



Full wwPDB EM Validation Report ⓘ

Jun 23, 2026 – 08:03 PM JST

PDB ID : 9XFL / pdb_00009xfl
EMDB ID : EMD-66736
Title : In vitro structure of bacterial 50S ribosomes
Authors : Wu, F.; Naschberger, A.
Deposited on : 2025-10-29
Resolution : 3.16 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:

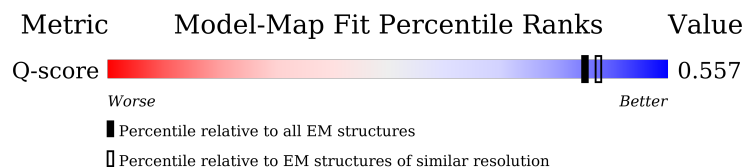
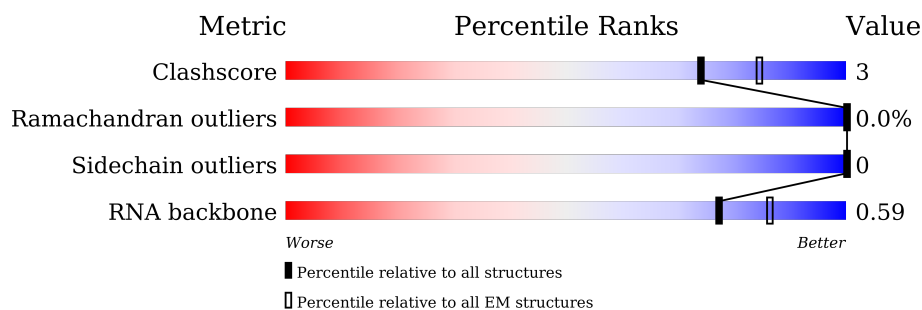
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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



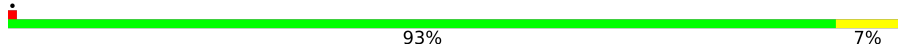
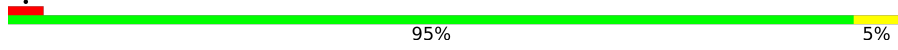
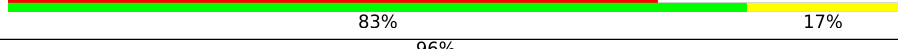
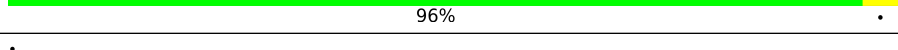
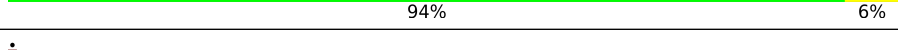
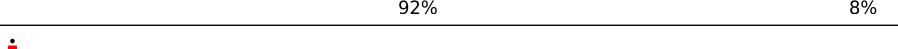
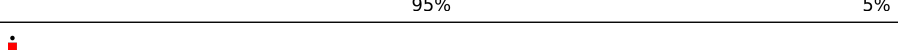
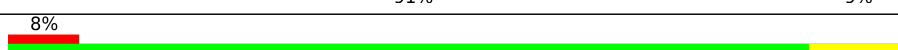
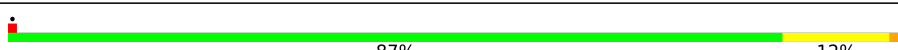
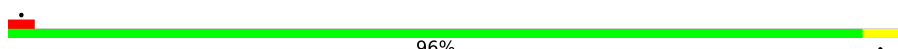
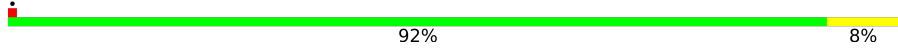
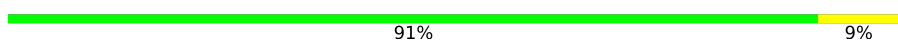
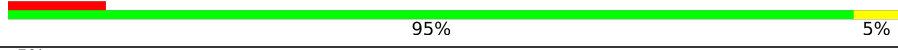
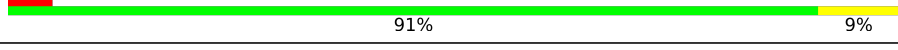
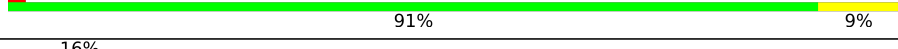
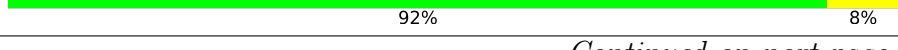
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14474 (2.66 - 3.66)

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	I	2904	6% 78% 19% .
2	J	118	. 78% 21% .
3	K	271	89% 11%

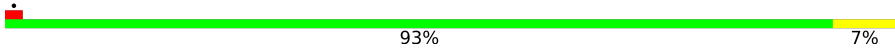
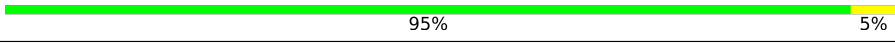
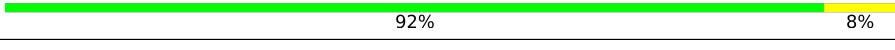
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	L	209	
5	M	201	
6	N	177	
7	O	176	
8	P	149	
9	Q	134	
10	R	142	
11	S	122	
12	T	144	
13	U	136	
14	V	120	
15	W	116	
16	X	114	
17	Y	117	
18	Z	103	
19	a	110	
20	b	93	
21	c	102	
22	d	94	
23	e	75	
24	f	77	
25	g	62	
26	h	58	
27	i	56	
28	j	50	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	k	46	 93%7%
30	l	64	 95%5%
31	m	38	 92%8%

2 Entry composition

There are 35 unique types of molecules in this entry. The entry contains 154215 atoms, of which 59930 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	I	2898	Total	C	H	N	O	P	0	0
			93473	27768	31244	11448	20115	2898		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	118	Total	C	H	N	O	P	0	0
			3810	1126	1281	464	821	118		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	K	271	Total	C	H	N	O	S	0	0
			4237	1288	2154	423	365	7		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	L	209	Total	C	H	N	O	S	0	0
			3182	979	1617	288	294	4		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	M	201	Total	C	H	N	O	S	0	0
			3171	974	1619	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	N	177	Total	C	H	N	O	S	0	0
			2855	899	1444	249	257	6		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	O	176	Total	C	H	N	O	S	0	0
			2694	832	1371	243	246	2		

- Molecule 8 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	P	149	Total	C	H	N	O	S	0	0
			2258	699	1148	197	213	1		

- Molecule 9 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Q	134	Total	C	H	N	O	S	0	0
			2007	619	1028	169	185	6		

- Molecule 10 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	R	142	Total	C	H	N	O	S	0	0
			2291	714	1162	212	199	4		

- Molecule 11 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	S	122	Total	C	H	N	O	S	0	0
			1950	587	1012	180	165	6		

- Molecule 12 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	T	144	Total	C	H	N	O	S	0	0
			2182	654	1129	207	190	2		

- Molecule 13 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	U	136	Total	C	H	N	O	S	0	0
			2222	686	1147	205	178	6		

- Molecule 14 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace	
14	V	120	Total	C	H	N	O	S	0	0
			1960	593	1000	196	166	5		

- Molecule 15 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	116	Total	C	H	N	O	0	0
			1815	552	923	178	162		

- Molecule 16 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	X	114	Total	C	H	N	O	S	0	0
			1879	574	962	179	163	1		

- Molecule 17 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Y	117	Total	C	H	N	O	0	0
			1967	604	1020	192	151		

- Molecule 18 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	Z	103	Total	C	H	N	O	S	0	0
			1655	516	839	153	145	2		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	a	110	Total	C	H	N	O	S	0	0
			1779	532	922	166	156	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms						AltConf	Trace
20	b	93	Total	C	H	N	O	S	0	0
			1546	466	807	139	132	2		

- Molecule 21 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	c	102	Total	C	H	N	O	0	0
			1611	492	831	146	142		

- Molecule 22 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	d	94	Total	C	H	N	O	S	0	0
			1533	479	780	137	134	3		

- Molecule 23 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	e	75	Total	C	H	N	O	S	0	0
			1167	356	592	116	102	1		

- Molecule 24 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms						AltConf	Trace
24	f	77	Total	C	H	N	O	S	0	0
			1277	388	652	129	106	2		

- Molecule 25 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace	
25	g	62	Total	C	H	N	O	S	0	0
			1032	308	531	98	94	1		

- Molecule 26 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms						AltConf	Trace
26	h	58	Total	C	H	N	O	S	0	0
			937	281	488	87	79	2		

- Molecule 27 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace	
27	i	56	Total	C	H	N	O	S	0	0
			902	269	458	94	80	1		

- Molecule 28 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	50	Total	C	H	N	O	0	0
			849	263	440	75	71		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace	
29	k	46	Total	C	H	N	O	S	0	0
			794	228	417	90	57	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms						AltConf	Trace
30	l	64	Total	C	H	N	O	S	0	0
			1076	323	572	105	74	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace	
31	m	38	Total	C	H	N	O	S	0	0
			642	185	340	65	48	4		

- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	I	170	Total	Mg	0
			170	170	
32	J	2	Total	Mg	0
			2	2	
32	K	1	Total	Mg	0
			1	1	
32	L	1	Total	Mg	0
			1	1	
32	T	1	Total	Mg	0
			1	1	
32	k	1	Total	Mg	0
			1	1	

- Molecule 33 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		AltConf
33	K	1	Total	Na	0
			1	1	

- Molecule 34 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
34	m	1	Total 1	Zn 1	0

- Molecule 35 is water.

Mol	Chain	Residues	Atoms		AltConf
35	I	2879	Total 2879	O 2879	0
35	J	27	Total 27	O 27	0
35	K	58	Total 58	O 58	0
35	L	40	Total 40	O 40	0
35	M	23	Total 23	O 23	0
35	N	4	Total 4	O 4	0
35	O	7	Total 7	O 7	0
35	P	2	Total 2	O 2	0
35	Q	5	Total 5	O 5	0
35	R	12	Total 12	O 12	0
35	S	14	Total 14	O 14	0
35	T	22	Total 22	O 22	0
35	U	15	Total 15	O 15	0
35	V	22	Total 22	O 22	0
35	W	5	Total 5	O 5	0
35	X	13	Total 13	O 13	0
35	Y	23	Total 23	O 23	0
35	Z	12	Total 12	O 12	0

Continued on next page...

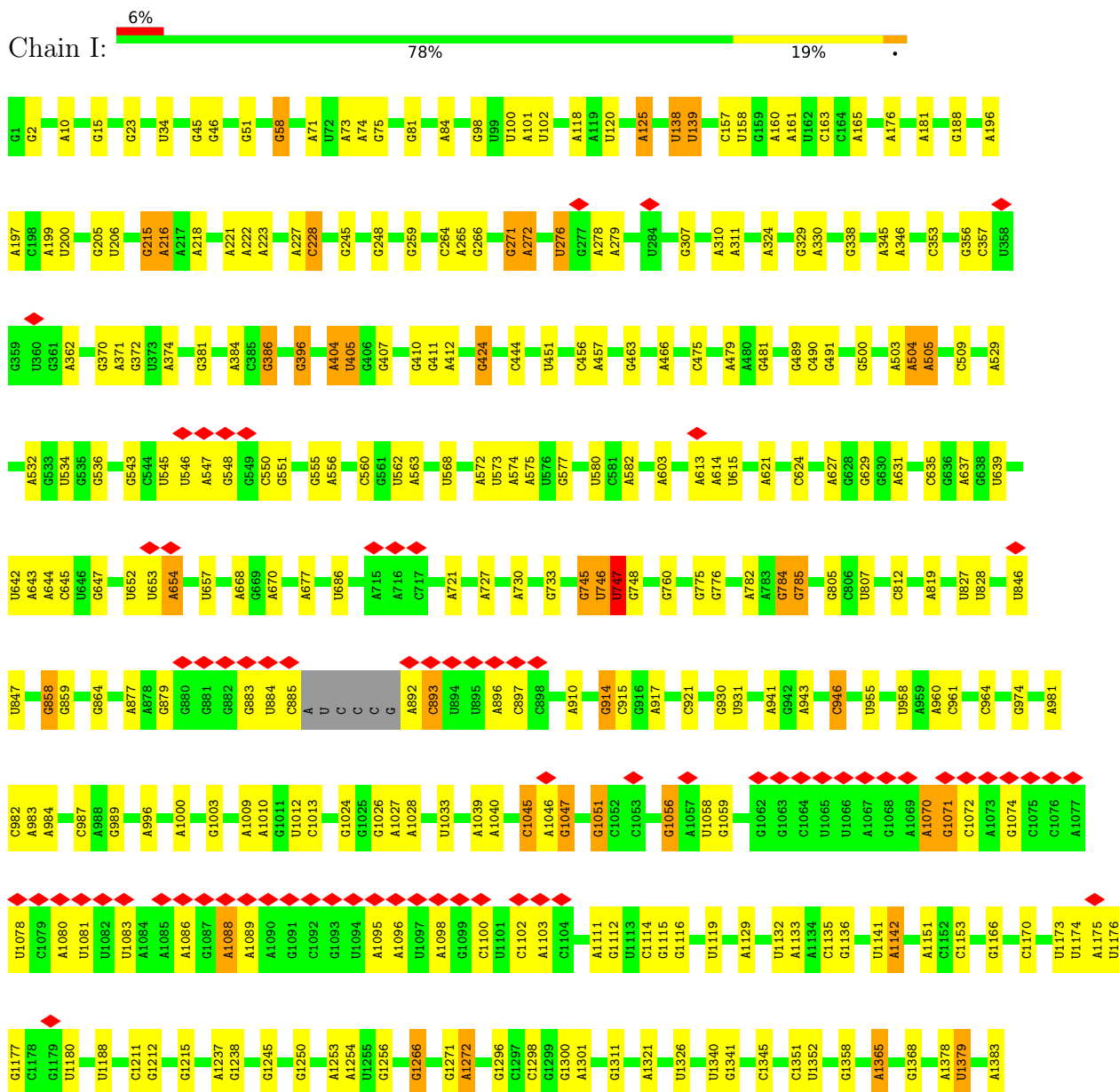
Continued from previous page...

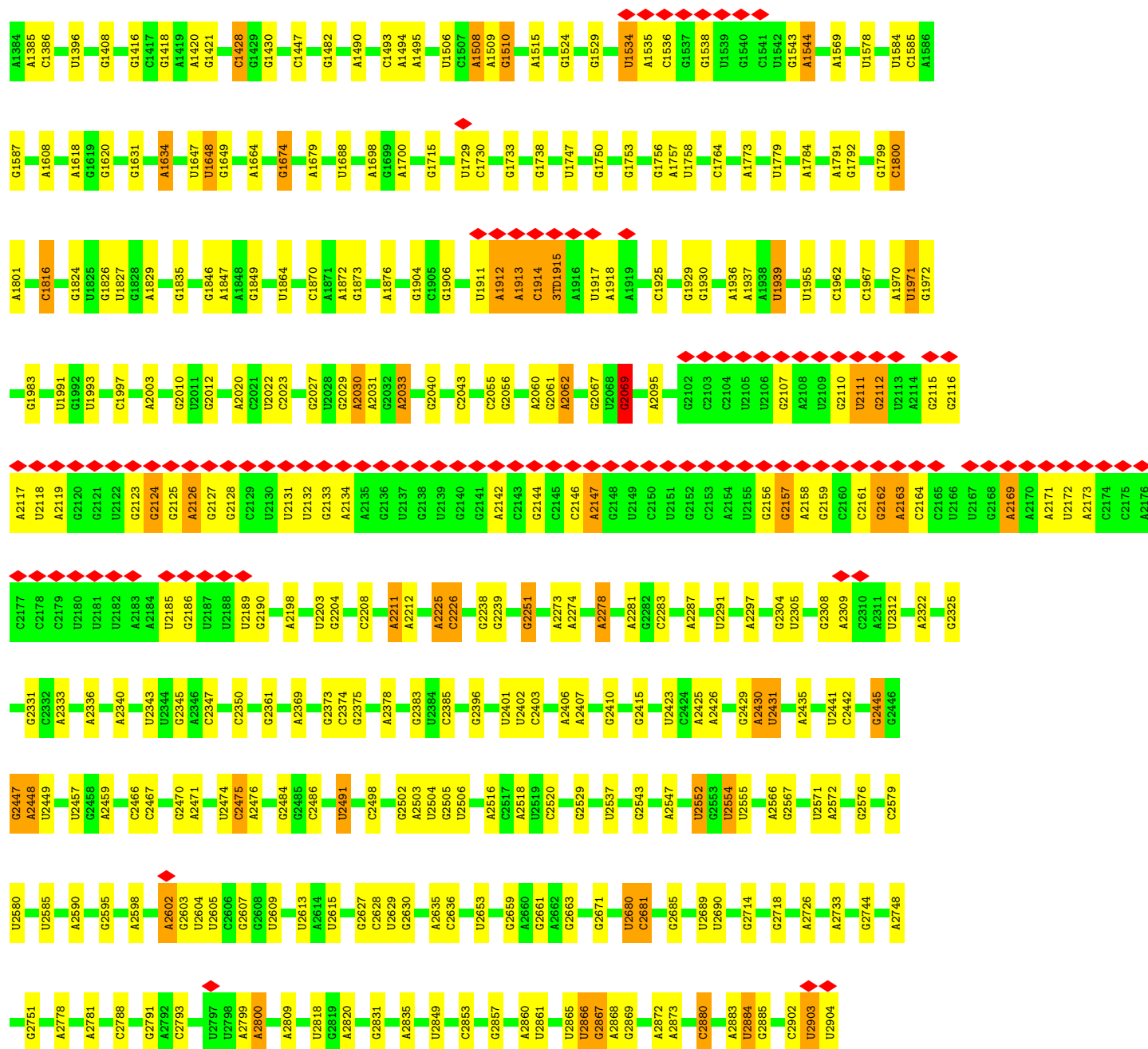
Mol	Chain	Residues	Atoms		AltConf
35	a	25	Total 25	O 25	0
35	b	5	Total 5	O 5	0
35	c	4	Total 4	O 4	0
35	d	2	Total 2	O 2	0
35	e	7	Total 7	O 7	0
35	f	14	Total 14	O 14	0
35	g	3	Total 3	O 3	0
35	h	7	Total 7	O 7	0
35	i	9	Total 9	O 9	0
35	j	1	Total 1	O 1	0
35	k	13	Total 13	O 13	0
35	l	8	Total 8	O 8	0
35	m	3	Total 3	O 3	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: 23S rRNA







