



Full wwPDB EM Validation Report ⓘ

Feb 3, 2024 – 04:31 PM EST

PDB ID : 1MJ1
EMDB ID : EMD-1004
Title : FITTING THE TERNARY COMPLEX OF EF-Tu/tRNA/GTP AND RIBOSOMAL PROTEINS INTO A 13 Å CRYO-EM MAP OF THE COLI 70S RIBOSOME
Authors : Stark, H.; Rodnina, M.V.; Wieden, H.-J.; Zemlin, F.; Wintermeyer, W.; Vanheul, M.
Deposited on : 2002-08-26
Resolution : 13.00 Å (reported)
Based on initial models : 1GIX, 1GIY, 1B23

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

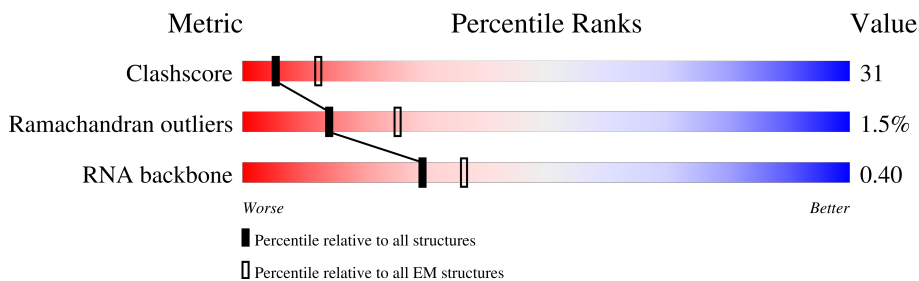
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 13.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	C	76	
1	D	76	
2	Q	41	
3	R	27	
4	A	405	
5	O	135	
6	P	126	
7	L	141	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5374 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called Phe-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	D	76	1652	746	294	536	76	0	0
1	C	76	1652	746	294	536	76	0	0

- Molecule 2 is a RNA chain called sarcin-ricin loop of 23SrRNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
2	Q	41	Total	P	0	41
			41	41		

- Molecule 3 is a RNA chain called helix 69 of 23S rRNA.

Mol	Chain	Residues	Atoms		AltConf	Trace
3	R	27	Total	P	0	27
			27	27		

- Molecule 4 is a protein called Elongation Factor Tu.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	A	405	1620	810	405	405	0	0

- Molecule 5 is a protein called S12 ribosomal protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
5	O	124	Total	C	0	124
			124	124		

- Molecule 6 is a protein called S13 ribosomal protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
6	P	125	Total 125	C 125	0	125

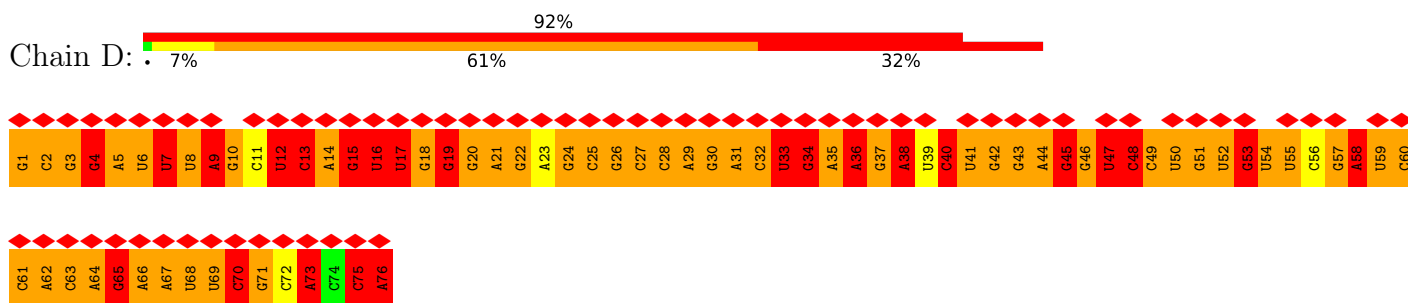
- Molecule 7 is a protein called L11 ribosomal protein.

Mol	Chain	Residues	Atoms		AltConf	Trace
7	L	133	Total 133	C 133	0	133

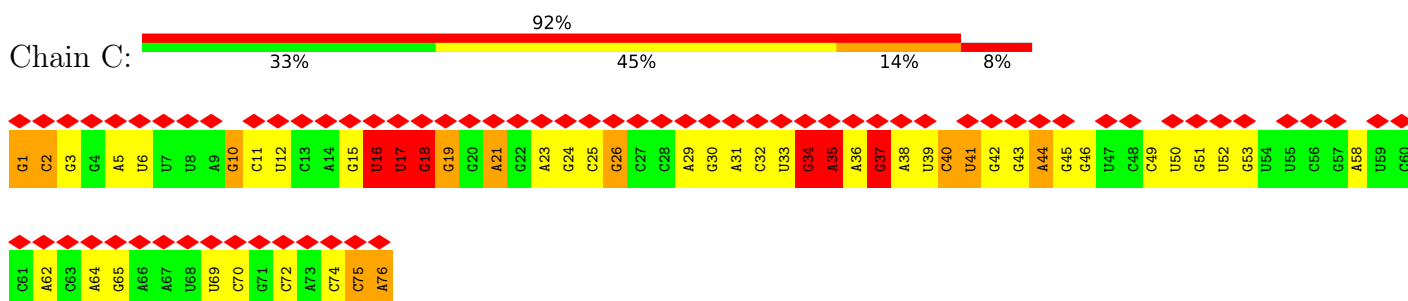
3 Residue-property plots [i](#)

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.

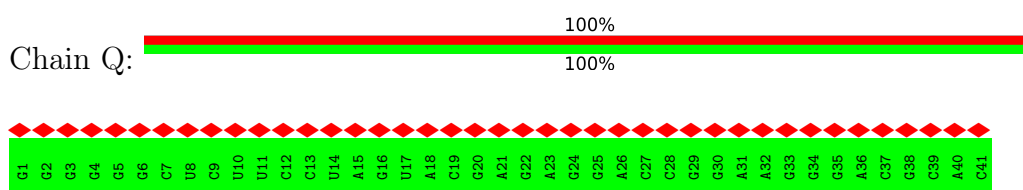
- Molecule 1: Phe-tRNA



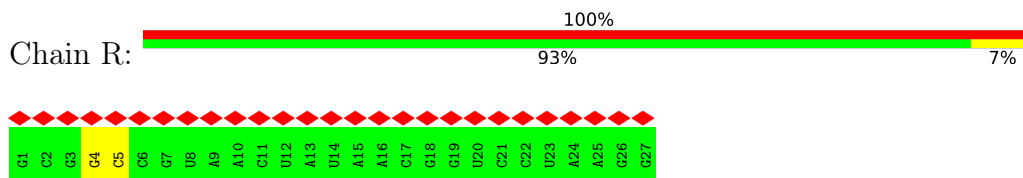
- Molecule 1: Phe-tRNA



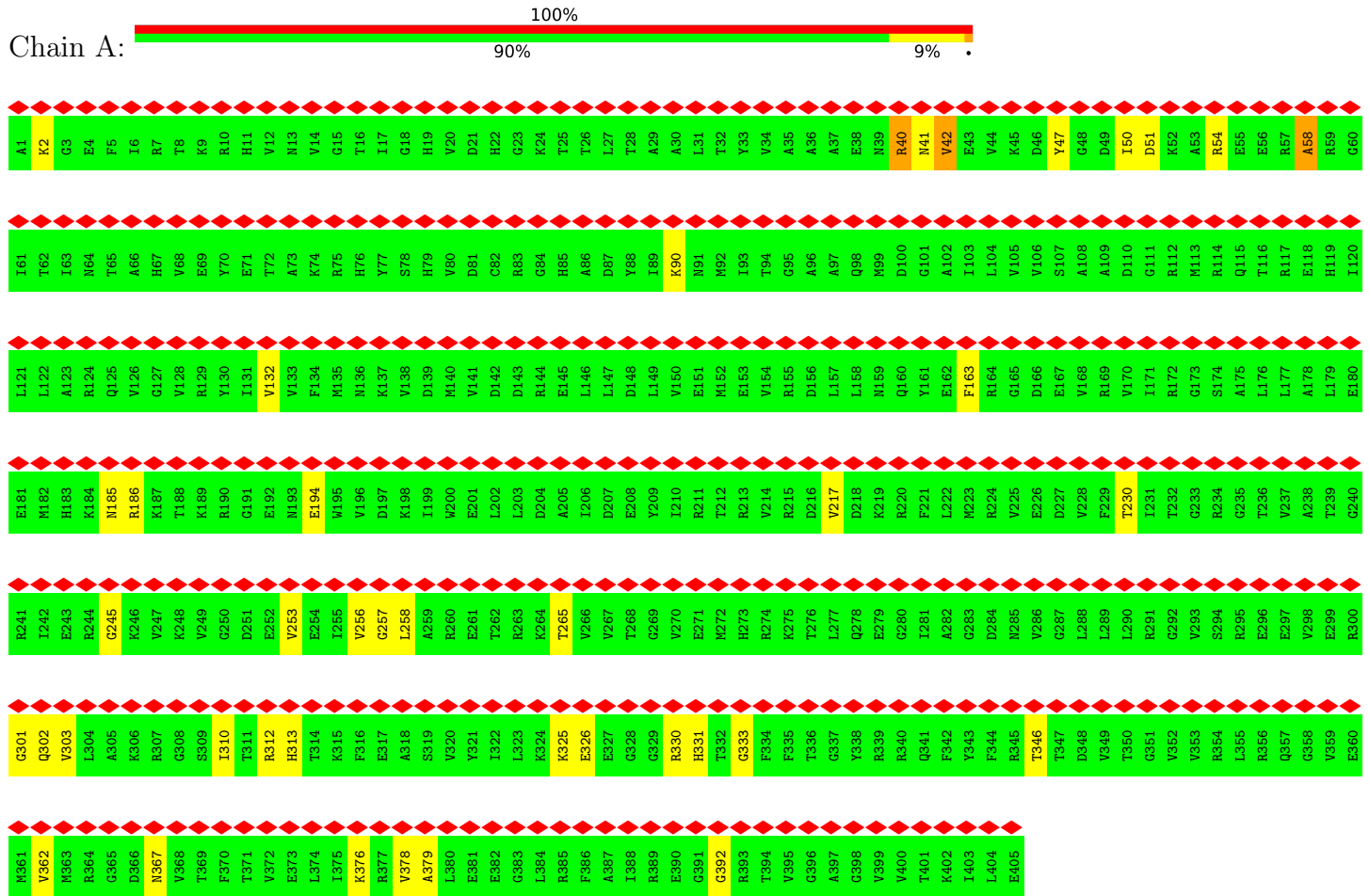
- Molecule 2: sarcin-ricin loop of 23SrRNA



