



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:18 AM UTC

PDB ID : 7QQ3 / pdb_00007qq3
EMDB ID : EMD-14121
Title : Cryo-EM structure of the E.coli 50S ribosomal subunit in complex with the antibiotic Myxovalargin A.
Authors : Koller, T.O.; Beckert, B.; Wilson, D.N.
Deposited on : 2022-01-06
Resolution : 2.10 Å(reported)
Based on initial model : 4YBB

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:

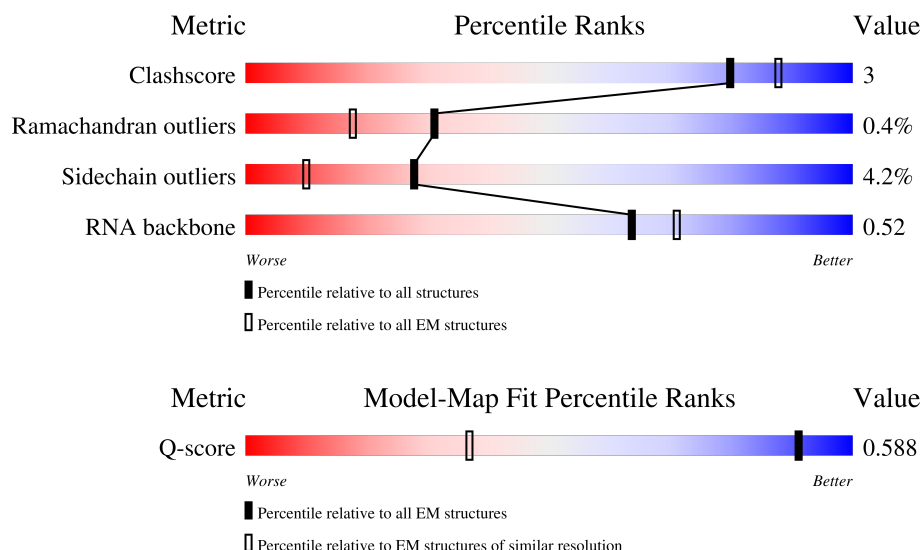
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.10 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	2317 (1.60 - 2.60)

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	19% 80% 18% .
2	J	120	59% 74% 22% ..
3	K	273	19% 97% ..

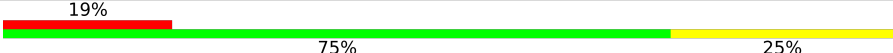
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Mol	Chain	Length	Quality of chain
4	L	209	50% 96% .
5	M	201	62% 98% .
6	O	177	90% 92% 7% ..
7	R	142	38% 94% 6%
8	S	123	47% 89% 8% ...
9	T	143	52% 92% 7% .
10	U	136	45% 94% 5% .
11	V	127	16% 90% 5% 6%
12	W	117	90% 91% 9% .
13	X	115	77% 91% 7% ..
14	Y	118	26% 94% 5% .
15	Z	103	67% 89% 11%
16	a	110	33% 96% .
17	b	100	53% 79% 13% . 7%
18	c	104	79% 86% 11% ..
19	d	94	76% 91% 9%
20	e	85	26% 81% 6% . 12%
21	f	78	33% 95% ..
22	g	63	63% 89% 10% .
23	h	59	49% 93% 5% .
24	i	57	37% 88% 9% ..
25	j	55	51% 89% 9%
26	k	46	11% 96% .
27	l	65	31% 95% ..
28	m	38	21% 100%

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Mol	Chain	Length	Quality of chain
29	B	16	 A horizontal bar chart showing the quality of chain B. The bar is divided into three segments: a red segment at the beginning labeled '19%', a green segment in the middle labeled '75%', and a yellow segment at the end labeled '25%'. The segments are stacked horizontally to represent the total length of the chain.

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 87594 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 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	2898	Total	C	N	O	P	0	0
			62225	27764	11448	20115	2898		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	118	Total	C	N	O	P	0	0
			2531	1127	465	821	118		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	K	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	209	Total	C	N	O	S	0	0
			1565	979	288	294	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	M	201	Total	C	N	O	S	0	0
			1552	974	283	290	5		

- Molecule 6 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O	176	Total	C	N	O	S	0	0
			1323	832	243	246	2		

- Molecule 7 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 8 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	122	Total	C	N	O	S	0	0
			938	587	180	165	6		

- Molecule 9 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 10 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	136	Total	C	N	O	S	0	0
			1074	686	205	177	6		

- Molecule 11 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	120	Total	C	N	O	S	0	0
			960	593	196	166	5		

- Molecule 12 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	116	Total	C	N	O	0	0
			892	552	178	162		

- Molecule 13 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	X	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 14 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	Y	117	Total	C	N	O	0	0
			947	604	192	151		

- Molecule 15 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms				AltConf	Trace
15	Z	103	Total	C	N	O	S	0
			816	516	153	145	2	0

- Molecule 16 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms				AltConf	Trace
16	a	110	Total	C	N	O	S	0
			857	532	166	156	3	0

- Molecule 17 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	b	93	Total	C	N	O	S	0
			738	466	139	131	2	0

- Molecule 18 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	c	102	Total	C	N	O		0
			779	492	146	141		0

- Molecule 19 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	d	94	Total	C	N	O	S	0
			753	479	137	134	3	0

- Molecule 20 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	e	75	Total	C	N	O	S	0
			569	353	113	102	1	0

- Molecule 21 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	f	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 22 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	g	62	Total	C	N	O	S	0	0
			501	308	98	94	1		

- Molecule 23 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	h	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 24 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	i	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 25 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	j	50	Total	C	N	O	0	0
			409	263	75	71		

- Molecule 26 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	k	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 27 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	l	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 28 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	m	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 29 is a protein called Myxovalargin A.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	B	16	Total	C	N	O	0	0
			119	81	21	17		

- Molecule 30 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	I	141	Total	Mg	0
			141	141	
30	J	3	Total	Mg	0
			3	3	
30	L	1	Total	Mg	0
			1	1	

- Molecule 31 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

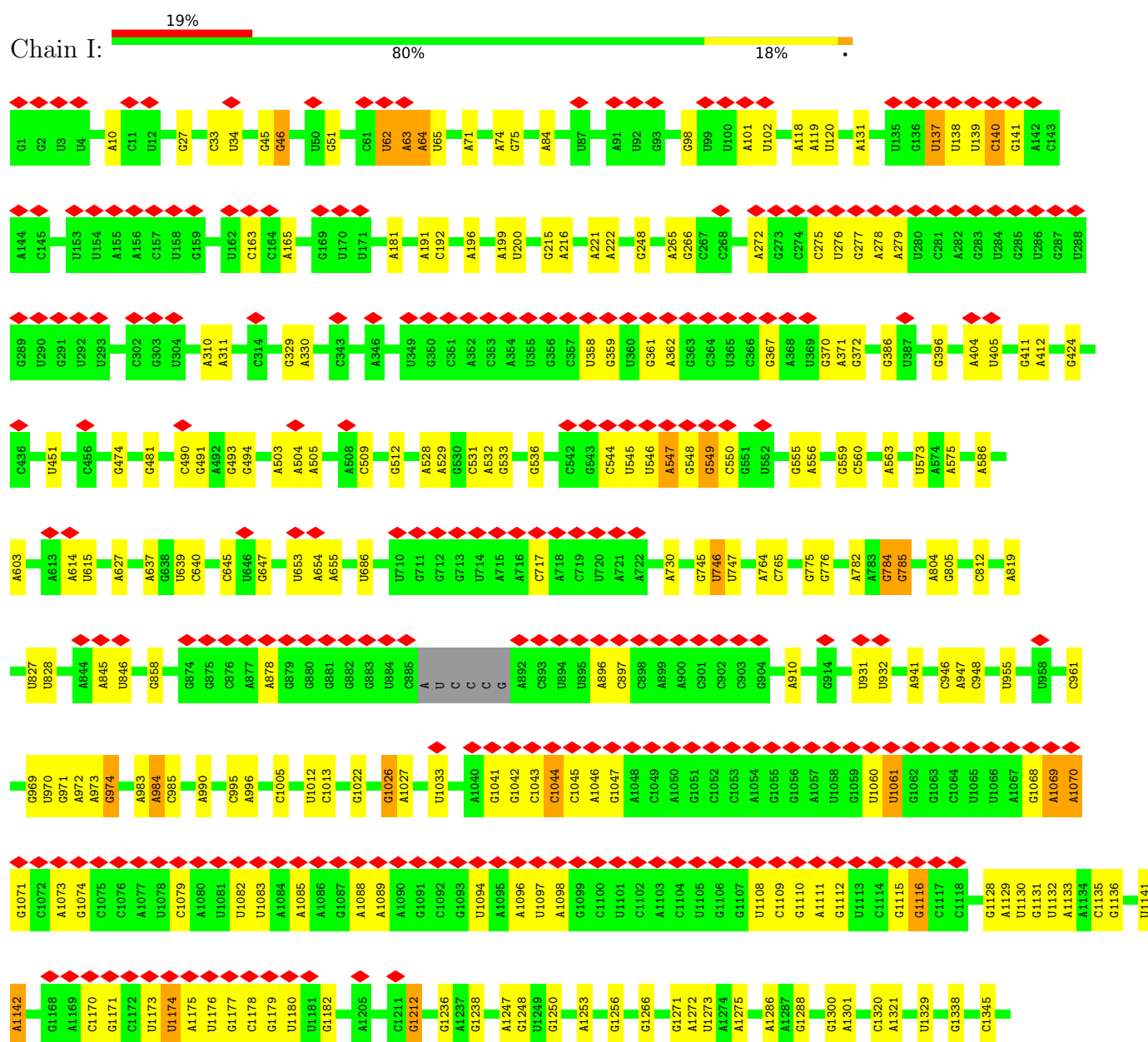
- Molecule 32 is water.

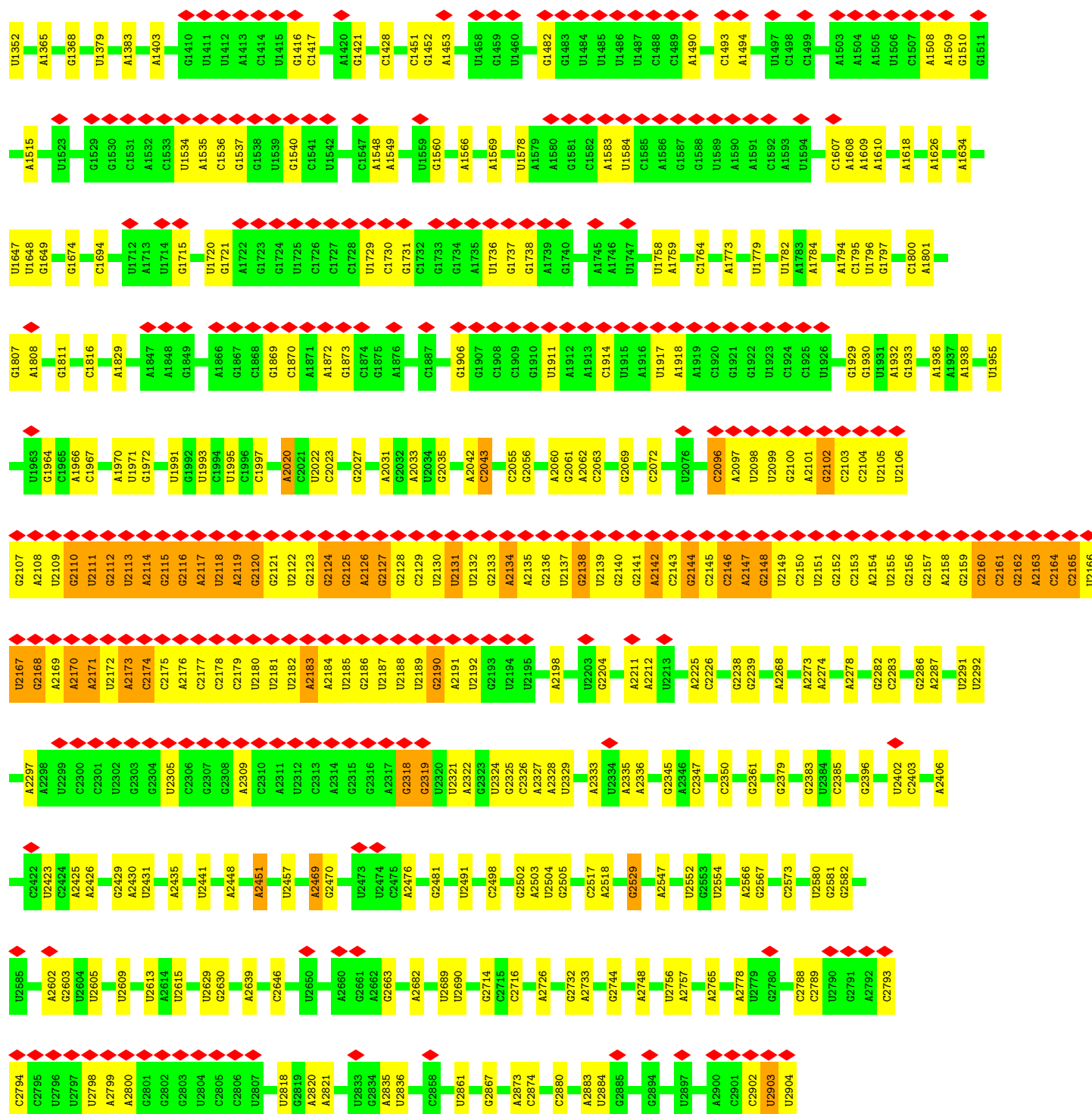
Mol	Chain	Residues	Atoms		AltConf
32	I	18	Total	O	0
			18	18	
32	B	10	Total	O	0
			10	10	

3 Residue-property plots

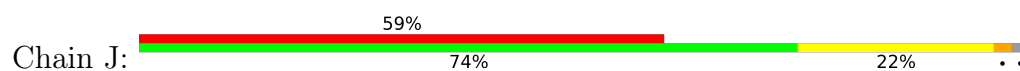
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