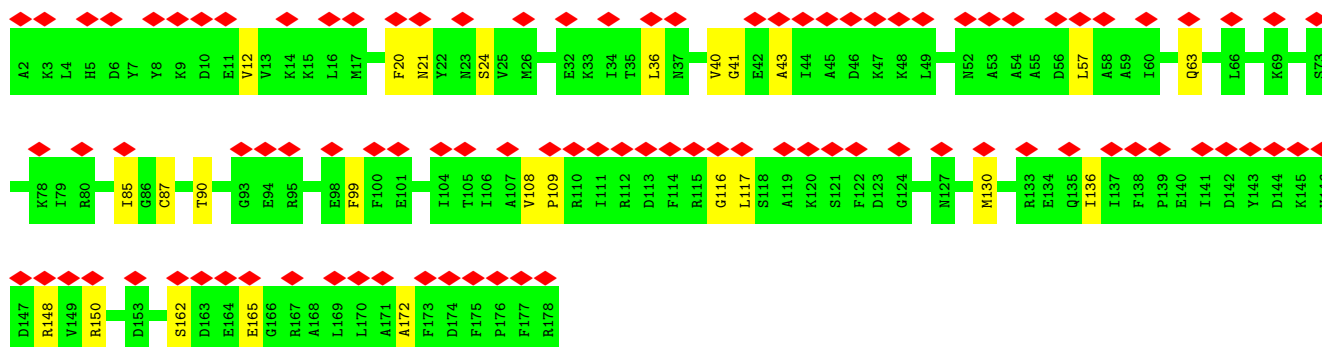
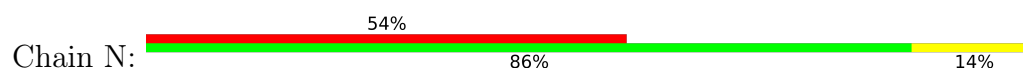
- Molecule 4: Large ribosomal subunit protein uL3



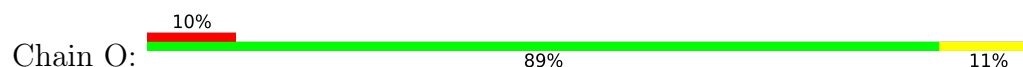
- Molecule 5: 50S ribosomal protein L4



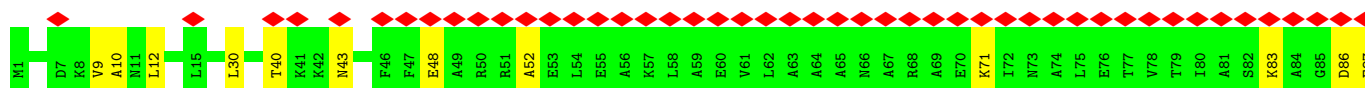
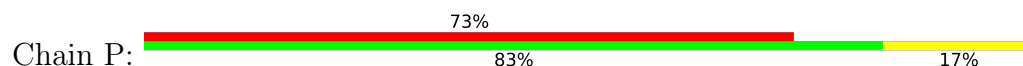
- Molecule 6: 50S ribosomal protein L5

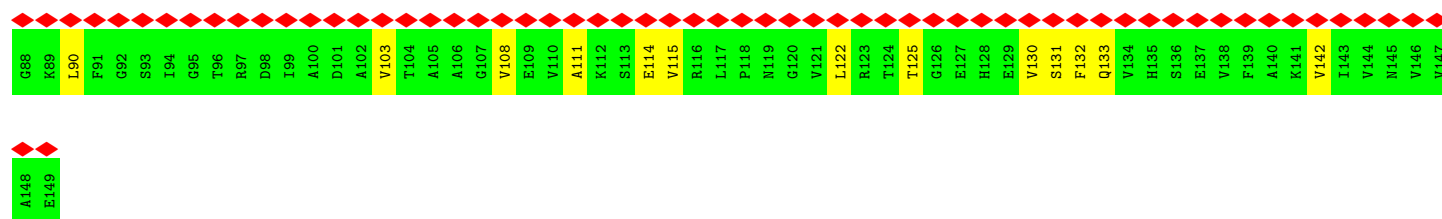


- Molecule 7: Large ribosomal subunit protein uL6

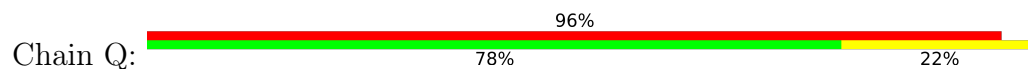


- Molecule 8: 50S ribosomal protein L9





• Molecule 9: 50S ribosomal protein L11



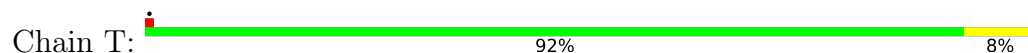
• Molecule 10: 50S ribosomal protein L13



• Molecule 11: Large ribosomal subunit protein uL14



• Molecule 12: 50S ribosomal protein L15



• Molecule 13: Large ribosomal subunit protein uL16

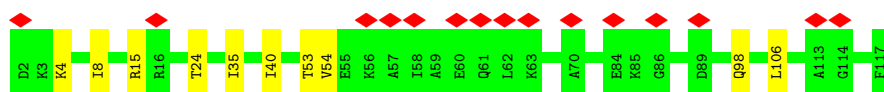




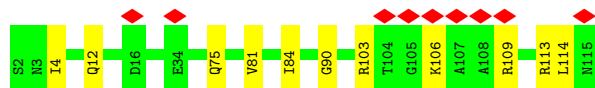
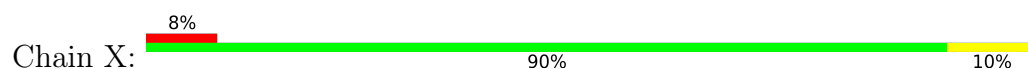
- Molecule 14: Large ribosomal subunit protein bL17



- Molecule 15: 50S ribosomal protein L18



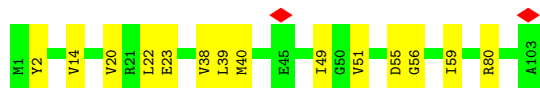
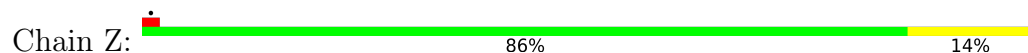
- Molecule 16: 50S ribosomal protein L19



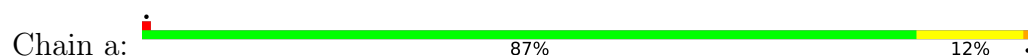
- Molecule 17: 50S ribosomal protein L20



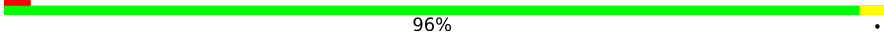
- Molecule 18: 50S ribosomal protein L21

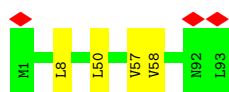


- Molecule 19: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L23

Chain b:  96%



- Molecule 21: Large ribosomal subunit protein uL24

Chain c:  6% 87% 13%

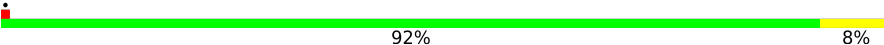


- Molecule 22: 50S ribosomal protein L25

Chain d:  88% 12%



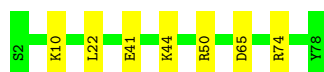
- Molecule 23: 50S ribosomal protein L27

Chain e:  92% 8%

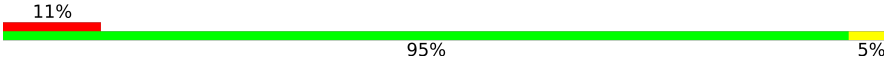


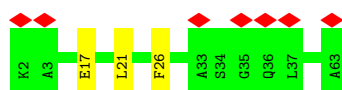
- Molecule 24: 50S ribosomal protein L28

Chain f:  91% 9%

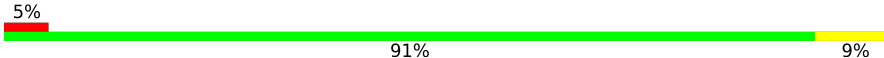


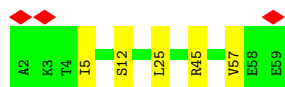
- Molecule 25: 50S ribosomal protein L29

Chain g:  11% 95% 5%



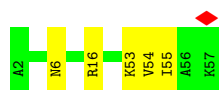
- Molecule 26: 50S ribosomal protein L30

Chain h:  5% 91% 9%



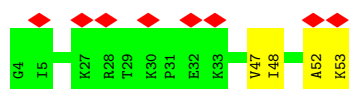
- Molecule 27: Large ribosomal subunit protein bL32

Chain i:  91% 9%



- Molecule 28: 50S ribosomal protein L33

Chain j:  16% 92% 8%



- Molecule 29: 50S ribosomal protein L34

Chain k:  93% 7%



- Molecule 30: 50S ribosomal protein L35

Chain l:  95% 5%



- Molecule 31: 50S ribosomal protein L36

Chain m:  92% 8%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	81081	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.031	Depositor
Minimum map value	-0.023	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0032	Depositor
Map size ($\text{\AA}$)	364.5, 364.5, 364.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.729, 0.729, 0.729	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: MG, 2MG, G7M, 4D4, H2U, OMG, OMC, PSU, ZN, 5MC, 1MG, NA, 3TD, OMU, 5MU, 2MA, 6MZ

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	I	0.22	0/69121	0.21	0/107828
2	J	0.15	0/2828	0.16	0/4410
3	K	0.19	0/2122	0.31	0/2852
4	L	0.18	0/1586	0.25	0/2134
5	M	0.15	0/1571	0.22	0/2113
6	N	0.10	0/1435	0.23	0/1926
7	O	0.10	0/1343	0.25	0/1816
8	P	0.09	0/1121	0.27	0/1515
9	Q	0.11	0/993	0.32	0/1341
10	R	0.17	0/1152	0.22	0/1551
11	S	0.16	0/947	0.25	0/1268
12	T	0.16	0/1062	0.24	0/1413
13	U	0.15	0/1081	0.23	0/1443
14	V	0.18	0/973	0.26	0/1301
15	W	0.12	0/902	0.23	0/1209
16	X	0.15	0/929	0.21	0/1242
17	Y	0.19	0/960	0.23	0/1278
18	Z	0.16	0/829	0.25	0/1107
19	a	0.18	0/864	0.26	0/1156
20	b	0.14	0/745	0.23	0/994
21	c	0.12	0/788	0.29	0/1051
22	d	0.12	0/766	0.21	0/1025
23	e	0.16	0/582	0.24	0/769
24	f	0.17	0/635	0.25	0/848
25	g	0.12	0/502	0.23	0/667
26	h	0.15	0/453	0.22	0/605
27	i	0.17	0/450	0.24	0/599
28	j	0.12	0/416	0.27	0/554
29	k	0.19	0/380	0.23	0/498
30	l	0.18	0/513	0.24	0/676
31	m	0.14	0/303	0.24	0/397

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
All	All	0.20	0/98352	0.22	0/147586

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	I	62229	31244	31318	257	0
2	J	2529	1281	1281	8	0
3	K	2083	2154	2154	23	0
4	L	1565	1617	1616	14	0
5	M	1552	1619	1619	7	0
6	N	1411	1444	1444	17	0
7	O	1323	1371	1371	13	0
8	P	1110	1148	1148	16	0
9	Q	979	1028	1028	24	0
10	R	1129	1162	1162	5	0
11	S	938	1012	1012	5	0
12	T	1053	1129	1129	9	0
13	U	1075	1147	1154	4	0
14	V	960	1000	1000	8	0
15	W	892	923	923	8	0
16	X	917	962	962	8	0
17	Y	947	1020	1019	7	0
18	Z	816	839	839	12	0
19	a	857	922	922	8	0
20	b	739	807	807	4	0
21	c	780	831	831	9	0
22	d	753	780	780	7	0
23	e	575	592	592	4	0
24	f	625	652	652	6	0
25	g	501	531	531	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	h	449	488	488	4	0
27	i	444	458	458	4	0
28	j	409	440	440	2	0
29	k	377	417	417	2	0
30	l	504	572	572	2	0
31	m	302	340	340	3	0
32	I	170	0	0	0	0
32	J	2	0	0	0	0
32	K	1	0	0	0	0
32	L	1	0	0	0	0
32	T	1	0	0	0	0
32	k	1	0	0	0	0
33	K	1	0	0	0	0
34	m	1	0	0	0	0
35	I	2879	0	0	90	0
35	J	27	0	0	2	0
35	K	58	0	0	0	0
35	L	40	0	0	1	0
35	M	23	0	0	1	0
35	N	4	0	0	0	0
35	O	7	0	0	0	0
35	P	2	0	0	0	0
35	Q	5	0	0	0	0
35	R	12	0	0	0	0
35	S	14	0	0	0	0
35	T	22	0	0	0	0
35	U	15	0	0	0	0
35	V	22	0	0	1	0
35	W	5	0	0	0	0
35	X	13	0	0	1	0
35	Y	23	0	0	0	0
35	Z	12	0	0	1	0
35	a	25	0	0	2	0
35	b	5	0	0	0	0
35	c	4	0	0	0	0
35	d	2	0	0	0	0
35	e	7	0	0	0	0
35	f	14	0	0	1	0
35	g	3	0	0	0	0
35	h	7	0	0	0	0
35	i	9	0	0	1	0
35	j	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	k	13	0	0	0	0
35	l	8	0	0	1	0
35	m	3	0	0	0	0
All	All	94285	59930	60009	451	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 3.