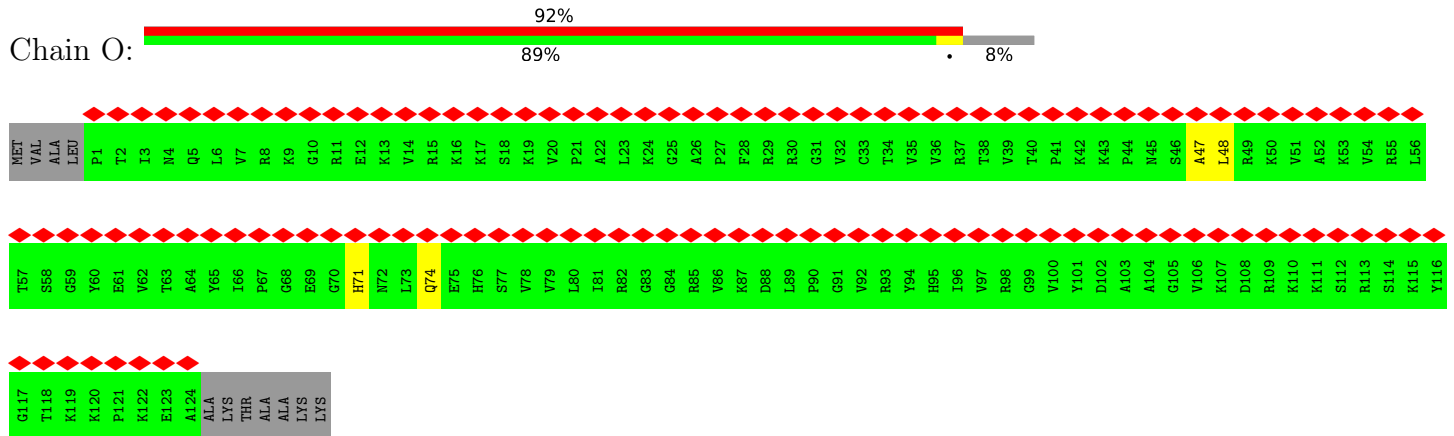
- Molecule 3: helix 69 of 23S rRNA



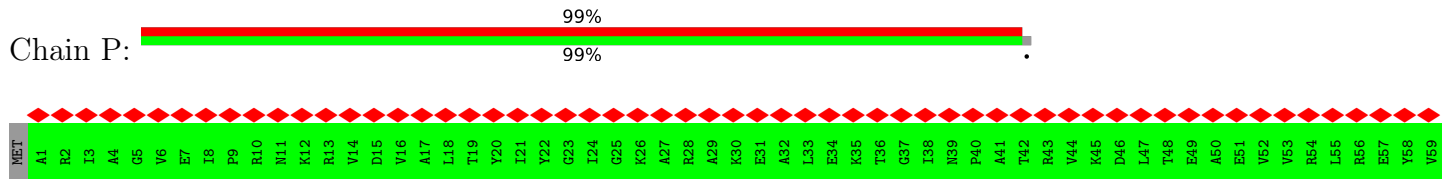
- Molecule 4: Elongation Factor Tu



• Molecule 5: S12 ribosomal protein



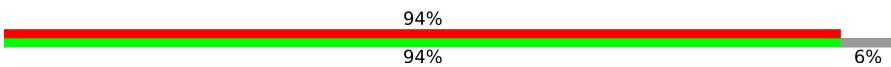
• Molecule 6: S13 ribosomal protein



E60 M61 N61 T62 M63 K64 L65 E66 G67 E68 L69 R70 A71 E72 V73 A74 A75 N76 I77 K78 R79 L80 M81 D82 I83 G84 C85 Y86 R87 G88 L89 R90 H91 R92 R93 G94 L95 P96 V97 R98 G99 Q100 R101 T102 R103 T104 N105 A106 T107 T108 R109 K110 G111 P112 R113 K114 T115 V116 A117 G118 K119

K120
 K121
 A122
 P123
 R124
 K125

• Molecule 7: L11 ribosomal protein

Chain L:  94% 94% 6%

MET
 ALA
 LYS
 LYS
 VAL
 VAL
 ALA
 ALA
 Q1 I2 I3 K3 L4 Q5 L6 P7 A8 G9 K10 A11 T12 P13 A14 P15 P16 V17 G18 P19 A20 L21 G22 Q23 H24 G25 V26 M27 I28 M29 E30 F31 C32 K33 R34 F35 N36 A37 E38 T39 A40 D41 K42 A43 G44 M45 I46 L47 P48 V49 V50 T52 V53

Y54 E55 D56 K57 S58 F59 T60 F61 I62 I63 K64 T65 P66 A68 S69 F70 L71 L72 K73 K74 A75 A76 G77 I78 E79 K80 G81 S82 S83 E84 P85 K86 R87 K88 I89 V90 G91 K92 V93 T94 R95 K96 I98 E99 E100 T101 A102 K103 T104 K105 M106 P107 D108 L109 M110 A111 M112 S113

L114
 E115
 A116
 A117
 M118
 K119
 I120
 I121
 E122
 G123
 T124
 A125
 K126
 S127
 M128
 G129
 I130
 E131
 V132
 V133
 ASP

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	24000	Depositor
Resolution determination method	Not provided	
CTF correction method	phase flip	Depositor
Microscope	FEI/PHILIPS CM200FEG/SOPHIE	Depositor
Voltage (kV)	120	Depositor
Electron dose ($e^-/\text{\AA}^2$)	15	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	58500	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	0.774	Depositor
Minimum map value	-0.481	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.046	Depositor
Recommended contour level	0.0411	Depositor
Map size (\AA)	360, 360, 360	wwPDB
Map dimensions	160, 160, 160	wwPDB
Map angles ($^\circ$)	90, 90, 90	wwPDB
Pixel spacing (\AA)	2.25, 2.25, 2.25	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: 5MC, YG, 2MG, PSU, M2G, 7MG, 1MA, H2U, 5MU, OMG, OMC

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	C	1.44	7/1487 (0.5%)	1.47	22/2315 (1.0%)
1	D	1.29	2/1487 (0.1%)	2.61	186/2315 (8.0%)
4	A	0.75	0/1618	1.34	8/2019 (0.4%)
All	All	1.19	9/4592 (0.2%)	1.91	216/6649 (3.2%)

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	C	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	74	C	O3'-P	-27.05	1.28	1.61
1	C	75	C	O3'-P	-25.57	1.30	1.61
1	C	44	A	O3'-P	-16.97	1.40	1.61
1	C	72	C	O3'-P	-15.88	1.42	1.61
1	C	35	A	O3'-P	8.16	1.71	1.61
1	C	1	G	OP3-P	-7.33	1.52	1.61
1	C	76	A	C2'-O2'	6.52	1.50	1.41
1	D	19	G	C2'-C1'	-5.46	1.47	1.53
1	D	47	U	C4-O4	5.15	1.27	1.23

