HD2	2.29	0.47
31:6:103:LEU:HD23	31:6:104:TRP:NE1	2.30	0.47
1:a:1027:A:C2	1:a:2488:G:H5'	2.50	0.47
30:3:16:ILE:HD13	30:3:25:VAL:HG22	1.97	0.47
3:c:29:PRO:HG2	3:c:34:LEU:HD11	1.97	0.47
16:p:91:ASP:C	16:p:91:ASP:OD1	2.57	0.47
22:v:37:ILE:HG21	22:v:80:ILE:HG21	1.97	0.47
1:a:191:A:H2'	1:a:192:C:C6	2.50	0.46
1:a:468:G:N7	28:1:39:ARG:NH2	2.56	0.46
1:a:2312:U:H5'	6:f:85:ILE:HD11	1.96	0.46
10:j:98:ARG:CZ	31:6:103:LEU:HD13	2.45	0.46
11:k:77:ILE:HD12	11:k:77:ILE:N	2.30	0.46
1:a:645:C:H2'	1:a:647:G:C8	2.51	0.46
1:a:1028:A:N6	1:a:1125:G:H2'	2.31	0.46
1:a:479:A:N3	1:a:481:G:H5''	2.30	0.46
2:b:32:U:C2	2:b:51:G:N2	2.83	0.46
1:a:1924:C:H2'	1:a:1925:C:O4'	2.16	0.46
1:a:2291:U:OP1	1:a:2380:C:O2'	2.32	0.46
1:a:2327:A:H2'	1:a:2328:A:C8	2.51	0.46
1:a:2615:U:C2	26:z:4:GLN:HA	2.50	0.46
25:y:5:ILE:HG22	25:y:59:GLU:HB3	1.96	0.46
1:a:2328:A:H2'	1:a:2329:U:C6	2.50	0.46
1:a:1340:U:OP1	19:s:19:LYS:NZ	2.43	0.46
33:Z:8:U:C5	33:Z:13:C:C5	3.03	0.46
1:a:1595:C:H2'	1:a:1596:A:O4'	2.16	0.46
13:m:13:ASN:C	13:m:13:ASN:OD1	2.58	0.46
1:a:703:U:H2'	1:a:704:G:O4'	2.16	0.46
1:a:984:A:N3	1:a:984:A:H2'	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:2532:G:O2'	1:a:2657:A:N1	2.44	0.46
18:r:7:HIS:HB2	18:r:50:VAL:HG22	1.98	0.46
1:a:2273:A:H2'	1:a:2274:A:C8	2.51	0.46
7:g:45:HIS:O	7:g:49:THR:O	2.34	0.46
20:t:36:VAL:HB	20:t:39:ILE:HG12	1.97	0.46
31:6:23:ILE:HD12	31:6:25:LEU:HD21	1.97	0.46
1:a:693:A:O2'	1:a:1353:A:N3	2.45	0.45
1:a:2522:U:O2'	1:a:2647:U:OP1	2.26	0.45
1:a:1542:U:H2'	1:a:1543:G:O4'	2.15	0.45
1:a:1577:C:H2'	1:a:1578:U:O4'	2.17	0.45
1:a:1754:A:O3'	15:o:103:ARG:NH2	2.48	0.45
1:a:1853:A:N1	1:a:2087:G:H1'	2.30	0.45
1:a:580:U:H2'	1:a:581:C:C6	2.52	0.45
1:a:1115:G:O2'	1:a:1116:G:H8	2.00	0.45
1:a:483:A:H5''	20:t:47:LYS:HD2	1.99	0.45
4:d:14:ILE:HA	15:o:12:GLN:HE22	1.81	0.45
16:p:97:ASP:OD2	17:q:13:ARG:NE	2.48	0.45
1:a:2314:A:H1'	6:f:155:THR:HG21	1.98	0.45
1:a:2585:U:O2	1:a:2585:U:O4'	2.35	0.45
13:m:24:MET:HE1	13:m:40:LYS:HD3	1.98	0.45
32:V:21:TYR:CE1	32:V:30:MET:HG3	2.52	0.45
3:c:155:ALA:HB2	3:c:162:VAL:HG23	1.98	0.45
1:a:1048:A:C8	1:a:1111:A:N1	2.85	0.45
1:a:1905:C:H5''	1:a:1906:G:OP1	2.17	0.45
9:i:43:GLU:O	9:i:44:TYR:C	2.60	0.45
1:a:644:A:H2'	1:a:645:C:O4'	2.17	0.44
3:c:5:LYS:HD2	3:c:17:VAL:HG22	2.00	0.44
12:l:53:MET:HG3	12:l:120:ALA:HB2	1.99	0.44
1:a:263:G:H2'	1:a:264:C:O4'	2.16	0.44
20:t:47:LYS:HE3	20:t:48:PRO:HD2	1.98	0.44
1:a:548:G:H2'	1:a:549:G:C1'	2.46	0.44
1:a:1474:U:C4	1:a:1475:G:C6	3.06	0.44
1:a:2191:A:N3	1:a:2191:A:H2'	2.32	0.44
5:e:168:ASP:OD2	5:e:170:ARG:NH1	2.50	0.44
1:a:1198:U:H5'	16:p:9:ILE:HD11	1.99	0.44
1:a:1859:U:H2'	1:a:1860:G:O4'	2.18	0.44
1:a:2491:U:H5''	1:a:2570:G:H5''	2.00	0.44
1:a:2293:G:H2'	1:a:2294:G:O4'	2.18	0.44
1:a:1048:A:C8	1:a:1111:A:C6	3.06	0.43
1:a:2469:A:H4'	12:l:55:ARG:CD	2.48	0.43
7:g:72:LEU:HD23	7:g:75:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:12:U:O2	1:a:12:U:H2'	2.17	0.43
1:a:2581:G:N3	1:a:2581:G:H2'	2.33	0.43
1:a:1021:A:H3'	1:a:1021:A:N3	2.32	0.43
1:a:1832:C:N4	1:a:1833:C:C4	2.87	0.43
1:a:5:A:H2'	1:a:6:A:C8	2.53	0.43
4:d:8:LYS:HB2	4:d:201:LEU:HD11	2.00	0.43
17:q:1:MET:HA	17:q:42:ALA:O	2.18	0.43
1:a:723:C:H2'	1:a:724:U:O4'	2.17	0.43
1:a:811:U:H2'	11:k:21:ARG:HA	1.99	0.43
6:f:50:LEU:HD11	6:f:67:ILE:HD12	2.00	0.43
1:a:1434:A:H2'	1:a:1435:G:C8	2.54	0.43
24:x:26:PHE:CE1	24:x:30:MET:HE3	2.53	0.43
1:a:276:U:O2'	1:a:278:A:N7	2.52	0.43
1:a:1328:A:H2'	1:a:1330:C:C5	2.54	0.43
1:a:1607:C:H4'	1:a:1608:A:O5'	2.19	0.43
6:f:12:VAL:HA	6:f:15:LYS:HE3	2.01	0.43
20:t:94:ARG:HB3	20:t:103:ILE:HD12	2.00	0.43
1:a:493:G:H2'	1:a:494:G:O4'	2.19	0.43
1:a:2063:C:O2	1:a:2450:A:N1	2.52	0.43
1:a:2291:U:H2'	1:a:2292:U:C6	2.54	0.43
16:p:76:TYR:CZ	16:p:80:ILE:HG13	2.54	0.43
1:a:24:G:O2'	18:r:77:ASP:HB3	2.19	0.43
1:a:829:A:N7	1:a:2248:C:H5'	2.34	0.42
6:f:65:PRO:HA	6:f:89:VAL:HG22	2.00	0.42
9:i:13:ARG:NH1	9:i:49:ASP:O	2.42	0.42
1:a:476:G:H4'	1:a:502:A:N1	2.34	0.42
7:g:89:LEU:HD22	7:g:162:VAL:HG22	2.01	0.42
10:j:1:MET:HE3	10:j:32:TYR:CE2	2.54	0.42
1:a:207:A:H2'	1:a:208:C:O4'	2.20	0.42
1:a:1730:C:O2'	1:a:1731:G:P	2.77	0.42
1:a:1799:G:N7	3:c:178:SER:OG	2.46	0.42
3:c:118:SER:HB2	3:c:129:THR:HB	2.00	0.42
26:z:55:ILE:O	26:z:55:ILE:HG13	2.19	0.42
4:d:48:ILE:HG23	4:d:84:LEU:HD11	2.01	0.42
6:f:138:PHE:HA	6:f:139:PRO:HD3	1.95	0.42
1:a:2365:G:N7	29:2:39:LYS:NZ	2.58	0.42
1:a:1541:C:H2'	1:a:1542:U:O4'	2.20	0.42
9:i:96:ARG:HD2	9:i:99:ARG:HG3	2.02	0.42
11:k:57:LEU:HD22	29:2:54:ASP:HB3	2.00	0.42
22:v:59:LEU:HD12	22:v:80:ILE:HD12	2.00	0.42
1:a:340:A:H2'	1:a:341:C:O4'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:f:61:SER:HB2	6:f:91:LEU:HD21	2.00	0.42
13:m:55:ALA:HA	13:m:80:PHE:CE2	2.55	0.42
14:n:99:TYR:OH	14:n:111:ARG:NH2	2.49	0.41
19:s:53:VAL:HG11	19:s:93:LEU:HB2	2.01	0.41
1:a:2552:OMU:H6	1:a:2552:OMU:O5'	2.19	0.41
1:a:2887:A:N3	26:z:27:SER:OG	2.50	0.41
1:a:639:U:H2'	1:a:640:C:C6	2.55	0.41
1:a:1736:U:H2'	1:a:1737:G:O4'	2.20	0.41
8:h:6:LEU:HD11	8:h:37:VAL:HG13	2.02	0.41
1:a:1664:A:N3	10:j:67:LYS:NZ	2.68	0.41
1:a:2020:A:H5'	26:z:9:THR:CG2	2.50	0.41
4:d:156:PHE:CE1	9:i:81:ILE:HD13	2.56	0.41
1:a:391:A:H1'	1:a:411:G:O4'	2.21	0.41
1:a:1721:G:H1'	1:a:1739:A:H61	1.86	0.41
1:a:2419:U:H4'	27:0:22:THR:HG21	2.03	0.41
6:f:152:LEU:HD12	6:f:152:LEU:C	2.45	0.41
26:z:52:ARG:CZ	26:z:54:VAL:HG12	2.50	0.41
1:a:488:G:O2'	1:a:491:G:N7	2.41	0.41
8:h:12:LEU:HD12	8:h:12:LEU:C	2.45	0.41
1:a:614:A:H3'	1:a:615:U:C5'	2.51	0.41
1:a:749:A:H4'	1:a:1271:G:N3	2.36	0.41
1:a:927:A:H2'	1:a:928:A:C8	2.55	0.41
1:a:1878:G:H2'	1:a:1879:C:O4'	2.21	0.41
1:a:1957:C:H5'	1:a:1984:G:O2'	2.21	0.41
7:g:35:ARG:NE	7:g:71:LEU:HD13	2.36	0.41
11:k:77:ILE:CD1	11:k:108:ALA:HB1	2.50	0.41
16:p:40:ILE:HG22	16:p:44:GLN:HE21	1.86	0.41
20:t:86:ARG:HG3	20:t:95:PHE:CD1	2.56	0.41
1:a:373:U:O2'	1:a:423:A:H1'	2.21	0.41
1:a:1721:G:H1'	1:a:1739:A:N6	2.35	0.41
1:a:2204:G:OP2	3:c:147:LYS:HE2	2.21	0.41
3:c:260:ASN:OD1	3:c:260:ASN:C	2.63	0.41
19:s:64:LYS:HD2	19:s:64:LYS:N	2.35	0.41
1:a:2395:C:H2'	1:a:2396:G:O4'	2.21	0.40
1:a:2622:U:O2'	1:a:2825:G:N7	2.53	0.40
17:q:41:ILE:HD12	17:q:103:ALA:HA	2.03	0.40
33:Z:16:U:H3'	33:Z:17:C:C5	2.56	0.40
1:a:146:A:H2'	1:a:147:C:O4'	2.21	0.40
1:a:1805:A:N3	3:c:50:THR:HB	2.36	0.40
1:a:2040:G:H2'	1:a:2041:U:O4'	2.21	0.40
1:a:2852:G:H2'	1:a:2853:C:O4'	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:d:62:LYS:N	4:d:63:PRO:CD	2.84	0.40
10:j:38:ILE:HD11	10:j:112:PHE:CZ	2.57	0.40
20:t:54:GLN:N	20:t:55:PRO:CD	2.84	0.40
31:6:67:LEU:HD11	31:6:83:GLY:HA2	2.04	0.40
1:a:901:C:H2'	1:a:902:C:O4'	2.21	0.40
1:a:1730:C:HO2'	1:a:1731:G:P	2.43	0.40
3:c:13:ARG:O	3:c:14:ARG:C	2.64	0.40
1:a:2038:G:H2'	1:a:2039:U:O4'	2.22	0.40
13:m:83:LEU:O	13:m:84:GLY:C	2.64	0.40
31:6:20:GLN:HB2	31:6:41:THR:HB	2.03	0.40
1:a:494:G:H4'	18:r:6:LYS:HB2	2.02	0.40
1:a:1713:A:C6	1:a:1716:U:H1'	2.57	0.40
1:a:1881:C:H2'	1:a:1882:U:O4'	2.22	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	
3	c	269/273 (98%)	261 (97%)	8 (3%)	0	100	100
4	d	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
5	e	199/201 (99%)	195 (98%)	4 (2%)	0	100	100
6	f	175/179 (98%)	167 (95%)	8 (5%)	0	100	100
7	g	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
8	h	39/149 (26%)	36 (92%)	3 (8%)	0	100	100
9	i	140/142 (99%)	139 (99%)	1 (1%)	0	100	100
10	j	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
11	k	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
12	l	132/136 (97%)	129 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	116/127 (91%)	112 (97%)	4 (3%)	0	100	100
14	n	114/117 (97%)	111 (97%)	3 (3%)	0	100	100
15	o	112/115 (97%)	108 (96%)	4 (4%)	0	100	100
16	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
17	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
18	r	108/110 (98%)	108 (100%)	0	0	100	100
19	s	91/100 (91%)	86 (94%)	5 (6%)	0	100	100
20	t	100/104 (96%)	93 (93%)	7 (7%)	0	100	100
21	u	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
22	v	76/85 (89%)	75 (99%)	1 (1%)	0	100	100
23	w	75/78 (96%)	75 (100%)	0	0	100	100
24	x	60/63 (95%)	59 (98%)	1 (2%)	0	100	100
25	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
26	z	54/57 (95%)	52 (96%)	2 (4%)	0	100	100
27	0	49/55 (89%)	49 (100%)	0	0	100	100
28	1	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
29	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
30	3	36/38 (95%)	36 (100%)	0	0	100	100
31	6	103/105 (98%)	97 (94%)	6 (6%)	0	100	100
32	V	93/142 (66%)	89 (96%)	4 (4%)	0	100	100
All	All	3254/3514 (93%)	3154 (97%)	100 (3%)	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	
3	c	216/218 (99%)	214 (99%)	2 (1%)	70	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	d	163/163 (100%)	163 (100%)	0	100	100
5	e	165/165 (100%)	165 (100%)	0	100	100
6	f	148/150 (99%)	148 (100%)	0	100	100
7	g	137/138 (99%)	136 (99%)	1 (1%)	76	81
8	h	32/114 (28%)	32 (100%)	0	100	100
9	i	116/116 (100%)	116 (100%)	0	100	100
10	j	103/104 (99%)	102 (99%)	1 (1%)	68	76
11	k	103/103 (100%)	103 (100%)	0	100	100
12	l	107/107 (100%)	106 (99%)	1 (1%)	70	78
13	m	98/103 (95%)	98 (100%)	0	100	100
14	n	86/87 (99%)	86 (100%)	0	100	100
15	o	99/100 (99%)	99 (100%)	0	100	100
16	p	89/90 (99%)	89 (100%)	0	100	100
17	q	84/84 (100%)	84 (100%)	0	100	100
18	r	93/93 (100%)	93 (100%)	0	100	100
19	s	80/84 (95%)	80 (100%)	0	100	100
20	t	83/85 (98%)	83 (100%)	0	100	100
21	u	78/78 (100%)	78 (100%)	0	100	100
22	v	58/63 (92%)	58 (100%)	0	100	100
23	w	67/68 (98%)	66 (98%)	1 (2%)	57	66
24	x	54/55 (98%)	54 (100%)	0	100	100
25	y	48/49 (98%)	48 (100%)	0	100	100
26	z	47/48 (98%)	47 (100%)	0	100	100
27	0	46/49 (94%)	46 (100%)	0	100	100
28	1	38/38 (100%)	38 (100%)	0	100	100
29	2	51/52 (98%)	51 (100%)	0	100	100
30	3	34/34 (100%)	34 (100%)	0	100	100
31	6	90/91 (99%)	90 (100%)	0	100	100
32	V	79/121 (65%)	79 (100%)	0	100	100
All	All	2692/2850 (94%)	2686 (100%)	6 (0%)	84	92