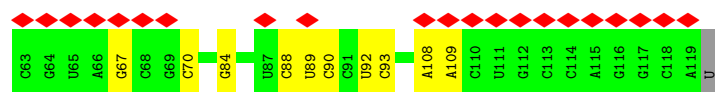
• Molecule 1: 23S ribosomal RNA



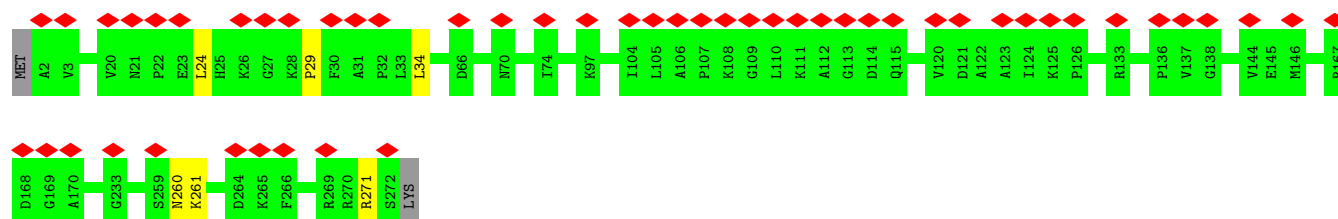


• Molecule 2: 5S ribosomal RNA

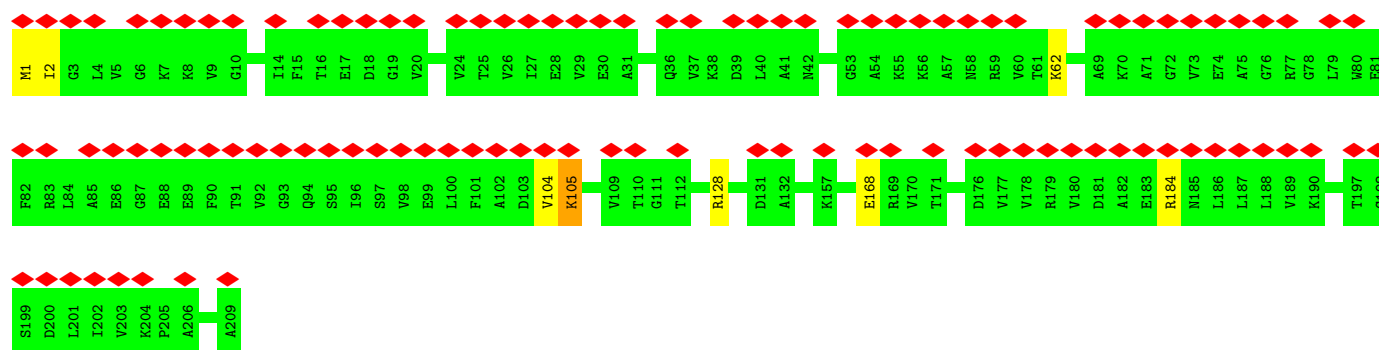




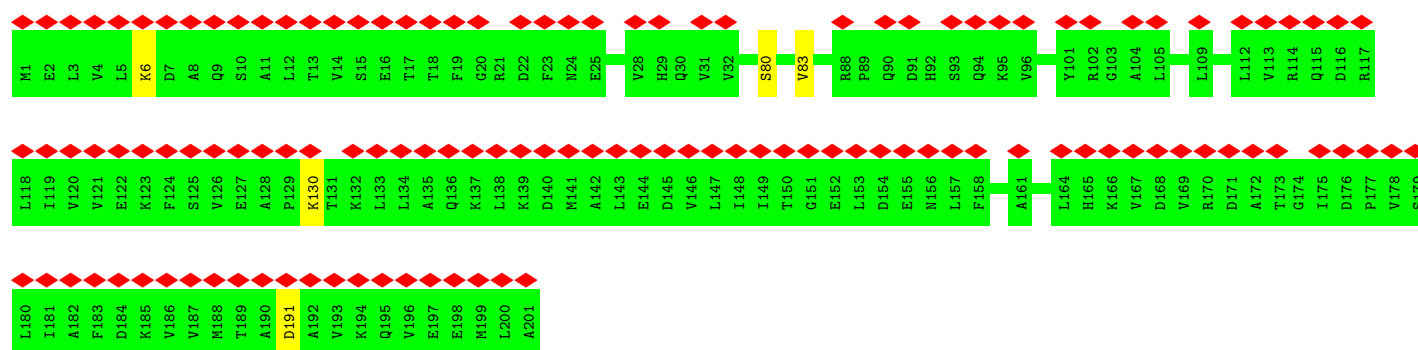
• Molecule 3: 50S ribosomal protein L2



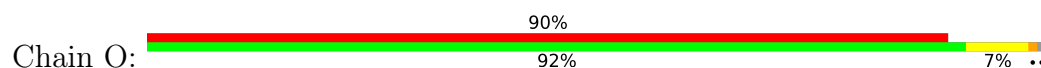
• Molecule 4: 50S ribosomal protein L3

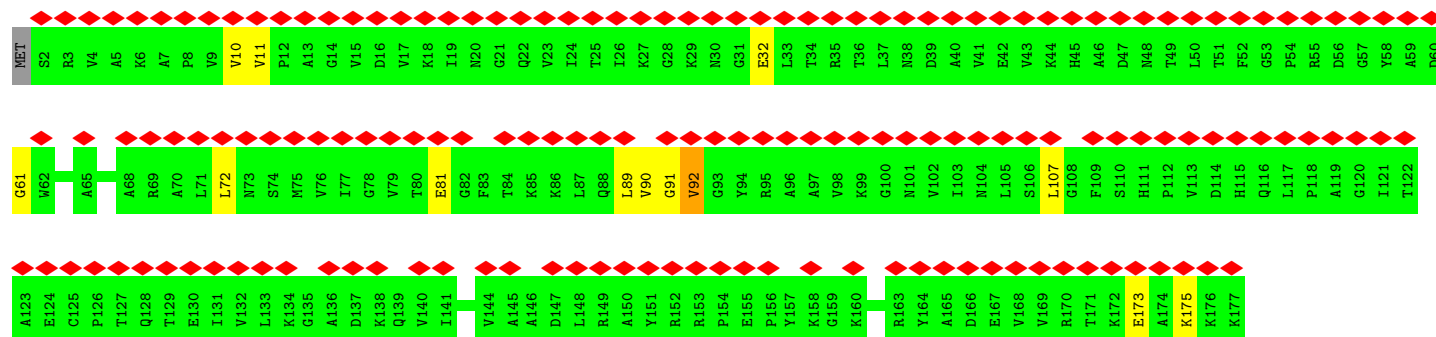


• Molecule 5: 50S ribosomal protein L4

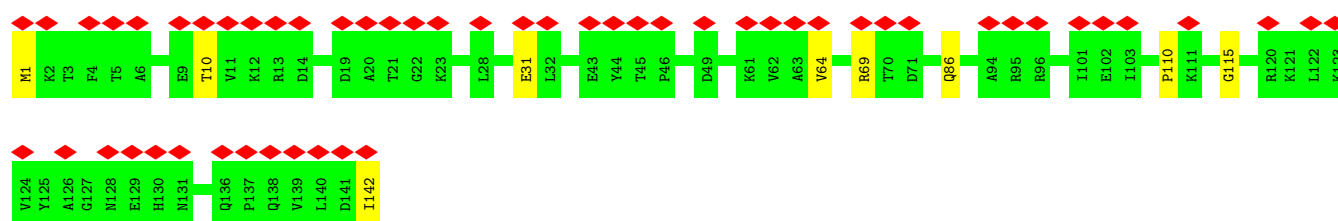
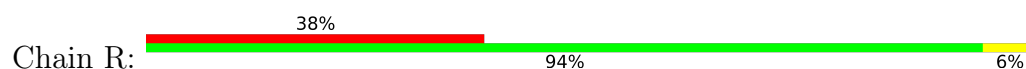


• Molecule 6: 50S ribosomal protein L6

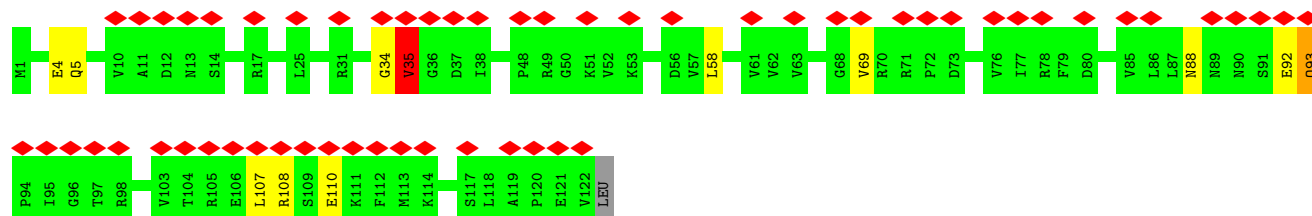
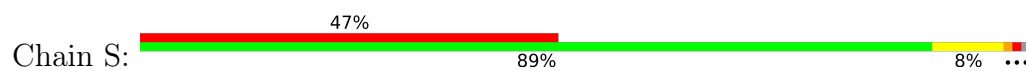




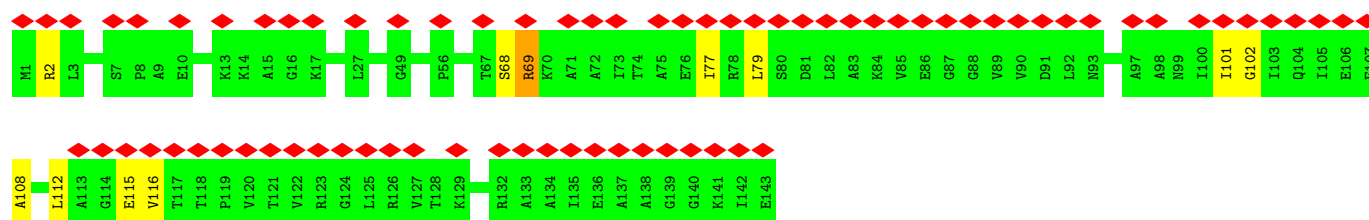
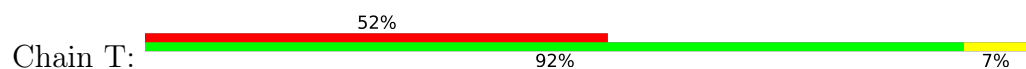
• Molecule 7: 50S ribosomal protein L13



• Molecule 8: 50S ribosomal protein L14

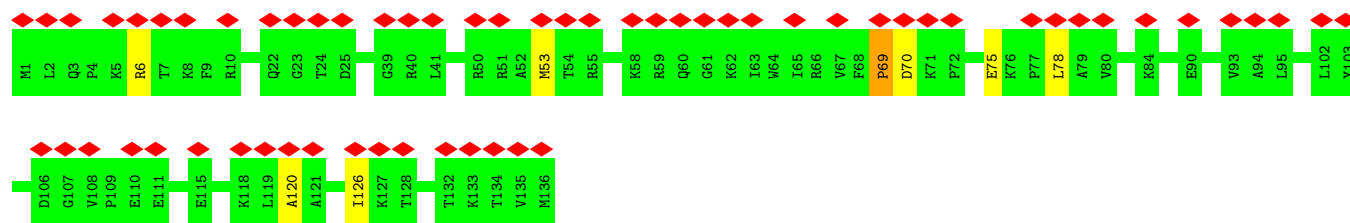


• Molecule 9: 50S ribosomal protein L15

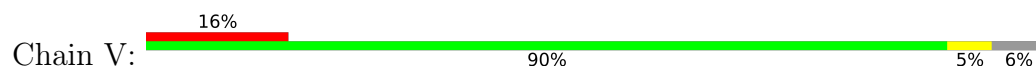


• Molecule 10: 50S ribosomal protein L16

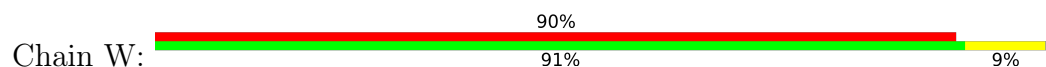




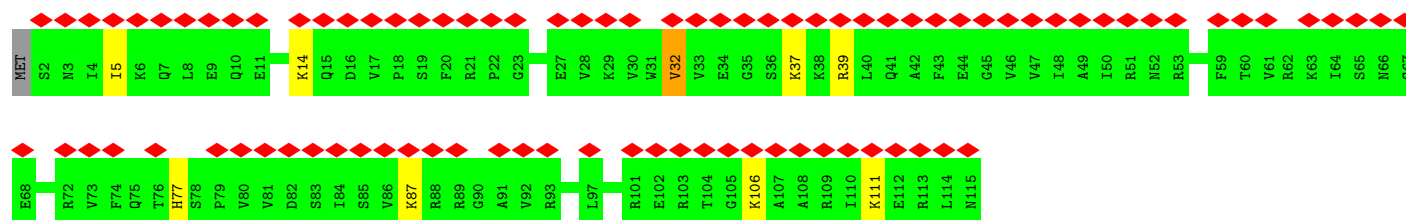
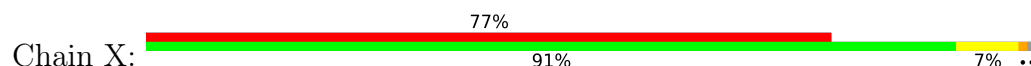
• Molecule 11: 50S ribosomal protein L17



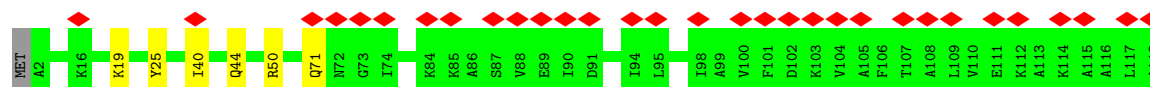
• Molecule 12: 50S ribosomal protein L18



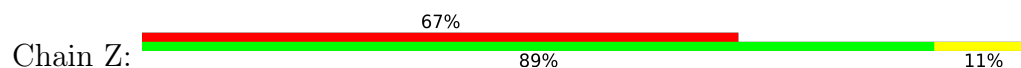
• Molecule 13: 50S ribosomal protein L19

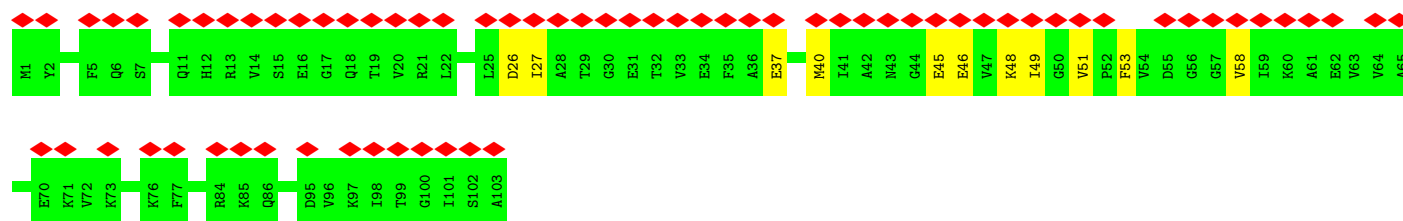


• Molecule 14: 50S ribosomal protein L20

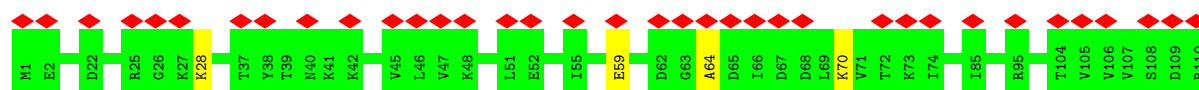


• Molecule 15: 50S ribosomal protein L21

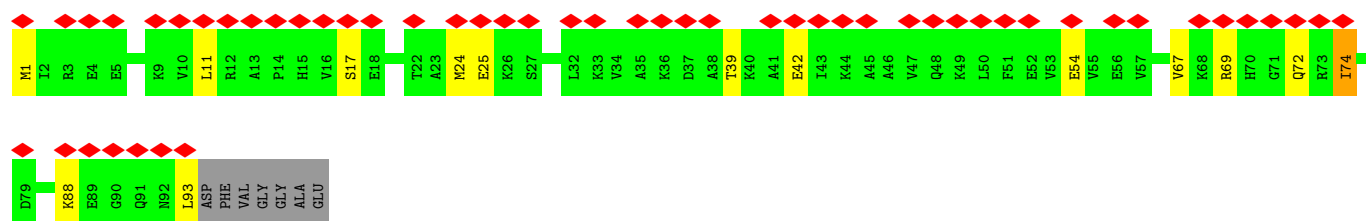
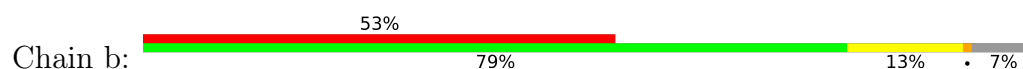




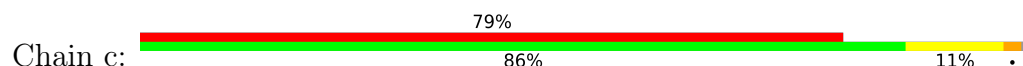
• Molecule 16: 50S ribosomal protein L22



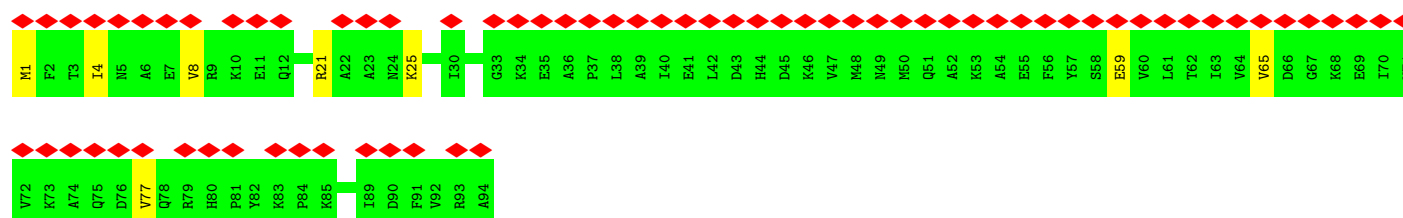
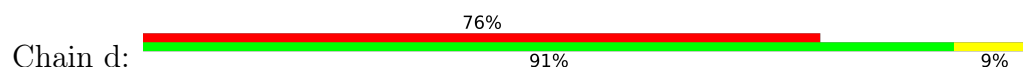
• Molecule 17: 50S ribosomal protein L23



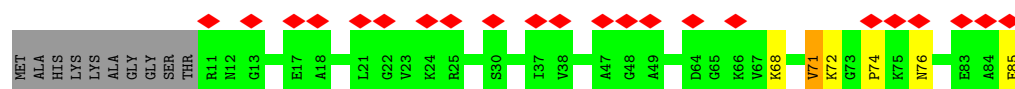
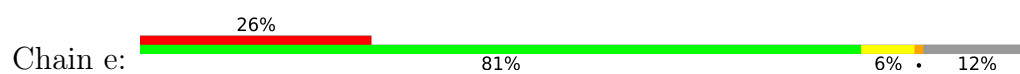
• Molecule 18: 50S ribosomal protein L24



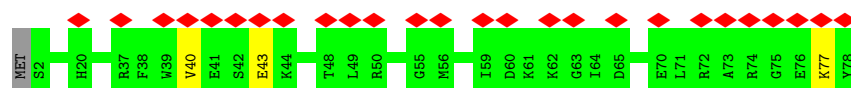
• Molecule 19: 50S ribosomal protein L25



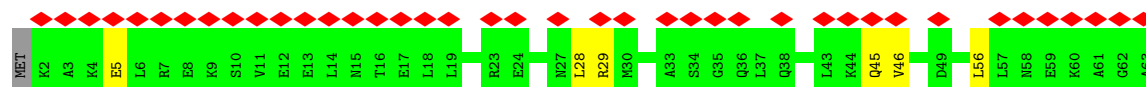
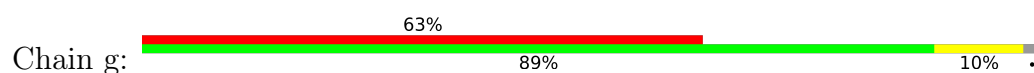
• Molecule 20: 50S ribosomal protein L27



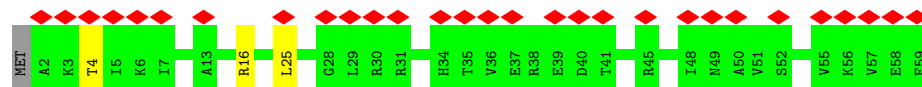
- Molecule 21: 50S ribosomal protein L28



