



## wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:46 PM UTC

PDB ID : 3JCS / pdb\_00003jcs  
EMDB ID : EMD-6583  
Title : 2.8 Angstrom cryo-EM structure of the large ribosomal subunit from the eukaryotic parasite Leishmania  
Authors : Shalev-Benami, M.; Zhang, Y.; Matzov, D.; Halfon, Y.; Zackay, A.; Rozenberg, H.; Zimmerman, E.; Bashan, A.; Jaffe, C.L.; Yonath, A.; Skiniotis, G.  
Deposited on : 2016-01-21  
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary 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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

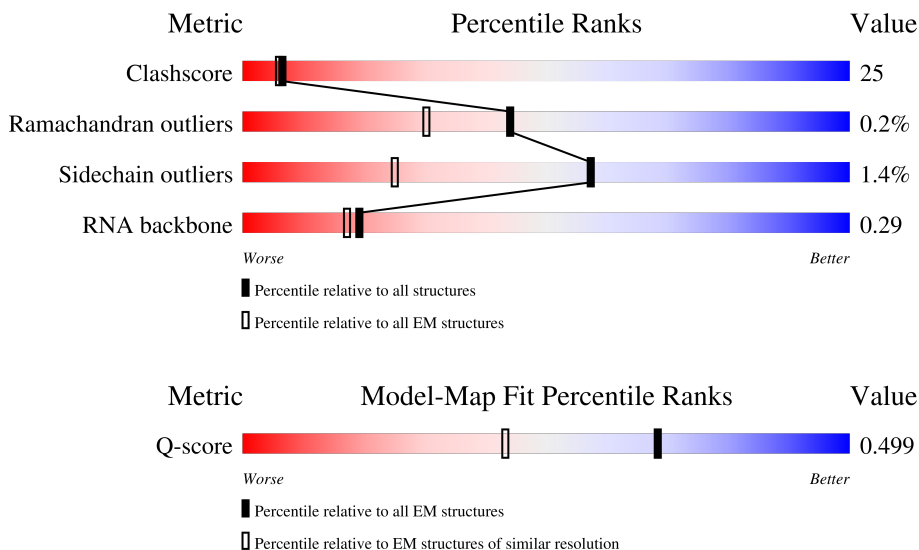
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 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 2.80 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	11806 ( 2.30 - 3.30 )

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	1	1782	
2	2	1527	
3	3	213	

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Mol	Chain	Length	Quality of chain
4	4	183	
5	5	133	
6	6	76	
7	7	171	
8	8	121	
9	A	260	
10	B	419	
11	C	373	
12	D	188	
13	E	190	
14	F	195	
15	G	348	
16	H	222	
17	I	220	
18	J	139	
19	K	233	
20	L	145	
21	M	204	
22	N	213	
23	O	305	
24	P	198	
25	Q	245	
26	R	179	
27	S	159	
28	T	166	

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Mol	Chain	Length	Quality of chain
29	U	129	
30	V	145	
31	W	143	
32	X	124	
33	Y	134	
34	Z	147	
35	a	127	
36	b	70	
37	c	252	
38	d	104	
39	e	183	
40	f	133	
41	g	144	
42	h	168	
43	i	105	
44	j	83	
45	k	83	
46	l	51	
47	m	92	
48	n	106	

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
1	OMU	1	36	-	-	X	-
1	OMG	1	959	-	-	X	-
2	OMU	2	1078	-	-	X	-

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
2	OMG	2	1079	-	-	X	-
2	OMG	2	1254	-	-	X	-
2	OMC	2	1318	-	-	X	-
2	OMC	2	443	-	-	X	-
2	A2M	2	527	-	-	X	-
2	OMU	2	667	-	-	X	-
2	OMG	2	71	-	-	X	-
7	OMU	7	7	-	-	X	-

## 2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 117257 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 26S alpha ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	1554	33313	14886	6081	10792	1554	0	0

- Molecule 2 is a RNA chain called 26S delta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	1119	23926	10702	4308	7797	1119	0	0

- Molecule 3 is a RNA chain called 26S gamma ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	3	184	3893	1740	662	1307	184	0	0

- Molecule 4 is a RNA chain called 26S delta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	4	149	3177	1418	570	1040	149	0	0

- Molecule 5 is a RNA chain called 26S epsilon ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	5	80	1708	763	310	555	80	0	0

- Molecule 6 is a RNA chain called 26S zeta ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	6	61	1288	577	225	425	61	0	0

- Molecule 7 is a RNA chain called 5.8S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	7	154	3280	1469	584	1074	153	0	0

- Molecule 8 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	8	119	2531	1132	450	830	119	0	0

- Molecule 9 is a protein called ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	A	245	1859	1158	384	307	10	2	0

- Molecule 10 is a protein called ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	B	396	3020	1908	592	508	12	2	0

- Molecule 11 is a protein called ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	301	2237	1413	428	384	12	1	0

- Molecule 12 is a protein called ribosomal protein L5.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	D	161	799	476	161	162	0	0

- Molecule 13 is a protein called ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	E	190	1509	953	276	272	8	0	0

- Molecule 14 is a protein called ribosomal protein L6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	137	Total	C	N	O	S	1	0
			1002	641	192	167	2		

- Molecule 15 is a protein called ribosomal protein L8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	226	Total	C	N	O	S	1	0
			1772	1113	353	299	7		

- Molecule 16 is a protein called ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	202	Total	C	N	O	S	0	0
			1596	1019	307	263	7		

- Molecule 17 is a protein called ribosomal protein L13e.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	132	Total	C	N	O	S	0	0
			1061	666	221	169	5		

- Molecule 18 is a protein called ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	128	Total	C	N	O	S	0	0
			924	588	171	160	5		

- Molecule 19 is a protein called ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	156	Total	C	N	O	S	0	0
			1061	661	212	184	4		

- Molecule 20 is a protein called ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	144	Total	C	N	O	S	0	0
			1096	691	223	177	5		

- Molecule 21 is a protein called ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	M	203	1714	1080	362	264	8	0	0

- Molecule 22 is a protein called ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	N	213	1714	1077	340	281	16	0	0

- Molecule 23 is a protein called ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	O	235	1557	986	300	268	3	0	0

- Molecule 24 is a protein called ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	P	195	1494	942	299	247	6	1	0

- Molecule 25 is a protein called ribosomal protein L19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	Q	156	1162	730	243	186	3	0	0

- Molecule 26 is a protein called ribosomal protein L20e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	R	131	1019	651	197	167	4	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	158	ILE	LEU	variant	UNP E9BRT7

- Molecule 27 is a protein called ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	S	149	1112	704	218	187	3	2	0

- Molecule 28 is a protein called ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	T	154	1221	763	241	206	11	2	0

- Molecule 29 is a protein called ribosomal protein L22e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
29	U	100	541	331	101	109	0	0

- Molecule 30 is a protein called ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	V	118	892	566	171	153	2	0	0

- Molecule 31 is a protein called ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	W	117	896	562	187	144	3	1	0

- Molecule 32 is a protein called ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	X	64	508	333	96	76	3	0	0

- Molecule 33 is a protein called ribosomal protein L27e.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
33	Y	132	914	589	174	151	0	0

- Molecule 34 is a protein called ribosomal protein L28e.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Z	79	Total	C	N	O	S	0	0
			538	329	111	95	3		

- Molecule 35 is a protein called ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	a	124	Total	C	N	O	S	0	0
			982	613	203	163	3		

- Molecule 36 is a protein called ribosomal protein L29e.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	b	65	Total	C	N	O	S	0	0
			503	309	113	80	1		

- Molecule 37 is a protein called ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	c	222	Total	C	N	O	S	0	0
			1732	1105	327	289	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	49	ALA	GLY	variant	UNP E9BI29

- Molecule 38 is a protein called ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	d	75	Total	C	N	O	S	0	0
			518	325	93	97	3		

- Molecule 39 is a protein called ribosomal protein L31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	e	112	Total	C	N	O	S	1	0
			824	531	155	136	2		

- Molecule 40 is a protein called ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	f	126	982	616	195	167	4	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
f	105	LYS	THR	variant	UNP E9BFJ5

- Molecule 41 is a protein called ribosomal protein L33e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	g	125	983	612	205	161	5	0	0

- Molecule 42 is a protein called ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	h	109	856	529	182	140	5	0	0

- Molecule 43 is a protein called ribosomal protein L36e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
43	i	63	494	316	100	76	2	1	0

- Molecule 44 is a protein called ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	j	78	639	385	149	99	6	0	0

- Molecule 45 is a protein called ribosomal protein L38e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	k	58	373	234	71	66	2	0	0

- Molecule 46 is a protein called ribosomal protein L39e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	l	50	457	294	98	64	1	1	0

- Molecule 47 is a protein called ribosomal protein L43e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	m	90	668	414	135	113	6	0	0

- Molecule 48 is a protein called ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	n	86	659	418	129	110	2	0	0

- Molecule 49 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
49	1	51	Total	Mg	0
			51	51	
49	2	25	Total	Mg	0
			25	25	
49	3	3	Total	Mg	0
			3	3	
49	4	2	Total	Mg	0
			2	2	
49	5	4	Total	Mg	0
			4	4	
49	7	9	Total	Mg	0
			9	9	
49	C	1	Total	Mg	0
			1	1	
49	K	1	Total	Mg	0
			1	1	
49	M	3	Total	Mg	0
			3	3	
49	V	1	Total	Mg	0
			1	1	
49	a	1	Total	Mg	0
			1	1	
49	f	2	Total	Mg	0
			2	2	

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Mol	Chain	Residues	Atoms		AltConf
49	g	1	Total 1	Mg 1	0
49	h	1	Total 1	Mg 1	0
49	j	4	Total 4	Mg 4	0