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	35	A	P-O3'-C3'	27.06	152.18	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	74	C	O3'-P-O5'	24.46	150.48	104.00
1	D	18	G	P-O3'-C3'	15.21	137.96	119.70
1	C	35	A	OP1-P-O3'	14.55	137.21	105.20
1	D	21	A	O4'-C1'-N9	14.50	119.80	108.20
1	D	47	U	P-O3'-C3'	14.39	136.97	119.70
1	C	72	C	O3'-P-O5'	13.95	130.51	104.00
1	C	75	C	P-O3'-C3'	12.69	134.92	119.70
1	C	76	A	O5'-P-OP2	-12.57	94.39	105.70
1	D	3	G	O4'-C1'-N9	11.96	117.77	108.20
1	C	1	G	P-O3'-C3'	11.10	133.02	119.70
1	D	7	U	P-O3'-C3'	-10.32	107.31	119.70
1	C	74	C	OP2-P-O3'	-10.19	82.79	105.20
1	C	35	A	OP2-P-O3'	-9.66	83.94	105.20
1	D	59	U	P-O3'-C3'	9.60	131.22	119.70
1	C	34	OMG	O3'-P-O5'	9.60	122.23	104.00
1	C	44	A	OP2-P-O3'	9.56	126.24	105.20
1	C	34	OMG	OP2-P-O3'	-9.31	84.72	105.20
1	D	57	G	O4'-C1'-N9	9.23	115.59	108.20
1	C	72	C	OP1-P-O3'	-8.97	85.46	105.20
1	D	68	U	C2-N3-C4	-8.86	121.68	127.00
1	D	69	U	C2-N3-C4	-8.85	121.69	127.00
1	D	12	U	C2-N3-C4	-8.83	121.70	127.00
1	D	68	U	N3-C4-C5	8.69	119.82	114.60
1	D	60	C	O4'-C1'-N1	8.66	115.13	108.20
1	D	12	U	N3-C4-C5	8.62	119.77	114.60
1	D	65	G	O4'-C1'-N9	8.60	115.08	108.20
1	D	33	U	C2-N3-C4	-8.42	121.95	127.00
1	C	18	G	C5'-C4'-O4'	-8.41	99.00	109.10
1	D	50	U	N3-C4-C5	8.36	119.62	114.60
1	D	21	A	N9-C1'-C2'	-8.31	102.86	112.00
1	D	32	OMC	P-O3'-C3'	8.30	129.66	119.70
1	D	6	U	C2-N3-C4	-8.27	122.04	127.00
1	D	33	U	N3-C4-C5	8.26	119.55	114.60
1	D	59	U	C2-N3-C4	-8.25	122.05	127.00
1	D	8	U	P-O3'-C3'	-8.21	109.84	119.70
1	D	12	U	C5-C4-O4	-8.20	120.98	125.90
1	D	3	G	N9-C1'-C2'	-8.18	103.00	112.00
1	D	7	U	C2-N3-C4	-8.17	122.10	127.00
1	C	74	C	P-O3'-C3'	-8.11	109.97	119.70
1	D	69	U	N3-C4-C5	8.10	119.46	114.60
1	D	50	U	C2-N3-C4	-8.06	122.17	127.00
1	D	41	U	N3-C4-C5	7.93	119.36	114.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	7	U	N3-C4-C5	7.92	119.35	114.60
1	D	6	U	N3-C4-C5	7.89	119.33	114.60
1	D	41	U	C2-N3-C4	-7.89	122.27	127.00
1	D	59	U	N3-C4-C5	7.85	119.31	114.60
1	C	72	C	P-O3'-C3'	-7.83	110.31	119.70
1	C	44	A	O3'-P-O5'	-7.83	89.13	104.00
1	D	8	U	N3-C4-C5	7.69	119.21	114.60
1	D	7	U	O4'-C1'-N1	7.68	114.34	108.20
1	C	75	C	O3'-P-O5'	7.60	118.43	104.00
1	D	66	A	O4'-C1'-N9	7.59	114.27	108.20
1	D	52	U	C2-N3-C4	-7.53	122.48	127.00
1	D	47	U	C2-N3-C4	-7.53	122.48	127.00
1	D	56	C	O4'-C1'-N1	7.50	114.20	108.20
1	D	52	U	N3-C4-C5	7.48	119.09	114.60
1	D	21	A	P-O3'-C3'	7.47	128.67	119.70
1	D	19	G	OP1-P-OP2	-7.46	108.41	119.60
1	D	8	U	C2-N3-C4	-7.44	122.53	127.00
1	C	75	C	O5'-P-OP1	-7.34	99.09	105.70
1	D	19	G	O4'-C1'-N9	-7.20	102.44	108.20
1	D	50	U	O4'-C1'-N1	7.17	113.93	108.20
1	D	36	A	N9-C1'-C2'	-7.15	104.13	112.00
1	D	75	C	P-O3'-C3'	7.14	128.27	119.70
1	D	61	C	P-O3'-C3'	7.10	128.22	119.70
1	D	53	G	N9-C1'-C2'	-7.05	104.25	112.00
1	D	22	G	OP1-P-OP2	-6.98	109.12	119.60
1	D	73	A	P-O3'-C3'	-6.97	111.34	119.70
1	D	73	A	N9-C1'-C2'	-6.92	104.38	112.00
1	D	69	U	P-O3'-C3'	6.91	127.99	119.70
1	D	15	G	N9-C1'-C2'	-6.82	104.50	112.00
1	D	47	U	N3-C4-C5	6.81	118.69	114.60
1	D	9	A	N1-C2-N3	-6.78	125.91	129.30
1	D	76	A	N1-C2-N3	-6.77	125.92	129.30
1	D	73	A	O4'-C1'-N9	6.72	113.58	108.20
1	D	64	A	N1-C2-N3	-6.60	126.00	129.30
1	D	31	A	O4'-C1'-N9	6.57	113.46	108.20
1	D	18	G	OP1-P-OP2	-6.57	109.75	119.60
1	D	29	A	N1-C2-N3	-6.55	126.02	129.30
1	D	73	A	N1-C2-N3	-6.49	126.05	129.30
1	D	2	C	O4'-C1'-N1	6.46	113.37	108.20
1	D	60	C	OP1-P-OP2	-6.42	109.97	119.60
1	D	31	A	N1-C2-N3	-6.40	126.10	129.30
1	D	11	C	OP1-P-OP2	-6.36	110.06	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	A	N1-C2-N3	-6.32	126.14	129.30
1	D	66	A	N9-C1'-C2'	-6.30	105.07	112.00
1	D	17	H2U	P-O3'-C3'	6.29	127.25	119.70
1	D	18	G	C5-C6-N1	6.29	114.65	111.50
1	D	36	A	N1-C2-N3	-6.27	126.17	129.30
4	A	163	PHE	N-CA-C	-6.26	94.11	111.00
1	D	61	C	N3-C4-C5	-6.24	119.40	121.90
1	D	65	G	C5-C6-N1	6.22	114.61	111.50
1	D	57	G	OP1-P-OP2	-6.19	110.31	119.60
1	D	67	A	N1-C2-N3	-6.16	126.22	129.30
1	D	56	C	N3-C4-C5	-6.15	119.44	121.90
1	D	9	A	OP1-P-OP2	-6.14	110.38	119.60
1	D	51	G	OP1-P-OP2	-6.14	110.39	119.60
1	D	52	U	OP1-P-OP2	-6.14	110.39	119.60
1	D	5	A	O5'-P-OP2	6.14	118.07	110.70
1	D	52	U	C5-C4-O4	-6.13	122.22	125.90
1	D	50	U	C5-C4-O4	-6.11	122.23	125.90
1	D	30	G	C5-C6-N1	6.11	114.55	111.50
1	D	35	A	N1-C2-N3	-6.10	126.25	129.30
1	D	43	G	C5-C6-N1	6.09	114.55	111.50
1	D	14	A	N1-C2-N3	-6.09	126.26	129.30
1	D	15	G	O4'-C1'-N9	6.06	113.05	108.20
1	D	42	G	C5-C6-N1	6.06	114.53	111.50
1	D	29	A	P-O3'-C3'	6.03	126.93	119.70
1	D	57	G	C5-C6-N1	6.02	114.51	111.50
1	D	76	A	OP1-P-OP2	-6.02	110.57	119.60
1	D	71	G	C5-C6-N1	6.01	114.51	111.50
1	D	44	A	N1-C2-N3	-6.01	126.30	129.30
1	D	20	G	C5-C6-N1	5.99	114.50	111.50
1	D	42	G	O4'-C1'-N9	5.99	113.00	108.20
1	D	53	G	C5-C6-N1	5.99	114.50	111.50
1	D	73	A	C6-N1-C2	5.98	122.19	118.60
1	D	36	A	O4'-C1'-N9	5.93	112.94	108.20
1	D	63	C	O4'-C1'-N1	5.93	112.94	108.20
1	D	66	A	N1-C2-N3	-5.92	126.34	129.30
1	C	15	G	N9-C1'-C2'	-5.91	105.50	112.00
1	D	53	G	O4'-C1'-N9	5.90	112.92	108.20
4	A	42	VAL	N-CA-C	-5.90	95.06	111.00
1	D	5	A	N1-C2-N3	-5.89	126.36	129.30
1	D	47	U	P-O5'-C5'	-5.88	111.49	120.90
1	D	21	A	N1-C2-N3	-5.86	126.37	129.30
1	D	63	C	N3-C4-C5	-5.86	119.56	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	28	C	O5'-P-OP2	5.83	117.69	110.70
1	D	70	C	O4'-C1'-N1	5.83	112.86	108.20
1	D	9	A	C6-N1-C2	5.82	122.09	118.60
1	D	35	A	C5-C6-N1	-5.79	114.80	117.70
1	D	69	U	OP1-P-OP2	-5.78	110.94	119.60
1	D	33	U	OP1-P-OP2	-5.76	110.96	119.60
1	D	48	C	N3-C4-C5	-5.74	119.60	121.90
1	D	59	U	OP1-P-OP2	-5.74	110.99	119.60
1	D	76	A	C6-N1-C2	5.72	122.03	118.60
1	D	76	A	C5-C6-N1	-5.72	114.84	117.70
1	D	3	G	C5-C6-N1	5.70	114.35	111.50
1	D	1	G	O4'-C1'-N9	5.70	112.76	108.20
1	D	23	A	N1-C2-N3	-5.68	126.46	129.30
1	D	1	G	C5-C6-N1	5.67	114.34	111.50
1	C	74	C	N1-C1'-C2'	5.66	121.36	114.00
1	D	48	C	OP1-P-OP2	-5.66	111.11	119.60
1	D	69	U	N1-C2-N3	5.66	118.29	114.90
1	D	12	U	O5'-P-OP2	5.65	117.48	110.70
1	D	13	C	OP1-P-OP2	-5.64	111.14	119.60
1	D	45	G	O4'-C1'-N9	5.63	112.70	108.20
1	D	29	A	C5-C6-N1	-5.62	114.89	117.70
1	D	62	A	C5-C6-N1	-5.61	114.90	117.70
1	D	75	C	OP1-P-OP2	-5.60	111.21	119.60
1	D	30	G	OP1-P-OP2	-5.59	111.21	119.60
1	D	21	A	C5-C6-N1	-5.59	114.90	117.70
1	D	9	A	C5-C6-N1	-5.56	114.92	117.70
1	D	48	C	P-O5'-C5'	-5.56	112.01	120.90
1	D	52	U	O4'-C1'-N1	5.55	112.64	108.20
1	D	73	A	C5-C6-N1	-5.50	114.95	117.70
1	D	60	C	N3-C4-C5	-5.47	119.71	121.90
1	D	75	C	N3-C4-C5	-5.43	119.73	121.90
1	D	31	A	C6-N1-C2	5.42	121.85	118.60
1	D	25	C	N3-C4-C5	-5.42	119.73	121.90
1	D	65	G	C6-N1-C2	-5.42	121.85	125.10
1	D	38	A	OP1-P-OP2	-5.41	111.48	119.60
4	A	185	ASN	CA-C-N	-5.40	105.32	117.20
1	D	69	U	C5-C4-O4	-5.37	122.68	125.90
4	A	132	VAL	N-CA-C	-5.35	96.55	111.00
1	D	29	A	C6-N1-C2	5.35	121.81	118.60
1	D	64	A	P-O3'-C3'	-5.33	113.30	119.70
1	D	62	A	N1-C2-N3	-5.32	126.64	129.30
1	D	35	A	C6-N1-C2	5.31	121.79	118.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	70	C	OP1-P-OP2	-5.31	111.63	119.60
1	D	59	U	N1-C2-N3	5.29	118.07	114.90
4	A	310	ILE	N-CA-C	5.29	125.27	111.00
1	D	62	A	C6-N1-C2	5.27	121.76	118.60
1	D	68	U	OP1-P-OP2	-5.27	111.69	119.60
1	D	72	C	OP1-P-OP2	-5.27	111.70	119.60
1	D	12	U	OP1-P-OP2	-5.26	111.71	119.60
1	D	51	G	C5-C6-N1	5.23	114.11	111.50
4	A	367	ASN	N-CA-C	-5.22	96.90	111.00
1	D	38	A	C6-N1-C2	5.21	121.73	118.60
1	D	22	G	C5-C6-N1	5.20	114.10	111.50
1	D	5	A	OP1-P-OP2	-5.19	111.81	119.60
1	D	47	U	N1-C2-N3	5.18	118.01	114.90
1	D	61	C	C2-N3-C4	5.18	122.49	119.90
1	D	70	C	N3-C4-C5	-5.16	119.83	121.90
1	D	47	U	O4'-C1'-N1	5.15	112.32	108.20
1	D	67	A	O5'-C5'-C4'	-5.15	101.92	111.70
1	D	47	U	C5-C4-O4	-5.14	122.82	125.90
1	D	11	C	N3-C4-C5	-5.14	119.85	121.90
1	D	63	C	N1-C1'-C2'	-5.13	106.35	112.00
1	D	66	A	P-O5'-C5'	-5.13	112.69	120.90
1	D	12	U	N1-C2-N3	5.13	117.98	114.90
1	D	36	A	C6-N1-C2	5.13	121.68	118.60
1	D	50	U	N1-C1'-C2'	-5.13	106.36	112.00
1	D	7	U	N1-C2-N3	5.12	117.97	114.90
1	D	44	A	C5-C6-N1	-5.11	115.14	117.70
1	D	4	G	OP1-P-OP2	-5.10	111.94	119.60
1	D	22	G	C6-N1-C2	-5.10	122.04	125.10
1	D	65	G	N9-C1'-C2'	-5.10	106.39	112.00
1	D	66	A	C5-C6-N1	-5.09	115.15	117.70
1	D	24	G	C5-C6-N1	5.08	114.04	111.50
1	D	59	U	O4'-C1'-N1	5.08	112.26	108.20
1	D	36	A	C5-C6-N1	-5.06	115.17	117.70
1	D	14	A	C5-C6-N1	-5.06	115.17	117.70
1	D	19	G	C5-C6-N1	5.05	114.03	111.50
1	D	31	A	C5-C6-N1	-5.04	115.18	117.70
1	D	2	C	OP1-P-OP2	-5.04	112.04	119.60
4	A	51	ASP	N-CA-C	-5.04	97.41	111.00
1	D	56	C	C2-N3-C4	5.03	122.42	119.90
1	D	53	G	OP1-P-OP2	-5.03	112.06	119.60
1	C	21	A	C5'-C4'-C3'	5.02	124.04	116.00
4	A	185	ASN	N-CA-C	5.02	124.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	73	A	OP1-P-OP2	-5.01	112.08	119.60
1	D	45	G	OP1-P-OP2	-5.01	112.09	119.60
1	D	73	A	N1-C6-N6	5.01	121.61	118.60
1	D	5	A	C5-C6-N1	-5.00	115.20	117.70
1	D	62	A	OP1-P-OP2	-5.00	112.09	119.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	18	G	Sidechain
1	C	19	G	Sidechain
1	C	62	A	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	C	1652	0	862	52	0
1	D	1652	0	859	149	0
2	Q	41	0	0	0	0
3	R	27	0	0	2	0
4	A	1620	0	481	53	0
5	O	124	0	0	5	0
6	P	125	0	0	0	0
7	L	133	0	0	0	0
All	All	5374	0	2202	232	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 31.