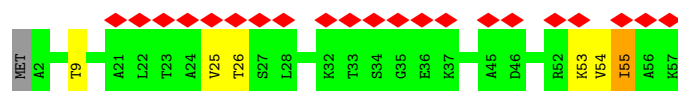
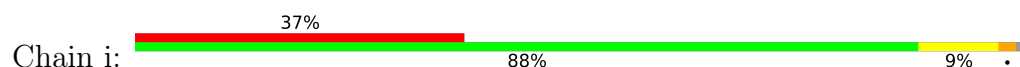
- Molecule 22: 50S ribosomal protein L29



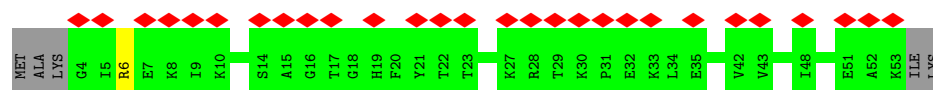
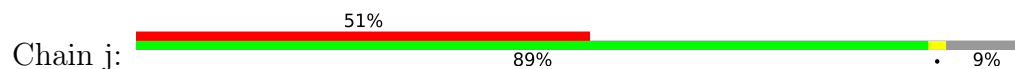
- Molecule 23: 50S ribosomal protein L30



- Molecule 24: 50S ribosomal protein L32

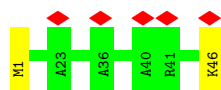


- Molecule 25: 50S ribosomal protein L33

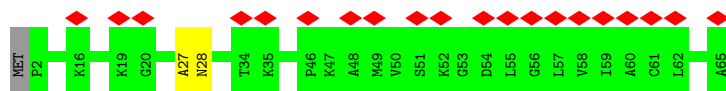
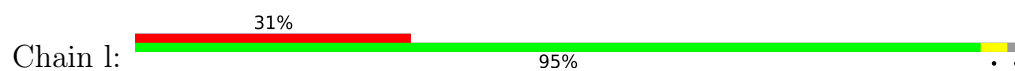


- Molecule 26: 50S ribosomal protein L34

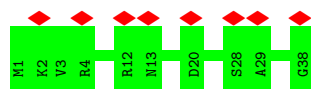




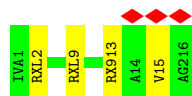
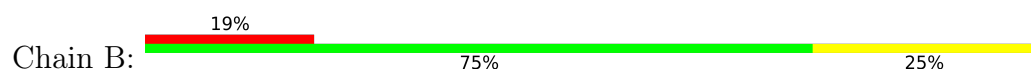
- Molecule 27: 50S ribosomal protein L35



- Molecule 28: 50S ribosomal protein L36



- Molecule 29: Myxovalargin A



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	580425	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.380	Depositor
Minimum map value	-0.163	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	298.08002, 298.08002, 298.08002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, MG, DVA, DHV, 5MU, OMU, ZN, IVA, RXL, RX9, 2MG, PSU, 1MG, MAA, IB9, DAR, 2MA, OMG, AG2, 5MC, OMC

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	I	0.38	0/69266	0.40	0/108061
2	J	0.30	0/2831	0.42	0/4415
3	K	0.51	0/2121	0.63	0/2852
4	L	0.26	0/1586	0.42	0/2134
5	M	0.25	0/1571	0.35	0/2113
6	O	0.20	0/1343	0.34	0/1816
7	R	0.28	0/1152	0.40	0/1551
8	S	0.26	0/947	0.43	0/1268
9	T	0.27	0/1052	0.44	0/1401
10	U	0.27	0/1093	0.39	0/1460
11	V	0.29	0/973	0.40	0/1301
12	W	0.20	0/902	0.34	0/1209
13	X	0.24	0/929	0.37	0/1242
14	Y	0.32	0/960	0.49	2/1278 (0.2%)
15	Z	0.29	0/829	0.51	0/1107
16	a	0.25	0/864	0.36	0/1156
17	b	0.25	0/744	0.42	0/994
18	c	0.22	0/787	0.40	0/1051
19	d	0.26	0/766	0.37	0/1025
20	e	0.30	0/576	0.53	0/762
21	f	0.25	0/635	0.39	0/848
22	g	0.22	0/502	0.38	0/667
23	h	0.23	0/453	0.34	0/605
24	i	0.27	0/450	0.43	0/599
25	j	0.24	0/416	0.39	0/554
26	k	0.29	0/380	0.44	0/498
27	l	0.27	0/513	0.40	0/676
28	m	0.28	0/303	0.38	0/397
29	B	0.17	0/10	0.75	0/11
All	All	0.36	0/94954	0.41	2/143051 (0.0%)

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
29	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Y	25	TYR	N-CA-C	6.24	119.68	109.76
14	Y	50	ARG	N-CA-C	-5.63	105.29	111.82