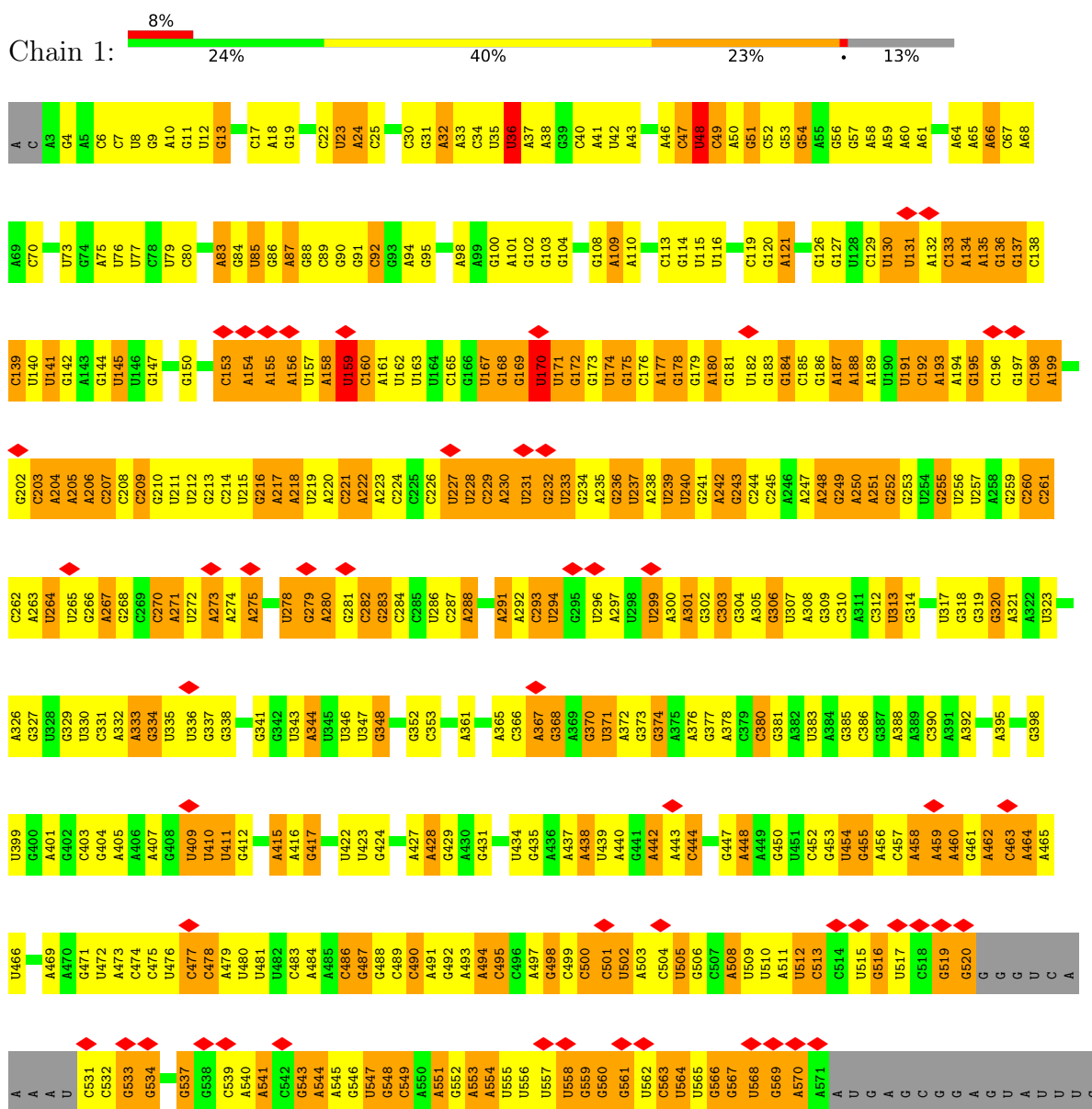
- Molecule 50 is water.

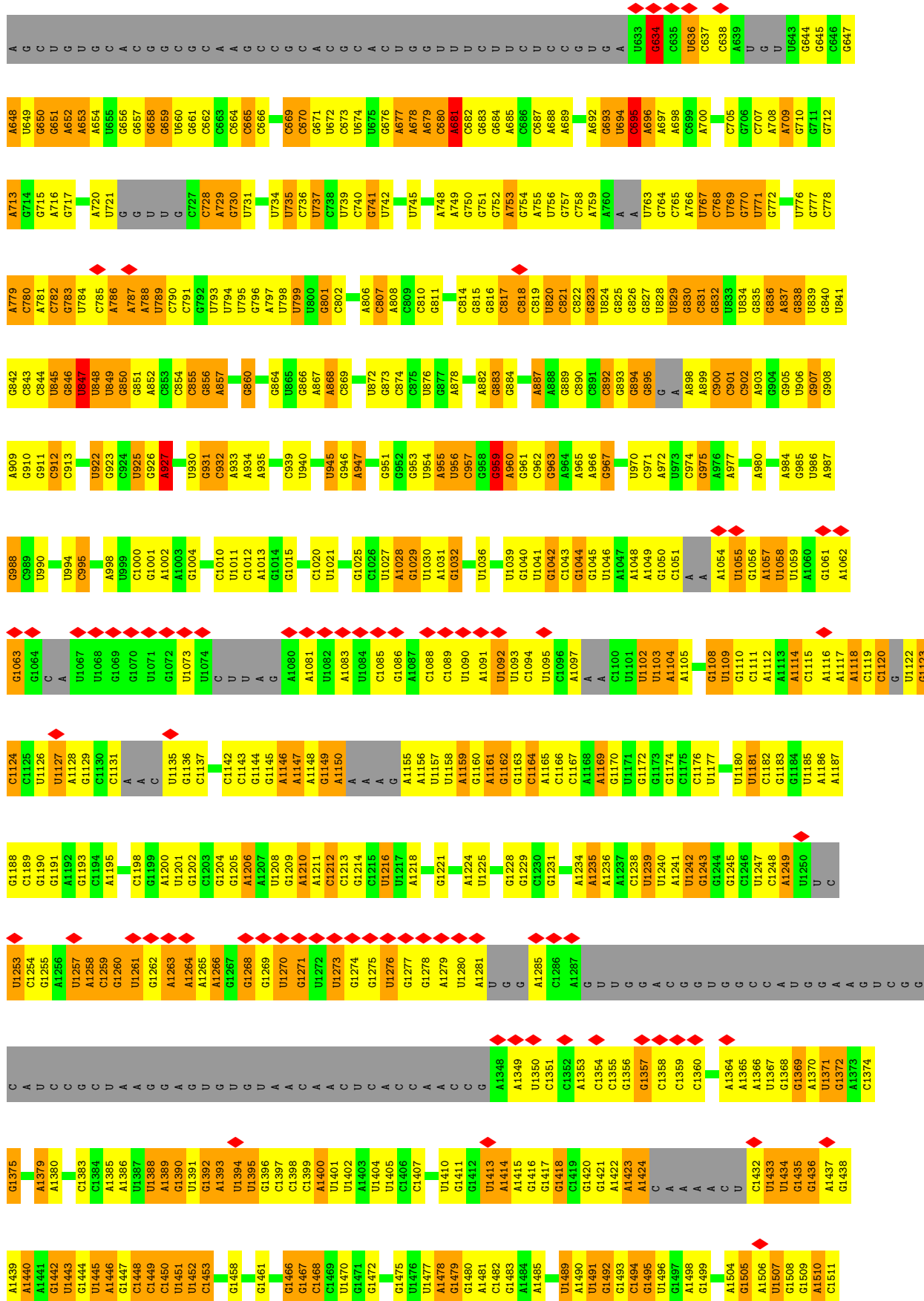
Mol	Chain	Residues	Atoms		AltConf
50	1	72	Total 72	O 72	0
50	2	40	Total 40	O 40	0
50	4	4	Total 4	O 4	0
50	5	4	Total 4	O 4	0
50	7	16	Total 16	O 16	0
50	8	1	Total 1	O 1	0
50	A	2	Total 2	O 2	0
50	G	1	Total 1	O 1	0
50	M	2	Total 2	O 2	0
50	i	1	Total 1	O 1	0
50	j	1	Total 1	O 1	0