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	c	79	GLU
3	c	116	ILE
7	g	76	VAL
10	j	86	LEU
12	l	78	LEU
23	w	41	GLU

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

Mol	Chain	Res	Type
3	c	134	ASN
5	e	136	GLN
7	g	22	GLN
7	g	30	ASN
8	h	2	GLN
9	i	47	HIS
9	i	80	HIS
9	i	128	ASN
12	l	13	HIS
12	l	60	GLN
15	o	12	GLN
16	p	44	GLN
17	q	66	HIS
18	r	7	HIS
18	r	31	GLN
18	r	40	ASN
20	t	54	GLN
21	u	24	ASN
21	u	49	ASN
23	w	6	GLN
23	w	17	ASN
24	x	27	ASN
26	z	6	ASN
29	2	31	HIS
32	V	74	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	2731/2904 (94%)	334 (12%)	0
2	b	118/120 (98%)	11 (9%)	0

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
33	Z	75/77 (97%)	17 (22%)	3 (4%)
All	All	2924/3101 (94%)	362 (12%)	3 (0%)

All (362) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	10	A
1	a	34	U
1	a	71	A
1	a	74	A
1	a	75	G
1	a	83	A
1	a	86	G
1	a	101	A
1	a	102	U
1	a	118	A
1	a	119	A
1	a	120	U
1	a	125	A
1	a	135	U
1	a	139	U
1	a	140	C
1	a	142	A
1	a	165	A
1	a	181	A
1	a	196	A
1	a	199	A
1	a	200	U
1	a	201	C
1	a	215	G
1	a	216	A
1	a	221	A
1	a	222	A
1	a	233	A
1	a	248	G
1	a	249	C
1	a	250	G
1	a	264	C
1	a	272	A
1	a	278	A
1	a	285	G
1	a	289	G

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Mol	Chain	Res	Type
1	a	304	U
1	a	310	A
1	a	311	A
1	a	329	G
1	a	330	A
1	a	356	G
1	a	361	G
1	a	362	A
1	a	367	G
1	a	386	G
1	a	404	A
1	a	405	U
1	a	411	G
1	a	412	A
1	a	420	C
1	a	425	G
1	a	451	U
1	a	456	C
1	a	481	G
1	a	491	G
1	a	504	A
1	a	505	A
1	a	509	C
1	a	530	G
1	a	531	C
1	a	532	A
1	a	544	C
1	a	545	U
1	a	546	U
1	a	547	A
1	a	549	G
1	a	563	A
1	a	564	C
1	a	573	U
1	a	575	A
1	a	586	A
1	a	592	A
1	a	603	A
1	a	614	A
1	a	615	U
1	a	627	A
1	a	637	A

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Mol	Chain	Res	Type
1	a	645	C
1	a	647	G
1	a	651	G
1	a	653	U
1	a	654	A
1	a	686	U
1	a	711	G
1	a	717	C
1	a	730	A
1	a	738	G
1	a	747	5MU
1	a	764	A
1	a	765	C
1	a	775	G
1	a	776	G
1	a	782	A
1	a	784	G
1	a	785	G
1	a	792	A
1	a	802	A
1	a	805	G
1	a	812	C
1	a	827	U
1	a	828	U
1	a	846	U
1	a	847	U
1	a	858	G
1	a	859	G
1	a	879	G
1	a	881	G
1	a	895	U
1	a	896	A
1	a	897	C
1	a	910	A
1	a	914	G
1	a	915	C
1	a	931	U
1	a	933	A
1	a	946	C
1	a	961	C
1	a	968	C
1	a	974	G