All (451) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:747:5MU:C5	1:I:747:5MU:C4	1.79	1.67
1:I:1939:5MU:C4	1:I:1939:5MU:C5	1.79	1.63
1:I:138:U:O2'	1:I:139:U:OP1	1.91	0.89
1:I:2069:G7M:N2	1:I:2442:C:O2	2.06	0.87
1:I:1095:A:H61	9:Q:9:VAL:HG13	1.38	0.87
1:I:1188:U:P	35:I:3244:HOH:O	2.33	0.86
1:I:1753:G:N2	1:I:1756:G:OP2	2.11	0.82
1:I:197:A:N6	1:I:2430:A:O2'	2.12	0.82
1:I:1237:A:OP2	35:I:3203:HOH:O	1.99	0.81
1:I:946:C:OP2	35:I:3204:HOH:O	2.01	0.79
1:I:572:A:OP2	18:Z:80:ARG:NH2	2.16	0.78
1:I:1272:A:N3	35:I:3247:HOH:O	2.16	0.78
1:I:2865:U:OP2	1:I:2866:U:O2'	2.00	0.77
1:I:410:G:OP2	35:I:3205:HOH:O	2.03	0.77
1:I:2040:G:N7	35:I:3248:HOH:O	2.16	0.77
1:I:1078:U:O2'	1:I:1088:A:OP1	2.02	0.77
1:I:2868:A:N1	35:I:3250:HOH:O	2.17	0.76
1:I:543:G:N7	35:I:3259:HOH:O	2.18	0.76
1:I:884:U:O4	1:I:892:A:N6	2.18	0.76
1:I:746:PSU:O2	35:I:3207:HOH:O	2.03	0.76
1:I:1177:G:N3	35:I:3253:HOH:O	2.18	0.76
1:I:1071:G:O6	1:I:1100:C:N4	2.19	0.75
1:I:2537:U:OP2	35:I:3206:HOH:O	2.03	0.75
1:I:81:G:N7	35:I:3265:HOH:O	2.19	0.75
6:N:148:ARG:O	6:N:150:ARG:NH1	2.19	0.75
35:I:5116:HOH:O	9:Q:117:MET:SD	2.45	0.75
1:I:2867:G:OP1	35:I:3209:HOH:O	2.05	0.75
1:I:2516:A:N7	35:I:3269:HOH:O	2.19	0.74
9:Q:55:ILE:HD11	9:Q:72:LYS:O	1.86	0.74
1:I:2274:A:N7	35:I:3272:HOH:O	2.20	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2543:G:OP1	35:I:3210:HOH:O	2.06	0.74
3:K:251:GLN:NE2	3:K:252:THR:O	2.21	0.74
1:I:2067:G:OP2	35:I:3212:HOH:O	2.06	0.73
1:I:2590:A:N3	35:I:3271:HOH:O	2.20	0.73
1:I:2003:A:OP2	35:I:3211:HOH:O	2.06	0.73
1:I:2799:A:O2'	1:I:2800:A:O5'	2.06	0.73
1:I:176:A:N7	35:I:3276:HOH:O	2.21	0.72
1:I:1211:C:O2	35:I:3217:HOH:O	2.07	0.72
1:I:1816:C:N4	3:K:35:GLU:OE1	2.22	0.72
1:I:1072:C:N4	1:I:1098:A:OP2	2.22	0.72
1:I:84:A:N1	1:I:98:G:O2'	2.22	0.72
1:I:879:G:N7	35:I:3289:HOH:O	2.23	0.72
1:I:1983:G:OP1	35:I:3220:HOH:O	2.08	0.72
1:I:1298:C:OP2	35:I:3219:HOH:O	2.08	0.72
1:I:1971:U:O2'	35:I:3218:HOH:O	2.07	0.72
18:Z:39:LEU:O	35:Z:201:HOH:O	2.08	0.71
1:I:1648:U:O2	35:I:3214:HOH:O	2.07	0.71
1:I:1849:G:O2'	35:I:3213:HOH:O	2.07	0.71
4:L:46:ARG:NH2	4:L:88:GLU:O	2.23	0.71
1:I:1351:C:OP2	35:I:3222:HOH:O	2.08	0.71
1:I:582:A:N3	35:I:3303:HOH:O	2.24	0.71
1:I:2520:C:OP1	35:I:3216:HOH:O	2.07	0.71
1:I:2281:A:N3	35:I:3293:HOH:O	2.23	0.71
1:I:1039:A:N7	35:I:3287:HOH:O	2.22	0.71
1:I:1166:G:N7	35:I:3299:HOH:O	2.24	0.71
1:I:1906:G:N2	1:I:1925:C:O2	2.24	0.71
1:I:1379:U:OP2	35:I:3223:HOH:O	2.08	0.70
1:I:1698:A:OP2	35:I:3221:HOH:O	2.08	0.70
1:I:23:G:N7	35:I:3301:HOH:O	2.24	0.70
1:I:1428:C:N3	35:I:3307:HOH:O	2.25	0.69
1:I:2062:A:OP2	35:I:3226:HOH:O	2.09	0.69
1:I:161:A:O2'	35:I:3231:HOH:O	2.10	0.69
1:I:2869:G:N7	35:I:3304:HOH:O	2.24	0.69
2:J:63:C:O2	35:J:301:HOH:O	2.08	0.69
1:I:1215:G:N7	35:I:3322:HOH:O	2.27	0.68
1:I:921:C:O2'	35:I:3236:HOH:O	2.12	0.68
9:Q:42:PHE:O	9:Q:46:THR:HG23	1.93	0.68
1:I:2607:G:OP1	35:I:3232:HOH:O	2.11	0.68
18:Z:55:ASP:OD1	18:Z:56:GLY:N	2.27	0.68
2:J:56:G:OP1	6:N:24:SER:OG	2.12	0.68
1:I:635:C:OP2	35:I:3230:HOH:O	2.10	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:536:G:OP2	35:I:3242:HOH:O	2.13	0.67
1:I:2751:G:N2	1:I:2751:G:OP1	2.27	0.67
1:I:733:G:O6	35:I:3229:HOH:O	2.10	0.67
1:I:1747:U:OP1	35:I:3233:HOH:O	2.11	0.67
1:I:2853:C:OP2	35:I:3237:HOH:O	2.12	0.67
2:J:116:G:N7	35:J:302:HOH:O	2.27	0.67
1:I:1071:G:O2'	1:I:1089:A:OP2	2.11	0.67
1:I:228:C:N4	1:I:2407:A:N3	2.41	0.66
1:I:2448:A:OP2	35:I:3238:HOH:O	2.12	0.66
1:I:958:U:OP1	35:I:3240:HOH:O	2.12	0.66
4:L:86:GLU:OE1	35:L:401:HOH:O	2.13	0.66
30:I:17:THR:O	35:I:101:HOH:O	2.13	0.66
1:I:784:G:O6	35:I:3228:HOH:O	2.10	0.66
3:K:29:PRO:HG2	3:K:34:LEU:HD11	1.77	0.66
1:I:1534:U:O4'	1:I:1538:G:N2	2.28	0.66
1:I:1904:G:N7	35:I:3328:HOH:O	2.28	0.66
1:I:1009:A:N3	1:I:1153:C:O2'	2.29	0.66
1:I:1430:G:OP2	35:I:3245:HOH:O	2.14	0.66
1:I:444:C:OP1	35:I:3243:HOH:O	2.13	0.66
1:I:1826:G:O2'	1:I:1971:U:OP2	2.14	0.66
1:I:2343:U:HO2'	1:I:2373:G:HO2'	1.44	0.65
1:I:381:G:N3	35:I:3344:HOH:O	2.29	0.65
1:I:2857:G:N2	1:I:2860:A:OP2	2.22	0.65
1:I:989:G:OP2	26:h:12:SER:OG	2.13	0.65
8:P:122:LEU:O	8:P:122:LEU:HD23	1.96	0.64
1:I:1188:U:OP2	35:I:3244:HOH:O	2.14	0.64
1:I:1529:G:N3	35:I:3346:HOH:O	2.29	0.64
9:Q:80:LEU:HD13	9:Q:138:LEU:HD11	1.79	0.64
1:I:500:G:N1	1:I:503:A:OP2	2.30	0.64
2:J:66:A:OP2	2:J:108:A:N6	2.30	0.64
1:I:534:U:O2'	17:Y:49:ASP:OD2	2.15	0.64
31:m:16:ILE:HD13	31:m:25:VAL:HG22	1.78	0.64
18:Z:14:VAL:HG12	18:Z:20:VAL:HG11	1.79	0.63
1:I:370:G:O2'	1:I:424:G:OP1	2.13	0.63
3:K:117:GLN:N	3:K:128:ASN:OD1	2.32	0.63
1:I:1028:A:N3	1:I:2486:C:O2'	2.28	0.63
1:I:1170:C:O2	35:I:3246:HOH:O	2.15	0.63
1:I:475:C:O2	1:I:479:A:N6	2.30	0.63
1:I:1800:C:OP2	3:K:182:ARG:NH2	2.32	0.62
3:K:107:PRO:HD2	3:K:110:LEU:HD22	1.81	0.62
5:M:16:GLU:O	5:M:20:GLY:N	2.32	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:624:C:O2'	1:I:657:U:OP1	2.19	0.61
1:I:1070:A:N7	1:I:1096:A:O2'	2.26	0.61
1:I:1056:G:N1	1:I:1102:C:OP2	2.32	0.61
11:S:14:SER:OG	11:S:86:LEU:HD12	2.01	0.61
1:I:1800:C:H5'	3:K:146:MET:HE1	1.83	0.61
1:I:748:G:O2'	35:I:3249:HOH:O	2.16	0.60
8:P:114:GLU:O	8:P:133:GLN:N	2.33	0.60
1:I:1266:G:OP1	27:i:16:ARG:NE	2.34	0.60
1:I:2685:G:OP1	11:S:78:ARG:NH2	2.35	0.60
1:I:568:U:H1'	1:I:2030:6MZ:H9C1	1.84	0.60
1:I:1792:G:C5'	3:K:204:VAL:HG13	2.32	0.60
14:V:33:ILE:HD13	14:V:114:GLU:HG2	1.82	0.60
1:I:1864:U:OP1	1:I:2410:G:O2'	2.18	0.60
1:I:807:U:OP2	12:T:41:ARG:NH2	2.35	0.60
5:M:69:ARG:NH2	35:M:301:HOH:O	2.36	0.59
12:T:79:LEU:HD11	12:T:112:LEU:HD12	1.84	0.59
1:I:356:G:N2	35:I:3408:HOH:O	2.36	0.59
7:O:100:GLY:O	7:O:101:ASN:OD1	2.21	0.58
3:K:51:THR:HG23	3:K:54:ILE:HD12	1.84	0.58
1:I:307:G:N1	1:I:310:A:OP2	2.36	0.58
1:I:943:A:N3	35:I:3372:HOH:O	2.32	0.58
1:I:2107:G:N2	35:I:3411:HOH:O	2.36	0.58
3:K:158:ALA:O	3:K:195:VAL:HG13	2.03	0.58
9:Q:101:ILE:HG12	9:Q:138:LEU:HD22	1.85	0.58
1:I:2474:U:OP2	1:I:2475:C:N4	2.27	0.58
1:I:1296:G:N7	35:I:3378:HOH:O	2.32	0.58
8:P:86:ASP:OD1	8:P:87:GLU:N	2.33	0.58
1:I:1058:U:H1'	9:Q:117:MET:HE1	1.85	0.58
1:I:1385:A:O2'	1:I:1396:U:O2	2.21	0.57
1:I:1447:C:O2'	1:I:1544:A:N3	2.35	0.57
1:I:357:C:OP2	35:I:3252:HOH:O	2.17	0.57
1:I:2467:C:OP1	31:m:8:LYS:NZ	2.37	0.57
1:I:1674:G:O2'	35:I:3227:HOH:O	2.10	0.57
17:Y:90:ILE:CD1	18:Z:40:MET:HE3	2.35	0.57
12:T:55:MET:HE1	12:T:59:ARG:HH21	1.70	0.57
1:I:2902:C:OP2	1:I:2903:U:O2'	2.16	0.57
7:O:72:LEU:HD13	7:O:75:MET:SD	2.44	0.57
1:I:1051:G:N1	35:I:3376:HOH:O	2.32	0.57
14:V:98:LEU:CD1	27:i:54:VAL:HG21	2.35	0.56
1:I:727:A:H2	3:K:9:THR:HG21	1.71	0.56
11:S:9:ASN:OD1	11:S:18:ARG:NH1	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:13:VAL:HG23	9:Q:24:VAL:HG13	1.86	0.56
16:X:106:LYS:O	16:X:109:ARG:NE	2.39	0.56
1:I:451:U:OP2	35:I:3254:HOH:O	2.18	0.55
4:L:3:GLY:O	4:L:4:LEU:HD12	2.07	0.55
1:I:227:A:O2'	1:I:228:C:OP2	2.17	0.55
2:J:47:C:O2'	15:W:98:GLN:OE1	2.24	0.55
1:I:1688:U:O2'	1:I:1700:A:N7	2.34	0.55
9:Q:74:PRO:O	9:Q:113:LYS:NZ	2.28	0.55
16:X:90:GLY:O	16:X:113:ARG:NH1	2.39	0.55
12:T:82:LEU:O	12:T:85:VAL:HG22	2.07	0.55
1:I:534:U:HO2'	17:Y:49:ASP:CG	2.15	0.54
31:m:16:ILE:CD1	31:m:25:VAL:HG22	2.38	0.54
1:I:562:U:OP2	35:I:3257:HOH:O	2.18	0.54
1:I:1114:C:N4	1:I:1115:G:O6	2.39	0.54
1:I:245:G:O2'	1:I:384:A:N1	2.31	0.54
1:I:1792:G:H5'	3:K:204:VAL:HG13	1.89	0.54
7:O:10:VAL:HG23	7:O:49:THR:HG22	1.89	0.54
7:O:32:GLU:C	7:O:33:LEU:HD12	2.33	0.54
27:i:53:LYS:NZ	27:i:55:ILE:O	2.37	0.54
1:I:960:A:OP2	35:I:3260:HOH:O	2.18	0.53
1:I:1365:A:OP2	35:I:3261:HOH:O	2.18	0.53
4:L:8:LYS:NZ	4:L:195:GLY:O	2.33	0.53
14:V:117:ASP:O	35:V:201:HOH:O	2.18	0.53
1:I:374:A:O2'	35:I:3258:HOH:O	2.18	0.53
4:L:12:THR:HG22	4:L:13:ARG:N	2.22	0.53
1:I:276:U:O2'	1:I:278:A:N7	2.41	0.53
1:I:1345:C:OP1	35:I:3256:HOH:O	2.18	0.53
5:M:106:LYS:HG3	5:M:200:LEU:HD23	1.89	0.53
1:I:259:G:O2'	1:I:621:A:O2'	2.25	0.53
1:I:2788:C:O2'	1:I:2809:A:N3	2.38	0.53
6:N:162:SER:N	6:N:165:GLU:OE2	2.40	0.53
24:f:41:GLU:OE2	24:f:44:LYS:NZ	2.27	0.53
15:W:4:LYS:O	15:W:8:ILE:HD12	2.08	0.53
2:J:76:G:OP1	22:d:9:ARG:NH1	2.41	0.53
8:P:125:THR:O	8:P:125:THR:HG22	2.08	0.53
18:Z:22:LEU:HD12	18:Z:23:GLU:O	2.09	0.53
20:b:8:LEU:HD23	20:b:50:LEU:HD21	1.91	0.53
5:M:106:LYS:CG	5:M:200:LEU:HD23	2.39	0.53
18:Z:14:VAL:CG1	18:Z:20:VAL:HG11	2.38	0.53
8:P:48:GLU:OE1	8:P:52:ALA:HB2	2.09	0.52
1:I:652:U:OP1	1:I:654:A:N6	2.41	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:a:95:ARG:O	35:a:201:HOH:O	2.18	0.52
27:i:6:ASN:ND2	35:i:102:HOH:O	2.42	0.52
10:R:4:PHE:O	17:Y:64:ARG:NH2	2.43	0.52
1:I:2866:U:H1'	1:I:2867:G:OP2	2.10	0.52
1:I:200:U:O2'	24:f:22:LEU:HD23	2.09	0.52
4:L:156:PHE:CE1	10:R:81:ILE:HD13	2.45	0.52
25:g:17:GLU:O	25:g:21:LEU:HD23	2.10	0.52
1:I:580:U:O3'	17:Y:31:VAL:HG13	2.10	0.52
1:I:2340:A:N3	35:I:3392:HOH:O	2.35	0.51
21:c:98:SER:O	21:c:99:ASN:OD1	2.29	0.51
1:I:2144:G:O2'	1:I:2147:A:N6	2.42	0.51
1:I:1074:G:OP1	1:I:2474:U:O2'	2.27	0.51
1:I:784:G:H5'	1:I:785:G:OP1	2.11	0.51
1:I:1779:U:OP2	1:I:1784:A:N6	2.32	0.51
3:K:51:THR:CG2	3:K:54:ILE:HD12	2.39	0.51
1:I:727:A:C2	3:K:9:THR:HG21	2.45	0.50
1:I:2012:G:OP2	35:I:3266:HOH:O	2.19	0.50
19:a:4:ILE:HD12	19:a:106:VAL:HG22	1.93	0.50
1:I:2555:U:OP2	35:I:3262:HOH:O	2.19	0.50
1:I:188:G:N7	35:I:3393:HOH:O	2.35	0.50
1:I:1237:A:OP1	35:I:3255:HOH:O	2.18	0.50
10:R:31:GLU:HG2	10:R:142:ILE:HG23	1.94	0.50
15:W:8:ILE:HD12	15:W:8:ILE:H	1.76	0.50
20:b:50:LEU:HD23	25:g:26:PHE:CZ	2.47	0.50
1:I:1058:U:N3	1:I:1081:U:O2	2.45	0.50
1:I:2653:U:OP2	35:I:3264:HOH:O	2.19	0.50
1:I:1045:C:O2	1:I:1047:G:N1	2.44	0.50
1:I:2134:A:N6	1:I:2157:G:O2'	2.45	0.50
16:X:103:ARG:NH1	35:X:203:HOH:O	2.44	0.50
1:I:1509:A:O2'	1:I:1510:G:OP2	2.26	0.50
12:T:77:ILE:CD1	12:T:108:ALA:HB1	2.42	0.50
15:W:24:THR:HG23	15:W:40:ILE:O	2.12	0.50
20:b:50:LEU:HD23	25:g:26:PHE:CE2	2.47	0.49
1:I:1750:G:O2'	1:I:2860:A:N1	2.41	0.49
1:I:1913:A:H3'	1:I:1914:C:H5'	1.93	0.49
1:I:2430:A:N3	1:I:2430:A:H2'	2.26	0.49
1:I:2331:G:O2'	1:I:2336:A:N1	2.38	0.49
21:c:72:ILE:HD11	21:c:83:VAL:HG22	1.93	0.49
9:Q:117:MET:HG2	9:Q:125:MET:HE3	1.95	0.49
6:N:36:LEU:HD21	6:N:99:PHE:CZ	2.48	0.49
18:Z:38:VAL:HG12	18:Z:59:ILE:HD12	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:386:G:N7	35:I:3399:HOH:O	2.35	0.49
1:I:2552:OMU:HM23	1:I:2554:U:C6	2.48	0.49
8:P:40:THR:HG22	8:P:43:ASN:OD1	2.13	0.49
1:I:223:A:N1	1:I:407:G:O2'	2.43	0.49
6:N:36:LEU:HD21	6:N:99:PHE:CE1	2.48	0.49
15:W:54:VAL:O	15:W:54:VAL:HG22	2.13	0.49
19:a:7:HIS:ND1	19:a:10:ALA:HB2	2.28	0.49
21:c:72:ILE:CD1	21:c:83:VAL:HG22	2.43	0.48
1:I:1024:G:OP2	1:I:1026:G:OP1	2.31	0.48
1:I:883:G:O6	1:I:893:C:N4	2.41	0.48
8:P:115:VAL:HG13	8:P:115:VAL:O	2.13	0.48
12:T:79:LEU:CD1	12:T:112:LEU:HD12	2.43	0.48
1:I:1086:A:O2'	1:I:1103:A:N1	2.45	0.48
7:O:98:VAL:HG12	7:O:100:GLY:H	1.78	0.48
23:e:33:ALA:N	23:e:64:ASP:OD1	2.44	0.48
28:j:52:ALA:O	28:j:53:LYS:C	2.57	0.48
1:I:2278:A:OP2	23:e:12:ASN:ND2	2.47	0.48
13:U:135:VAL:HG23	13:U:135:VAL:O	2.14	0.48
1:I:463:G:N2	1:I:466:A:OP2	2.36	0.48
4:L:12:THR:HG22	4:L:13:ARG:H	1.78	0.48
6:N:12:VAL:HG13	6:N:172:ALA:CB	2.44	0.48
12:T:77:ILE:HD13	12:T:108:ALA:HB1	1.96	0.48
7:O:10:VAL:O	7:O:10:VAL:HG13	2.14	0.48
1:I:215:G:O3'	1:I:216:A:H4'	2.13	0.47
1:I:2471:A:OP2	35:I:3270:HOH:O	2.20	0.47
5:M:15:SER:HB3	5:M:18:THR:HG22	1.96	0.47
6:N:57:LEU:HD12	6:N:87:CYS:SG	2.54	0.47
7:O:9:VAL:O	7:O:50:LEU:N	2.46	0.47
1:I:125:A:OP2	29:k:19:ARG:NH1	2.43	0.47
1:I:864:G:O2'	1:I:914:G:O6	2.32	0.47
4:L:177:VAL:HG13	4:L:177:VAL:O	2.15	0.47
1:I:574:A:N7	35:I:3400:HOH:O	2.35	0.47
1:I:1358:G:OP2	35:I:3274:HOH:O	2.20	0.47
1:I:2134:A:OP2	1:I:2157:G:N2	2.48	0.47
1:I:2430:A:O2'	1:I:2431:U:H5'	2.15	0.47
1:I:160:A:N3	1:I:2208:C:O2'	2.44	0.47
1:I:642:U:O2'	1:I:644:A:N7	2.41	0.47
1:I:1141:U:H4'	1:I:1142:A:O4'	2.14	0.47
1:I:2134:A:OP2	1:I:2156:G:N1	2.48	0.47
1:I:2484:G:O2'	13:U:123:LYS:O	2.31	0.47
1:I:2659:G:OP2	35:I:3273:HOH:O	2.20	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2880:C:O3'	14:V:90:ARG:NH2	2.47	0.47
8:P:132:PHE:CE2	8:P:142:VAL:HG22	2.50	0.47
1:I:745:1MG:O2'	1:I:748:G:O2'	2.31	0.47
1:I:2029:G:N1	1:I:2033:A:OP2	2.41	0.47
8:P:71:LYS:HB2	8:P:108:VAL:HG21	1.96	0.47
19:a:29:VAL:HG13	19:a:55:ILE:HD11	1.96	0.47
19:a:64:ALA:O	19:a:65:ASP:OD1	2.32	0.47
26:h:5:ILE:HD11	26:h:57:VAL:HG21	1.96	0.47
1:I:964:C:O2'	1:I:2273:A:N3	2.44	0.47
1:I:1311:G:OP2	1:I:1311:G:N2	2.35	0.47
9:Q:80:LEU:HD11	9:Q:136:MET:CE	2.45	0.47
1:I:58:G:O2'	1:I:73:A:N1	2.38	0.46
24:f:50:ARG:NE	35:f:101:HOH:O	2.40	0.46
1:I:2304:G:H22	1:I:2312:U:H3	1.63	0.46
1:I:2680:U:O2'	1:I:2681:C:P	2.73	0.46
1:I:555:G:HO2'	1:I:556:A:H8	1.63	0.46
16:X:114:LEU:HD23	16:X:114:LEU:H	1.80	0.46
1:I:205:G:O2'	1:I:206:U:OP2	2.28	0.46
1:I:577:G:O2'	1:I:1254:A:OP1	2.33	0.46
21:c:74:ASN:O	21:c:75:ALA:HB3	2.16	0.46
8:P:103:VAL:HG22	8:P:103:VAL:O	2.16	0.46
14:V:2:ARG:NH1	14:V:5:LYS:O	2.49	0.46
22:d:4:ILE:CG2	22:d:42:LEU:HD22	2.46	0.46
1:I:1420:A:O2'	1:I:2211:A:N7	2.49	0.46
19:a:109:ASP:OD1	19:a:110:ARG:N	2.48	0.46
1:I:138:U:HO2'	1:I:139:U:P	2.30	0.46
3:K:270:ARG:NH1	3:K:271:ARG:HG2	2.31	0.46
1:I:2125:G:H2'	1:I:2126:A:O4'	2.17	0.45
1:I:2595:G:N2	1:I:2598:A:OP2	2.40	0.45
1:I:1508:A:O2'	1:I:1509:A:O4'	2.35	0.45
1:I:2576:G:O2'	1:I:2579:C:OP2	2.26	0.45
16:X:81:VAL:HG11	16:X:84:ILE:HD11	1.98	0.45
1:I:205:G:HO2'	1:I:206:U:P	2.37	0.45
1:I:1792:G:H5''	3:K:204:VAL:HG13	1.96	0.45
9:Q:122:ILE:HA	9:Q:125:MET:HE1	1.97	0.45
7:O:96:ALA:N	7:O:128:GLN:O	2.48	0.45
10:R:96:ARG:O	10:R:96:ARG:HG3	2.16	0.45
16:X:4:ILE:HD12	16:X:4:ILE:H	1.82	0.45
2:J:5:U:O2'	2:J:27:C:O2	2.35	0.45
1:I:2635:A:O2'	4:L:81:GLU:OE2	2.30	0.45
22:d:63:ILE:HD12	22:d:72:VAL:HG21	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:629:G:N3	1:I:639:U:O2'	2.48	0.45
7:O:155:GLU:OE2	7:O:158:LYS:N	2.45	0.45
8:P:111:ALA:O	8:P:115:VAL:HG12	2.16	0.45
1:I:1824:G:O2'	3:K:252:THR:HG21	2.17	0.45
1:I:2865:U:P	1:I:2866:U:HO2'	2.34	0.45
6:N:63:GLN:NE2	6:N:90:THR:O	2.48	0.45
1:I:1912:A:C6	1:I:1918:A:C2	3.04	0.44
13:U:28:PHE:N	13:U:104:GLU:OE1	2.49	0.44
15:W:106:LEU:C	15:W:106:LEU:HD23	2.42	0.44
21:c:98:SER:O	21:c:99:ASN:CG	2.60	0.44
1:I:668:A:H2'	1:I:670:A:H62	1.82	0.44
5:M:131:THR:HG22	5:M:160:ALA:O	2.17	0.44
8:P:83:LYS:O	8:P:90:LEU:HD12	2.17	0.44
8:P:9:VAL:HG12	8:P:10:ALA:N	2.32	0.44
9:Q:15:ALA:HB1	9:Q:46:THR:HG21	1.98	0.44
1:I:2571:U:O2'	4:L:151:THR:O	2.35	0.44
1:I:2627:G:O2'	1:I:2781:A:N1	2.44	0.44
7:O:101:ASN:O	7:O:102:VAL:HG23	2.18	0.44
13:U:78:LEU:HD23	13:U:79:ALA:N	2.32	0.44
1:I:858:G:OP1	23:e:78:LYS:NZ	2.35	0.44
22:d:2:PHE:HB2	22:d:61:LEU:HD22	1.99	0.44
26:h:5:ILE:HD12	26:h:45:ARG:NH2	2.33	0.44
6:N:40:VAL:HG21	6:N:43:ALA:HB2	1.99	0.44
9:Q:80:LEU:HB2	9:Q:138:LEU:HD11	1.98	0.44
1:I:643:A:N1	1:I:2369:A:O2'	2.51	0.44
1:I:2185:U:H2'	1:I:2186:G:C8	2.53	0.43
2:J:8:C:OP1	15:W:15:ARG:NH2	2.43	0.43
15:W:35:ILE:HG22	15:W:53:THR:HG23	1.98	0.43
29:k:21:ARG:NH1	29:k:30:VAL:HG11	2.33	0.43
1:I:987:C:O2'	1:I:1000:A:N3	2.44	0.43
1:I:2680:U:O2'	1:I:2681:C:O5'	2.36	0.43
6:N:20:PHE:O	6:N:21:ASN:OD1	2.35	0.43
8:P:12:LEU:HD11	8:P:30:LEU:HD11	2.00	0.43
1:I:930:G:H1'	26:h:25:LEU:HD21	2.00	0.43
1:I:2602:A:H2'	1:I:2602:A:N3	2.34	0.43
1:I:760:G:N7	35:I:3413:HOH:O	2.36	0.43
1:I:2225:A:H1'	1:I:2226:C:OP2	2.19	0.43
6:N:40:VAL:HG13	6:N:41:GLY:N	2.34	0.43
1:I:2162:G:C4'	1:I:2163:A:OP1	2.66	0.43
18:Z:40:MET:HE2	18:Z:49:ILE:HG12	1.99	0.43
21:c:36:VAL:HG12	21:c:37:GLU:N	2.34	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:C:H2'	1:I:158:U:O4'	2.18	0.43
1:I:1071:G:N3	1:I:1089:A:O2'	2.42	0.43
1:I:1620:G:N7	35:I:3415:HOH:O	2.37	0.43
19:a:72:THR:HG21	19:a:108:SER:HB3	1.99	0.43
1:I:1080:A:O2'	9:Q:128:SER:N	2.51	0.43
3:K:157:SER:O	3:K:195:VAL:HG11	2.18	0.43
9:Q:88:SER:OG	9:Q:89:GLY:N	2.52	0.43
1:I:2831:G:OP2	4:L:59:ARG:NH2	2.43	0.43
1:I:1679:A:N3	35:I:3410:HOH:O	2.36	0.42
1:I:2124:G:H2'	1:I:2125:G:O4'	2.18	0.42
9:Q:33:VAL:CG2	9:Q:61:VAL:HG21	2.48	0.42
10:R:142:ILE:HG22	10:R:142:ILE:OXT	2.19	0.42
1:I:2291:U:O2'	1:I:2374:C:O2	2.38	0.42
4:L:13:ARG:NH1	16:X:75:GLN:OE1	2.50	0.42
1:I:984:A:N3	1:I:984:A:H2'	2.33	0.42
1:I:1003:G:O2'	1:I:1010:A:N1	2.46	0.42
1:I:1129:A:N6	1:I:2491:U:OP1	2.51	0.42
19:a:15:GLN:NE2	35:a:204:HOH:O	2.51	0.42
1:I:218:A:OP2	35:I:3279:HOH:O	2.21	0.42
1:I:1059:G:H4'	9:Q:113:LYS:HE2	2.00	0.42
1:I:2375:G:N2	1:I:2378:A:OP2	2.44	0.42
6:N:136:ILE:HG22	6:N:136:ILE:O	2.19	0.42
14:V:67:PHE:O	14:V:71:ARG:N	2.48	0.42
22:d:40:ILE:HD12	22:d:42:LEU:HD21	2.01	0.42
5:M:188:MET:HE2	5:M:193:VAL:HG22	2.01	0.42
1:I:2119:A:N6	1:I:2169:A:N7	2.67	0.42
30:l:31:HIS:ND1	30:l:32:ILE:HG13	2.35	0.42
1:I:396:G:OP2	24:f:10:LYS:NZ	2.48	0.42
1:I:504:A:H1'	1:I:505:A:P	2.60	0.42
1:I:1245:G:OP1	12:T:13:LYS:NZ	2.52	0.42
9:Q:21:SER:HB2	9:Q:22:PRO:HD3	2.01	0.42
17:Y:109:LEU:HD11	18:Z:40:MET:HE1	2.01	0.42
21:c:13:VAL:HG21	21:c:39:ILE:HD12	2.01	0.42
24:f:65:ASP:OD1	24:f:65:ASP:N	2.52	0.42
1:I:324:A:N6	1:I:338:G:O2'	2.49	0.42
1:I:1799:G:OP1	3:K:258:ARG:NH1	2.42	0.42
3:K:155:ALA:HB2	3:K:162:VAL:HG23	2.01	0.42
24:f:74:ARG:O	24:f:74:ARG:HG2	2.20	0.42
1:I:2831:G:O2'	1:I:2884:U:OP1	2.37	0.42
3:K:130:LEU:HD11	3:K:135:ILE:HG13	2.02	0.42
7:O:38:ASN:OD1	7:O:39:ASP:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:130:VAL:HG12	8:P:131:SER:N	2.35	0.42
18:Z:2:TYR:CD1	18:Z:2:TYR:C	2.98	0.42
21:c:54:GLN:N	21:c:55:PRO:CD	2.83	0.42
1:I:404:A:C4'	1:I:405:U:OP2	2.68	0.41
1:I:545:U:O2	1:I:545:U:O5'	2.37	0.41
7:O:33:LEU:HD13	7:O:79:VAL:HG12	2.01	0.41
7:O:127:THR:HG22	7:O:128:GLN:N	2.35	0.41
14:V:106:ASP:OD1	14:V:106:ASP:N	2.53	0.41
1:I:1095:A:N6	9:Q:9:VAL:HG13	2.19	0.41
1:I:2636:C:H4'	4:L:81:GLU:OE1	2.20	0.41
20:b:57:VAL:HG22	20:b:58:VAL:N	2.35	0.41
1:I:631:A:N3	1:I:2415:G:O2'	2.47	0.41
1:I:2111:U:H4'	1:I:2112:G:OP2	2.20	0.41
1:I:2251:OMG:HM23	1:I:2251:OMG:H1'	1.92	0.41
1:I:1408:G:O6	35:I:3282:HOH:O	2.21	0.41
3:K:263:THR:O	3:K:267:ILE:HD12	2.21	0.41
1:I:560:C:O2'	17:Y:48:ARG:NH1	2.54	0.41
1:I:1827:U:OP1	1:I:1971:U:O2'	2.32	0.41
6:N:116:GLY:O	6:N:117:LEU:HD22	2.20	0.41
9:Q:28:LEU:HD11	9:Q:38:PHE:CG	2.56	0.41
21:c:72:ILE:HD12	21:c:96:PHE:CE1	2.55	0.41
28:j:47:VAL:HG12	28:j:48:ILE:N	2.36	0.41
1:I:1266:G:O2'	1:I:2012:G:O6	2.32	0.41
1:I:1846:G:H2'	1:I:1847:A:O4'	2.21	0.41
11:S:49:ARG:HD2	11:S:49:ARG:O	2.21	0.41
12:T:135:ILE:HG22	12:T:140:GLY:HA3	2.03	0.41
18:Z:51:VAL:HG23	18:Z:51:VAL:O	2.21	0.41
1:I:1421:G:N2	1:I:1495:A:N1	2.61	0.41
1:I:1664:A:N3	11:S:67:LYS:NZ	2.69	0.41
1:I:2447:G:H4'	1:I:2448:A:O5'	2.20	0.41
1:I:2572:A:OP2	4:L:149:ASN:O	2.38	0.41
3:K:141:VAL:CG2	3:K:190:ALA:HB1	2.50	0.41
6:N:108:VAL:N	6:N:109:PRO:CD	2.84	0.41
14:V:61:ALA:O	14:V:65:LEU:HD23	2.20	0.41
1:I:1326:U:O2'	1:I:2010:G:O2'	2.37	0.41
1:I:2628:C:OP2	35:I:3283:HOH:O	2.22	0.41
1:I:981:A:OP2	1:I:982:C:N4	2.42	0.41
22:d:26:PHE:CE2	22:d:89:ILE:HD12	2.56	0.41
6:N:85:ILE:O	6:N:85:ILE:HG13	2.22	0.40
6:N:117:LEU:HD11	6:N:130:MET:HE2	2.03	0.40
23:e:56:ASP:OD1	23:e:58:THR:HG22	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:271:G:C4'	1:I:272:A:OP1	2.69	0.40
1:I:2552:OMU:O5'	1:I:2552:OMU:H6	2.21	0.40
9:Q:80:LEU:HD12	9:Q:80:LEU:C	2.46	0.40
22:d:65:VAL:O	22:d:65:VAL:HG23	2.20	0.40
1:I:1631:G:N2	1:I:1634:A:OP2	2.36	0.40
8:P:132:PHE:N	8:P:142:VAL:HG23	2.35	0.40
16:X:12:GLN:HG2	16:X:12:GLN:O	2.22	0.40
1:I:138:U:O2'	1:I:139:U:P	2.78	0.40
6:N:20:PHE:O	6:N:21:ASN:C	2.65	0.40
9:Q:49:ILE:CG2	9:Q:50:GLU:N	2.84	0.40
9:Q:59:ILE:O	9:Q:59:ILE:HG13	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	K	269/271 (99%)	264 (98%)	5 (2%)	0	100	100
4	L	207/209 (99%)	202 (98%)	5 (2%)	0	100	100
5	M	199/201 (99%)	199 (100%)	0	0	100	100
6	N	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
7	O	174/176 (99%)	170 (98%)	4 (2%)	0	100	100
8	P	147/149 (99%)	145 (99%)	2 (1%)	0	100	100
9	Q	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
10	R	140/142 (99%)	140 (100%)	0	0	100	100
11	S	120/122 (98%)	119 (99%)	1 (1%)	0	100	100
12	T	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
13	U	133/136 (98%)	132 (99%)	1 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	V	118/120 (98%)	117 (99%)	1 (1%)	0	100	100
15	W	114/116 (98%)	114 (100%)	0	0	100	100
16	X	112/114 (98%)	112 (100%)	0	0	100	100
17	Y	115/117 (98%)	115 (100%)	0	0	100	100
18	Z	101/103 (98%)	100 (99%)	1 (1%)	0	100	100
19	a	108/110 (98%)	106 (98%)	1 (1%)	1 (1%)	14	43
20	b	91/93 (98%)	89 (98%)	2 (2%)	0	100	100
21	c	100/102 (98%)	96 (96%)	4 (4%)	0	100	100
22	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
23	e	73/75 (97%)	72 (99%)	1 (1%)	0	100	100
24	f	75/77 (97%)	73 (97%)	2 (3%)	0	100	100
25	g	60/62 (97%)	58 (97%)	2 (3%)	0	100	100
26	h	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	i	54/56 (96%)	54 (100%)	0	0	100	100
28	j	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
29	k	44/46 (96%)	44 (100%)	0	0	100	100
30	l	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
31	m	36/38 (95%)	36 (100%)	0	0	100	100
All	All	3297/3356 (98%)	3245 (98%)	51 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	a	64	ALA