### 3 Residue-property plots

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

- Molecule 1: 26S alpha ribosomal RNA



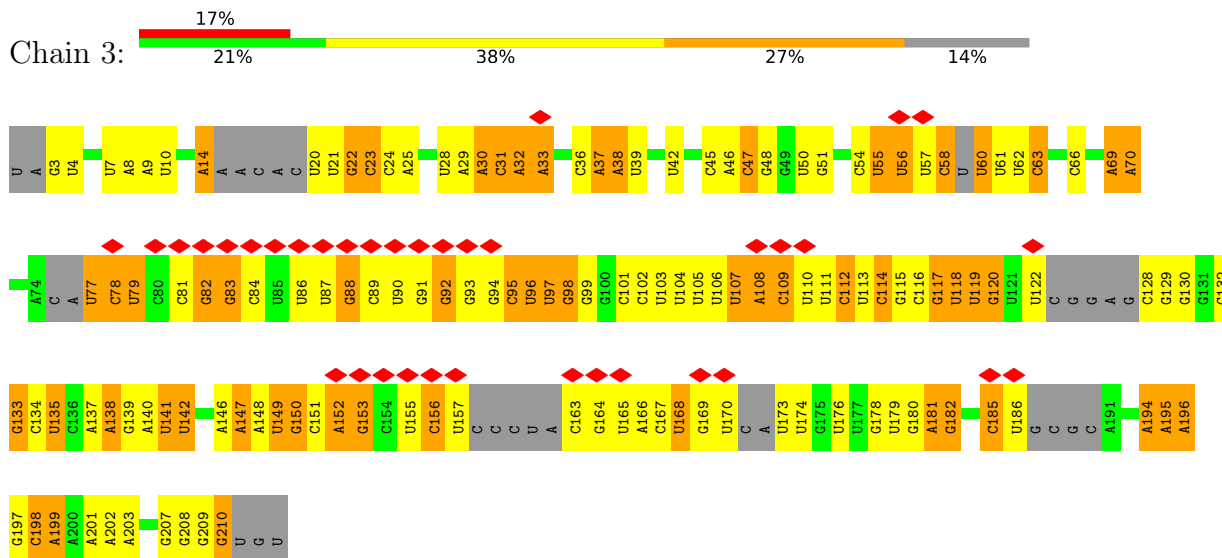




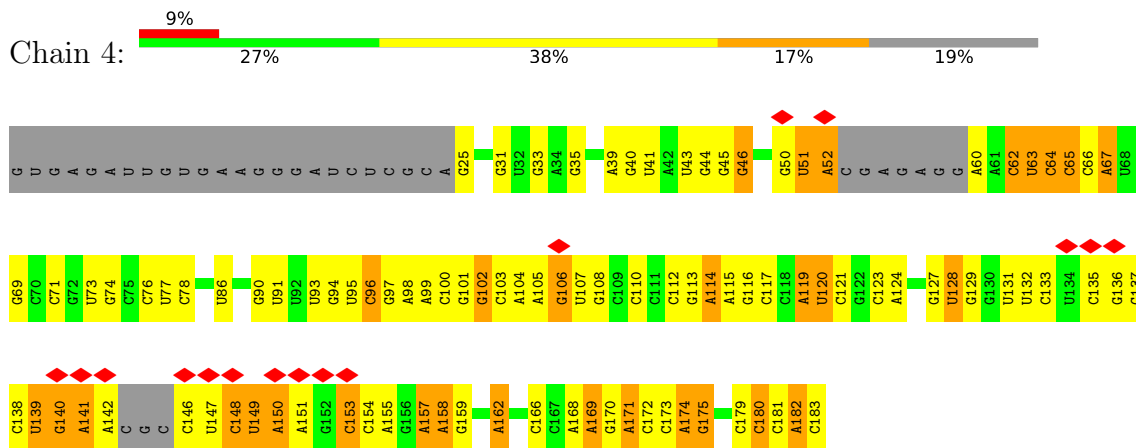


G U A G A G U A C U U G G G U A C A C G C U U C C A U U C A C C

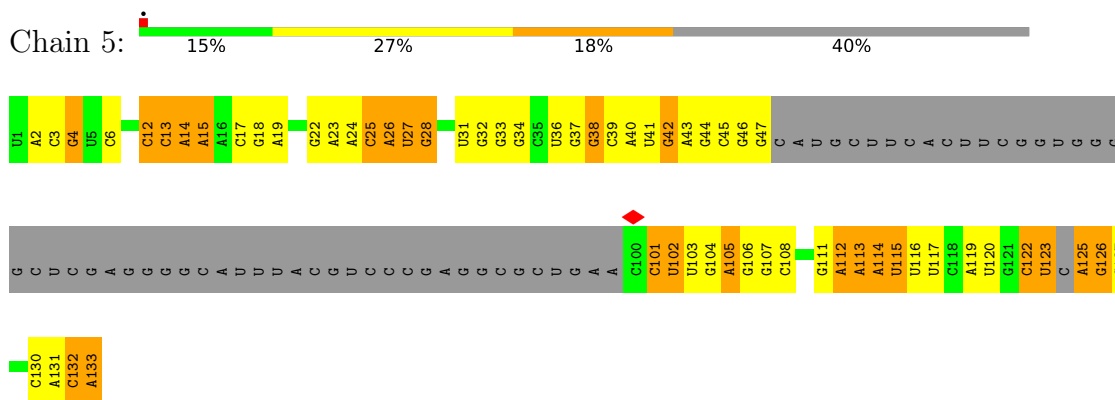
• Molecule 3: 26S gamma ribosomal RNA



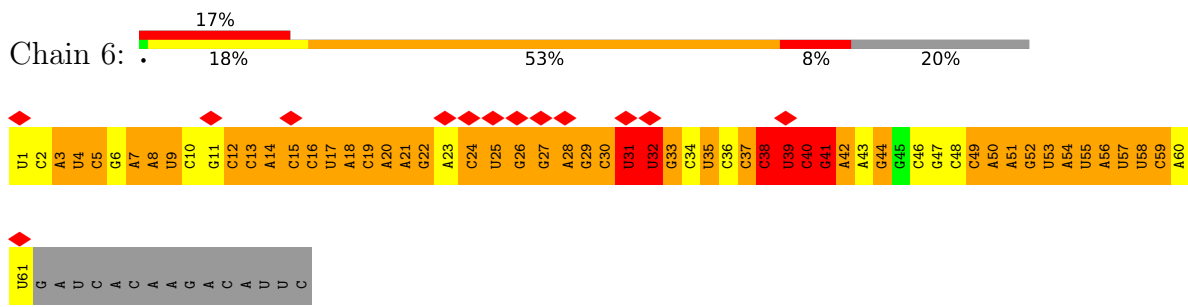
• Molecule 4: 26S delta ribosomal RNA



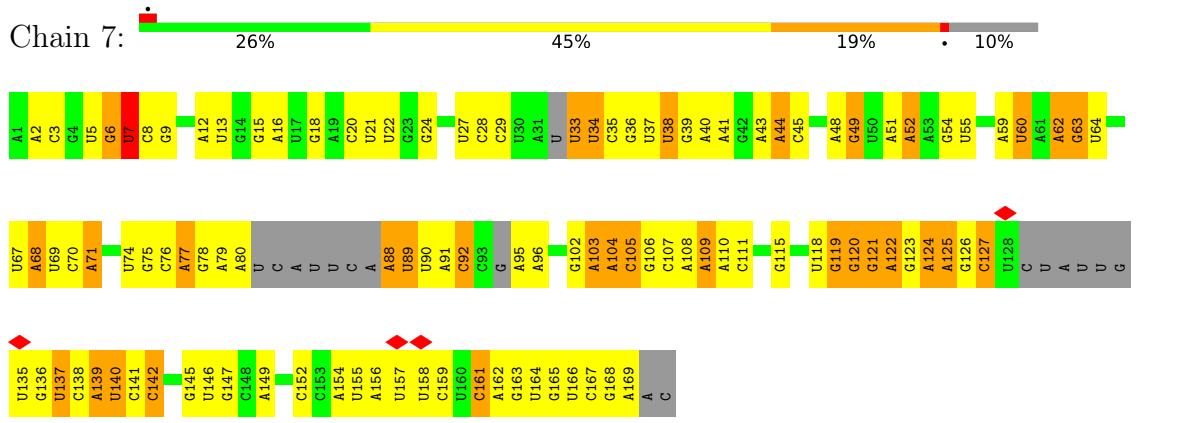
• Molecule 5: 26S epsilon ribosomal RNA



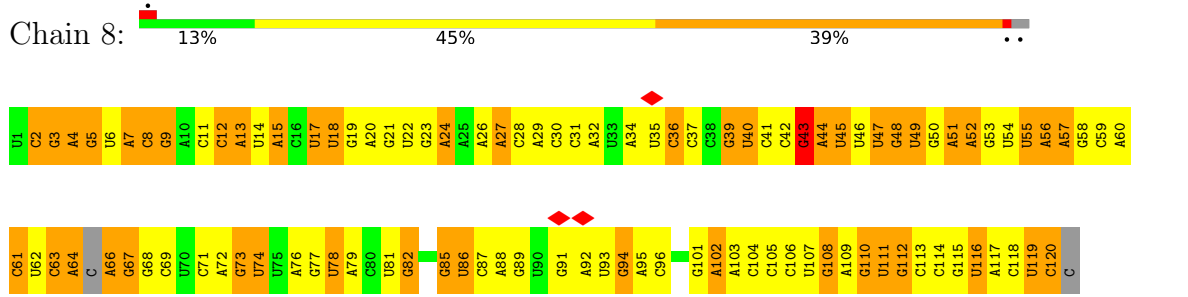
• Molecule 6: 26S zeta ribosomal RNA



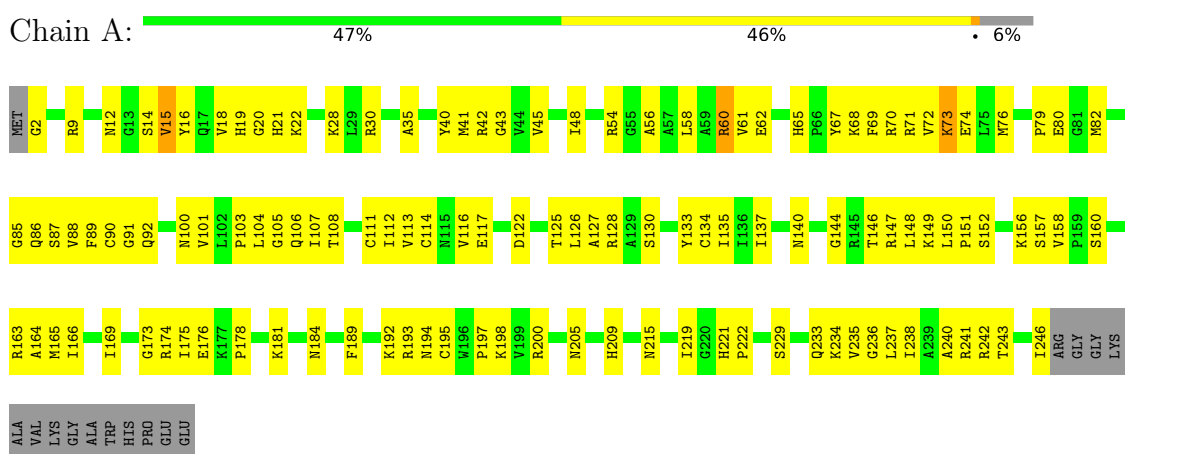
• Molecule 7: 5.8S ribosomal RNA



