



## Full wwPDB EM Validation Report ⓘ

Jun 3, 2024 – 04:05 pm BST

PDB ID : 8P8U  
EMDB ID : EMD-17552  
Title : Yeast 60S ribosomal subunit  
Authors : Rabl, J.; Banerjee, A.; Boehringer, D.; Zavolan, M.  
Deposited on : 2023-06-02  
Resolution : 2.23 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](mailto: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:

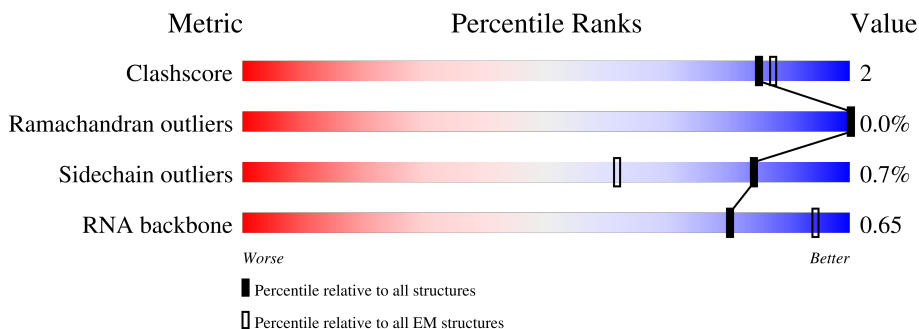
EMDB validation analysis : 0.0.1.dev92  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.2

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.23 Å.

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





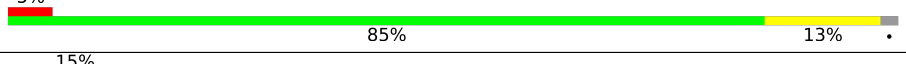
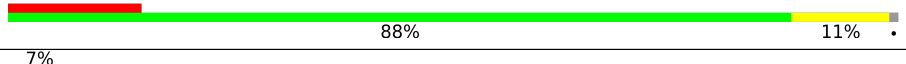
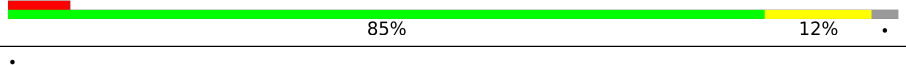
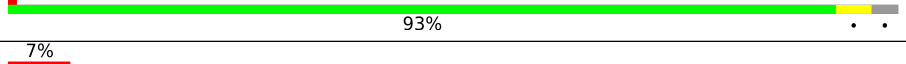

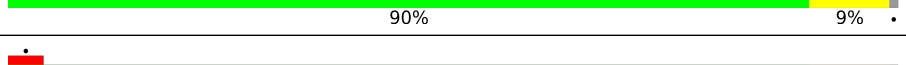
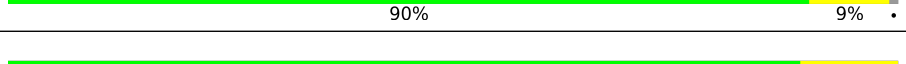
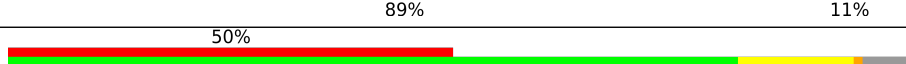
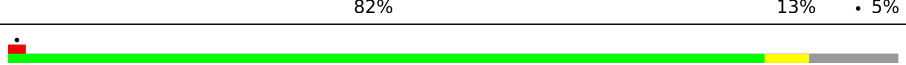
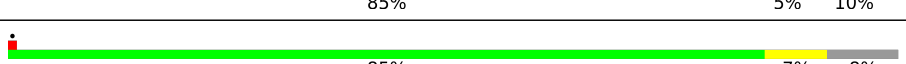
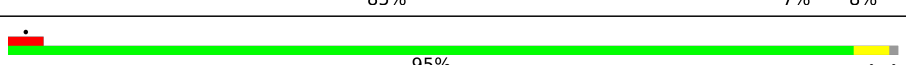
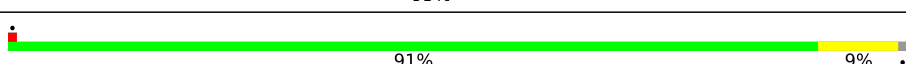
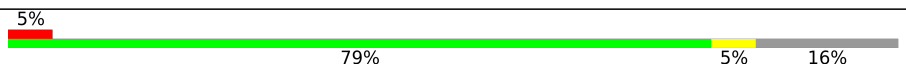
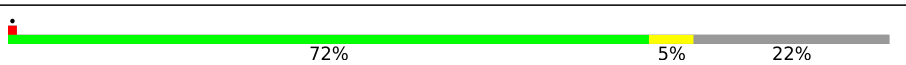
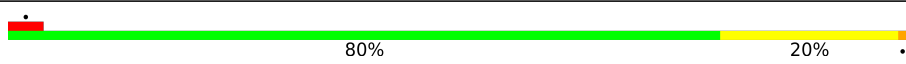
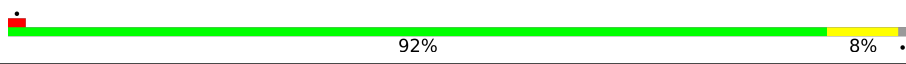

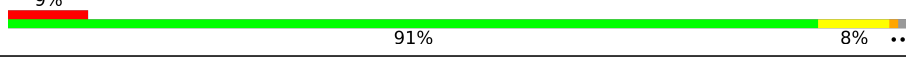
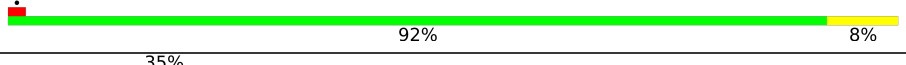
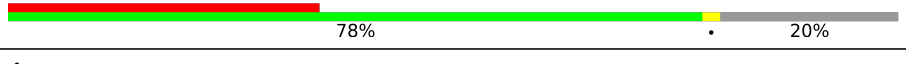
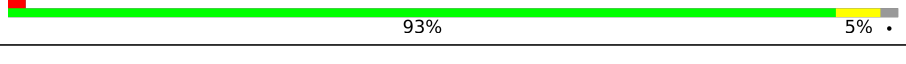


Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	2	51	<p>96%</p>
2	LK	244	<p>86% 5% 9%</p>
3	QX	142	<p>79% 6% 15%</p>
4	RM	78	<p>33% 91% 8%</p>
5	A	3396	<p>5% 72% 16% 10%</p>
6	LL	256	<p>11% 80% 8% 12%</p>
7	QY	127	<p>91% 6%</p>


Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	RO	128	
9	JT	199	
10	LM	191	
11	QZ	136	
12	RQ	106	
13	JU	138	
14	LN	221	
15	RA	149	
16	RT	92	
17	JV	204	
18	LO	174	
19	RB	59	
20	QO	184	
21	JW	199	
22	QP	186	
23	RC	105	
24	QQ	189	
25	LD	158	
26	QS	172	
27	RD	113	
28	QT	160	
29	LE	121	
30	QU	121	
31	RE	130	
32	QV	137	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
33	LF	254	
34	QW	155	
35	RF	107	
36	LG	387	
37	RG	121	
38	LH	362	
39	RH	120	
40	LI	297	
41	RI	100	
42	LJ	176	
43	RJ	88	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CL	RQ	202	-	-	X	-

## 2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 119919 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 protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	2	50	436	272	97	65	2	0	0

- Molecule 2 is a protein called 60S ribosomal protein L7-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	LK	222	1784	1151	324	308	1	0	0

- Molecule 3 is a protein called 60S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	QX	120	959	617	168	172	2	0	0

- Molecule 4 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	RM	77	612	391	115	106	0	0

- Molecule 5 is a RNA chain called 25S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	3045	65135	29094	11742	21254	3045	0	0

- Molecule 6 is a protein called 60S ribosomal protein L8-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	LL	226	1757	1125	314	315	3	0	0

- Molecule 7 is a protein called 60S ribosomal protein L26-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
7	QY	124	976	614	190	172	0	0

- Molecule 8 is a protein called Ubiquitin-60S ribosomal protein L40.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	RO	49	392	241	82	64	5	0	0

- Molecule 9 is a protein called 60S ribosomal protein L13-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	JT	189	1515	946	311	258	0	0

- Molecule 10 is a protein called 60S ribosomal protein L9-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	LM	188	1493	948	271	270	4	0	0

- Molecule 11 is a protein called 60S ribosomal protein L27-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	QZ	135	1092	710	202	180	0	0

- Molecule 12 is a protein called 60S ribosomal protein L42-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	RQ	103	827	520	167	135	5	0	0

- Molecule 13 is a protein called 60S ribosomal protein L14-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	JU	134	1039	666	196	175	2	0	0

- Molecule 14 is a protein called 60S ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LN	204	Total	C	N	O	S	0	0
			1664	1056	315	287	6		

- Molecule 15 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	RA	148	Total	C	N	O	S	0	0
			1173	749	231	190	3		

- Molecule 16 is a protein called 60S ribosomal protein L43-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	RT	91	Total	C	N	O	S	0	0
			694	429	138	121	6		

- Molecule 17 is a protein called 60S ribosomal protein L15-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	JV	203	Total	C	N	O	S	0	0
			1720	1077	361	281	1		

- Molecule 18 is a protein called 60S ribosomal protein L11-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LO	165	Total	C	N	O	S	0	0
			1319	828	246	241	4		

- Molecule 19 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	RB	53	Total	C	N	O	0	0
			429	268	93	68		

- Molecule 20 is a protein called 60S ribosomal protein L17-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	QO	169	Total	C	N	O	0	0
			1336	830	267	239		

- Molecule 21 is a protein called 60S ribosomal protein L16-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	JW	197	Total	C	N	O	S	0	0
			1555	1003	289	262	1		

- Molecule 22 is a protein called 60S ribosomal protein L18-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	QP	185	Total	C	N	O	S	0	0
			1441	908	290	241	2		

- Molecule 23 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	RC	88	Total	C	N	O	S	0	0
			677	439	115	122	1		

- Molecule 24 is a protein called 60S ribosomal protein L19-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	QQ	147	Total	C	N	O	0	0
			1185	738	250	197		

- Molecule 25 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LD	158	Total	C	N	O	P	0	0
			3353	1500	586	1109	158		

- Molecule 26 is a protein called 60S ribosomal protein L20-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	QS	171	Total	C	N	O	S	0	0
			1437	925	266	243	3		

- Molecule 27 is a protein called 60S ribosomal protein L31-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	RD	98	Total	C	N	O	S	0	0
			796	511	153	131	1		

- Molecule 28 is a protein called 60S ribosomal protein L21-A.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	QT	159	Total	C	N	O	S	0	0
			1276	805	246	221	4		

- Molecule 29 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LE	121	Total	C	N	O	P	0	0
			2579	1152	461	845	121		

- Molecule 30 is a protein called 60S ribosomal protein L22-A.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	QU	97	Total	C	N	O	0	0
			766	496	126	144		

- Molecule 31 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	RE	127	Total	C	N	O	S	0	0
			1020	647	205	167	1		

- Molecule 32 is a protein called 60S ribosomal protein L23-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	QV	129	Total	C	N	O	S	0	0
			963	607	180	169	7		

- Molecule 33 is a protein called 60S ribosomal protein L2-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LF	244	Total	C	N	O	S	0	0
			1855	1156	375	323	1		

- Molecule 34 is a protein called 60S ribosomal protein L24-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	QW	61	Total	C	N	O	S	0	0
			509	328	100	80	1		

- Molecule 35 is a protein called 60S ribosomal protein L33-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	RF	106	Total	C	N	O	S	0	0
			850	540	165	144	1		

- Molecule 36 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LG	386	Total	C	N	O	S	0	0
			3075	1950	584	533	8		

- Molecule 37 is a protein called 60S ribosomal protein L34-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	RG	103	Total	C	N	O	S	0	0
			811	503	167	137	4		

- Molecule 38 is a protein called 60S ribosomal protein L4-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	LH	361	Total	C	N	O	S	0	0
			2748	1729	522	494	3		

- Molecule 39 is a protein called 60S ribosomal protein L35-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	RH	119	Total	C	N	O	S	0	0
			969	615	186	167	1		

- Molecule 40 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LI	285	Total	C	N	O	S	0	0
			2293	1450	399	442	2		

- Molecule 41 is a protein called 60S ribosomal protein L36-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	RI	99	Total	C	N	O	S	0	0
			771	481	156	132	2		

- Molecule 42 is a protein called 60S ribosomal protein L6-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	LJ	156	Total	C	N	O	S	0	0
			1239	800	222	216	1		

- Molecule 43 is a protein called 60S ribosomal protein L37-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	RJ	85	Total	C	N	O	S	0	0
			670	408	146	111	5		

- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	A	126	Total	Mg	0
			126	126	
44	QO	1	Total	Mg	0
			1	1	
44	LD	1	Total	Mg	0
			1	1	
44	LE	1	Total	Mg	0
			1	1	

- Molecule 45 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

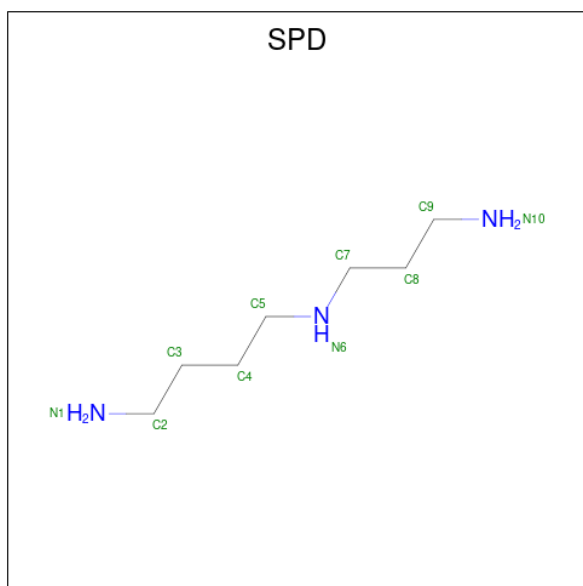
Mol	Chain	Residues	Atoms		AltConf
45	A	20	Total	Cl	0
			20	20	
45	RQ	1	Total	Cl	0
			1	1	
45	JV	1	Total	Cl	0
			1	1	
45	QO	1	Total	Cl	0
			1	1	
45	LG	1	Total	Cl	0
			1	1	

- Molecule 46 is SPERMINE (three-letter code: SPM) (formula: C<sub>10</sub>H<sub>26</sub>N<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
46	A	1	Total	C	N	0
			14	10	4	

- Molecule 47 is SPERMIDINE (three-letter code: SPD) (formula:  $C_7H_{19}N_3$ ).



Mol	Chain	Residues	Atoms			AltConf
47	A	1	Total	C	N	0
			10	7	3	

- Molecule 48 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
48	RO	1	Total 1	Zn 1	0
48	RQ	1	Total 1	Zn 1	0
48	RT	1	Total 1	Zn 1	0
48	RG	1	Total 1	Zn 1	0
48	RJ	1	Total 1	Zn 1	0

- Molecule 49 is water.

Mol	Chain	Residues	Atoms		AltConf
49	QX	1	Total 1	O 1	0
49	A	517	Total 517	O 517	0
49	RQ	1	Total 1	O 1	0
49	RA	2	Total 2	O 2	0
49	JV	2	Total 2	O 2	0
49	QO	1	Total 1	O 1	0
49	JW	2	Total 2	O 2	0
49	QQ	1	Total 1	O 1	0
49	LD	3	Total 3	O 3	0
49	LE	3	Total 3	O 3	0
49	RE	1	Total 1	O 1	0
49	LF	4	Total 4	O 4	0
49	LG	5	Total 5	O 5	0
49	LH	2	Total 2	O 2	0
49	LI	1	Total 1	O 1	0

*Continued on next page...*

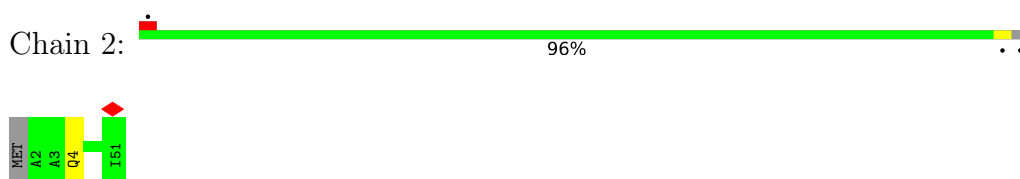
*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>AltConf</b>
49	RJ	1	Total	O	0
			1	1	

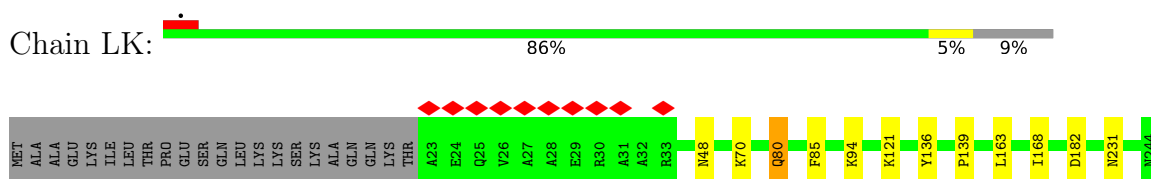
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

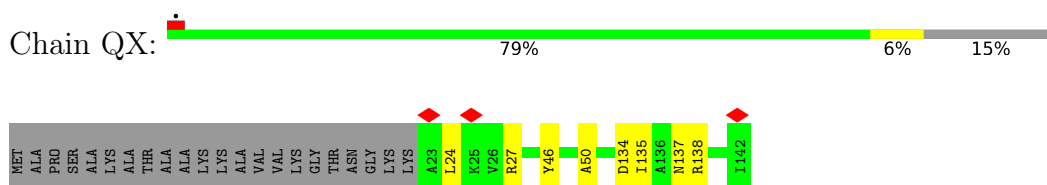
- Molecule 1: 60S ribosomal protein L39



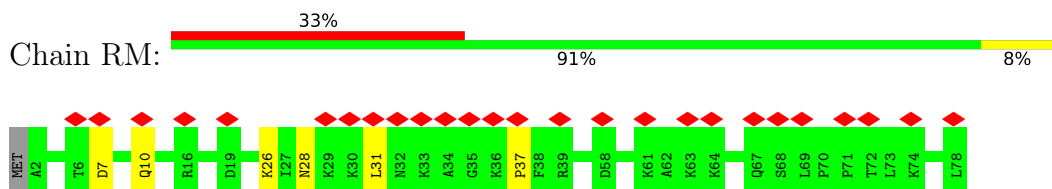
- Molecule 2: 60S ribosomal protein L7-A



