



Full wwPDB EM Validation Report ⓘ

Dec 10, 2022 – 08:15 am GMT

PDB ID : 4CXG
EMDB ID : EMD-2623
Title : Regulation of the mammalian elongation cycle by 40S subunit rolling: a eukaryotic-specific ribosome rearrangement
Authors : Budkevich, T.V.; Giesebrecht, J.; Behrmann, E.; Loerke, J.; Ramrath, D.J.F.; Mielke, T.; Ismer, J.; Hildebrand, P.; Tung, C.-S.; Nierhaus, K.H.; Sanbonmatsu, K.Y.; Spahn, C.M.T.
Deposited on : 2014-04-07
Resolution : 8.70 Å(reported)

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

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

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.dev43
Mogul : 1.8.4, 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) : 2.31.3

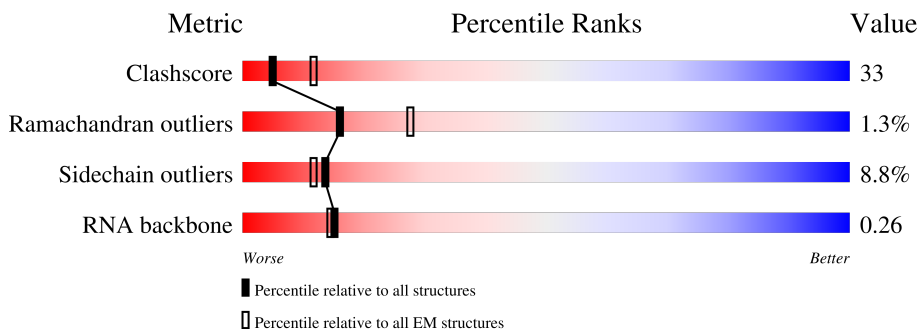
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.70 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	1	135	
2	2	50	
3	A	437	
4	X	143	
5	Y	76	
6	a	48	
7	b	17	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	c	19	
9	x	28	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	2MG	Y	10	-	-	X	-
5	M2G	Y	26	-	-	X	-

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 12269 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 18S RRNA - H44.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	135	2890	1288	527	940	135	0	0

- Molecule 2 is a RNA chain called 28S RRNA - H89.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	50	1057	471	176	360	50	0	0

- Molecule 3 is a protein called ELONGATION FACTOR 1A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	427	3272	2104	570	585	13	0	0

- Molecule 4 is a protein called 40S RIBOSOMAL PROTEIN US12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	X	134	1046	663	205	176	2	0	0

- Molecule 5 is a RNA chain called TRANSFER RNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	P	S		
5	Y	76	1636	737	290	532	76	1	0	0

- Molecule 6 is a RNA chain called 18S RRNA - H5-H14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	a	48	1024	458	192	326	48	0	0

- Molecule 7 is a RNA chain called 18S RRNA - H8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	b	17	363	162	63	121	17	0	0

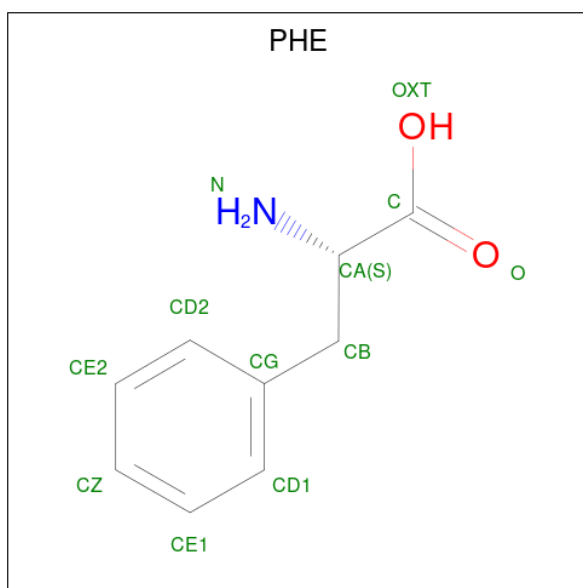
- Molecule 8 is a RNA chain called 28S RRNA - H95.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	c	19	410	183	78	130	19	0	0

- Molecule 9 is a RNA chain called MESSENGER RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
9	x	28	560	252	56	224	28	0	0

- Molecule 10 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).

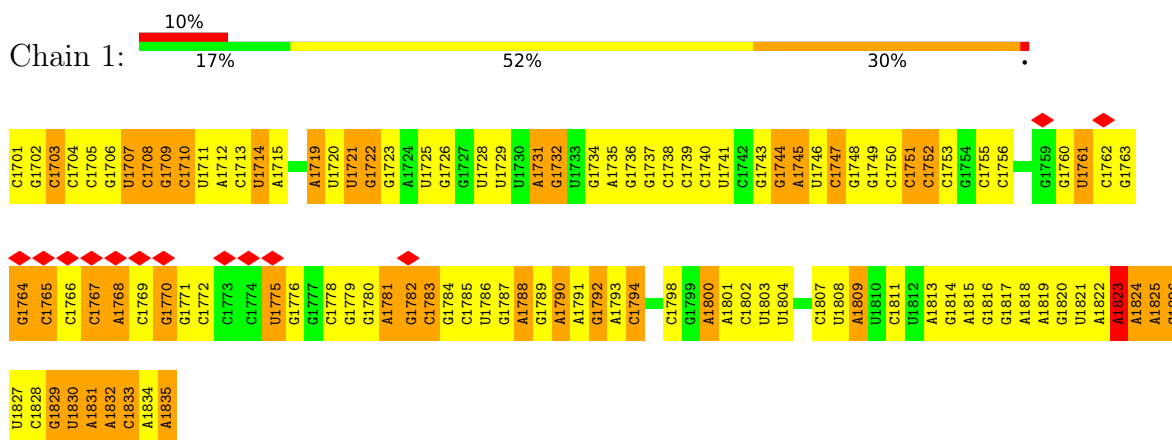


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
10	Y	1	11	9	1	1	0

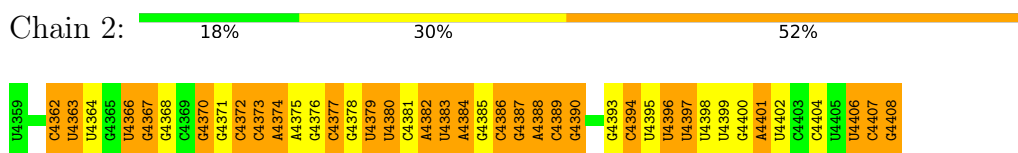
3 Residue-property plots

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.

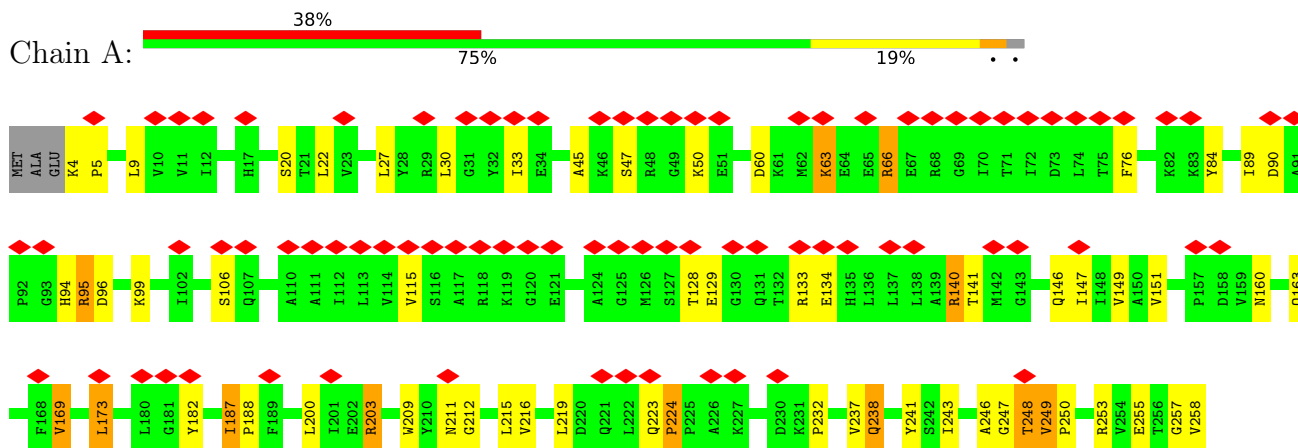
• Molecule 1: 18S RRNA - H44

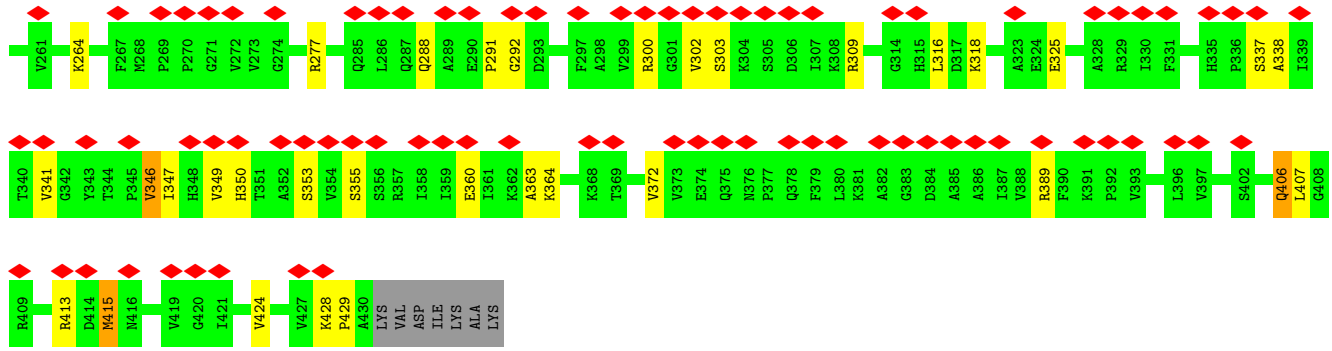


• Molecule 2: 28S RRNA - H89

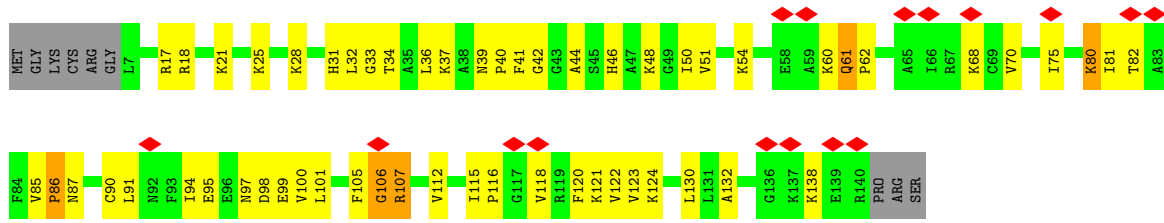


• Molecule 3: ELONGATION FACTOR 1A

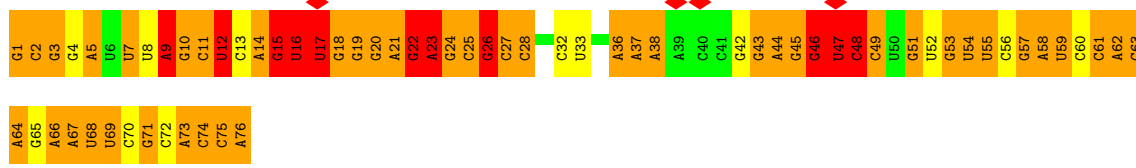




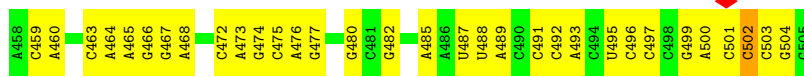
• Molecule 4: 40S RIBOSOMAL PROTEIN US12