• Molecule 8: 5S ribosomal RNA

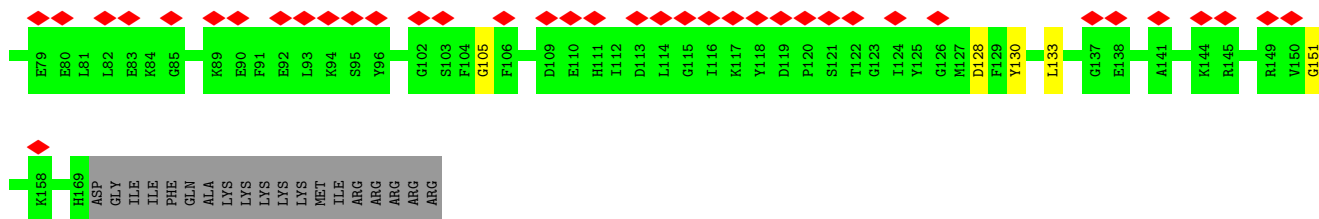


• Molecule 9: ribosomal protein L2

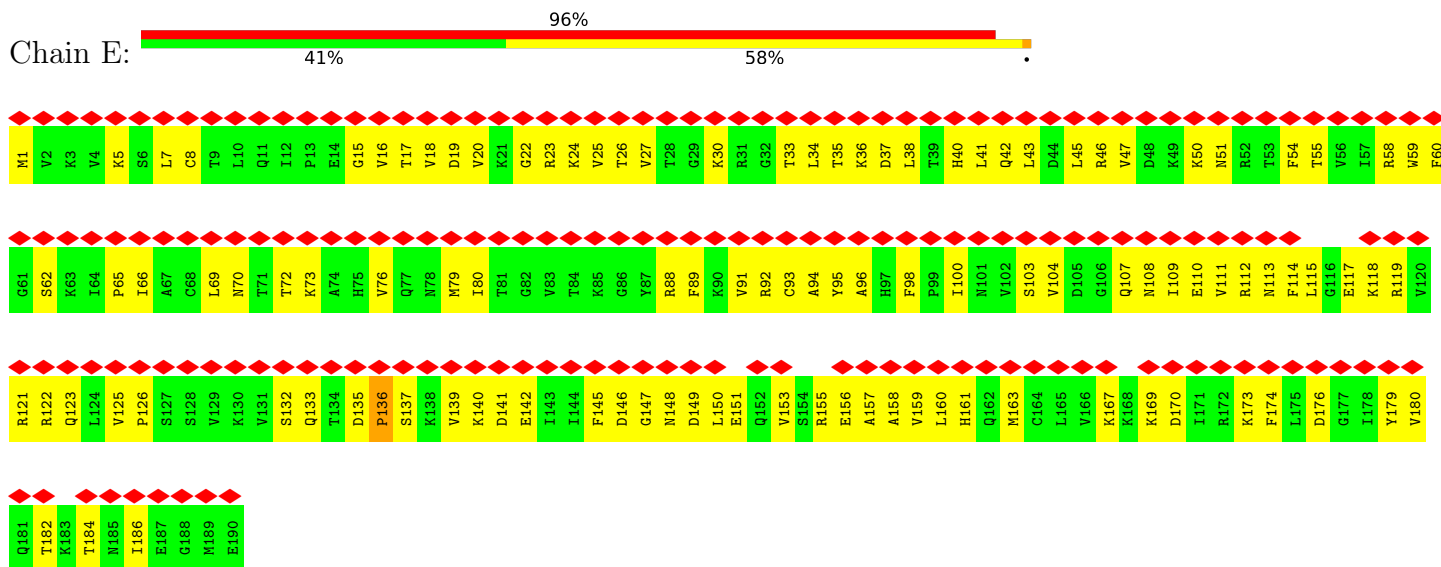


• Molecule 10: ribosomal protein L3

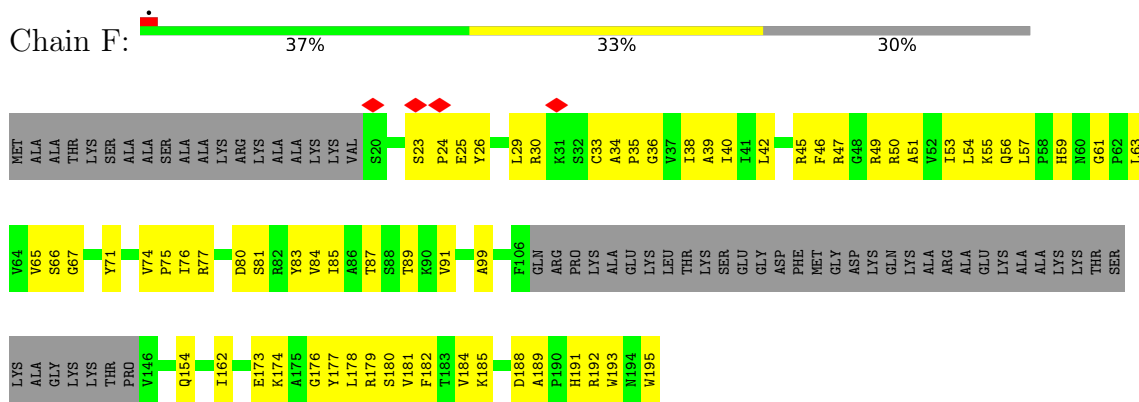




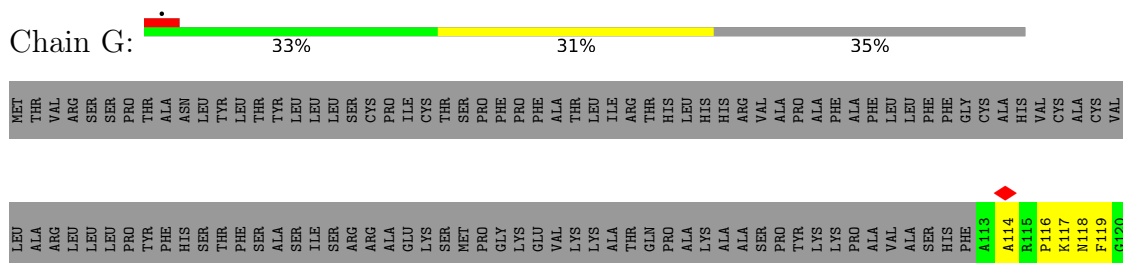
• Molecule 13: ribosomal protein L6

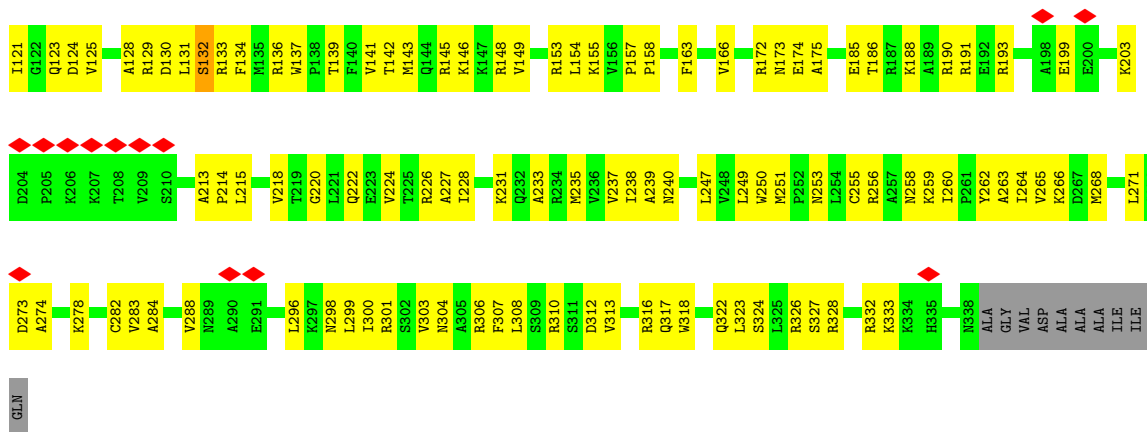


• Molecule 14: ribosomal protein L6e



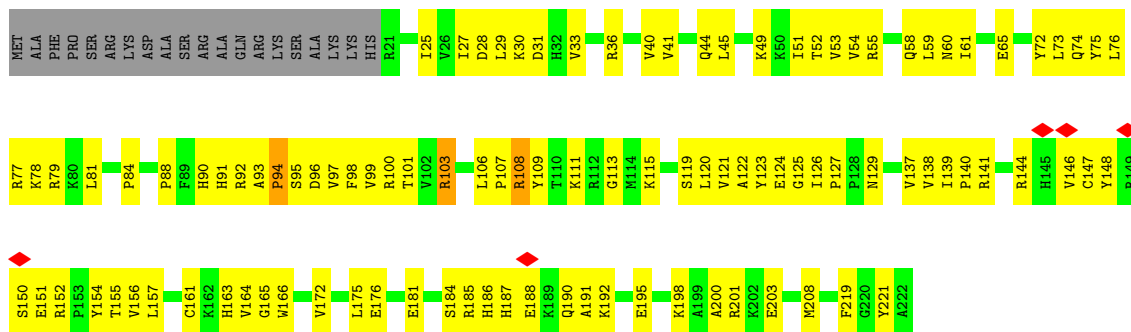
• Molecule 15: ribosomal protein L8e





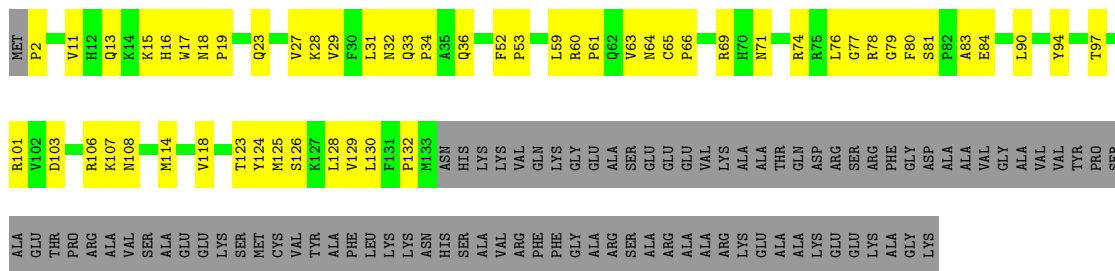
• Molecule 16: ribosomal protein L13

Chain H: 44% 46% 9%



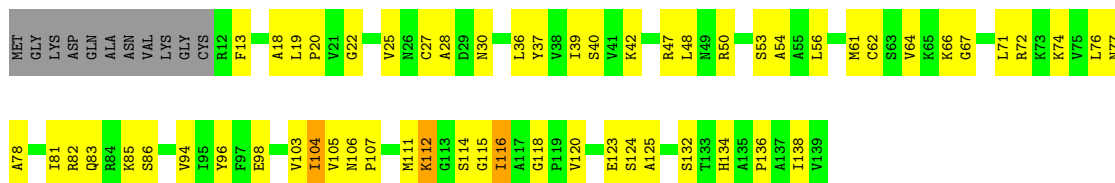
• Molecule 17: ribosomal protein L13e