All (232) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:258:LEU:O	4:A:376:LYS:CA	1.70	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:G:N2	1:C:2:C:H41	1.22	1.38
1:C:1:G:N2	1:C:2:C:N4	1.77	1.31
1:D:50:U:O2'	4:A:331:HIS:N	1.71	1.22
1:D:12:U:O2'	5:O:48:LEU:CA	1.92	1.18
1:C:25:C:O3'	1:C:26:M2G:P	2.12	1.07
4:A:258:LEU:O	4:A:376:LYS:C	1.79	1.06
1:D:37:YG:H101	1:D:37:YG:N20	1.76	0.99
1:D:1:G:H2'	1:D:2:C:H6	1.27	0.98
1:C:41:U:H6	1:C:41:U:H5'	1.34	0.91
1:C:33:U:C2	1:C:35:A:H5'	2.06	0.91
1:C:1:G:H22	1:C:2:C:N4	1.65	0.90
1:D:1:G:H2'	1:D:2:C:C6	2.08	0.89
1:D:3:G:O2'	1:D:4:G:H5'	1.74	0.87
1:D:47:U:H2'	1:D:50:U:OP1	1.75	0.87
1:D:52:U:C4'	4:A:326:GLU:CA	2.52	0.87
4:A:90:LYS:CA	4:A:346:THR:N	2.39	0.86
1:D:38:A:H2'	1:D:39:PSU:O4'	1.76	0.85
4:A:301:GLY:CA	4:A:379:ALA:H	1.90	0.85
4:A:301:GLY:O	4:A:378:VAL:C	2.14	0.85
1:D:37:YG:H101	1:D:37:YG:HN2	1.40	0.84
1:D:52:U:O4'	4:A:326:GLU:CA	2.25	0.84
1:D:66:A:H3'	4:A:392:GLY:N	1.53	0.84
1:C:10:2MG:C5	1:C:26:M2G:HM12	2.12	0.83
1:D:68:U:H2'	1:D:69:U:H6	1.44	0.82
1:D:12:U:H1'	5:O:47:ALA:CA	2.09	0.82
1:C:25:C:H2'	1:C:26:M2G:O4'	1.80	0.82
1:D:14:A:C3'	1:D:15:G:H5'	2.10	0.82
1:C:33:U:O2	1:C:35:A:H3'	1.80	0.82
1:D:30:G:O2'	1:D:31:A:H5'	1.81	0.81
1:D:75:C:H2'	1:D:75:C:O2	1.80	0.80
1:C:1:G:H22	1:C:2:C:H41	1.25	0.80
4:A:301:GLY:O	4:A:379:ALA:N	2.15	0.79
1:D:37:YG:H31	1:D:37:YG:C2'	2.13	0.79
1:D:37:YG:H243	1:D:37:YG:O17	1.83	0.79
1:D:75:C:H4'	1:D:76:A:OP1	1.85	0.77
1:C:1:G:H21	1:C:2:C:N4	1.80	0.77
4:A:301:GLY:HA2	4:A:379:ALA:H	1.49	0.76
4:A:301:GLY:O	4:A:312:ARG:CA	2.33	0.76
1:D:34:OMG:N3	1:D:34:OMG:H2'	1.98	0.76
1:D:76:A:O3'	4:A:230:THR:O	2.03	0.76
1:D:51:G:C4'	4:A:325:LYS:CA	2.64	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:A:C2'	1:D:15:G:H5'	2.16	0.75
4:A:258:LEU:H	4:A:313:HIS:C	1.90	0.75
4:A:301:GLY:CA	4:A:379:ALA:N	2.50	0.74
1:C:10:2MG:C4	1:C:26:M2G:HM12	2.22	0.74
1:D:70:C:H2'	1:D:71:G:H8	1.52	0.74
1:D:42:G:O2'	1:D:43:G:H5'	1.87	0.73
1:D:68:U:H2'	1:D:69:U:C6	2.23	0.73
1:C:37:YG:H31	1:C:37:YG:C1'	2.19	0.73
1:D:34:OMG:H5''	1:D:35:A:OP2	1.88	0.73
1:C:10:2MG:C5	1:C:26:M2G:CM1	2.71	0.73
1:D:35:A:H2'	1:D:36:A:C1'	2.18	0.73
1:D:51:G:H4'	4:A:325:LYS:CA	2.19	0.72
1:D:37:YG:H31	1:D:37:YG:C1'	2.19	0.72
1:C:37:YG:H31	1:C:37:YG:C2'	2.20	0.72
1:C:11:C:H4'	3:R:5:C:P	2.29	0.72
1:D:16:H2U:H51	1:D:16:H2U:OP1	1.90	0.72
1:C:34:OMG:H8	1:C:34:OMG:OP1	1.71	0.72
4:A:258:LEU:N	4:A:313:HIS:O	2.23	0.71
1:C:37:YG:N20	1:C:37:YG:H101	2.06	0.71
1:D:52:U:H4'	4:A:326:GLU:CA	2.22	0.69
1:C:37:YG:H31	1:C:37:YG:H1'	1.74	0.69
1:D:1:G:C6	1:D:73:A:C2	2.82	0.68
1:C:1:G:N2	1:C:2:C:C4	2.61	0.68
1:D:54:5MU:H73	1:D:55:PSU:C2	2.29	0.68
4:A:301:GLY:HA2	4:A:379:ALA:N	2.09	0.67
1:D:28:C:C2	1:D:29:A:C8	2.82	0.67
4:A:257:GLY:HA3	4:A:312:ARG:O	1.96	0.66
1:C:44:A:C2'	1:C:45:G:H5'	2.25	0.66
4:A:302:GLN:CA	4:A:312:ARG:CA	2.75	0.65
1:C:26:M2G:HM22	1:C:44:A:C2	2.32	0.65
1:C:12:U:OP1	3:R:4:G:P	2.55	0.65
1:D:70:C:C2	1:D:71:G:C8	2.84	0.65
4:A:47:TYR:O	4:A:50:ILE:N	2.27	0.64
4:A:303:VAL:N	4:A:312:ARG:N	2.45	0.64
1:D:28:C:N3	1:D:29:A:N7	2.46	0.64
1:D:16:H2U:H51	1:D:16:H2U:P	2.38	0.64
1:D:31:A:O2'	1:D:32:OMC:H5''	1.98	0.64
1:D:5:A:O2'	1:D:6:U:H5'	1.99	0.63
4:A:54:ARG:O	4:A:58:ALA:N	2.30	0.63
1:D:43:G:O2'	1:D:44:A:H5'	1.99	0.62
1:D:51:G:H4'	4:A:330:ARG:O	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:37:YG:C2'	1:D:38:A:H5'	2.29	0.62
1:C:40:5MC:H2'	1:C:41:U:H5'	1.82	0.62
1:D:26:M2G:O2'	1:D:27:C:H5'	2.00	0.61
1:D:12:U:O2	5:O:47:ALA:CA	2.48	0.61
4:A:90:LYS:CA	4:A:346:THR:CA	2.78	0.61
1:C:37:YG:H101	1:C:37:YG:C21	2.30	0.61
1:D:28:C:O2'	1:D:29:A:H5'	2.01	0.60
1:C:41:U:H5'	1:C:41:U:C6	2.27	0.60
1:C:44:A:O2'	1:C:45:G:H5'	2.00	0.60
1:D:37:YG:H31	1:D:37:YG:H1'	1.83	0.60
1:D:76:A:O3'	4:A:230:THR:CA	2.49	0.60
1:C:41:U:H6	1:C:41:U:C5'	2.13	0.60
1:D:14:A:H2'	1:D:15:G:H5'	1.84	0.59
1:D:29:A:O2'	1:D:30:G:H5'	2.02	0.59
1:D:41:U:O2'	1:D:42:G:H5'	2.02	0.59
1:D:16:H2U:H4'	1:D:17:H2U:OP1	2.02	0.59
1:D:19:G:C4	1:D:57:G:N2	2.71	0.59
1:D:50:U:O2'	1:D:51:G:H5'	2.03	0.59
1:D:24:G:C6	1:D:25:C:C4	2.90	0.58
1:C:41:U:H2'	1:C:42:G:O4'	2.03	0.58
4:A:253:VAL:N	4:A:265:THR:O	2.29	0.58
4:A:257:GLY:HA3	4:A:312:ARG:C	2.23	0.58
1:D:37:YG:O2'	1:D:38:A:H5'	2.04	0.57
1:C:64:A:H2'	1:C:65:G:O4'	2.04	0.57
1:C:44:A:H2'	1:C:45:G:O4'	2.04	0.57
1:D:50:U:O2'	4:A:331:HIS:CA	2.52	0.57
1:D:66:A:H2'	1:D:67:A:C8	2.40	0.57
1:D:34:OMG:H3'	1:D:35:A:H8	1.69	0.56
1:D:10:2MG:N3	1:D:10:2MG:H2'	2.20	0.56
4:A:302:GLN:C	4:A:312:ARG:CA	2.73	0.56
1:D:26:M2G:HM22	1:D:44:A:C2	2.41	0.56
4:A:302:GLN:C	4:A:312:ARG:N	2.59	0.56
1:D:47:U:H2'	1:D:47:U:O2	2.06	0.55
1:D:34:OMG:H3'	1:D:35:A:C8	2.42	0.55
1:C:29:A:O2'	1:C:30:G:H5'	2.06	0.55
1:D:24:G:C6	1:D:25:C:N3	2.75	0.55
1:D:19:G:H4'	1:D:20:G:OP2	2.07	0.55
1:D:50:U:HO2'	4:A:331:HIS:H	1.52	0.55
1:D:7:U:H4'	1:D:8:U:OP2	2.06	0.55
1:D:2:C:H2'	1:D:2:C:O2	2.06	0.54
1:C:16:H2U:H1'	1:C:17:H2U:OP2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:A:H2'	1:D:67:A:H8	1.72	0.54
1:D:9:A:C2	1:D:45:G:C6	2.96	0.54
1:D:66:A:H8	4:A:392:GLY:CA	2.19	0.53
1:D:51:G:H1'	4:A:325:LYS:O	2.08	0.53
1:D:66:A:C8	4:A:392:GLY:HA3	2.43	0.53
4:A:333:GLY:HA2	4:A:362:VAL:O	2.09	0.53
1:D:67:A:O2'	1:D:68:U:H5'	2.09	0.53
1:D:24:G:C5	1:D:25:C:C4	2.97	0.52
1:D:53:G:H2'	1:D:53:G:N3	2.23	0.52
4:A:40:ARG:C	4:A:42:VAL:H	2.13	0.52
1:D:31:A:C2'	1:D:32:OMC:H5''	2.40	0.52
1:D:66:A:H8	4:A:392:GLY:HA3	1.74	0.52
1:D:50:U:HO2'	4:A:331:HIS:N	2.01	0.51
1:D:33:U:C2'	1:D:34:OMG:O5'	2.59	0.51
1:C:69:U:H2'	1:C:70:C:C6	2.46	0.51
1:D:37:YG:H31	1:D:37:YG:H2'	1.90	0.51
1:D:69:U:H5'	5:O:71:HIS:CA	2.40	0.51
4:A:217:VAL:O	4:A:245:GLY:HA2	2.11	0.50
1:D:51:G:OP1	4:A:331:HIS:O	2.28	0.50
1:C:40:5MC:H2'	1:C:41:U:C5'	2.40	0.50
4:A:301:GLY:HA3	4:A:379:ALA:H	1.72	0.50
1:D:35:A:C2'	1:D:36:A:O4'	2.60	0.50
1:D:29:A:C6	1:D:42:G:C6	3.00	0.49
1:D:33:U:H2'	1:D:34:OMG:O5'	2.13	0.49
1:D:28:C:C4	1:D:29:A:N7	2.80	0.49
1:D:76:A:H8	1:D:76:A:OP2	1.95	0.49
1:C:23:A:O2'	1:C:24:G:H5'	2.12	0.49
1:D:37:YG:H32	1:D:38:A:O4'	2.12	0.49
1:D:51:G:C4'	4:A:330:ARG:O	2.60	0.49
1:D:42:G:O2'	1:D:43:G:C5'	2.59	0.49
1:D:76:A:OP2	1:D:76:A:C8	2.65	0.49
1:C:30:G:O2'	1:C:31:A:H5'	2.12	0.49
1:D:37:YG:O6	1:D:37:YG:H132	2.13	0.48
1:C:16:H2U:O2'	1:C:17:H2U:OP2	2.21	0.48
1:D:47:U:C2'	1:D:50:U:OP1	2.55	0.47
1:D:75:C:O2	1:D:75:C:C2'	2.51	0.47
1:D:16:H2U:OP1	1:D:16:H2U:C5	2.61	0.47
1:D:65:G:O2'	1:D:66:A:H5'	2.15	0.47
4:A:90:LYS:CA	4:A:346:THR:H	2.26	0.47
1:D:31:A:H2'	1:D:32:OMC:C5'	2.45	0.47
1:D:70:C:O3'	5:O:74:GLN:CA	2.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:YG:H31	1:C:37:YG:O2'	2.15	0.47
1:D:35:A:H2'	1:D:36:A:H1'	1.95	0.47
4:A:301:GLY:C	4:A:379:ALA:N	2.68	0.47
1:D:8:U:C4	1:D:13:C:C4	3.04	0.46
1:D:31:A:N1	1:D:39:PSU:O2	2.48	0.46
1:D:32:OMC:H2'	1:D:33:U:C6	2.50	0.46
1:D:76:A:O3'	4:A:230:THR:C	2.54	0.46
1:D:35:A:H2'	1:D:36:A:O4'	2.16	0.46
1:D:1:G:C2'	1:D:2:C:H6	2.14	0.46
1:D:30:G:O2'	1:D:31:A:C5'	2.61	0.46
1:D:31:A:C2	1:D:40:5MC:N3	2.84	0.46
1:D:70:C:N3	1:D:71:G:N7	2.64	0.46
1:D:37:YG:H2'	1:D:37:YG:C3	2.45	0.46
1:D:51:G:H2'	1:D:52:U:C6	2.51	0.46
1:D:61:C:H2'	1:D:62:A:H8	1.80	0.46
4:A:303:VAL:CA	4:A:312:ARG:N	2.79	0.46
1:C:33:U:O2	1:C:35:A:H5'	2.13	0.45
1:D:5:A:O2'	1:D:6:U:C5'	2.64	0.45
1:D:70:C:H2'	1:D:71:G:C8	2.41	0.45
1:C:23:A:H2'	1:C:24:G:C8	2.52	0.45
1:D:34:OMG:O3'	1:D:34:OMG:HM23	2.16	0.45
1:D:16:H2U:H2'	1:D:16:H2U:H62	1.67	0.44
1:D:37:YG:H243	1:D:37:YG:C16	2.46	0.44
1:C:50:U:O2'	1:C:51:G:H5'	2.17	0.44
1:D:2:C:O2	1:D:2:C:C2'	2.66	0.44
1:D:43:G:HO2'	1:D:44:A:H5'	1.81	0.44
1:D:3:G:N2	1:D:71:G:C4	2.86	0.44
4:A:256:VAL:O	4:A:312:ARG:O	2.35	0.44
1:C:16:H2U:C2'	1:C:17:H2U:OP2	2.65	0.44
1:D:3:G:C2'	1:D:4:G:H5'	2.47	0.43
1:D:63:C:H2'	1:D:64:A:C8	2.53	0.43
1:D:9:A:H4'	1:D:10:2MG:OP2	2.18	0.43
1:D:28:C:H2'	1:D:29:A:H8	1.84	0.43
1:C:50:U:C2'	1:C:51:G:H5'	2.48	0.43
1:D:33:U:O2'	1:D:35:A:N7	2.43	0.43
1:C:43:G:H2'	1:C:44:A:C8	2.53	0.43
1:D:70:C:O2'	1:D:71:G:H5'	2.19	0.42
1:C:34:OMG:H3'	1:C:35:A:H5''	2.00	0.42
1:C:44:A:C2'	1:C:45:G:C5'	2.96	0.42
1:D:1:G:C4	1:D:2:C:C6	3.07	0.42
1:D:12:U:C2'	1:D:13:C:O5'	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:H2U:C2'	1:D:16:H2U:O5'	2.68	0.42
1:D:66:A:C3'	4:A:392:GLY:N	2.27	0.42
1:D:3:G:N1	1:D:71:G:C6	2.88	0.42
1:C:32:OMC:H6	1:C:32:OMC:O5'	2.01	0.42
1:D:12:U:H2'	1:D:13:C:O5'	2.20	0.41
1:D:5:A:C2'	1:D:6:U:O5'	2.68	0.41
1:D:14:A:C6	1:D:22:G:N3	2.88	0.41
1:D:61:C:H2'	1:D:62:A:C8	2.54	0.41
1:C:37:YG:H32	1:C:38:A:O4'	2.20	0.41
4:A:40:ARG:O	4:A:42:VAL:N	2.45	0.41
1:D:30:G:HO2'	1:D:31:A:H5'	1.81	0.41
1:D:14:A:C5	1:D:22:G:C2	3.09	0.41
1:D:19:G:C5	1:D:57:G:N2	2.88	0.41
1:D:19:G:C8	1:D:57:G:N2	2.89	0.41
1:C:52:U:O2'	1:C:53:G:H5'	2.20	0.41
1:D:31:A:C2'	1:D:32:OMC:C5'	2.98	0.41
1:D:35:A:C2'	1:D:36:A:C1'	2.95	0.41
1:D:7:U:C4'	1:D:8:U:OP2	2.68	0.40
1:D:26:M2G:C2'	1:D:27:C:O5'	2.69	0.40
1:D:47:U:H4'	1:D:48:C:OP2	2.20	0.40
1:D:30:G:C2'	1:D:31:A:O5'	2.69	0.40
1:D:66:A:C8	4:A:392:GLY:CA	3.01	0.40
1:D:47:U:O2	1:D:47:U:C2'	2.69	0.40
1:D:58:1MA:H4'	1:D:59:U:OP1	2.21	0.40
1:C:5:A:H2'	1:C:6:U:O4'	2.21	0.40
1:C:39:PSU:N1	1:C:40:5MC:HM52	2.36	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	
4	A	401/405 (99%)	371 (92%)	24 (6%)	6 (2%)	10	46