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
29	B	15	DHV	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	62225	0	31309	327	0
2	J	2531	0	1280	8	0
3	K	2082	0	2154	2	0
4	L	1565	0	1616	2	0
5	M	1552	0	1619	0	0
6	O	1323	0	1371	2	0
7	R	1129	0	1162	2	0
8	S	938	0	1012	4	0
9	T	1043	0	1122	4	0
10	U	1074	0	1157	1	0
11	V	960	0	1000	2	0
12	W	892	0	923	3	0
13	X	917	0	962	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	Y	947	0	1019	2	0
15	Z	816	0	839	2	0
16	a	857	0	922	1	0
17	b	738	0	807	7	0
18	c	779	0	831	5	0
19	d	753	0	780	1	0
20	e	569	0	581	3	0
21	f	625	0	652	0	0
22	g	501	0	531	2	0
23	h	449	0	488	0	0
24	i	444	0	458	2	0
25	j	409	0	440	1	0
26	k	377	0	418	0	0
27	l	504	0	572	1	0
28	m	302	0	340	0	0
29	B	119	0	102	0	0
30	I	141	0	0	0	0
30	J	3	0	0	0	0
30	L	1	0	0	0	0
31	m	1	0	0	0	0
32	B	10	0	0	0	0
32	I	18	0	0	0	0
All	All	87594	0	56467	377	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 (377) 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:2119:A:H61	1:I:2167:U:H1'	1.29	0.97
1:I:2124:G:H3'	1:I:2125:G:H8	1.29	0.96
1:I:2133:G:H2'	1:I:2157:G:H22	1.32	0.93
1:I:2159:G:H2'	1:I:2160:C:C6	2.05	0.90
1:I:2111:U:H1'	1:I:2118:U:H4'	1.53	0.90
1:I:2175:C:H2'	1:I:2176:A:C8	2.11	0.83
1:I:2160:C:H2'	1:I:2161:C:C2	2.13	0.83
1:I:2163:A:H3'	1:I:2164:C:H4'	1.61	0.83
1:I:2127:G:H2'	1:I:2128:G:C8	2.14	0.83
1:I:2149:U:H2'	1:I:2150:C:C6	2.15	0.82
1:I:2116:G:H2'	1:I:2117:A:H2	1.45	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2106:U:H2'	1:I:2183:A:N1	1.95	0.81
1:I:2114:A:C4	1:I:2167:U:H4'	2.17	0.80
1:I:2116:G:H2'	1:I:2117:A:C2	2.17	0.80
1:I:2151:U:H2'	1:I:2152:G:H8	1.47	0.80
1:I:2134:A:H1'	1:I:2159:G:H1'	1.65	0.79
1:I:2139:U:H2'	1:I:2140:G:C8	2.18	0.78
1:I:62:U:O2	1:I:63:A:N6	2.16	0.78
1:I:2149:U:H2'	1:I:2150:C:H6	1.47	0.78
1:I:2151:U:H2'	1:I:2152:G:C8	2.19	0.78
1:I:2119:A:N6	1:I:2167:U:H1'	1.98	0.78
1:I:2115:G:H4'	1:I:2166:U:H1'	1.64	0.77
1:I:2112:G:P	1:I:2169:A:H61	2.06	0.77
1:I:2137:U:H2'	1:I:2138:G:C8	2.19	0.77
1:I:2138:G:H2'	1:I:2139:U:C6	2.21	0.76
1:I:2173:A:H3'	1:I:2174:C:H6	1.49	0.76
1:I:2185:U:H2'	1:I:2186:G:C8	2.21	0.75
1:I:2105:U:H2'	1:I:2106:U:C6	2.21	0.74
1:I:2176:A:H2'	1:I:2177:C:C6	2.24	0.73
1:I:2096:C:H2'	1:I:2097:A:C8	2.25	0.72
1:I:2134:A:H2'	1:I:2135:A:C8	2.25	0.72
1:I:2173:A:H3'	1:I:2174:C:C6	2.23	0.72
1:I:2102:G:H1	1:I:2186:G:H1	1.39	0.71
1:I:2128:G:H4'	1:I:2174:C:H4'	1.72	0.71
1:I:2152:G:H2'	1:I:2153:C:C6	2.25	0.71
1:I:2179:C:H2'	1:I:2180:U:H6	1.53	0.71
1:I:2125:G:H22	1:I:2171:A:P	2.14	0.70
1:I:2135:A:H2'	1:I:2136:G:O4'	1.90	0.70
1:I:2124:G:H3'	1:I:2125:G:C8	2.19	0.70
1:I:2101:A:H2'	1:I:2102:G:C8	2.28	0.69
1:I:2139:U:H2'	1:I:2140:G:H8	1.54	0.69
1:I:2104:C:H42	1:I:2185:U:H3	1.42	0.68
1:I:2140:G:H2'	1:I:2141:G:C8	2.28	0.68
1:I:2111:U:C5	1:I:2145:C:H1'	2.29	0.67
1:I:2125:G:N2	1:I:2173:A:H62	1.92	0.67
1:I:2115:G:H2'	1:I:2117:A:OP2	1.93	0.67
1:I:2096:C:H2'	1:I:2097:A:H8	1.58	0.67
1:I:2121:G:H2'	1:I:2122:U:C6	2.30	0.67
1:I:2112:G:N3	1:I:2112:G:H2'	2.09	0.67
1:I:2126:A:N1	1:I:2163:A:H8	1.91	0.67
1:I:140:C:O3'	1:I:141:G:N2	2.28	0.67
1:I:2133:G:H2'	1:I:2157:G:N2	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2116:G:H5'	1:I:2165:C:N3	2.11	0.66
1:I:2177:C:H3'	1:I:2178:C:C6	2.31	0.66
2:J:84:G:H1	2:J:92:U:H3	1.44	0.66
1:I:2108:A:H3'	1:I:2109:U:C6	2.31	0.65
1:I:2191:A:H2'	1:I:2192:U:C6	2.32	0.65
1:I:2177:C:H2'	1:I:2178:C:O4'	1.97	0.65
1:I:2108:A:C2	1:I:2182:U:H1'	2.32	0.65
18:c:16:GLY:O	18:c:18:ASP:N	2.29	0.64
1:I:2185:U:H2'	1:I:2186:G:H8	1.63	0.64
1:I:2135:A:H3'	1:I:2136:G:H8	1.63	0.64
1:I:2108:A:H3'	1:I:2109:U:H6	1.63	0.64
1:I:2125:G:H21	1:I:2173:A:H62	1.46	0.64
1:I:2124:G:C2	1:I:2125:G:H1'	2.32	0.64
1:I:2143:C:H2'	1:I:2144:G:O4'	1.98	0.64
1:I:2122:U:H2'	1:I:2123:G:C8	2.33	0.63
1:I:2150:C:H2'	1:I:2151:U:C6	2.34	0.63
1:I:2170:A:H1'	1:I:2171:A:C8	2.33	0.63
1:I:1173:U:H2'	1:I:1174:U:H4'	1.80	0.62
1:I:2104:C:H2'	1:I:2105:U:O4'	1.99	0.62
1:I:2143:C:H3'	1:I:2144:G:H8	1.64	0.62
1:I:2178:C:H2'	1:I:2179:C:C5	2.35	0.62
1:I:2125:G:H2'	1:I:2173:A:H61	1.65	0.62
1:I:1041:G:N2	1:I:1042:G:N7	2.45	0.62
1:I:2177:C:H3'	1:I:2178:C:H6	1.65	0.62
1:I:2128:G:H2'	1:I:2129:C:O4'	2.00	0.61
1:I:2148:G:H2'	1:I:2149:U:C6	2.35	0.61
1:I:2116:G:N7	1:I:2164:C:H5''	2.15	0.61
1:I:2138:G:H2'	1:I:2139:U:H6	1.65	0.61
1:I:947:A:H2'	1:I:948:C:C6	2.36	0.61
9:T:68:SER:O	9:T:69:ARG:HB2	2.01	0.60
1:I:2156:G:H3'	1:I:2157:G:C8	2.36	0.60
1:I:2176:A:H2'	1:I:2177:C:H6	1.66	0.60
1:I:2179:C:H2'	1:I:2180:U:C6	2.36	0.59
1:I:547:A:N1	1:I:549:G:N1	2.51	0.59
1:I:2144:G:O2'	1:I:2145:C:H2'	2.01	0.59
1:I:2175:C:H2'	1:I:2176:A:H8	1.63	0.59
1:I:2111:U:H5''	1:I:2145:C:N3	2.18	0.59
1:I:2116:G:H5'	1:I:2165:C:C4	2.37	0.59
1:I:2156:G:H3'	1:I:2157:G:H8	1.67	0.59
1:I:2152:G:H2'	1:I:2153:C:H6	1.68	0.59
1:I:2148:G:H2'	1:I:2149:U:H6	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:948:C:H1'	1:I:984:A:C8	2.38	0.58
1:I:2136:G:N2	1:I:2156:G:H1'	2.19	0.58
1:I:2118:U:C5	1:I:2149:U:H1'	2.39	0.58
1:I:2105:U:H3	1:I:2184:A:H61	1.51	0.58
1:I:2144:G:H2'	1:I:2146:C:C5	2.38	0.57
1:I:2111:U:H5	1:I:2145:C:H1'	1.68	0.57
15:Z:48:LYS:HG3	15:Z:49:ILE:H	1.68	0.57
1:I:2124:G:H1	1:I:2174:C:N4	2.02	0.57
1:I:2134:A:H2'	1:I:2135:A:H8	1.66	0.57
1:I:2104:C:N4	1:I:2185:U:H3	2.02	0.57
1:I:2168:G:H2'	1:I:2169:A:C8	2.40	0.57
1:I:1779:U:H5	1:I:1784:A:N7	2.02	0.56
1:I:2113:U:H3'	1:I:2113:U:OP2	2.06	0.56
1:I:2120:G:H2'	1:I:2121:G:C8	2.39	0.56
1:I:2144:G:HO2'	1:I:2145:C:H6	1.53	0.56
16:a:59:GLU:HA	16:a:64:ALA:HA	1.88	0.56
1:I:2188:U:H2'	1:I:2189:U:O4'	2.06	0.56
1:I:2144:G:C2	1:I:2146:C:C2	2.93	0.56
1:I:2126:A:H1'	1:I:2127:G:H5''	1.87	0.56
12:W:33:ARG:O	12:W:34:HIS:HB2	2.05	0.55
1:I:2140:G:H2'	1:I:2141:G:H8	1.70	0.55
1:I:2135:A:O2'	1:I:2160:C:H4'	2.06	0.55
1:I:2100:G:H3'	1:I:2101:A:H8	1.72	0.54
1:I:2451:A:H5''	1:I:2451:A:H8	1.70	0.54
1:I:2107:G:H8	1:I:2107:G:P	2.31	0.54
1:I:2135:A:C2	1:I:2136:G:H1'	2.42	0.54
2:J:14:U:H5''	2:J:70:C:O2	2.08	0.54
1:I:2136:G:H2'	1:I:2137:U:H6	1.72	0.54
1:I:2163:A:N3	1:I:2163:A:H2'	2.22	0.54
22:g:45:GLN:O	22:g:46:VAL:HB	2.08	0.54
1:I:1178:C:N4	1:I:1179:G:O6	2.41	0.53
1:I:2131:U:H4'	1:I:2132:U:H2'	1.90	0.53
1:I:2150:C:H2'	1:I:2151:U:H6	1.74	0.53
1:I:2161:C:H2'	1:I:2164:C:N3	2.24	0.53
1:I:2121:G:H2'	1:I:2122:U:H6	1.74	0.53
1:I:2124:G:H1	1:I:2174:C:H42	1.55	0.53
1:I:2136:G:H2'	1:I:2137:U:C6	2.43	0.53
1:I:2144:G:H1'	1:I:2147:A:H61	1.72	0.53
1:I:2153:C:H2'	1:I:2154:A:C8	2.43	0.53
24:i:25:VAL:O	24:i:26:THR:HB	2.09	0.53
1:I:974:G:H8	1:I:990:A:H62	1.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2110:G:C6	1:I:2120:G:C8	2.98	0.52
1:I:2141:G:H2'	1:I:2142:A:O4'	2.09	0.52
1:I:2168:G:H3'	1:I:2169:A:H8	1.75	0.52
14:Y:40:ILE:O	14:Y:44:GLN:HG3	2.10	0.52
18:c:97:LYS:O	18:c:98:SER:CB	2.58	0.51
1:I:2126:A:H4'	1:I:2127:G:OP1	2.09	0.51
1:I:2153:C:H2'	1:I:2154:A:H8	1.75	0.51
18:c:4:LYS:O	18:c:94:ARG:NH1	2.44	0.51
1:I:2098:U:H2'	1:I:2099:U:C6	2.45	0.51
1:I:2137:U:H2'	1:I:2138:G:H8	1.71	0.51
1:I:2100:G:H2'	1:I:2101:A:O4'	2.10	0.51
1:I:2105:U:H2'	1:I:2106:U:H6	1.70	0.51
1:I:2124:G:N2	1:I:2175:C:C2	2.80	0.50
1:I:45:G:H5''	1:I:46:G:H5'	1.92	0.50
1:I:2114:A:C5	1:I:2167:U:H4'	2.46	0.50
1:I:2127:G:H2'	1:I:2128:G:H8	1.70	0.50
1:I:27:G:N2	1:I:512:G:H1'	2.26	0.50
1:I:2130:U:O2'	1:I:2134:A:H5''	2.12	0.50
9:T:101:ILE:HG13	9:T:102:GLY:H	1.76	0.50
1:I:2102:G:N2	1:I:2186:G:H22	2.10	0.50
1:I:2108:A:H2'	1:I:2109:U:O4'	2.12	0.50
1:I:2191:A:H2'	1:I:2192:U:H6	1.76	0.50
1:I:2185:U:C2	1:I:2186:G:C8	2.99	0.50
2:J:92:U:H2'	2:J:93:C:C6	2.46	0.50
1:I:2107:G:H22	1:I:2182:U:H2'	1.76	0.49
1:I:2161:C:O2'	1:I:2162:G:H8	1.95	0.49
1:I:2144:G:H1'	1:I:2147:A:N6	2.28	0.49
17:b:54:GLU:HG2	17:b:88:LYS:HB2	1.95	0.49
1:I:974:G:H2'	1:I:974:G:N3	2.27	0.49
1:I:2123:G:H2'	1:I:2124:G:O4'	2.13	0.49
1:I:2166:U:N3	1:I:2170:A:N1	2.61	0.49
1:I:2143:C:H42	1:I:2148:G:H1	1.60	0.49
1:I:969:G:H2'	1:I:970:U:C6	2.48	0.49
1:I:2162:G:OP2	1:I:2162:G:H3'	2.13	0.49
1:I:2164:C:OP1	1:I:2166:U:H5	1.96	0.49
1:I:2189:U:H2'	1:I:2190:G:H8	1.78	0.49
2:J:12:A:C2	20:e:74:PRO:HB3	2.48	0.48
1:I:1141:U:H4'	1:I:1142:A:O4'	2.13	0.48
1:I:2097:A:H2'	1:I:2098:U:C6	2.48	0.48
1:I:2108:A:H2	1:I:2182:U:H1'	1.78	0.48
1:I:1069:A:O2'	1:I:1074:G:O6	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2155:U:H2'	1:I:2156:G:O4'	2.13	0.48
1:I:2115:G:C4	1:I:2117:A:C8	3.02	0.48
1:I:2133:G:C5	1:I:2157:G:N1	2.82	0.48
1:I:2156:G:H2'	1:I:2157:G:O4'	2.13	0.48
1:I:2165:C:H41	1:I:2171:A:N6	2.12	0.48
1:I:2110:G:H2'	1:I:2120:G:OP2	2.14	0.48
1:I:2153:C:C2	1:I:2154:A:C8	3.01	0.48
1:I:2122:U:C2	1:I:2123:G:C8	3.02	0.48
1:I:2155:U:H2'	1:I:2156:G:C8	2.49	0.47
18:c:7:ARG:O	18:c:25:VAL:HB	2.14	0.47
1:I:1068:G:O2'	1:I:1070:A:N6	2.44	0.47
1:I:2110:G:H5'	1:I:2145:C:N4	2.29	0.47
1:I:2119:A:C4	1:I:2171:A:C2	3.02	0.47
1:I:2171:A:H5'	1:I:2174:C:H41	1.79	0.47
1:I:2131:U:C4	1:I:2133:G:C4	3.01	0.47
1:I:2107:G:H1	1:I:2182:U:H2'	1.78	0.47
1:I:2127:G:H2'	1:I:2128:G:O4'	2.14	0.47
1:I:2128:G:C4'	1:I:2174:C:H4'	2.41	0.47
1:I:2142:A:H3'	1:I:2143:C:H6	1.80	0.47
1:I:1796:U:H2'	1:I:1797:G:H8	1.79	0.47
1:I:2154:A:H2'	1:I:2155:U:H6	1.80	0.47
10:U:53:MET:HG3	10:U:120:ALA:HB2	1.95	0.47
1:I:1178:C:H2'	1:I:1179:G:C8	2.49	0.47
1:I:1794:A:H2'	1:I:1795:C:C6	2.49	0.47
1:I:2118:U:H1'	1:I:2145:C:H41	1.80	0.47
1:I:2122:U:H2'	1:I:2123:G:H8	1.76	0.47
1:I:2105:U:H3	1:I:2184:A:N6	2.12	0.47
1:I:2134:A:H2'	1:I:2135:A:O4'	2.14	0.47
1:I:2144:G:H2'	1:I:2146:C:H5	1.80	0.47
17:b:54:GLU:H	17:b:54:GLU:CD	2.23	0.47
1:I:639:U:H2'	1:I:640:C:C6	2.50	0.47
6:O:91:GLY:O	6:O:92:VAL:HB	2.15	0.47
1:I:2147:A:H3'	1:I:2148:G:O4'	2.15	0.47
20:e:71:VAL:O	20:e:72:LYS:HD2	2.15	0.47
1:I:1995:U:OP1	4:L:128:ARG:CZ	2.63	0.46
1:I:2158:A:H1'	1:I:2159:G:N9	2.30	0.46
1:I:2318:G:O2'	1:I:2319:G:OP1	2.23	0.46
1:I:27:G:C2	1:I:512:G:N3	2.83	0.46
1:I:2100:G:H3'	1:I:2101:A:C8	2.49	0.46
1:I:2469:A:N6	1:I:2481:G:O2'	2.48	0.46
15:Z:49:ILE:HB	15:Z:51:VAL:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2138:G:H1	1:I:2153:C:H42	1.63	0.46
1:I:2168:G:H3'	1:I:2169:A:C8	2.51	0.46
3:K:260:ASN:O	3:K:261:LYS:HB2	2.16	0.46
1:I:358:U:H2'	1:I:359:G:H8	1.79	0.46
1:I:2104:C:H2'	1:I:2105:U:C6	2.51	0.46
1:I:2154:A:H2'	1:I:2155:U:C6	2.49	0.46
1:I:2157:G:H2'	1:I:2158:A:H2	1.80	0.46
18:c:3:ALA:O	18:c:4:LYS:HB2	2.15	0.46
1:I:2106:U:N3	1:I:2184:A:C6	2.83	0.46
1:I:2134:A:N7	1:I:2157:G:O2'	2.42	0.46
1:I:2181:U:H2'	1:I:2182:U:O4'	2.17	0.46
1:I:2129:C:H2'	1:I:2130:U:C6	2.51	0.45
1:I:2110:G:H5'	1:I:2145:C:H42	1.81	0.45
1:I:2115:G:N3	1:I:2117:A:N7	2.64	0.45
1:I:2163:A:H5''	1:I:2171:A:H8	1.82	0.45
1:I:2318:G:HO2'	1:I:2319:G:P	2.37	0.45
1:I:2123:G:C5	1:I:2124:G:C5	3.04	0.45
2:J:12:A:H8	2:J:12:A:OP2	1.99	0.45
1:I:1212:G:H1'	1:I:1236:G:N2	2.31	0.45
1:I:2102:G:H3'	1:I:2103:C:C6	2.52	0.45
1:I:2116:G:C6	1:I:2171:A:C6	3.04	0.45
1:I:2107:G:C5	1:I:2183:A:C6	3.04	0.45
1:I:2119:A:C6	1:I:2170:A:C2	3.04	0.45
1:I:2124:G:N3	1:I:2125:G:H1'	2.31	0.45
13:X:14:LYS:HD3	13:X:77:HIS:HA	1.99	0.45
1:I:2122:U:H2'	1:I:2123:G:O4'	2.17	0.45
1:I:2123:G:H2'	1:I:2124:G:C8	2.52	0.45
1:I:2127:G:C2'	1:I:2128:G:C8	2.96	0.45
1:I:2158:A:H1'	1:I:2159:G:C1'	2.47	0.45
1:I:2107:G:C2	1:I:2108:A:H1'	2.52	0.45
1:I:2114:A:H2	1:I:2166:U:O2	1.99	0.45
1:I:2120:G:C5	1:I:2121:G:C5	3.05	0.45
1:I:2902:C:C6	1:I:2903:U:H2'	2.51	0.45
1:I:528:A:C2	1:I:2043:C:H4'	2.52	0.45
1:I:1796:U:H2'	1:I:1797:G:C8	2.52	0.45
2:J:92:U:H2'	2:J:93:C:H6	1.81	0.45
1:I:2127:G:C8	1:I:2162:G:C2	3.05	0.44
1:I:2162:G:H1'	1:I:2163:A:OP1	2.17	0.44
1:I:2529:G:H4'	6:O:175:LYS:HG2	1.99	0.44
1:I:2135:A:H3'	1:I:2136:G:C8	2.49	0.44
1:I:2138:G:C2	1:I:2154:A:C2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:1043:C:H2'	1:I:1044:C:C2	2.52	0.44
1:I:2157:G:N2	1:I:2158:A:N1	2.65	0.44
7:R:110:PRO:O	7:R:115:GLY:HA3	2.17	0.44
1:I:1338:G:O3'	17:b:17:SER:HB2	2.18	0.44
1:I:2114:A:N3	1:I:2114:A:H2'	2.32	0.44
1:I:2120:G:H2'	1:I:2121:G:O4'	2.18	0.44
1:I:2123:G:H3'	1:I:2124:G:H8	1.81	0.44
1:I:2142:A:C3'	1:I:2143:C:H6	2.30	0.44
1:I:2147:A:C8	1:I:2148:G:H1'	2.52	0.44
1:I:2149:U:O2'	1:I:2150:C:H5'	2.18	0.44
1:I:1212:G:N3	1:I:1236:G:C2	2.86	0.44
1:I:2101:A:H2	1:I:2188:U:O4	2.01	0.44
1:I:2125:G:H2'	1:I:2125:G:N3	2.33	0.44
1:I:2124:G:C6	1:I:2125:G:C4	3.06	0.44
1:I:2143:C:H3'	1:I:2144:G:C8	2.50	0.44
1:I:2113:U:OP2	1:I:2115:G:N2	2.51	0.44
2:J:12:A:H2'	20:e:76:ASN:OD1	2.18	0.44
1:I:1171:G:N2	1:I:1178:C:N3	2.62	0.44
1:I:2100:G:C6	1:I:2190:G:C6	3.06	0.44
1:I:2106:U:C2	1:I:2183:A:N1	2.86	0.44
1:I:2123:G:C2	1:I:2176:A:N3	2.86	0.44
4:L:104:VAL:O	4:L:105:LYS:HB2	2.17	0.44
1:I:2109:U:H1'	1:I:2181:U:O2	2.18	0.43
1:I:2125:G:H2'	1:I:2173:A:N6	2.32	0.43
1:I:2139:U:H3	1:I:2152:G:H1	1.65	0.43
1:I:2273:A:H2'	1:I:2274:A:C8	2.53	0.43
1:I:2107:G:H2'	1:I:2108:A:O4'	2.18	0.43
1:I:2117:A:C5	1:I:2119:A:N7	2.86	0.43
1:I:2145:C:H3'	1:I:2146:C:C6	2.53	0.43
1:I:84:A:N1	1:I:98:G:O2'	2.47	0.43
1:I:2147:A:N6	1:I:2148:G:H21	2.17	0.43
1:I:63:A:H2'	1:I:64:A:O4'	2.19	0.43
1:I:2102:G:H3'	1:I:2103:C:H6	1.83	0.43
1:I:2118:U:C6	1:I:2149:U:H1'	2.53	0.43
1:I:559:G:O2'	1:I:560:C:H5'	2.19	0.43
1:I:1115:G:O2'	1:I:1116:G:H5'	2.18	0.43
1:I:2102:G:H22	1:I:2186:G:H22	1.66	0.43
1:I:2177:C:C4	1:I:2178:C:C2	3.07	0.43
1:I:2328:A:H2'	1:I:2329:U:C6	2.54	0.43
11:V:33:ILE:HD13	11:V:114:GLU:HB3	2.01	0.43
1:I:559:G:C2'	1:I:560:C:H5'	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2115:G:N3	1:I:2117:A:C8	2.87	0.43
11:V:86:ARG:HH21	11:V:117:ASP:HB2	1.84	0.43
1:I:2114:A:N6	1:I:2115:G:H21	2.17	0.42
13:X:32:VAL:HG23	13:X:39:ARG:HG3	2.01	0.42
1:I:64:A:H2'	1:I:65:U:C6	2.54	0.42
1:I:971:G:H2'	1:I:972:A:O4'	2.19	0.42
9:T:77:ILE:HD13	9:T:108:ALA:HB1	2.00	0.42
1:I:2161:C:H2'	1:I:2164:C:C4	2.54	0.42
14:Y:40:ILE:HG22	14:Y:44:GLN:OE1	2.20	0.42
1:I:137:U:H2'	1:I:140:C:H42	1.85	0.42
1:I:1736:U:H2'	1:I:1737:G:O4'	2.20	0.42
1:I:1932:A:H2'	1:I:1933:G:O4'	2.20	0.42
1:I:2097:A:H2'	1:I:2098:U:O4'	2.19	0.42
1:I:2144:G:N3	1:I:2148:G:N2	2.66	0.42
8:S:88:ASN:HB3	8:S:92:GLU:O	2.18	0.42
1:I:544:C:H2'	1:I:545:U:O4'	2.20	0.42
1:I:2113:U:O4	1:I:2168:G:H8	2.01	0.42
1:I:2286:G:OP2	25:j:6:ARG:NH2	2.53	0.42
1:I:2291:U:H2'	1:I:2292:U:C6	2.55	0.42
1:I:2020:A:H5'	24:i:9:THR:CG2	2.50	0.42
1:I:2162:G:H4'	1:I:2173:A:O4'	2.19	0.42
1:I:2167:U:H3	1:I:2169:A:H3'	1.84	0.42
27:l:27:ALA:O	27:l:28:ASN:HB2	2.19	0.42
1:I:1026:G:H2'	1:I:1027:A:C8	2.55	0.41
1:I:2117:A:N1	1:I:2171:A:N6	2.67	0.41
1:I:2133:G:C2'	1:I:2157:G:H22	2.17	0.41
2:J:34:A:N6	2:J:44:G:H1'	2.34	0.41
1:I:1115:G:C4	1:I:1116:G:C8	3.08	0.41
1:I:1720:U:H2'	1:I:1721:G:O4'	2.20	0.41
19:d:21:ARG:HA	19:d:25:LYS:O	2.20	0.41
1:I:141:G:C6	17:b:1:MET:HG3	2.54	0.41
1:I:2165:C:N4	1:I:2171:A:N6	2.68	0.41
8:S:92:GLU:O	8:S:93:GLN:HB2	2.18	0.41
1:I:2143:C:H2'	1:I:2143:C:O2	2.21	0.41
1:I:2134:A:H62	1:I:2157:G:C1'	2.33	0.41
1:I:2140:G:H1	1:I:2151:U:H3	1.68	0.41
1:I:2180:U:C5	1:I:2181:U:N3	2.88	0.41
1:I:2297:A:N1	1:I:2321:U:H5	2.18	0.41
1:I:2168:G:C6	1:I:2169:A:C6	3.09	0.41
1:I:2788:C:H2'	1:I:2789:C:C6	2.56	0.41
17:b:11:LEU:O	22:g:29:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:2116:G:C5	1:I:2171:A:N6	2.89	0.41
7:R:31:GLU:HG3	7:R:142:ILE:HG13	2.02	0.41
12:W:33:ARG:HG2	12:W:34:HIS:CD2	2.55	0.41
1:I:2130:U:C2	1:I:2159:G:N1	2.88	0.41
1:I:2142:A:H3'	1:I:2143:C:C6	2.56	0.41
1:I:2146:C:H4'	1:I:2147:A:N9	2.36	0.41
1:I:1069:A:C5	1:I:1096:A:H4'	2.55	0.41
1:I:2106:U:H2'	1:I:2183:A:C2	2.53	0.41
1:I:2118:U:H1'	1:I:2145:C:N4	2.35	0.41
1:I:2155:U:C4	1:I:2156:G:C5	3.08	0.41
1:I:2155:U:H3'	1:I:2156:G:H8	1.84	0.41
1:I:2163:A:H4'	1:I:2170:A:O2'	2.20	0.41
1:I:2165:C:H2'	1:I:2166:U:C6	2.56	0.41
12:W:31:THR:OG1	12:W:33:ARG:O	2.37	0.41
17:b:39:THR:HG23	17:b:42:GLU:H	1.86	0.41
1:I:1061:U:O3'	1:I:1070:A:H4'	2.21	0.41
1:I:1548:A:H2'	1:I:1549:A:C8	2.57	0.41
1:I:2119:A:C5	1:I:2169:A:C6	3.09	0.41
1:I:2178:C:H2'	1:I:2179:C:C4	2.56	0.41
8:S:4:GLU:O	8:S:5:GLN:HB2	2.20	0.41
1:I:784:G:H5'	1:I:785:G:OP1	2.21	0.40
1:I:2110:G:C6	1:I:2180:U:N3	2.89	0.40
1:I:2116:G:C8	1:I:2164:C:C6	3.09	0.40
8:S:34:GLY:O	8:S:35:VAL:C	2.64	0.40
1:I:493:G:H2'	1:I:494:G:O4'	2.21	0.40
1:I:1171:G:H1	1:I:1177:G:H1	1.69	0.40
1:I:2113:U:P	1:I:2115:G:H22	2.43	0.40
1:I:2140:G:C2	1:I:2141:G:C4	3.09	0.40
3:K:29:PRO:HG2	3:K:34:LEU:HD11	2.02	0.40
1:I:191:A:H2'	1:I:192:C:C6	2.56	0.40
1:I:2116:G:H1	1:I:2173:A:P	2.44	0.40
1:I:2154:A:H2'	1:I:2155:U:O4'	2.21	0.40
17:b:69:ARG:HG2	17:b:74:ILE:HG23	2.04	0.40
1:I:528:A:N1	1:I:2042:A:H2'	2.36	0.40
1:I:2102:G:N2	1:I:2187:U:O2	2.53	0.40
1:I:2134:A:C2	1:I:2159:G:H4'	2.56	0.40
1:I:2140:G:C6	1:I:2152:G:C6	3.09	0.40
9:T:79:LEU:HD11	9:T:112:LEU:HD12	2.04	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	269/273 (98%)	260 (97%)	9 (3%)	0	100	100
4	L	207/209 (99%)	198 (96%)	9 (4%)	0	100	100
5	M	199/201 (99%)	192 (96%)	5 (2%)	2 (1%)	12	9
6	O	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	11	8
7	R	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
8	S	120/123 (98%)	108 (90%)	10 (8%)	2 (2%)	7	3
9	T	141/143 (99%)	134 (95%)	6 (4%)	1 (1%)	18	15
10	U	134/136 (98%)	129 (96%)	4 (3%)	1 (1%)	18	15
11	V	118/127 (93%)	114 (97%)	4 (3%)	0	100	100
12	W	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
13	X	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
14	Y	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
15	Z	101/103 (98%)	94 (93%)	6 (6%)	1 (1%)	12	9
16	a	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
17	b	91/100 (91%)	88 (97%)	3 (3%)	0	100	100
18	c	100/104 (96%)	88 (88%)	10 (10%)	2 (2%)	6	2
19	d	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
20	e	73/85 (86%)	72 (99%)	1 (1%)	0	100	100
21	f	75/78 (96%)	75 (100%)	0	0	100	100
22	g	60/63 (95%)	56 (93%)	4 (7%)	0	100	100
23	h	56/59 (95%)	54 (96%)	2 (4%)	0	100	100
24	i	54/57 (95%)	52 (96%)	1 (2%)	1 (2%)	6	3
25	j	48/55 (87%)	46 (96%)	2 (4%)	0	100	100
26	k	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
27	l	62/65 (95%)	60 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
28	m	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
29	B	2/16 (12%)	1 (50%)	1 (50%)	0	100	100
All	All	2845/2954 (96%)	2731 (96%)	102 (4%)	12 (0%)	31	28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	O	61	GLY
8	S	35	VAL
10	U	69	PRO
24	i	55	ILE
18	c	17	LYS
8	S	93	GLN
5	M	80	SER
5	M	83	VAL
6	O	92	VAL
15	Z	53	PHE
9	T	69	ARG
18	c	98	SER