Chain I: 35% 25% 40%



• Molecule 18: ribosomal protein L14

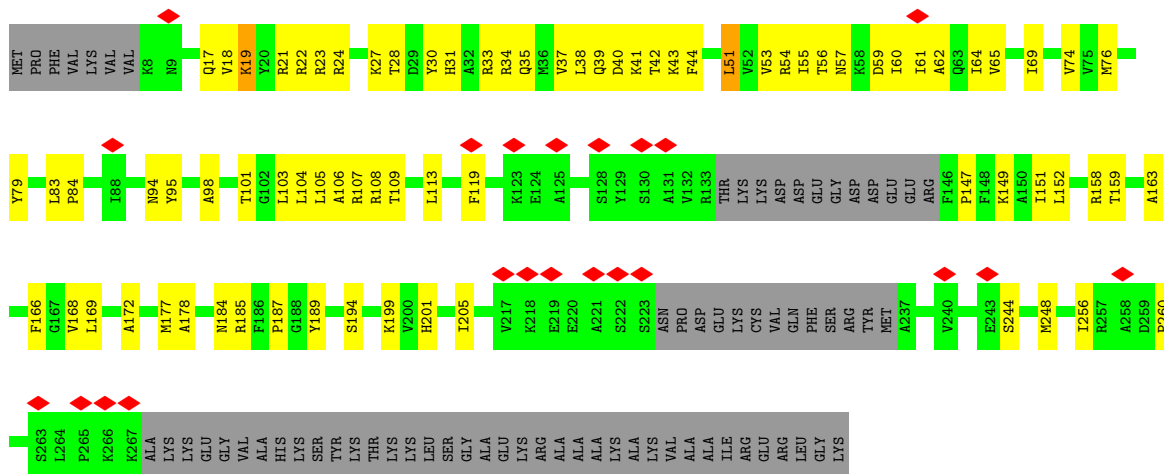
Chain J: 50% 40% 8%







• Molecule 23: ribosomal protein L18

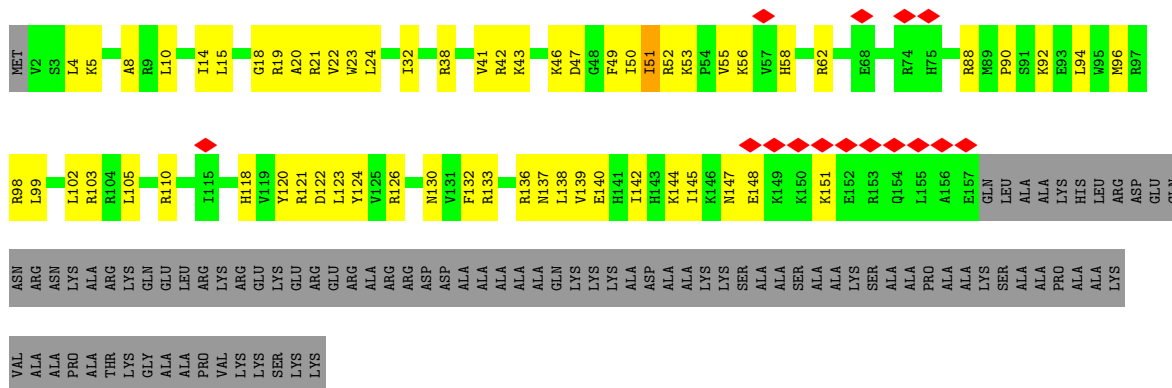


• Molecule 24: ribosomal protein L18e

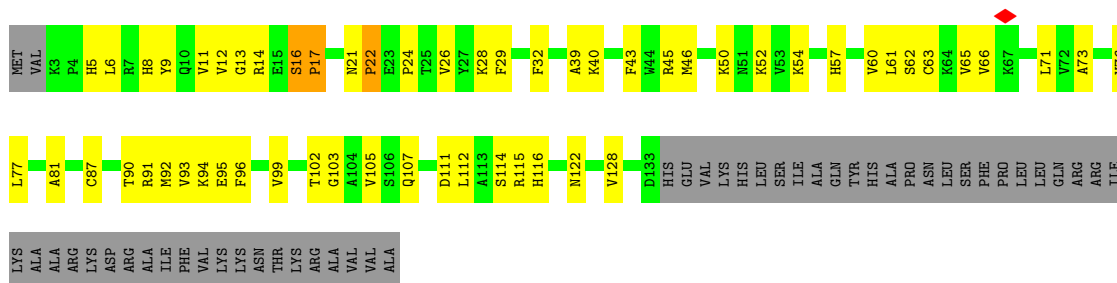


• Molecule 25: ribosomal protein L19e

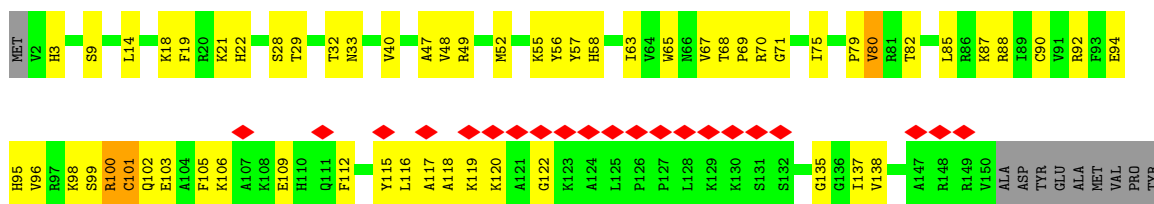




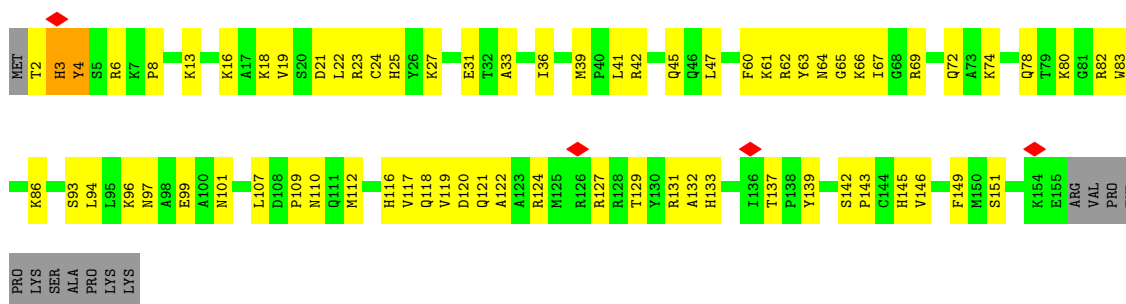
• Molecule 26: ribosomal protein L20e



• Molecule 27: ribosomal protein L21e

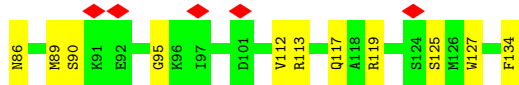


• Molecule 28: ribosomal protein L22

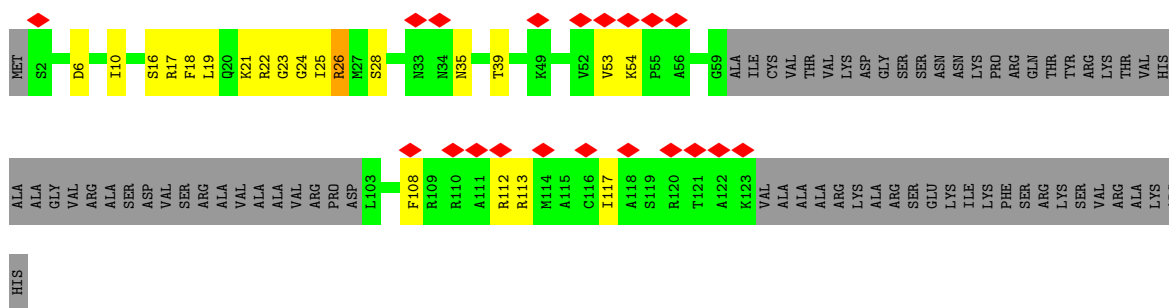
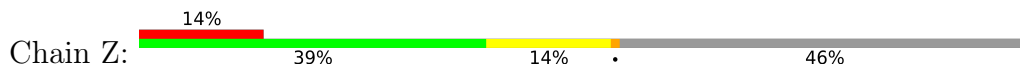