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	2	LYS
4	A	41	ASN
4	A	40	ARG
4	A	194	GLU
4	A	58	ALA
4	A	186	ARG

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	75/76 (98%)	13 (17%)	3 (4%)
1	D	75/76 (98%)	29 (38%)	3 (4%)
2	Q	0/41	-	-
3	R	0/27	-	-
All	All	150/220 (68%)	42 (28%)	6 (4%)

All (42) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	D	4	G
1	D	7	U
1	D	9	A
1	D	12	U
1	D	13	C
1	D	15	G
1	D	16	H2U
1	D	17	H2U
1	D	18	G
1	D	19	G
1	D	21	A
1	D	27	C
1	D	33	U

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Mol	Chain	Res	Type
1	D	34	OMG
1	D	36	A
1	D	38	A
1	D	40	5MC
1	D	45	G
1	D	46	7MG
1	D	47	U
1	D	48	C
1	D	49	5MC
1	D	53	G
1	D	58	1MA
1	D	60	C
1	D	65	G
1	D	70	C
1	D	73	A
1	D	76	A
1	C	2	C
1	C	3	G
1	C	17	H2U
1	C	18	G
1	C	19	G
1	C	21	A
1	C	34	OMG
1	C	35	A
1	C	36	A
1	C	37	YG
1	C	41	U
1	C	75	C
1	C	76	A

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	D	16	H2U
1	D	47	U
1	D	75	C
1	C	16	H2U
1	C	18	G
1	C	35	A

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

28 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	H2U	D	16	1	18,21,22	0.91	0	21,30,33	1.14	1 (4%)
1	5MU	D	54	1	19,22,23	0.78	0	28,32,35	1.63	5 (17%)
1	5MC	D	40	1	18,22,23	0.56	0	26,32,35	0.87	1 (3%)
1	PSU	C	55	1	18,21,22	0.74	0	22,30,33	0.86	0
1	5MC	C	40	1	18,22,23	0.45	0	26,32,35	0.70	1 (3%)
1	H2U	D	17	1	18,21,22	0.60	0	21,30,33	0.79	0
1	H2U	C	17	1	18,21,22	0.67	1 (5%)	21,30,33	0.98	1 (4%)
1	OMG	C	34	1	18,26,27	1.04	2 (11%)	19,38,41	0.86	1 (5%)
1	OMG	D	34	1	18,26,27	1.31	2 (11%)	19,38,41	2.11	2 (10%)
1	H2U	C	16	1	18,21,22	0.74	1 (5%)	21,30,33	1.14	2 (9%)
1	5MU	C	54	1	19,22,23	0.51	0	28,32,35	0.64	0
1	M2G	D	26	1	20,27,28	1.26	3 (15%)	22,40,43	1.52	2 (9%)
1	YG	D	37	1	31,42,43	2.34	9 (29%)	33,62,65	2.55	14 (42%)
1	1MA	D	58	1	16,25,26	1.52	3 (18%)	18,37,40	0.64	0
1	1MA	C	58	1	16,25,26	2.83	4 (25%)	18,37,40	2.21	5 (27%)
1	2MG	D	10	1	18,26,27	1.06	2 (11%)	16,38,41	2.03	2 (12%)
1	PSU	D	39	1	18,21,22	0.49	0	22,30,33	0.64	0
1	M2G	C	26	1	20,27,28	1.21	2 (10%)	22,40,43	0.78	0
1	YG	C	37	1	31,42,43	0.92	1 (3%)	33,62,65	2.59	10 (30%)
1	PSU	D	55	1	18,21,22	0.72	1 (5%)	22,30,33	1.00	1 (4%)
1	7MG	D	46	1	22,26,27	3.48	2 (9%)	29,39,42	1.71	3 (10%)
1	OMC	D	32	1	19,22,23	1.06	1 (5%)	26,31,34	1.79	1 (3%)
1	5MC	D	49	1	18,22,23	0.56	0	26,32,35	1.05	2 (7%)
1	PSU	C	39	1	18,21,22	0.71	0	22,30,33	0.68	0
1	2MG	C	10	1	18,26,27	1.09	1 (5%)	16,38,41	0.74	0
1	7MG	C	46	1	22,26,27	1.08	2 (9%)	29,39,42	1.20	3 (10%)
1	5MC	C	49	1	18,22,23	0.76	0	26,32,35	0.72	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	C	32	1	19,22,23	0.46	0	26,31,34	0.57	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	H2U	D	16	1	-	4/7/38/39	0/2/2/2
1	5MU	D	54	1	-	0/7/25/26	0/2/2/2
1	5MC	D	40	1	-	2/7/25/26	0/2/2/2
1	PSU	C	55	1	-	0/7/25/26	0/2/2/2
1	5MC	C	40	1	-	1/7/25/26	0/2/2/2
1	H2U	D	17	1	-	6/7/38/39	0/2/2/2
1	H2U	C	17	1	-	0/7/38/39	0/2/2/2
1	OMG	C	34	1	-	1/5/27/28	0/3/3/3
1	OMG	D	34	1	-	3/5/27/28	0/3/3/3
1	H2U	C	16	1	-	4/7/38/39	0/2/2/2
1	5MU	C	54	1	-	0/7/25/26	0/2/2/2
1	M2G	D	26	1	-	0/7/29/30	0/3/3/3
1	YG	D	37	1	-	12/20/42/43	0/3/4/4
1	1MA	D	58	1	-	1/3/25/26	0/3/3/3
1	1MA	C	58	1	-	0/3/25/26	0/3/3/3
1	2MG	D	10	1	-	1/5/27/28	0/3/3/3
1	PSU	D	39	1	-	1/7/25/26	0/2/2/2
1	M2G	C	26	1	-	0/7/29/30	0/3/3/3
1	YG	C	37	1	-	7/20/42/43	0/3/4/4
1	PSU	D	55	1	-	0/7/25/26	0/2/2/2
1	7MG	D	46	1	-	4/7/37/38	0/3/3/3
1	OMC	D	32	1	-	1/9/27/28	0/2/2/2
1	5MC	D	49	1	-	3/7/25/26	0/2/2/2
1	PSU	C	39	1	-	0/7/25/26	0/2/2/2
1	2MG	C	10	1	-	0/5/27/28	0/3/3/3
1	7MG	C	46	1	-	2/7/37/38	0/3/3/3
1	5MC	C	49	1	-	0/7/25/26	0/2/2/2
1	OMC	C	32	1	-	0/9/27/28	0/2/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	46	7MG	C8-N9	-15.70	1.37	1.46
1	C	58	1MA	C6-N6	8.08	1.48	1.27
1	D	37	YG	C2-N2	6.91	1.48	1.35
1	C	58	1MA	C2-N3	6.87	1.37	1.29
1	D	37	YG	O23-C21	4.95	1.43	1.34
1	D	37	YG	C3-N3	-4.55	1.36	1.46
1	D	37	YG	O18-C16	3.97	1.42	1.33
1	D	32	OMC	O2'-CM2	-3.84	1.28	1.42
1	D	58	1MA	C2-N3	3.60	1.33	1.29
1	D	34	OMG	O2'-CM2	-3.60	1.29	1.42
1	D	46	7MG	C5-N7	3.50	1.39	1.35
1	D	37	YG	O4'-C1'	3.40	1.45	1.41
1	D	37	YG	C12-N1	-3.31	1.30	1.36
1	D	37	YG	O6-C6	3.19	1.26	1.22
1	C	26	M2G	C5-C6	-3.12	1.41	1.47
1	C	10	2MG	C5-C6	-3.07	1.41	1.47
1	C	46	7MG	C4-N9	2.93	1.41	1.37
1	D	26	M2G	C2-N3	2.80	1.34	1.30
1	C	46	7MG	C5-N7	2.76	1.38	1.35
1	D	37	YG	C14-C15	-2.64	1.47	1.53
1	C	26	M2G	C8-N7	-2.60	1.30	1.35
1	C	16	H2U	C2-N1	2.54	1.39	1.35
1	D	34	OMG	C5-C6	-2.47	1.42	1.47
1	D	37	YG	C4-N3	-2.44	1.35	1.40
1	C	58	1MA	C8-N7	-2.35	1.31	1.35
1	D	10	2MG	C5-C6	-2.29	1.42	1.47
1	D	26	M2G	C5-C6	-2.26	1.42	1.47
1	C	34	OMG	C8-N7	-2.25	1.31	1.35
1	D	26	M2G	C8-N7	-2.22	1.31	1.35
1	D	58	1MA	C8-N7	-2.21	1.31	1.35
1	D	10	2MG	C8-N7	-2.18	1.31	1.35
1	C	58	1MA	C5-C4	-2.17	1.37	1.43
1	C	37	YG	C8-N7	-2.15	1.31	1.35
1	D	55	PSU	O4'-C1'	-2.04	1.41	1.43
1	D	58	1MA	C6-N6	2.01	1.32	1.27
1	C	34	OMG	C5-C6	-2.01	1.43	1.47
1	C	17	H2U	C2-N1	2.01	1.38	1.35