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	K	216/216 (100%)	216 (100%)	0	100	100
4	L	164/164 (100%)	164 (100%)	0	100	100
5	M	165/165 (100%)	165 (100%)	0	100	100
6	N	148/148 (100%)	148 (100%)	0	100	100
7	O	137/137 (100%)	137 (100%)	0	100	100
8	P	114/114 (100%)	114 (100%)	0	100	100
9	Q	104/104 (100%)	104 (100%)	0	100	100
10	R	116/116 (100%)	116 (100%)	0	100	100
11	S	103/103 (100%)	103 (100%)	0	100	100
12	T	103/103 (100%)	103 (100%)	0	100	100
13	U	108/108 (100%)	108 (100%)	0	100	100
14	V	100/100 (100%)	100 (100%)	0	100	100
15	W	86/86 (100%)	86 (100%)	0	100	100
16	X	99/99 (100%)	99 (100%)	0	100	100
17	Y	89/89 (100%)	89 (100%)	0	100	100
18	Z	84/84 (100%)	84 (100%)	0	100	100
19	a	93/93 (100%)	93 (100%)	0	100	100
20	b	80/80 (100%)	80 (100%)	0	100	100
21	c	83/83 (100%)	83 (100%)	0	100	100
22	d	78/78 (100%)	78 (100%)	0	100	100
23	e	57/57 (100%)	57 (100%)	0	100	100
24	f	67/67 (100%)	67 (100%)	0	100	100
25	g	54/54 (100%)	54 (100%)	0	100	100
26	h	48/48 (100%)	48 (100%)	0	100	100
27	i	47/47 (100%)	47 (100%)	0	100	100
28	j	45/45 (100%)	45 (100%)	0	100	100
29	k	38/38 (100%)	38 (100%)	0	100	100
30	l	51/51 (100%)	51 (100%)	0	100	100
31	m	34/34 (100%)	34 (100%)	0	100	100
All	All	2711/2711 (100%)	2711 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19)

such sidechains are listed below:

Mol	Chain	Res	Type
3	K	90	ASN
3	K	143	ASN
3	K	153	GLN
4	L	150	GLN
4	L	173	GLN
6	N	52	ASN
7	O	73	ASN
7	O	104	ASN
8	P	128	HIS
13	U	13	HIS
14	V	9	GLN
15	W	38	GLN
19	a	9	HIS
21	c	74	ASN
22	d	44	HIS
24	f	36	HIS
25	g	27	ASN
25	g	39	GLN
27	i	6	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2896/2904 (99%)	359 (12%)	18 (0%)
2	J	117/118 (99%)	17 (14%)	0
All	All	3013/3022 (99%)	376 (12%)	18 (0%)

All (376) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	G
1	I	10	A
1	I	15	G
1	I	34	U
1	I	45	G
1	I	46	G
1	I	51	G
1	I	58	G
1	I	71	A
1	I	74	A
1	I	75	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	101	A
1	I	102	U
1	I	118	A
1	I	120	U
1	I	125	A
1	I	139	U
1	I	163	C
1	I	165	A
1	I	181	A
1	I	196	A
1	I	199	A
1	I	215	G
1	I	216	A
1	I	221	A
1	I	222	A
1	I	228	C
1	I	248	G
1	I	264	C
1	I	265	A
1	I	266	G
1	I	272	A
1	I	276	U
1	I	279	A
1	I	311	A
1	I	329	G
1	I	330	A
1	I	345	A
1	I	346	A
1	I	353	C
1	I	362	A
1	I	371	A
1	I	372	G
1	I	386	G
1	I	396	G
1	I	405	U
1	I	411	G
1	I	412	A
1	I	424	G
1	I	456	C
1	I	457	A
1	I	481	G
1	I	489	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	490	C
1	I	491	G
1	I	504	A
1	I	505	A
1	I	509	C
1	I	529	A
1	I	532	A
1	I	546	U
1	I	547	A
1	I	548	G
1	I	550	C
1	I	551	G
1	I	563	A
1	I	573	U
1	I	575	A
1	I	603	A
1	I	613	A
1	I	614	A
1	I	615	U
1	I	627	A
1	I	637	A
1	I	645	C
1	I	647	G
1	I	653	U
1	I	654	A
1	I	677	A
1	I	686	U
1	I	721	A
1	I	730	A
1	I	747	5MU
1	I	775	G
1	I	776	G
1	I	782	A
1	I	784	G
1	I	785	G
1	I	805	G
1	I	812	C
1	I	819	A
1	I	827	U
1	I	828	U
1	I	846	U
1	I	847	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	858	G
1	I	859	G
1	I	877	A
1	I	885	C
1	I	893	C
1	I	896	A
1	I	897	C
1	I	910	A
1	I	914	G
1	I	915	C
1	I	917	A
1	I	931	U
1	I	941	A
1	I	946	C
1	I	961	C
1	I	974	G
1	I	983	A
1	I	996	A
1	I	1012	U
1	I	1013	C
1	I	1027	A
1	I	1033	U
1	I	1040	A
1	I	1045	C
1	I	1046	A
1	I	1047	G
1	I	1051	G
1	I	1056	G
1	I	1070	A
1	I	1071	G
1	I	1083	U
1	I	1088	A
1	I	1111	A
1	I	1112	G
1	I	1116	G
1	I	1119	U
1	I	1132	U
1	I	1133	A
1	I	1135	C
1	I	1136	G
1	I	1142	A
1	I	1151	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	1173	U
1	I	1174	U
1	I	1175	A
1	I	1176	U
1	I	1180	U
1	I	1212	G
1	I	1238	G
1	I	1250	G
1	I	1253	A
1	I	1256	G
1	I	1266	G
1	I	1271	G
1	I	1272	A
1	I	1300	G
1	I	1301	A
1	I	1321	A
1	I	1340	U
1	I	1341	G
1	I	1352	U
1	I	1365	A
1	I	1368	G
1	I	1378	A
1	I	1379	U
1	I	1383	A
1	I	1386	C
1	I	1416	G
1	I	1418	G
1	I	1428	C
1	I	1482	G
1	I	1490	A
1	I	1493	C
1	I	1494	A
1	I	1506	U
1	I	1508	A
1	I	1510	G
1	I	1515	A
1	I	1524	G
1	I	1534	U
1	I	1535	A
1	I	1536	C
1	I	1544	A
1	I	1569	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	1578	U
1	I	1584	U
1	I	1585	C
1	I	1587	G
1	I	1608	A
1	I	1634	A
1	I	1647	U
1	I	1648	U
1	I	1649	G
1	I	1674	G
1	I	1715	G
1	I	1729	U
1	I	1730	C
1	I	1733	G
1	I	1738	G
1	I	1758	U
1	I	1764	C
1	I	1773	A
1	I	1791	A
1	I	1800	C
1	I	1801	A
1	I	1816	C
1	I	1829	A
1	I	1870	C
1	I	1872	A
1	I	1873	G
1	I	1876	A
1	I	1912	A
1	I	1913	A
1	I	1914	C
1	I	1915	3TD
1	I	1929	G
1	I	1930	G
1	I	1936	A
1	I	1937	A
1	I	1955	U
1	I	1967	C
1	I	1970	A
1	I	1971	U
1	I	1972	G
1	I	1991	U
1	I	1993	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	1997	C
1	I	2020	A
1	I	2022	U
1	I	2023	C
1	I	2027	G
1	I	2031	A
1	I	2033	A
1	I	2043	C
1	I	2055	C
1	I	2056	G
1	I	2060	A
1	I	2061	G
1	I	2062	A
1	I	2069	G7M
1	I	2095	A
1	I	2110	G
1	I	2111	U
1	I	2112	G
1	I	2115	G
1	I	2116	G
1	I	2117	A
1	I	2118	U
1	I	2123	G
1	I	2124	G
1	I	2126	A
1	I	2127	G
1	I	2128	G
1	I	2131	U
1	I	2132	U
1	I	2133	G
1	I	2142	A
1	I	2146	C
1	I	2147	A
1	I	2157	G
1	I	2158	A
1	I	2159	G
1	I	2161	C
1	I	2162	G
1	I	2163	A
1	I	2164	C
1	I	2169	A
1	I	2171	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	2172	U
1	I	2173	A
1	I	2189	U
1	I	2190	G
1	I	2198	A
1	I	2203	U
1	I	2204	G
1	I	2211	A
1	I	2212	A
1	I	2225	A
1	I	2226	C
1	I	2238	G
1	I	2239	G
1	I	2278	A
1	I	2283	C
1	I	2287	A
1	I	2297	A
1	I	2305	U
1	I	2308	G
1	I	2309	A
1	I	2322	A
1	I	2325	G
1	I	2333	A
1	I	2345	G
1	I	2347	C
1	I	2350	C
1	I	2361	G
1	I	2383	G
1	I	2385	C
1	I	2396	G
1	I	2401	U
1	I	2402	U
1	I	2403	C
1	I	2406	A
1	I	2423	U
1	I	2425	A
1	I	2426	A
1	I	2429	G
1	I	2430	A
1	I	2431	U
1	I	2435	A
1	I	2441	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	2445	2MG
1	I	2448	A
1	I	2459	A
1	I	2466	C
1	I	2470	G
1	I	2475	C
1	I	2476	A
1	I	2491	U
1	I	2502	G
1	I	2505	G
1	I	2506	U
1	I	2518	A
1	I	2529	G
1	I	2547	A
1	I	2554	U
1	I	2566	A
1	I	2567	G
1	I	2585	U
1	I	2602	A
1	I	2603	G
1	I	2609	U
1	I	2613	U
1	I	2615	U
1	I	2629	U
1	I	2630	G
1	I	2661	G
1	I	2663	G
1	I	2671	G
1	I	2681	C
1	I	2689	U
1	I	2690	U
1	I	2714	G
1	I	2718	G
1	I	2726	A
1	I	2733	A
1	I	2744	G
1	I	2748	A
1	I	2778	A
1	I	2791	G
1	I	2793	C
1	I	2800	A
1	I	2818	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	2820	A
1	I	2835	A
1	I	2849	U
1	I	2861	U
1	I	2867	G
1	I	2872	A
1	I	2873	A
1	I	2880	C
1	I	2883	A
1	I	2884	U
1	I	2885	G
1	I	2904	U
2	J	3	C
2	J	9	G
2	J	15	A
2	J	16	G
2	J	17	C
2	J	24	G
2	J	25	U
2	J	32	U
2	J	35	C
2	J	56	G
2	J	67	G
2	J	88	C
2	J	89	U
2	J	90	C
2	J	99	A
2	J	109	A
2	J	119	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	100	U
1	I	138	U
1	I	271	G
1	I	404	A
1	I	489	G
1	I	504	A
1	I	784	G
1	I	1543	G
1	I	1757	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	2162	G
1	I	2225	A
1	I	2401	U
1	I	2402	U
1	I	2425	A
1	I	2447	G
1	I	2680	U
1	I	2866	U
1	I	2903	U