• Molecule 5: TRANSFER RNA



• Molecule 6: 18S RRNA - H5-H14

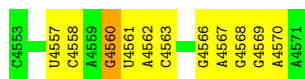


• Molecule 7: 18S RRNA - H8

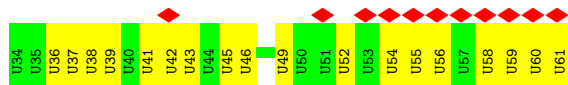


• Molecule 8: 28S RRNA - H95





- Molecule 9: MESSENGER RNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	79705	Depositor
Resolution determination method	Not provided	
CTF correction method	DEFOCUS GROUP	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	65520	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	12.311	Depositor
Minimum map value	-5.352	Depositor
Average map value	0.238	Depositor
Map value standard deviation	0.963	Depositor
Recommended contour level	3.0	Depositor
Map size (\AA)	453.6, 453.6, 453.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.26, 1.26, 1.26	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: M2G, H2U, MIA, OMC, 5MC, PSU, 2MG, 7MG, 5MU, 1MA

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	1	0.33	0/3232	0.77	0/5039
2	2	0.34	0/1177	0.81	0/1831
3	A	0.44	0/3346	0.62	0/4542
4	X	0.46	0/1063	0.70	0/1421
5	Y	0.48	1/1550 (0.1%)	1.94	65/2410 (2.7%)
6	a	0.37	0/1145	0.83	1/1782 (0.1%)
7	b	0.35	0/405	0.78	0/629
8	c	0.35	0/459	0.86	1/714 (0.1%)
9	x	0.42	1/615 (0.2%)	1.25	11/948 (1.2%)
All	All	0.40	2/12992 (0.0%)	1.00	78/19316 (0.4%)

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	1	0	1
5	Y	1	1
9	x	1	0
All	All	2	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	1	G	OP3-P	-5.77	1.54	1.61
9	x	60	U	O3'-P	5.07	1.67	1.61

All (78) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	22	G	O4'-C1'-N9	29.56	131.85	108.20
5	Y	21	A	N9-C1'-C2'	-20.07	87.90	114.00
5	Y	22	G	N9-C1'-C2'	-18.97	89.33	114.00
5	Y	71	G	O4'-C1'-N9	-17.30	94.36	108.20
5	Y	48	C	O4'-C1'-N1	15.16	120.33	108.20
5	Y	18	G	O4'-C1'-N9	14.46	119.77	108.20
5	Y	47	U	N1-C1'-C2'	13.15	131.10	114.00
5	Y	19	G	O5'-P-OP1	-12.69	94.28	105.70
5	Y	47	U	O4'-C1'-N1	12.69	118.35	108.20
9	x	58	U	P-O5'-C5'	12.68	141.18	120.90
5	Y	19	G	N9-C1'-C2'	-12.49	97.77	114.00
5	Y	59	U	O4'-C1'-N1	11.24	117.19	108.20
5	Y	7	U	N1-C1'-C2'	-11.16	99.49	114.00
5	Y	61	C	O4'-C1'-N1	11.03	117.02	108.20
5	Y	3	G	N9-C1'-C2'	-10.69	100.10	114.00
5	Y	23	A	O4'-C1'-N9	10.39	116.52	108.20
9	x	59	U	P-O5'-C5'	10.22	137.25	120.90
5	Y	23	A	N9-C1'-C2'	9.70	126.62	114.00
5	Y	73	A	N9-C1'-C2'	-9.40	101.66	112.00
9	x	58	U	C4'-C3'-O3'	9.33	131.65	113.00
5	Y	66	A	O4'-C1'-N9	-9.24	100.81	108.20
5	Y	56	C	O4'-C1'-N1	-9.13	100.89	108.20
5	Y	18	G	N9-C1'-C2'	-8.86	102.26	112.00
5	Y	36	A	C2'-C3'-O3'	8.83	128.93	109.50
9	x	60	U	C5'-C4'-C3'	8.38	129.40	116.00
5	Y	74	C	O4'-C1'-N1	-8.21	101.64	108.20
5	Y	21	A	C3'-C2'-O2'	-7.92	90.33	113.30
5	Y	5	A	O4'-C1'-N9	7.70	114.36	108.20
5	Y	3	G	O4'-C1'-N9	7.63	114.31	108.20
5	Y	1	G	O4'-C1'-N9	-7.41	102.27	108.20
5	Y	7	U	O4'-C1'-N1	7.29	114.03	108.20
5	Y	63	C	OP1-P-O3'	-7.12	89.53	105.20
5	Y	53	G	O4'-C1'-N9	-7.11	102.51	108.20
5	Y	62	A	O4'-C1'-N9	-7.07	102.54	108.20
5	Y	9	A	O4'-C1'-N9	7.05	113.84	108.20
5	Y	64	A	OP1-P-OP2	7.00	130.10	119.60
5	Y	15	G	O4'-C1'-N9	-6.84	102.73	108.20
5	Y	65	G	O5'-P-OP2	-6.83	99.55	105.70
5	Y	68	U	O4'-C1'-N1	6.78	113.62	108.20
5	Y	22	G	C4'-C3'-O3'	6.77	126.54	113.00
5	Y	69	U	C2'-C3'-O3'	6.71	124.44	113.70
5	Y	21	A	P-O5'-C5'	-6.70	110.19	120.90
5	Y	3	G	O3'-P-O5'	6.69	116.71	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	15	G	N9-C1'-C2'	6.59	122.57	114.00
5	Y	62	A	OP2-P-O3'	6.53	119.57	105.20
5	Y	2	C	OP2-P-O3'	6.49	119.48	105.20
5	Y	75	C	O5'-P-OP1	6.48	118.48	110.70
9	x	60	U	O5'-C5'-C4'	6.48	124.01	111.70
9	x	59	U	O3'-P-O5'	-6.42	91.80	104.00
5	Y	7	U	O5'-P-OP2	6.33	118.29	110.70
5	Y	18	G	OP1-P-O3'	6.31	119.09	105.20
5	Y	20	G	N9-C1'-C2'	-6.30	105.07	112.00
5	Y	63	C	N1-C1'-C2'	-6.17	105.21	112.00
5	Y	64	A	OP2-P-O3'	6.17	118.78	105.20
5	Y	69	U	O5'-P-OP2	6.16	118.10	110.70
5	Y	51	G	N9-C1'-C2'	6.16	122.01	114.00
9	x	59	U	C4'-C3'-O3'	6.15	125.30	113.00
9	x	58	U	O3'-P-O5'	6.14	115.66	104.00
6	a	502	C	C3'-C2'-C1'	-6.07	96.64	101.50
8	c	4560	G	C3'-C2'-C1'	-6.06	96.66	101.50
5	Y	3	G	O5'-P-OP2	-6.04	100.26	105.70
5	Y	24	G	N9-C1'-C2'	-5.97	105.44	112.00
5	Y	61	C	O5'-P-OP1	-5.90	100.39	105.70
5	Y	57	G	O4'-C1'-N9	-5.82	103.55	108.20
5	Y	11	C	N1-C1'-C2'	-5.76	105.66	112.00
5	Y	69	U	O3'-P-O5'	-5.76	93.06	104.00
9	x	60	U	P-O5'-C5'	-5.75	111.70	120.90
5	Y	22	G	O5'-P-OP2	-5.74	100.53	105.70
5	Y	23	A	OP2-P-O3'	5.62	117.58	105.20
9	x	58	U	C2'-C3'-O3'	5.53	122.54	113.70
5	Y	71	G	C2'-C3'-O3'	5.52	122.53	113.70
5	Y	69	U	P-O3'-C3'	-5.51	113.08	119.70
5	Y	70	C	N1-C1'-C2'	-5.51	105.94	112.00
5	Y	52	U	O5'-P-OP2	-5.44	100.80	105.70
5	Y	12	U	O4'-C1'-N1	-5.31	103.95	108.20
5	Y	23	A	O5'-P-OP2	-5.26	100.97	105.70
9	x	58	U	N1-C1'-C2'	5.26	120.83	114.00
5	Y	22	G	OP1-P-O3'	5.21	116.65	105.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	Y	36	A	C3'
9	x	58	U	C3'

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	1823	A	Sidechain
5	Y	33	U	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	1	2890	0	1462	156	0
2	2	1057	0	535	67	0
3	A	3272	0	3292	88	0
4	X	1046	0	1110	48	0
5	Y	1636	0	848	145	0
6	a	1024	0	525	0	0
7	b	363	0	182	0	0
8	c	410	0	207	0	0
9	x	560	0	281	0	0
10	Y	11	0	8	0	0
All	All	12269	0	8450	464	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 33.

All (464) 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)
3:A:249:VAL:CG1	5:Y:76:A:N3	1.70	1.51
3:A:249:VAL:HG11	5:Y:76:A:C2	1.58	1.38
3:A:249:VAL:CG1	5:Y:76:A:C2	2.08	1.37
3:A:243:ILE:O	5:Y:76:A:N6	1.62	1.29
3:A:415:MET:CE	5:Y:51:G:H21	1.46	1.28
3:A:249:VAL:HG11	5:Y:76:A:N3	0.92	1.24
3:A:241:TYR:CG	5:Y:76:A:H4'	1.72	1.22
3:A:247:GLY:H	5:Y:76:A:N6	1.37	1.19
3:A:415:MET:CE	5:Y:51:G:N2	2.05	1.17
3:A:247:GLY:N	5:Y:76:A:N6	1.94	1.12