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Mol	Chain	Res	Type
1	a	983	A
1	a	984	A
1	a	985	C
1	a	996	A
1	a	1005	C
1	a	1012	U
1	a	1013	C
1	a	1022	G
1	a	1026	G
1	a	1033	U
1	a	1040	A
1	a	1046	A
1	a	1047	G
1	a	1109	C
1	a	1111	A
1	a	1112	G
1	a	1115	G
1	a	1116	G
1	a	1128	G
1	a	1129	A
1	a	1132	U
1	a	1133	A
1	a	1134	A
1	a	1135	C
1	a	1136	G
1	a	1142	A
1	a	1143	A
1	a	1171	G
1	a	1172	C
1	a	1187	G
1	a	1210	G
1	a	1253	A
1	a	1256	G
1	a	1271	G
1	a	1272	A
1	a	1273	U
1	a	1300	G
1	a	1301	A
1	a	1345	C
1	a	1352	U
1	a	1365	A
1	a	1379	U

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Mol	Chain	Res	Type
1	a	1383	A
1	a	1411	U
1	a	1416	G
1	a	1419	A
1	a	1427	A
1	a	1428	C
1	a	1452	G
1	a	1453	A
1	a	1478	G
1	a	1482	G
1	a	1483	G
1	a	1493	C
1	a	1497	U
1	a	1498	C
1	a	1508	A
1	a	1510	G
1	a	1515	A
1	a	1523	U
1	a	1529	G
1	a	1534	U
1	a	1535	A
1	a	1536	C
1	a	1537	G
1	a	1569	A
1	a	1578	U
1	a	1583	A
1	a	1584	U
1	a	1585	C
1	a	1586	A
1	a	1608	A
1	a	1644	C
1	a	1647	U
1	a	1648	U
1	a	1649	G
1	a	1674	G
1	a	1686	C
1	a	1715	G
1	a	1729	U
1	a	1730	C
1	a	1731	G
1	a	1732	C
1	a	1738	G

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Mol	Chain	Res	Type
1	a	1742	U
1	a	1744	A
1	a	1764	C
1	a	1773	A
1	a	1800	C
1	a	1801	A
1	a	1807	G
1	a	1808	A
1	a	1816	C
1	a	1829	A
1	a	1839	G
1	a	1842	G
1	a	1847	A
1	a	1848	A
1	a	1858	A
1	a	1862	G
1	a	1872	A
1	a	1873	G
1	a	1906	G
1	a	1911	PSU
1	a	1920	C
1	a	1922	G
1	a	1929	G
1	a	1930	G
1	a	1931	U
1	a	1937	A
1	a	1938	A
1	a	1955	U
1	a	1960	A
1	a	1965	C
1	a	1967	C
1	a	1970	A
1	a	1971	U
1	a	1972	G
1	a	1987	A
1	a	1991	U
1	a	1993	U
1	a	2020	A
1	a	2023	C
1	a	2031	A
1	a	2033	A
1	a	2043	C

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Mol	Chain	Res	Type
1	a	2055	C
1	a	2056	G
1	a	2060	A
1	a	2061	G
1	a	2062	A
1	a	2069	G7M
1	a	2093	G
1	a	2192	U
1	a	2198	A
1	a	2203	U
1	a	2204	G
1	a	2211	A
1	a	2221	G
1	a	2223	G
1	a	2225	A
1	a	2238	G
1	a	2244	U
1	a	2268	A
1	a	2282	G
1	a	2283	C
1	a	2287	A
1	a	2305	U
1	a	2307	G
1	a	2308	G
1	a	2312	U
1	a	2322	A
1	a	2325	G
1	a	2335	A
1	a	2340	A
1	a	2347	C
1	a	2361	G
1	a	2366	A
1	a	2372	U
1	a	2383	G
1	a	2385	C
1	a	2402	U
1	a	2403	C
1	a	2406	A
1	a	2424	C
1	a	2425	A
1	a	2429	G
1	a	2430	A

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Mol	Chain	Res	Type
1	a	2431	U
1	a	2435	A
1	a	2441	U
1	a	2448	A
1	a	2459	A
1	a	2474	U
1	a	2476	A
1	a	2491	U
1	a	2502	G
1	a	2505	G
1	a	2506	U
1	a	2507	C
1	a	2518	A
1	a	2529	G
1	a	2547	A
1	a	2566	A
1	a	2567	G
1	a	2573	C
1	a	2574	G
1	a	2602	A
1	a	2603	G
1	a	2609	U
1	a	2613	U
1	a	2629	U
1	a	2660	A
1	a	2661	G
1	a	2663	G
1	a	2689	U
1	a	2690	U
1	a	2714	G
1	a	2726	A
1	a	2744	G
1	a	2748	A
1	a	2757	A
1	a	2765	A
1	a	2790	U
1	a	2791	G
1	a	2793	C
1	a	2798	U
1	a	2799	A
1	a	2820	A
1	a	2821	A

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Mol	Chain	Res	Type
1	a	2867	G
1	a	2868	A
1	a	2884	U
1	a	2899	A
2	b	35	C
2	b	37	C
2	b	44	G
2	b	45	A
2	b	56	G
2	b	57	A
2	b	58	A
2	b	89	U
2	b	90	C
2	b	99	A
2	b	109	A
33	Z	5	C
33	Z	9	A
33	Z	17	C
33	Z	18	G
33	Z	19	U
33	Z	20	U
33	Z	21	A
33	Z	29	U
33	Z	31	C
33	Z	46	G
33	Z	47	U
33	Z	53	G
33	Z	58	A
33	Z	64	G
33	Z	69	U
33	Z	71	C
33	Z	76	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
33	Z	18	G
33	Z	19	U
33	Z	48	C

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

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
1	5MU	a	747	1	19,22,23	0.50	0	28,32,35	0.60	1 (3%)
1	PSU	a	2605	1	18,21,22	0.88	2 (11%)	22,30,33	0.89	1 (4%)
1	PSU	a	1911	1	18,21,22	0.94	1 (5%)	22,30,33	0.65	0
1	OMU	a	2552	1	19,22,23	0.41	0	26,31,34	0.59	0
1	H2U	a	2449	1	18,21,22	0.92	2 (11%)	21,30,33	1.11	2 (9%)
1	OMC	a	2498	34,1	19,22,23	0.46	0	26,31,34	0.68	0
1	PSU	a	2504	1	18,21,22	1.08	1 (5%)	22,30,33	0.92	1 (4%)
1	PSU	a	2457	1	18,21,22	1.02	2 (11%)	22,30,33	0.64	0
12	4D4	l	81	12	9,11,12	0.72	0	8,13,15	0.74	0
1	6MZ	a	1618	1	22,25,26	0.58	0	30,36,39	0.74	0
1	OMG	a	2251	33,1	23,26,27	0.41	0	33,38,41	0.52	0
1	2MG	a	1835	1	23,26,27	0.40	0	32,38,41	0.60	0
1	PSU	a	2604	1	18,21,22	0.82	1 (5%)	22,30,33	0.83	1 (4%)
1	PSU	a	746	34,1	18,21,22	1.13	2 (11%)	22,30,33	0.88	0
1	1MG	a	745	1	22,26,27	0.81	1 (4%)	33,39,42	0.75	1 (3%)
12	MS6	l	82	12	5,7,8	0.42	0	2,7,9	1.17	0
1	2MA	a	2503	34,1	22,25,26	0.98	3 (13%)	33,37,40	1.42	5 (15%)
4	MEQ	d	150	4	8,9,10	0.64	0	5,10,12	0.68	0
1	5MC	a	1962	1	18,22,23	0.41	0	26,32,35	0.89	1 (3%)
1	2MG	a	2445	1	23,26,27	0.60	0	32,38,41	0.62	0
1	PSU	a	955	1	18,21,22	0.91	0	22,30,33	0.92	1 (4%)
1	PSU	a	2580	1	18,21,22	0.93	0	22,30,33	1.05	1 (4%)
1	6MZ	a	2030	1	22,25,26	0.94	1 (4%)	30,36,39	0.90	1 (3%)
1	G7M	a	2069	1	23,26,27	0.96	1 (4%)	35,39,42	0.91	2 (5%)
1	5MU	a	1939	1	19,22,23	0.44	0	28,32,35	0.53	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
1	5MU	a	747	1	-	0/7/25/26	0/2/2/2
1	PSU	a	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	a	1911	1	-	2/7/25/26	0/2/2/2
1	OMU	a	2552	1	-	0/9/27/28	0/2/2/2
1	H2U	a	2449	1	-	0/7/38/39	0/2/2/2
1	OMC	a	2498	34,1	-	0/9/27/28	0/2/2/2
1	PSU	a	2504	1	-	1/7/25/26	0/2/2/2
1	PSU	a	2457	1	-	0/7/25/26	0/2/2/2
12	4D4	l	81	12	-	2/11/12/14	-
1	6MZ	a	1618	1	-	0/9/27/28	0/3/3/3
1	OMG	a	2251	33,1	-	0/9/27/28	0/3/3/3
1	2MG	a	1835	1	-	0/9/27/28	0/3/3/3
1	PSU	a	2604	1	-	0/7/25/26	0/2/2/2
1	PSU	a	746	34,1	-	1/7/25/26	0/2/2/2
1	1MG	a	745	1	-	0/7/25/26	0/3/3/3
12	MS6	l	82	12	-	1/4/6/8	-
1	2MA	a	2503	34,1	-	3/7/25/26	0/3/3/3
4	MEQ	d	150	4	-	5/8/9/11	-
1	5MC	a	1962	1	-	0/7/25/26	0/2/2/2
1	2MG	a	2445	1	-	0/9/27/28	0/3/3/3
1	PSU	a	955	1	-	0/7/25/26	0/2/2/2
1	PSU	a	2580	1	-	0/7/25/26	0/2/2/2
1	6MZ	a	2030	1	-	2/9/27/28	0/3/3/3
1	G7M	a	2069	1	-	2/7/25/26	0/3/3/3
1	5MU	a	1939	1	-	0/7/25/26	0/2/2/2