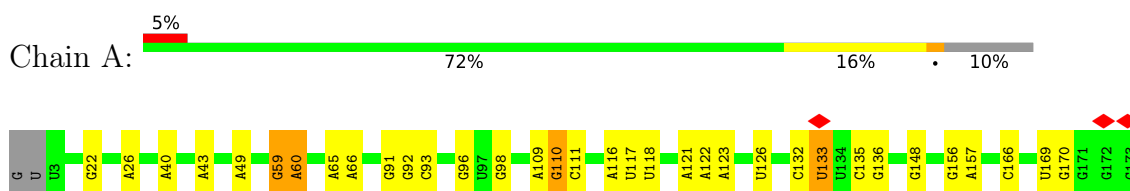
- Molecule 3: 60S ribosomal protein L25

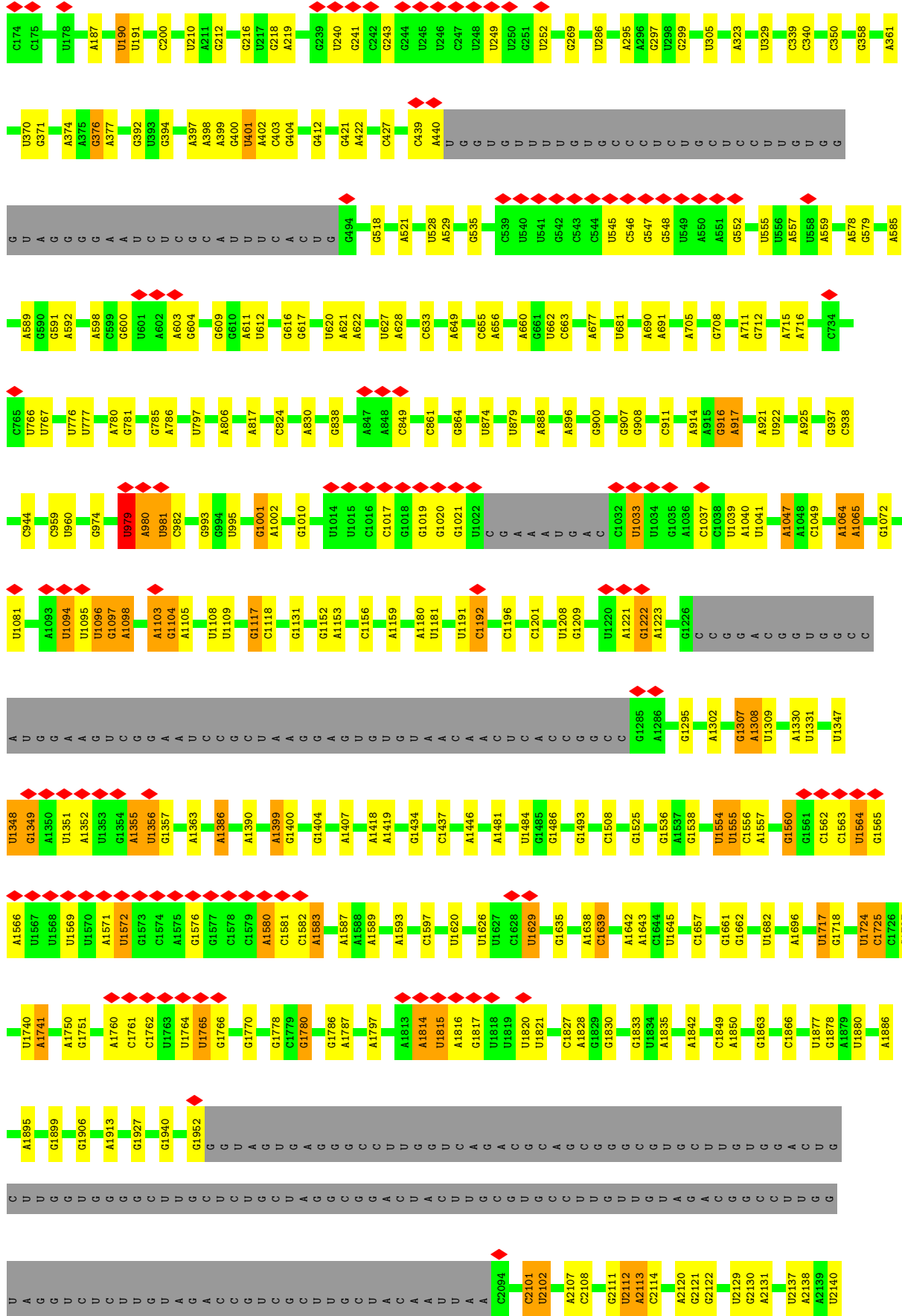


- Molecule 4: 60S ribosomal protein L38

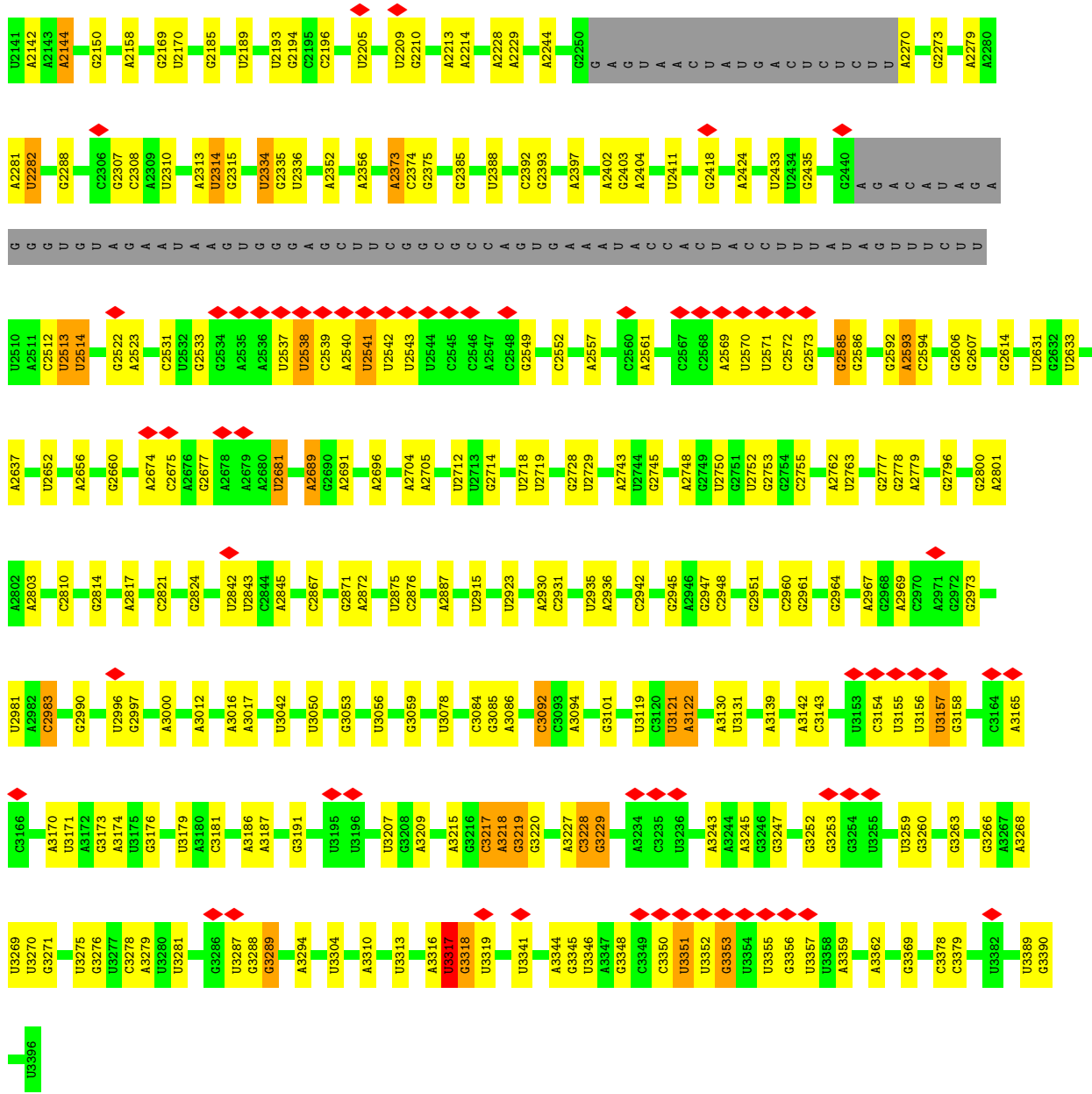


- Molecule 5: 25S rRNA

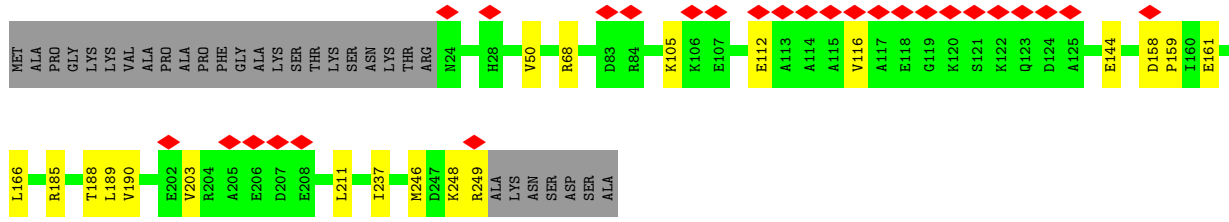
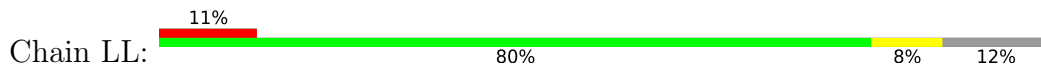








• Molecule 6: 60S ribosomal protein L8-A



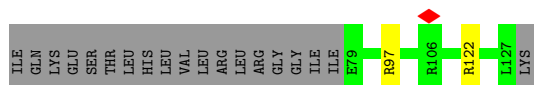
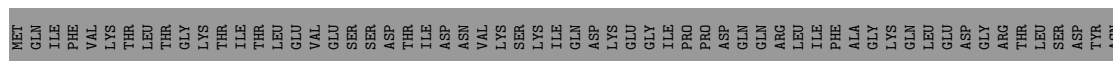
• Molecule 7: 60S ribosomal protein L26-A

Chain QY:  91% 6%




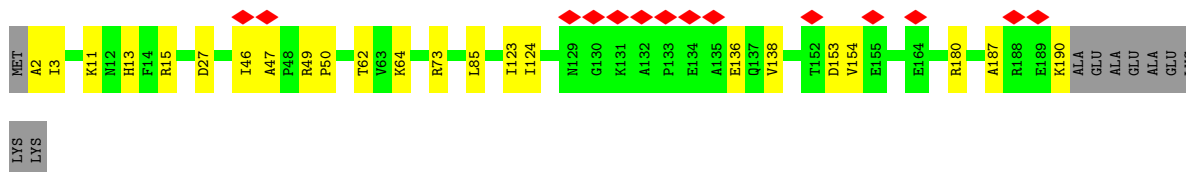
• Molecule 8: Ubiquitin-60S ribosomal protein L40

Chain RO:  37% 62%




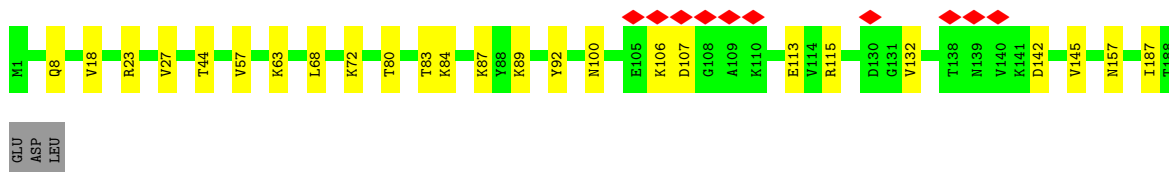
• Molecule 9: 60S ribosomal protein L13-A

Chain JT:  7% 83% 12% 5%




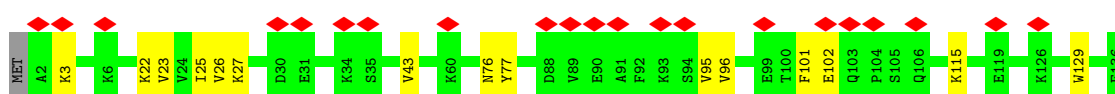
• Molecule 10: 60S ribosomal protein L9-A

Chain LM:  5% 85% 13%




• Molecule 11: 60S ribosomal protein L27-A

Chain QZ:  15% 88% 11%

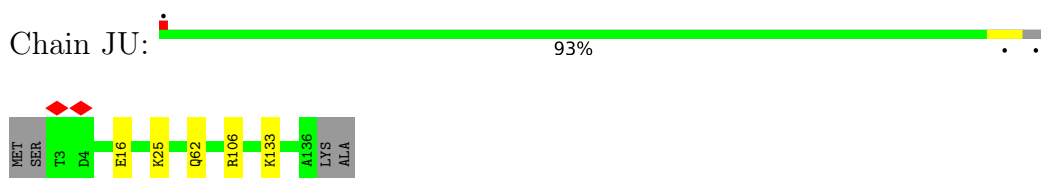


• Molecule 12: 60S ribosomal protein L42-A

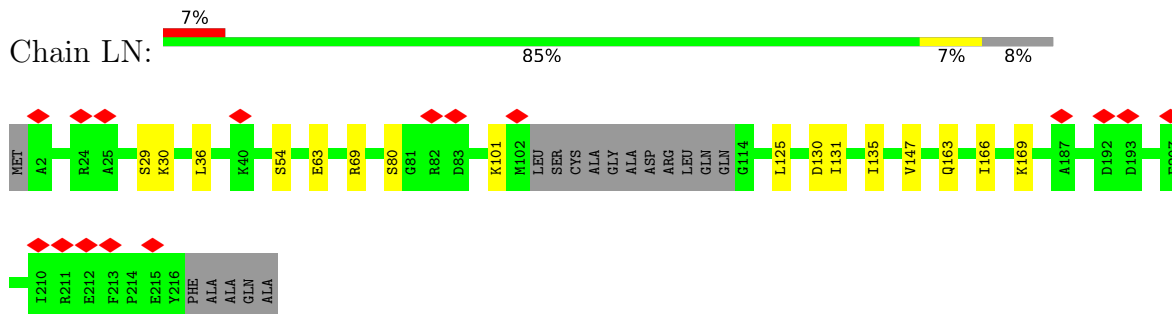
Chain RQ:  7% 85% 12%



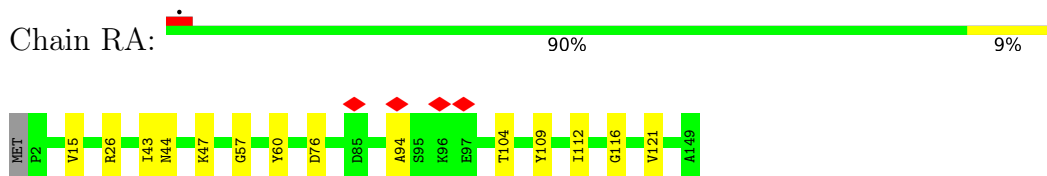
- Molecule 13: 60S ribosomal protein L14-A



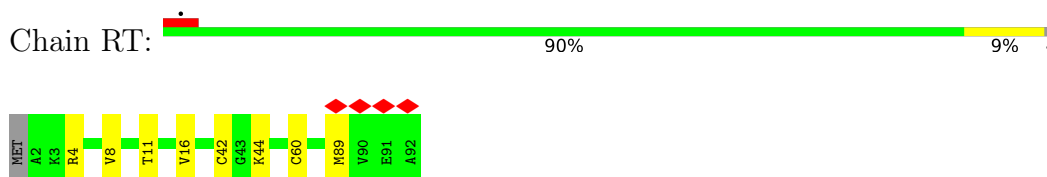
- Molecule 14: 60S ribosomal protein L10



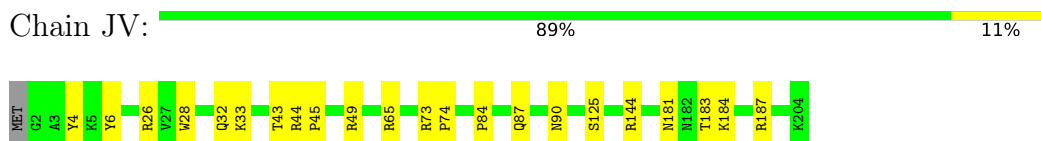
- Molecule 15: 60S ribosomal protein L28



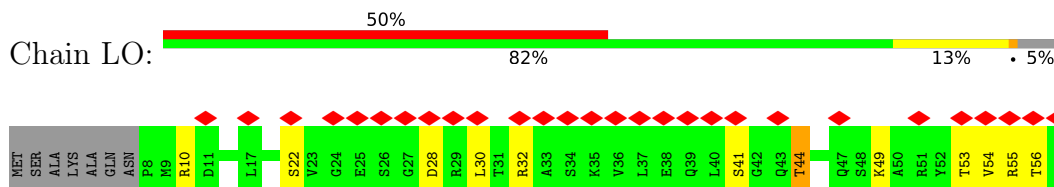
- Molecule 16: 60S ribosomal protein L43-A

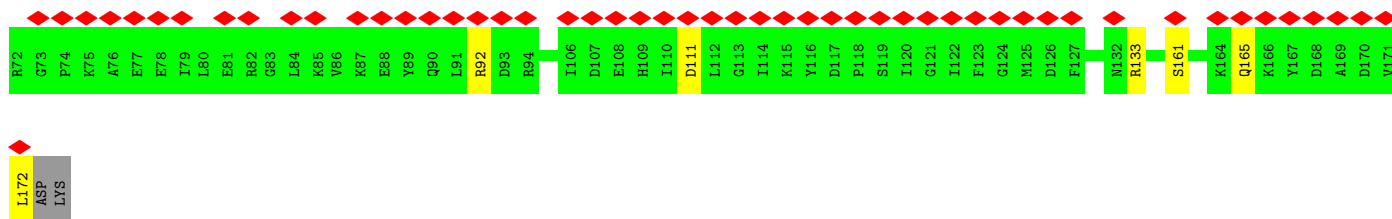


- Molecule 17: 60S ribosomal protein L15-A

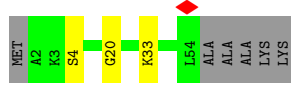
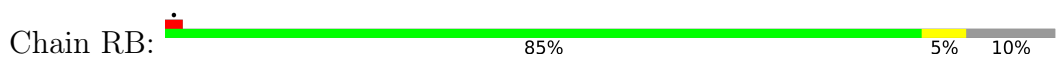


- Molecule 18: 60S ribosomal protein L11-A

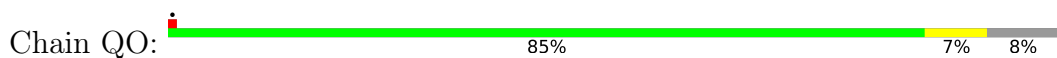




- Molecule 19: 60S ribosomal protein L29



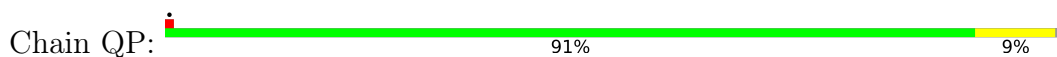
- Molecule 20: 60S ribosomal protein L17-A



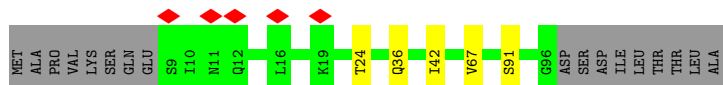
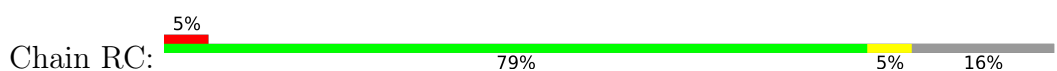
- Molecule 21: 60S ribosomal protein L16-A