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	YG	C11-C12-N1	8.52	111.34	106.53
1	D	32	OMC	CM2-O2'-C2'	8.28	136.25	114.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	34	OMG	CM2-O2'-C2'	8.21	136.06	114.52
1	D	46	7MG	N9-C8-N7	7.36	113.90	103.38
1	D	10	2MG	CM2-N2-C2	-6.81	108.82	123.86
1	D	37	YG	C3-N3-C4	6.61	128.44	116.71
1	C	37	YG	C24-O23-C21	6.28	123.08	115.66
1	D	37	YG	C24-O23-C21	-5.45	109.23	115.66
1	D	37	YG	O23-C21-N20	5.35	120.20	110.80
1	C	58	1MA	CM1-N1-C6	-5.21	112.38	120.27
1	C	37	YG	C3-N3-C4	5.00	125.59	116.71
1	D	54	5MU	C5-C4-N3	4.57	119.21	115.31
1	C	58	1MA	CM1-N1-C2	4.55	130.13	120.55
1	C	37	YG	O23-C21-N20	4.38	118.50	110.80
1	D	26	M2G	CM2-N2-CM1	4.32	129.14	115.77
1	C	58	1MA	N1-C2-N3	4.25	130.98	126.02
1	D	37	YG	C4-N3-C2	-4.19	109.44	122.15
1	C	46	7MG	C4-C5-N7	3.98	111.06	105.53
1	D	26	M2G	CM1-N2-C2	-3.80	112.63	120.55
1	D	54	5MU	C4-N3-C2	-3.70	122.57	127.35
1	D	37	YG	O18-C16-C15	3.68	120.94	111.52
1	D	37	YG	O23-C21-O22	-3.63	119.24	124.58
1	D	46	7MG	C4-C5-N7	3.60	110.52	105.53
1	C	37	YG	C4-N3-C2	-3.40	111.85	122.15
1	C	37	YG	O23-C21-O22	-3.35	119.66	124.58
1	D	37	YG	C11-C12-N1	-3.01	104.83	106.53
1	D	54	5MU	C2'-C1'-N1	-2.91	104.96	113.22
1	D	10	2MG	O6-C6-N1	-2.91	117.21	120.65
1	C	37	YG	C19-O18-C16	2.90	122.50	115.94
1	D	16	H2U	O5'-C5'-C4'	-2.88	99.19	108.99
1	D	54	5MU	O4'-C1'-N1	2.88	114.94	108.36
1	C	16	H2U	C4-N3-C2	2.81	128.13	125.79
1	D	37	YG	C5-C6-N1	2.80	118.13	113.96
1	C	46	7MG	N9-C8-N7	2.77	107.34	103.38
1	C	46	7MG	CM7-N7-C5	2.75	133.50	126.40
1	C	58	1MA	N1-C6-N6	2.67	126.57	119.77
1	D	37	YG	O22-C21-N20	-2.62	120.56	124.85
1	C	37	YG	C3-N3-C2	2.60	122.56	120.13
1	D	34	OMG	O6-C6-N1	-2.58	117.60	120.65
1	D	49	5MC	C1'-N1-C6	2.57	125.40	121.12
1	C	49	5MC	C5-C6-N1	-2.54	120.72	123.34
1	C	40	5MC	C5-C6-N1	-2.51	120.75	123.34
1	D	49	5MC	O4'-C1'-N1	2.49	114.06	108.36
1	D	55	PSU	O4'-C1'-C2'	2.46	108.61	105.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	37	YG	O6-C6-C5	2.46	128.53	124.17
1	D	37	YG	C14-C15-N20	2.40	115.73	110.88
1	C	37	YG	O18-C16-C15	2.37	117.59	111.52
1	D	40	5MC	C5-C4-N3	-2.37	119.12	121.67
1	C	16	H2U	O3'-C3'-C2'	2.36	119.47	111.82
1	C	17	H2U	C4-N3-C2	2.34	127.74	125.79
1	D	37	YG	O17-C16-C15	-2.24	117.26	123.92
1	C	34	OMG	O6-C6-C5	2.23	128.73	124.37
1	D	37	YG	C4-C5-C6	-2.22	116.25	121.16
1	D	46	7MG	C6-C5-C4	-2.20	118.08	122.62
1	C	58	1MA	O4'-C1'-C2'	-2.15	103.79	106.93
1	D	37	YG	C3-N3-C2	2.12	122.11	120.13
1	D	54	5MU	N3-C2-N1	2.07	117.64	114.89
1	D	37	YG	C16-C15-N20	-2.01	106.09	110.72

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	16	H2U	O4'-C1'-N1-C6
1	D	16	H2U	C2'-C1'-N1-C2
1	D	16	H2U	C2'-C1'-N1-C6
1	D	17	H2U	O4'-C1'-N1-C6
1	D	17	H2U	C2'-C1'-N1-C6
1	D	32	OMC	C1'-C2'-O2'-CM2
1	D	34	OMG	C3'-C2'-O2'-CM2
1	D	37	YG	C12-C13-C14-C15
1	D	37	YG	C13-C14-C15-N20
1	D	37	YG	C16-C15-N20-C21
1	D	37	YG	O22-C21-N20-C15
1	D	37	YG	O23-C21-N20-C15
1	D	37	YG	N20-C21-O23-C24
1	D	37	YG	O22-C21-O23-C24
1	D	40	5MC	O4'-C4'-C5'-O5'
1	D	46	7MG	C2'-C1'-N9-C8
1	D	49	5MC	O4'-C4'-C5'-O5'
1	C	16	H2U	O4'-C1'-N1-C2
1	C	16	H2U	O4'-C1'-N1-C6
1	C	16	H2U	C2'-C1'-N1-C6
1	C	37	YG	C12-C13-C14-C15
1	C	37	YG	C15-C16-O18-C19
1	C	46	7MG	C2'-C1'-N9-C8

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Mol	Chain	Res	Type	Atoms
1	C	37	YG	O17-C16-O18-C19
1	D	37	YG	O17-C16-O18-C19
1	D	37	YG	C15-C16-O18-C19
1	D	17	H2U	C3'-C4'-C5'-O5'
1	D	40	5MC	C3'-C4'-C5'-O5'
1	D	49	5MC	C3'-C4'-C5'-O5'
1	D	17	H2U	O4'-C4'-C5'-O5'
1	D	46	7MG	O4'-C4'-C5'-O5'
1	D	46	7MG	C3'-C4'-C5'-O5'
1	C	16	H2U	C2'-C1'-N1-C2
1	D	17	H2U	C2'-C1'-N1-C2
1	C	37	YG	C13-C14-C15-C16
1	D	37	YG	C13-C14-C15-C16
1	D	34	OMG	O4'-C4'-C5'-O5'
1	D	17	H2U	O4'-C1'-N1-C2
1	D	10	2MG	C4'-C5'-O5'-P
1	D	16	H2U	O4'-C1'-N1-C2
1	D	49	5MC	C4'-C5'-O5'-P
1	C	34	OMG	C4'-C5'-O5'-P
1	C	46	7MG	C2'-C1'-N9-C4
1	D	37	YG	N20-C15-C16-O18
1	C	40	5MC	O4'-C4'-C5'-O5'
1	D	34	OMG	C3'-C4'-C5'-O5'
1	D	39	PSU	O4'-C4'-C5'-O5'
1	C	37	YG	C14-C15-C16-O18
1	C	37	YG	C13-C14-C15-N20
1	D	46	7MG	O4'-C1'-N9-C8
1	C	37	YG	C14-C15-C16-O17
1	D	58	1MA	O4'-C4'-C5'-O5'
1	D	37	YG	N20-C15-C16-O17

There are no ring outliers.

21 monomers are involved in 63 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	16	H2U	6	0
1	D	54	5MU	1	0
1	D	40	5MC	1	0
1	C	40	5MC	3	0
1	D	17	H2U	1	0
1	C	17	H2U	3	0
1	C	34	OMG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	34	OMG	7	0
1	C	16	H2U	3	0
1	D	26	M2G	3	0
1	D	37	YG	13	0
1	D	58	1MA	1	0
1	D	10	2MG	2	0
1	D	39	PSU	2	0
1	C	26	M2G	6	0
1	C	37	YG	7	0
1	D	55	PSU	1	0
1	D	32	OMC	5	0
1	C	39	PSU	1	0
1	C	10	2MG	3	0
1	C	32	OMC	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	4
4	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	311:THR	C	312:ARG	N	8.60

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	25:C	O3'	26:M2G	P	2.12
1	C	75:C	O3'	76:A	P	1.30
1	C	74:C	O3'	75:C	P	1.28
1	C	36:A	O3'	37:YG	P	1.18

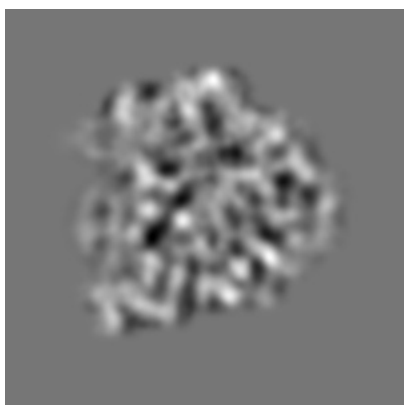
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-1004. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections [i](#)

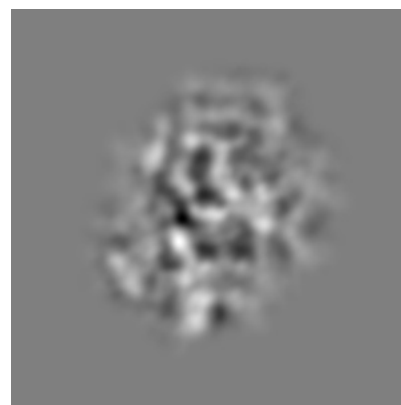
6.1.1 Primary map



X



Y



Z

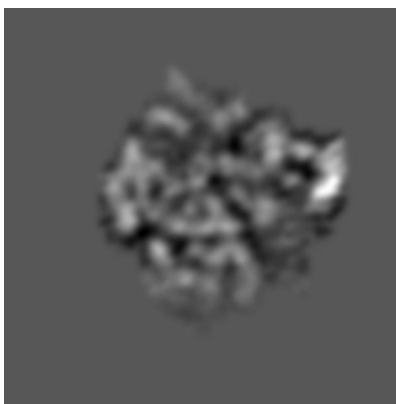
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 80



Y Index: 80



Z Index: 80

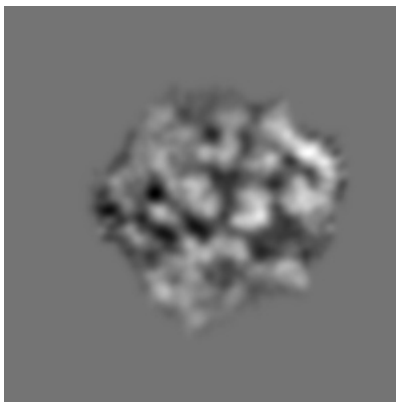
The images above show central slices of the map in three orthogonal directions.