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	1911	PSU	C6-C5	3.66	1.39	1.35
1	a	2069	G7M	C8-N7	3.49	1.39	1.33
1	a	2030	6MZ	C8-N9	-3.33	1.31	1.37
1	a	2504	PSU	C6-C5	3.09	1.38	1.35
1	a	746	PSU	C6-C5	3.00	1.38	1.35
1	a	2457	PSU	C6-C5	2.88	1.38	1.35
1	a	2449	H2U	C2-N3	-2.76	1.33	1.38
1	a	2604	PSU	C6-C5	2.74	1.38	1.35
1	a	745	1MG	C1'-N9	-2.63	1.40	1.47
1	a	2605	PSU	C6-C5	2.43	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	2503	2MA	C6-N6	-2.41	1.28	1.34
1	a	2457	PSU	C4-C5	-2.25	1.37	1.44
1	a	2605	PSU	C4-C5	-2.25	1.37	1.44
1	a	746	PSU	C6-N1	-2.08	1.32	1.36
1	a	2449	H2U	C2-N1	-2.06	1.32	1.35
1	a	2503	2MA	C5-C6	-2.06	1.35	1.41
1	a	2503	2MA	C6-N1	2.02	1.37	1.35

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	2503	2MA	CM2-C2-N1	4.30	123.86	117.15
1	a	2449	H2U	N3-C2-N1	3.30	120.14	116.65
1	a	2503	2MA	C5-C4-N3	-3.16	123.63	127.19
1	a	2580	PSU	C3'-C2'-C1'	2.73	104.81	101.64
1	a	1962	5MC	C5-C6-N1	-2.64	120.62	123.34
1	a	2449	H2U	O2-C2-N1	-2.64	119.80	123.11
1	a	2605	PSU	C2'-C3'-C4'	-2.46	97.85	102.64
1	a	2069	G7M	N9-C8-N7	-2.40	106.28	112.21
1	a	2030	6MZ	C4-C5-N7	-2.29	107.83	110.62
1	a	2504	PSU	C5-C6-N1	-2.23	118.77	122.11
1	a	2069	G7M	CN7-N7-C5	-2.19	124.05	126.77
1	a	2604	PSU	C2'-C3'-C4'	-2.18	98.40	102.64
1	a	2503	2MA	N3-C4-N9	2.12	129.93	126.99
1	a	2503	2MA	CM2-C2-N3	-2.11	113.86	117.15
1	a	2503	2MA	O3'-C3'-C2'	-2.10	105.02	111.82
1	a	745	1MG	O3'-C3'-C4'	-2.06	105.08	111.05
1	a	747	5MU	O3'-C3'-C4'	-2.04	105.14	111.05
1	a	955	PSU	C2'-C3'-C4'	-2.02	98.72	102.64

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	1911	PSU	C3'-C4'-C5'-O5'
1	a	1911	PSU	O4'-C4'-C5'-O5'
4	d	150	MEQ	OE1-CD-NE2-CE
4	d	150	MEQ	OE1-CD-CG-CB
4	d	150	MEQ	NE2-CD-CG-CB
1	a	2030	6MZ	O4'-C4'-C5'-O5'
4	d	150	MEQ	CG-CD-NE2-CE
1	a	2069	G7M	C4'-C5'-O5'-P

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Mol	Chain	Res	Type	Atoms
12	l	82	MS6	CB-CG-SD-CE
12	l	81	4D4	CG-CD-NE-CZ
4	d	150	MEQ	CA-CB-CG-CD
1	a	2030	6MZ	C3'-C4'-C5'-O5'
1	a	2503	2MA	O4'-C1'-N9-C8
1	a	2504	PSU	O4'-C4'-C5'-O5'
1	a	746	PSU	O4'-C1'-C5-C6
1	a	2069	G7M	O4'-C4'-C5'-O5'
1	a	2503	2MA	O4'-C4'-C5'-O5'
1	a	2503	2MA	C4'-C5'-O5'-P
12	l	81	4D4	O-C-CA-CB

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	2552	OMU	1	0
1	a	2030	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 206 ligands modelled in this entry, 205 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	ASP	Z	101	33	6,7,8	0.96	0	5,8,10	0.91	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	ASP	Z	101	33	-	4/5/6/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	Z	101	ASP	C-CA-CB-CG
36	Z	101	ASP	N-CA-CB-CG
36	Z	101	ASP	CA-CB-CG-OD1
36	Z	101	ASP	CA-CB-CG-OD2

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](#)

There are no chain breaks in this entry.

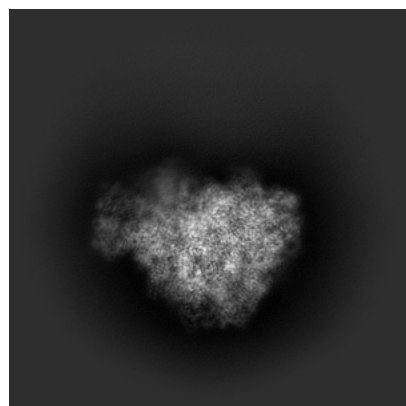
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57973. These allow visual inspection of the internal detail of the map and identification of artifacts.

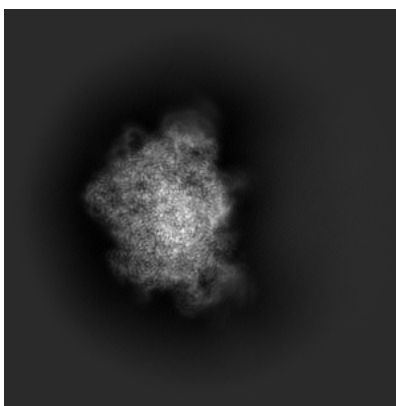
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

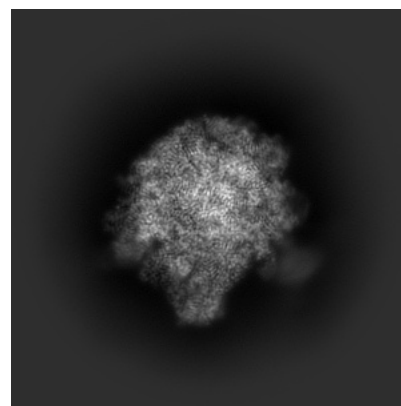
6.1.1 Primary map



X

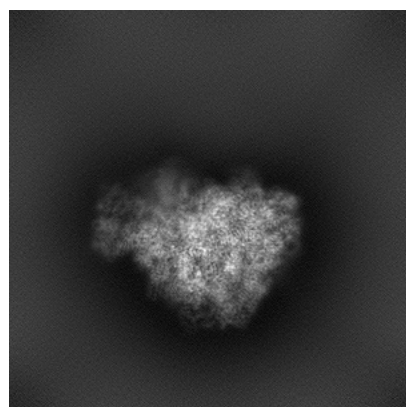


Y

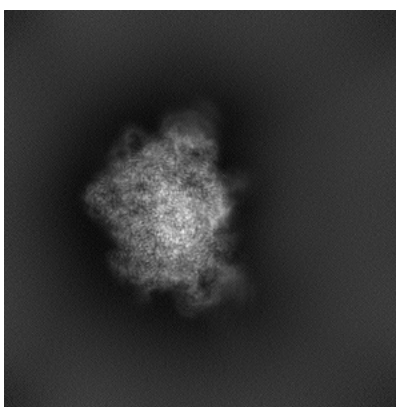


Z

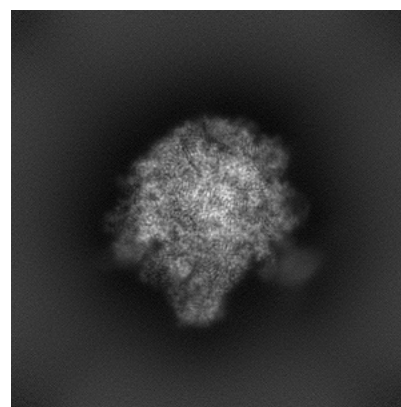
6.1.2 Raw map



X



Y

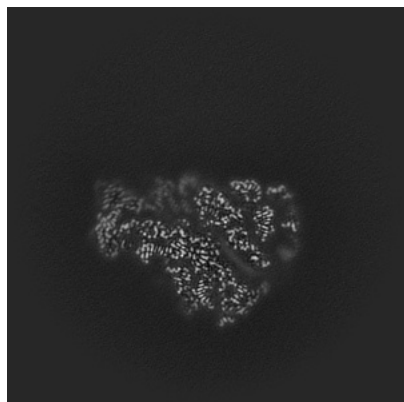


Z

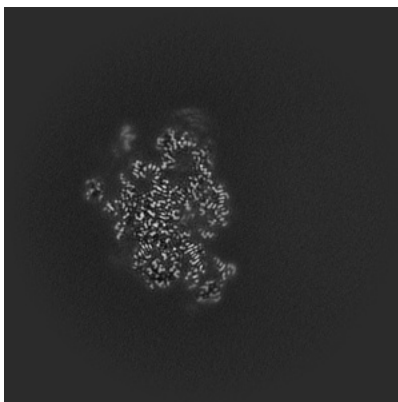
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