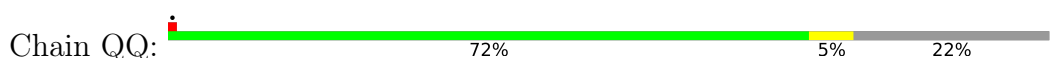
- Molecule 22: 60S ribosomal protein L18-A

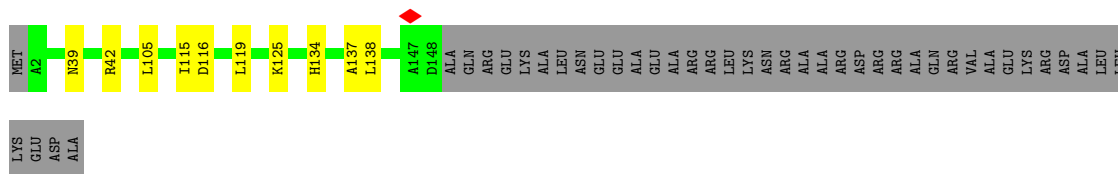


- Molecule 23: 60S ribosomal protein L30

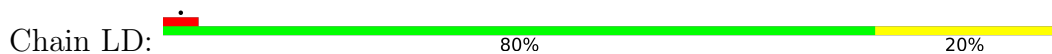


- Molecule 24: 60S ribosomal protein L19-A

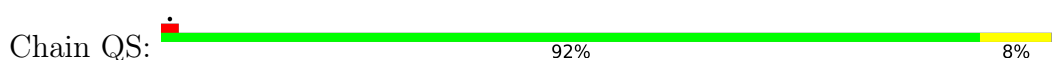




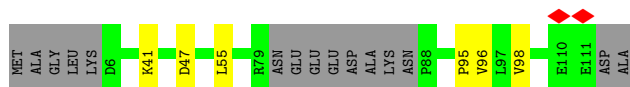
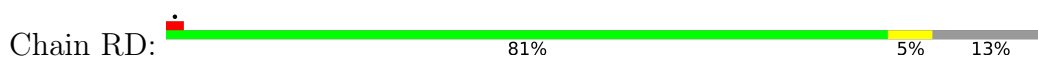
- Molecule 25: 5.8S rRNA



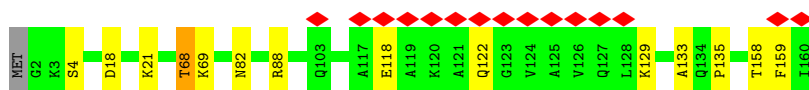
- Molecule 26: 60S ribosomal protein L20-A



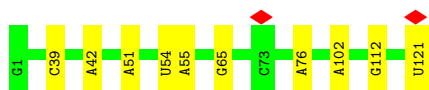
- Molecule 27: 60S ribosomal protein L31-A



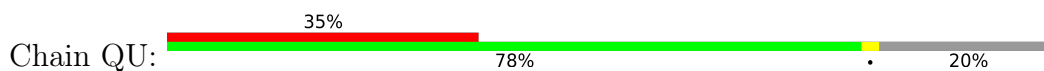
- Molecule 28: 60S ribosomal protein L21-A

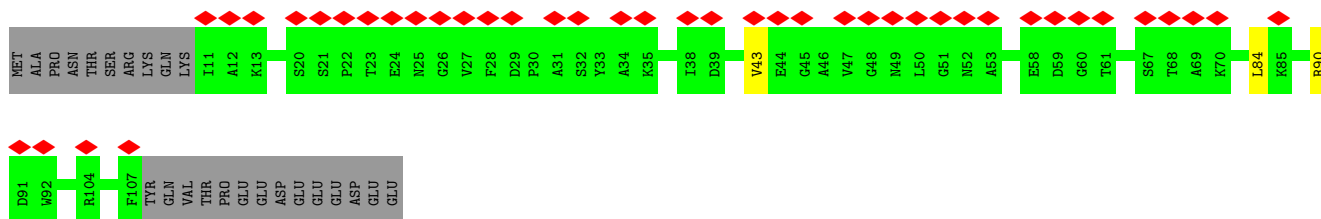


- Molecule 29: 5S rRNA



- Molecule 30: 60S ribosomal protein L22-A

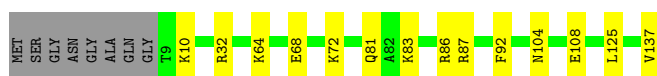
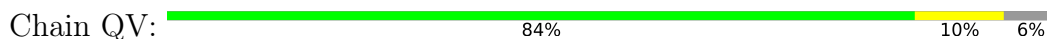




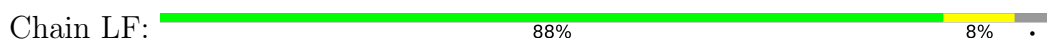
• Molecule 31: 60S ribosomal protein L32



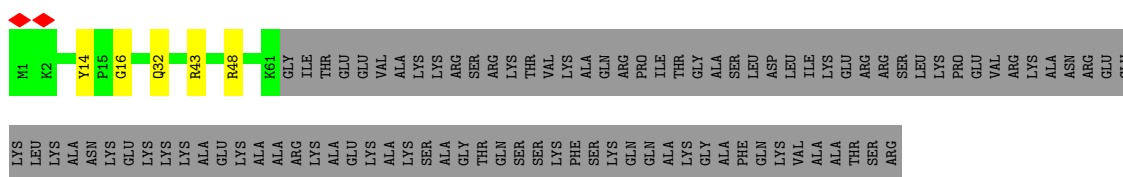
• Molecule 32: 60S ribosomal protein L23-A



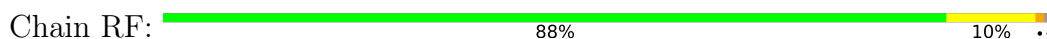
• Molecule 33: 60S ribosomal protein L2-A



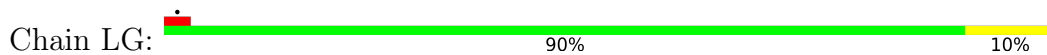
• Molecule 34: 60S ribosomal protein L24-A

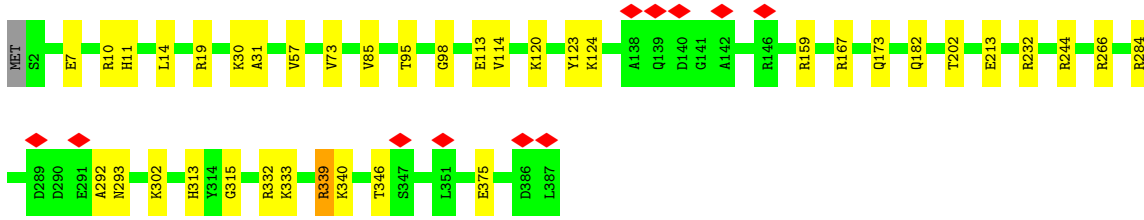


• Molecule 35: 60S ribosomal protein L33-A

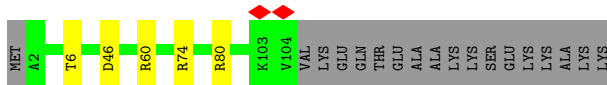
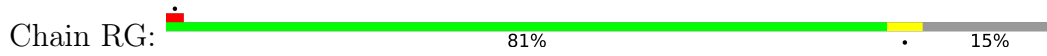


• Molecule 36: 60S ribosomal protein L3

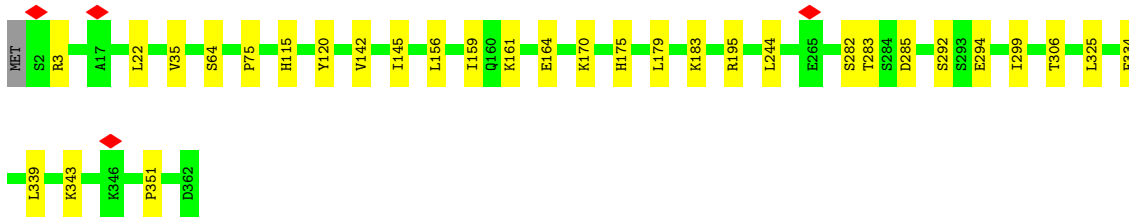




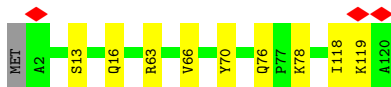
- Molecule 37: 60S ribosomal protein L34-A



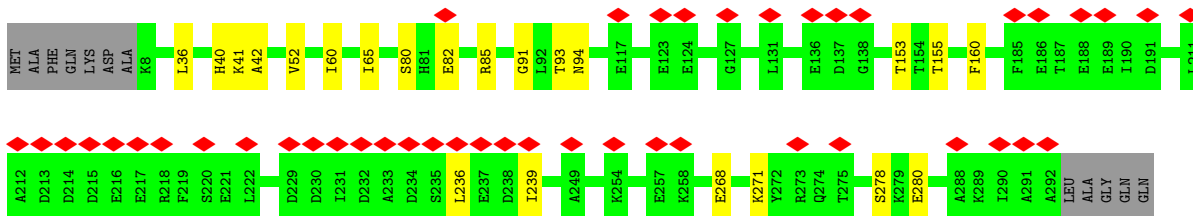
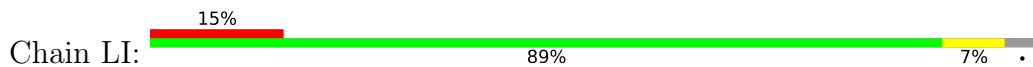
- Molecule 38: 60S ribosomal protein L4-A



- Molecule 39: 60S ribosomal protein L35-A

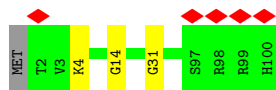


- Molecule 40: 60S ribosomal protein L5

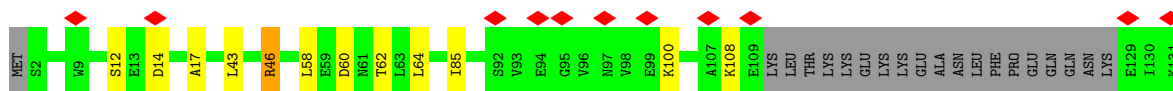
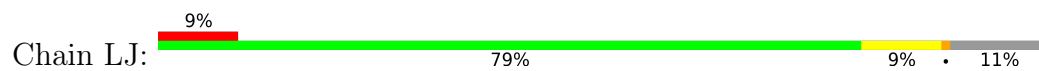


- Molecule 41: 60S ribosomal protein L36-A





- Molecule 42: 60S ribosomal protein L6-A



- Molecule 43: 60S ribosomal protein L37-A





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	264900	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 ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.654	Depositor
Minimum map value	-1.239	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	503.99997, 503.99997, 503.99997	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.84, 0.84, 0.84	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: SPD, CL, SPM, MG, ZN

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	2	0.23	0/443	0.55	0/588
2	LK	0.25	0/1821	0.47	0/2451
3	QX	0.23	0/974	0.48	0/1314
4	RM	0.24	0/618	0.52	0/826
5	A	0.19	0/72907	0.70	6/113661 (0.0%)
6	LL	0.24	0/1789	0.45	0/2418
7	QY	0.23	0/987	0.51	0/1318
8	RO	0.23	0/398	0.54	0/529
9	JT	0.24	0/1540	0.54	0/2068
10	LM	0.24	0/1514	0.48	0/2039
11	QZ	0.24	0/1118	0.47	0/1497
12	RQ	0.24	0/839	0.51	0/1108
13	JU	0.23	0/1054	0.48	0/1420
14	LN	0.24	0/1699	0.50	0/2277
15	RA	0.23	0/1204	0.50	0/1612
16	RT	0.23	0/701	0.54	0/934
17	JV	0.23	0/1757	0.55	0/2354
18	LO	0.23	0/1340	0.51	0/1796
19	RB	0.24	0/440	0.48	0/586
20	QO	0.23	0/1358	0.52	0/1824
21	JW	0.24	0/1585	0.47	0/2128
22	QP	0.24	0/1465	0.54	0/1965
23	RC	0.24	0/685	0.42	0/918
24	QQ	0.22	0/1202	0.51	0/1605
25	LD	0.18	0/3746	0.68	0/5832
26	QS	0.24	0/1473	0.51	0/1980
27	RD	0.23	0/809	0.51	0/1084
28	QT	0.24	0/1300	0.50	0/1743
29	LE	0.17	0/2883	0.67	0/4491
30	QU	0.25	0/781	0.44	0/1058
31	RE	0.23	0/1041	0.50	0/1394
32	QV	0.25	0/978	0.52	0/1316

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	LF	0.24	0/1889	0.54	0/2539
34	QW	0.24	0/521	0.50	0/691
35	RF	0.24	0/868	0.52	0/1168
36	LG	0.23	0/3146	0.51	0/4228
37	RG	0.23	0/821	0.55	0/1097
38	LH	0.23	0/2800	0.50	0/3790
39	RH	0.23	0/978	0.48	0/1301
40	LI	0.24	0/2342	0.48	0/3160
41	RI	0.23	0/778	0.52	0/1034
42	LJ	0.24	0/1260	0.47	0/1694
43	RJ	0.24	0/685	0.56	0/908
All	All	0.21	0/128537	0.64	6/189744 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	922	U	C2-N1-C1'	6.43	125.42	117.70
5	A	979	U	P-O3'-C3'	5.90	126.78	119.70
5	A	922	U	N1-C2-O2	5.43	126.60	122.80
5	A	3317	U	OP2-P-O3'	5.15	116.54	105.20
5	A	922	U	N3-C2-O2	-5.14	118.60	122.20
5	A	3317	U	P-O3'-C3'	5.08	125.79	119.70

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	2	436	0	475	1	0
2	LK	1784	0	1862	9	0
3	QX	959	0	1023	7	0
4	RM	612	0	682	3	0
5	A	65135	0	32730	208	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	LL	1757	0	1834	13	0
7	QY	976	0	1064	5	0
8	RO	392	0	420	1	0
9	JT	1515	0	1586	21	0
10	LM	1493	0	1566	13	0
11	QZ	1092	0	1155	8	0
12	RQ	827	0	897	9	0
13	JU	1039	0	1131	4	0
14	LN	1664	0	1706	8	0
15	RA	1173	0	1215	9	0
16	RT	694	0	734	5	0
17	JV	1720	0	1779	14	0
18	LO	1319	0	1353	14	0
19	RB	429	0	450	3	0
20	QO	1336	0	1364	8	0
21	JW	1555	0	1659	3	0
22	QP	1441	0	1543	12	0
23	RC	677	0	732	3	0
24	QQ	1185	0	1269	7	0
25	LD	3353	0	1695	8	0
26	QS	1437	0	1475	6	0
27	RD	796	0	854	3	0
28	QT	1276	0	1323	12	0
29	LE	2579	0	1304	1	0
30	QU	766	0	782	2	0
31	RE	1020	0	1090	4	0
32	QV	963	0	1015	7	0
33	LF	1855	0	1919	12	0
34	QW	509	0	537	3	0
35	RF	850	0	880	8	0
36	LG	3075	0	3142	23	0
37	RG	811	0	869	3	0
38	LH	2748	0	2859	18	0
39	RH	969	0	1078	9	0
40	LI	2293	0	2246	13	0
41	RI	771	0	849	2	0
42	LJ	1239	0	1326	12	0
43	RJ	670	0	673	4	0
44	A	126	0	0	0	0
44	LD	1	0	0	0	0
44	LE	1	0	0	0	0
44	QO	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	A	20	0	0	8	0
45	JV	1	0	0	0	0
45	LG	1	0	0	1	0
45	QO	1	0	0	0	0
45	RQ	1	0	0	2	0
46	A	14	0	26	0	0
47	A	10	0	19	1	0
48	RG	1	0	0	0	0
48	RJ	1	0	0	0	0
48	RO	1	0	0	0	0
48	RQ	1	0	0	0	0
48	RT	1	0	0	0	0
49	A	517	0	0	1	0
49	JV	2	0	0	0	0
49	JW	2	0	0	0	0
49	LD	3	0	0	0	0
49	LE	3	0	0	0	0
49	LF	4	0	0	0	0
49	LG	5	0	0	0	0
49	LH	2	0	0	0	0
49	LI	1	0	0	0	0
49	QO	1	0	0	0	0
49	QQ	1	0	0	0	0
49	QX	1	0	0	0	0
49	RA	2	0	0	0	0
49	RE	1	0	0	0	0
49	RJ	1	0	0	0	0
49	RQ	1	0	0	0	0
All	All	119919	0	86190	436	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (436) 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)
16:RT:42:CYS:HB3	16:RT:60:CYS:SG	1.90	1.10
9:JT:47:ALA:HB3	9:JT:49:ARG:HG2	1.57	0.84
5:A:2967:A:N6	45:A:3515:CL:CL	2.49	0.81
8:RO:97:ARG:HE	8:RO:122:ARG:HB3	1.47	0.79
5:A:888:A:N6	45:A:3520:CL:CL	2.53	0.78