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

6.3.1 Primary map



X Index: 76



Y Index: 74

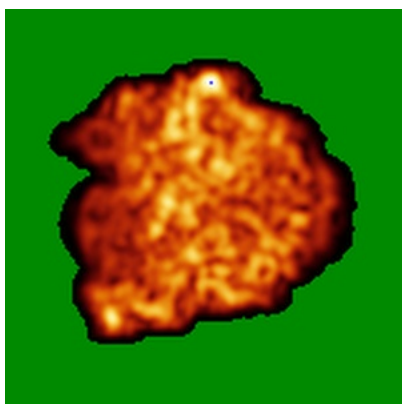


Z Index: 99

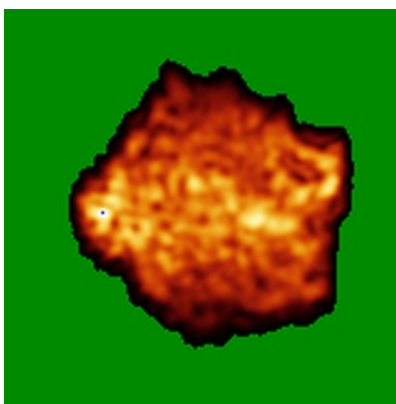
The images above show the largest variance slices of the map in three orthogonal directions.

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

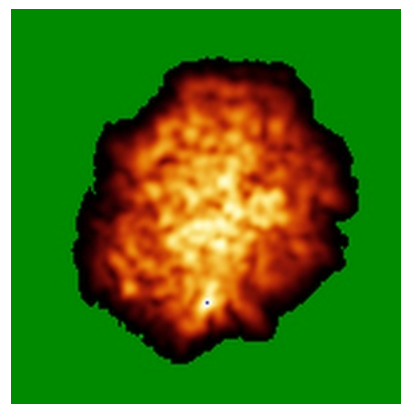
6.4.1 Primary map



X



Y

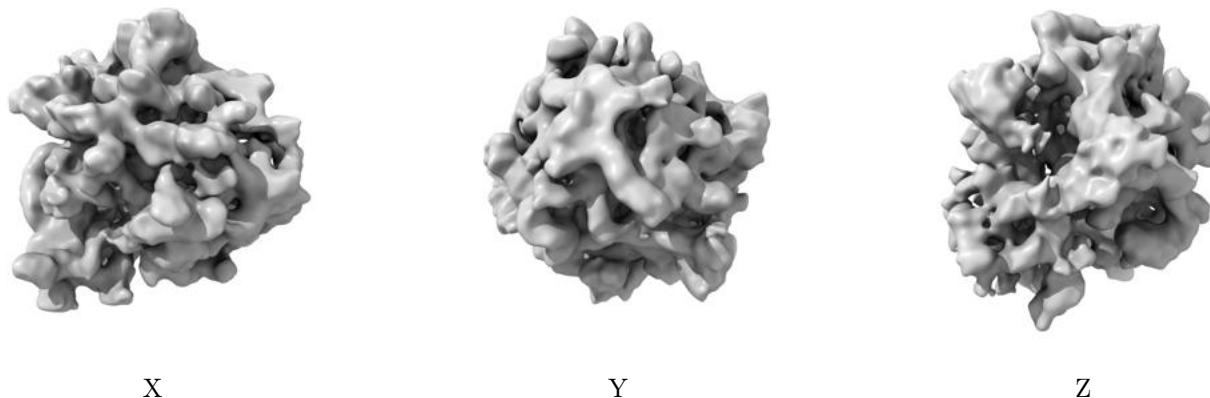


Z

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 0.0411. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

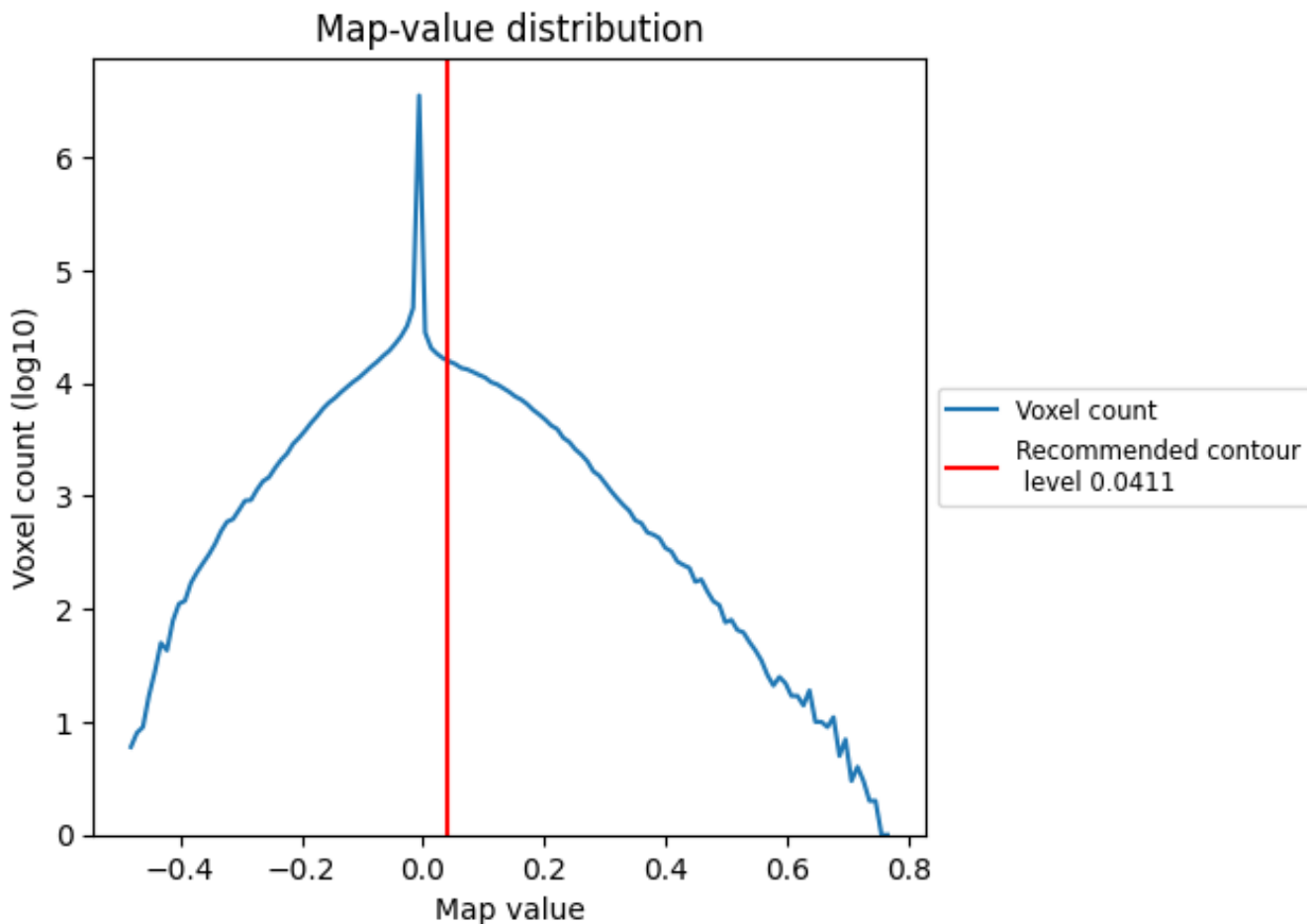
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

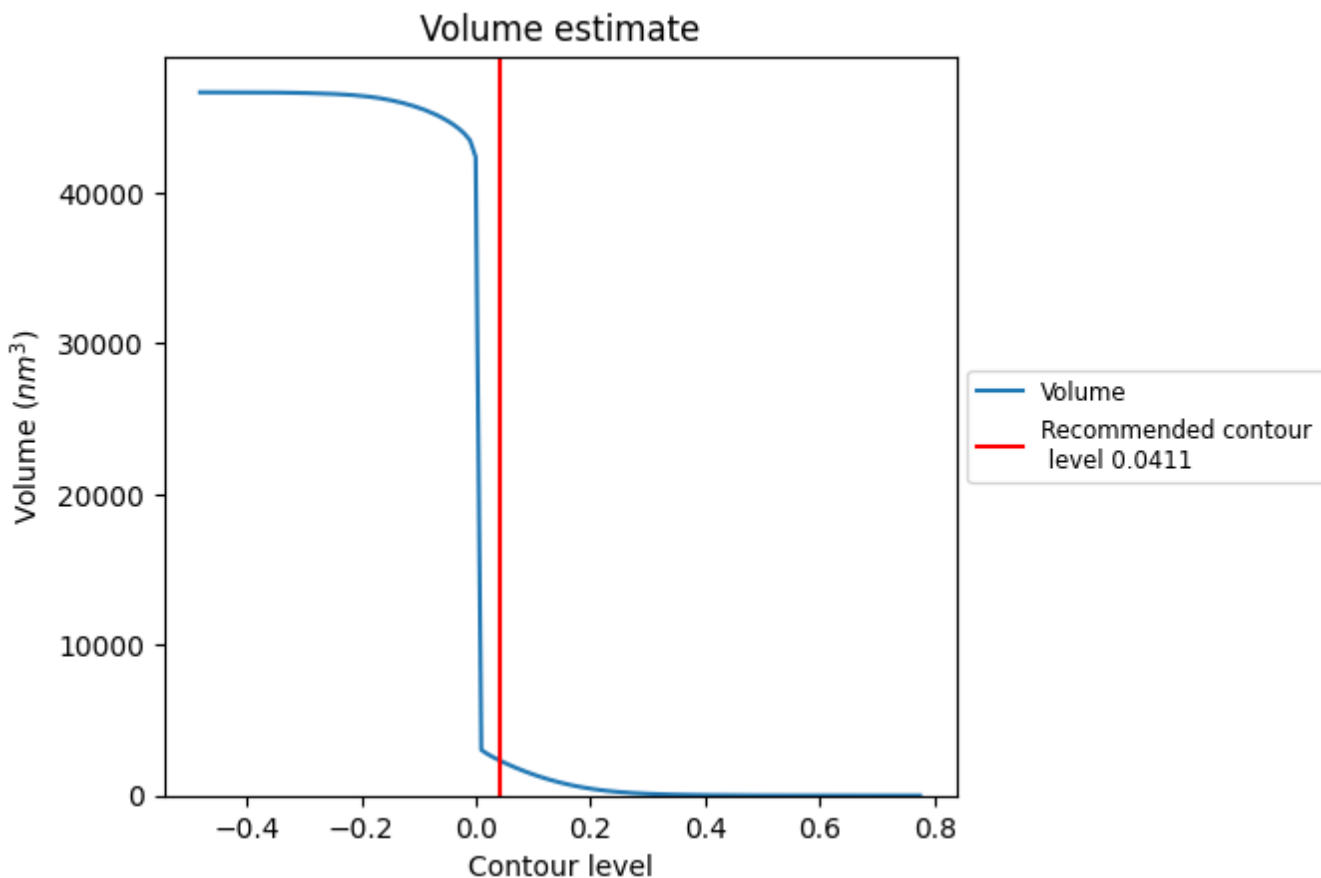
This section contains the results of statistical analysis of the map.

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.