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

25 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMC	I	2498	1	19,22,23	3.12	8 (42%)	26,31,34	0.74	0
1	2MA	I	2503	32,1	22,25,26	3.72	8 (36%)	33,37,40	2.31	8 (24%)
1	PSU	I	2504	1	18,21,22	4.02	6 (33%)	22,30,33	1.87	6 (27%)
1	PSU	I	1911	1	18,21,22	4.21	6 (33%)	22,30,33	1.86	6 (27%)
1	1MG	I	745	1	22,26,27	2.60	7 (31%)	33,39,42	2.65	8 (24%)
1	6MZ	I	1618	1	22,25,26	3.29	4 (18%)	30,36,39	2.38	11 (36%)
1	5MU	I	1939	1	19,22,23	7.22	8 (42%)	28,32,35	3.43	10 (35%)
1	PSU	I	2605	1	18,21,22	3.99	7 (38%)	22,30,33	1.80	5 (22%)
1	6MZ	I	2030	1	22,25,26	3.26	5 (22%)	30,36,39	2.45	12 (40%)
1	PSU	I	2580	1	18,21,22	3.93	8 (44%)	22,30,33	2.00	6 (27%)
1	G7M	I	2069	1	23,26,27	2.88	8 (34%)	35,39,42	2.65	11 (31%)
1	3TD	I	1915	1	18,22,23	4.19	6 (33%)	22,32,35	1.53	2 (9%)
1	PSU	I	1917	1	18,21,22	0.90	1 (5%)	22,30,33	0.62	0
1	5MU	I	747	1	19,22,23	7.21	8 (42%)	28,32,35	3.52	10 (35%)
1	PSU	I	2604	1	18,21,22	3.98	6 (33%)	22,30,33	2.00	6 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	2MG	I	1835	1	23,26,27	2.85	8 (34%)	32,38,41	2.24	12 (37%)
1	2MG	I	2445	1	23,26,27	2.75	8 (34%)	32,38,41	2.20	12 (37%)
1	PSU	I	955	1	18,21,22	3.95	7 (38%)	22,30,33	2.05	6 (27%)
1	H2U	I	2449	1	18,21,22	2.97	5 (27%)	21,30,33	2.09	5 (23%)
1	PSU	I	746	1	18,21,22	4.01	6 (33%)	22,30,33	1.69	5 (22%)
1	PSU	I	2457	1	18,21,22	3.98	7 (38%)	22,30,33	1.98	6 (27%)
1	OMU	I	2552	1	19,22,23	3.10	8 (42%)	26,31,34	1.72	4 (15%)
1	OMG	I	2251	1	23,26,27	2.91	8 (34%)	33,38,41	2.13	10 (30%)
13	4D4	U	81	13	9,11,12	2.41	2 (22%)	8,13,15	0.85	0
1	5MC	I	1962	1	18,22,23	3.62	8 (44%)	26,32,35	1.05	2 (7%)

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	OMC	I	2498	1	-	0/9/27/28	0/2/2/2
1	2MA	I	2503	32,1	-	2/7/25/26	0/3/3/3
1	PSU	I	2504	1	-	0/7/25/26	0/2/2/2
1	PSU	I	1911	1	-	1/7/25/26	0/2/2/2
1	1MG	I	745	1	-	0/7/25/26	0/3/3/3
1	6MZ	I	1618	1	-	1/9/27/28	0/3/3/3
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2
1	6MZ	I	2030	1	-	1/9/27/28	0/3/3/3
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	G7M	I	2069	1	-	3/7/25/26	0/3/3/3
1	3TD	I	1915	1	-	3/7/25/26	0/2/2/2
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2604	1	-	0/7/25/26	0/2/2/2
1	2MG	I	1835	1	-	0/9/27/28	0/3/3/3
1	2MG	I	2445	1	-	2/9/27/28	0/3/3/3
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	H2U	I	2449	1	-	0/7/38/39	0/2/2/2
1	PSU	I	746	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	I	2251	1	-	0/9/27/28	0/3/3/3
13	4D4	U	81	13	-	1/11/12/14	-
1	5MC	I	1962	1	-	2/7/25/26	0/2/2/2

All (163) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	747	5MU	C4-C5	20.88	1.79	1.44
1	I	1939	5MU	C4-C5	20.80	1.79	1.44
1	I	1939	5MU	C6-N1	15.31	1.64	1.38
1	I	747	5MU	C6-N1	15.10	1.63	1.38
1	I	1618	6MZ	C6-N6	13.59	1.48	1.34
1	I	2030	6MZ	C6-N6	13.40	1.48	1.34
1	I	1915	3TD	C6-C5	12.35	1.49	1.35
1	I	747	5MU	C6-C5	-12.15	1.14	1.34
1	I	1939	5MU	C6-C5	-11.95	1.14	1.34
1	I	1939	5MU	C4-N3	-11.82	1.16	1.38
1	I	2503	2MA	C4-N3	11.72	1.49	1.34
1	I	747	5MU	C4-N3	-11.62	1.17	1.38
1	I	1911	PSU	C6-C5	11.17	1.48	1.35
1	I	746	PSU	C6-C5	10.78	1.47	1.35
1	I	2457	PSU	C6-C5	10.68	1.47	1.35
1	I	2504	PSU	C6-C5	10.65	1.47	1.35
1	I	2604	PSU	C6-C5	10.63	1.47	1.35
1	I	2605	PSU	C6-C5	10.61	1.47	1.35
1	I	955	PSU	C6-C5	10.51	1.47	1.35
1	I	2580	PSU	C6-C5	10.46	1.47	1.35
1	I	1911	PSU	C2-N1	9.60	1.49	1.36
1	I	1962	5MC	C6-C5	9.22	1.49	1.34
1	I	2504	PSU	C2-N1	9.18	1.49	1.36
1	I	2457	PSU	C2-N1	9.10	1.49	1.36
1	I	746	PSU	C2-N1	9.05	1.49	1.36
1	I	955	PSU	C2-N1	9.04	1.49	1.36
1	I	1915	3TD	C2-N1	9.02	1.48	1.37
1	I	2605	PSU	C2-N1	9.02	1.48	1.36
1	I	2604	PSU	C2-N1	9.01	1.48	1.36
1	I	2449	H2U	C2-N1	8.98	1.48	1.35
1	I	2580	PSU	C2-N1	8.95	1.48	1.36
1	I	2552	OMU	C2-N1	7.28	1.50	1.38
1	I	2251	OMG	C4-N3	7.24	1.51	1.34
1	I	1835	2MG	C2-N3	7.23	1.45	1.31
1	I	2069	G7M	C4-N3	6.77	1.50	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1962	5MC	C4-N3	6.76	1.45	1.34
1	I	2503	2MA	C2-N3	6.75	1.46	1.34
1	I	2445	2MG	C2-N3	6.74	1.44	1.31
1	I	1835	2MG	C4-N3	6.67	1.50	1.34
1	I	2552	OMU	C2-N3	6.62	1.49	1.38
1	I	1911	PSU	C2-N3	6.59	1.48	1.37
1	I	2251	OMG	C2-N2	6.55	1.49	1.34
1	I	2498	OMC	C2-N3	6.41	1.49	1.36
1	I	2069	G7M	C2-N2	6.40	1.49	1.34
1	I	2498	OMC	C6-C5	6.34	1.49	1.35
1	I	2445	2MG	C4-N3	6.32	1.49	1.34
1	I	2449	H2U	C2-N3	6.24	1.49	1.38
1	I	2504	PSU	C2-N3	6.19	1.48	1.37
1	I	2605	PSU	C2-N3	6.17	1.48	1.37
1	I	746	PSU	C2-N3	6.17	1.48	1.37
1	I	2604	PSU	C2-N3	6.16	1.48	1.37
1	I	745	1MG	C2-N3	6.13	1.45	1.34
1	I	1962	5MC	C2-N3	6.13	1.48	1.36
1	I	745	1MG	C4-N3	6.12	1.48	1.34
13	U	81	4D4	CZ-NE	6.11	1.45	1.33
1	I	955	PSU	C2-N3	6.10	1.48	1.37
1	I	745	1MG	C2-N2	6.07	1.45	1.34
1	I	2457	PSU	C2-N3	6.07	1.47	1.37
1	I	2580	PSU	C2-N3	6.02	1.47	1.37
1	I	2251	OMG	C2-N3	5.91	1.47	1.33
1	I	2498	OMC	C4-N4	5.87	1.47	1.33
1	I	2503	2MA	C2-N1	5.76	1.44	1.34
1	I	2552	OMU	C6-C5	5.71	1.48	1.35
1	I	1915	3TD	C6-N1	5.70	1.45	1.36
1	I	2503	2MA	C6-N1	5.67	1.43	1.35
1	I	2069	G7M	C5-N7	-5.62	1.32	1.39
1	I	1835	2MG	C2-N2	5.48	1.45	1.33
1	I	2445	2MG	C2-N2	5.33	1.45	1.33
1	I	2069	G7M	C2-N3	5.12	1.45	1.33
1	I	2498	OMC	C4-N3	5.12	1.44	1.34
1	I	1915	3TD	C2-N3	4.97	1.49	1.38
1	I	2445	2MG	C2-N1	4.97	1.44	1.36
1	I	1835	2MG	C2-N1	4.96	1.44	1.36
1	I	2449	H2U	C4-N3	4.86	1.45	1.37
1	I	1911	PSU	C6-N1	4.79	1.44	1.36
1	I	746	PSU	C6-N1	4.57	1.43	1.36
1	I	2504	PSU	C6-N1	4.51	1.43	1.36

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	1962	5MC	C6-N1	4.51	1.45	1.38
1	I	2604	PSU	C6-N1	4.42	1.43	1.36
1	I	2457	PSU	C6-N1	4.42	1.43	1.36
1	I	2605	PSU	C6-N1	4.42	1.43	1.36
1	I	955	PSU	C6-N1	4.38	1.43	1.36
1	I	2580	PSU	C6-N1	4.33	1.43	1.36
1	I	2498	OMC	C2-N1	4.31	1.49	1.40
1	I	2251	OMG	O6-C6	-4.30	1.15	1.23
1	I	1911	PSU	C4-N3	4.29	1.46	1.38
1	I	2503	2MA	C5-C6	4.27	1.52	1.41
1	I	1962	5MC	C2-N1	4.22	1.49	1.40
1	I	2552	OMU	C4-N3	4.08	1.45	1.38
1	I	1962	5MC	C4-N4	4.07	1.44	1.34
1	I	746	PSU	C4-N3	3.95	1.46	1.38
1	I	2504	PSU	C4-N3	3.93	1.46	1.38
1	I	2251	OMG	C6-N1	3.92	1.46	1.38
1	I	2605	PSU	C4-N3	3.86	1.46	1.38
1	I	955	PSU	C4-N3	3.82	1.45	1.38
1	I	747	5MU	C2-N3	3.81	1.44	1.38
1	I	2604	PSU	C4-N3	3.81	1.45	1.38
1	I	2069	G7M	C5-C6	3.79	1.54	1.43
1	I	1939	5MU	C2-N3	3.76	1.44	1.38
1	I	2457	PSU	C4-N3	3.74	1.45	1.38
1	I	2552	OMU	O4-C4	-3.71	1.17	1.24
1	I	2580	PSU	C4-N3	3.68	1.45	1.38
1	I	2030	6MZ	C5-C4	-3.68	1.32	1.39
1	I	2030	6MZ	C5-N7	-3.66	1.32	1.39
1	I	1618	6MZ	C8-N9	-3.64	1.31	1.37
1	I	1618	6MZ	C5-C4	-3.62	1.32	1.39
1	I	1618	6MZ	C5-N7	-3.58	1.32	1.39
1	I	2030	6MZ	C8-N9	-3.58	1.31	1.37
1	I	1917	PSU	C6-C5	3.51	1.39	1.35
1	I	2503	2MA	C6-N6	-3.50	1.25	1.34
1	I	1939	5MU	C2-N1	3.23	1.43	1.38
1	I	2498	OMC	C6-N1	3.13	1.45	1.38
1	I	747	5MU	C2-N1	3.13	1.43	1.38
1	I	745	1MG	C5-N7	-3.07	1.33	1.39
1	I	1915	3TD	C4-N3	3.04	1.47	1.40
1	I	2503	2MA	C5-N7	-3.02	1.33	1.39
1	I	1835	2MG	C5-N7	-3.02	1.33	1.39
1	I	2251	OMG	C5-N7	-2.98	1.33	1.39
1	I	2552	OMU	O2-C2	-2.96	1.17	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	745	1MG	C5-C6	2.92	1.53	1.45
1	I	2445	2MG	C5-N7	-2.91	1.33	1.39
1	I	2069	G7M	O6-C6	-2.90	1.18	1.23
1	I	1939	5MU	O4-C4	-2.77	1.18	1.23
1	I	2251	OMG	C5-C6	2.65	1.54	1.44
1	I	747	5MU	O4-C4	-2.65	1.18	1.23
13	U	81	4D4	CZ-NH1	2.60	1.45	1.34
1	I	1939	5MU	O2-C2	-2.60	1.18	1.23
1	I	2069	G7M	C2-N1	2.60	1.44	1.37
1	I	1962	5MC	O2-C2	-2.59	1.18	1.23
1	I	2580	PSU	O4-C4	-2.58	1.18	1.23
1	I	2449	H2U	O2-C2	-2.58	1.18	1.23
1	I	2605	PSU	O4-C4	-2.57	1.18	1.23
1	I	2069	G7M	C6-N1	2.57	1.43	1.38
1	I	747	5MU	O2-C2	-2.57	1.18	1.23
1	I	2552	OMU	C6-N1	2.53	1.44	1.38
1	I	2552	OMU	C5-C4	2.53	1.49	1.43
1	I	2498	OMC	O2-C2	-2.51	1.19	1.23
1	I	2457	PSU	O4-C4	-2.51	1.18	1.23
1	I	955	PSU	O4-C4	-2.50	1.18	1.23
1	I	2604	PSU	O4-C4	-2.46	1.18	1.23
1	I	2504	PSU	O4-C4	-2.45	1.18	1.23
1	I	1915	3TD	O2-C2	-2.41	1.18	1.23
1	I	2445	2MG	C5-C6	2.40	1.53	1.44
1	I	2498	OMC	C5-C4	2.37	1.48	1.42
1	I	1835	2MG	C5-C6	2.36	1.53	1.44
1	I	745	1MG	O6-C6	-2.30	1.18	1.23
1	I	2503	2MA	C4-N9	-2.28	1.32	1.37
1	I	745	1MG	C4-N9	-2.27	1.32	1.38
1	I	1911	PSU	O4-C4	-2.27	1.19	1.23
1	I	746	PSU	O4-C4	-2.25	1.19	1.23
1	I	1835	2MG	O6-C6	-2.25	1.19	1.23
1	I	2445	2MG	O6-C6	-2.18	1.19	1.23
1	I	2251	OMG	C2-N1	2.14	1.43	1.37
1	I	1835	2MG	C6-N1	2.13	1.42	1.38
1	I	2445	2MG	C6-N1	2.11	1.42	1.38
1	I	2580	PSU	O4'-C1'	-2.10	1.40	1.43
1	I	2580	PSU	O2-C2	-2.08	1.19	1.23
1	I	1962	5MC	CM5-C5	2.06	1.55	1.50
1	I	2030	6MZ	C6-N1	-2.05	1.31	1.35
1	I	955	PSU	O2-C2	-2.05	1.19	1.23
1	I	2605	PSU	O4'-C1'	-2.03	1.41	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2449	H2U	O4-C4	-2.02	1.19	1.23
1	I	2457	PSU	O2-C2	-2.01	1.19	1.23