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:415:MET:HE3	5:Y:51:G:H21	1.05	1.08
3:A:249:VAL:HG12	5:Y:76:A:C2	1.86	1.07
3:A:241:TYR:CD1	5:Y:76:A:H4'	1.90	1.07
1:1:1833:C:H6	1:1:1833:C:H5'	1.18	1.05
1:1:1768:A:H2'	1:1:1769:C:H5'	1.38	1.04
5:Y:45:G:H5'	5:Y:45:G:H8	1.24	1.03
3:A:415:MET:CE	5:Y:64:A:H1'	1.91	1.01
1:1:1750:C:H2'	1:1:1751:C:H5'	1.48	0.95
5:Y:42:G:C2'	5:Y:43:G:H5'	1.97	0.95
1:1:1832:A:H2'	1:1:1833:C:H5''	1.46	0.94
1:1:1766:C:H3'	1:1:1767:C:C5	2.04	0.93
3:A:415:MET:HE1	5:Y:51:G:N2	1.83	0.93
5:Y:27:C:H2'	5:Y:28:C:C6	2.04	0.92
3:A:415:MET:SD	5:Y:64:A:H1'	2.10	0.91
3:A:241:TYR:HB3	5:Y:76:A:O4'	1.70	0.91
3:A:337:SER:HB3	5:Y:53:G:OP1	1.72	0.90
5:Y:42:G:H2'	5:Y:43:G:H5'	1.53	0.89
5:Y:11:C:H2'	5:Y:12:U:H6	1.37	0.89
5:Y:26:M2G:H2'	5:Y:27:C:N1	1.89	0.88
3:A:241:TYR:HB3	5:Y:76:A:C4'	2.03	0.87
1:1:1765:C:H2'	1:1:1766:C:O4'	1.74	0.86
1:1:1768:A:C2'	1:1:1769:C:H5'	2.05	0.86
1:1:1781:A:H1'	1:1:1782:G:OP2	1.76	0.85
3:A:243:ILE:O	5:Y:76:A:C6	2.21	0.85
5:Y:25:C:H2'	5:Y:26:M2G:O4'	1.76	0.85
5:Y:11:C:H2'	5:Y:12:U:C6	2.11	0.85
1:1:1825:A:H2'	1:1:1826:G:H5''	1.59	0.84
1:1:1832:A:C2'	1:1:1833:C:H5''	2.06	0.84
1:1:1775:U:H2'	1:1:1776:G:H8	1.42	0.84
5:Y:15:G:C2'	5:Y:16:H2U:H5'	2.08	0.84
1:1:1833:C:H5'	1:1:1833:C:C6	2.11	0.83
1:1:1766:C:H3'	1:1:1767:C:C6	2.12	0.83
4:X:87:ASN:HB2	4:X:90:CYS:SG	2.19	0.83
3:A:415:MET:HE1	5:Y:64:A:H1'	1.57	0.82
5:Y:23:A:H2'	5:Y:24:G:H8	1.43	0.82
5:Y:13:C:H2'	5:Y:14:A:H8	1.43	0.82
3:A:241:TYR:CB	5:Y:76:A:H4'	2.10	0.81
5:Y:24:G:H2'	5:Y:25:C:H6	1.46	0.81
3:A:415:MET:SD	5:Y:64:A:C1'	2.69	0.80
5:Y:26:M2G:H2'	5:Y:27:C:C6	2.16	0.80
5:Y:23:A:H2'	5:Y:24:G:C8	2.16	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1743:G:H1'	1:1:1792:G:N2	1.97	0.80
1:1:1769:C:H2'	1:1:1770:G:H8	1.47	0.79
3:A:241:TYR:CB	5:Y:76:A:C4'	2.60	0.79
5:Y:26:M2G:H2'	5:Y:27:C:C1'	2.13	0.79
5:Y:27:C:H2'	5:Y:28:C:H6	1.45	0.79
1:1:1769:C:H2'	1:1:1770:G:C8	2.17	0.78
5:Y:25:C:H2'	5:Y:26:M2G:C4'	2.13	0.78
3:A:247:GLY:N	5:Y:76:A:C6	2.51	0.78
3:A:241:TYR:CG	5:Y:76:A:C4'	2.64	0.78
4:X:61:GLN:HB3	4:X:62:PRO:CD	2.13	0.78
5:Y:45:G:H5'	5:Y:45:G:C8	2.16	0.78
3:A:249:VAL:CG1	5:Y:76:A:C4	2.67	0.77
1:1:1833:C:H6	1:1:1833:C:C5'	1.97	0.77
1:1:1787:G:H2'	1:1:1788:A:C8	2.19	0.76
1:1:1725:U:H2'	1:1:1726:G:C8	2.20	0.76
5:Y:15:G:O2'	5:Y:16:H2U:H5'	1.86	0.75
3:A:241:TYR:CD1	5:Y:76:A:C4'	2.69	0.75
3:A:337:SER:CB	5:Y:53:G:OP1	2.34	0.74
1:1:1755:C:H2'	1:1:1756:C:C6	2.21	0.74
1:1:1825:A:O5'	1:1:1825:A:H8	1.70	0.74
2:2:4374:A:H2'	2:2:4382:A:C2	2.21	0.74
3:A:415:MET:SD	5:Y:51:G:N2	2.60	0.74
1:1:1771:G:H2'	1:1:1772:C:C6	2.23	0.73
1:1:1787:G:H2'	1:1:1788:A:H8	1.53	0.73
3:A:241:TYR:CD1	5:Y:76:A:C5'	2.71	0.73
1:1:1807:C:H2'	1:1:1808:U:C6	2.24	0.73
2:2:4374:A:H2'	2:2:4382:A:N1	2.04	0.73
2:2:4399:U:C2'	2:2:4400:G:H5'	2.20	0.72
2:2:4373:C:H3'	2:2:4373:C:O2	1.90	0.72
1:1:1731:A:H2'	1:1:1732:G:C8	2.24	0.71
1:1:1704:C:H1'	1:1:1832:A:N1	2.05	0.71
1:1:1815:A:H3'	1:1:1816:G:H8	1.54	0.71
2:2:4367:G:H2'	2:2:4368:G:H8	1.55	0.71
4:X:51:VAL:HG13	4:X:70:VAL:HG13	1.73	0.71
5:Y:45:G:H8	5:Y:45:G:C5'	2.02	0.71
1:1:1784:G:H2'	1:1:1785:C:C6	2.26	0.70
2:2:4400:G:H2'	2:2:4401:A:C8	2.26	0.70
5:Y:43:G:O3'	5:Y:44:A:O4'	2.09	0.70
1:1:1736:G:H2'	1:1:1737:G:C8	2.27	0.70
2:2:4384:A:N3	2:2:4384:A:H2'	2.08	0.69
1:1:1764:G:N3	1:1:1764:G:H3'	2.07	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1780:G:P	1:1:1781:A:H5''	2.33	0.69
1:1:1814:G:O5'	1:1:1814:G:H8	1.75	0.69
1:1:1721:U:H4'	1:1:1722:G:O5'	1.93	0.69
5:Y:10:2MG:N2	5:Y:26:M2G:H1'	2.08	0.69
1:1:1750:C:C2'	1:1:1751:C:H5'	2.23	0.68
2:2:4399:U:H2'	2:2:4400:G:H5'	1.75	0.68
5:Y:1:G:C2'	5:Y:2:C:H5'	2.23	0.68
5:Y:44:A:O2'	5:Y:45:G:H5'	1.93	0.68
4:X:100:VAL:CG1	4:X:122:VAL:HG13	2.24	0.68
5:Y:42:G:O2'	5:Y:43:G:H5'	1.93	0.68
1:1:1750:C:H2'	1:1:1751:C:C5'	2.23	0.68
5:Y:24:G:H2'	5:Y:25:C:C6	2.29	0.68
1:1:1746:U:H2'	1:1:1747:C:C6	2.30	0.67
2:2:4373:C:H2'	2:2:4374:A:O4'	1.95	0.67
5:Y:1:G:O2'	5:Y:2:C:H5'	1.95	0.67
5:Y:17:H2U:H4'	5:Y:18:G:H5''	1.75	0.67
2:2:4383:U:H3'	2:2:4383:U:H6	1.60	0.66
1:1:1778:C:H2'	1:1:1779:G:C8	2.31	0.66
3:A:20:SER:OG	3:A:90:ASP:OD2	2.13	0.65
1:1:1721:U:H1'	1:1:1722:G:OP2	1.96	0.65
1:1:1743:G:H1'	1:1:1792:G:H22	1.61	0.65
4:X:46:HIS:HB3	4:X:101:LEU:HD11	1.77	0.65
5:Y:19:G:H4'	5:Y:20:G:C4	2.30	0.65
5:Y:25:C:N3	5:Y:26:M2G:C8	2.65	0.65
5:Y:16:H2U:H4'	5:Y:17:H2U:OP2	1.96	0.65
3:A:255:GLU:HB3	3:A:406:GLN:HG3	1.79	0.65
4:X:112:VAL:HB	4:X:115:ILE:HD13	1.78	0.65
3:A:241:TYR:CB	5:Y:76:A:O4'	2.44	0.64
1:1:1767:C:C2'	1:1:1768:A:H5'	2.27	0.64
1:1:1778:C:H2'	1:1:1779:G:H8	1.62	0.64
4:X:51:VAL:HG22	4:X:70:VAL:HG11	1.79	0.63
5:Y:7:U:H4'	5:Y:8:U:OP2	1.97	0.63
1:1:1767:C:O2'	1:1:1768:A:H5'	1.98	0.63
3:A:415:MET:HE3	5:Y:51:G:N2	1.87	0.63
1:1:1734:G:O5'	1:1:1734:G:H8	1.81	0.63
4:X:132:ALA:O	4:X:138:LYS:HB2	1.99	0.63
5:Y:25:C:C2	5:Y:26:M2G:C8	2.86	0.63
1:1:1775:U:H2'	1:1:1776:G:C8	2.30	0.63
1:1:1768:A:H2'	1:1:1769:C:C5'	2.23	0.63
1:1:1825:A:O5'	1:1:1825:A:C8	2.52	0.62
1:1:1832:A:C3'	1:1:1833:C:H5''	2.29	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:TYR:HD1	5:Y:76:A:H5'	1.63	0.62
3:A:415:MET:SD	5:Y:64:A:O4'	2.57	0.62
1:1:1714:U:H3'	1:1:1715:A:C8	2.34	0.62
4:X:61:GLN:HB3	4:X:62:PRO:HD3	1.80	0.62
1:1:1835:A:H2'	1:1:1835:A:N3	2.14	0.62
2:2:4384:A:H5'	2:2:4385:G:OP2	1.99	0.62
5:Y:10:2MG:HM22	5:Y:26:M2G:O2'	2.00	0.62
3:A:169:VAL:HG23	3:A:173:LEU:HD22	1.81	0.62
2:2:4400:G:H2'	2:2:4401:A:H8	1.64	0.62
1:1:1808:U:H2'	1:1:1809:A:C8	2.35	0.61
1:1:1741:U:O4	1:1:1793:A:C2	2.54	0.61
2:2:4383:U:H3'	2:2:4383:U:C6	2.34	0.61
1:1:1820:G:H2'	1:1:1821:U:C6	2.36	0.61
2:2:4377:C:H3'	2:2:4378:G:H8	1.66	0.61
1:1:1714:U:H3'	1:1:1715:A:H8	1.66	0.60
2:2:4387:G:H4'	2:2:4387:G:OP1	2.00	0.60
2:2:4394:C:H2'	2:2:4395:U:O4'	2.02	0.60
5:Y:10:2MG:N2	5:Y:26:M2G:O2'	2.33	0.60
1:1:1751:C:C2'	1:1:1752:C:H5'	2.32	0.60
3:A:203:ARG:NH2	3:A:212:GLY:O	2.30	0.60
4:X:105:PHE:CZ	4:X:121:LYS:HD2	2.37	0.60
5:Y:18:G:OP2	5:Y:58:1MA:HM11	2.02	0.60
1:1:1782:G:N3	1:1:1783:C:N4	2.49	0.59
5:Y:10:2MG:HN2	5:Y:26:M2G:H1'	1.66	0.59
1:1:1771:G:H2'	1:1:1772:C:H6	1.66	0.59
5:Y:26:M2G:C2'	5:Y:27:C:C6	2.85	0.59
3:A:253:ARG:HE	3:A:292:GLY:HA2	1.68	0.59
2:2:4370:G:H2'	2:2:4371:G:H5'	1.83	0.59
2:2:4372:C:H42	2:2:4390:G:H1	1.49	0.58
5:Y:10:2MG:CM2	5:Y:26:M2G:O2'	2.51	0.58
1:1:1784:G:H2'	1:1:1785:C:H6	1.68	0.58
2:2:4363:U:O2'	2:2:4364:U:H5'	2.03	0.58
4:X:41:PHE:HE1	4:X:120:PHE:CE1	2.21	0.58
5:Y:25:C:O2'	5:Y:26:M2G:H5'	2.03	0.58
1:1:1701:C:H4'	1:1:1701:C:OP2	2.02	0.58
1:1:1828:C:H3'	1:1:1829:G:H8	1.68	0.58
2:2:4381:C:C2'	2:2:4382:A:H5'	2.33	0.58
2:2:4384:A:H3'	2:2:4385:G:H8	1.68	0.58
1:1:1800:A:H3'	1:1:1801:A:H8	1.66	0.57
1:1:1800:A:H5''	1:1:1801:A:OP2	2.04	0.57
1:1:1828:C:H3'	1:1:1829:G:C8	2.40	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:4379:U:H2'	2:2:4379:U:O2	2.03	0.57
5:Y:25:C:C4	5:Y:26:M2G:C8	2.92	0.57
1:1:1790:A:C2'	1:1:1791:A:H5'	2.35	0.57
4:X:123:VAL:O	4:X:130:LEU:HG	2.04	0.56
1:1:1802:C:H2'	1:1:1803:U:O4'	2.05	0.56
3:A:63:LYS:NZ	5:Y:74:C:OP1	2.37	0.56
3:A:94:HIS:HD2	3:A:96:ASP:HB2	1.69	0.56
2:2:4406:U:H2'	2:2:4406:U:O2	2.05	0.56
3:A:248:THR:HG21	3:A:302:VAL:O	2.06	0.56
5:Y:43:G:H2'	5:Y:44:A:C4	2.41	0.56
1:1:1746:U:H2'	1:1:1747:C:H6	1.70	0.56
1:1:1783:C:H2'	1:1:1783:C:O2	2.05	0.56
1:1:1830:U:H1'	1:1:1831:A:OP2	2.06	0.56
1:1:1791:A:H2'	1:1:1792:G:O4'	2.06	0.55
1:1:1821:U:H2'	1:1:1822:A:C8	2.41	0.55
3:A:360:GLU:HG2	3:A:389:ARG:HE	1.71	0.55
1:1:1739:C:H6	1:1:1739:C:O5'	1.89	0.55
2:2:4396:U:H4'	2:2:4397:U:OP1	2.05	0.55
4:X:68:LYS:HB2	4:X:85:VAL:HB	1.87	0.55
5:Y:16:H2U:H62	5:Y:16:H2U:O2'	2.02	0.55
1:1:1755:C:H2'	1:1:1756:C:H6	1.67	0.55
5:Y:10:2MG:CM2	5:Y:26:M2G:O3'	2.54	0.55
1:1:1835:A:N3	1:1:1835:A:C2'	2.69	0.54
2:2:4367:G:H2'	2:2:4368:G:C8	2.40	0.54
5:Y:45:G:C8	5:Y:45:G:C5'	2.85	0.54
4:X:32:LEU:HD22	4:X:34:THR:HB	1.89	0.54
2:2:4379:U:O2	2:2:4379:U:C2'	2.55	0.54
1:1:1815:A:H3'	1:1:1816:G:C8	2.40	0.54
2:2:4388:A:H3'	2:2:4389:C:O4'	2.07	0.54
3:A:94:HIS:CD2	3:A:96:ASP:H	2.25	0.54
5:Y:10:2MG:HM21	5:Y:26:M2G:O3'	2.07	0.54
4:X:90:CYS:O	4:X:94:ILE:HG13	2.07	0.54
2:2:4383:U:C6	2:2:4383:U:C3'	2.89	0.53
4:X:61:GLN:HB3	4:X:62:PRO:HD2	1.90	0.53
3:A:95:ARG:HH21	3:A:129:GLU:HB3	1.73	0.53
5:Y:46:7MG:H4'	5:Y:47:U:OP2	2.07	0.53
4:X:39:ASN:OD1	4:X:41:PHE:HB2	2.07	0.53
1:1:1752:C:C2'	1:1:1753:C:H5'	2.39	0.53
3:A:363:ALA:HB1	3:A:372:VAL:HG13	1.90	0.53
3:A:94:HIS:CD2	3:A:96:ASP:HB2	2.43	0.53
4:X:95:GLU:HB2	4:X:98:ASP:OD2	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1825:A:H2'	1:1:1826:G:C5'	2.34	0.53
2:2:4364:U:H2'	2:2:4364:U:O2	2.08	0.53
3:A:337:SER:OG	5:Y:53:G:OP1	2.27	0.53
5:Y:10:2MG:C2	5:Y:26:M2G:O2'	2.61	0.52
2:2:4374:A:C8	2:2:4382:A:C2	2.97	0.52
3:A:94:HIS:HD2	3:A:96:ASP:H	1.55	0.52
4:X:36:LEU:O	4:X:42:GLY:HA2	2.09	0.52
1:1:1714:U:H6	1:1:1714:U:O5'	1.91	0.52
5:Y:9:A:H5'	5:Y:46:7MG:H1'	1.90	0.52
1:1:1822:A:C6	1:1:1823:A:C6	2.97	0.52
5:Y:13:C:C2	5:Y:14:A:C8	2.98	0.52
5:Y:14:A:C2'	5:Y:15:G:H5'	2.40	0.52
5:Y:25:C:C2'	5:Y:26:M2G:H5'	2.40	0.52
1:1:1747:C:H2'	1:1:1748:G:C8	2.44	0.52
4:X:82:THR:OG1	4:X:118:VAL:HG22	2.09	0.52
5:Y:44:A:O2'	5:Y:45:G:C8	2.62	0.52
5:Y:11:C:C6	5:Y:12:U:H5	2.27	0.52
5:Y:11:C:H6	5:Y:11:C:O5'	1.93	0.52
5:Y:14:A:C5	5:Y:22:G:C2	2.98	0.52
1:1:1705:C:H2'	1:1:1706:G:C8	2.45	0.52
1:1:1743:G:H21	1:1:1791:A:H62	1.56	0.52
4:X:32:LEU:C	4:X:34:THR:H	2.14	0.51
1:1:1767:C:C6	1:1:1767:C:H3'	2.46	0.51
2:2:4402:U:O5'	2:2:4402:U:H6	1.92	0.51
1:1:1761:U:H3	1:1:1771:G:H1	1.58	0.51
1:1:1782:G:O4'	1:1:1782:G:P	2.68	0.51