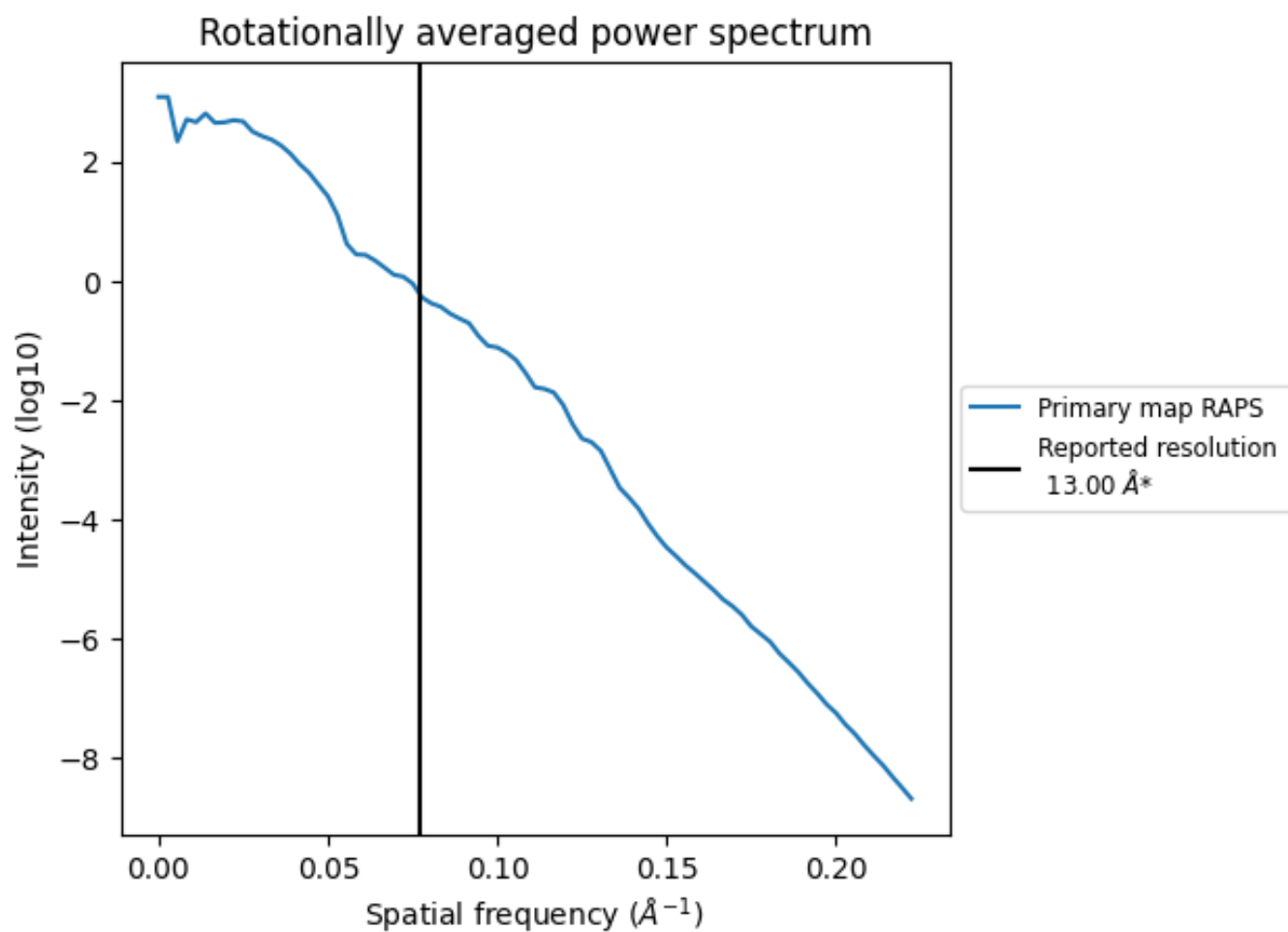
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2333 nm^3 ; this corresponds to an approximate mass of 2107 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.077\AA^{-1}

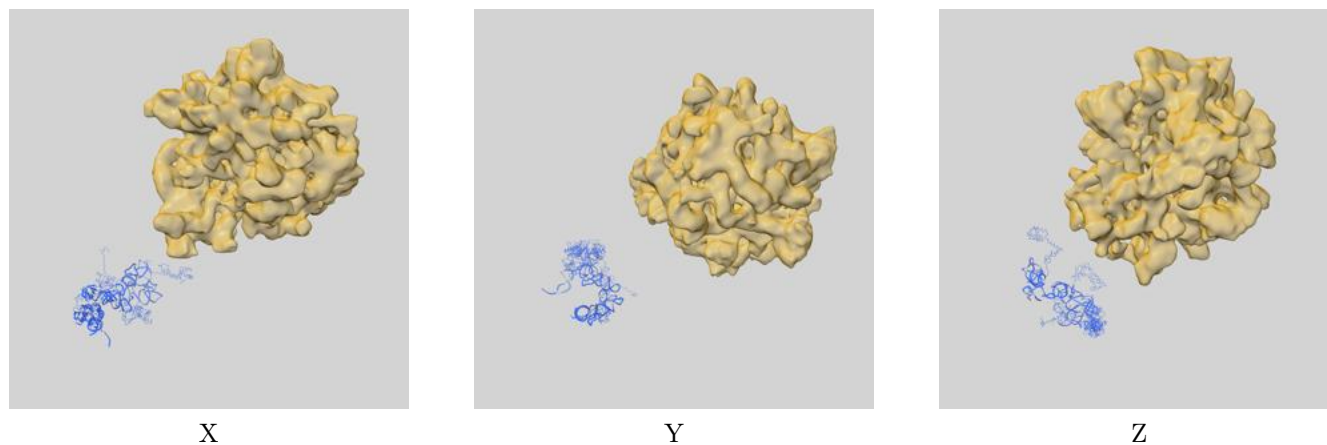
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-1004 and PDB model 1MJ1. Per-residue inclusion information can be found in section 3 on page 5.

9.1 Map-model overlay [i](#)



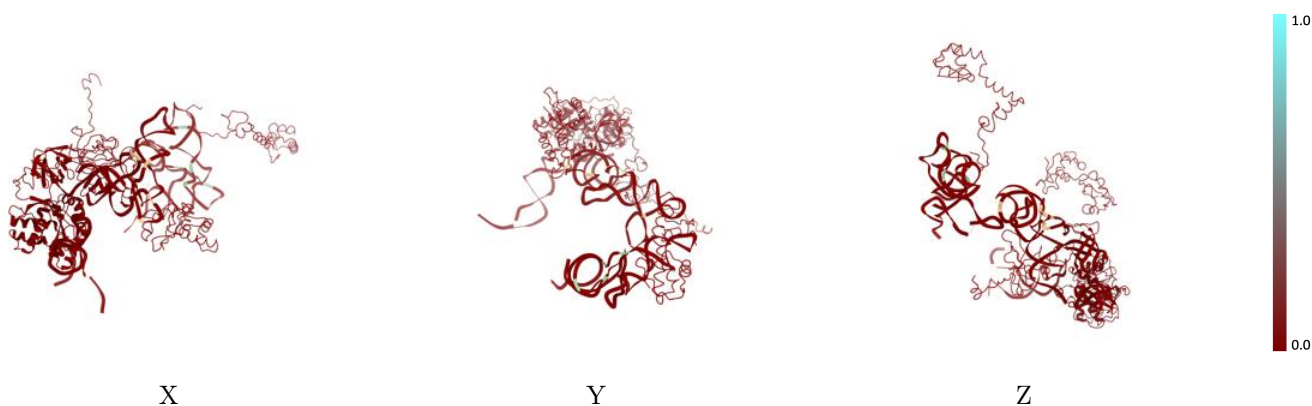
The images above show the 3D surface view of the map at the recommended contour level 0.0411 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



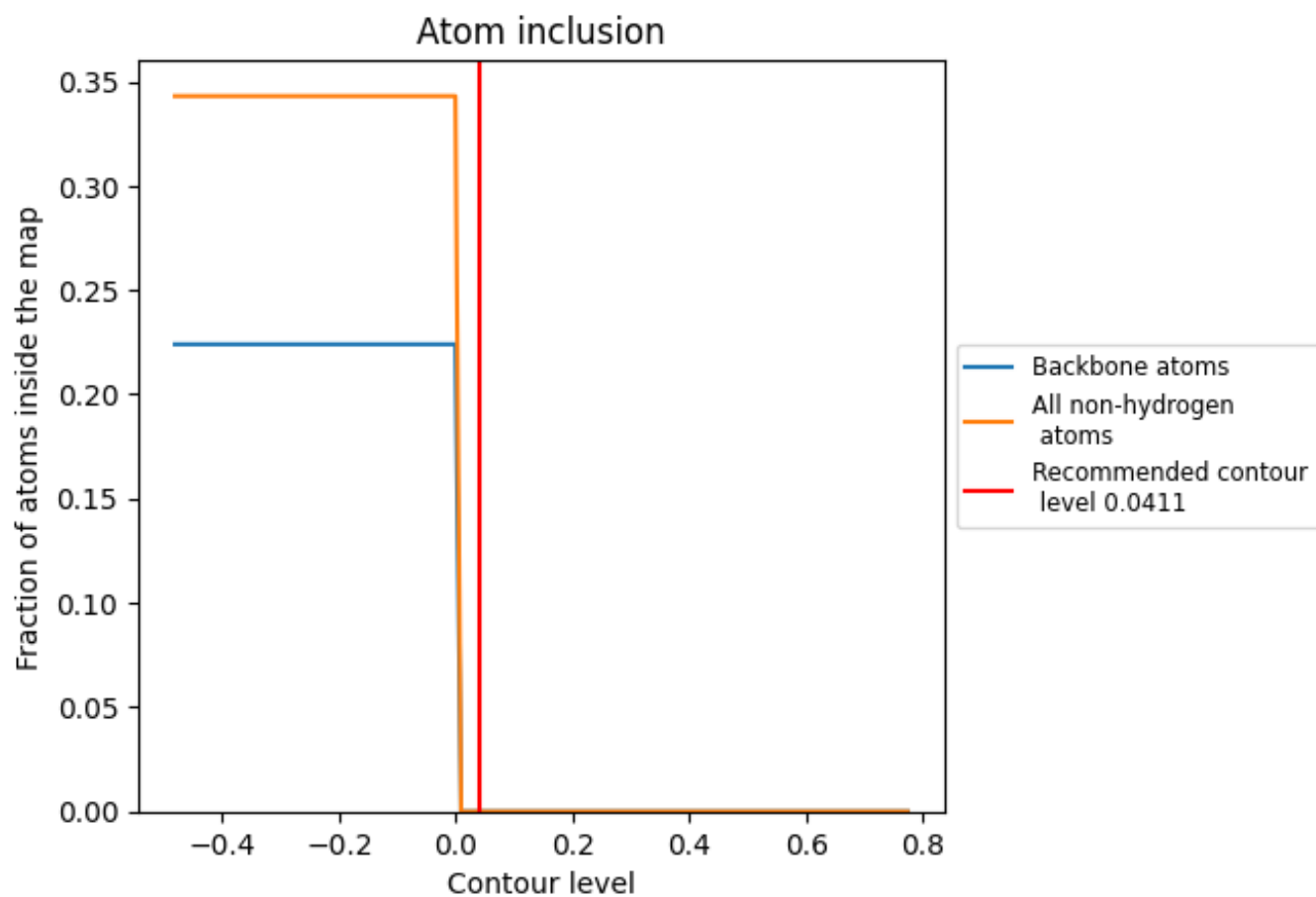
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0411).



















9.4 Atom inclusion [i](#)



At the recommended contour level, 0% of all backbone atoms, 0% 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 (0.0411) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.0000	 -0.0030
A	 0.0000	 0.0040
C	 0.0000	 -0.0060
D	 0.0000	 -0.0060
L	 0.0000	 0.0000
O	 0.0000	 0.0130
P	 0.0000	 -0.0120
Q	 0.0000	 0.0000
R	 0.0000	 -0.0410