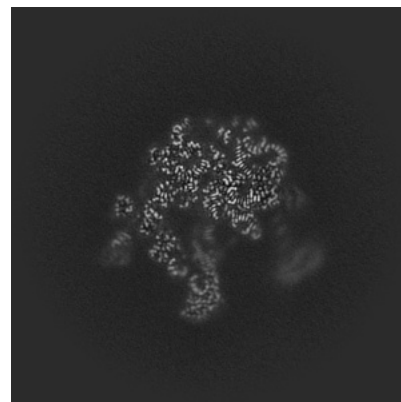
6.2.1 Primary map



X Index: 256

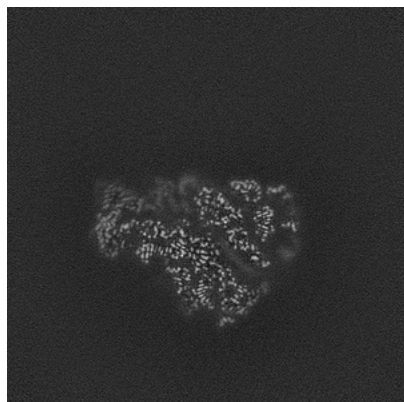


Y Index: 256

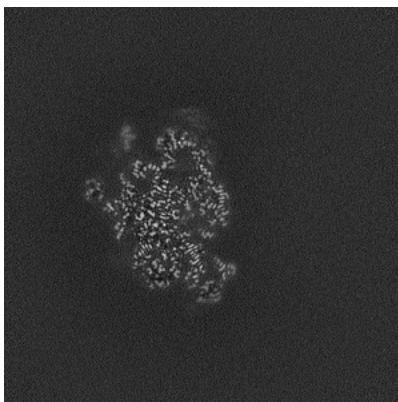


Z Index: 256

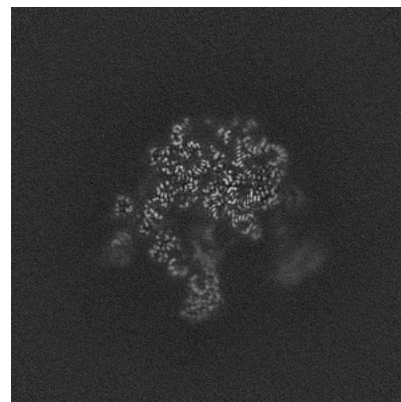
6.2.2 Raw map



X Index: 256



Y Index: 256

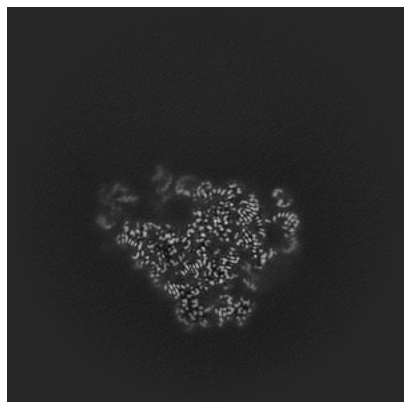


Z Index: 256

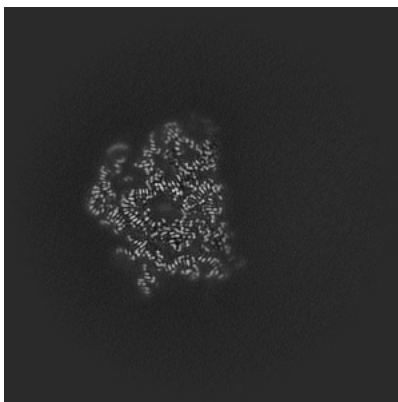
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

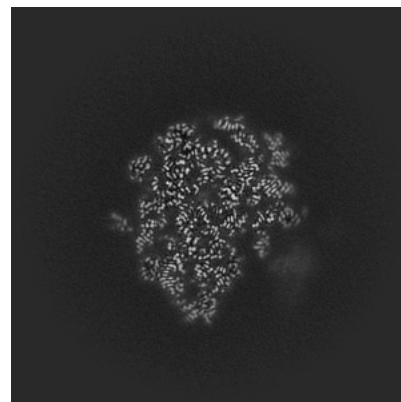
6.3.1 Primary map



X Index: 269

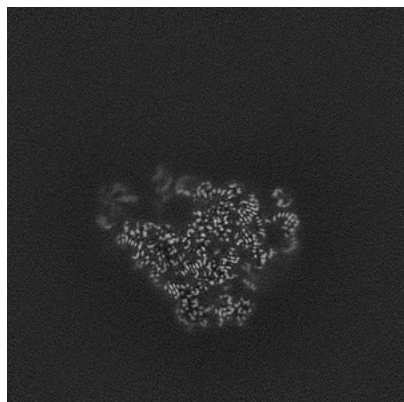


Y Index: 278

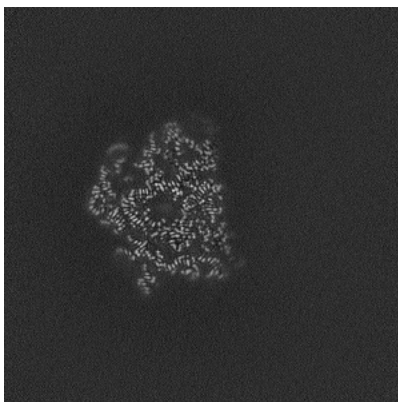


Z Index: 221

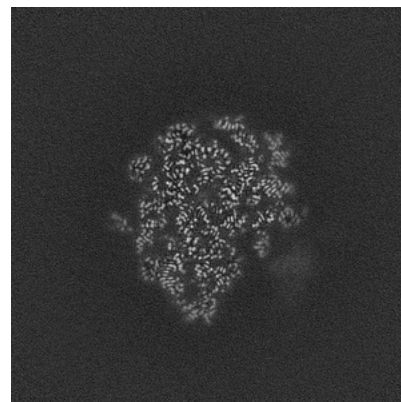
6.3.2 Raw map



X Index: 269



Y Index: 278



Z Index: 221

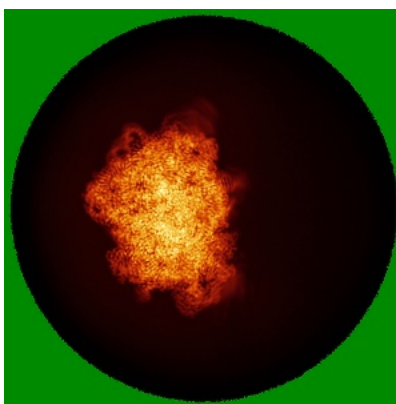
The images above show the largest variance slices of the map in three orthogonal directions.

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

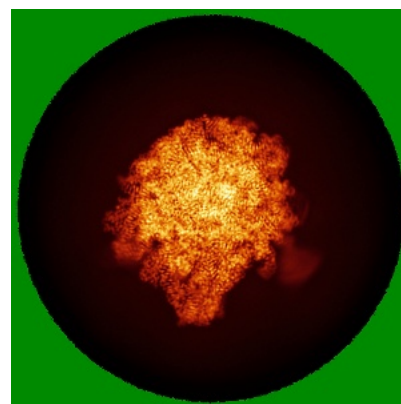
6.4.1 Primary map



X

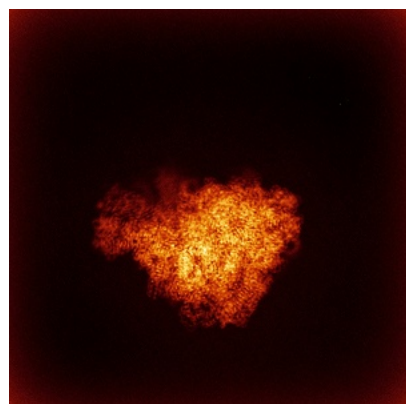


Y

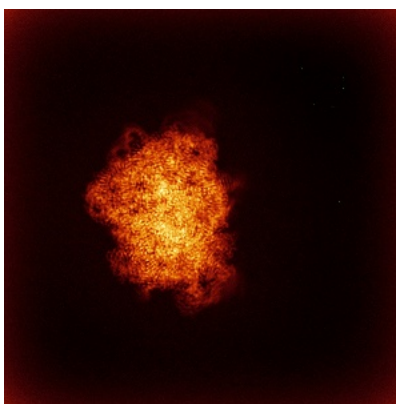


Z

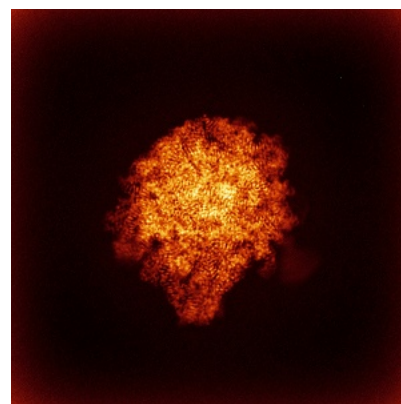
6.4.2 Raw map



X



Y

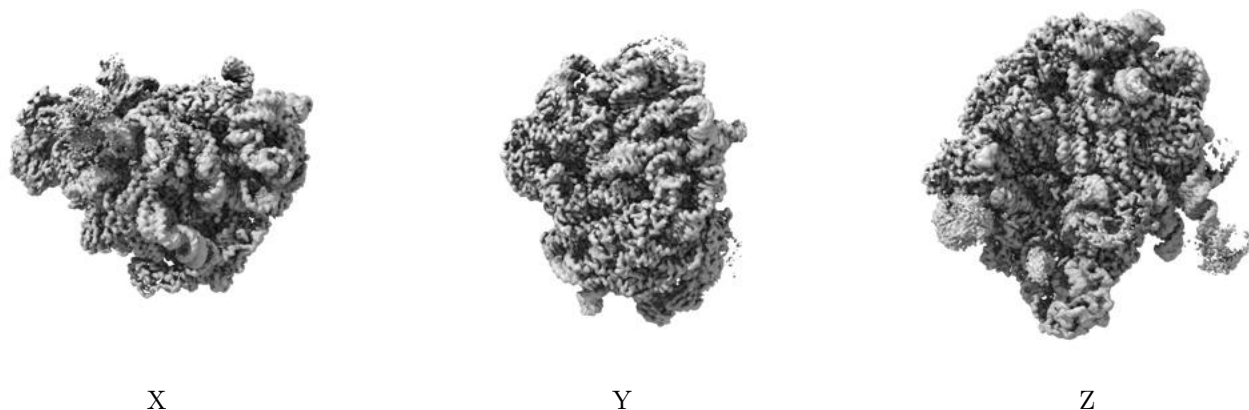


Z

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.