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1939	5MU	C5-C4-N3	10.36	124.15	115.31
1	I	747	5MU	C5-C4-N3	10.33	124.13	115.31
1	I	745	1MG	C1'-N9-C8	-9.12	100.72	126.70
1	I	747	5MU	C5-C6-N1	-8.97	114.11	123.34
1	I	1939	5MU	C5-C6-N1	-8.82	114.27	123.34
1	I	745	1MG	C1'-N9-C4	7.95	150.11	126.50
1	I	747	5MU	C4-N3-C2	-7.41	117.75	127.35
1	I	2449	H2U	C4-N3-C2	-7.22	119.80	125.79
1	I	1939	5MU	C4-N3-C2	-7.21	118.01	127.35
1	I	2069	G7M	CN7-N7-C5	6.63	135.01	126.77
1	I	2069	G7M	C1'-N9-C4	6.59	146.08	126.50
1	I	2069	G7M	C1'-N9-C8	-6.20	105.79	126.74
1	I	2445	2MG	C2-N3-C4	6.14	119.66	112.04
1	I	2503	2MA	C5-C4-N3	-6.11	120.32	127.19
1	I	1835	2MG	C2-N3-C4	6.03	119.52	112.04
1	I	2503	2MA	N9-C8-N7	-5.93	105.80	113.91
1	I	2030	6MZ	C9-N6-C6	-5.47	118.16	122.87
1	I	1618	6MZ	N1-C2-N3	-5.41	120.14	128.60
1	I	2552	OMU	C4-N3-C2	-5.31	119.57	126.58
1	I	1618	6MZ	C5-C4-N3	-5.30	119.84	126.75
1	I	2030	6MZ	C5-C4-N3	-5.27	119.87	126.75
1	I	2030	6MZ	N1-C2-N3	-5.26	120.38	128.60
1	I	2069	G7M	CN7-N7-C8	-5.22	116.79	124.84
1	I	2251	OMG	C5-C4-N3	-5.06	120.26	128.46
1	I	2503	2MA	N3-C4-N9	5.05	133.99	126.99
1	I	2503	2MA	C4-N9-C8	5.01	111.16	105.73
1	I	1835	2MG	C5-C4-N3	-4.92	120.49	128.46
1	I	1939	5MU	N3-C2-N1	4.89	121.38	114.89
1	I	955	PSU	C4-N3-C2	-4.88	119.31	126.34
1	I	747	5MU	N3-C2-N1	4.85	121.33	114.89
1	I	955	PSU	N1-C2-N3	4.76	120.52	115.13
1	I	2457	PSU	C4-N3-C2	-4.75	119.49	126.34
1	I	747	5MU	C5M-C5-C6	-4.75	116.51	122.85
1	I	1915	3TD	N1-C2-N3	4.74	119.88	116.14
1	I	2580	PSU	C4-N3-C2	-4.69	119.58	126.34
1	I	2251	OMG	C1'-N9-C4	-4.64	112.71	126.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2445	2MG	C5-C4-N3	-4.64	120.94	128.46
1	I	2604	PSU	C4-N3-C2	-4.63	119.67	126.34
1	I	2457	PSU	N1-C2-N3	4.60	120.34	115.13
1	I	2580	PSU	N1-C2-N3	4.60	120.34	115.13
1	I	745	1MG	C5-C4-N3	-4.59	121.01	128.46
1	I	2604	PSU	N1-C2-N3	4.58	120.32	115.13
1	I	2504	PSU	C4-N3-C2	-4.55	119.78	126.34
1	I	2251	OMG	C2-N3-C4	4.50	120.31	112.30
1	I	2605	PSU	C4-N3-C2	-4.46	119.91	126.34
1	I	1911	PSU	C4-N3-C2	-4.40	120.00	126.34
1	I	2445	2MG	C2-N1-C6	-4.39	119.43	124.48
1	I	746	PSU	C4-N3-C2	-4.36	120.06	126.34
1	I	2030	6MZ	N9-C8-N7	-4.32	108.00	113.91
1	I	1618	6MZ	N9-C8-N7	-4.32	108.01	113.91
1	I	2069	G7M	C2-N3-C4	4.28	119.93	112.30
1	I	1835	2MG	C2-N1-C6	-4.27	119.56	124.48
1	I	2504	PSU	N1-C2-N3	4.27	119.97	115.13
1	I	1915	3TD	C4-N3-C2	-4.19	120.06	124.61
1	I	1939	5MU	C5M-C5-C6	-4.16	117.30	122.85
1	I	747	5MU	O4-C4-C5	-4.14	120.10	124.90
1	I	2605	PSU	N1-C2-N3	4.13	119.80	115.13
1	I	1911	PSU	N1-C2-N3	4.11	119.78	115.13
1	I	1618	6MZ	C4-C5-C6	4.10	119.99	116.81
1	I	1618	6MZ	C9-N6-C6	-4.09	119.35	122.87
1	I	2251	OMG	C1'-N9-C8	4.06	138.25	126.70
1	I	746	PSU	N1-C2-N3	4.06	119.72	115.13
1	I	2069	G7M	C5-C6-N1	3.96	120.06	111.79
1	I	2030	6MZ	C4-C5-C6	3.92	119.85	116.81
1	I	1835	2MG	C1'-N9-C8	-3.88	115.64	126.70
1	I	1939	5MU	O4-C4-C5	-3.88	120.41	124.90
1	I	747	5MU	C6-C5-C4	3.81	121.22	118.03
1	I	2069	G7M	C5-C4-N3	-3.75	120.97	128.15
1	I	2069	G7M	O6-C6-C5	-3.68	119.77	128.06
1	I	2503	2MA	C5-N7-C8	3.65	108.70	103.51
1	I	1939	5MU	C6-C5-C4	3.64	121.08	118.03
1	I	2552	OMU	N3-C2-N1	3.56	119.62	114.89
1	I	2552	OMU	C5-C4-N3	3.56	120.17	114.84
1	I	955	PSU	C6-C5-C4	3.55	120.68	118.20
1	I	745	1MG	C2-N3-C4	3.54	119.94	111.98
1	I	1618	6MZ	C2-N3-C4	3.51	120.05	111.75
1	I	2604	PSU	C6-C5-C4	3.49	120.64	118.20
1	I	2030	6MZ	C2-N3-C4	3.44	119.88	111.75

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2445	2MG	C1'-N9-C8	-3.34	117.19	126.70
1	I	955	PSU	C6-N1-C2	-3.34	119.27	122.68
1	I	2604	PSU	C6-N1-C2	-3.34	119.27	122.68
1	I	2445	2MG	N9-C8-N7	-3.33	107.13	113.39
1	I	1962	5MC	C5-C6-N1	-3.31	119.93	123.34
1	I	2580	PSU	C6-C5-C4	3.31	120.51	118.20
1	I	1835	2MG	N9-C4-N3	3.31	132.58	125.94
1	I	2580	PSU	C6-N1-C2	-3.28	119.32	122.68
1	I	2457	PSU	C6-C5-C4	3.28	120.49	118.20
1	I	2251	OMG	N9-C4-N3	3.27	132.50	125.94
1	I	2457	PSU	C6-N1-C2	-3.26	119.35	122.68
1	I	1911	PSU	C6-C5-C4	3.25	120.47	118.20
1	I	1618	6MZ	N3-C4-N9	3.23	132.41	127.08
1	I	745	1MG	N9-C8-N7	-3.23	107.31	113.39
1	I	1835	2MG	N9-C8-N7	-3.20	107.36	113.39
1	I	2504	PSU	C6-N1-C2	-3.19	119.42	122.68
1	I	747	5MU	C5M-C5-C4	3.19	122.27	118.77
1	I	2449	H2U	N3-C2-N1	3.17	120.00	116.65
1	I	2251	OMG	N9-C8-N7	-3.14	107.47	113.39
1	I	2605	PSU	C6-N1-C2	-3.10	119.51	122.68
1	I	2449	H2U	C5-C4-N3	3.10	120.14	116.65
1	I	2552	OMU	O4-C4-C5	-3.10	119.70	125.16
1	I	2030	6MZ	C5-N7-C8	3.09	107.90	103.51
1	I	2251	OMG	C2-N1-C6	-3.06	119.52	125.10
1	I	2503	2MA	N3-C2-N1	-3.04	120.12	125.72
1	I	1911	PSU	C6-N1-C2	-3.04	119.57	122.68
1	I	2069	G7M	C2-N1-C6	-2.99	119.65	125.10
1	I	2030	6MZ	N3-C4-N9	2.96	131.96	127.08
1	I	2504	PSU	C6-C5-C4	2.96	120.27	118.20
1	I	746	PSU	C6-N1-C2	-2.96	119.66	122.68
1	I	955	PSU	O2-C2-N1	-2.91	119.59	122.79
1	I	1835	2MG	C1'-N9-C4	2.89	135.09	126.50
1	I	2604	PSU	O2-C2-N1	-2.89	119.61	122.79
1	I	1618	6MZ	C5-N7-C8	2.88	107.61	103.51
1	I	747	5MU	O2-C2-N1	-2.84	119.02	122.79
1	I	2580	PSU	O2-C2-N1	-2.81	119.70	122.79
1	I	745	1MG	N9-C4-N3	2.79	131.54	125.94
1	I	2251	OMG	C5-C6-N1	2.76	120.20	113.19
1	I	2445	2MG	N9-C4-N3	2.76	131.47	125.94
1	I	1835	2MG	C5-C6-N1	2.74	120.16	113.19
1	I	2445	2MG	C5-C6-N1	2.73	120.13	113.19
1	I	2449	H2U	C5-C6-N1	2.69	120.48	111.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	745	1MG	C5-C6-N1	2.67	120.08	114.91
1	I	2457	PSU	O2-C2-N1	-2.61	119.92	122.79
1	I	1939	5MU	C5M-C5-C4	2.60	121.62	118.77
1	I	2605	PSU	C6-C5-C4	2.59	120.01	118.20
1	I	1835	2MG	O6-C6-C5	-2.58	119.76	126.60
1	I	2504	PSU	O2-C2-N1	-2.55	119.98	122.79
1	I	1911	PSU	O2-C2-N1	-2.54	119.99	122.79
1	I	2030	6MZ	C4-N9-C1'	-2.53	120.56	126.59
1	I	2445	2MG	CM2-N2-C2	-2.52	118.30	123.86
1	I	2605	PSU	O2-C2-N1	-2.51	120.03	122.79
1	I	2449	H2U	O2-C2-N1	-2.50	119.96	123.11
1	I	2251	OMG	O6-C6-C5	-2.49	119.99	126.60
1	I	2445	2MG	O6-C6-C5	-2.47	120.04	126.60
1	I	1939	5MU	O4-C4-N3	-2.44	115.44	120.12
1	I	2445	2MG	C1'-N9-C4	2.38	133.59	126.50
1	I	2580	PSU	O4'-C1'-C2'	2.35	108.45	105.14
1	I	2503	2MA	N6-C6-N1	2.34	120.33	117.03
1	I	1835	2MG	N1-C2-N3	-2.33	120.35	123.95
1	I	2445	2MG	N1-C2-N3	-2.33	120.35	123.95
1	I	1618	6MZ	C4-N9-C8	2.32	108.25	105.73
1	I	2069	G7M	N9-C4-N3	2.32	130.60	125.94
1	I	746	PSU	O2-C2-N1	-2.32	120.24	122.79
1	I	1939	5MU	O2-C2-N1	-2.31	119.72	122.79
1	I	1618	6MZ	C4-N9-C1'	-2.27	121.19	126.59
1	I	747	5MU	O4-C4-N3	-2.27	115.77	120.12
1	I	1911	PSU	O4'-C1'-C2'	2.23	108.29	105.14
1	I	1835	2MG	CM2-N2-C2	-2.22	118.95	123.86
1	I	746	PSU	C6-C5-C4	2.22	119.75	118.20
1	I	2604	PSU	O4'-C1'-C2'	2.21	108.26	105.14
1	I	2251	OMG	C8-N7-C5	2.14	108.12	104.24
1	I	1962	5MC	CM5-C5-C6	-2.13	120.00	122.85
1	I	2030	6MZ	C4-C5-N7	-2.11	108.05	110.62
1	I	955	PSU	O4'-C1'-C2'	2.09	108.09	105.14
1	I	2445	2MG	C8-N7-C5	2.09	108.02	104.24
1	I	2457	PSU	O4'-C1'-C2'	2.08	108.08	105.14
1	I	2503	2MA	C6-C5-C4	2.08	119.98	117.18
1	I	1618	6MZ	C5-C6-N1	2.06	120.40	118.20
1	I	2030	6MZ	C5-C4-N9	2.05	108.17	105.78
1	I	1835	2MG	C8-N7-C5	2.05	107.95	104.24
1	I	2504	PSU	O4'-C1'-C2'	2.03	108.00	105.14
1	I	745	1MG	C8-N7-C5	2.01	107.87	104.24
1	I	2069	G7M	N2-C2-N1	2.00	120.98	116.71

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2030	6MZ	C5-C6-N1	2.00	120.33	118.20

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	I	1618	6MZ	N1-C6-N6-C9
1	I	1915	3TD	C3'-C4'-C5'-O5'
1	I	1915	3TD	O4'-C4'-C5'-O5'
1	I	2503	2MA	O4'-C4'-C5'-O5'
1	I	2445	2MG	C3'-C4'-C5'-O5'
1	I	2503	2MA	C3'-C4'-C5'-O5'
1	I	2445	2MG	O4'-C4'-C5'-O5'
1	I	2069	G7M	O4'-C4'-C5'-O5'
1	I	2069	G7M	C4'-C5'-O5'-P
1	I	2030	6MZ	O4'-C4'-C5'-O5'
1	I	1962	5MC	O4'-C4'-C5'-O5'
1	I	1911	PSU	O4'-C1'-C5-C4
1	I	1915	3TD	O4'-C1'-C5-C4
1	I	2069	G7M	C3'-C4'-C5'-O5'
1	I	1962	5MC	C3'-C4'-C5'-O5'
13	U	81	4D4	O-C-CA-CB

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	745	1MG	1	0
1	I	1939	5MU	1	0
1	I	2030	6MZ	1	0
1	I	2069	G7M	1	0
1	I	747	5MU	1	0
1	I	746	PSU	1	0
1	I	2552	OMU	2	0
1	I	2251	OMG	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 178 ligands modelled in this entry, 178 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

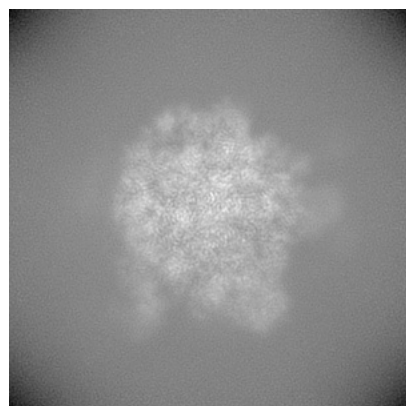
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-66736. These allow visual inspection of the internal detail of the map and identification of artifacts.

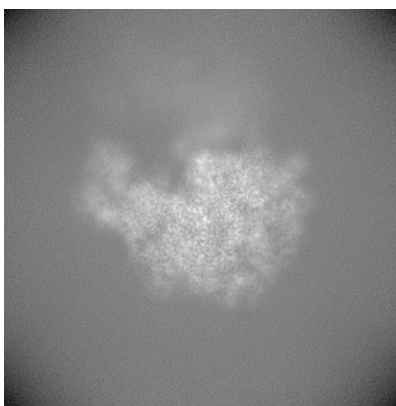
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

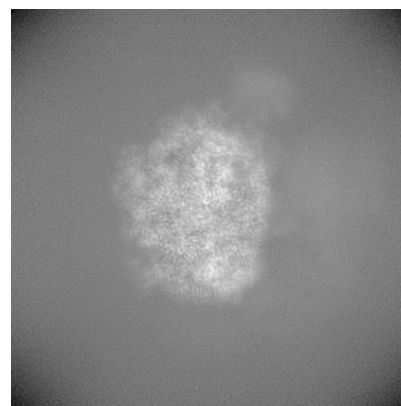
6.1.1 Primary map



X

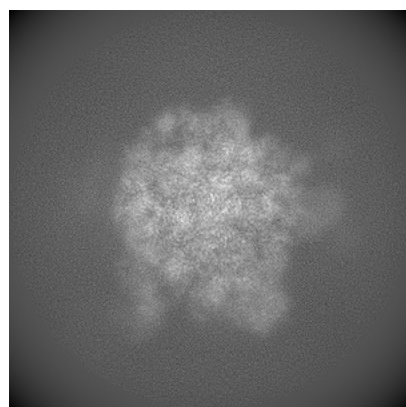


Y

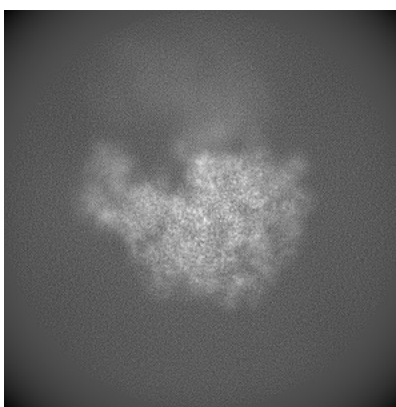


Z

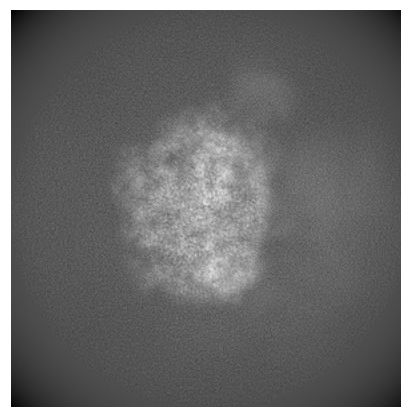
6.1.2 Raw map



X



Y

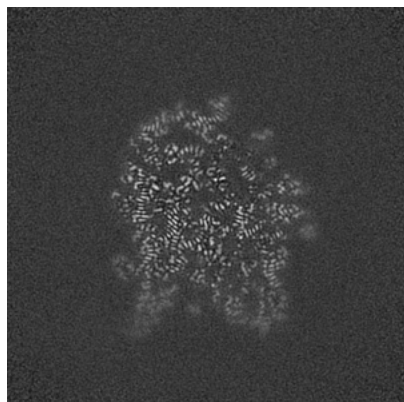


Z

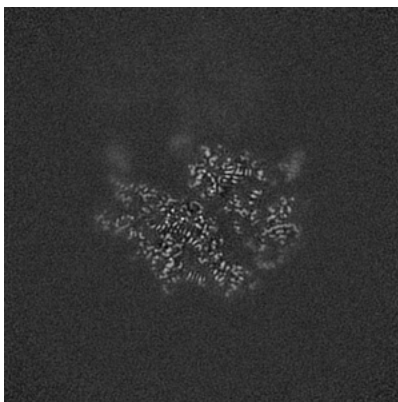
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