2:2:4387:G:C8	2:2:4387:G:H5''	2.45	0.51
3:A:241:TYR:CD1	5:Y:76:A:H5'	2.40	0.51
4:X:18:ARG:O	4:X:21:LYS:HB3	2.10	0.51
4:X:50:ILE:HG23	4:X:97:ASN:HA	1.92	0.51
5:Y:10:2MG:C6	5:Y:11:C:C4	2.99	0.51
5:Y:37:MIA:H121	5:Y:38:A:N1	2.26	0.51
1:1:1790:A:O2'	1:1:1791:A:H5'	2.11	0.51
3:A:257:GLY:O	3:A:291:PRO:HD3	2.11	0.51
5:Y:66:A:O2'	5:Y:67:A:H5'	2.11	0.51
2:2:4362:C:H5'	2:2:4363:U:OP2	2.11	0.51
2:2:4373:C:O2	2:2:4373:C:C3'	2.58	0.51
3:A:249:VAL:HG13	5:Y:76:A:N3	2.07	0.51
4:X:122:VAL:O	4:X:130:LEU:HD11	2.11	0.50
5:Y:14:A:C6	5:Y:22:G:C2	2.99	0.50
5:Y:25:C:C4	5:Y:26:M2G:N7	2.79	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1814:G:O5'	1:1:1814:G:C8	2.62	0.50
1:1:1818:A:O5'	1:1:1818:A:H8	1.94	0.50
1:1:1823:A:H4'	1:1:1824:A:O5'	2.11	0.50
2:2:4397:U:H2'	2:2:4398:U:H5'	1.93	0.50
5:Y:48:C:N4	5:Y:59:U:C5	2.79	0.50
3:A:146:GLN:NE2	3:A:223:GLN:O	2.42	0.50
4:X:100:VAL:HG11	4:X:122:VAL:HG13	1.94	0.50
2:2:4374:A:C8	2:2:4382:A:N1	2.79	0.50
4:X:54:LYS:HD2	4:X:91:LEU:HD11	1.94	0.50
2:2:4371:G:H2'	2:2:4372:C:C6	2.47	0.50
1:1:1704:C:C1'	1:1:1832:A:N1	2.75	0.49
5:Y:48:C:N4	5:Y:59:U:C4	2.80	0.49
1:1:1709:G:OP2	1:1:1709:G:H8	1.94	0.49
5:Y:11:C:C2	5:Y:12:U:C5	3.00	0.49
1:1:1788:A:N3	1:1:1788:A:H2'	2.27	0.49
4:X:123:VAL:HA	4:X:130:LEU:CD1	2.42	0.49
1:1:1781:A:C4	1:1:1782:G:N2	2.81	0.49
1:1:1704:C:H1'	1:1:1832:A:C6	2.48	0.49
1:1:1707:U:C2'	1:1:1708:C:H5'	2.42	0.49
2:2:4367:G:C4	2:2:4368:G:C8	3.01	0.49
2:2:4399:U:O2'	2:2:4400:G:H5'	2.13	0.49
3:A:232:PRO:HB3	3:A:318:LYS:HD2	1.94	0.49
5:Y:24:G:C5	5:Y:25:C:C5	3.00	0.49
2:2:4386:C:H2'	2:2:4386:C:O2	2.12	0.49
5:Y:24:G:C4	5:Y:25:C:C6	3.01	0.49
2:2:4408:G:H8	2:2:4408:G:H5''	1.78	0.48
5:Y:14:A:C4	5:Y:22:G:N2	2.81	0.48
5:Y:14:A:N3	5:Y:14:A:H2'	2.28	0.48
5:Y:23:A:C2	5:Y:24:G:C5	3.00	0.48
1:1:1731:A:H2'	1:1:1732:G:H8	1.75	0.48
5:Y:10:2MG:C2	5:Y:26:M2G:H1'	2.48	0.48
5:Y:14:A:H2'	5:Y:15:G:H5'	1.95	0.48
5:Y:22:G:C6	5:Y:23:A:N7	2.81	0.48
1:1:1714:U:C3'	1:1:1715:A:H8	2.27	0.48
3:A:347:ILE:O	3:A:353:SER:HA	2.14	0.48
4:X:86:PRO:HB3	4:X:121:LYS:NZ	2.29	0.48
1:1:1762:C:H2'	1:1:1763:G:C8	2.48	0.48
1:1:1769:C:C6	1:1:1769:C:O5'	2.67	0.48
3:A:238:GLN:O	3:A:309:ARG:NE	2.41	0.48
3:A:140:ARG:HG2	3:A:182:TYR:CZ	2.49	0.48
5:Y:26:M2G:H3'	5:Y:27:C:H6	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:14:A:N6	5:Y:22:G:C6	2.82	0.48
4:X:48:LYS:HD3	4:X:99:GLU:OE2	2.14	0.48
4:X:100:VAL:HA	4:X:124:LYS:O	2.12	0.48
5:Y:25:C:H2'	5:Y:26:M2G:C5'	2.43	0.48
5:Y:27:C:O2'	5:Y:28:C:H5'	2.13	0.48
2:2:4371:G:H2'	2:2:4372:C:H6	1.79	0.48
4:X:100:VAL:HG13	4:X:122:VAL:HG13	1.95	0.48
1:1:1825:A:C8	1:1:1825:A:H3'	2.49	0.47
5:Y:59:U:C5	5:Y:60:C:N4	2.82	0.47
3:A:215:LEU:O	3:A:219:LEU:HG	2.14	0.47
4:X:51:VAL:HG13	4:X:70:VAL:CG1	2.43	0.47
1:1:1712:A:H2'	1:1:1713:C:C6	2.50	0.47
1:1:1829:G:C8	1:1:1829:G:O5'	2.68	0.47
1:1:1743:G:O2'	1:1:1744:G:H5'	2.14	0.47
2:2:4393:G:O2'	2:2:4394:C:H5'	2.15	0.47
2:2:4401:A:H8	2:2:4401:A:OP2	1.96	0.47
4:X:25:LYS:O	4:X:28:LYS:HB3	2.14	0.47
1:1:1822:A:N1	1:1:1823:A:C6	2.82	0.47
3:A:277:ARG:NH2	3:A:300:ARG:HG3	2.28	0.47
1:1:1771:G:O2'	1:1:1772:C:H5'	2.14	0.47
1:1:1803:U:H2'	1:1:1804:U:C6	2.50	0.47
1:1:1824:A:N3	1:1:1824:A:H5''	2.29	0.47
2:2:4398:U:H6	2:2:4398:U:OP2	1.98	0.47
2:2:4407:C:O2'	2:2:4408:G:P	2.73	0.47
1:1:1751:C:H2'	1:1:1752:C:H5'	1.96	0.47
3:A:140:ARG:HG2	3:A:182:TYR:CE2	2.50	0.47
4:X:106:GLY:O	4:X:107:ARG:O	2.33	0.47
1:1:1767:C:H3'	1:1:1767:C:H6	1.80	0.47
2:2:4393:G:H2'	2:2:4394:C:C6	2.50	0.46
5:Y:18:G:O6	5:Y:55:PSU:H1'	2.15	0.46
1:1:1752:C:O2'	1:1:1753:C:H5'	2.15	0.46
2:2:4374:A:H2'	2:2:4382:A:C6	2.49	0.46
5:Y:26:M2G:H3'	5:Y:27:C:C6	2.50	0.46
1:1:1767:C:C6	1:1:1767:C:C3'	2.99	0.46
3:A:187:ILE:HA	3:A:188:PRO:HD3	1.73	0.46
2:2:4388:A:H3'	2:2:4389:C:C5'	2.46	0.46
1:1:1778:C:H6	1:1:1778:C:O5'	1.99	0.46
2:2:4383:U:H6	2:2:4383:U:C3'	2.27	0.46
4:X:61:GLN:CB	4:X:62:PRO:CD	2.89	0.46
1:1:1766:C:H2'	1:1:1766:C:O2	2.15	0.46
1:1:1780:G:OP2	1:1:1781:A:C8	2.69	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:98:ASP:O	4:X:100:VAL:HG23	2.16	0.46
5:Y:24:G:C6	5:Y:25:C:C4	3.04	0.46
1:1:1704:C:O5'	1:1:1704:C:H6	1.98	0.46
1:1:1709:G:H2'	1:1:1710:C:H5''	1.97	0.46
3:A:246:ALA:C	5:Y:76:A:C6	2.75	0.46
5:Y:22:G:N1	5:Y:23:A:N7	2.64	0.46
5:Y:58:1MA:HM12	5:Y:61:C:H1'	1.97	0.46
1:1:1738:C:H6	1:1:1738:C:O5'	1.99	0.45
4:X:68:LYS:CB	4:X:85:VAL:HB	2.45	0.45
1:1:1782:G:C2	1:1:1783:C:N4	2.84	0.45
1:1:1808:U:H6	1:1:1808:U:O5'	1.99	0.45
2:2:4388:A:C8	2:2:4388:A:H5''	2.51	0.45
1:1:1781:A:HO2'	1:1:1782:G:P	2.38	0.45
3:A:60:ASP:O	3:A:66:ARG:HD3	2.15	0.45
5:Y:15:G:H2'	5:Y:16:H2U:H5'	1.92	0.45
2:2:4381:C:C3'	2:2:4382:A:H5'	2.47	0.45
2:2:4388:A:H3'	2:2:4389:C:C4'	2.47	0.45
4:X:41:PHE:HB3	4:X:44:ALA:HB3	1.99	0.45
5:Y:44:A:O2'	5:Y:45:G:H8	1.99	0.45
5:Y:59:U:C2'	5:Y:60:C:H5'	2.47	0.45
1:1:1750:C:C6	1:1:1750:C:O5'	2.70	0.45
5:Y:71:G:C2'	5:Y:72:C:H5'	2.47	0.45
1:1:1747:C:H2'	1:1:1748:G:H8	1.82	0.44
1:1:1815:A:O5'	1:1:1815:A:H8	2.01	0.44
2:2:4397:U:H4'	2:2:4397:U:OP2	2.17	0.44
3:A:216:VAL:HA	3:A:219:LEU:HD12	1.99	0.44
5:Y:14:A:C6	5:Y:22:G:N1	2.85	0.44
5:Y:25:C:C2'	5:Y:26:M2G:C5'	2.95	0.44
5:Y:59:U:O2'	5:Y:60:C:H5'	2.16	0.44
2:2:4366:U:C2'	2:2:4367:G:H5'	2.47	0.44
1:1:1745:A:H3'	1:1:1745:A:N3	2.32	0.44
5:Y:28:C:C6	5:Y:28:C:OP2	2.70	0.44
1:1:1721:U:C4'	1:1:1722:G:O5'	2.64	0.44
5:Y:44:A:C8	5:Y:44:A:OP2	2.70	0.44
1:1:1794:C:H6	1:1:1794:C:O5'	2.00	0.44
5:Y:62:A:C2'	5:Y:63:C:H5'	2.47	0.44
3:A:200:LEU:O	3:A:216:VAL:HG23	2.18	0.44
3:A:325:GLU:OE2	3:A:389:ARG:HD2	2.17	0.44
5:Y:17:H2U:C4'	5:Y:18:G:H5''	2.43	0.44
1:1:1762:C:H2'	1:1:1763:G:H8	1.82	0.44
2:2:4377:C:C6	2:2:4377:C:C5'	3.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:32:LEU:O	4:X:34:THR:N	2.51	0.44
1:1:1829:G:H8	1:1:1829:G:O5'	2.01	0.44
1:1:1831:A:C2'	1:1:1832:A:H5'	2.48	0.44
3:A:341:VAL:HG22	3:A:360:GLU:HA	1.99	0.44
1:1:1833:C:C6	1:1:1833:C:C5'	2.85	0.43
3:A:84:TYR:HE1	3:A:224:PRO:HG3	1.83	0.43
5:Y:13:C:C2	5:Y:14:A:N7	2.86	0.43
1:1:1739:C:O5'	1:1:1739:C:C6	2.70	0.43
1:1:1766:C:H5'	1:1:1767:C:OP2	2.18	0.43
1:1:1769:C:O5'	1:1:1769:C:H6	2.00	0.43
3:A:45:ALA:HB1	3:A:50:LYS:O	2.19	0.43
4:X:87:ASN:HB2	4:X:90:CYS:HG	1.81	0.43
5:Y:62:A:H2'	5:Y:63:C:O4'	2.18	0.43
1:1:1765:C:H2'	1:1:1766:C:C1'	2.46	0.43
1:1:1830:U:C6	1:1:1830:U:O5'	2.71	0.43
3:A:163:GLN:HB2	3:A:209:TRP:CD2	2.53	0.43
5:Y:8:U:O2	5:Y:15:G:O6	2.36	0.43
3:A:346:VAL:HA	3:A:355:SER:HA	2.01	0.43
2:2:4377:C:H5''	2:2:4377:C:H6	1.83	0.43
3:A:76:PHE:CD2	3:A:89:ILE:HG12	2.53	0.43
4:X:123:VAL:HA	4:X:130:LEU:HD12	2.00	0.43
1:1:1781:A:O2'	1:1:1782:G:P	2.76	0.43
3:A:337:SER:OG	3:A:338:ALA:N	2.51	0.43
1:1:1748:G:H1	1:1:1786:U:H3	1.67	0.43
2:2:4384:A:H3'	2:2:4385:G:C8	2.53	0.43
2:2:4401:A:C8	2:2:4401:A:OP2	2.71	0.43
1:1:1719:A:O5'	1:1:1719:A:H8	2.02	0.43
3:A:115:VAL:HG13	3:A:151:VAL:HA	2.00	0.43
3:A:163:GLN:HB2	3:A:209:TRP:CE2	2.54	0.43
4:X:60:LYS:O	4:X:61:GLN:HB2	2.19	0.43
1:1:1703:C:H3'	1:1:1704:C:C5	2.54	0.43
1:1:1739:C:H2'	1:1:1740:C:O4'	2.19	0.43
4:X:32:LEU:CD2	4:X:34:THR:HB	2.49	0.43
1:1:1703:C:C4	1:1:1704:C:C4	3.06	0.42
3:A:4:LYS:HA	3:A:5:PRO:HD3	1.90	0.42
4:X:80:LYS:H	4:X:80:LYS:HG3	1.71	0.42
3:A:264:LYS:HE3	3:A:264:LYS:HB2	1.71	0.42
2:2:4396:U:P	2:2:4396:U:H6	2.43	0.42
2:2:4399:U:H2'	2:2:4400:G:C5'	2.45	0.42
3:A:264:LYS:HG2	3:A:316:LEU:HD21	2.00	0.42
1:1:1829:G:C4	1:1:1830:U:H5	2.37	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:187:ILE:O	3:A:187:ILE:HG12	2.18	0.42
1:1:1746:U:H6	1:1:1746:U:O5'	2.02	0.42
1:1:1766:C:C5	1:1:1767:C:N4	2.88	0.42
1:1:1782:G:H1'	1:1:1783:C:C5	2.54	0.42
1:1:1782:G:O2'	1:1:1783:C:C6	2.68	0.42
3:A:134:GLU:OE2	3:A:413:ARG:NH2	2.50	0.42
1:1:1822:A:C3'	1:1:1823:A:H5''	2.50	0.42
1:1:1829:G:H2'	1:1:1829:G:N3	2.35	0.41
3:A:169:VAL:O	3:A:173:LEU:HB2	2.19	0.41
5:Y:53:G:H2'	5:Y:54:5MU:O4'	2.20	0.41
1:1:1764:G:N3	1:1:1764:G:C3'	2.80	0.41
3:A:428:LYS:HA	3:A:429:PRO:HD3	1.91	0.41
2:2:4395:U:H3'	2:2:4396:U:C5	2.55	0.41
1:1:1711:U:H2'	1:1:1712:A:C8	2.55	0.41
4:X:39:ASN:HB2	4:X:40:PRO:HD2	2.02	0.41
5:Y:8:U:H5'	5:Y:49:5MC:OP2	2.20	0.41
3:A:223:GLN:HA	3:A:224:PRO:HD3	1.92	0.41
4:X:41:PHE:HE1	4:X:120:PHE:CD1	2.38	0.41
5:Y:26:M2G:C2'	5:Y:27:C:C1'	2.94	0.41
1:1:1745:A:C2	1:1:1746:U:C5	3.08	0.41
1:1:1790:A:H2'	1:1:1791:A:H5'	2.03	0.41
3:A:349:VAL:HG22	3:A:350:HIS:CD2	2.55	0.41
4:X:132:ALA:HA	4:X:138:LYS:HG3	2.03	0.41
1:1:1731:A:C6	1:1:1732:G:C6	3.09	0.41
1:1:1743:G:C2'	1:1:1744:G:H5'	2.51	0.41
2:2:4397:U:C6	2:2:4397:U:H5'	2.56	0.41
5:Y:11:C:H2'	5:Y:12:U:C5	2.50	0.41
3:A:27:LEU:HB3	3:A:33:ILE:HD13	2.02	0.41
5:Y:60:C:H6	5:Y:60:C:H2'	1.50	0.41
2:2:4380:U:OP2	2:2:4381:C:C5	2.74	0.40
3:A:277:ARG:HH21	3:A:300:ARG:HG3	1.86	0.40
1:1:1721:U:H4'	1:1:1721:U:OP1	2.21	0.40
1:1:1781:A:C2	1:1:1782:G:N2	2.89	0.40
2:2:4381:C:H2'	2:2:4382:A:H5'	2.03	0.40
5:Y:14:A:C5	5:Y:22:G:N2	2.89	0.40
5:Y:44:A:O4'	5:Y:44:A:P	2.79	0.40
2:2:4377:C:H3'	2:2:4378:G:C8	2.51	0.40
2:2:4406:U:O2	2:2:4406:U:C2'	2.70	0.40
3:A:249:VAL:HA	3:A:250:PRO:HD2	1.84	0.40
4:X:86:PRO:HB3	4:X:121:LYS:HZ2	1.86	0.40
1:1:1787:G:C2'	1:1:1788:A:H8	2.27	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:1825:A:C8	1:1:1825:A:C3'	3.03	0.40
5:Y:24:G:H2'	5:Y:25:C:O5'	2.22	0.40
5:Y:43:G:C5'	5:Y:44:A:OP1	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	425/437 (97%)	413 (97%)	12 (3%)	0	100	100
4	X	132/143 (92%)	120 (91%)	5 (4%)	7 (5%)	2	19
All	All	557/580 (96%)	533 (96%)	17 (3%)	7 (1%)	16	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	X	61	GLN
4	X	106	GLY
4	X	107	ARG
4	X	116	PRO
4	X	33	GLY
4	X	86	PRO
4	X	75	ILE