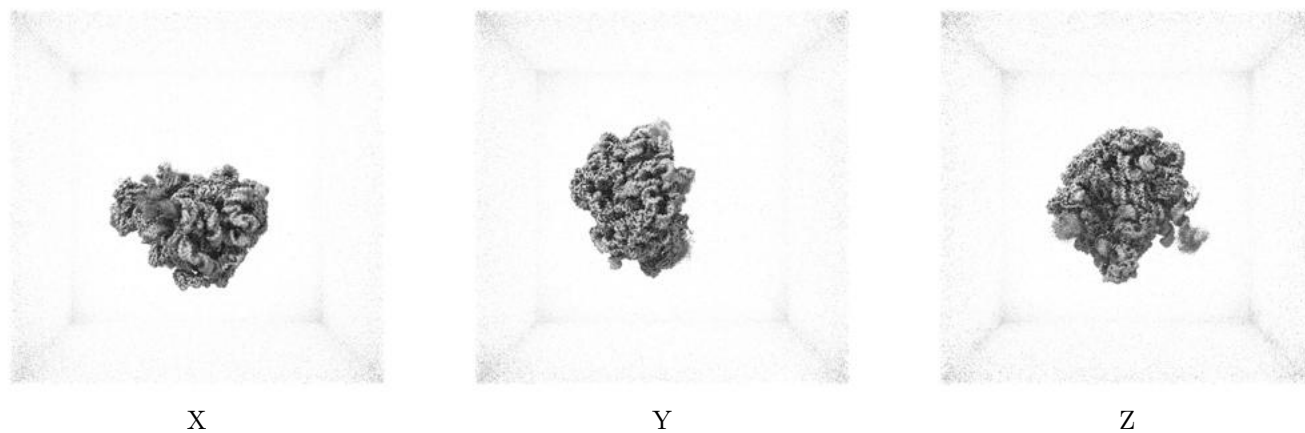
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

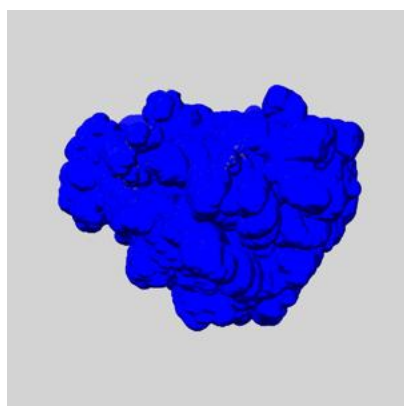
6.6 Mask visualisation [i](#)

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

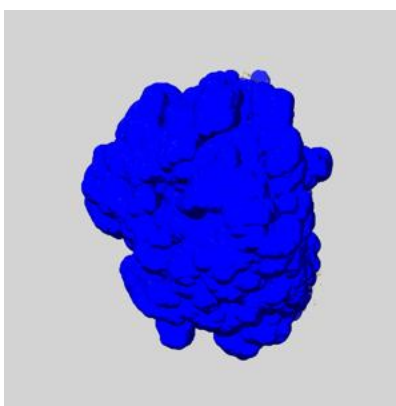
A mask typically either:

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

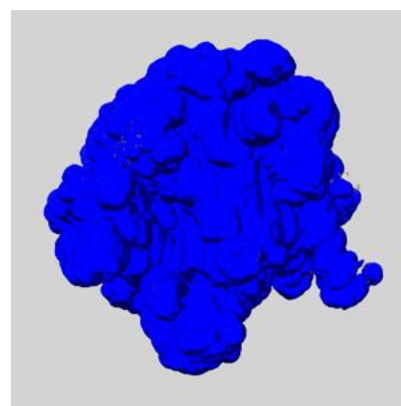
6.6.1 emd_57973_msk_1.map [i](#)



X

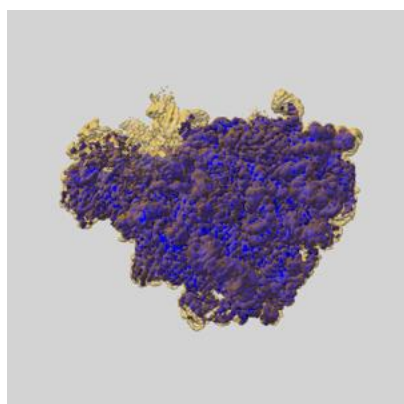


Y

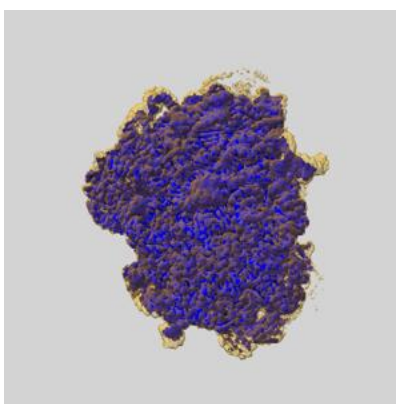


Z

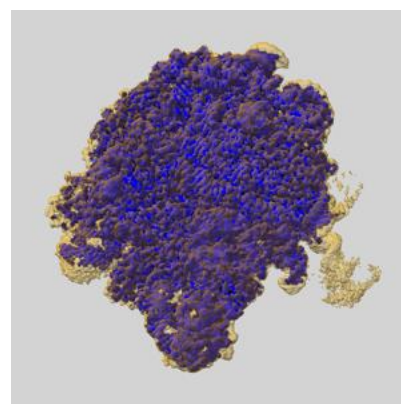
6.6.2 emd_57973_msk_2.map [i](#)