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3042:U:OP2	5:A:3092:C:N4	2.21	0.72
40:LI:40:HIS:HD2	40:LI:42:ALA:H	1.36	0.72
5:A:838:G:O6	16:RT:4:ARG:NH2	2.23	0.72
15:RA:57:GLY:HA3	22:QP:170:ARG:HD2	1.72	0.72
5:A:979:U:O2'	5:A:980:A:OP2	2.08	0.71
3:QX:50:ALA:HB1	39:RH:66:VAL:HG11	1.73	0.70
5:A:2185:G:O2'	5:A:2314:U:OP2	2.09	0.69
5:A:3218:A:O2'	5:A:3219:G:OP2	2.10	0.69
5:A:2969:A:N7	33:LF:215:ASN:ND2	2.40	0.69
5:A:1019:G:H1	5:A:1033:U:H3	1.41	0.68
5:A:1635:G:N2	5:A:1638:A:OP2	2.27	0.67
20:QO:122:ALA:HB3	20:QO:143:PRO:HB2	1.77	0.67
38:LH:283:THR:HG22	38:LH:285:ASP:H	1.59	0.67
40:LI:91:GLY:O	40:LI:94:ASN:ND2	2.28	0.66
36:LG:10:ARG:NH1	36:LG:11:HIS:O	2.29	0.65
5:A:824:C:H5''	33:LF:21:ARG:HD3	1.77	0.65
38:LH:170:LYS:HD2	38:LH:175:HIS:HB2	1.77	0.65
5:A:3351:U:O2'	5:A:3353:G:N2	2.29	0.65
19:RB:33:LYS:O	28:QT:88:ARG:NH1	2.30	0.64
5:A:974:G:H5'	22:QP:16:ARG:HG3	1.79	0.64
5:A:2675:C:N4	18:LO:22:SER:OG	2.30	0.64
5:A:2514:U:O2	5:A:2593:A:N6	2.31	0.63
18:LO:49:LYS:HB3	18:LO:62:ASN:HA	1.80	0.63
5:A:1407:A:N6	45:A:3512:CL:CL	2.65	0.63
5:A:2282:U:OP1	5:A:2973:G:O2'	2.16	0.63
15:RA:76:ASP:HB3	15:RA:116:GLY:HA3	1.80	0.63
15:RA:104:THR:HG22	15:RA:109:TYR:HB2	1.79	0.63
9:JT:62:THR:HG22	9:JT:64:LYS:H	1.63	0.62
22:QP:62:VAL:HG13	22:QP:66:ARG:HD2	1.81	0.62
38:LH:334:PHE:HA	38:LH:339:LEU:HD23	1.81	0.62
5:A:2712:U:HO2'	5:A:2743:A:HO2'	1.46	0.62
5:A:3268:A:OP1	42:LJ:46:ARG:NH2	2.32	0.61
26:QS:8:GLN:HB3	26:QS:64:ILE:HD11	1.83	0.61
5:A:1682:U:O4	30:QU:90:ARG:NH1	2.34	0.61
10:LM:100:ASN:HB2	10:LM:115:ARG:HB2	1.82	0.61
38:LH:3:ARG:NH1	38:LH:22:LEU:O	2.33	0.61
5:A:358:G:N2	5:A:361:A:OP2	2.34	0.61
5:A:1152:G:OP2	5:A:1152:G:N2	2.32	0.61
26:QS:12:ARG:HH21	26:QS:22:PRO:HD2	1.65	0.61
35:RF:14:LEU:HD11	35:RF:31:LYS:HB2	1.83	0.60
18:LO:10:ARG:O	18:LO:133:ARG:NH1	2.34	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:RH:13:SER:H	39:RH:16:GLN:HE21	1.50	0.60
24:QQ:134:HIS:HD2	24:QQ:137:ALA:H	1.50	0.60
5:A:1814:A:H4'	5:A:1815:U:H5'	1.84	0.59
23:RC:24:THR:HB	23:RC:91:SER:HB3	1.84	0.59
9:JT:46:ILE:HG23	9:JT:47:ALA:H	1.67	0.59
5:A:3348:G:H1	5:A:3357:U:H3	1.49	0.58
32:QV:68:GLU:O	32:QV:72:LYS:NZ	2.36	0.58
5:A:3350:C:H2'	5:A:3351:U:H2'	1.85	0.58
2:LK:163:LEU:HA	2:LK:168:ILE:HD11	1.83	0.58
9:JT:123:ILE:HG22	39:RH:118:ILE:HG12	1.85	0.58
43:RJ:63:ARG:O	43:RJ:68:LYS:NZ	2.29	0.58
15:RA:104:THR:HG21	15:RA:112:ILE:HD11	1.86	0.58
5:A:1486:G:H21	37:RG:6:THR:HG22	1.69	0.58
5:A:3310:A:N6	45:A:3437:CL:CL	2.63	0.57
27:RD:41:LYS:NZ	27:RD:47:ASP:OD1	2.37	0.57
5:A:1103:A:N6	5:A:1363:A:O2'	2.38	0.57
5:A:3191:G:H5''	21:JW:176:LYS:HE2	1.87	0.57
5:A:297:G:OP2	5:A:297:G:N2	2.36	0.57
5:A:91:G:OP2	5:A:93:C:N4	2.36	0.56
10:LM:8:GLN:HB3	10:LM:72:LYS:HD2	1.87	0.56
5:A:3275:U:O2'	35:RF:99:ARG:NH1	2.39	0.56
32:QV:104:ASN:OD1	32:QV:108:GLU:N	2.36	0.56
5:A:1386:A:OP2	31:RE:80:LYS:NZ	2.39	0.56
3:QX:135:ILE:HD12	3:QX:138:ARG:HH21	1.70	0.56
5:A:2112:U:H4'	5:A:2113:A:O5'	2.06	0.56
9:JT:27:ASP:HB3	25:LD:29:U:H5''	1.88	0.56
2:LK:94:LYS:NZ	5:A:1156:C:OP2	2.39	0.55
5:A:2964:G:N2	5:A:2967:A:OP2	2.29	0.55
4:RM:31:LEU:HA	4:RM:37:PRO:HA	1.88	0.55
5:A:216:G:OP1	7:QY:16:ARG:NH1	2.40	0.55
21:JW:61:ALA:HA	21:JW:70:PRO:HD2	1.89	0.55
24:QQ:39:ASN:OD1	24:QQ:42:ARG:NH1	2.39	0.55
26:QS:5:LYS:HE2	26:QS:63:GLN:HB3	1.88	0.55
5:A:2424:A:OP1	17:JV:90:ASN:ND2	2.36	0.55
20:QO:56:ARG:NH2	20:QO:75:GLU:OE2	2.37	0.55
5:A:3000:A:O3'	36:LG:120:LYS:NZ	2.39	0.55
5:A:3218:A:H2'	5:A:3278:C:H5	1.71	0.55
36:LG:85:VAL:HG22	36:LG:202:THR:HG22	1.88	0.55
17:JV:33:LYS:O	17:JV:65:ARG:NH2	2.39	0.55
37:RG:46:ASP:OD1	37:RG:80:ARG:NH1	2.38	0.54
5:A:1348:U:P	22:QP:39:ARG:HH22	2.30	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1404:G:N2	5:A:1407:A:OP2	2.34	0.54
32:QV:10:LYS:HB2	32:QV:125:LEU:HD11	1.89	0.54
40:LI:268:GLU:HA	40:LI:271:LYS:HE2	1.89	0.54
5:A:1778:G:O2'	5:A:1780:G:OP2	2.23	0.54
5:A:3139:A:OP2	36:LG:30:LYS:NZ	2.30	0.54
5:A:1192:C:N4	5:A:1302:A:OP2	2.39	0.54
5:A:1626:U:H3	5:A:1817:G:H1	1.54	0.54
5:A:3092:C:O2'	5:A:3094:A:OP2	2.20	0.54
3:QX:134:ASP:HA	3:QX:137:ASN:HD21	1.73	0.54
6:LL:203:VAL:HG21	6:LL:211:LEU:HD22	1.90	0.54
5:A:2631:U:OP2	28:QT:4:SER:OG	2.24	0.54
5:A:2745:G:N2	5:A:2748:A:OP2	2.39	0.54
33:LF:117:GLU:HG2	33:LF:124:GLY:H	1.73	0.53
5:A:3217:C:H6	5:A:3266:G:H21	1.55	0.53
20:QO:60:PHE:HB3	20:QO:64:ASN:HB3	1.89	0.53
32:QV:87:ARG:HH22	32:QV:137:VAL:HG21	1.73	0.53
11:QZ:22:LYS:NZ	11:QZ:129:TRP:O	2.35	0.53
34:QW:14:TYR:OH	36:LG:375:GLU:OE2	2.26	0.53
5:A:1191:U:H4'	5:A:1192:C:H5''	1.90	0.53
5:A:2111:G:H5'	34:QW:48:ARG:HE	1.72	0.53
14:LN:54:SER:HB2	14:LN:135:ILE:HD11	1.90	0.53
9:JT:153:ASP:OD1	9:JT:154:VAL:N	2.41	0.53
40:LI:60:ILE:HB	40:LI:80:SER:HB3	1.91	0.53
5:A:412:G:OP1	20:QO:62:ARG:NH1	2.41	0.53
5:A:585:A:H5''	35:RF:70:LYS:HE2	1.91	0.53
5:A:3218:A:H5''	5:A:3219:G:C4	2.44	0.53
45:A:3471:CL:CL	33:LF:6:ARG:HB2	2.46	0.53
11:QZ:3:LYS:NZ	23:RC:36:GLN:O	2.37	0.53
24:QQ:134:HIS:CD2	24:QQ:137:ALA:H	2.27	0.53
36:LG:284:ARG:NH1	36:LG:293:ASN:O	2.42	0.52
3:QX:46:TYR:OH	39:RH:78:LYS:NZ	2.42	0.52
5:A:1724:U:O4	24:QQ:125:LYS:NZ	2.39	0.52
14:LN:36:LEU:HD21	14:LN:69:ARG:HD2	1.92	0.52
17:JV:183:THR:HG22	17:JV:187:ARG:HB2	1.91	0.52
5:A:110:G:OP2	9:JT:73:ARG:NH2	2.39	0.52
5:A:1940:G:H21	5:A:3362:A:H8	1.57	0.52
5:A:1118:C:N4	45:A:3421:CL:CL	2.60	0.52
5:A:627:U:H4'	5:A:1399:A:H1'	1.92	0.52
5:A:3121:U:H1'	5:A:3122:A:H5''	1.90	0.51
38:LH:156:LEU:HD12	38:LH:159:ILE:HD12	1.92	0.51
5:A:22:G:H5''	43:RJ:43:LYS:HG2	1.92	0.51

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LM:92:TYR:HB2	10:LM:142:ASP:HB3	1.92	0.51
36:LG:213:GLU:OE2	36:LG:340:LYS:NZ	2.40	0.51
5:A:1835:A:N6	45:A:3484:CL:CL	2.67	0.51
5:A:900:G:H1'	5:A:1589:A:N6	2.26	0.51
5:A:1639:C:OP2	37:RG:74:ARG:NH1	2.43	0.51
5:A:2193:U:H5'	5:A:2194:G:H5'	1.93	0.51
9:JT:3:ILE:HG22	15:RA:44:ASN:HD22	1.76	0.50
5:A:1493:G:OP2	5:A:1493:G:N2	2.39	0.50
9:JT:124:ILE:HD13	39:RH:119:LYS:HB2	1.93	0.50
36:LG:14:LEU:N	45:LG:401:CL:CL	2.72	0.50
5:A:1094:U:H4'	5:A:1096:U:H5''	1.93	0.50
5:A:3217:C:C5	5:A:3220:G:H1'	2.47	0.50
10:LM:87:LYS:HE2	10:LM:187:ILE:HA	1.93	0.50
18:LO:92:ARG:HA	18:LO:172:LEU:HB2	1.93	0.50
22:QP:125:ASP:OD2	38:LH:282:SER:OG	2.20	0.50
36:LG:31:ALA:O	36:LG:339:ARG:NH1	2.43	0.50
5:A:394:G:N1	5:A:397:A:OP2	2.45	0.50
5:A:1717:U:H2'	5:A:1718:G:C8	2.47	0.50
18:LO:54:VAL:HG13	18:LO:56:THR:H	1.77	0.50
22:QP:165:ILE:HD11	22:QP:172:PHE:HB3	1.94	0.50
5:A:3209:A:C4	13:JU:106:ARG:HD3	2.47	0.50
10:LM:18:VAL:HG22	10:LM:27:VAL:HG12	1.93	0.50
35:RF:37:THR:HG22	35:RF:39:GLN:H	1.76	0.50
38:LH:292:SER:OG	38:LH:294:GLU:OE1	2.29	0.50
40:LI:236:LEU:HA	40:LI:239:ILE:HG12	1.93	0.50
5:A:3317:U:H4'	5:A:3318:G:H5'	1.94	0.50
19:RB:20:GLY:HA3	28:QT:82:ASN:HB2	1.93	0.50
32:QV:32:ARG:HH21	32:QV:64:LYS:HB3	1.77	0.49
2:LK:70:LYS:HG2	38:LH:351:PRO:HB3	1.94	0.49
12:RQ:45:ARG:NH1	45:RQ:202:CL:CL	2.77	0.49
40:LI:52:VAL:HG21	40:LI:65:ILE:HD12	1.94	0.49
5:A:518:G:OP2	5:A:518:G:N2	2.34	0.49
5:A:3288:G:HO2'	5:A:3289:G:H8	1.58	0.49
10:LM:57:VAL:HG23	10:LM:68:LEU:HD13	1.94	0.49
2:LK:121:LYS:HB2	28:QT:133:ALA:HB3	1.94	0.49
5:A:2915:U:C5	36:LG:7:GLU:HG2	2.48	0.49
5:A:1564:U:H2'	5:A:1565:G:H8	1.78	0.49
5:A:3271:G:C5	42:LJ:108:LYS:HE3	2.47	0.49
5:A:3313:U:H4'	36:LG:173:GLN:HG3	1.94	0.49
5:A:633:C:O2'	35:RF:21:ARG:O	2.30	0.49
5:A:2945:G:O2'	5:A:2948:C:OP2	2.25	0.48

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:LF:104:LEU:HD22	33:LF:136:ILE:HD11	1.95	0.48
5:A:1629:U:O3'	11:QZ:115:LYS:NZ	2.46	0.48
5:A:3227:A:O3'	13:JU:133:LYS:NZ	2.46	0.48
5:A:627:U:H2'	5:A:628:A:C8	2.49	0.48
5:A:3050:U:O2'	34:QW:16:GLY:O	2.30	0.48
10:LM:80:THR:HA	10:LM:83:THR:HG22	1.94	0.48
11:QZ:25:ILE:HA	11:QZ:43:VAL:HG12	1.94	0.48
18:LO:28:ASP:OD2	18:LO:32:ARG:NH1	2.46	0.48
18:LO:53:THR:HG23	18:LO:60:ARG:HA	1.94	0.48
36:LG:313:HIS:O	36:LG:333:LYS:HE3	2.13	0.48
5:A:1877:U:H5''	5:A:1878:G:O4'	2.14	0.48
5:A:2763:U:O2	47:A:3504:SPD:N1	2.47	0.48
5:A:3217:C:N3	20:QO:182:ILE:HD12	2.28	0.48
5:A:1108:U:H2'	5:A:1109:U:C6	2.49	0.48
5:A:2352:A:H5''	20:QO:83:TRP:O	2.13	0.48
5:A:3350:C:H42	5:A:3353:G:H1	1.62	0.48
7:QY:55:GLU:HB2	7:QY:108:LYS:HB3	1.95	0.48
7:QY:5:SER:HB3	7:QY:8:VAL:HG12	1.96	0.48
12:RQ:46:LYS:HE2	12:RQ:54:THR:HB	1.96	0.48
36:LG:159:ARG:HG2	36:LG:182:GLN:HG2	1.96	0.48
5:A:981:U:H2'	5:A:982:C:C6	2.48	0.48
5:A:1098:A:OP2	28:QT:129:LYS:HA	2.14	0.48
36:LG:57:VAL:HG22	36:LG:73:VAL:HG22	1.96	0.48
22:QP:180:ARG:NH1	22:QP:185:LYS:H	2.12	0.48
33:LF:113:VAL:HG12	33:LF:166:ILE:HD13	1.94	0.48
2:LK:85:PHE:HB2	2:LK:139:PRO:HG3	1.96	0.47
5:A:916:G:H5'	5:A:917:A:OP1	2.14	0.47
5:A:2681:U:H5'	18:LO:65:ILE:HD11	1.94	0.47
13:JU:16:GLU:HB3	26:QS:149:LYS:HG2	1.96	0.47
31:RE:123:LYS:HA	31:RE:126:LEU:HD12	1.96	0.47
5:A:3218:A:H2'	5:A:3278:C:C5	2.48	0.47
20:QO:67:ILE:HD11	20:QO:80:LYS:HB3	1.96	0.47
5:A:427:C:OP2	31:RE:15:LYS:NZ	2.42	0.47
5:A:1913:A:N3	5:A:2120:A:H2'	2.29	0.47
5:A:2433:U:H1'	17:JV:125:SER:HB2	1.95	0.47
5:A:1347:U:H2'	5:A:1355:A:H61	1.79	0.47
4:RM:26:LYS:NZ	4:RM:28:ASN:OD1	2.41	0.47
5:A:1222:G:HO2'	5:A:1223:A:P	2.37	0.47
3:QX:27:ARG:HD3	6:LL:50:VAL:HG21	1.96	0.47
5:A:979:U:HO2'	5:A:980:A:P	2.35	0.47
5:A:2108:C:H1'	5:A:3344:A:C8	2.50	0.47

Continued on next page...