• Molecule 29: ribosomal protein L22e

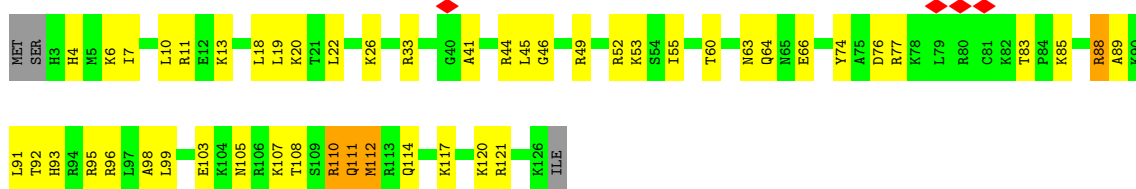




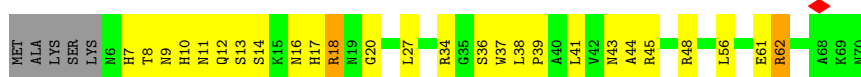
• Molecule 34: ribosomal protein L28e



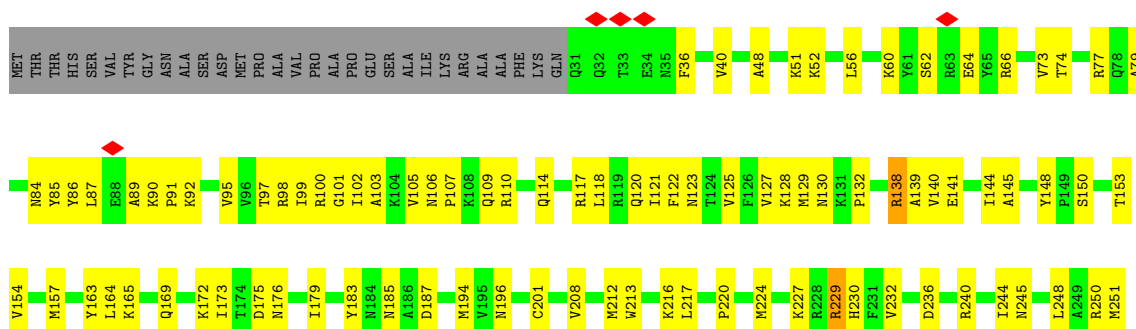
• Molecule 35: ribosomal protein L29



• Molecule 36: ribosomal protein L29e



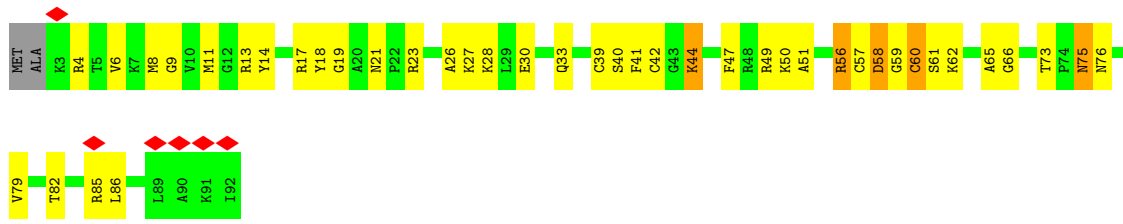
• Molecule 37: ribosomal protein L30



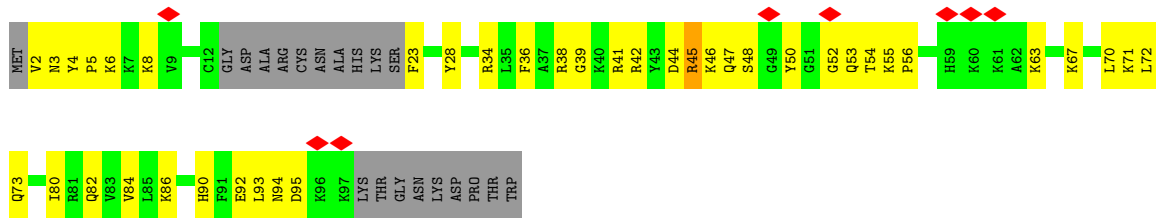




• Molecule 47: ribosomal protein L43e



• Molecule 48: ribosomal protein L44e



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	107134	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	25000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.231	Depositor
Minimum map value	-0.118	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size ( $\text{\AA}$ )	384.0, 384.0, 384.0	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0, 1.0, 1.0	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, A2M, OMG, H2U, OMC, OMU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	1	0.37	9/36881 (0.0%)	0.41	2/57466 (0.0%)
2	2	0.30	0/26109	0.38	1/40668 (0.0%)
3	3	0.25	0/4337	0.37	0/6734
4	4	0.33	0/3549	0.37	0/5525
5	5	0.34	0/1908	0.41	0/2967
6	6	0.41	2/1437 (0.1%)	0.77	6/2234 (0.3%)
7	7	0.37	0/3615	0.37	0/5622
8	8	0.25	0/2828	0.38	2/4401 (0.0%)
9	A	0.41	0/1903	0.60	1/2559 (0.0%)
10	B	0.38	0/3086	0.58	0/4176
11	C	0.40	0/2284	0.61	0/3092
12	D	0.15	0/800	0.41	0/1111
13	E	0.24	0/1529	0.65	0/2056
14	F	0.33	0/1023	0.62	1/1390 (0.1%)
15	G	0.34	0/1798	0.66	1/2423 (0.0%)
16	H	0.37	0/1628	0.61	0/2194
17	I	0.36	0/1084	0.60	0/1454
18	J	0.36	0/941	0.67	2/1277 (0.2%)
19	K	0.31	0/1077	0.79	2/1475 (0.1%)
20	L	0.37	0/1123	0.56	0/1505
21	M	0.45	0/1754	0.60	0/2342
22	N	0.24	0/1747	0.62	1/2338 (0.0%)
23	O	0.25	0/1583	0.52	0/2157
24	P	0.35	0/1519	0.61	0/2040
25	Q	0.31	0/1179	0.66	0/1588
26	R	0.32	0/1044	0.70	5/1415 (0.4%)
27	S	0.34	0/1142	0.63	0/1547
28	T	0.39	0/1249	0.67	1/1679 (0.1%)
29	U	0.16	0/545	0.47	0/754
30	V	0.36	0/907	0.54	0/1227
31	W	0.32	0/910	0.64	0/1224
32	X	0.30	0/527	0.58	0/716

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	Y	0.28	0/934	0.57	0/1274
34	Z	0.24	0/545	0.49	0/739
35	a	0.29	0/992	0.57	0/1326
36	b	0.32	0/514	0.60	0/690
37	c	0.37	0/1763	0.57	0/2374
38	d	0.22	0/525	0.51	0/719
39	e	0.33	0/838	0.58	0/1131
40	f	0.40	0/1002	0.63	0/1346
41	g	0.42	0/1003	0.56	0/1352
42	h	0.33	0/868	0.62	0/1160
43	i	0.29	0/499	0.55	0/662
44	j	0.45	0/651	0.65	0/869
45	k	0.21	0/378	0.53	0/518
46	l	0.39	0/470	0.57	0/627
47	m	0.36	0/680	0.64	1/913 (0.1%)
48	n	0.29	0/667	0.64	0/889
All	All	0.34	11/125375 (0.0%)	0.48	26/185945 (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
9	A	0	1
10	B	0	2
13	E	0	1
15	G	0	1
16	H	0	1
19	K	0	3
26	R	0	1
27	S	0	1
28	T	0	1
40	f	0	1
All	All	0	13

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	634	G	C1'-N9	-6.97	1.37	1.48
1	1	159	U	C1'-N1	6.37	1.58	1.48
1	1	568	U	C1'-N1	6.26	1.57	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	564	U	C1'-N1	6.14	1.57	1.48
1	1	565	U	C1'-N1	6.11	1.57	1.48

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1575	A	OP1-P-O3'	-9.59	79.22	108.00
15	G	326	ARG	N-CA-C	8.68	120.51	111.14
26	R	22	PRO	N-CA-CB	8.61	112.29	103.25
6	6	41	G	C2'-C3'-O3'	8.54	122.30	109.50
18	J	112	LYS	N-CA-C	8.27	128.41	110.80

There are no chirality outliers.