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	A	344/372 (92%)	309 (90%)	35 (10%)	7	25
4	X	108/115 (94%)	103 (95%)	5 (5%)	27	52
All	All	452/487 (93%)	412 (91%)	40 (9%)	13	31

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	9	LEU
3	A	22	LEU
3	A	30	LEU
3	A	47	SER
3	A	63	LYS
3	A	66	ARG
3	A	95	ARG
3	A	99	LYS
3	A	106	SER
3	A	128	THR
3	A	133	ARG
3	A	140	ARG
3	A	141	THR
3	A	147	ILE
3	A	149	VAL
3	A	160	ASN
3	A	169	VAL
3	A	173	LEU
3	A	187	ILE
3	A	203	ARG
3	A	211	ASN
3	A	224	PRO
3	A	237	VAL
3	A	238	GLN
3	A	248	THR
3	A	249	VAL
3	A	258	VAL
3	A	288	GLN
3	A	303	SER
3	A	346	VAL
3	A	364	LYS
3	A	406	GLN
3	A	407	LEU
3	A	415	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	424	VAL
4	X	17	ARG
4	X	31	HIS
4	X	37	LYS
4	X	80	LYS
4	X	81	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	94	HIS
3	A	287	GLN
3	A	315	HIS
3	A	348	HIS
4	X	31	HIS
4	X	61	GLN
4	X	73	GLN
4	X	77	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	134/135 (99%)	57 (42%)	7 (5%)
2	2	49/50 (98%)	28 (57%)	4 (8%)
5	Y	74/76 (97%)	29 (39%)	7 (9%)
6	a	47/48 (97%)	32 (68%)	0
7	b	16/17 (94%)	10 (62%)	0
8	c	18/19 (94%)	11 (61%)	0
9	x	27/28 (96%)	15 (55%)	0
All	All	365/373 (97%)	182 (49%)	18 (4%)