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2150:G:O2'	5:A:2189:U:OP1	2.30	0.47
17:JV:43:THR:HG23	17:JV:44:ARG:HG3	1.96	0.47
42:LJ:100:LYS:NZ	42:LJ:137:ASP:OD2	2.41	0.47
5:A:3215:A:H5''	35:RF:2:ALA:HB2	1.97	0.47
17:JV:28:TRP:O	17:JV:32:GLN:HG2	2.15	0.47
27:RD:55:LEU:HB2	27:RD:95:PRO:HD3	1.97	0.47
5:A:1564:U:H2'	5:A:1565:G:C8	2.50	0.47
5:A:2213:A:H2'	5:A:2214:A:C8	2.50	0.47
22:QP:38:ARG:HH12	22:QP:39:ARG:HH21	1.63	0.47
5:A:59:G:H4'	5:A:60:A:H4'	1.97	0.46
5:A:1927:G:C8	16:RT:16:VAL:HG12	2.51	0.46
5:A:2196:C:O2'	5:A:2270:A:N3	2.39	0.46
9:JT:46:ILE:HG23	9:JT:47:ALA:N	2.30	0.46
28:QT:118:GLU:O	28:QT:122:GLN:NE2	2.47	0.46
5:A:1863:G:N1	5:A:1866:C:OP2	2.44	0.46
14:LN:130:ASP:OD1	14:LN:131:ILE:N	2.40	0.46
21:JW:37:ARG:HD2	21:JW:108:ILE:HD11	1.97	0.46
5:A:132:C:H2'	5:A:133:U:H5''	1.95	0.46
5:A:711:A:N6	45:A:3440:CL:CL	2.79	0.46
5:A:1538:G:H21	5:A:1583:A:H62	1.64	0.46
24:QQ:105:LEU:HD23	24:QQ:138:LEU:HD23	1.97	0.46
5:A:598:A:H4'	38:LH:325:LEU:HD13	1.96	0.46
5:A:2356:A:H61	5:A:2983:C:H5	1.60	0.46
32:QV:86:ARG:HB2	32:QV:92:PHE:CE1	2.51	0.46
4:RM:7:ASP:HB3	4:RM:10:GLN:HG2	1.97	0.46
14:LN:30:LYS:HG3	14:LN:63:GLU:HG3	1.98	0.46
5:A:655:C:H2'	5:A:656:A:C8	2.51	0.46
17:JV:84:PRO:HA	17:JV:87:GLN:HG3	1.97	0.46
5:A:1064:A:H4'	5:A:1065:A:O5'	2.15	0.46
36:LG:292:ALA:HB2	36:LG:302:LYS:HD3	1.98	0.46
5:A:911:C:H5''	33:LF:15:ILE:HD13	1.98	0.46
5:A:2592:G:H4'	5:A:2594:C:C2	2.50	0.46
5:A:2138:A:C4	43:RJ:3:LYS:HB3	2.51	0.46
35:RF:49:ILE:HD11	35:RF:71:VAL:HG22	1.98	0.45
5:A:2129:U:H2'	5:A:2130:G:C8	2.52	0.45
17:JV:181:ASN:OD1	17:JV:184:LYS:NZ	2.50	0.45
28:QT:18:ASP:HB2	28:QT:21:LYS:HB2	1.97	0.45
31:RE:79:VAL:HG13	31:RE:111:ARG:HG2	1.97	0.45
39:RH:70:TYR:HB3	39:RH:76:GLN:HG2	1.97	0.45
5:A:2373:A:N3	5:A:2824:G:O2'	2.43	0.45
9:JT:3:ILE:HG22	15:RA:44:ASN:ND2	2.31	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:LL:189:LEU:HD12	6:LL:190:VAL:HG13	1.99	0.45
5:A:1355:A:H4'	5:A:1356:U:O5'	2.15	0.45
5:A:1571:A:H2'	5:A:1572:U:O4'	2.16	0.45
5:A:3228:C:H4'	5:A:3229:G:O5'	2.16	0.45
10:LM:83:THR:HG23	10:LM:84:LYS:HG3	1.99	0.45
10:LM:132:VAL:HG11	10:LM:157:ASN:HD22	1.81	0.45
38:LH:161:LYS:HB2	38:LH:164:GLU:HG2	1.99	0.45
12:RQ:65:THR:O	12:RQ:87:ARG:NH1	2.50	0.45
32:QV:81:GLN:HE21	32:QV:83:LYS:HB3	1.81	0.45
5:A:1104:G:H2'	5:A:1105:A:C8	2.52	0.45
11:QZ:76:ASN:OD1	11:QZ:77:TYR:N	2.50	0.45
5:A:3157:U:H4'	5:A:3158:G:H5'	1.99	0.45
18:LO:111:ASP:OD1	18:LO:111:ASP:N	2.50	0.45
5:A:371:G:N1	5:A:374:A:OP2	2.44	0.45
5:A:2960:C:H2'	5:A:2961:G:C8	2.51	0.45
5:A:123:A:OP1	6:LL:105:LYS:NZ	2.40	0.44
5:A:1020:G:C2	5:A:1021:G:H1'	2.52	0.44
5:A:2538:U:O2'	5:A:2541:U:O4	2.29	0.44
42:LJ:148:GLU:HA	42:LJ:151:LYS:HZ3	1.82	0.44
5:A:1727:G:OP1	16:RT:44:LYS:NZ	2.49	0.44
5:A:3356:G:H2'	5:A:3357:U:C6	2.52	0.44
5:A:1047:A:N3	5:A:2633:U:O2'	2.51	0.44
5:A:3084:C:H2'	5:A:3085:G:O4'	2.18	0.44
42:LJ:43:LEU:HD11	42:LJ:85:ILE:HG13	1.98	0.44
5:A:2514:U:OP1	5:A:2586:G:N2	2.51	0.44
5:A:2981:U:OP2	36:LG:244:ARG:NH2	2.46	0.44
5:A:3379:C:H4'	36:LG:315:GLY:HA2	1.99	0.44
18:LO:161:SER:O	18:LO:165:GLN:HG2	2.18	0.44
5:A:1390:A:N6	5:A:1418:A:O2'	2.50	0.44
9:JT:11:LYS:O	9:JT:13:HIS:HD2	1.99	0.44
10:LM:113:GLU:OE2	10:LM:115:ARG:NE	2.45	0.44
23:RC:42:ILE:HD11	23:RC:67:VAL:HG22	2.00	0.44
25:LD:103:G:OP2	25:LD:105:A:O2'	2.35	0.44
5:A:1895:A:O2'	5:A:3053:G:H4'	2.17	0.44
9:JT:49:ARG:HB2	9:JT:50:PRO:HD2	1.99	0.44
12:RQ:103:ALA:HB1	18:LO:60:ARG:HE	1.82	0.44
5:A:2718:U:OP1	12:RQ:13:LYS:NZ	2.49	0.44
14:LN:80:SER:HB3	14:LN:147:VAL:HG11	1.99	0.44
5:A:1039:U:H2'	5:A:1040:A:C8	2.53	0.43
6:LL:185:ARG:O	6:LL:188:THR:OG1	2.31	0.43
38:LH:35:VAL:HG21	38:LH:244:LEU:HD21	2.00	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:528:U:H2'	5:A:529:A:C8	2.53	0.43
5:A:864:G:N7	49:A:3640:HOH:O	2.36	0.43
5:A:1307:G:O2'	5:A:1308:A:OP2	2.34	0.43
5:A:1740:U:H1'	5:A:1741:A:H2	1.83	0.43
5:A:2137:U:OP2	5:A:2142:A:N6	2.44	0.43
20:QO:126:ARG:HA	20:QO:140:GLU:HG2	2.00	0.43
6:LL:161:GLU:OE2	17:JV:26:ARG:NH1	2.48	0.43
11:QZ:26:VAL:HG12	11:QZ:27:LYS:HG3	1.99	0.43
5:A:616:G:H2'	5:A:617:G:C8	2.53	0.43
6:LL:144:GLU:OE2	17:JV:6:TYR:OH	2.25	0.43
12:RQ:8:ARG:HG2	12:RQ:10:THR:HG23	2.00	0.43
18:LO:44:THR:HG23	29:LE:39:C:H4'	2.00	0.43
3:QX:24:LEU:HD13	5:A:2585:G:C6	2.53	0.43
5:A:600:G:N2	5:A:603:A:OP2	2.45	0.43
5:A:993:G:N3	5:A:2637:A:H2'	2.34	0.43
5:A:1097:G:H4'	5:A:1098:A:O5'	2.18	0.43
10:LM:89:LYS:HG2	10:LM:145:VAL:HG22	2.00	0.43
25:LD:81:U:H4'	25:LD:82:U:H5'	2.01	0.43
26:QS:13:ARG:NH1	26:QS:50:LYS:O	2.52	0.43
40:LI:153:THR:HG23	40:LI:160:PHE:HZ	1.84	0.43
5:A:400:G:H4'	5:A:401:U:H5''	2.01	0.43
5:A:1348:U:O2	5:A:1349:G:N2	2.50	0.43
5:A:2392:C:O2'	36:LG:266:ARG:NH2	2.51	0.43
5:A:2748:A:H1'	40:LI:36:LEU:HD23	2.01	0.43
12:RQ:71:ARG:HD3	12:RQ:80:ARG:HD3	1.99	0.43
18:LO:60:ARG:HG2	18:LO:63:GLU:HG3	2.00	0.43
42:LJ:12:SER:OG	42:LJ:14:ASP:OD1	2.25	0.43
5:A:148:G:OP2	17:JV:4:TYR:OH	2.24	0.43
15:RA:94:ALA:HB2	15:RA:121:VAL:HG22	2.00	0.43
33:LF:138:GLY:HA3	33:LF:147:ARG:NH2	2.34	0.43
35:RF:59:VAL:HG23	35:RF:60:ARG:H	1.83	0.43
38:LH:343:LYS:HE2	38:LH:343:LYS:HB3	1.91	0.43
5:A:1786:G:H2'	5:A:1787:A:C8	2.54	0.43
25:LD:142:C:H2'	25:LD:143:U:C6	2.54	0.43
30:QU:84:LEU:HD23	30:QU:90:ARG:HD2	2.01	0.43
2:LK:80:GLN:H	2:LK:80:GLN:HG2	1.67	0.43
5:A:370:U:H4'	5:A:404:G:H5'	2.01	0.43
5:A:797:U:H5''	9:JT:2:ALA:HB1	2.00	0.43
5:A:938:C:OP2	15:RA:26:ARG:NH1	2.51	0.43
5:A:1554:U:H4'	5:A:1555:U:OP1	2.16	0.43
5:A:1117:G:OP1	19:RB:4:SER:HB2	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:3016:A:H2'	5:A:3017:A:C8	2.54	0.42
6:LL:166:LEU:HD23	6:LL:166:LEU:HA	1.88	0.42
9:JT:50:PRO:HA	9:JT:138:VAL:O	2.19	0.42
14:LN:169:LYS:HD2	28:QT:159:PHE:HA	2.01	0.42
26:QS:141:LYS:HD2	26:QS:144:LEU:HD12	2.01	0.42
40:LI:82:GLU:O	40:LI:85:ARG:HG2	2.20	0.42
24:QQ:115:ILE:HD12	24:QQ:119:LEU:HD23	2.01	0.42
36:LG:113:GLU:OE2	36:LG:167:ARG:NH1	2.41	0.42
36:LG:123:TYR:CZ	36:LG:124:LYS:HG3	2.53	0.42
40:LI:41:LYS:HA	40:LI:41:LYS:HD3	1.83	0.42
5:A:340:C:OP2	38:LH:195:ARG:NH1	2.43	0.42
5:A:1899:G:O2'	5:A:2334:U:O4	2.25	0.42
5:A:3346:U:H3	5:A:3359:A:H61	1.68	0.42
15:RA:43:ILE:O	15:RA:47:LYS:HG2	2.19	0.42
38:LH:159:ILE:HG23	38:LH:164:GLU:HG3	2.01	0.42
36:LG:346:THR:O	36:LG:346:THR:OG1	2.36	0.42
5:A:190:U:H2'	7:QY:60:ARG:HH22	1.85	0.42
5:A:2138:A:HO2'	43:RJ:2:GLY:N	2.17	0.42
16:RT:8:VAL:O	16:RT:11:THR:OG1	2.38	0.42
33:LF:103:PRO:HA	33:LF:163:ARG:HA	2.02	0.42
41:RI:4:LYS:HD3	41:RI:14:GLY:HA3	2.00	0.42
42:LJ:58:LEU:HD21	42:LJ:64:LEU:HB2	2.02	0.42
2:LK:80:GLN:HG3	28:QT:135:PRO:HB2	2.02	0.42
3:QX:24:LEU:HD11	25:LD:151:C:C5	2.55	0.42
5:A:3170:A:H2'	5:A:3171:U:C6	2.54	0.42
33:LF:2:GLY:HA2	33:LF:207:VAL:HG23	2.00	0.42
2:LK:136:TYR:CZ	2:LK:231:ASN:HB2	2.54	0.42
5:A:1597:C:H5'	5:A:1696:A:H1'	2.00	0.42
38:LH:64:SER:HA	38:LH:75:PRO:HA	2.02	0.42
5:A:708:G:N2	5:A:711:A:OP2	2.47	0.42
5:A:1764:U:H3'	5:A:1765:U:H5''	2.02	0.42
5:A:2514:U:C6	6:LL:68:ARG:HB3	2.54	0.42
14:LN:29:SER:HB2	14:LN:125:LEU:HD12	2.01	0.42
24:QQ:116:ASP:OD1	24:QQ:116:ASP:N	2.53	0.42
5:A:1724:U:H1'	5:A:1725:C:C6	2.55	0.41
5:A:1761:C:O2'	5:A:1762:C:H5''	2.19	0.41
5:A:3218:A:HO2'	5:A:3219:G:P	2.42	0.41
11:QZ:101:PHE:O	11:QZ:102:GLU:HG2	2.20	0.41
14:LN:166:ILE:HG21	28:QT:158:THR:HG21	2.02	0.41
36:LG:19:ARG:HB2	36:LG:232:ARG:NH2	2.35	0.41
42:LJ:60:ASP:OD1	42:LJ:62:THR:OG1	2.32	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:4:GLN:HE22	5:A:1833:G:H21	1.68	0.41
5:A:2585:G:H2'	5:A:2585:G:N3	2.35	0.41
6:LL:112:GLU:O	6:LL:116:VAL:HG12	2.20	0.41
42:LJ:100:LYS:HE3	42:LJ:100:LYS:HB3	1.88	0.41
5:A:126:U:OP1	17:JV:144:ARG:NH1	2.48	0.41
5:A:1525:G:H5'	5:A:1830:G:OP2	2.20	0.41
5:A:2557:A:OP1	33:LF:69:TYR:OH	2.33	0.41
5:A:2930:A:H2'	5:A:2931:C:C6	2.55	0.41
9:JT:136:GLU:HB3	39:RH:119:LYS:NZ	2.36	0.41
5:A:911:C:OP2	33:LF:9:ARG:HD2	2.21	0.41
6:LL:158:ASP:HB2	6:LL:159:PRO:HD3	2.01	0.41
12:RQ:28:TYR:HB3	12:RQ:69:VAL:HB	2.03	0.41
25:LD:110:C:O2'	25:LD:112:U:OP2	2.27	0.41
42:LJ:172:HIS:CD2	42:LJ:173:MET:HG2	2.55	0.41
5:A:212:G:OP2	7:QY:2:ALA:N	2.53	0.41
10:LM:106:LYS:HG2	10:LM:107:ASP:OD2	2.21	0.41
22:QP:39:ARG:HG2	38:LH:299:ILE:HB	2.01	0.41
25:LD:97:A:OP1	39:RH:63:ARG:NH2	2.46	0.41
38:LH:179:LEU:O	38:LH:183:LYS:HG2	2.21	0.41
5:A:59:G:H2'	25:LD:33:A:O2'	2.21	0.41
5:A:1560:G:N1	5:A:1580:A:N1	2.68	0.41
5:A:2144:A:H1'	5:A:2281:A:H61	1.85	0.41
42:LJ:148:GLU:HA	42:LJ:151:LYS:NZ	2.35	0.41
5:A:96:G:H5'	9:JT:15:ARG:CZ	2.51	0.41
5:A:2513:U:O2'	5:A:2514:U:O5'	2.39	0.41
5:A:2689:A:H2'	5:A:2689:A:N3	2.34	0.41
38:LH:142:VAL:HG12	38:LH:145:ILE:HD12	2.02	0.41
5:A:374:A:O2'	5:A:376:G:H5'	2.21	0.41
5:A:662:U:H2'	5:A:663:C:C6	2.55	0.41
9:JT:46:ILE:HG12	9:JT:49:ARG:HE	1.85	0.41
17:JV:45:PRO:O	17:JV:49:ARG:HG3	2.21	0.41
28:QT:69:LYS:HA	40:LI:40:HIS:CD2	2.55	0.41
5:A:1827:C:H2'	5:A:1828:A:C8	2.56	0.41
5:A:2101:C:HO2'	5:A:2102:U:H6	1.68	0.41
5:A:2228:A:H2'	5:A:2229:A:C8	2.55	0.41
5:A:2660:G:OP1	5:A:2750:U:O2'	2.39	0.41
18:LO:41:SER:HB2	18:LO:71:VAL:HG11	2.03	0.41
22:QP:148:GLU:O	22:QP:151:ARG:HG2	2.21	0.41
27:RD:96:VAL:HG12	27:RD:98:VAL:HG13	2.02	0.41
5:A:98:G:N7	9:JT:13:HIS:HE1	2.18	0.40
5:A:1001:G:N3	5:A:1041:U:H5'	2.36	0.40

*Continued on next page...*



Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1661:G:H2'	5:A:1662:G:C8	2.56	0.40
5:A:3252:G:H2'	5:A:3253:G:C8	2.56	0.40
22:QP:123:THR:OG1	22:QP:125:ASP:OD1	2.26	0.40
39:RH:119:LYS:HA	39:RH:119:LYS:HE2	2.03	0.40
5:A:377:A:H1'	5:A:392:G:N2	2.36	0.40
6:LL:246:MET:O	6:LL:249:ARG:HG2	2.21	0.40
12:RQ:45:ARG:HD3	45:RQ:202:CL:CL	2.58	0.40
2:LK:48:ASN:ND2	2:LK:182:ASP:OD2	2.54	0.40
5:A:591:G:O2'	42:LJ:17:ALA:O	2.33	0.40
22:QP:96:PHE:HA	22:QP:97:PRO:HD3	1.92	0.40
36:LG:95:THR:HB	36:LG:98:GLY:O	2.21	0.40
40:LI:278:SER:OG	40:LI:280:GLU:OE1	2.37	0.40
9:JT:187:ALA:O	9:JT:190:LYS:HG2	2.21	0.40
5:A:299:G:C4	41:RI:31:GLY:HA3	2.56	0.40
5:A:2779:A:O2'	9:JT:180:ARG:NH2	2.53	0.40
5:A:3186:A:N3	10:LM:44:THR:OG1	2.51	0.40
6:LL:68:ARG:HD3	6:LL:237:ILE:O	2.22	0.40
11:QZ:95:VAL:HG13	11:QZ:96:VAL:HG23	2.04	0.40
13:JU:25:LYS:HE3	13:JU:62:GLN:NE2	2.37	0.40
17:JV:73:ARG:HA	17:JV:74:PRO:HD3	1.91	0.40
28:QT:68:THR:O	40:LI:41:LYS:HB2	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	48/51 (94%)	48 (100%)	0	0	100	100
2	LK	220/244 (90%)	215 (98%)	5 (2%)	0	100	100
3	QX	118/142 (83%)	117 (99%)	1 (1%)	0	100	100
4	RM	75/78 (96%)	73 (97%)	2 (3%)	0	100	100

Continued on next page...



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	LL	224/256 (88%)	219 (98%)	5 (2%)	0	100	100
7	QY	122/127 (96%)	122 (100%)	0	0	100	100
8	RO	47/128 (37%)	47 (100%)	0	0	100	100
9	JT	187/199 (94%)	176 (94%)	11 (6%)	0	100	100
10	LM	186/191 (97%)	177 (95%)	9 (5%)	0	100	100
11	QZ	133/136 (98%)	125 (94%)	8 (6%)	0	100	100
12	RQ	101/106 (95%)	94 (93%)	7 (7%)	0	100	100
13	JU	132/138 (96%)	128 (97%)	4 (3%)	0	100	100
14	LN	200/221 (90%)	194 (97%)	6 (3%)	0	100	100
15	RA	146/149 (98%)	131 (90%)	14 (10%)	1 (1%)	22	20
16	RT	89/92 (97%)	88 (99%)	1 (1%)	0	100	100
17	JV	201/204 (98%)	196 (98%)	5 (2%)	0	100	100
18	LO	163/174 (94%)	158 (97%)	5 (3%)	0	100	100
19	RB	51/59 (86%)	49 (96%)	2 (4%)	0	100	100
20	QO	165/184 (90%)	164 (99%)	1 (1%)	0	100	100
21	JW	195/199 (98%)	194 (100%)	1 (0%)	0	100	100
22	QP	183/186 (98%)	177 (97%)	6 (3%)	0	100	100
23	RC	86/105 (82%)	86 (100%)	0	0	100	100
24	QQ	145/189 (77%)	145 (100%)	0	0	100	100
26	QS	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
27	RD	94/113 (83%)	94 (100%)	0	0	100	100
28	QT	157/160 (98%)	152 (97%)	5 (3%)	0	100	100
30	QU	95/121 (78%)	95 (100%)	0	0	100	100
31	RE	125/130 (96%)	125 (100%)	0	0	100	100
32	QV	127/137 (93%)	125 (98%)	2 (2%)	0	100	100
33	LF	242/254 (95%)	230 (95%)	12 (5%)	0	100	100
34	QW	59/155 (38%)	58 (98%)	1 (2%)	0	100	100
35	RF	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
36	LG	384/387 (99%)	376 (98%)	8 (2%)	0	100	100
37	RG	101/121 (84%)	99 (98%)	2 (2%)	0	100	100
38	LH	359/362 (99%)	348 (97%)	11 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	RH	117/120 (98%)	116 (99%)	1 (1%)	0	100	100
40	LI	283/297 (95%)	278 (98%)	5 (2%)	0	100	100
41	RI	97/100 (97%)	94 (97%)	3 (3%)	0	100	100
42	LJ	152/176 (86%)	151 (99%)	1 (1%)	0	100	100
43	RJ	83/88 (94%)	81 (98%)	2 (2%)	0	100	100
All	All	5965/6558 (91%)	5809 (97%)	155 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	RA	15	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	45/46 (98%)	45 (100%)	0	100	100
2	LK	186/205 (91%)	185 (100%)	1 (0%)	88	92
3	QX	104/118 (88%)	104 (100%)	0	100	100
4	RM	68/69 (99%)	68 (100%)	0	100	100
6	LL	182/208 (88%)	181 (100%)	1 (0%)	88	92
7	QY	107/110 (97%)	106 (99%)	1 (1%)	78	84
8	RO	44/116 (38%)	44 (100%)	0	100	100
9	JT	152/159 (96%)	151 (99%)	1 (1%)	84	88
10	LM	168/171 (98%)	166 (99%)	2 (1%)	71	78
11	QZ	115/116 (99%)	114 (99%)	1 (1%)	78	84
12	RQ	88/91 (97%)	88 (100%)	0	100	100
13	JU	106/109 (97%)	106 (100%)	0	100	100
14	LN	176/187 (94%)	174 (99%)	2 (1%)	73	80