X



Y

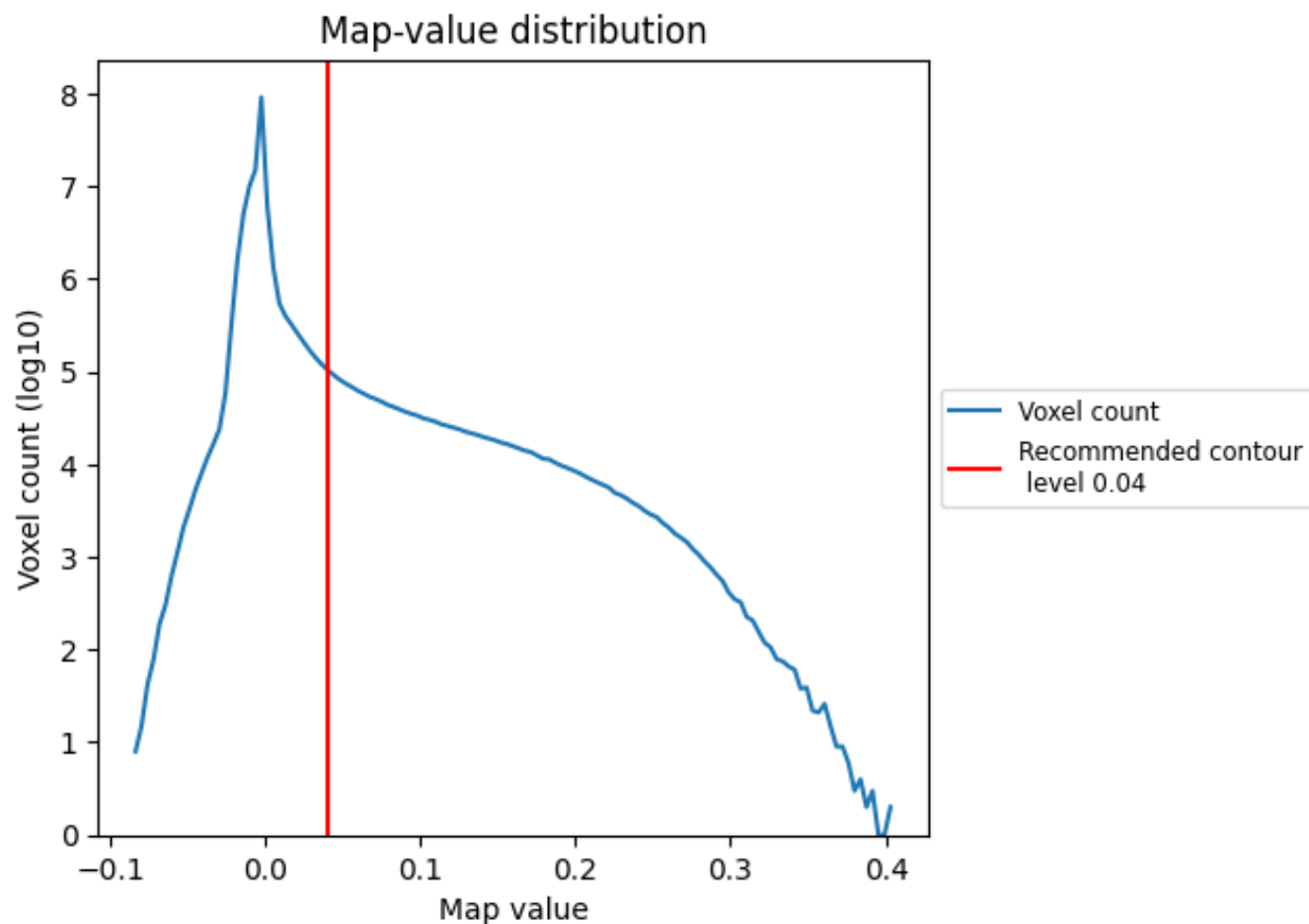


Z

7 Map analysis [i](#)

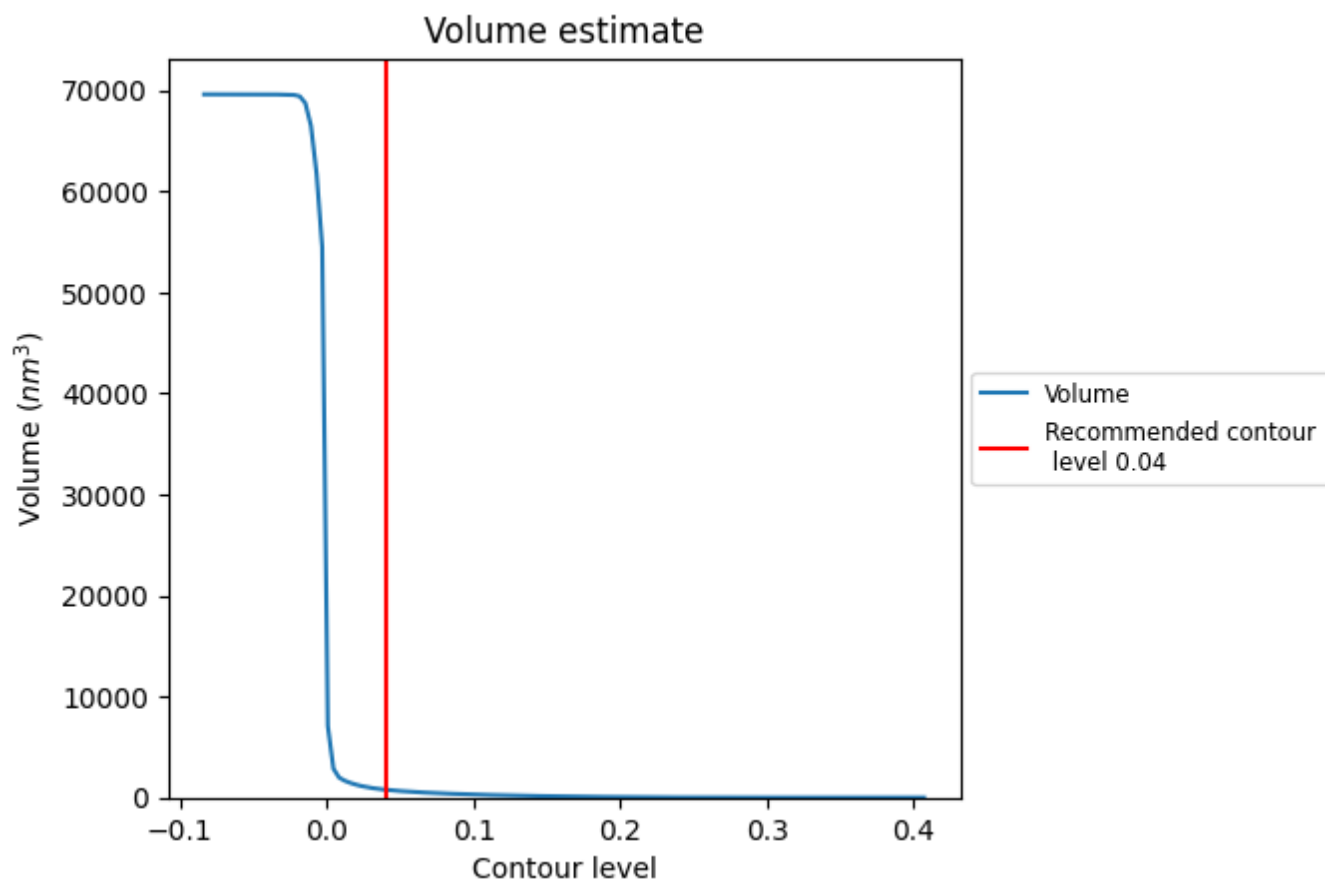
This section contains the results of statistical analysis of the map.

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.

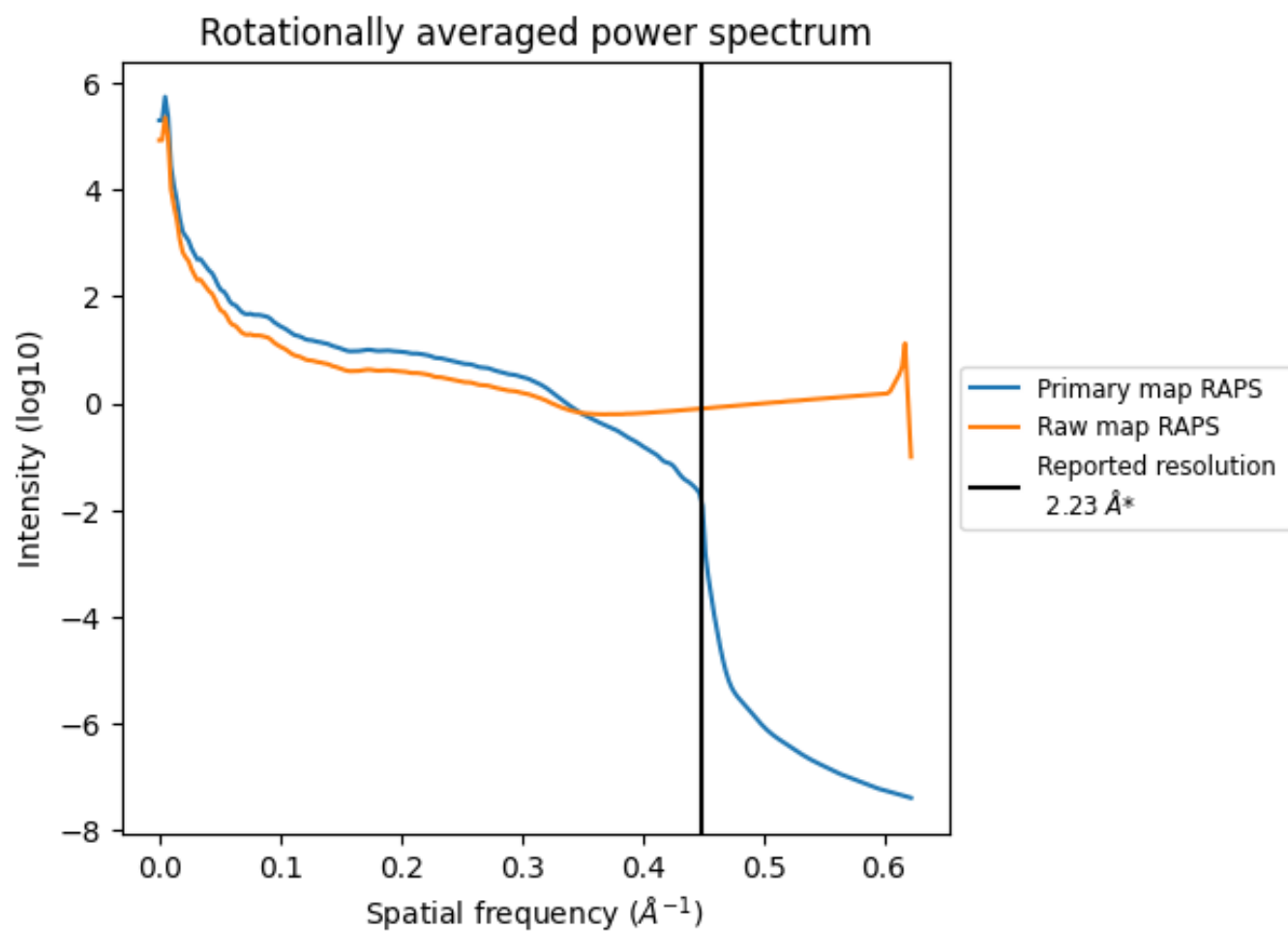
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 778 nm³; this corresponds to an approximate mass of 703 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 ⓘ

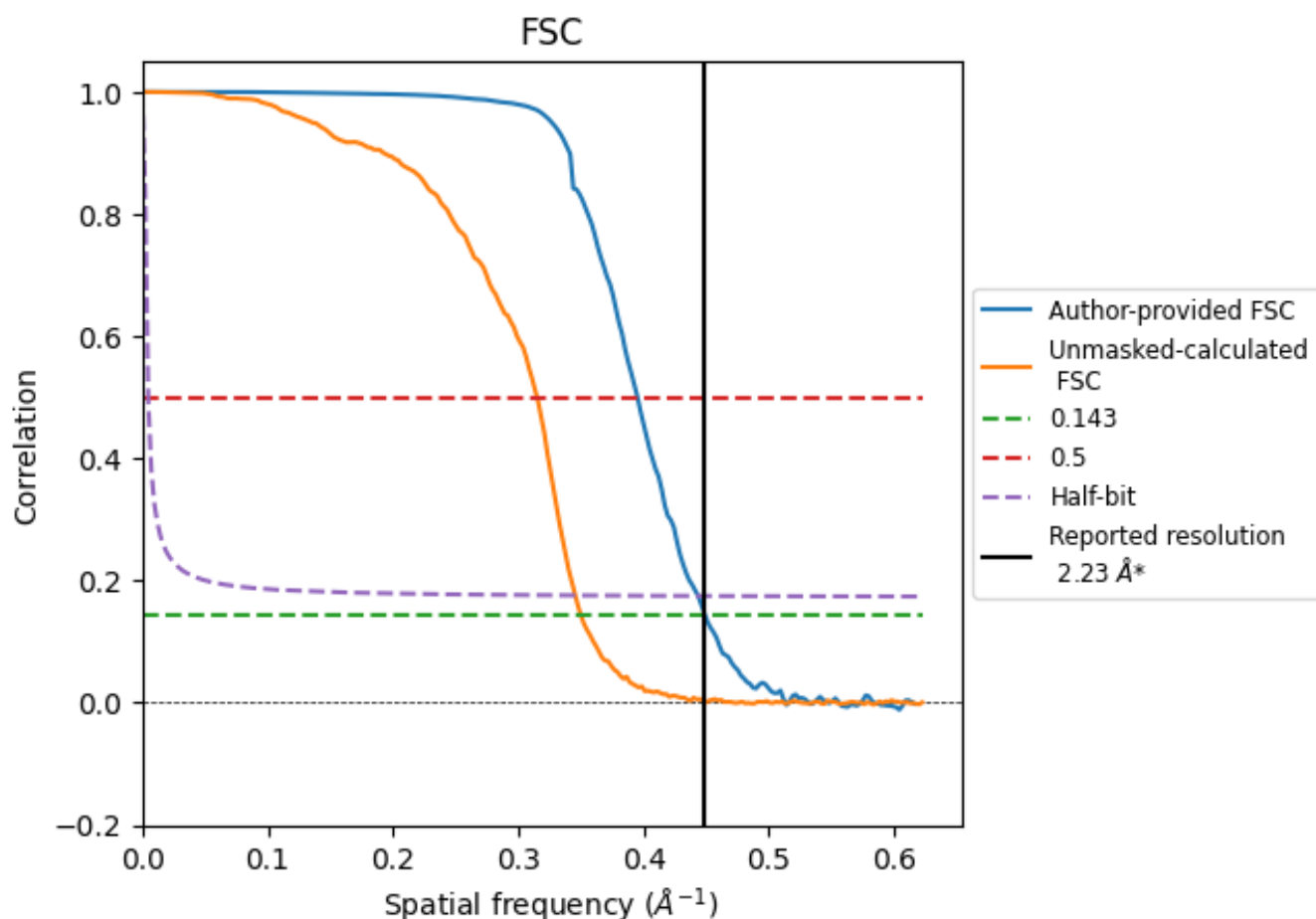


*Reported resolution corresponds to spatial frequency of 0.448 \AA^{-1}

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 0.448 \AA^{-1}

8.2 Resolution estimates [i](#)

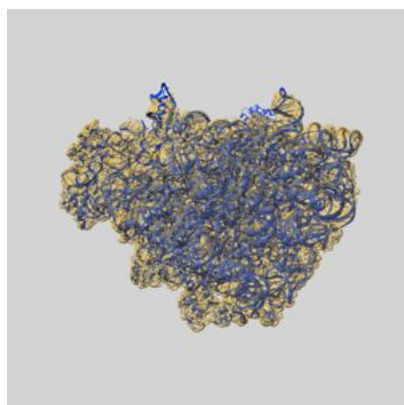
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.23	-	-
Author-provided FSC curve	2.23	2.53	2.25
Unmasked-calculated*	2.86	3.17	2.89

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.86 differs from the reported value 2.23 by more than 10 %

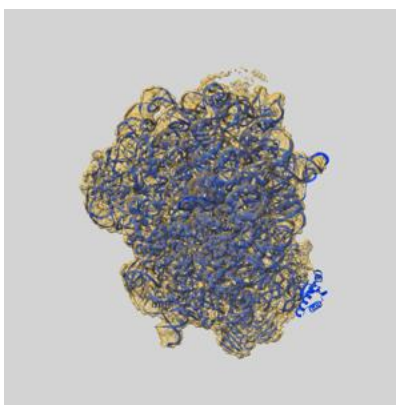
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57973 and PDB model 30QZ. Per-residue inclusion information can be found in section [3](#) on page [12](#).