All (182) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	1702	G
1	1	1703	C
1	1	1707	U
1	1	1708	C
1	1	1709	G
1	1	1710	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1714	U
1	1	1719	A
1	1	1720	U
1	1	1721	U
1	1	1722	G
1	1	1723	G
1	1	1728	U
1	1	1729	U
1	1	1731	A
1	1	1732	G
1	1	1735	A
1	1	1744	G
1	1	1745	A
1	1	1747	C
1	1	1749	G
1	1	1751	C
1	1	1752	C
1	1	1760	G
1	1	1761	U
1	1	1764	G
1	1	1765	C
1	1	1767	C
1	1	1768	A
1	1	1770	G
1	1	1775	U
1	1	1781	A
1	1	1782	G
1	1	1783	C
1	1	1788	A
1	1	1789	G
1	1	1790	A
1	1	1792	G
1	1	1794	C
1	1	1798	C
1	1	1800	A
1	1	1809	A
1	1	1811	C
1	1	1813	A
1	1	1817	G
1	1	1819	A
1	1	1823	A
1	1	1824	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	1	1825	A
1	1	1826	G
1	1	1827	U
1	1	1829	G
1	1	1831	A
1	1	1832	A
1	1	1833	C
1	1	1834	A
1	1	1835	A
2	2	4362	C
2	2	4363	U
2	2	4366	U
2	2	4367	G
2	2	4370	G
2	2	4372	C
2	2	4373	C
2	2	4375	A
2	2	4376	G
2	2	4377	C
2	2	4379	U
2	2	4380	U
2	2	4382	A
2	2	4383	U
2	2	4384	A
2	2	4386	C
2	2	4387	G
2	2	4388	A
2	2	4389	C
2	2	4390	G
2	2	4394	C
2	2	4396	U
2	2	4397	U
2	2	4401	A
2	2	4404	C
2	2	4406	U
2	2	4407	C
2	2	4408	G
5	Y	4	G
5	Y	5	A
5	Y	9	A
5	Y	12	U
5	Y	14	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	Y	15	G
5	Y	16	H2U
5	Y	17	H2U
5	Y	21	A
5	Y	22	G
5	Y	23	A
5	Y	25	C
5	Y	27	C
5	Y	28	C
5	Y	36	A
5	Y	38	A
5	Y	43	G
5	Y	44	A
5	Y	45	G
5	Y	46	7MG
5	Y	47	U
5	Y	48	C
5	Y	57	G
5	Y	67	A
5	Y	68	U
5	Y	69	U
5	Y	73	A
5	Y	75	C
5	Y	76	A
6	a	459	C
6	a	460	A
6	a	463	C
6	a	464	A
6	a	465	A
6	a	466	G
6	a	467	G
6	a	468	A
6	a	472	C
6	a	473	A
6	a	474	G
6	a	475	C
6	a	476	A
6	a	477	G
6	a	480	G
6	a	482	G
6	a	485	A
6	a	487	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	a	488	U
6	a	489	A
6	a	491	C
6	a	492	C
6	a	493	A
6	a	495	U
6	a	496	C
6	a	497	C
6	a	499	G
6	a	500	A
6	a	501	C
6	a	502	C
6	a	503	C
6	a	504	G
7	b	152	U
7	b	153	G
7	b	158	A
7	b	160	U
7	b	161	U
7	b	162	C
7	b	163	U
7	b	164	A
7	b	166	A
7	b	167	G
8	c	4557	U
8	c	4558	C
8	c	4560	G
8	c	4561	U
8	c	4562	A
8	c	4563	C
8	c	4566	G
8	c	4567	A
8	c	4568	G
8	c	4569	G
8	c	4570	A
9	x	36	U
9	x	37	U
9	x	38	U
9	x	39	U
9	x	41	U
9	x	42	U
9	x	43	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	x	45	U
9	x	46	U
9	x	49	U
9	x	52	U
9	x	54	U
9	x	55	U
9	x	56	U
9	x	61	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1721	U
1	1	1781	A
1	1	1823	A
1	1	1824	A
1	1	1830	U
1	1	1833	C
1	1	1834	A
2	2	4374	A
2	2	4387	G
2	2	4388	A
2	2	4396	U
5	Y	3	G
5	Y	16	H2U
5	Y	21	A
5	Y	22	G
5	Y	26	M2G
5	Y	45	G
5	Y	46	7MG

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

11 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
5	5MC	Y	49	5	18,22,23	0.55	1 (5%)	26,32,35	1.70	4 (15%)
5	PSU	Y	55	5	18,21,22	0.75	0	22,30,33	0.97	1 (4%)
5	1MA	Y	58	5	16,25,26	1.40	2 (12%)	18,37,40	1.09	2 (11%)
5	M2G	Y	26	5	20,27,28	1.32	3 (15%)	22,40,43	1.13	2 (9%)
5	MIA	Y	37	5	24,31,32	1.01	2 (8%)	26,44,47	1.73	4 (15%)
5	2MG	Y	10	5	18,26,27	1.02	2 (11%)	16,38,41	1.12	2 (12%)
5	OMC	Y	32	5	19,22,23	0.34	0	26,31,34	0.64	1 (3%)
5	H2U	Y	17	5	18,21,22	0.70	1 (5%)	21,30,33	2.02	5 (23%)
5	7MG	Y	46	5	22,26,27	3.47	3 (13%)	29,39,42	1.94	6 (20%)
5	5MU	Y	54	5	19,22,23	4.45	1 (5%)	28,32,35	3.51	5 (17%)
5	H2U	Y	16	5	18,21,22	0.72	0	21,30,33	2.09	4 (19%)

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
5	5MC	Y	49	5	-	0/7/25/26	0/2/2/2
5	PSU	Y	55	5	-	2/7/25/26	0/2/2/2
5	1MA	Y	58	5	-	2/3/25/26	0/3/3/3
5	M2G	Y	26	5	-	2/7/29/30	0/3/3/3
5	MIA	Y	37	5	-	3/11/33/34	0/3/3/3
5	2MG	Y	10	5	-	2/5/27/28	0/3/3/3
5	OMC	Y	32	5	-	0/9/27/28	0/2/2/2
5	H2U	Y	17	5	-	6/7/38/39	0/2/2/2
5	7MG	Y	46	5	-	2/7/37/38	0/3/3/3
5	5MU	Y	54	5	-	0/7/25/26	0/2/2/2
5	H2U	Y	16	5	-	6/7/38/39	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	54	5MU	C5M-C5	-19.32	1.02	1.50
5	Y	46	7MG	C8-N9	-15.42	1.37	1.46
5	Y	46	7MG	CM7-N7	3.60	1.58	1.45
5	Y	58	1MA	C2-N3	3.58	1.33	1.29
5	Y	46	7MG	C5-N7	3.29	1.39	1.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Y	26	M2G	O4'-C1'	2.82	1.45	1.41
5	Y	26	M2G	C2-N2	2.81	1.40	1.35
5	Y	58	1MA	C6-N6	2.72	1.34	1.27
5	Y	10	2MG	C8-N7	-2.42	1.30	1.35
5	Y	26	M2G	C5-C6	-2.36	1.42	1.47
5	Y	10	2MG	C5-C6	-2.31	1.42	1.47
5	Y	17	H2U	C2-N1	2.25	1.38	1.35
5	Y	37	MIA	C2-S10	2.04	1.77	1.75
5	Y	49	5MC	CM5-C5	-2.03	1.45	1.50
5	Y	37	MIA	C8-N7	-2.00	1.31	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	54	5MU	C5M-C5-C4	12.63	132.67	118.77
5	Y	54	5MU	C5M-C5-C6	-11.43	107.58	122.85
5	Y	49	5MC	CM5-C5-C6	7.10	132.33	122.85
5	Y	17	H2U	C4-N3-C2	-6.88	120.08	125.79
5	Y	46	7MG	N9-C8-N7	6.71	112.97	103.38
5	Y	54	5MU	O2'-C2'-C3'	-5.68	93.45	111.82
5	Y	16	H2U	O4'-C1'-N1	5.11	116.25	109.30
5	Y	37	MIA	C11-S10-C2	4.82	105.87	102.27
5	Y	16	H2U	C4-N3-C2	-4.60	121.97	125.79
5	Y	16	H2U	O2-C2-N1	-4.59	117.34	123.11
5	Y	46	7MG	O4'-C1'-N9	4.29	115.14	109.30
5	Y	37	MIA	C5-C6-N1	-4.13	117.38	120.81
5	Y	37	MIA	C12-N6-C6	3.89	128.30	122.55
5	Y	46	7MG	C4-C5-N7	3.59	110.52	105.53
5	Y	37	MIA	C2-N3-C4	-3.31	110.76	115.32
5	Y	17	H2U	N3-C2-N1	3.30	120.14	116.65
5	Y	54	5MU	O4'-C1'-N1	-3.04	101.42	108.36
5	Y	26	M2G	C2'-C3'-C4'	2.97	108.42	102.64
5	Y	17	H2U	O2-C2-N1	-2.94	119.42	123.11
5	Y	46	7MG	O3'-C3'-C4'	2.72	118.93	111.05
5	Y	58	1MA	N1-C2-N3	2.69	129.16	126.02
5	Y	17	H2U	O3'-C3'-C4'	-2.59	103.55	111.05
5	Y	16	H2U	O4-C4-C5	-2.53	116.76	122.17
5	Y	46	7MG	O3'-C3'-C2'	-2.49	103.76	111.82
5	Y	58	1MA	C5-C6-N1	2.48	117.59	113.90
5	Y	10	2MG	CM2-N2-C2	-2.46	118.42	123.86
5	Y	49	5MC	C5-C6-N1	-2.45	120.82	123.34
5	Y	46	7MG	O2'-C2'-C1'	2.43	118.13	110.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	32	OMC	CM2-O2'-C2'	-2.34	108.39	114.52
5	Y	26	M2G	C8-N7-C5	2.28	107.34	102.99
5	Y	55	PSU	C6-C5-C4	2.27	119.78	118.20
5	Y	10	2MG	O6-C6-C5	2.18	128.64	124.37
5	Y	49	5MC	O3'-C3'-C4'	2.12	117.19	111.05
5	Y	17	H2U	O4-C4-C5	-2.11	117.67	122.17
5	Y	54	5MU	C6-C5-C4	2.05	119.75	118.03
5	Y	49	5MC	O2'-C2'-C3'	2.03	118.39	111.82

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	Y	16	H2U	O4'-C1'-N1-C6
5	Y	16	H2U	C2'-C1'-N1-C2
5	Y	17	H2U	O4'-C4'-C5'-O5'
5	Y	17	H2U	C3'-C4'-C5'-O5'
5	Y	37	MIA	C5-C6-N6-C12
5	Y	46	7MG	O4'-C4'-C5'-O5'
5	Y	46	7MG	C3'-C4'-C5'-O5'
5	Y	16	H2U	O4'-C4'-C5'-O5'
5	Y	16	H2U	C3'-C4'-C5'-O5'
5	Y	26	M2G	O4'-C4'-C5'-O5'
5	Y	58	1MA	O4'-C4'-C5'-O5'
5	Y	58	1MA	C3'-C4'-C5'-O5'
5	Y	17	H2U	C2'-C1'-N1-C6
5	Y	37	MIA	N1-C6-N6-C12
5	Y	16	H2U	C2'-C1'-N1-C6
5	Y	10	2MG	C3'-C4'-C5'-O5'
5	Y	10	2MG	O4'-C4'-C5'-O5'
5	Y	17	H2U	O4'-C1'-N1-C2
5	Y	17	H2U	C4'-C5'-O5'-P
5	Y	17	H2U	C2'-C1'-N1-C2
5	Y	37	MIA	N6-C12-C13-C14
5	Y	55	PSU	O4'-C1'-C5-C4
5	Y	26	M2G	C3'-C4'-C5'-O5'
5	Y	55	PSU	O4'-C1'-C5-C6
5	Y	16	H2U	O4'-C1'-N1-C2

There are no ring outliers.