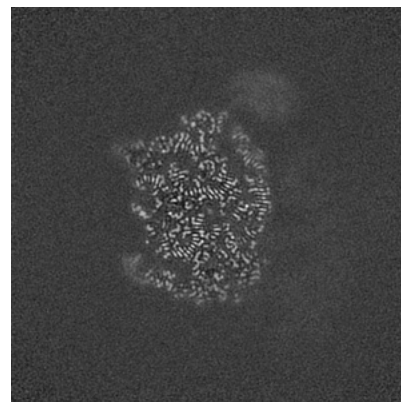
6.2.1 Primary map



X Index: 250

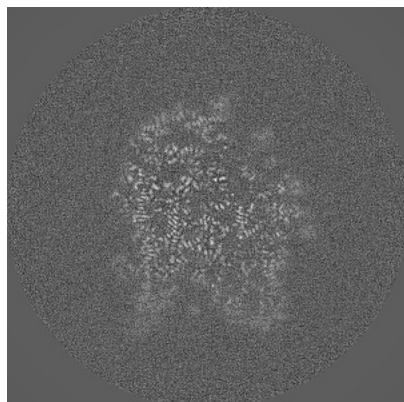


Y Index: 250

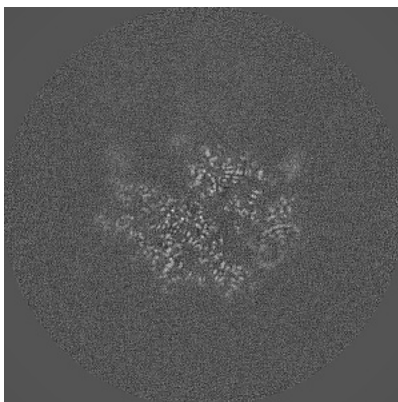


Z Index: 250

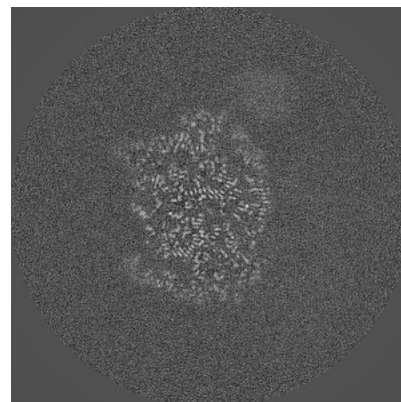
6.2.2 Raw map



X Index: 250



Y Index: 250

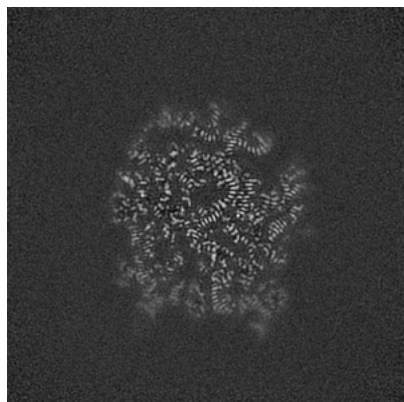


Z Index: 250

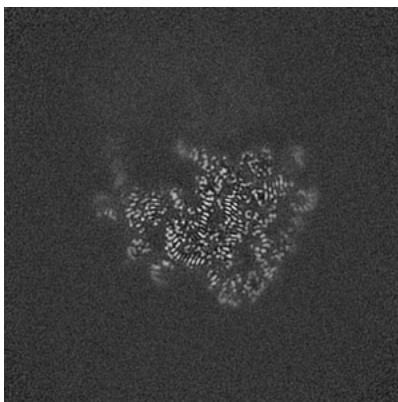
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

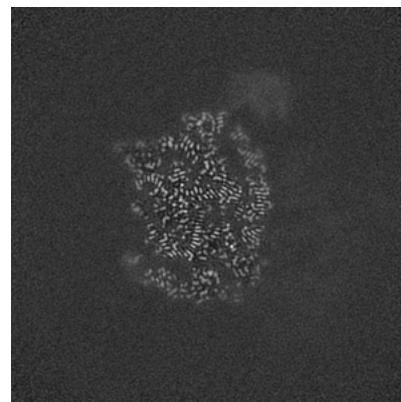
6.3.1 Primary map



X Index: 241

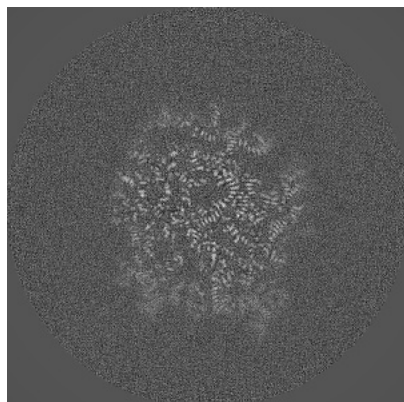


Y Index: 270

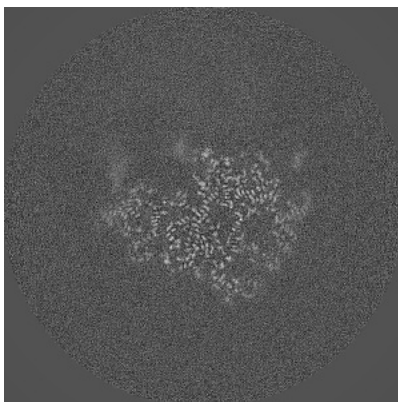


Z Index: 248

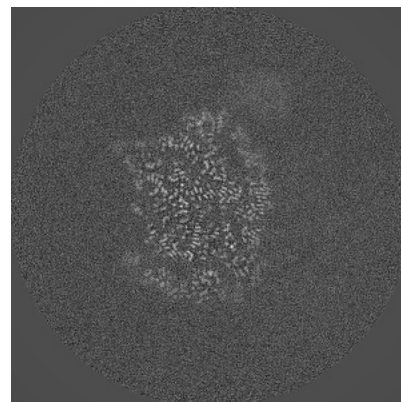
6.3.2 Raw map



X Index: 241



Y Index: 261

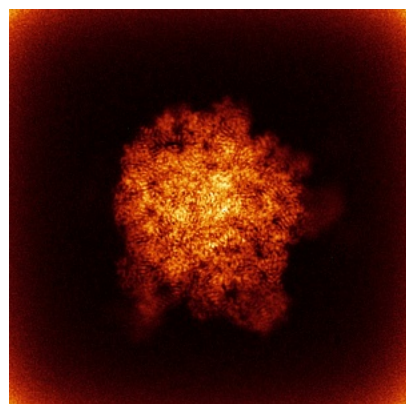


Z Index: 248

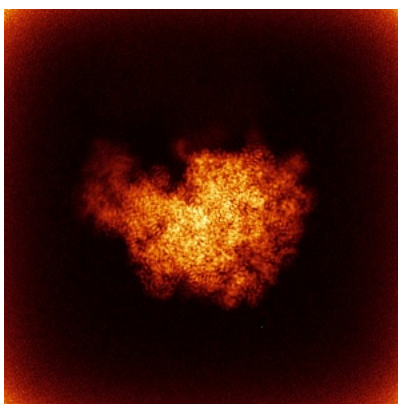
The images above show the largest variance slices of the map in three orthogonal directions.

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

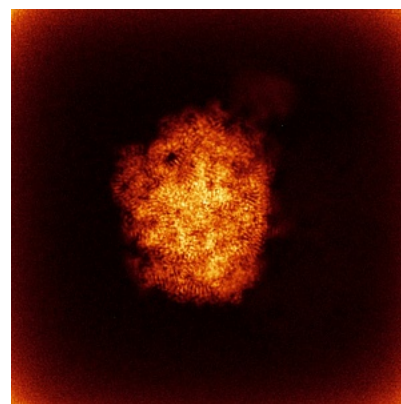
6.4.1 Primary map



X

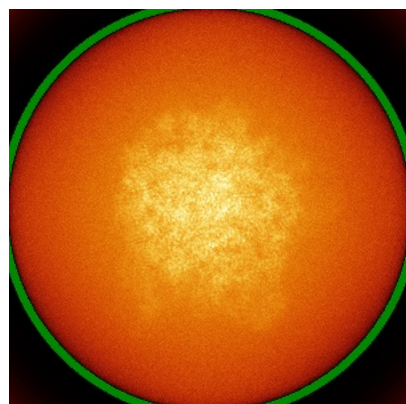


Y

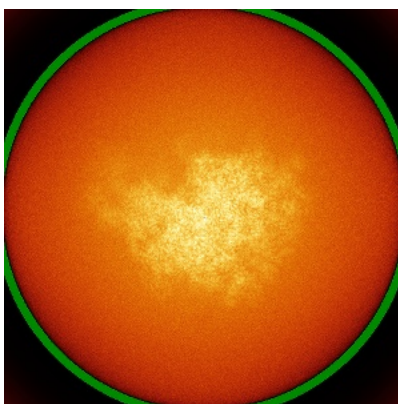


Z

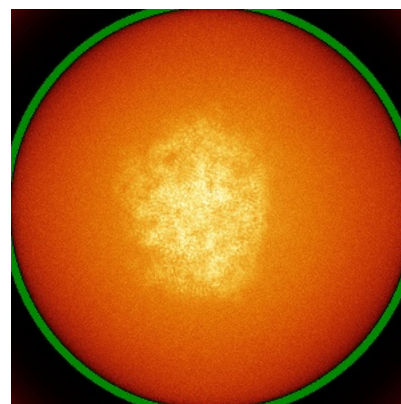
6.4.2 Raw map



X



Y

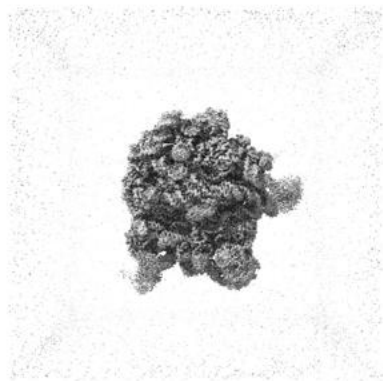


Z

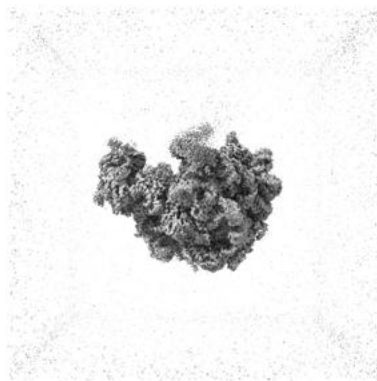
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

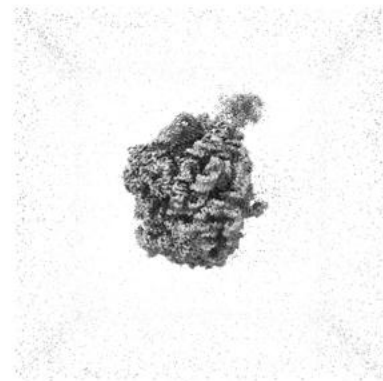
6.5.1 Primary map



X



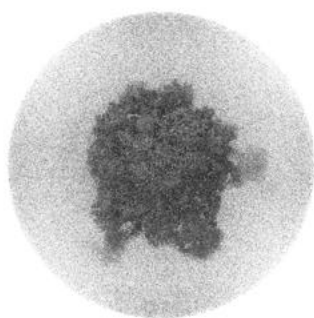
Y



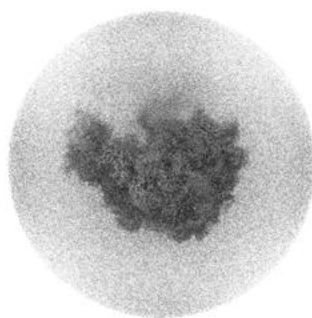
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

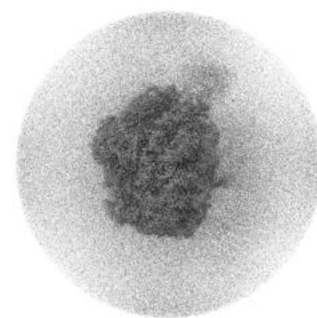
6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

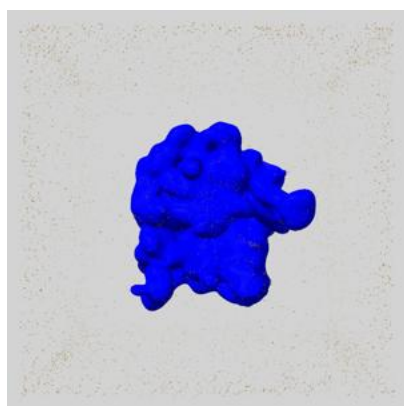
6.6 Mask visualisation [i](#)

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

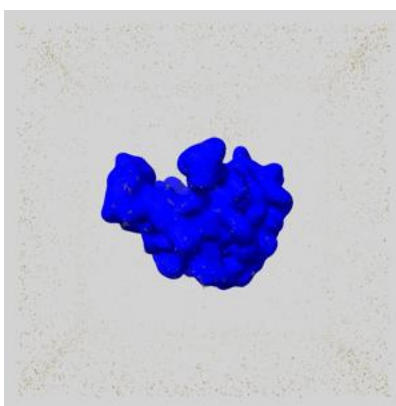
A mask typically either:

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

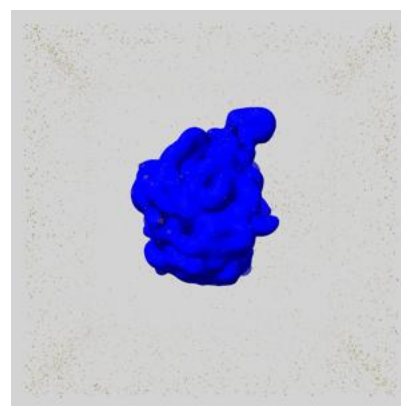
6.6.1 emd_66736_msk_1.map [i](#)



X



Y

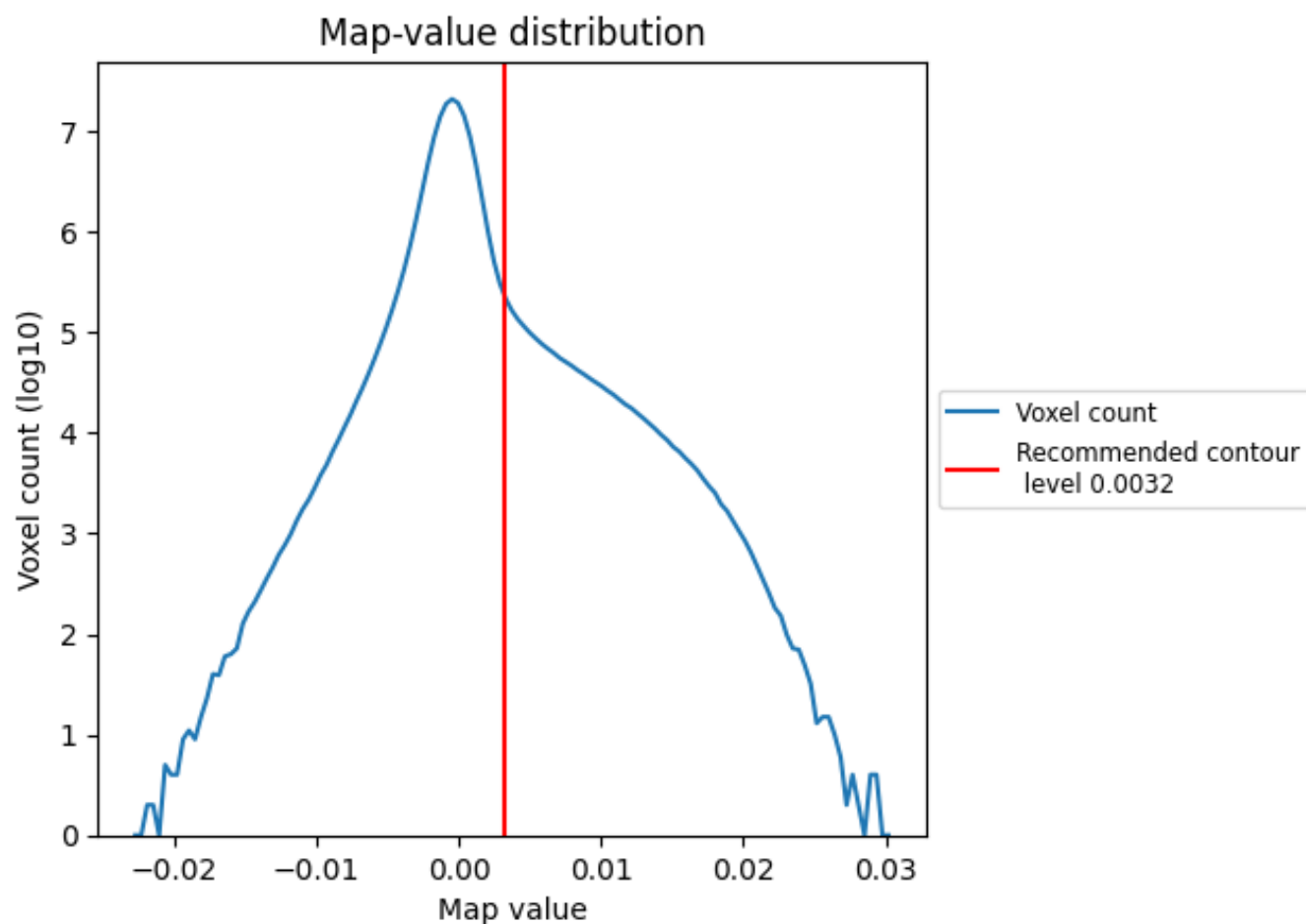


Z

7 Map analysis [i](#)

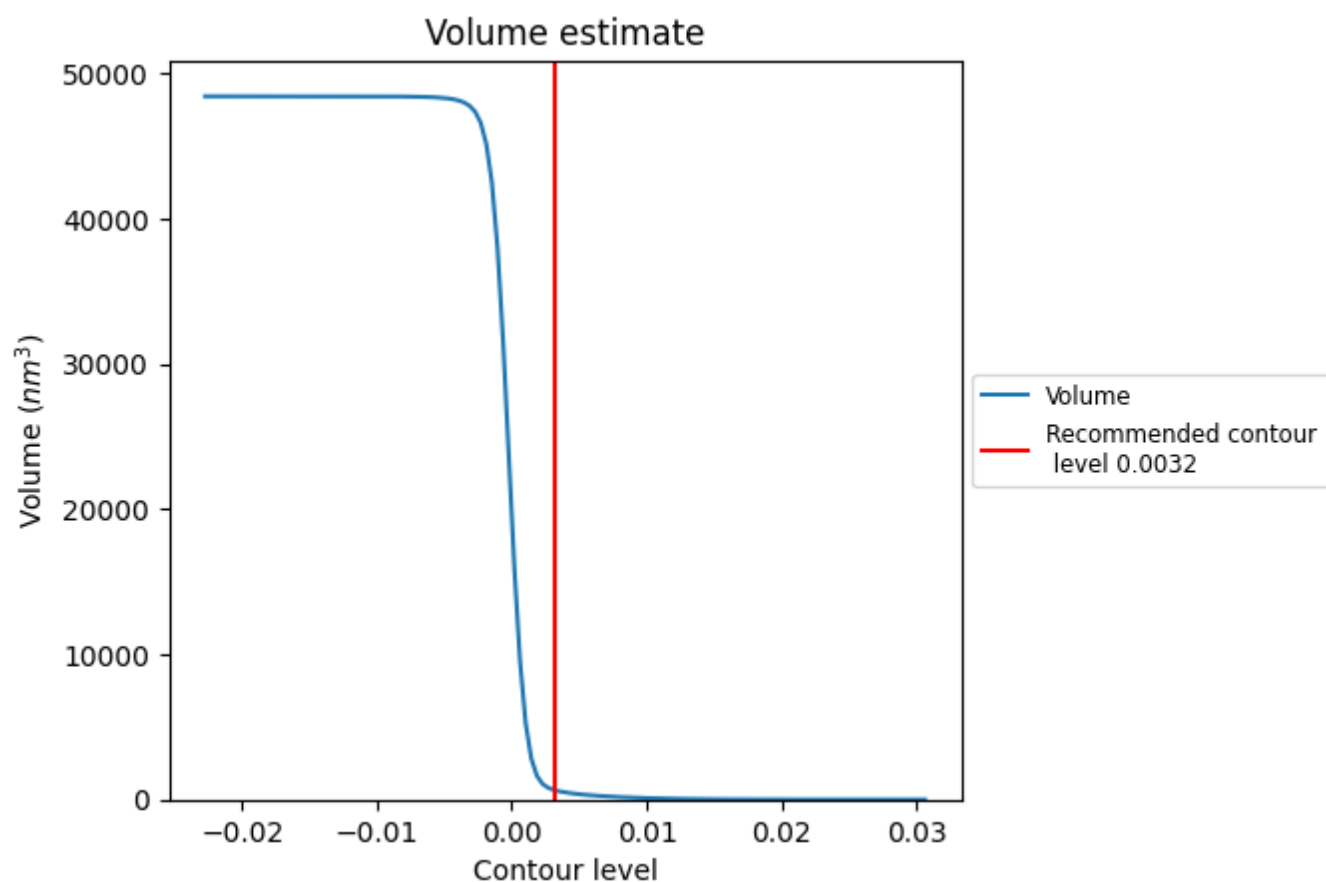
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