5 of 13 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	A	60[B]	ARG	Mainchain
10	B	337	GLY	Peptide
10	B	373	GLY	Peptide
13	E	136	PRO	Peptide
15	G	114	ALA	Peptide

## 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	33313	0	16798	1225	0
2	2	23926	0	12113	785	0
3	3	3893	0	1971	165	0
4	4	3177	0	1611	111	0
5	5	1708	0	867	64	0
6	6	1288	0	657	205	0
7	7	3280	0	1664	113	0
8	8	2531	0	1281	155	0
9	A	1859	0	1901	138	0
10	B	3020	0	3003	180	0
11	C	2237	0	2231	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	799	0	374	5	0
13	E	1509	0	1595	124	0
14	F	1002	0	994	56	0
15	G	1772	0	1853	109	0
16	H	1596	0	1683	139	0
17	I	1061	0	1123	67	0
18	J	924	0	934	62	0
19	K	1061	0	939	210	0
20	L	1096	0	1096	58	0
21	M	1714	0	1793	107	0
22	N	1714	0	1786	112	0
23	O	1557	0	1351	87	0
24	P	1494	0	1554	92	0
25	Q	1162	0	1130	75	0
26	R	1019	0	981	54	0
27	S	1112	0	1051	67	0
28	T	1221	0	1230	98	0
29	U	541	0	295	9	0
30	V	892	0	903	50	0
31	W	896	0	915	39	0
32	X	508	0	477	27	0
33	Y	914	0	813	49	0
34	Z	538	0	479	25	0
35	a	982	0	1029	57	0
36	b	503	0	500	31	0
37	c	1732	0	1768	82	0
38	d	518	0	462	15	0
39	e	824	0	839	35	0
40	f	982	0	985	62	0
41	g	983	0	1006	81	0
42	h	856	0	873	88	0
43	i	494	0	535	20	0
44	j	639	0	641	44	0
45	k	373	0	302	11	0
46	l	457	0	484	28	0
47	m	668	0	648	58	0
48	n	659	0	672	52	0
49	1	51	0	0	0	0
49	2	25	0	0	0	0
49	3	3	0	0	0	0
49	4	2	0	0	0	0
49	5	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	7	9	0	0	0	0
49	C	1	0	0	0	0
49	K	1	0	0	0	0
49	M	3	0	0	0	0
49	V	1	0	0	0	0
49	a	1	0	0	0	0
49	f	2	0	0	0	0
49	g	1	0	0	0	0
49	h	1	0	0	0	0
49	j	4	0	0	0	0
50	1	72	0	0	18	0
50	2	40	0	0	17	0
50	4	4	0	0	1	0
50	5	4	0	0	0	0
50	7	16	0	0	2	0
50	8	1	0	0	1	0
50	A	2	0	0	1	0
50	G	1	0	0	0	0
50	M	2	0	0	0	0
50	i	1	0	0	0	0
50	j	1	0	0	0	0
All	All	117257	0	80190	4605	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 25.

The worst 5 of 4605 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:57:U:H2'	3:3:58:C:C5	1.26	1.62
19:K:89:VAL:CG1	26:R:73:ALA:HB2	1.26	1.56
19:K:89:VAL:HG12	26:R:73:ALA:CB	1.38	1.50
24:P:17:HIS:CE1	24:P:18:HIS:HD1	1.29	1.50
25:Q:23:TRP:CE3	25:Q:51:ILE:CD1	2.02	1.42

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	
9	A	245/260 (94%)	220 (90%)	25 (10%)	0	100	100
10	B	396/419 (94%)	352 (89%)	43 (11%)	1 (0%)	36	66
11	C	300/373 (80%)	269 (90%)	31 (10%)	0	100	100
12	D	159/188 (85%)	136 (86%)	23 (14%)	0	100	100
13	E	188/190 (99%)	160 (85%)	28 (15%)	0	100	100
14	F	134/195 (69%)	112 (84%)	22 (16%)	0	100	100
15	G	225/348 (65%)	205 (91%)	18 (8%)	2 (1%)	14	41
16	H	200/222 (90%)	175 (88%)	24 (12%)	1 (0%)	24	55
17	I	130/220 (59%)	120 (92%)	10 (8%)	0	100	100
18	J	126/139 (91%)	115 (91%)	11 (9%)	0	100	100
19	K	154/233 (66%)	136 (88%)	17 (11%)	1 (1%)	21	51
20	L	142/145 (98%)	127 (89%)	15 (11%)	0	100	100
21	M	201/204 (98%)	187 (93%)	14 (7%)	0	100	100
22	N	211/213 (99%)	186 (88%)	25 (12%)	0	100	100
23	O	229/305 (75%)	205 (90%)	24 (10%)	0	100	100
24	P	194/198 (98%)	179 (92%)	15 (8%)	0	100	100
25	Q	154/245 (63%)	141 (92%)	13 (8%)	0	100	100
26	R	130/179 (73%)	104 (80%)	25 (19%)	1 (1%)	16	44
27	S	149/159 (94%)	125 (84%)	22 (15%)	2 (1%)	9	31
28	T	154/166 (93%)	127 (82%)	27 (18%)	0	100	100
29	U	98/129 (76%)	81 (83%)	17 (17%)	0	100	100
30	V	116/145 (80%)	99 (85%)	17 (15%)	0	100	100
31	W	116/143 (81%)	106 (91%)	10 (9%)	0	100	100
32	X	62/124 (50%)	59 (95%)	3 (5%)	0	100	100
33	Y	130/134 (97%)	111 (85%)	19 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Z	75/147 (51%)	65 (87%)	10 (13%)	0	100	100
35	a	122/127 (96%)	105 (86%)	17 (14%)	0	100	100
36	b	63/70 (90%)	53 (84%)	10 (16%)	0	100	100
37	c	220/252 (87%)	190 (86%)	30 (14%)	0	100	100
38	d	71/104 (68%)	63 (89%)	8 (11%)	0	100	100
39	e	111/183 (61%)	92 (83%)	19 (17%)	0	100	100
40	f	124/133 (93%)	110 (89%)	14 (11%)	0	100	100
41	g	123/144 (85%)	112 (91%)	11 (9%)	0	100	100
42	h	106/168 (63%)	91 (86%)	15 (14%)	0	100	100
43	i	62/105 (59%)	57 (92%)	5 (8%)	0	100	100
44	j	76/83 (92%)	68 (90%)	8 (10%)	0	100	100
45	k	56/83 (68%)	52 (93%)	4 (7%)	0	100	100
46	l	49/51 (96%)	46 (94%)	2 (4%)	1 (2%)	6	21
47	m	88/92 (96%)	71 (81%)	16 (18%)	1 (1%)	11	36
48	n	82/106 (77%)	66 (80%)	16 (20%)	0	100	100
All	All	5771/7124 (81%)	5078 (88%)	683 (12%)	10 (0%)	44	72

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	G	132	SER
26	R	22	PRO
27	S	101	CYS
47	m	40	SER
10	B	380	LYS

### 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	
9	A	188/204 (92%)	187 (100%)	1 (0%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	B	296/352 (84%)	292 (99%)	4 (1%)	59	85
11	C	222/302 (74%)	222 (100%)	0	100	100
12	D	4/163 (2%)	4 (100%)	0	100	100
13	E	172/172 (100%)	172 (100%)	0	100	100
14	F	92/154 (60%)	92 (100%)	0	100	100
15	G	179/292 (61%)	179 (100%)	0	100	100
16	H	166/188 (88%)	164 (99%)	2 (1%)	63	87
17	I	114/181 (63%)	114 (100%)	0	100	100
18	J	91/111 (82%)	89 (98%)	2 (2%)	45	78
19	K	79/195 (40%)	70 (89%)	9 (11%)	5	19
20	L	105/115 (91%)	105 (100%)	0	100	100
21	M	179/180 (99%)	177 (99%)	2 (1%)	65	87
22	N	178/179 (99%)	178 (100%)	0	100	100
23	O	103/242 (43%)	101 (98%)	2 (2%)	50	81
24	P	149/164 (91%)	147 (99%)	2 (1%)	61	86
25	Q	100/196 (51%)	99 (99%)	1 (1%)	68	88
26	R	98/158 (62%)	98 (100%)	0	100	100
27	S	100/133 (75%)	100 (100%)	0	100	100
28	T	125/144 (87%)	125 (100%)	0	100	100
29	U	13/114 (11%)	13 (100%)	0	100	100
30	V	86/124 (69%)	84 (98%)	2 (2%)	44	78
31	W	87/122 (71%)	86 (99%)	1 (1%)	65	87
32	X	48/104 (46%)	46 (96%)	2 (4%)	26	61
33	Y	70/115 (61%)	70 (100%)	0	100	100
34	Z	44/119 (37%)	43 (98%)	1 (2%)	44	78
35	a	99/117 (85%)	93 (94%)	6 (6%)	17	46
36	b	48/58 (83%)	46 (96%)	2 (4%)	26	61
37	c	168/209 (80%)	166 (99%)	2 (1%)	63	87
38	d	47/90 (52%)	45 (96%)	2 (4%)	26	60
39	e	79/156 (51%)	79 (100%)	0	100	100
40	f	97/114 (85%)	94 (97%)	3 (3%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
41	g	98/121 (81%)	97 (99%)	1 (1%)	68	88
42	h	85/145 (59%)	83 (98%)	2 (2%)	43	77
43	i	47/89 (53%)	47 (100%)	0	100	100
44	j	63/70 (90%)	61 (97%)	2 (3%)	34	70
45	k	26/74 (35%)	26 (100%)	0	100	100
46	l	46/47 (98%)	45 (98%)	1 (2%)	45	78
47	m	63/74 (85%)	58 (92%)	5 (8%)	11	35
48	n	64/92 (70%)	63 (98%)	1 (2%)	55	83
All	All	4118/5979 (69%)	4060 (99%)	58 (1%)	57	85

5 of 58 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	X	37	ARG
47	m	58	ASP
35	a	112	MET
47	m	56	ARG
44	j	22	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such sidechains are listed below:

Mol	Chain	Res	Type
40	f	28	GLN
41	g	80	HIS
18	J	134	HIS
18	J	77	ASN
42	h	51	HIS

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	1535/1782 (86%)	588 (38%)	57 (3%)
2	2	1106/1527 (72%)	446 (40%)	28 (2%)
3	3	178/213 (83%)	85 (47%)	10 (5%)
4	4	146/183 (79%)	48 (32%)	5 (3%)
5	5	78/133 (58%)	30 (38%)	4 (5%)
6	6	60/76 (78%)	48 (80%)	15 (25%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	7	151/171 (88%)	51 (33%)	2 (1%)
8	8	118/121 (97%)	55 (46%)	5 (4%)
All	All	3372/4206 (80%)	1351 (40%)	126 (3%)