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	216/218 (99%)	214 (99%)	2 (1%)	70	78
4	L	164/164 (100%)	158 (96%)	6 (4%)	30	33
5	M	165/165 (100%)	162 (98%)	3 (2%)	51	60
6	O	137/138 (99%)	128 (93%)	9 (7%)	15	13
7	R	116/116 (100%)	111 (96%)	5 (4%)	26	27
8	S	103/104 (99%)	97 (94%)	6 (6%)	18	16
9	T	102/102 (100%)	99 (97%)	3 (3%)	37	42
10	U	109/109 (100%)	103 (94%)	6 (6%)	19	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	V	100/103 (97%)	98 (98%)	2 (2%)	48	56
12	W	86/87 (99%)	79 (92%)	7 (8%)	11	8
13	X	99/100 (99%)	93 (94%)	6 (6%)	17	15
14	Y	89/90 (99%)	87 (98%)	2 (2%)	45	53
15	Z	84/84 (100%)	77 (92%)	7 (8%)	10	8
16	a	93/93 (100%)	91 (98%)	2 (2%)	45	53
17	b	80/84 (95%)	74 (92%)	6 (8%)	12	10
18	c	83/85 (98%)	79 (95%)	4 (5%)	23	23
19	d	78/78 (100%)	72 (92%)	6 (8%)	12	9
20	e	56/63 (89%)	53 (95%)	3 (5%)	20	18
21	f	67/68 (98%)	64 (96%)	3 (4%)	24	25
22	g	54/55 (98%)	51 (94%)	3 (6%)	19	18
23	h	48/49 (98%)	45 (94%)	3 (6%)	16	14
24	i	47/48 (98%)	44 (94%)	3 (6%)	16	14
25	j	45/49 (92%)	45 (100%)	0	100	100
26	k	38/38 (100%)	36 (95%)	2 (5%)	20	19
27	l	51/52 (98%)	51 (100%)	0	100	100
28	m	34/34 (100%)	34 (100%)	0	100	100
29	B	1/1 (100%)	1 (100%)	0	100	100
All	All	2345/2377 (99%)	2246 (96%)	99 (4%)	28	28

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	K	24	LEU
3	K	271	ARG
4	L	1	MET
4	L	2	ILE
4	L	62	LYS
4	L	105	LYS
4	L	168	GLU
4	L	184	ARG
5	M	6	LYS
5	M	130	LYS
5	M	191	ASP

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Mol	Chain	Res	Type
6	O	10	VAL
6	O	11	VAL
6	O	32	GLU
6	O	72	LEU
6	O	81	GLU
6	O	89	LEU
6	O	90	VAL
6	O	107	LEU
6	O	173	GLU
7	R	1	MET
7	R	10	THR
7	R	64	VAL
7	R	69	ARG
7	R	86	GLN
8	S	35	VAL
8	S	58	LEU
8	S	69	VAL
8	S	107	LEU
8	S	108	ARG
8	S	110	GLU
9	T	2	ARG
9	T	115	GLU
9	T	116	VAL
10	U	6	ARG
10	U	69	PRO
10	U	70	ASP
10	U	75	GLU
10	U	78	LEU
10	U	126	ILE
11	V	65	LEU
11	V	74	GLU
12	W	17	LYS
12	W	47	VAL
12	W	56	LYS
12	W	63	LYS
12	W	76	LYS
12	W	85	LYS
12	W	87	ILE
13	X	5	ILE
13	X	32	VAL
13	X	37	LYS
13	X	87	LYS

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Mol	Chain	Res	Type
13	X	106	LYS
13	X	111	LYS
14	Y	19	LYS
14	Y	71	GLN
15	Z	26	ASP
15	Z	27	ILE
15	Z	37	GLU
15	Z	40	MET
15	Z	45	GLU
15	Z	46	GLU
15	Z	58	VAL
16	a	28	LYS
16	a	70	LYS
17	b	24	MET
17	b	25	GLU
17	b	67	VAL
17	b	72	GLN
17	b	74	ILE
17	b	93	LEU
18	c	18	ASP
18	c	34	VAL
18	c	35	ILE
18	c	74	ASN
19	d	1	MET
19	d	4	ILE
19	d	8	VAL
19	d	59	GLU
19	d	65	VAL
19	d	77	VAL
20	e	68	LYS
20	e	71	VAL
20	e	85	GLU
21	f	40	VAL
21	f	43	GLU
21	f	77	LYS
22	g	5	GLU
22	g	28	LEU
22	g	56	LEU
23	h	4	THR
23	h	16	ARG
23	h	25	LEU
24	i	53	LYS

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Mol	Chain	Res	Type
24	i	54	VAL
24	i	55	ILE
26	k	1	MET
26	k	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
3	K	25	HIS
3	K	86	ASN
4	L	42	ASN
4	L	130	GLN
4	L	173	GLN
6	O	104	ASN
7	R	47	HIS
14	Y	71	GLN
17	b	28	ASN
17	b	72	GLN
20	e	57	HIS
21	f	36	HIS
22	g	58	ASN
23	h	20	HIS
27	l	28	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	2896/2904 (99%)	423 (14%)	50 (1%)
2	J	117/120 (97%)	23 (19%)	4 (3%)
All	All	3013/3024 (99%)	446 (14%)	54 (1%)

All (446) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	10	A
1	I	34	U
1	I	46	G
1	I	51	G
1	I	62	U
1	I	63	A

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Mol	Chain	Res	Type
1	I	64	A
1	I	71	A
1	I	74	A
1	I	75	G
1	I	101	A
1	I	102	U
1	I	118	A
1	I	119	A
1	I	120	U
1	I	131	A
1	I	137	U
1	I	138	U
1	I	139	U
1	I	140	C
1	I	163	C
1	I	165	A
1	I	181	A
1	I	196	A
1	I	199	A
1	I	200	U
1	I	215	G
1	I	216	A
1	I	221	A
1	I	222	A
1	I	248	G
1	I	265	A
1	I	266	G
1	I	272	A
1	I	275	C
1	I	276	U
1	I	277	G
1	I	278	A
1	I	279	A
1	I	311	A
1	I	329	G
1	I	330	A
1	I	361	G
1	I	362	A
1	I	367	G
1	I	370	G
1	I	371	A
1	I	372	G

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Mol	Chain	Res	Type
1	I	386	G
1	I	396	G
1	I	404	A
1	I	405	U
1	I	411	G
1	I	412	A
1	I	424	G
1	I	451	U
1	I	481	G
1	I	490	C
1	I	491	G
1	I	503	A
1	I	504	A
1	I	505	A
1	I	509	C
1	I	529	A
1	I	531	C
1	I	532	A
1	I	533	G
1	I	536	G
1	I	546	U
1	I	547	A
1	I	548	G
1	I	549	G
1	I	550	C
1	I	555	G
1	I	556	A
1	I	563	A
1	I	573	U
1	I	575	A
1	I	586	A
1	I	603	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	655	A
1	I	686	U
1	I	717	C

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Mol	Chain	Res	Type
1	I	730	A
1	I	746	PSU
1	I	747	5MU
1	I	764	A
1	I	765	C
1	I	775	G
1	I	776	G
1	I	782	A
1	I	784	G
1	I	785	G
1	I	804	A
1	I	805	G
1	I	812	C
1	I	819	A
1	I	827	U
1	I	828	U
1	I	845	A
1	I	846	U
1	I	858	G
1	I	878	A
1	I	896	A
1	I	897	C
1	I	910	A
1	I	931	U
1	I	932	U
1	I	941	A
1	I	946	C
1	I	961	C
1	I	974	G
1	I	983	A
1	I	984	A
1	I	985	C
1	I	995	C
1	I	996	A
1	I	1005	C
1	I	1012	U
1	I	1013	C
1	I	1022	G
1	I	1026	G
1	I	1033	U
1	I	1044	C
1	I	1045	C

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Mol	Chain	Res	Type
1	I	1046	A
1	I	1047	G
1	I	1060	U
1	I	1061	U
1	I	1069	A
1	I	1070	A
1	I	1071	G
1	I	1073	A
1	I	1079	C
1	I	1082	U
1	I	1083	U
1	I	1085	A
1	I	1088	A
1	I	1089	A
1	I	1094	U
1	I	1097	U
1	I	1098	A
1	I	1108	U
1	I	1109	C
1	I	1110	G
1	I	1111	A
1	I	1112	G
1	I	1116	G
1	I	1128	G
1	I	1129	A
1	I	1130	U
1	I	1131	G
1	I	1132	U
1	I	1133	A
1	I	1135	C
1	I	1136	G
1	I	1142	A
1	I	1170	C
1	I	1174	U
1	I	1175	A
1	I	1176	U
1	I	1180	U
1	I	1182	G
1	I	1212	G
1	I	1238	G
1	I	1247	A
1	I	1248	G

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Mol	Chain	Res	Type
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	1273	U
1	I	1275	A
1	I	1300	G
1	I	1301	A
1	I	1321	A
1	I	1329	U
1	I	1345	C
1	I	1352	U
1	I	1365	A
1	I	1368	G
1	I	1379	U
1	I	1383	A
1	I	1403	A
1	I	1416	G
1	I	1417	C
1	I	1421	G
1	I	1428	C
1	I	1452	G
1	I	1453	A
1	I	1482	G
1	I	1490	A
1	I	1493	C
1	I	1494	A
1	I	1508	A
1	I	1509	A
1	I	1510	G
1	I	1515	A
1	I	1534	U
1	I	1535	A
1	I	1536	C
1	I	1537	G
1	I	1540	G
1	I	1560	G
1	I	1566	A
1	I	1569	A
1	I	1578	U

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Mol	Chain	Res	Type
1	I	1583	A
1	I	1584	U
1	I	1607	C
1	I	1608	A
1	I	1609	A
1	I	1610	A
1	I	1618	A
1	I	1626	A
1	I	1634	A
1	I	1647	U
1	I	1648	U
1	I	1649	G
1	I	1674	G
1	I	1694	C
1	I	1715	G
1	I	1729	U
1	I	1730	C
1	I	1731	G
1	I	1738	G
1	I	1758	U
1	I	1759	A
1	I	1764	C
1	I	1773	A
1	I	1782	U
1	I	1800	C
1	I	1801	A
1	I	1807	G
1	I	1808	A
1	I	1811	G
1	I	1816	C
1	I	1829	A
1	I	1869	G
1	I	1870	C
1	I	1872	A
1	I	1873	G
1	I	1906	G
1	I	1914	C
1	I	1929	G
1	I	1930	G
1	I	1936	A
1	I	1938	A
1	I	1955	U

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Mol	Chain	Res	Type
1	I	1964	G
1	I	1966	A
1	I	1967	C
1	I	1970	A
1	I	1971	U
1	I	1972	G
1	I	1991	U
1	I	1993	U
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	2063	C
1	I	2069	G
1	I	2072	C
1	I	2096	C
1	I	2102	G
1	I	2110	G
1	I	2111	U
1	I	2112	G
1	I	2113	U
1	I	2114	A
1	I	2115	G
1	I	2116	G
1	I	2117	A
1	I	2118	U
1	I	2119	A
1	I	2120	G
1	I	2124	G
1	I	2125	G
1	I	2126	A
1	I	2127	G
1	I	2131	U

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Mol	Chain	Res	Type
1	I	2134	A
1	I	2138	G
1	I	2142	A
1	I	2144	G
1	I	2146	C
1	I	2147	A
1	I	2148	G
1	I	2160	C
1	I	2161	C
1	I	2162	G
1	I	2163	A
1	I	2164	C
1	I	2165	C
1	I	2167	U
1	I	2168	G
1	I	2170	A
1	I	2171	A
1	I	2172	U
1	I	2173	A
1	I	2174	C
1	I	2183	A
1	I	2190	G
1	I	2198	A
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	2268	A
1	I	2278	A
1	I	2282	G
1	I	2283	C
1	I	2287	A
1	I	2305	U
1	I	2309	A
1	I	2319	G
1	I	2322	A
1	I	2324	U
1	I	2325	G
1	I	2326	C

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Mol	Chain	Res	Type
1	I	2327	A
1	I	2333	A
1	I	2335	A
1	I	2336	A
1	I	2345	G
1	I	2347	C
1	I	2350	C
1	I	2361	G
1	I	2379	G
1	I	2383	G
1	I	2385	C
1	I	2396	G
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
1	I	2448	A
1	I	2451	A
1	I	2469	A
1	I	2470	G
1	I	2476	A
1	I	2491	U
1	I	2502	G
1	I	2505	G
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	2573	C
1	I	2582	G
1	I	2602	A
1	I	2603	G
1	I	2609	U

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Mol	Chain	Res	Type
1	I	2613	U
1	I	2615	U
1	I	2629	U
1	I	2630	G
1	I	2639	A
1	I	2646	C
1	I	2663	G
1	I	2682	A
1	I	2689	U
1	I	2690	U
1	I	2714	G
1	I	2716	C
1	I	2726	A
1	I	2732	G
1	I	2733	A
1	I	2744	G
1	I	2748	A
1	I	2757	A
1	I	2765	A
1	I	2778	A
1	I	2793	C
1	I	2794	C
1	I	2798	U
1	I	2799	A
1	I	2800	A
1	I	2818	U
1	I	2820	A
1	I	2821	A
1	I	2835	A
1	I	2836	U
1	I	2861	U
1	I	2867	G
1	I	2873	A
1	I	2874	C
1	I	2880	C
1	I	2883	A
1	I	2884	U
1	I	2903	U
1	I	2904	U
2	J	9	G
2	J	13	G
2	J	14	U

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Mol	Chain	Res	Type
2	J	15	A
2	J	16	G
2	J	24	G
2	J	25	U
2	J	32	U
2	J	35	C
2	J	40	U
2	J	41	G
2	J	44	G
2	J	45	A
2	J	52	A
2	J	53	A
2	J	56	G
2	J	57	A
2	J	67	G
2	J	88	C
2	J	89	U
2	J	90	C
2	J	108	A
2	J	109	A

All (54) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	33	C
1	I	62	U
1	I	101	A
1	I	137	U
1	I	199	A
1	I	221	A
1	I	278	A
1	I	310	A
1	I	404	A
1	I	474	G
1	I	503	A
1	I	532	A
1	I	549	G
1	I	555	G
1	I	614	A
1	I	764	A
1	I	784	G
1	I	973	A