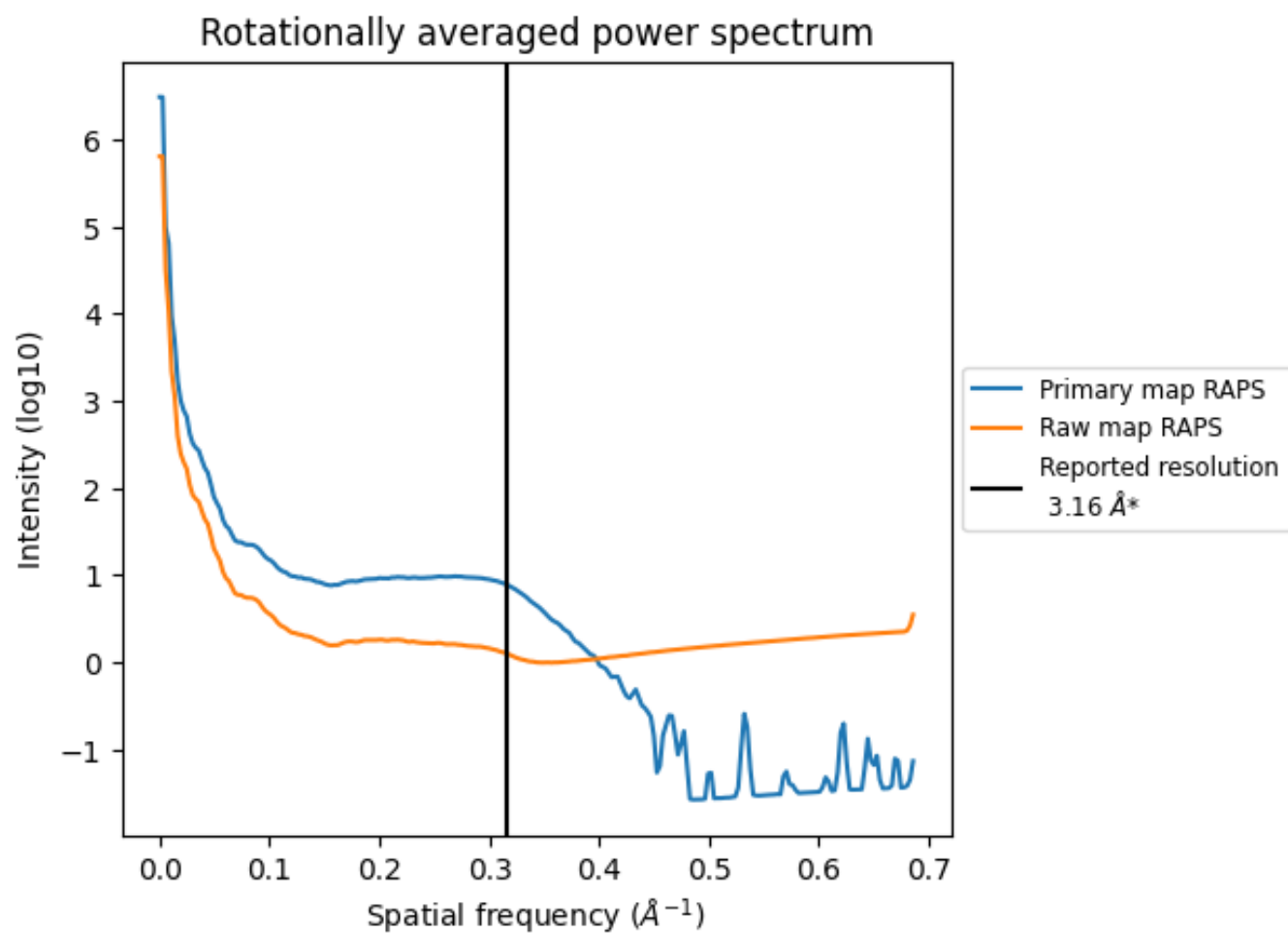
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 642 nm³; this corresponds to an approximate mass of 580 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

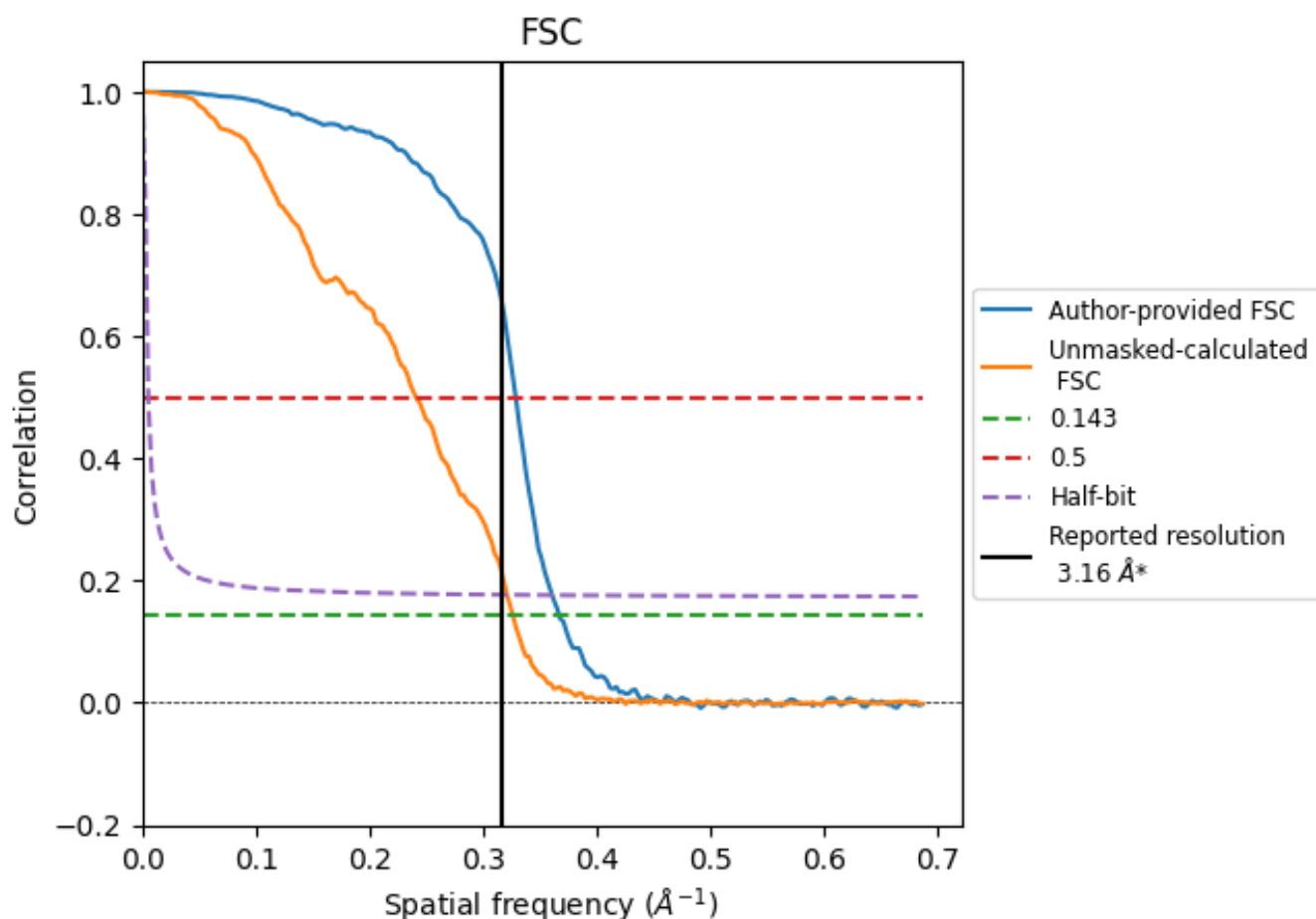


*Reported resolution corresponds to spatial frequency of 0.316 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.316 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

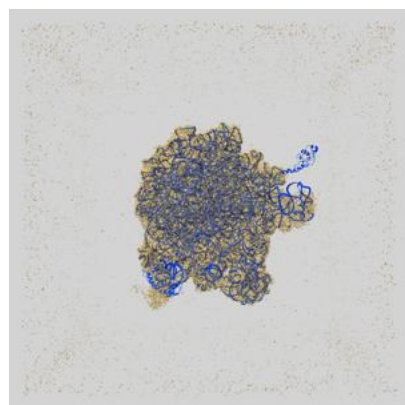
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.16	-	-
Author-provided FSC curve	2.73	3.04	2.77
Unmasked-calculated*	3.07	4.15	3.12

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 2.73 differs from the reported value 3.16 by more than 10 %

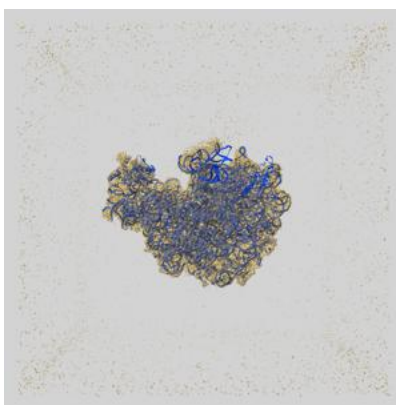
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-66736 and PDB model 9XFL. Per-residue inclusion information can be found in section [3](#) on page [12](#).

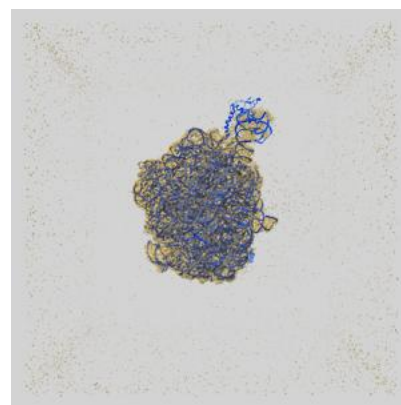
9.1 Map-model overlay [i](#)



X



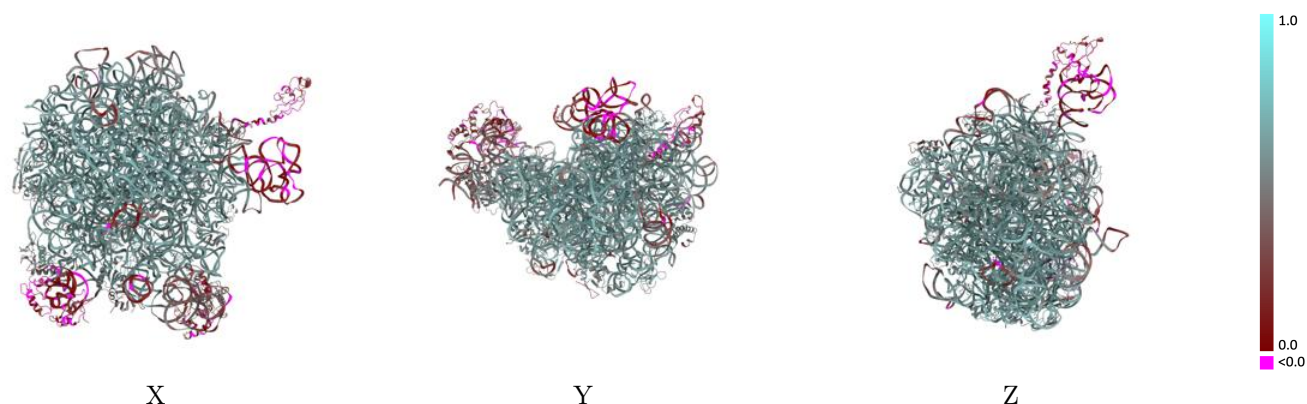
Y



Z

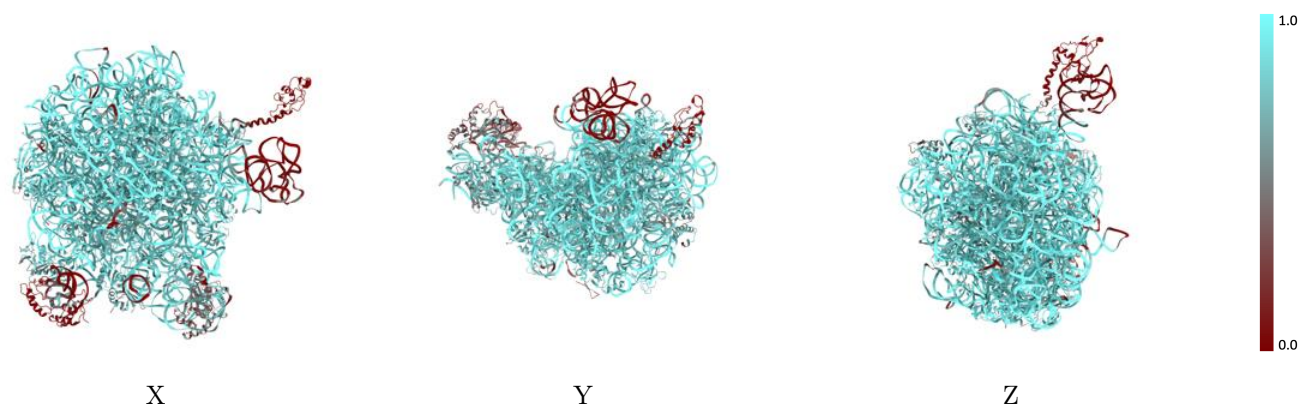
The images above show the 3D surface view of the map at the recommended contour level 0.0032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



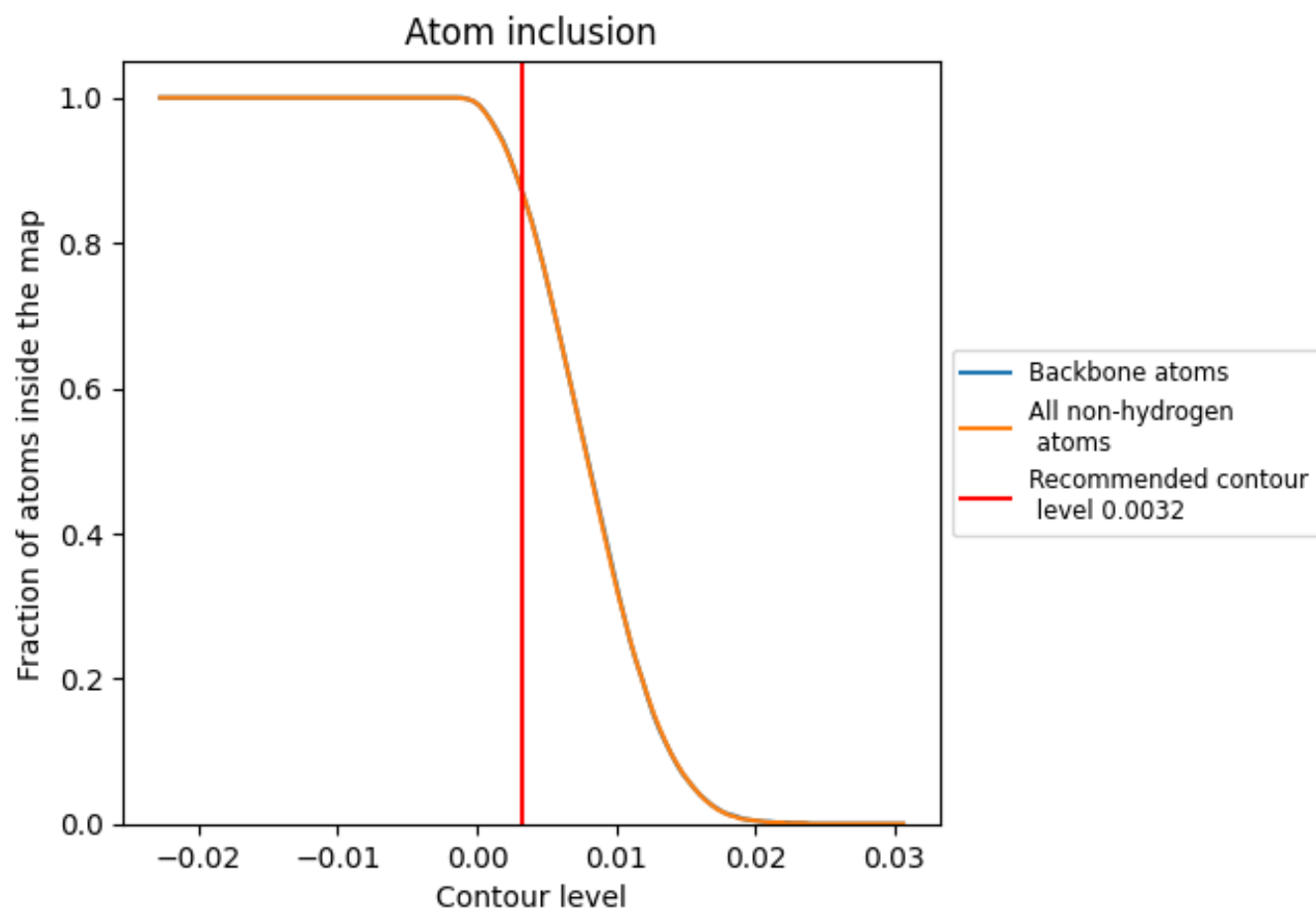
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0032).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 87% 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 (0.0032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8740	 0.5570
I	 0.9180	 0.5770
J	 0.8790	 0.4700
K	 0.9220	 0.6080
L	 0.9150	 0.6120
M	 0.8450	 0.5620
N	 0.3650	 0.2330
O	 0.7160	 0.4580
P	 0.2270	 0.2060
Q	 0.0520	 0.0550
R	 0.9200	 0.6040
S	 0.8830	 0.5670
T	 0.8940	 0.5950
U	 0.8840	 0.5760
V	 0.9400	 0.6180
W	 0.6840	 0.4080
X	 0.8220	 0.5490
Y	 0.9340	 0.6300
Z	 0.8720	 0.5780
a	 0.8900	 0.6010
b	 0.8300	 0.5530
c	 0.8010	 0.5350
d	 0.7660	 0.4930
e	 0.8960	 0.5960
f	 0.9130	 0.6000
g	 0.7530	 0.4870
h	 0.8790	 0.5760
i	 0.9090	 0.6110
j	 0.7080	 0.5090
k	 0.9440	 0.6400
l	 0.9570	 0.6350
m	 0.9010	 0.5820