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	RA	118/119 (99%)	117 (99%)	1 (1%)	81	87
16	RT	71/72 (99%)	70 (99%)	1 (1%)	67	74
17	JV	175/176 (99%)	175 (100%)	0	100	100
18	LO	143/150 (95%)	140 (98%)	3 (2%)	53	60
19	RB	44/47 (94%)	44 (100%)	0	100	100
20	QO	135/146 (92%)	135 (100%)	0	100	100
21	JW	160/162 (99%)	158 (99%)	2 (1%)	69	76
22	QP	150/151 (99%)	150 (100%)	0	100	100
23	RC	73/88 (83%)	73 (100%)	0	100	100
24	QQ	122/154 (79%)	122 (100%)	0	100	100
26	QS	155/156 (99%)	153 (99%)	2 (1%)	69	76
27	RD	85/97 (88%)	85 (100%)	0	100	100
28	QT	136/137 (99%)	135 (99%)	1 (1%)	84	88
30	QU	84/107 (78%)	83 (99%)	1 (1%)	71	78
31	RE	109/111 (98%)	109 (100%)	0	100	100
32	QV	101/105 (96%)	101 (100%)	0	100	100
33	LF	187/196 (95%)	185 (99%)	2 (1%)	73	80
34	QW	54/129 (42%)	52 (96%)	2 (4%)	34	38
35	RF	90/91 (99%)	89 (99%)	1 (1%)	73	80
36	LG	319/323 (99%)	316 (99%)	3 (1%)	78	84
37	RG	88/103 (85%)	87 (99%)	1 (1%)	73	80
38	LH	288/289 (100%)	285 (99%)	3 (1%)	76	82
39	RH	104/105 (99%)	104 (100%)	0	100	100
40	LI	237/245 (97%)	235 (99%)	2 (1%)	81	87
41	RI	81/82 (99%)	81 (100%)	0	100	100
42	LJ	134/153 (88%)	133 (99%)	1 (1%)	84	88
43	RJ	69/71 (97%)	69 (100%)	0	100	100
All	All	5053/5470 (92%)	5018 (99%)	35 (1%)	84	88

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	LK	80	GLN

Continued on next page...

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	LL	248	LYS
7	QY	74	TYR
9	JT	85	LEU
10	LM	23	ARG
10	LM	63	LYS
11	QZ	23	VAL
14	LN	101	LYS
14	LN	163	GLN
15	RA	60	TYR
16	RT	89	MET
18	LO	30	LEU
18	LO	44	THR
18	LO	55	ARG
21	JW	84	LEU
21	JW	117	ARG
26	QS	45	LEU
26	QS	172	TYR
28	QT	68	THR
30	QU	43	VAL
33	LF	143	GLU
33	LF	217	GLN
34	QW	32	GLN
34	QW	43	ARG
35	RF	59	VAL
36	LG	114	VAL
36	LG	332	ARG
36	LG	339	ARG
37	RG	60	ARG
38	LH	115	HIS
38	LH	120	TYR
38	LH	306	THR
40	LI	93	THR
40	LI	155	THR
42	LJ	46	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	LK	52	GLN
3	QX	65	GLN
3	QX	137	ASN
6	LL	77	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	LL	138	HIS
9	JT	13	HIS
9	JT	114	GLN
10	LM	157	ASN
11	QZ	79	HIS
11	QZ	123	GLN
12	RQ	3	ASN
13	JU	62	GLN
13	JU	119	GLN
14	LN	59	GLN
14	LN	163	GLN
15	RA	39	HIS
15	RA	44	ASN
16	RT	25	GLN
16	RT	32	GLN
16	RT	34	HIS
17	JV	15	GLN
18	LO	43	GLN
24	QQ	58	HIS
24	QQ	134	HIS
26	QS	88	HIS
27	RD	56	ASN
28	QT	49	GLN
28	QT	122	GLN
28	QT	134	GLN
33	LF	217	GLN
34	QW	32	GLN
36	LG	173	GLN
36	LG	198	HIS
37	RG	98	GLN
38	LH	116	ASN
38	LH	160	GLN
39	RH	16	GLN
39	RH	68	GLN
39	RH	104	GLN
40	LI	40	HIS
40	LI	264	GLN

### 5.3.3 RNA

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
25	LD	157/158 (99%)	20 (12%)	1 (0%)
29	LE	120/121 (99%)	9 (7%)	0
5	A	3038/3396 (89%)	390 (12%)	24 (0%)
All	All	3315/3675 (90%)	419 (12%)	25 (0%)

All (419) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	A	26	A
5	A	40	A
5	A	43	A
5	A	49	A
5	A	59	G
5	A	60	A
5	A	65	A
5	A	66	A
5	A	92	G
5	A	109	A
5	A	110	G
5	A	111	C
5	A	116	A
5	A	117	U
5	A	118	U
5	A	121	A
5	A	122	A
5	A	133	U
5	A	135	C
5	A	136	G
5	A	156	G
5	A	157	A
5	A	166	C
5	A	170	G
5	A	187	A
5	A	190	U
5	A	191	U
5	A	200	C
5	A	210	U
5	A	218	G
5	A	219	A
5	A	240	U
5	A	241	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	243	G
5	A	249	U
5	A	252	U
5	A	269	G
5	A	286	U
5	A	295	A
5	A	305	U
5	A	323	A
5	A	329	U
5	A	339	C
5	A	350	C
5	A	376	G
5	A	398	A
5	A	399	A
5	A	401	U
5	A	402	A
5	A	403	C
5	A	421	G
5	A	422	A
5	A	439	C
5	A	440	A
5	A	521	A
5	A	535	G
5	A	545	U
5	A	546	C
5	A	547	G
5	A	548	G
5	A	552	G
5	A	555	U
5	A	557	A
5	A	559	A
5	A	578	A
5	A	579	G
5	A	589	A
5	A	592	A
5	A	604	G
5	A	609	G
5	A	611	A
5	A	612	U
5	A	620	U
5	A	621	A
5	A	622	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	649	A
5	A	660	A
5	A	677	A
5	A	681	U
5	A	690	A
5	A	691	A
5	A	705	A
5	A	712	G
5	A	715	A
5	A	716	A
5	A	766	U
5	A	767	U
5	A	776	U
5	A	777	U
5	A	780	A
5	A	781	G
5	A	785	G
5	A	786	A
5	A	806	A
5	A	817	A
5	A	830	A
5	A	849	C
5	A	861	C
5	A	874	U
5	A	879	U
5	A	896	A
5	A	907	G
5	A	908	G
5	A	914	A
5	A	916	G
5	A	917	A
5	A	921	A
5	A	925	A
5	A	937	G
5	A	944	C
5	A	959	C
5	A	960	U
5	A	979	U
5	A	980	A
5	A	981	U
5	A	995	U
5	A	1001	G

*Continued on next page...*



*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	1002	A
5	A	1010	G
5	A	1017	C
5	A	1033	U
5	A	1037	C
5	A	1047	A
5	A	1049	C
5	A	1064	A
5	A	1065	A
5	A	1072	G
5	A	1081	U
5	A	1094	U
5	A	1095	U
5	A	1096	U
5	A	1097	G
5	A	1098	A
5	A	1103	A
5	A	1104	G
5	A	1117	G
5	A	1131	G
5	A	1153	A
5	A	1159	A
5	A	1180	A
5	A	1181	U
5	A	1192	C
5	A	1196	C
5	A	1201	C
5	A	1208	U
5	A	1209	G
5	A	1221	A
5	A	1222	G
5	A	1295	G
5	A	1307	G
5	A	1308	A
5	A	1309	U
5	A	1330	A
5	A	1331	U
5	A	1348	U
5	A	1349	G
5	A	1351	U
5	A	1352	A
5	A	1356	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	1357	G
5	A	1386	A
5	A	1399	A
5	A	1400	G
5	A	1419	A
5	A	1434	G
5	A	1437	C
5	A	1446	A
5	A	1481	A
5	A	1484	U
5	A	1508	C
5	A	1536	G
5	A	1555	U
5	A	1556	C
5	A	1557	A
5	A	1560	G
5	A	1562	C
5	A	1563	C
5	A	1564	U
5	A	1566	A
5	A	1569	U
5	A	1572	U
5	A	1576	G
5	A	1580	A
5	A	1581	C
5	A	1582	C
5	A	1583	A
5	A	1587	A
5	A	1593	A
5	A	1620	U
5	A	1629	U
5	A	1639	C
5	A	1642	A
5	A	1643	A
5	A	1645	U
5	A	1657	C
5	A	1717	U
5	A	1724	U
5	A	1725	C
5	A	1741	A
5	A	1750	A
5	A	1751	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	1760	A
5	A	1765	U
5	A	1766	G
5	A	1770	G
5	A	1780	G
5	A	1797	A
5	A	1814	A
5	A	1816	A
5	A	1820	U
5	A	1821	U
5	A	1842	A
5	A	1849	C
5	A	1850	A
5	A	1880	U
5	A	1886	A
5	A	1906	G
5	A	1952	G
5	A	2101	C
5	A	2102	U
5	A	2107	A
5	A	2112	U
5	A	2113	A
5	A	2114	C
5	A	2121	G
5	A	2122	G
5	A	2131	A
5	A	2140	U
5	A	2144	A
5	A	2158	A
5	A	2169	G
5	A	2170	U
5	A	2205	U
5	A	2209	U
5	A	2210	G
5	A	2244	A
5	A	2273	G
5	A	2279	A
5	A	2282	U
5	A	2288	G
5	A	2307	G
5	A	2308	C
5	A	2310	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	2313	A
5	A	2314	U
5	A	2315	G
5	A	2334	U
5	A	2335	G
5	A	2336	U
5	A	2373	A
5	A	2374	C
5	A	2375	G
5	A	2385	G
5	A	2388	U
5	A	2393	G
5	A	2397	A
5	A	2402	A
5	A	2403	G
5	A	2404	A
5	A	2411	U
5	A	2418	G
5	A	2435	G
5	A	2513	U
5	A	2514	U
5	A	2522	G
5	A	2523	A
5	A	2531	C
5	A	2533	G
5	A	2537	U
5	A	2538	U
5	A	2539	C
5	A	2540	A
5	A	2541	U
5	A	2542	U
5	A	2543	U
5	A	2549	G
5	A	2552	C
5	A	2561	A
5	A	2569	A
5	A	2570	U
5	A	2571	U
5	A	2572	C
5	A	2573	G
5	A	2585	G
5	A	2593	A

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	2606	G
5	A	2607	G
5	A	2614	G
5	A	2652	U
5	A	2656	A
5	A	2674	A
5	A	2677	G
5	A	2681	U
5	A	2689	A
5	A	2691	A
5	A	2696	A
5	A	2704	A
5	A	2705	A
5	A	2714	G
5	A	2719	U
5	A	2728	G
5	A	2729	U
5	A	2752	U
5	A	2753	G
5	A	2755	C
5	A	2762	A
5	A	2777	G
5	A	2778	G
5	A	2796	G
5	A	2800	G
5	A	2801	A
5	A	2803	A
5	A	2810	C
5	A	2814	G
5	A	2817	A
5	A	2821	C
5	A	2842	U
5	A	2843	U
5	A	2845	A
5	A	2867	C
5	A	2871	G
5	A	2872	A
5	A	2875	U
5	A	2876	C
5	A	2887	A
5	A	2923	U
5	A	2935	U

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	2936	A
5	A	2942	C
5	A	2947	G
5	A	2951	G
5	A	2983	C
5	A	2990	G
5	A	2996	U
5	A	2997	G
5	A	3012	A
5	A	3056	U
5	A	3059	G
5	A	3078	U
5	A	3086	A
5	A	3092	C
5	A	3101	G
5	A	3119	U
5	A	3122	A
5	A	3130	A
5	A	3131	U
5	A	3142	A
5	A	3143	C
5	A	3154	C
5	A	3155	U
5	A	3156	U
5	A	3157	U
5	A	3165	A
5	A	3173	G
5	A	3174	A
5	A	3176	G
5	A	3179	U
5	A	3181	C
5	A	3187	A
5	A	3207	U
5	A	3217	C
5	A	3218	A
5	A	3219	G
5	A	3229	G
5	A	3243	A
5	A	3245	A
5	A	3247	G
5	A	3259	U
5	A	3260	G

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	A	3263	G
5	A	3270	U
5	A	3276	G
5	A	3279	A
5	A	3281	U
5	A	3287	U
5	A	3289	G
5	A	3294	A
5	A	3304	U
5	A	3316	A
5	A	3318	G
5	A	3319	U
5	A	3341	U
5	A	3345	G
5	A	3352	U
5	A	3353	G
5	A	3355	U
5	A	3369	G
5	A	3378	C
5	A	3389	U
5	A	3390	G
25	LD	23	U
25	LD	34	U
25	LD	35	C
25	LD	59	A
25	LD	62	C
25	LD	63	G
25	LD	80	A
25	LD	81	U
25	LD	84	C
25	LD	86	U
25	LD	87	G
25	LD	90	U
25	LD	95	G
25	LD	104	A
25	LD	106	C
25	LD	111	A
25	LD	113	U
25	LD	125	U
25	LD	126	A
25	LD	152	G
29	LE	42	A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
29	LE	51	A
29	LE	54	U
29	LE	55	A
29	LE	65	G
29	LE	76	A
29	LE	102	A
29	LE	112	G
29	LE	121	U

All (25) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	A	169	U
5	A	547	G
5	A	916	G
5	A	979	U
5	A	1064	A
5	A	1097	G
5	A	1103	A
5	A	1307	G
5	A	1355	A
5	A	1554	U
5	A	1562	C
5	A	1815	U
5	A	2101	C
5	A	2112	U
5	A	2209	U
5	A	2512	C
5	A	2537	U
5	A	2541	U
5	A	3121	U
5	A	3218	A
5	A	3228	C
5	A	3269	U
5	A	3317	U
5	A	3351	U
25	LD	85	G

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

There are no non-standard protein/DNA/RNA residues in this entry.



## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 160 ligands modelled in this entry, 158 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
47	SPD	A	3504	-	9,9,9	0.27	0	8,8,8	0.32	0
46	SPM	A	3468	-	13,13,13	0.36	0	12,12,12	0.85	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
47	SPD	A	3504	-	-	0/7/7/7	-
46	SPM	A	3468	-	-	1/11/11/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	3468	SPM	C12-C11-N10-C9

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	A	3504	SPD	1	0

## 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.

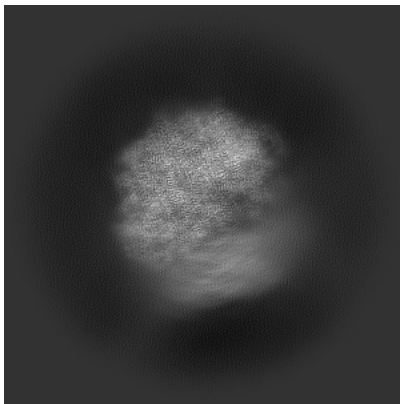
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17552. These allow visual inspection of the internal detail of the map and identification of artifacts.

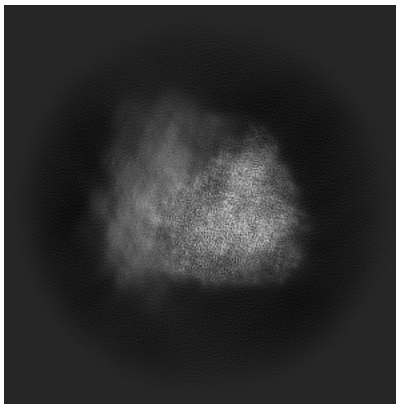
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

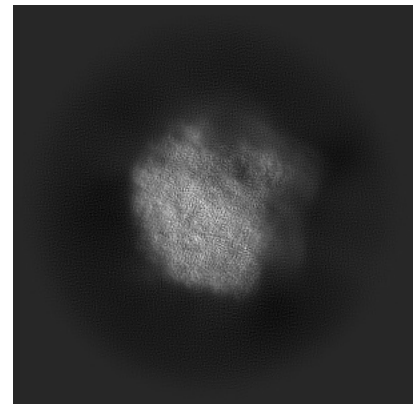
#### 6.1.1 Primary map



X

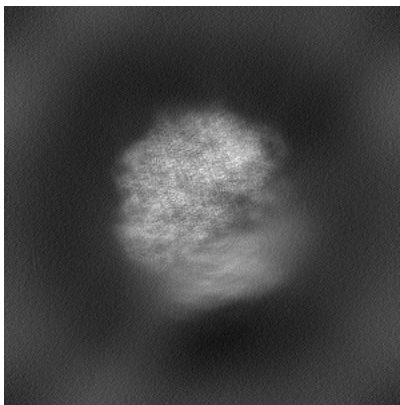


Y

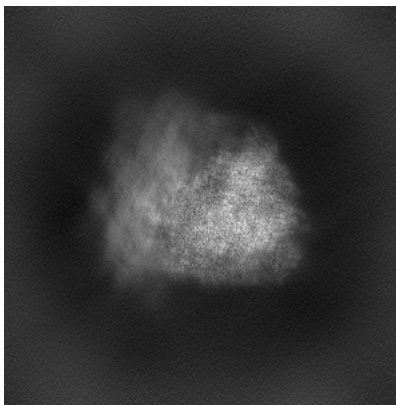


Z

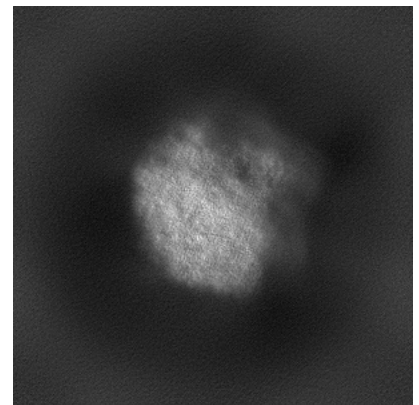
#### 6.1.2 Raw map



X



Y

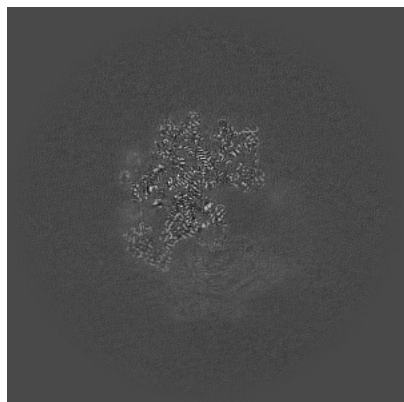


Z

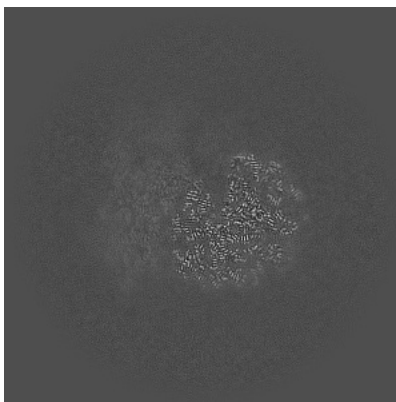
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