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Mol	Chain	Res	Type
1	I	984	A
1	I	1046	A
1	I	1069	A
1	I	1088	A
1	I	1128	G
1	I	1286	A
1	I	1288	G
1	I	1320	C
1	I	1451	C
1	I	1490	A
1	I	1536	C
1	I	1608	A
1	I	1647	U
1	I	1730	C
1	I	1918	A
1	I	2035	G
1	I	2126	A
1	I	2160	C
1	I	2162	G
1	I	2164	C
1	I	2171	A
1	I	2282	G
1	I	2318	G
1	I	2324	U
1	I	2326	C
1	I	2425	A
1	I	2430	A
1	I	2517	C
1	I	2581	G
1	I	2756	U
1	I	2873	A
1	I	2903	U
2	J	14	U
2	J	52	A
2	J	88	C
2	J	108	A

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

30 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
29	RXL	B	9	29	5,6,7	1.32	1 (20%)	5,7,9	1.59	1 (20%)
1	2MA	I	2503	1,30	22,25,26	3.84	10 (45%)	32,37,40	2.31	9 (28%)
29	RX9	B	13	29	6,7,8	2.15	2 (33%)	4,8,10	1.58	1 (25%)
1	OMU	I	2552	1	19,22,23	2.90	8 (42%)	25,31,34	1.90	5 (20%)
1	5MC	I	1962	1	19,22,23	0.72	0	26,32,35	0.62	0
1	OMG	I	2251	1	23,26,27	0.60	0	32,38,41	0.48	0
1	PSU	I	2605	1	18,21,22	1.09	2 (11%)	21,30,33	2.00	4 (19%)
1	PSU	I	746	1,30	18,21,22	1.06	1 (5%)	21,30,33	1.93	4 (19%)
1	5MU	I	747	1	19,22,23	0.65	0	27,32,35	0.46	0
29	IB9	B	7	29	11,12,13	0.25	0	12,15,17	0.54	0
1	PSU	I	2504	1	18,21,22	1.13	3 (16%)	21,30,33	2.06	6 (28%)
1	2MG	I	2445	1	23,26,27	0.72	0	33,38,41	0.54	0
1	1MG	I	745	1	23,26,27	3.08	8 (34%)	33,39,42	2.22	11 (33%)
29	MAA	B	4	29	4,5,6	0.48	0	2,5,7	0.62	0
1	5MU	I	1939	1	19,22,23	0.68	0	27,32,35	0.60	0
1	PSU	I	1911	1	18,21,22	1.09	1 (5%)	21,30,33	1.99	5 (23%)
29	DHV	B	15	29	5,7,8	0.62	0	7,10,12	0.76	0
1	2MG	I	1835	1	23,26,27	0.55	0	33,38,41	0.49	0
29	RXL	B	2	29	5,6,7	1.51	1 (20%)	5,7,9	1.28	1 (20%)
1	PSU	I	1917	1	18,21,22	1.09	1 (5%)	21,30,33	2.04	6 (28%)
1	PSU	I	955	1	18,21,22	1.03	1 (5%)	21,30,33	1.94	4 (19%)
1	PSU	I	2580	1	18,21,22	1.12	2 (11%)	21,30,33	2.12	6 (28%)
1	PSU	I	2457	1	18,21,22	1.10	2 (11%)	21,30,33	1.99	5 (23%)
1	OMC	I	2498	1,30	19,22,23	0.76	1 (5%)	25,31,34	0.59	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	RXL	B	9	29	-	0/0/6/8	-
1	2MA	I	2503	1,30	-	0/7/25/26	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	RX9	B	13	29	-	2/2/8/10	-
1	OMU	I	2552	1	-	0/9/27/28	0/2/2/2
1	5MC	I	1962	1	-	0/7/25/26	0/2/2/2
1	OMG	I	2251	1	-	0/9/27/28	0/3/3/3
1	PSU	I	2605	1	-	0/7/25/26	0/2/2/2
1	PSU	I	746	1,30	-	2/7/25/26	0/2/2/2
1	5MU	I	747	1	-	0/7/25/26	0/2/2/2
29	IB9	B	7	29	-	0/7/7/8	0/1/1/1
1	PSU	I	2504	1	-	2/7/25/26	0/2/2/2
1	2MG	I	2445	1	-	1/9/27/28	0/3/3/3
1	1MG	I	745	1	-	0/7/25/26	0/3/3/3
29	MAA	B	4	29	-	0/2/4/6	-
1	5MU	I	1939	1	-	0/7/25/26	0/2/2/2
1	PSU	I	1911	1	-	0/7/25/26	0/2/2/2
29	DHV	B	15	29	-	0/4/8/10	-
1	2MG	I	1835	1	-	0/9/27/28	0/3/3/3
29	RXL	B	2	29	-	0/0/6/8	-
1	PSU	I	1917	1	-	0/7/25/26	0/2/2/2
1	PSU	I	955	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2580	1	-	0/7/25/26	0/2/2/2
1	PSU	I	2457	1	-	0/7/25/26	0/2/2/2
1	OMC	I	2498	1,30	-	0/9/27/28	0/2/2/2

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2503	2MA	C4-N3	12.06	1.49	1.34
1	I	745	1MG	C2-N3	8.36	1.46	1.33
1	I	2503	2MA	C2-N1	6.59	1.45	1.34
1	I	2552	OMU	C2-N1	6.52	1.48	1.38
1	I	2503	2MA	C2-N3	6.51	1.45	1.34
1	I	2552	OMU	C2-N3	6.44	1.49	1.38
1	I	745	1MG	C4-N3	6.01	1.48	1.34
1	I	745	1MG	C2-N2	5.84	1.44	1.34
1	I	2552	OMU	C6-C5	5.36	1.47	1.35
1	I	2503	2MA	C5-N7	-4.73	1.30	1.39
1	I	2503	2MA	C6-N1	4.68	1.41	1.35
1	I	2503	2MA	C5-C6	4.53	1.53	1.41
1	I	745	1MG	O6-C6	-4.51	1.13	1.23
29	B	13	RX9	CB-CA	4.08	1.40	1.34
1	I	745	1MG	C2-N1	3.90	1.44	1.37
1	I	745	1MG	C5-C6	3.89	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	2552	OMU	C4-N3	3.80	1.45	1.38
1	I	745	1MG	C5-N7	-3.52	1.32	1.39
1	I	1911	PSU	C6-C5	3.41	1.39	1.35
1	I	2552	OMU	O4-C4	-3.32	1.18	1.24
1	I	1917	PSU	C6-C5	3.31	1.39	1.35
1	I	2503	2MA	C6-N6	-3.22	1.26	1.34
1	I	2457	PSU	C6-C5	3.07	1.38	1.35
1	I	2504	PSU	C6-C5	3.06	1.38	1.35
1	I	2605	PSU	C6-C5	3.04	1.38	1.35
1	I	746	PSU	C6-C5	2.97	1.38	1.35
1	I	2552	OMU	O2-C2	-2.95	1.17	1.23
1	I	2580	PSU	C6-C5	2.91	1.38	1.35
1	I	955	PSU	C6-C5	2.83	1.38	1.35
1	I	2503	2MA	C4-N9	-2.66	1.32	1.37
1	I	2552	OMU	C6-N1	2.63	1.44	1.38
29	B	2	RXL	CA-N	2.61	1.42	1.36
29	B	13	RX9	CA-N	2.59	1.42	1.36
1	I	745	1MG	C8-N9	-2.59	1.31	1.37
29	B	9	RXL	CA-N	2.45	1.42	1.36
1	I	2580	PSU	O4'-C1'	-2.41	1.40	1.43
1	I	2503	2MA	C8-N9	-2.17	1.33	1.37
1	I	2504	PSU	C4-C5	-2.14	1.38	1.44
1	I	2504	PSU	O4'-C1'	-2.13	1.40	1.43
1	I	2552	OMU	C5-C4	2.11	1.48	1.43
1	I	2503	2MA	C5-C4	-2.06	1.35	1.39
1	I	2605	PSU	C4-C5	-2.01	1.38	1.44
1	I	2457	PSU	O4'-C1'	-2.01	1.41	1.43
1	I	2498	OMC	C4-N3	-2.00	1.30	1.34

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	2503	2MA	C5-C4-N3	-7.92	118.84	127.18
1	I	2552	OMU	C4-N3-C2	-5.96	119.21	126.61
1	I	745	1MG	C5-C4-N3	-5.91	118.98	128.39
1	I	2580	PSU	N1-C2-N3	5.27	120.73	115.17
1	I	2504	PSU	N1-C2-N3	5.24	120.69	115.17
1	I	2605	PSU	C4-N3-C2	-5.22	119.19	126.37
1	I	2504	PSU	C4-N3-C2	-5.13	119.31	126.37
1	I	2605	PSU	N1-C2-N3	5.11	120.56	115.17
1	I	746	PSU	C4-N3-C2	-5.11	119.33	126.37
1	I	2457	PSU	N1-C2-N3	5.10	120.55	115.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	955	PSU	C4-N3-C2	-5.07	119.39	126.37
1	I	1917	PSU	C4-N3-C2	-5.03	119.44	126.37
1	I	1911	PSU	C4-N3-C2	-5.01	119.46	126.37
1	I	955	PSU	N1-C2-N3	5.00	120.44	115.17
1	I	2503	2MA	N3-C4-N9	5.00	133.34	126.99
1	I	2457	PSU	C4-N3-C2	-4.97	119.53	126.37
1	I	1917	PSU	N1-C2-N3	4.97	120.41	115.17
1	I	2580	PSU	C4-N3-C2	-4.91	119.61	126.37
1	I	746	PSU	N1-C2-N3	4.91	120.35	115.17
1	I	1911	PSU	N1-C2-N3	4.79	120.22	115.17
1	I	745	1MG	C1'-N9-C4	-4.36	113.59	126.49
1	I	2552	OMU	N3-C2-N1	4.22	120.39	114.89
1	I	745	1MG	C1'-N9-C8	4.12	138.43	126.73
1	I	745	1MG	C2-N3-C4	4.11	121.22	111.98
1	I	745	1MG	N2-C2-N1	3.98	121.99	118.79
1	I	2503	2MA	N9-C8-N7	-3.98	108.29	113.94
1	I	2552	OMU	C5-C4-N3	3.76	120.06	114.80
1	I	745	1MG	N9-C4-N3	3.68	133.31	125.95
1	I	2503	2MA	N3-C2-N1	-3.22	120.08	125.77
1	I	745	1MG	C5-C6-N1	3.21	120.95	115.02
1	I	746	PSU	O2-C2-N1	-3.14	119.55	122.79
1	I	2503	2MA	C5-N7-C8	2.98	108.13	103.45
1	I	2552	OMU	O4-C4-C5	-2.92	120.13	125.16
1	I	2503	2MA	C6-C5-C4	2.87	121.10	117.18
1	I	745	1MG	N9-C8-N7	-2.87	108.08	113.40
1	I	2457	PSU	O2-C2-N1	-2.85	119.85	122.79
1	I	2580	PSU	O2-C2-N1	-2.84	119.86	122.79
1	I	1911	PSU	O2-C2-N1	-2.84	119.86	122.79
29	B	13	RX9	O-C-CA	-2.81	120.25	125.53
1	I	1917	PSU	O2-C2-N1	-2.77	119.93	122.79
1	I	2580	PSU	C6-N1-C2	-2.70	120.19	122.69
1	I	2580	PSU	O4'-C1'-C2'	2.64	108.81	105.15
29	B	9	RXL	O-C-CA	-2.63	120.59	125.53
1	I	2504	PSU	O2-C2-N1	-2.58	120.12	122.79
1	I	955	PSU	O2-C2-N1	-2.54	120.17	122.79
1	I	745	1MG	C2-N1-C6	-2.51	118.89	120.99
1	I	2503	2MA	C4-N9-C1'	-2.49	120.81	126.63
1	I	2552	OMU	O2-C2-N1	-2.47	119.58	122.80
1	I	1917	PSU	C6-C5-C4	2.46	119.83	118.17
1	I	2457	PSU	C6-N1-C2	-2.41	120.45	122.69
1	I	2504	PSU	C6-N1-C2	-2.41	120.46	122.69
29	B	2	RXL	O-C-CA	-2.40	121.04	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	1911	PSU	O4'-C1'-C2'	2.37	108.43	105.15
1	I	955	PSU	C6-N1-C2	-2.36	120.50	122.69
1	I	1917	PSU	C6-N1-C2	-2.34	120.52	122.69
1	I	2580	PSU	C3'-C2'-C1'	2.30	104.40	101.69
1	I	1917	PSU	O4'-C1'-C2'	2.24	108.25	105.15
1	I	2605	PSU	O2-C2-N1	-2.23	120.49	122.79
1	I	1911	PSU	C6-N1-C2	-2.23	120.63	122.69
1	I	2504	PSU	C6-C5-C4	2.19	119.65	118.17
1	I	2605	PSU	C6-N1-C2	-2.19	120.66	122.69
1	I	2504	PSU	O4'-C1'-C2'	2.15	108.12	105.15
1	I	745	1MG	C8-N7-C5	2.11	108.01	104.26
1	I	745	1MG	O6-C6-C5	-2.10	119.19	124.59
1	I	2503	2MA	C1'-N9-C8	2.08	131.70	127.09
1	I	2457	PSU	O4'-C1'-C2'	2.06	108.01	105.15
1	I	746	PSU	C6-N1-C2	-2.05	120.79	122.69
1	I	2503	2MA	C4-C5-N7	-2.02	108.27	110.58

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	B	13	RX9	CG2-CB-CG1-CD1
1	I	2504	PSU	O4'-C4'-C5'-O5'
1	I	2504	PSU	C3'-C4'-C5'-O5'
29	B	13	RX9	CA-CB-CG1-CD1
1	I	746	PSU	O4'-C1'-C5-C6
1	I	2445	2MG	C3'-C4'-C5'-O5'
1	I	746	PSU	C2'-C1'-C5-C6

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 146 ligands modelled in this entry, 146 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

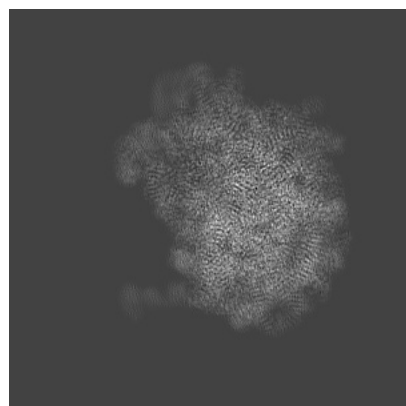
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14121. These allow visual inspection of the internal detail of the map and identification of artifacts.

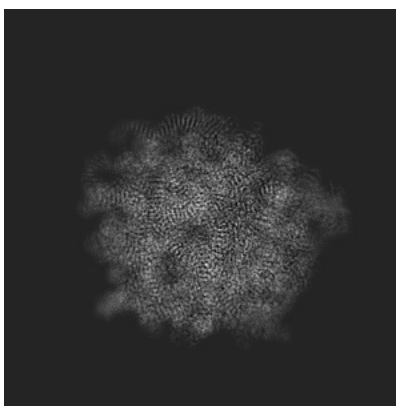
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

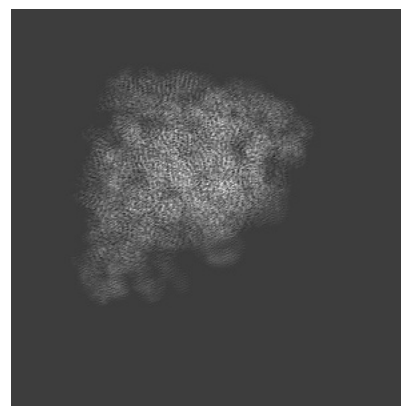
6.1.1 Primary map



X

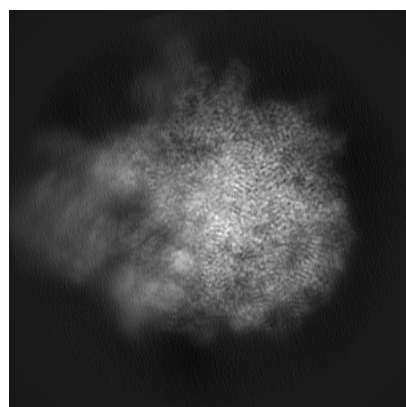


Y

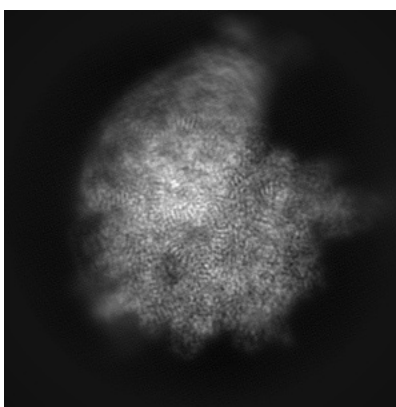


Z

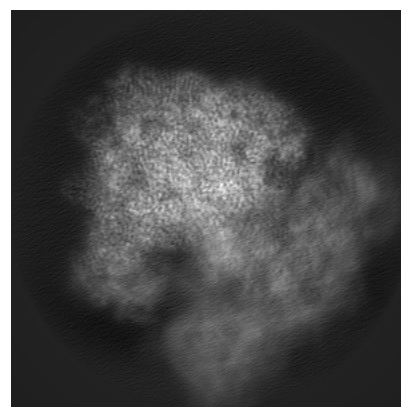
6.1.2 Raw map



X



Y

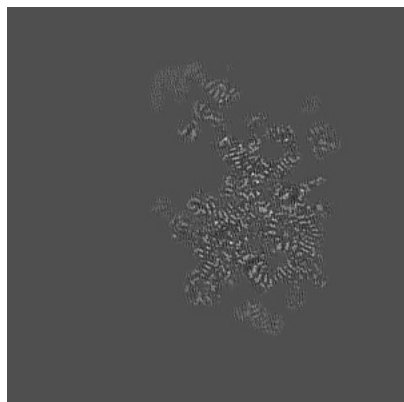


Z

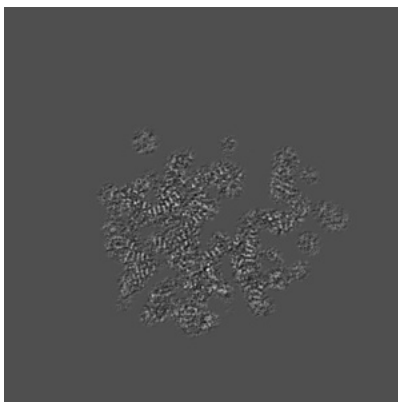
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 180