10 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	Y	49	5MC	1	0
5	Y	55	PSU	1	0
5	Y	58	1MA	2	0
5	Y	26	M2G	26	0
5	Y	37	MIA	1	0
5	Y	10	2MG	10	0
5	Y	17	H2U	3	0
5	Y	46	7MG	2	0
5	Y	54	5MU	1	0
5	Y	16	H2U	5	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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
10	PHE	Y	77	5	10,11,12	1.11	1 (10%)	10,13,15	2.49	2 (20%)

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
10	PHE	Y	77	5	-	0/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	Y	77	PHE	CA-N	-3.02	1.39	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	Y	77	PHE	CG-CB-CA	-5.52	102.92	114.10
10	Y	77	PHE	CB-CA-C	-5.51	101.14	111.47

There are no chirality outliers.

There are no torsion outliers.

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.

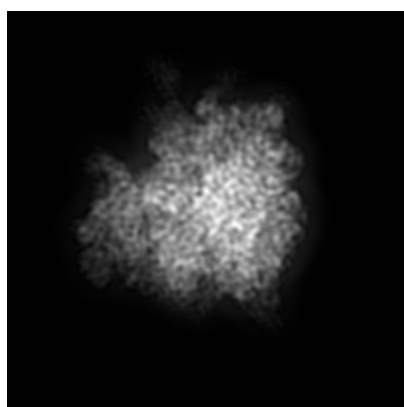
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2623. These allow visual inspection of the internal detail of the map and identification of artifacts.

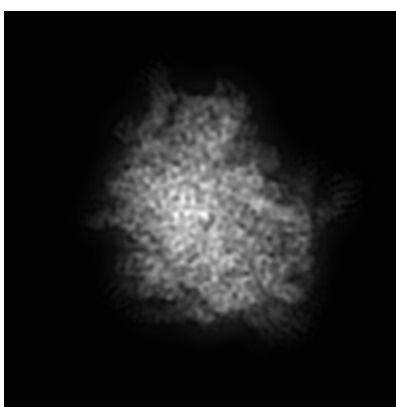
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

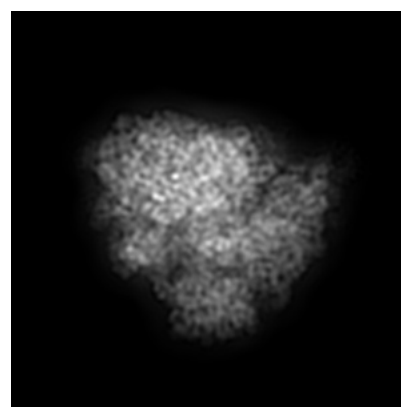
6.1.1 Primary map



X



Y

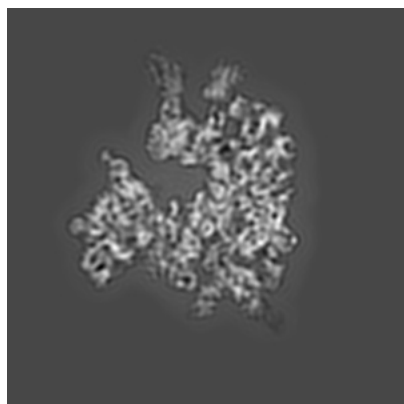


Z

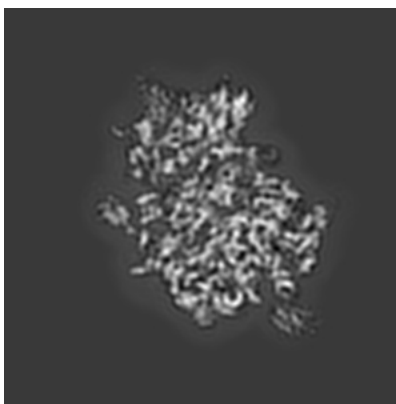
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

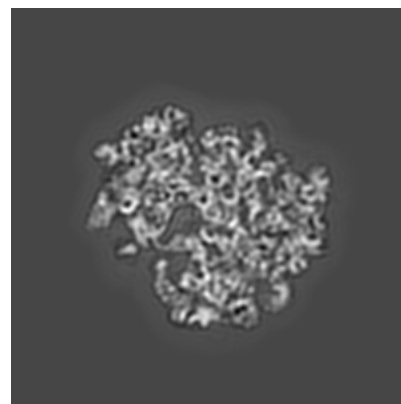
6.2.1 Primary map



X Index: 180



Y Index: 180

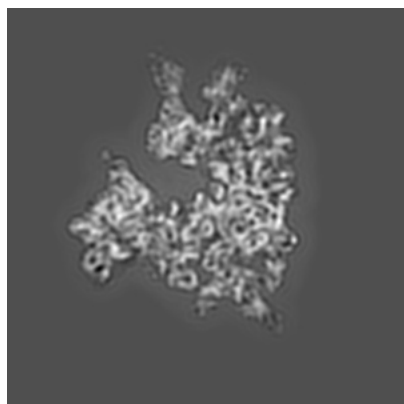


Z Index: 180

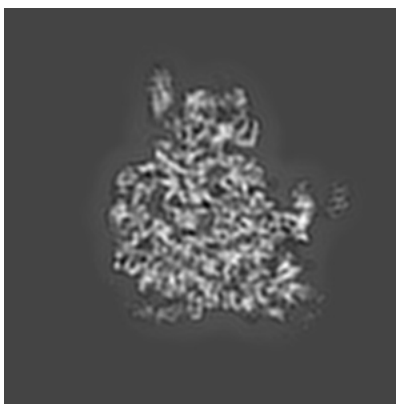
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

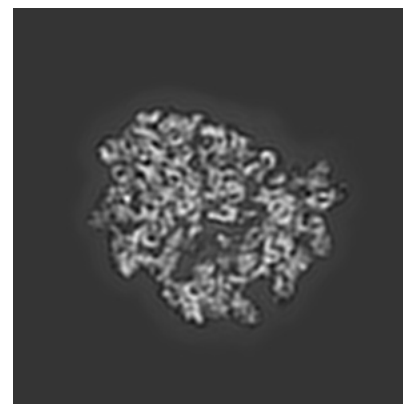
6.3.1 Primary map



X Index: 178



Y Index: 206



Z Index: 189

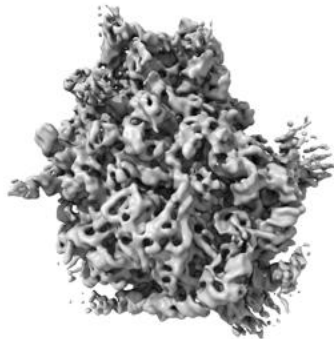
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

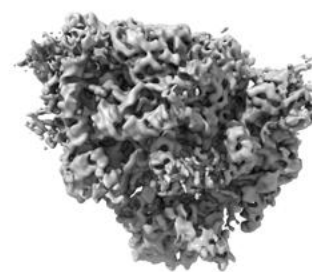
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