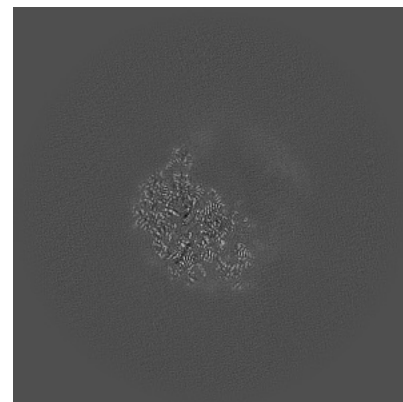
### 6.2.1 Primary map



X Index: 300

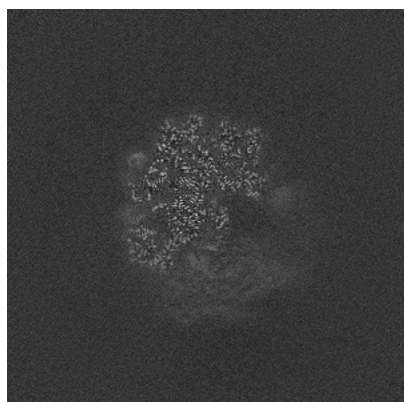


Y Index: 300

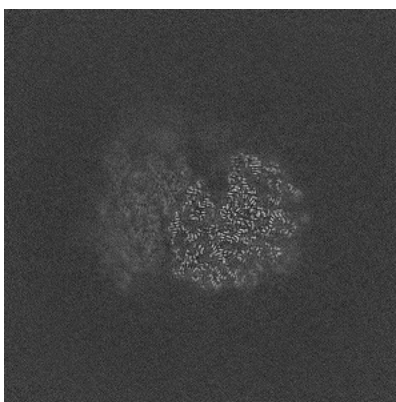


Z Index: 300

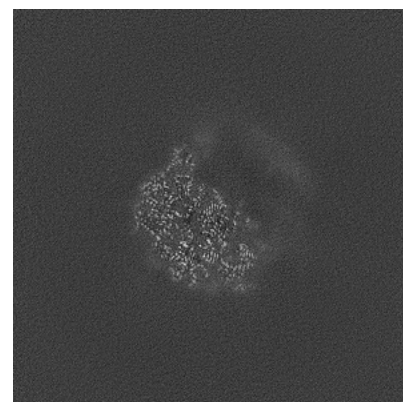
### 6.2.2 Raw map



X Index: 300



Y Index: 300

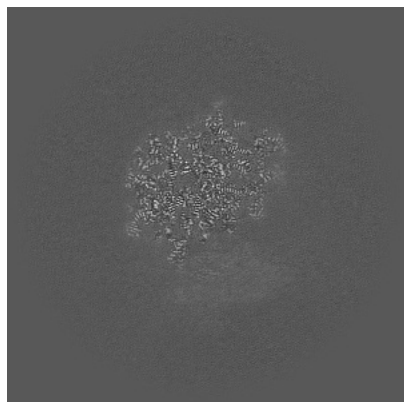


Z Index: 300

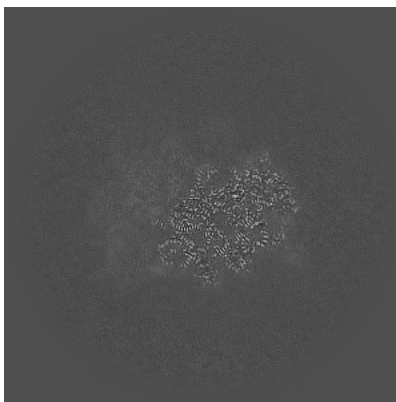
The images above show central slices of the map in three orthogonal directions.

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

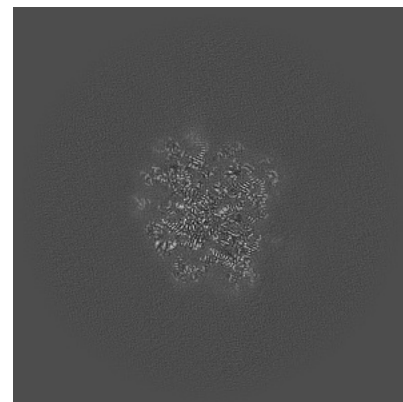
### 6.3.1 Primary map



X Index: 261

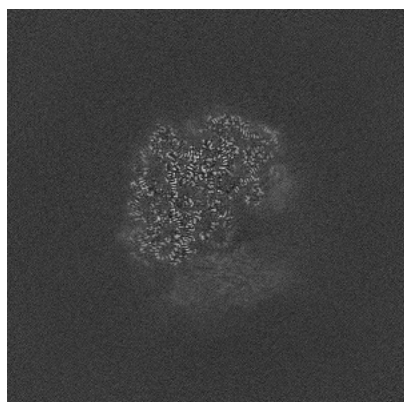


Y Index: 273

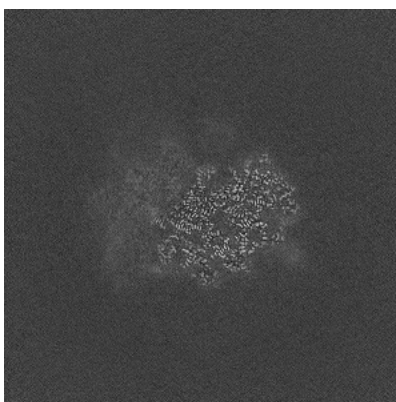


Z Index: 360

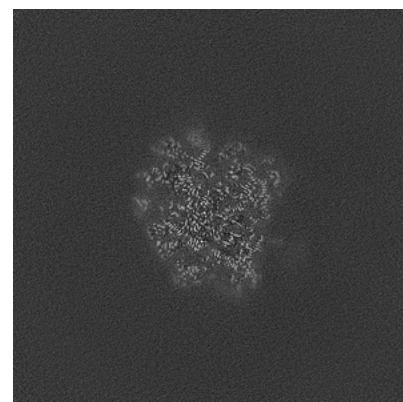
### 6.3.2 Raw map



X Index: 276



Y Index: 276



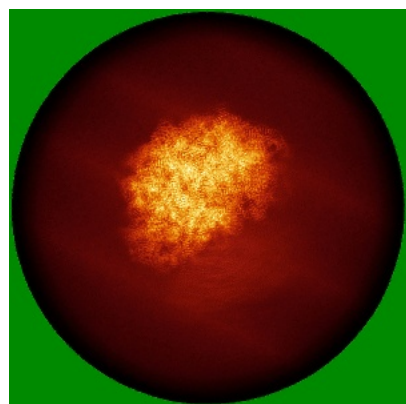
Z Index: 360

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

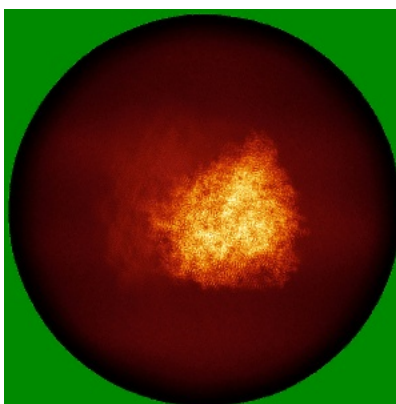


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

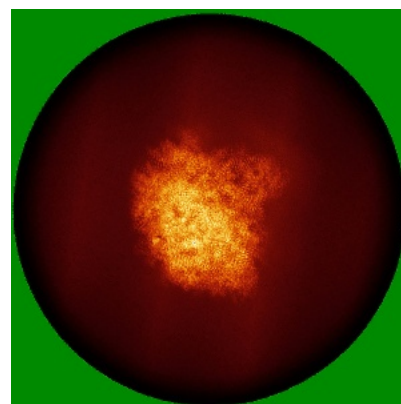
### 6.4.1 Primary map



X

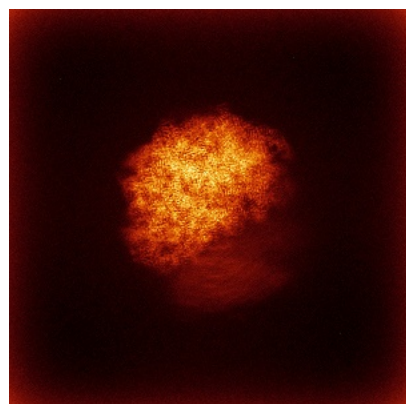


Y

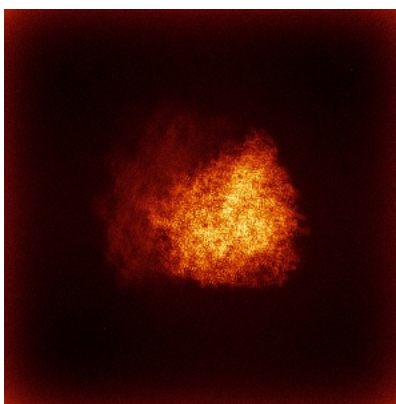


Z

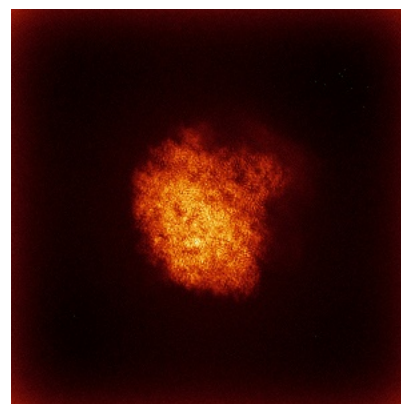
### 6.4.2 Raw map



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 0.3. 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.

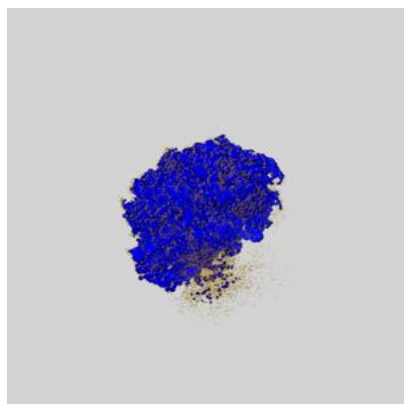
## 6.6 Mask visualisation [i](#)

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

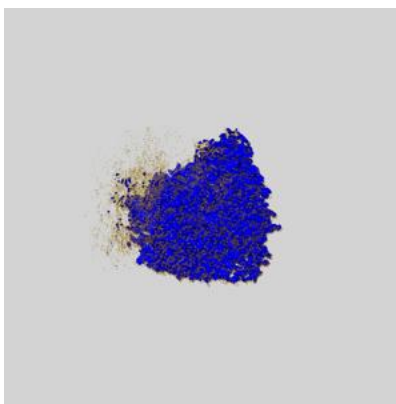
A mask typically either:

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

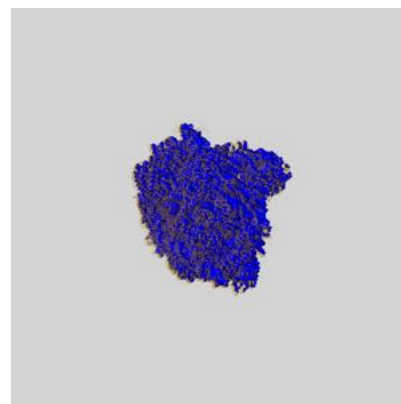
### 6.6.1 emd\_17552\_msk\_1.map [i](#)



X



Y



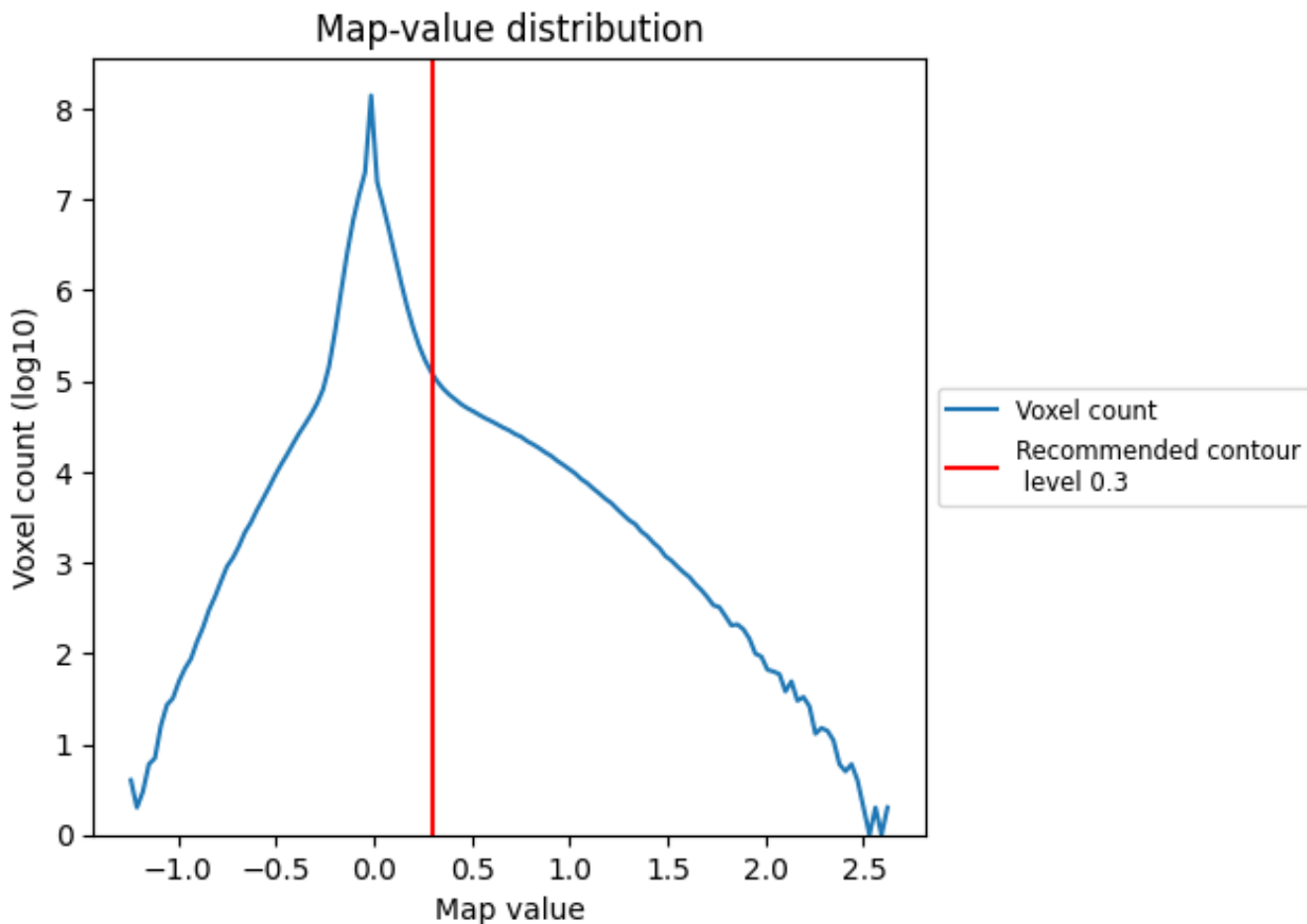
Z



## 7 Map analysis [i](#)

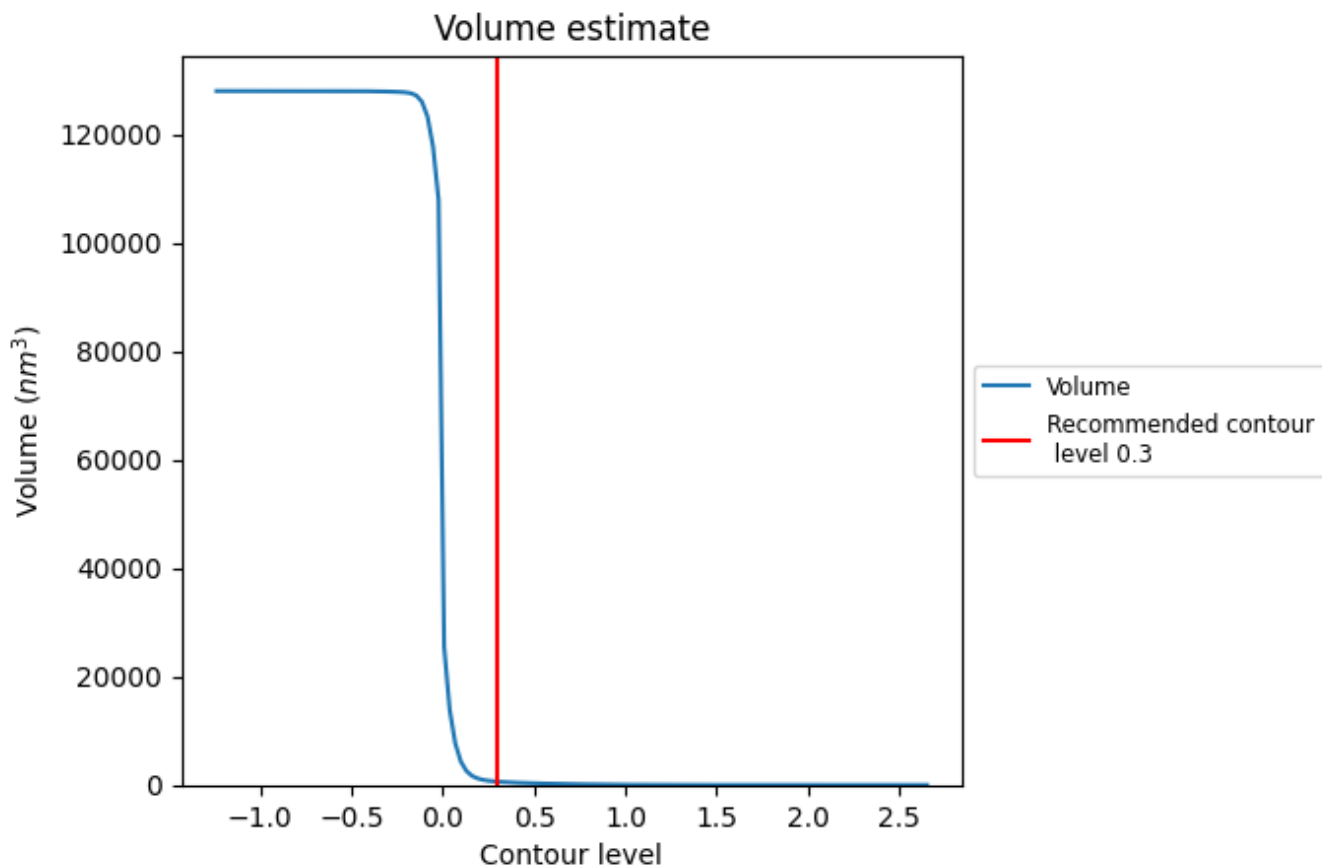
This section contains the results of statistical analysis of the map.