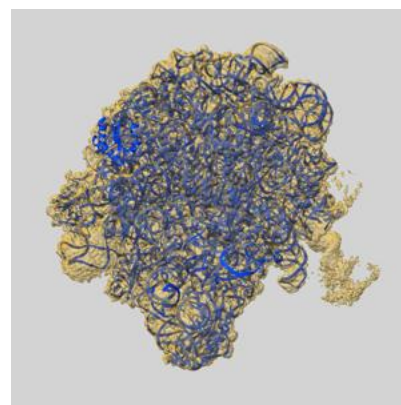
9.1 Map-model overlay [i](#)



X



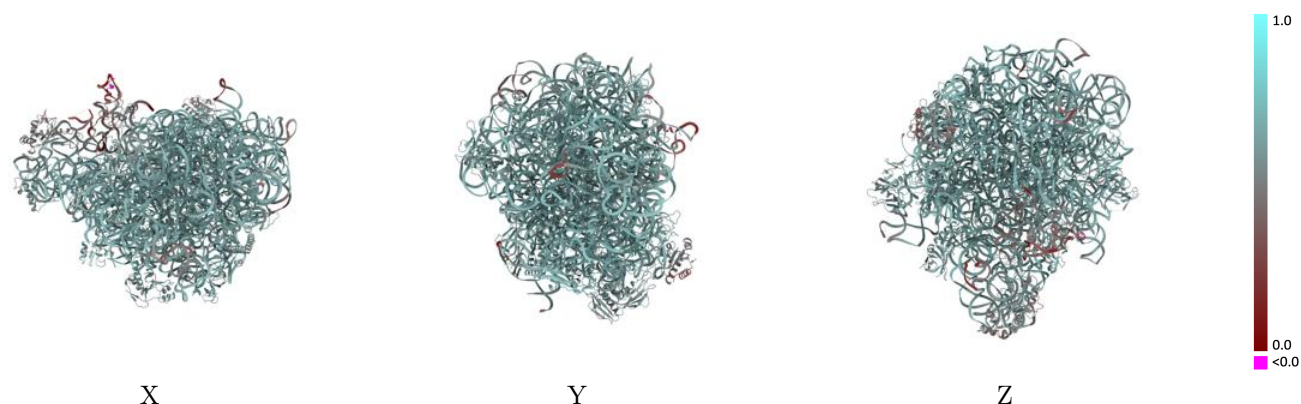
Y



Z

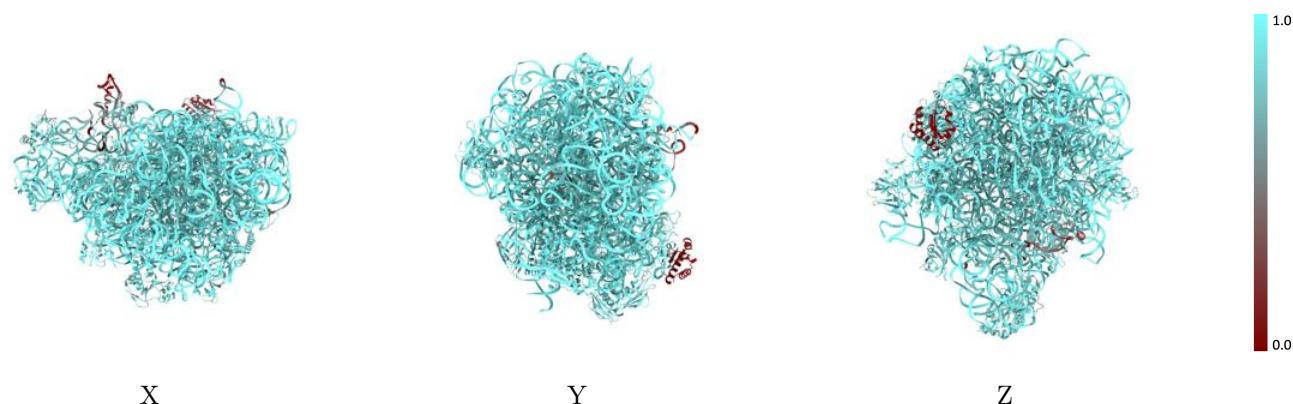
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



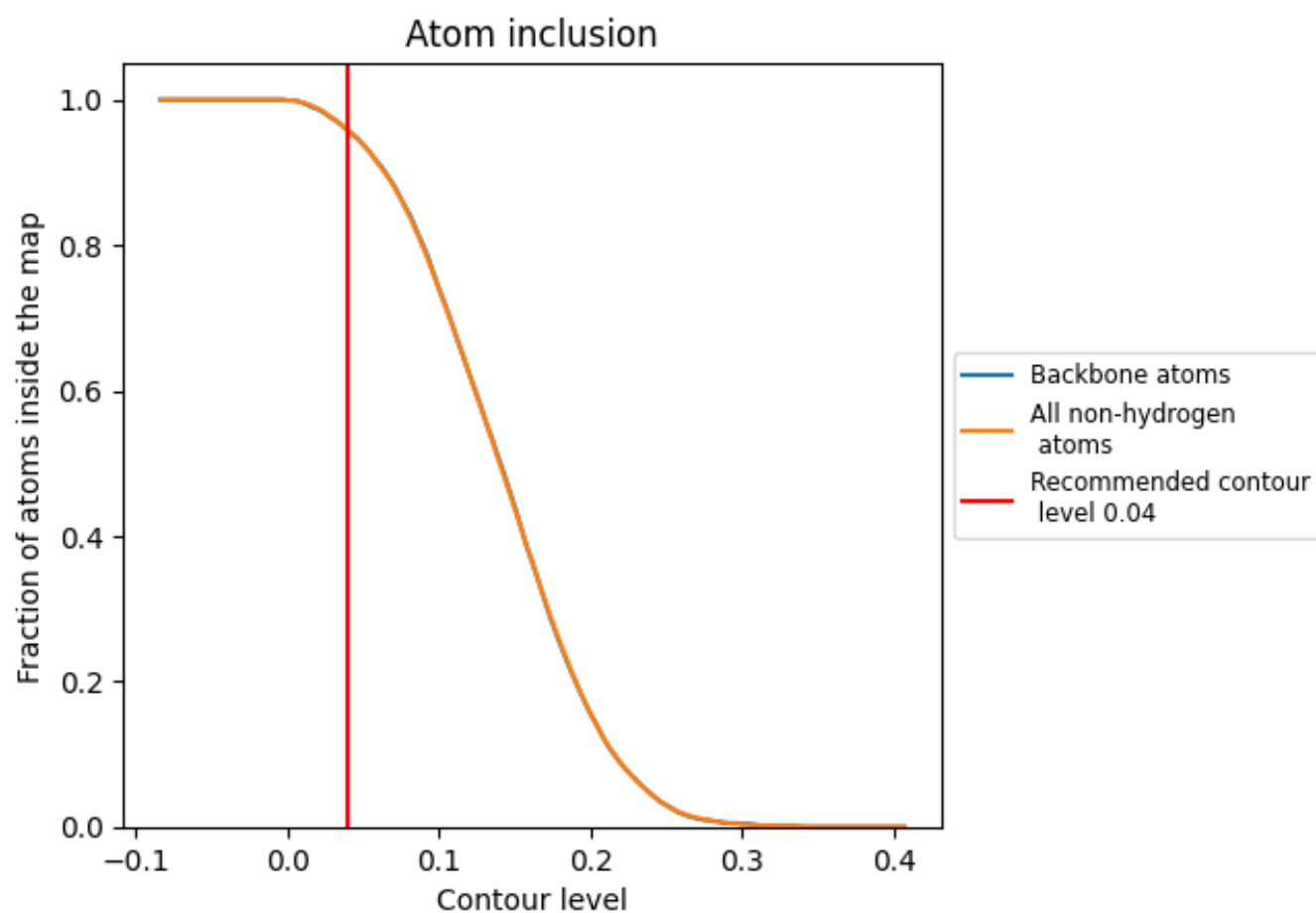
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).





































































9.4 Atom inclusion [i](#)



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

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9590	 0.6240
0	 0.9240	 0.6170
1	 0.9690	 0.6640
2	 0.9820	 0.6630
3	 0.9560	 0.6390
6	 0.0300	 0.4280
V	 0.5650	 0.4080
Z	 0.6820	 0.4060
a	 0.9930	 0.6390
b	 0.9970	 0.6070
c	 0.9700	 0.6470
d	 0.9590	 0.6420
e	 0.9330	 0.6230
f	 0.8140	 0.4830
g	 0.8870	 0.5560
h	 0.8730	 0.5550
i	 0.9590	 0.6440
j	 0.9320	 0.6230
k	 0.9590	 0.6390
l	 0.9520	 0.6350
m	 0.9840	 0.6530
n	 0.9300	 0.5910
o	 0.9170	 0.6220
p	 0.9810	 0.6620
q	 0.9410	 0.6330
r	 0.9430	 0.6340
s	 0.9270	 0.6220
t	 0.9110	 0.5870
u	 0.9130	 0.6100
v	 0.9370	 0.6450
w	 0.9620	 0.6410
x	 0.8920	 0.5820
y	 0.9310	 0.6250
z	 0.9490	 0.6400