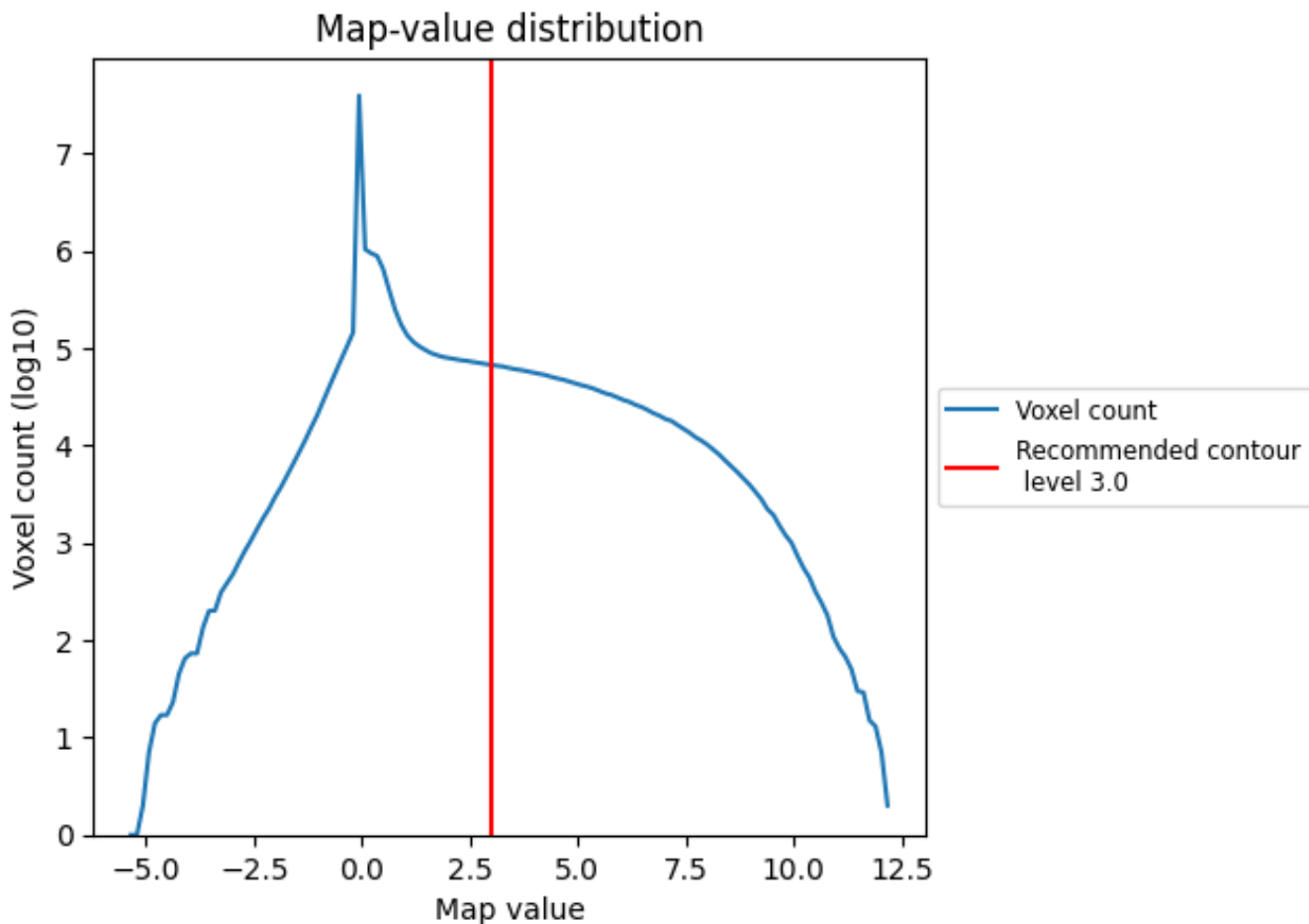
6.5 Mask visualisation

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

7 Map analysis [i](#)

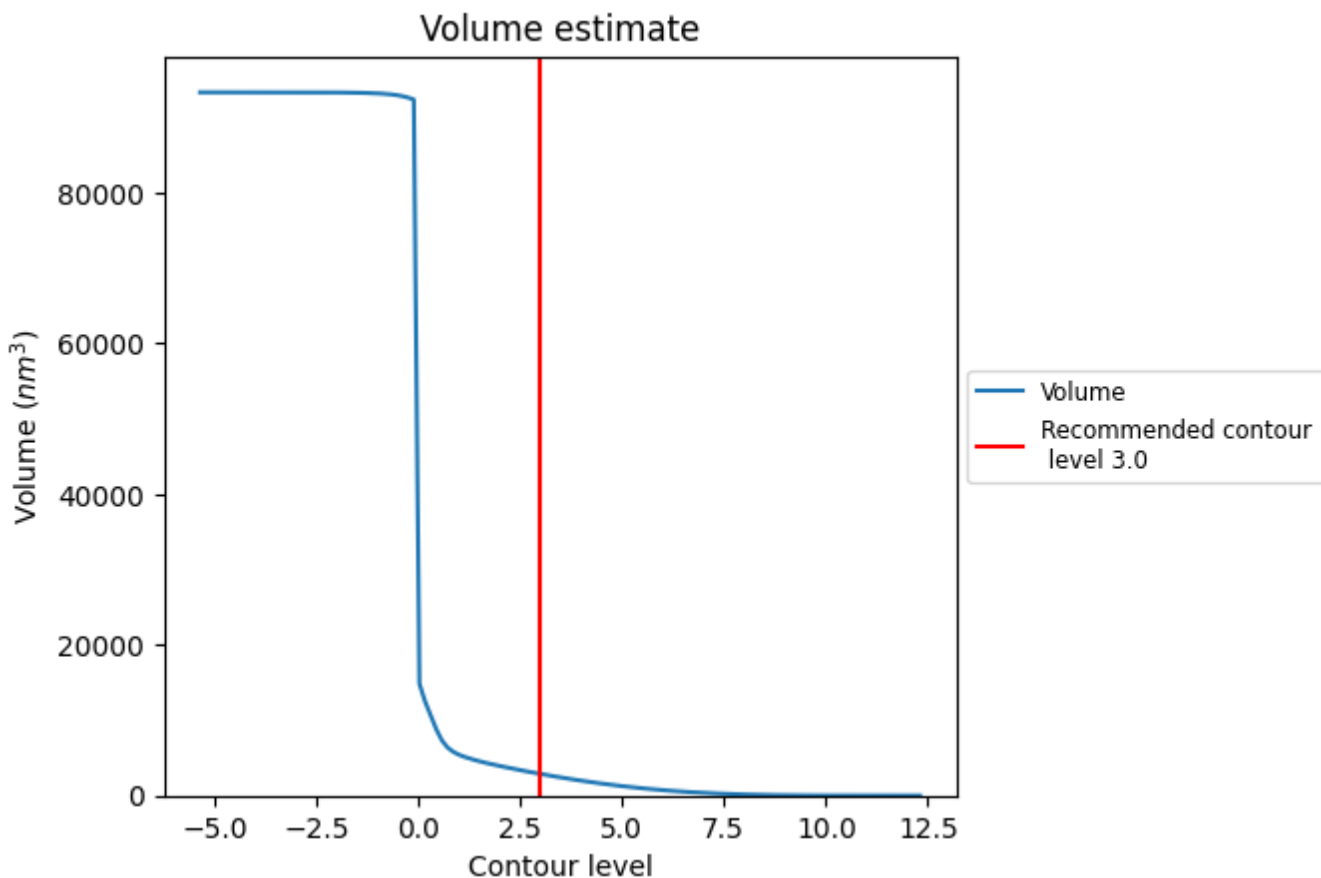
This section contains the results of statistical analysis of the map.

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.

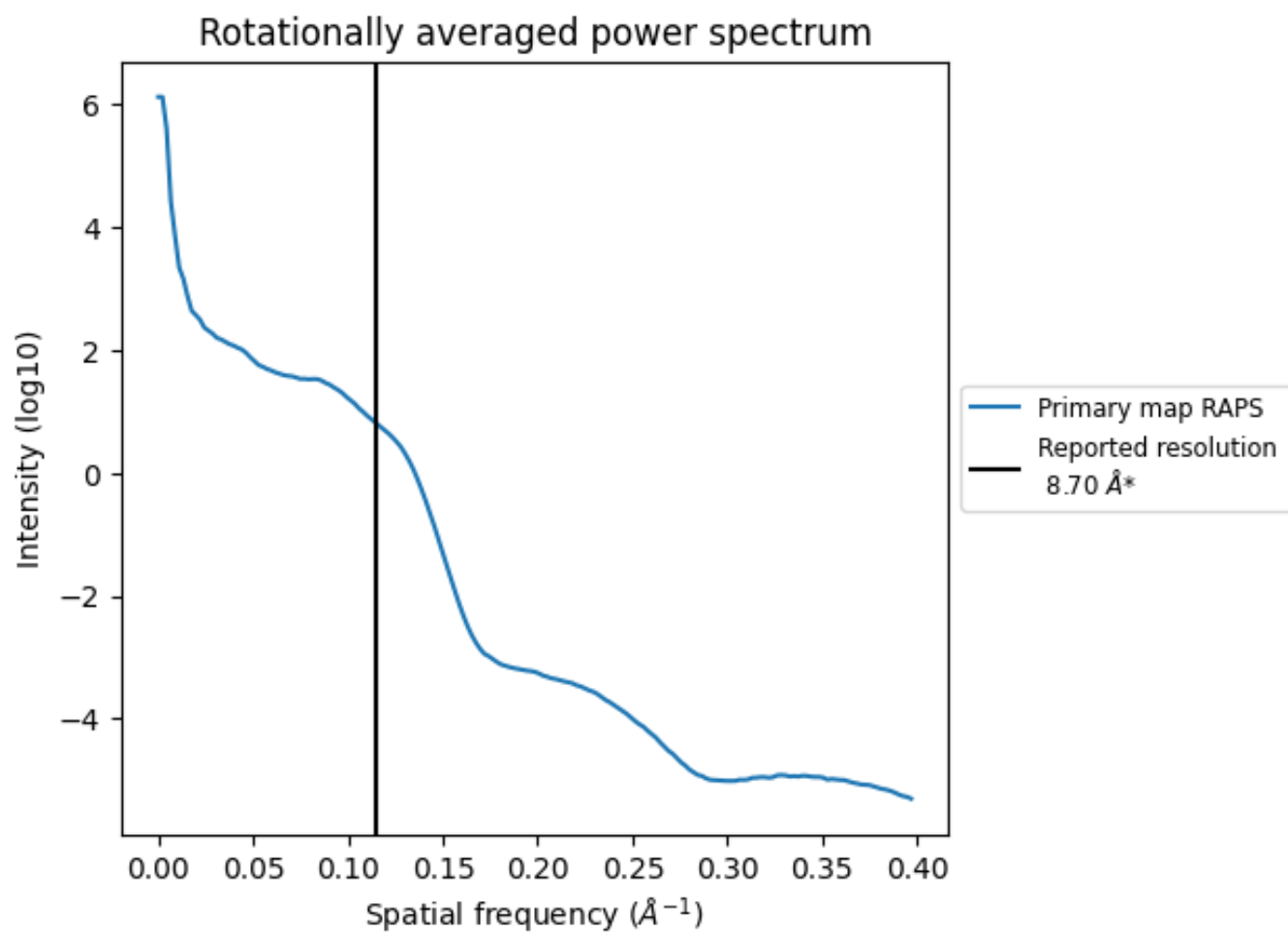
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2869 nm^3 ; this corresponds to an approximate mass of 2591 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 0.115\AA^{-1}

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

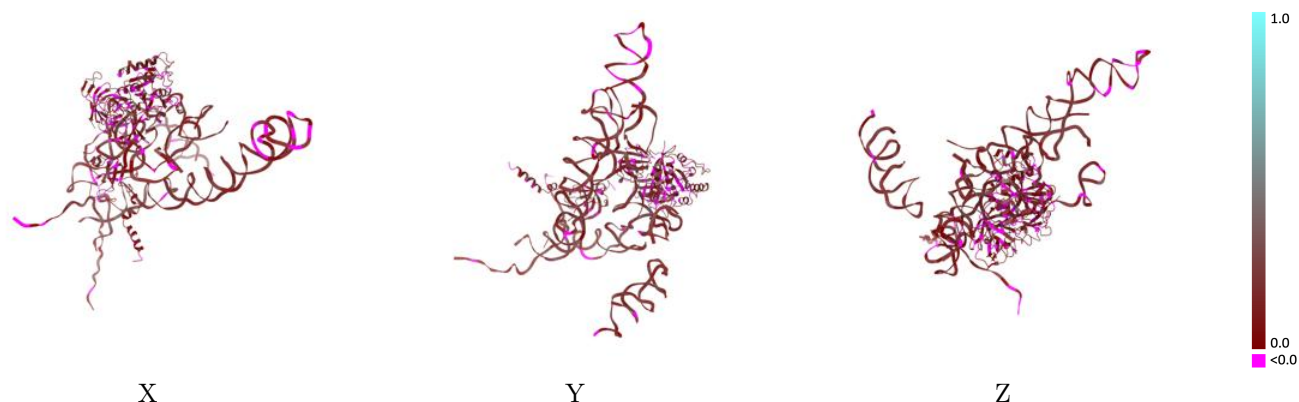
This section contains information regarding the fit between EMDB map EMD-2623 and PDB model 4CXG. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 3.0 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](#)



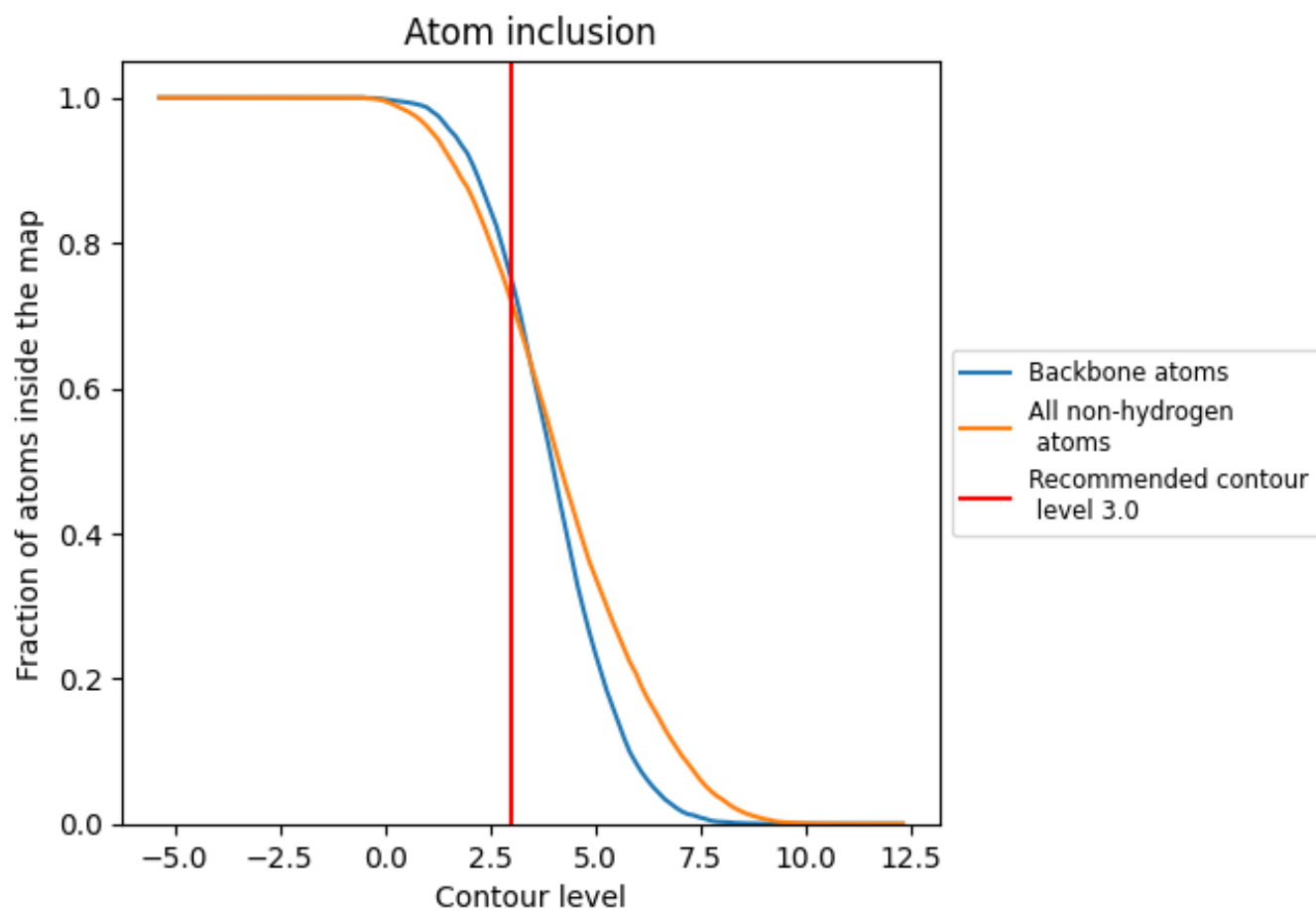
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (3.0).





















9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 72% 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 (3.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7210	 0.1410
1	 0.8045	 0.1650
2	 0.9262	 0.1890
A	 0.5059	 0.0980
X	 0.6305	 0.1110
Y	 0.8002	 0.1500
a	 0.9131	 0.1670
b	 0.8705	 0.1970
c	 0.9390	 0.1790
x	 0.4625	 0.0970