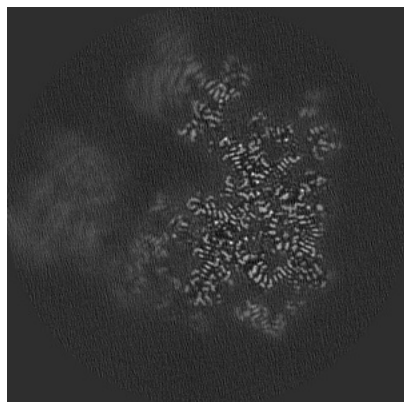


Y Index: 180

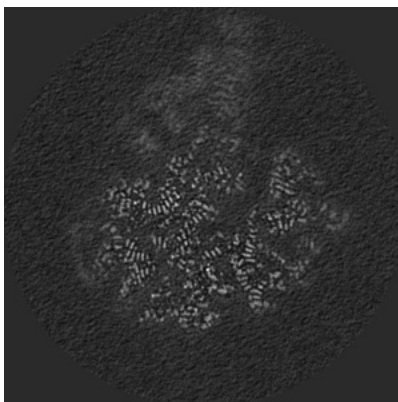


Z Index: 180

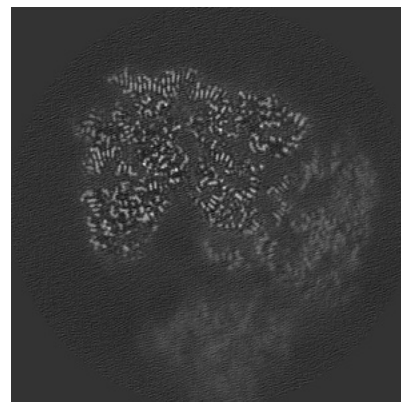
6.2.2 Raw map



X Index: 180



Y Index: 180

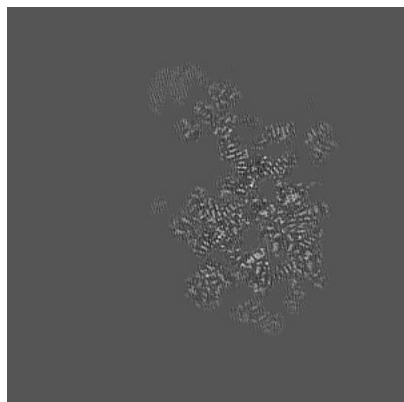


Z Index: 180

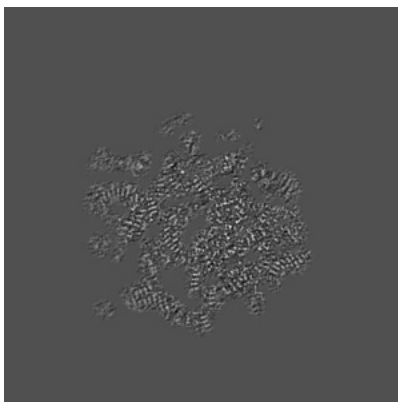
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

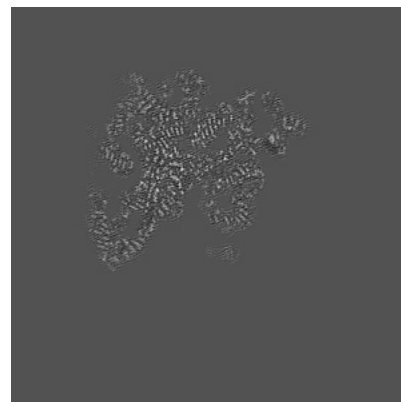
6.3.1 Primary map



X Index: 183

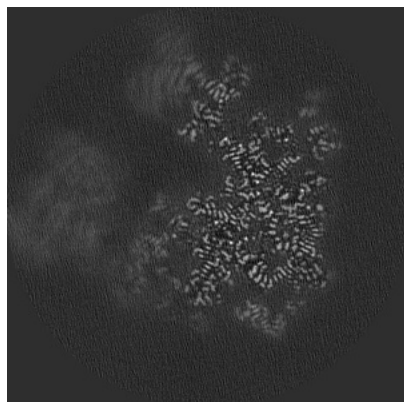


Y Index: 220

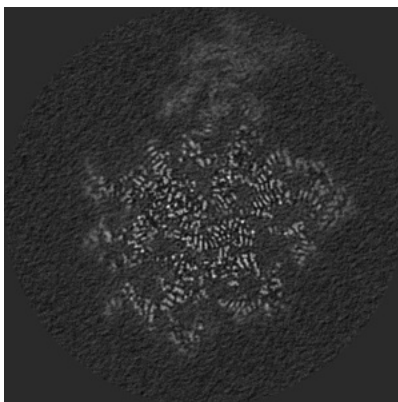


Z Index: 188

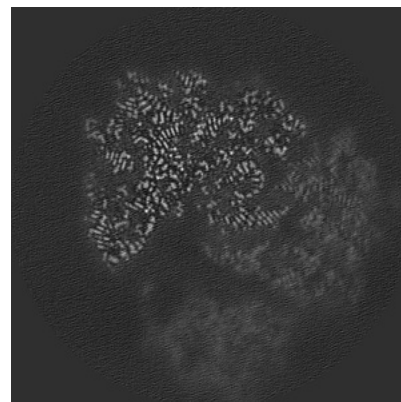
6.3.2 Raw map



X Index: 180



Y Index: 201

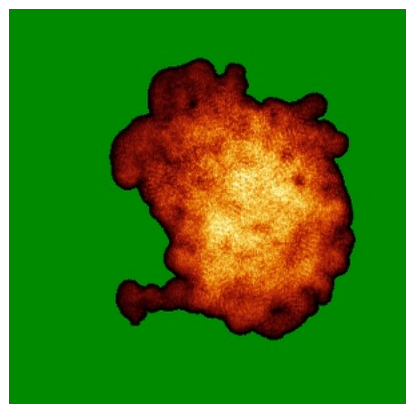


Z Index: 187

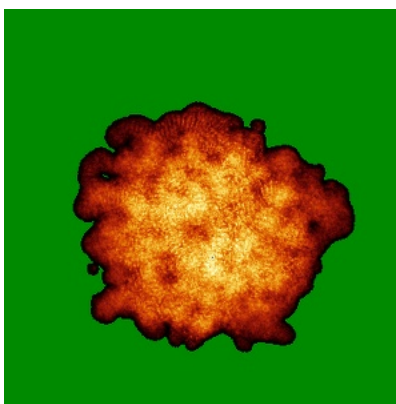
The images above show the largest variance slices of the map in three orthogonal directions.

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

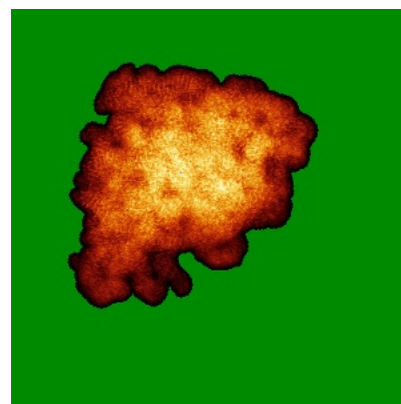
6.4.1 Primary map



X

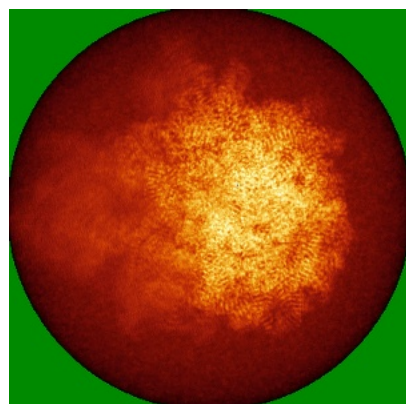


Y

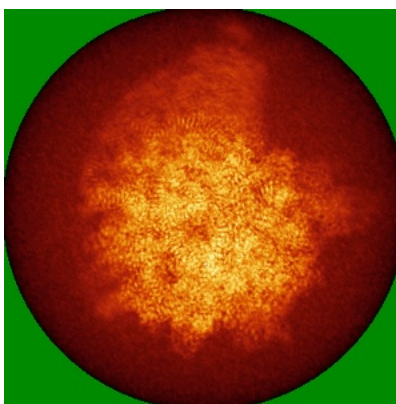


Z

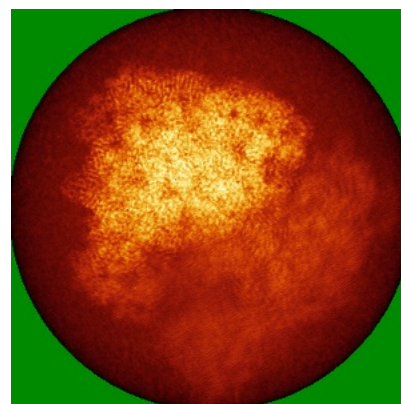
6.4.2 Raw map



X



Y

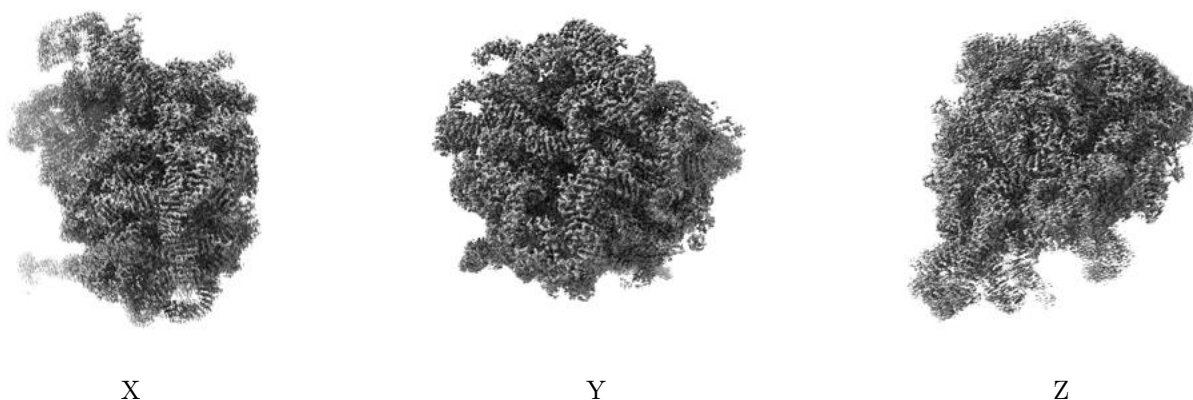


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

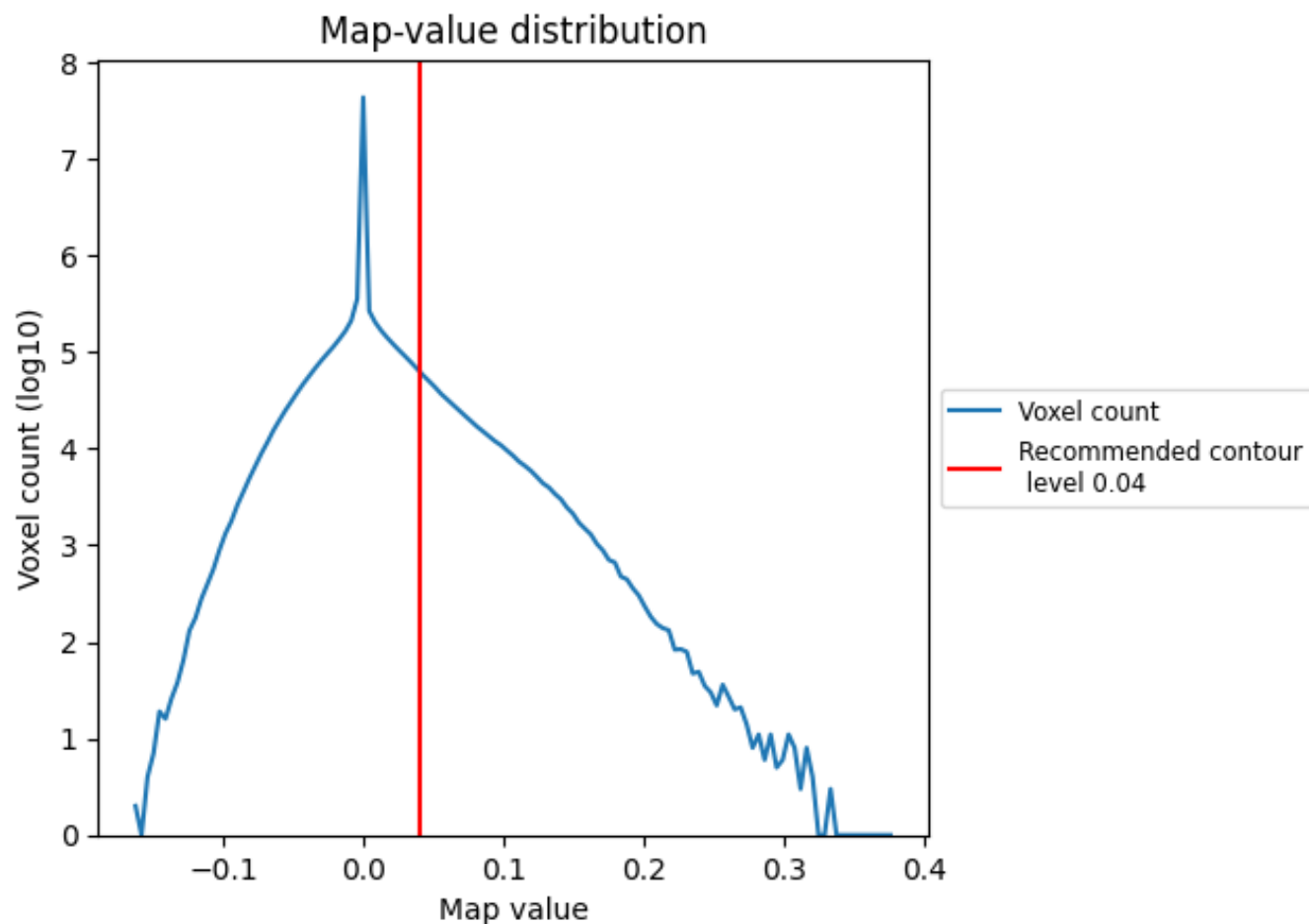
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

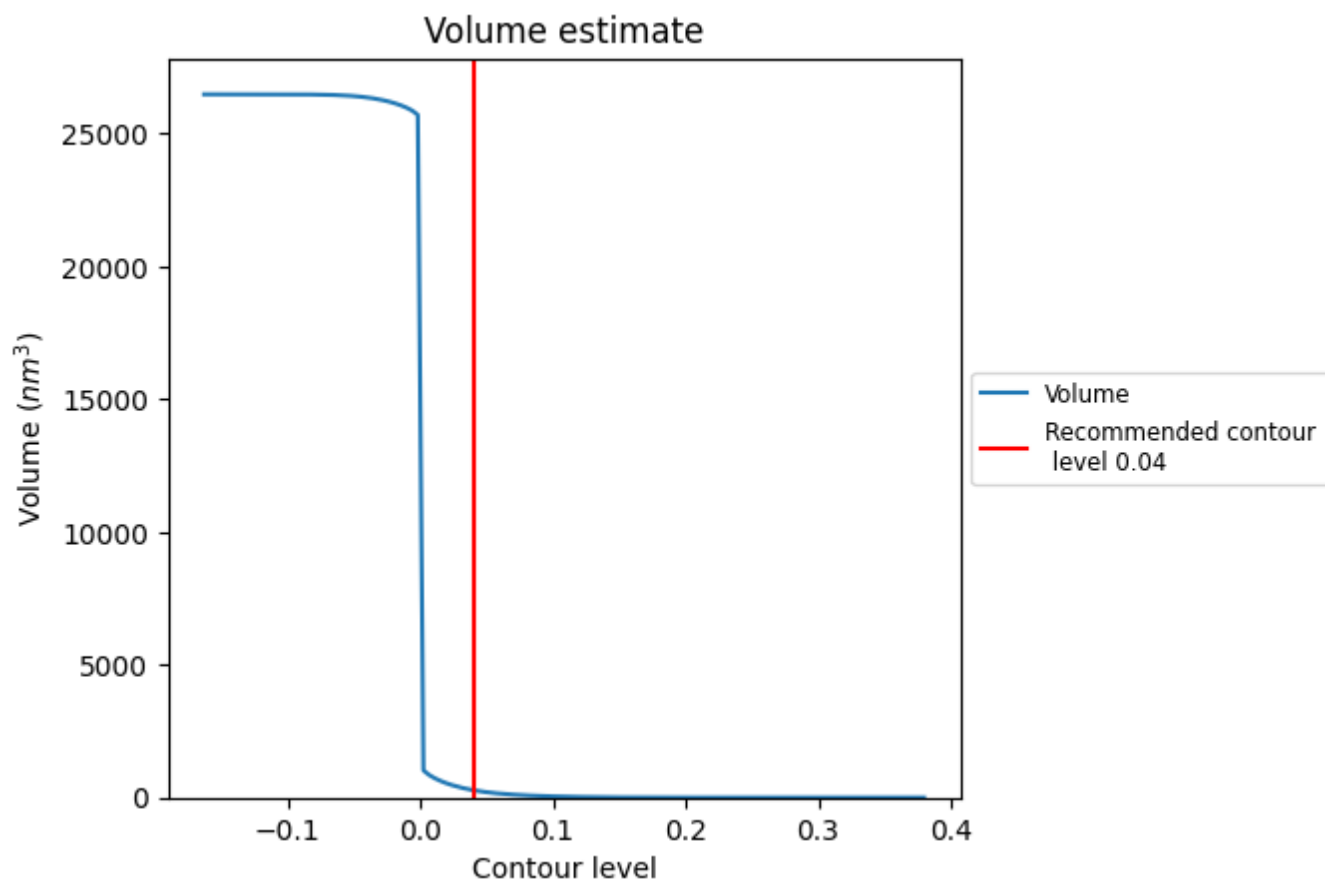
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