### 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.

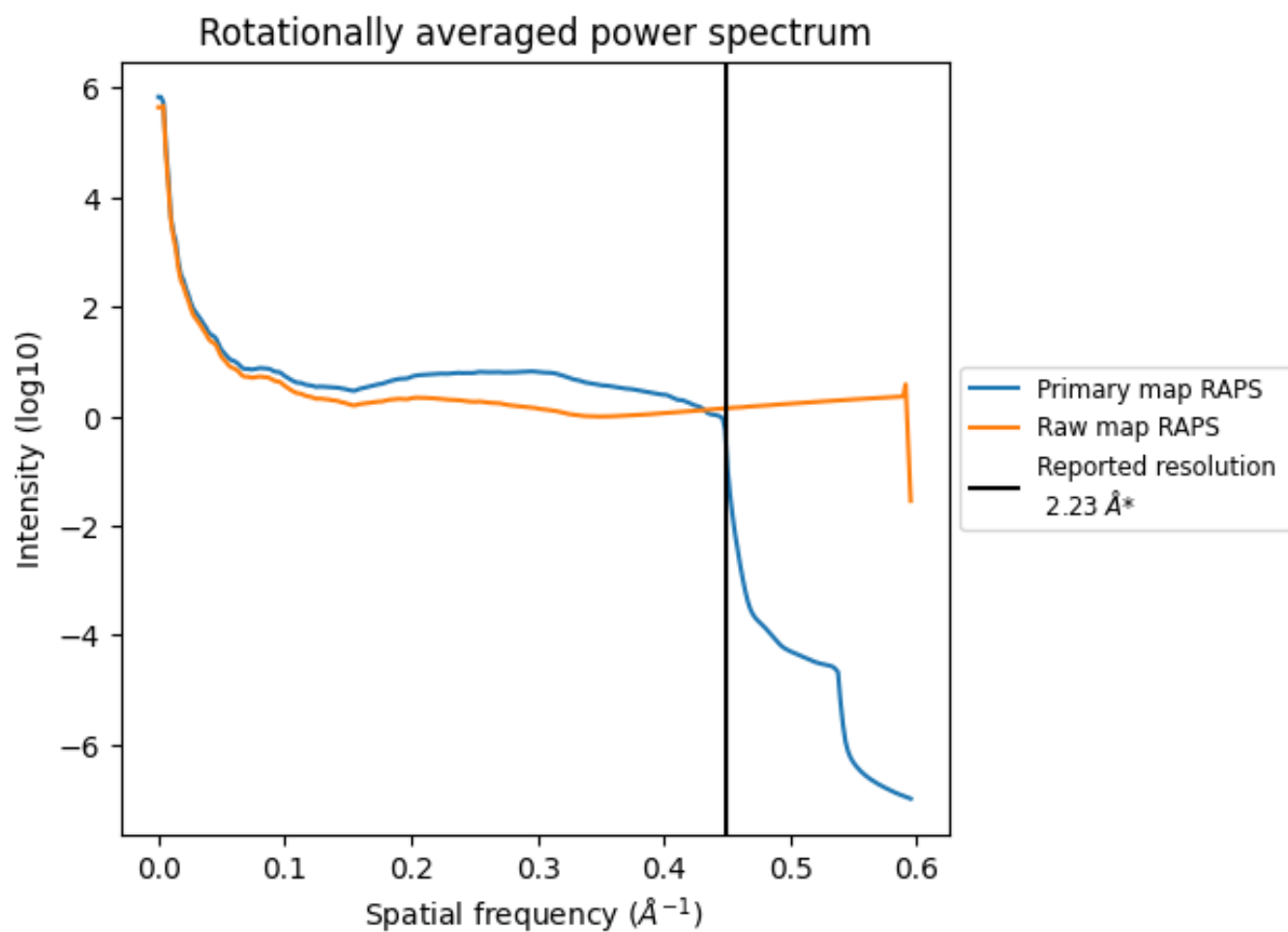
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is  $610 \text{ nm}^3$ ; this corresponds to an approximate mass of 551 kDa.

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

### 7.3 Rotationally averaged power spectrum i

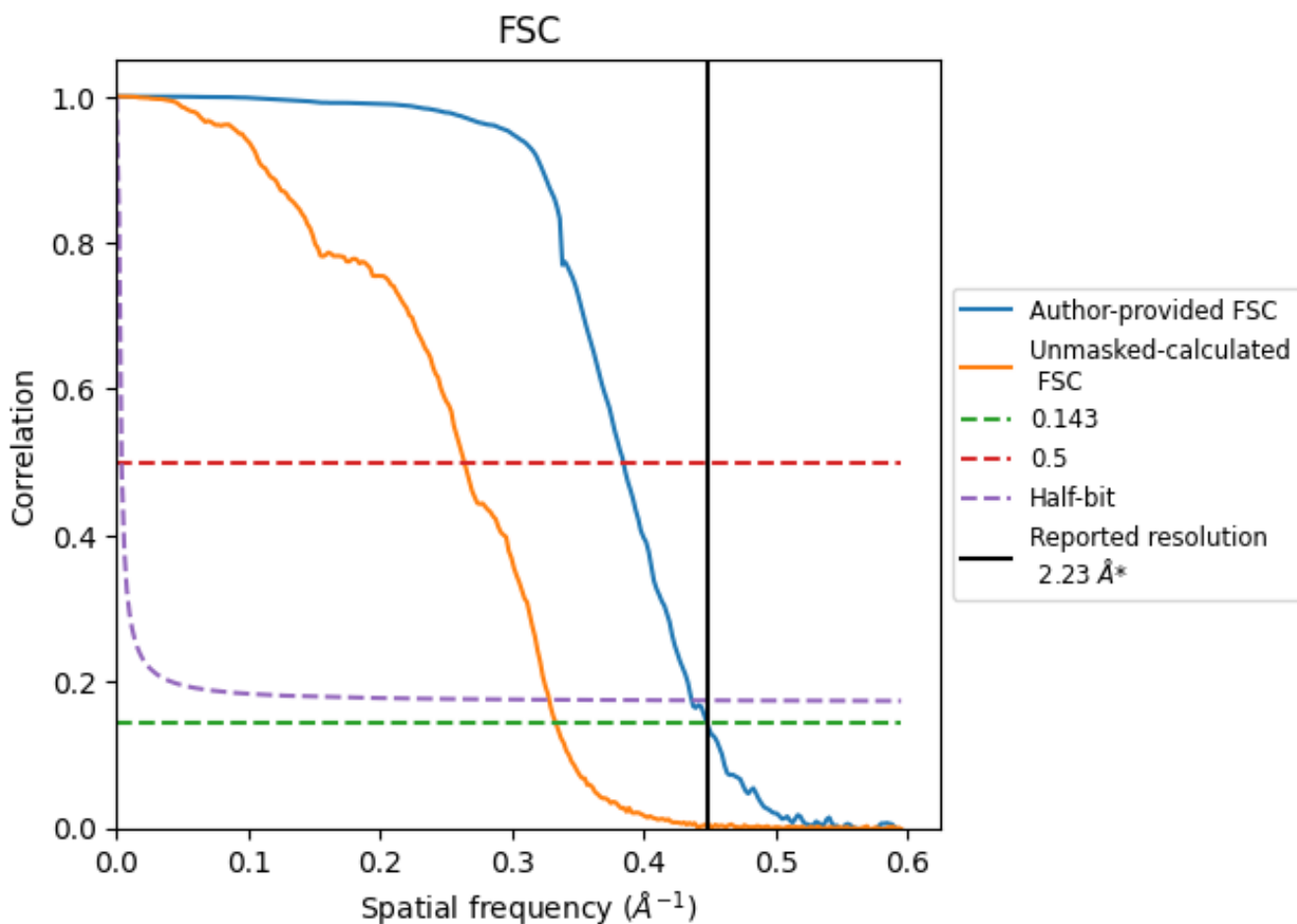


\*Reported resolution corresponds to spatial frequency of 0.448 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.448 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

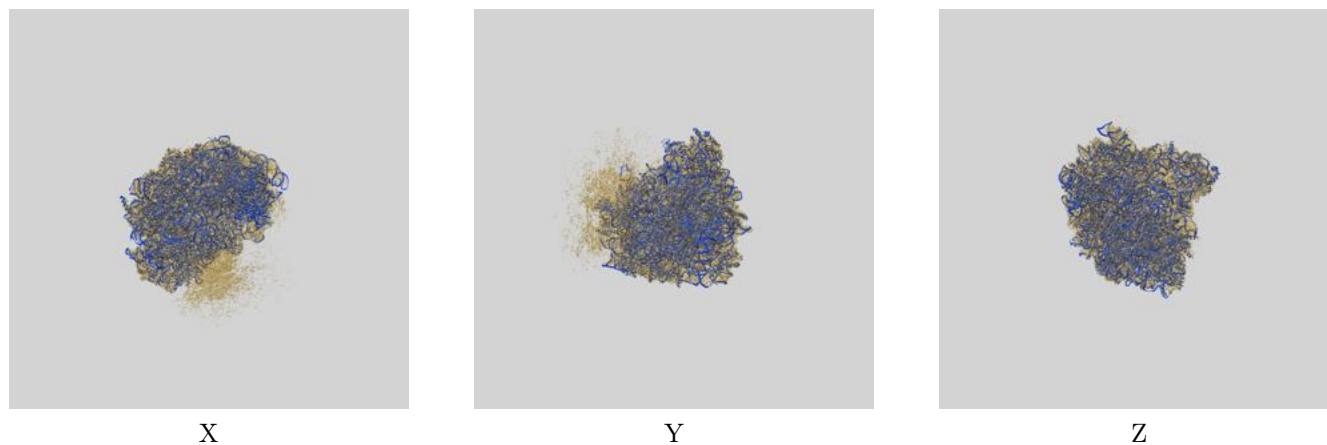
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.23	-	-
Author-provided FSC curve	2.23	2.60	2.29
Unmasked-calculated*	3.00	3.79	3.05

\*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 3.00 differs from the reported value 2.23 by more than 10 %

## 9 Map-model fit [i](#)

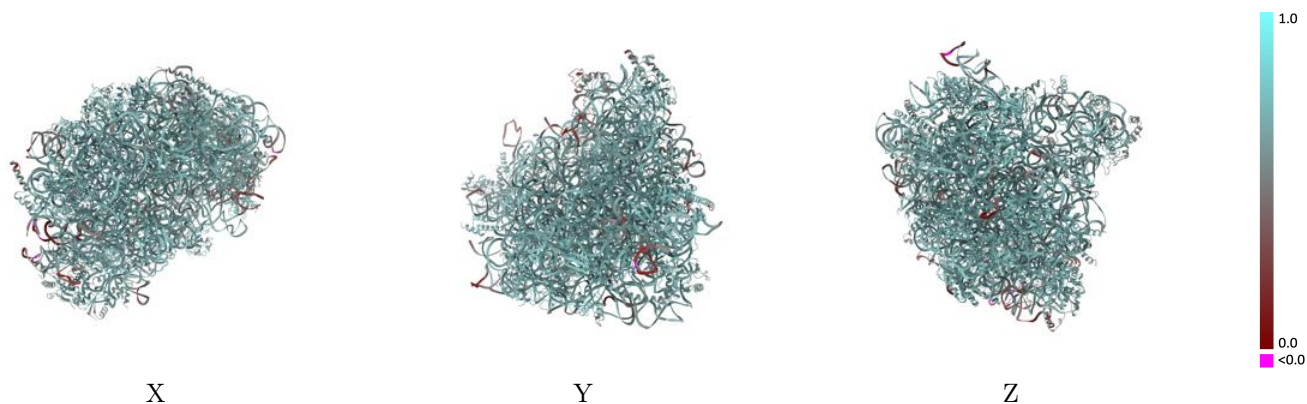
This section contains information regarding the fit between EMDB map EMD-17552 and PDB model 8P8U. Per-residue inclusion information can be found in section 3 on page 15.

### 9.1 Map-model overlay [i](#)



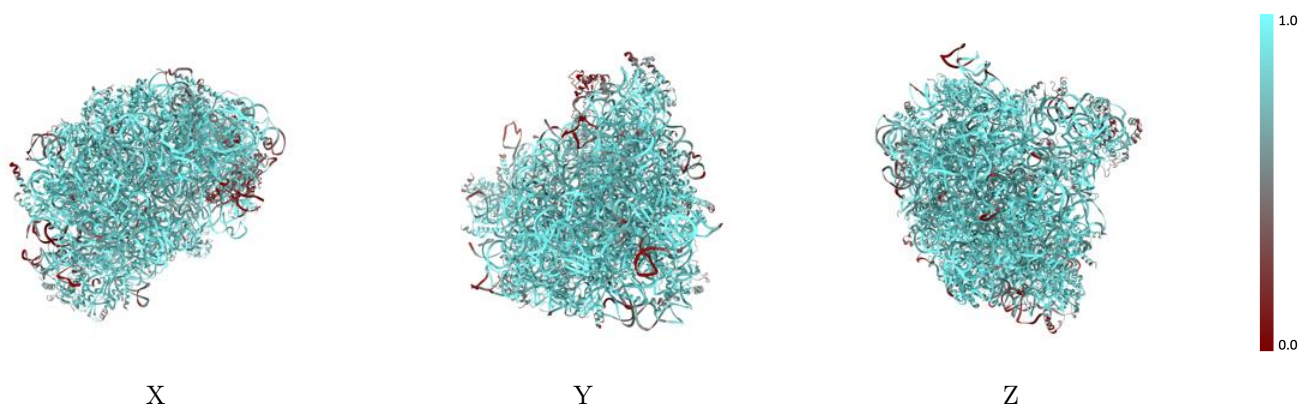
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



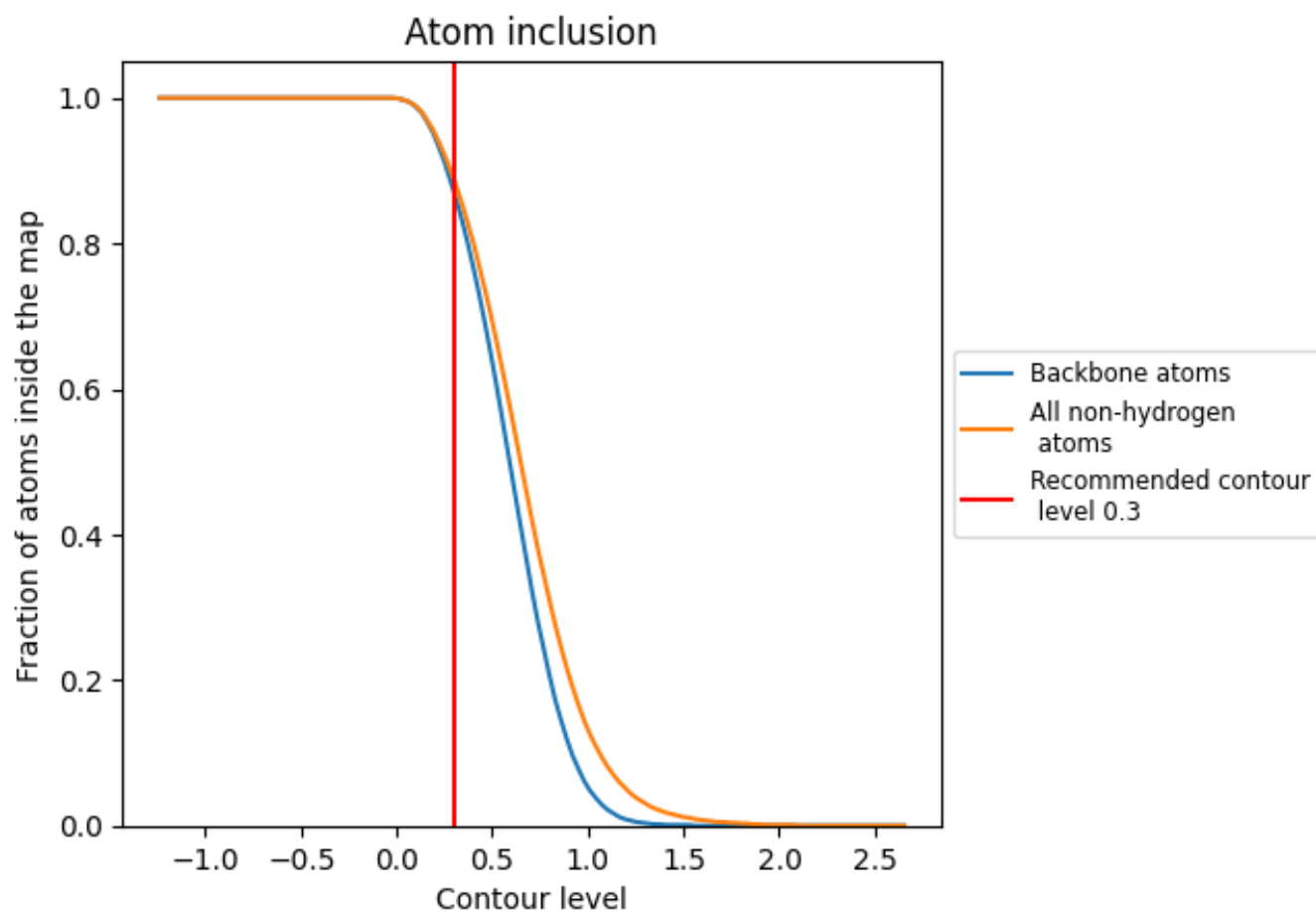
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.3).

## 9.4 Atom inclusion [i](#)









































































At the recommended contour level, 87% of all backbone atoms, 89% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8870	 0.6530
2	 0.9540	 0.6960
A	 0.9060	 0.6490
JT	 0.8660	 0.6550
JU	 0.8730	 0.6610
JV	 0.9780	 0.7020
JW	 0.9160	 0.6780
LD	 0.9400	 0.6640
LE	 0.9330	 0.6560
LF	 0.9430	 0.6920
LG	 0.8990	 0.6770
LH	 0.9090	 0.6760
LI	 0.7250	 0.6020
LJ	 0.7680	 0.6210
LK	 0.9090	 0.6770
LL	 0.8110	 0.6270
LM	 0.8260	 0.6410
LN	 0.8290	 0.6540
LO	 0.4170	 0.5220
QO	 0.9390	 0.6950
QP	 0.9440	 0.6870
QQ	 0.9150	 0.6820
QS	 0.9150	 0.6780
QT	 0.8560	 0.6490
QU	 0.4990	 0.5740
QV	 0.9050	 0.6790
QW	 0.8580	 0.6680
QX	 0.8910	 0.6620
QY	 0.9030	 0.6740
QZ	 0.7090	 0.6000
RA	 0.9200	 0.6790
RB	 0.8660	 0.6310
RC	 0.7790	 0.6250
RD	 0.9090	 0.6750
RE	 0.9390	 0.6930



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
RF	 0.9600	 0.6940
RG	 0.9070	 0.6800
RH	 0.8760	 0.6590
RI	 0.8230	 0.6230
RJ	 0.9720	 0.7070
RM	 0.5740	 0.5640
RO	 0.9000	 0.6640
RQ	 0.8280	 0.6490
RT	 0.8690	 0.6700