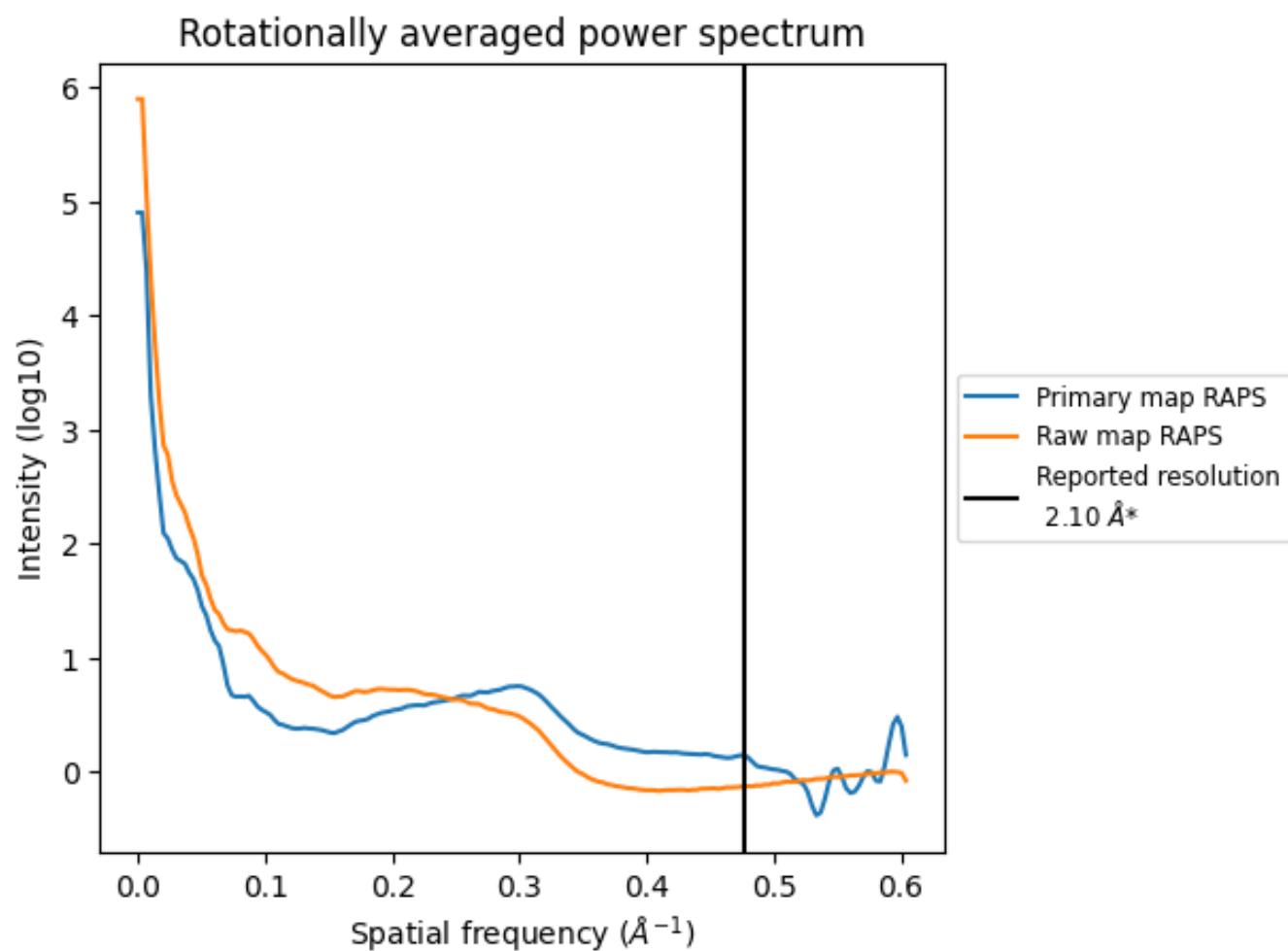
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 278 nm^3 ; this corresponds to an approximate mass of 251 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 ⓘ

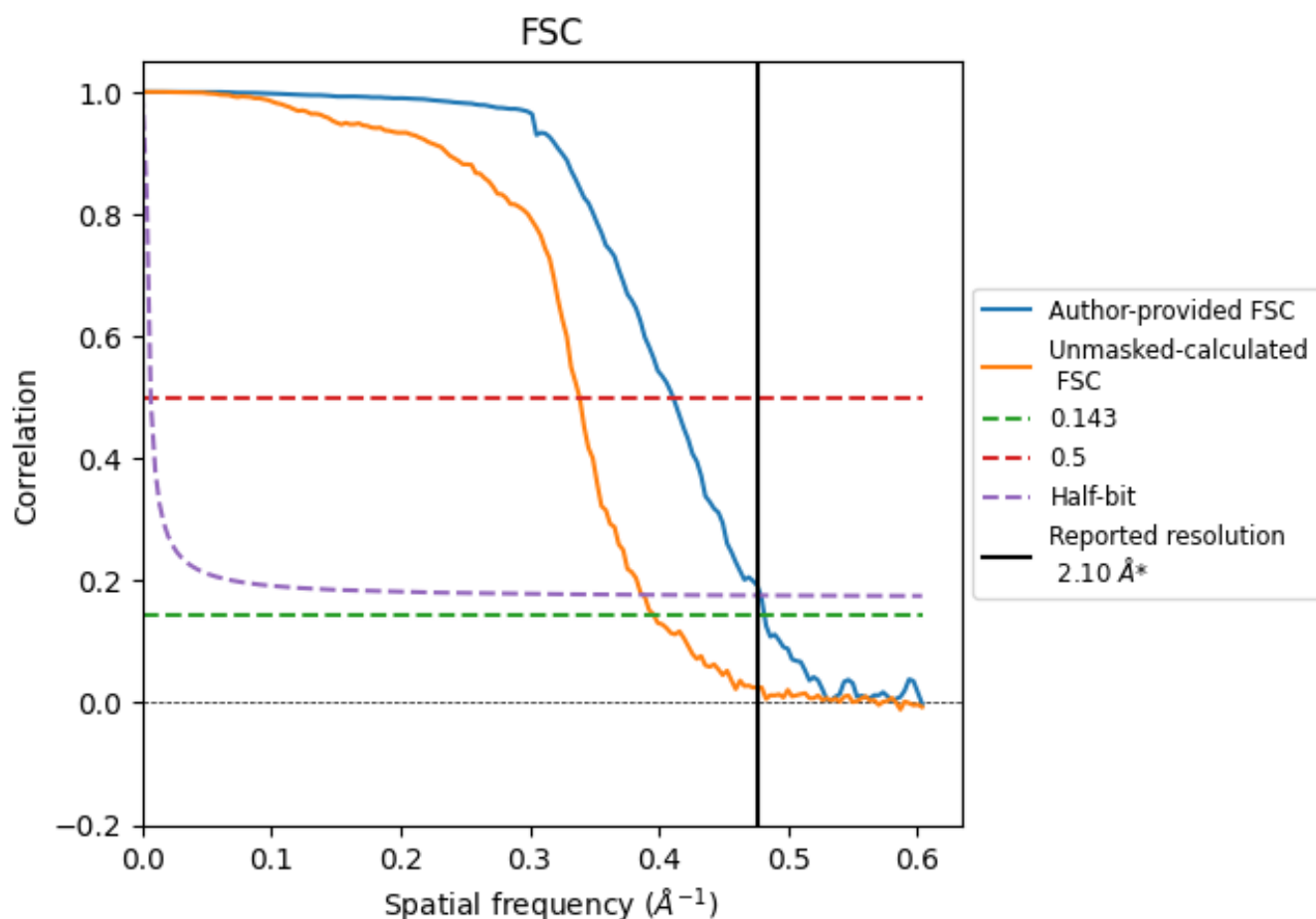


*Reported resolution corresponds to spatial frequency of 0.476 Å⁻¹

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 0.476 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

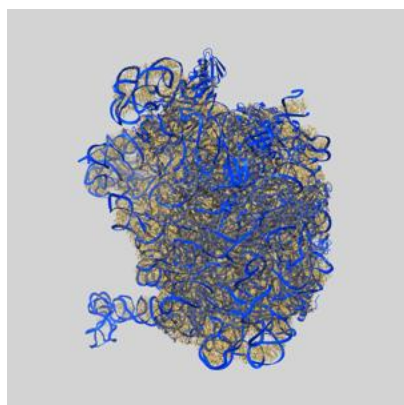
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.10	-	-
Author-provided FSC curve	2.08	2.43	2.09
Unmasked-calculated*	2.52	2.95	2.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.52 differs from the reported value 2.1 by more than 10 %

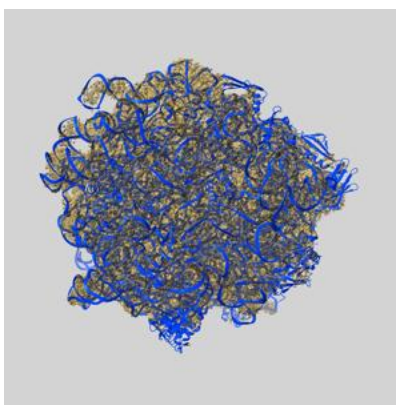
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14121 and PDB model 7QQ3. Per-residue inclusion information can be found in section 3 on page 10.

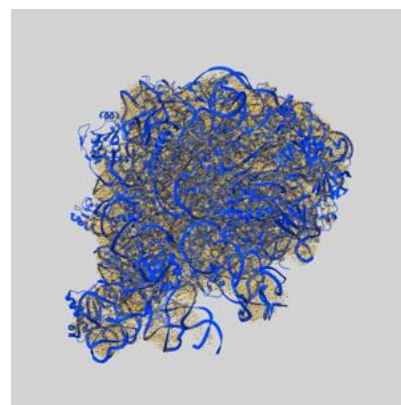
9.1 Map-model overlay [i](#)



X



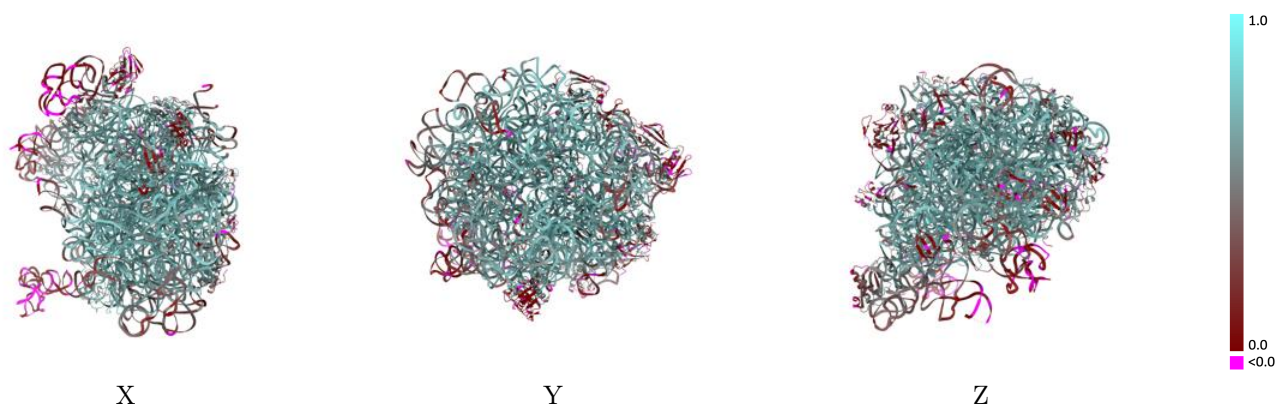
Y



Z

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

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

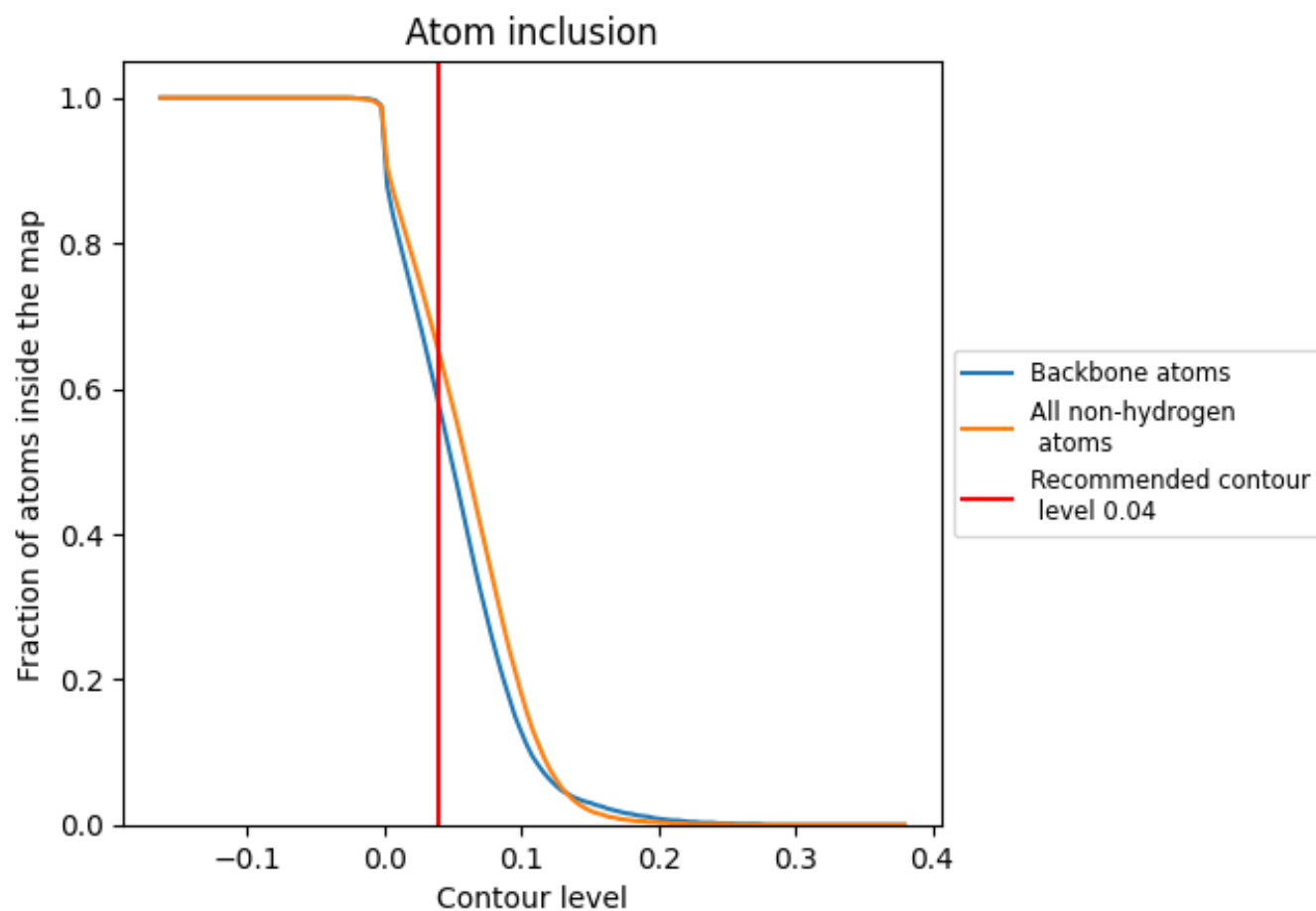


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 58% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.6500	 0.5880
B	 0.8160	 0.7220
I	 0.7320	 0.6190
J	 0.4260	 0.4840
K	 0.7230	 0.6650
L	 0.4420	 0.5070
M	 0.3370	 0.3710
O	 0.1050	 0.2590
R	 0.5430	 0.5980
S	 0.4350	 0.5330
T	 0.4410	 0.4990
U	 0.4590	 0.5640
V	 0.7150	 0.6780
W	 0.1510	 0.3500
X	 0.1980	 0.3610
Y	 0.6570	 0.6530
Z	 0.3010	 0.4230
a	 0.5690	 0.5880
b	 0.3910	 0.4900
c	 0.1750	 0.3440
d	 0.2210	 0.3630
e	 0.6020	 0.6440
f	 0.5790	 0.6100
g	 0.3230	 0.4350
h	 0.4070	 0.5210
i	 0.5980	 0.6110
j	 0.3620	 0.4980
k	 0.8680	 0.7220
l	 0.6310	 0.6650
m	 0.6140	 0.6200