5 of 1351 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	4	G
1	1	10	A
1	1	13	G
1	1	23	U
1	1	24	A

5 of 126 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	2	29	C
6	6	29	G
2	2	815	G
6	6	24	C
6	6	58	U

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

44 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
2	A2M	2	1186	2	22,25,26	1.47	4 (18%)	30,36,39	2.12	10 (33%)
1	OMC	1	695	1	19,22,23	0.90	1 (5%)	25,31,34	1.23	2 (8%)
1	OMU	1	36	1	19,22,23	1.34	3 (15%)	25,31,34	1.96	6 (24%)
2	OMG	2	71	2	23,26,27	1.25	3 (13%)	32,38,41	2.11	7 (21%)
2	OMG	2	655	2	23,26,27	1.23	3 (13%)	32,38,41	2.04	6 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMG	1	1526	1	23,26,27	1.21	3 (13%)	32,38,41	2.04	6 (18%)
1	A2M	1	955	1	22,25,26	1.50	6 (27%)	30,36,39	2.15	10 (33%)
2	OMC	2	554	2	19,22,23	0.83	0	25,31,34	1.04	1 (4%)
2	OMC	2	443	2	19,22,23	0.84	0	25,31,34	0.90	0
2	OMG	2	571	2	23,26,27	1.20	4 (17%)	32,38,41	2.16	7 (21%)
2	OMG	2	1079	2	23,26,27	1.20	3 (13%)	32,38,41	1.99	5 (15%)
2	OMC	2	1398	2	19,22,23	0.85	0	25,31,34	1.08	1 (4%)
2	OMU	2	1153	2	19,22,23	1.32	3 (15%)	25,31,34	2.11	6 (24%)
2	OMG	2	534	2	23,26,27	1.20	3 (13%)	32,38,41	2.10	6 (18%)
1	OMU	1	48	1	19,22,23	1.38	3 (15%)	25,31,34	1.95	6 (24%)
2	OMU	2	1078	2	19,22,23	1.30	2 (10%)	25,31,34	1.93	6 (24%)
2	OMC	2	1160	2	19,22,23	0.84	0	25,31,34	1.01	1 (4%)
2	OMU	2	656	2	19,22,23	1.25	3 (15%)	25,31,34	2.09	6 (24%)
1	A2M	1	927	1	22,25,26	1.51	5 (22%)	30,36,39	2.14	9 (30%)
1	OMG	1	1628	1	23,26,27	1.22	4 (17%)	32,38,41	2.15	7 (21%)
1	OMU	1	847	1	19,22,23	1.28	3 (15%)	25,31,34	1.92	6 (24%)
2	OMC	2	1318	2	19,22,23	0.84	0	25,31,34	1.03	2 (8%)
1	OMG	1	856	1	23,26,27	1.22	4 (17%)	32,38,41	2.22	7 (21%)
1	A2M	1	678	1,2	22,25,26	1.49	4 (18%)	30,36,39	2.08	9 (30%)
2	OMC	2	583	2	19,22,23	0.86	0	25,31,34	1.06	1 (4%)
2	A2M	2	628	2	22,25,26	1.48	5 (22%)	30,36,39	2.13	10 (33%)
2	OMG	2	1254	2	23,26,27	1.22	3 (13%)	32,38,41	2.05	7 (21%)
2	A2M	2	527	2	22,25,26	1.47	5 (22%)	30,36,39	2.18	9 (30%)
2	H2U	2	1404	2	18,21,22	1.11	2 (11%)	19,30,33	1.03	1 (5%)
2	A2M	2	382	2	22,25,26	1.46	5 (22%)	30,36,39	2.03	8 (26%)
2	OMU	2	667	2	19,22,23	1.28	3 (15%)	25,31,34	1.94	6 (24%)
7	A2M	7	162	1,7	22,25,26	1.50	4 (18%)	30,36,39	2.14	9 (30%)
2	OMC	2	1249	2	19,22,23	0.84	0	25,31,34	1.04	1 (4%)
1	OMG	1	959	1	23,26,27	1.24	3 (13%)	32,38,41	2.09	8 (25%)
2	A2M	2	591	2	22,25,26	1.48	5 (22%)	30,36,39	2.11	9 (30%)
1	A2M	1	681	1	22,25,26	1.45	5 (22%)	30,36,39	2.10	9 (30%)
2	OMG	2	1230	2	23,26,27	1.21	3 (13%)	32,38,41	2.09	7 (21%)
7	OMU	7	7	1,7	19,22,23	1.27	3 (15%)	25,31,34	2.25	6 (24%)
1	OMG	1	1542	1,2	23,26,27	1.23	3 (13%)	32,38,41	2.06	7 (21%)
1	A2M	1	1541	1,2	22,25,26	1.48	5 (22%)	30,36,39	2.04	8 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	OMC	1	1529	1	19,22,23	0.86	0	25,31,34	1.02	1 (4%)
2	OMG	2	641	2	23,26,27	1.24	4 (17%)	32,38,41	2.05	7 (21%)
2	A2M	2	572	2	22,25,26	1.49	4 (18%)	30,36,39	2.10	9 (30%)
1	OMU	1	845	1	19,22,23	1.35	4 (21%)	25,31,34	2.09	6 (24%)

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
2	A2M	2	1186	2	-	3/9/27/28	0/3/3/3
1	OMC	1	695	1	-	0/9/27/28	0/2/2/2
1	OMU	1	36	1	-	2/9/27/28	0/2/2/2
2	OMG	2	71	2	-	2/9/27/28	0/3/3/3
2	OMG	2	655	2	-	0/9/27/28	0/3/3/3
1	OMG	1	1526	1	-	1/9/27/28	0/3/3/3
1	A2M	1	955	1	-	3/9/27/28	0/3/3/3
2	OMC	2	554	2	-	2/9/27/28	0/2/2/2
2	OMC	2	443	2	-	5/9/27/28	0/2/2/2
2	OMG	2	571	2	-	2/9/27/28	0/3/3/3
2	OMG	2	1079	2	-	2/9/27/28	0/3/3/3
2	OMC	2	1398	2	-	0/9/27/28	0/2/2/2
2	OMU	2	1153	2	-	2/9/27/28	0/2/2/2
2	OMG	2	534	2	-	0/9/27/28	0/3/3/3
1	OMU	1	48	1	-	3/9/27/28	0/2/2/2
2	OMU	2	1078	2	-	0/9/27/28	0/2/2/2
2	OMC	2	1160	2	-	0/9/27/28	0/2/2/2
2	OMU	2	656	2	-	4/9/27/28	0/2/2/2
1	A2M	1	927	1	-	1/9/27/28	0/3/3/3
1	OMG	1	1628	1	-	0/9/27/28	0/3/3/3
1	OMU	1	847	1	-	3/9/27/28	0/2/2/2
2	OMC	2	1318	2	-	2/9/27/28	0/2/2/2
1	OMG	1	856	1	-	0/9/27/28	0/3/3/3
1	A2M	1	678	1,2	-	2/9/27/28	0/3/3/3
2	OMC	2	583	2	-	2/9/27/28	0/2/2/2
2	A2M	2	628	2	-	0/9/27/28	0/3/3/3
2	OMG	2	1254	2	-	4/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A2M	2	527	2	-	2/9/27/28	0/3/3/3
2	H2U	2	1404	2	-	3/7/38/39	0/2/2/2
2	A2M	2	382	2	-	1/9/27/28	0/3/3/3
2	OMU	2	667	2	-	3/9/27/28	0/2/2/2
7	A2M	7	162	1,7	-	3/9/27/28	0/3/3/3
2	OMC	2	1249	2	-	3/9/27/28	0/2/2/2
1	OMG	1	959	1	-	1/9/27/28	0/3/3/3
2	A2M	2	591	2	-	3/9/27/28	0/3/3/3
1	A2M	1	681	1	-	3/9/27/28	0/3/3/3
2	OMG	2	1230	2	-	3/9/27/28	0/3/3/3
7	OMU	7	7	1,7	-	4/9/27/28	0/2/2/2
1	OMG	1	1542	1,2	-	2/9/27/28	0/3/3/3
1	A2M	1	1541	1,2	-	3/9/27/28	0/3/3/3
1	OMC	1	1529	1	-	2/9/27/28	0/2/2/2
2	OMG	2	641	2	-	2/9/27/28	0/3/3/3
2	A2M	2	572	2	-	2/9/27/28	0/3/3/3
1	OMU	1	845	1	-	0/9/27/28	0/2/2/2

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	162	A2M	C5-C4	4.67	1.47	1.39
2	2	572	A2M	C5-C4	4.53	1.47	1.39
2	2	1186	A2M	C5-C4	4.45	1.47	1.39
1	1	927	A2M	C5-C4	4.44	1.47	1.39
2	2	591	A2M	C5-C4	4.42	1.47	1.39

The worst 5 of 261 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	959	OMG	C5-C4-N3	-6.35	118.29	128.39
2	2	1254	OMG	C5-C4-N3	-6.22	118.49	128.39
2	2	71	OMG	C5-C4-N3	-6.13	118.63	128.39
2	2	655	OMG	C5-C4-N3	-6.08	118.72	128.39
1	1	856	OMG	C2'-C1'-N9	-6.02	102.82	114.24

There are no chirality outliers.

5 of 85 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1	48	OMU	O4'-C4'-C5'-O5'
1	1	681	A2M	O4'-C4'-C5'-O5'
1	1	681	A2M	C3'-C4'-C5'-O5'
1	1	1541	A2M	C1'-C2'-O2'-CM'
2	2	382	A2M	C1'-C2'-O2'-CM'

There are no ring outliers.

41 monomers are involved in 194 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	2	1186	A2M	3	0
1	1	695	OMC	3	0
1	1	36	OMU	14	0
2	2	71	OMG	11	0
2	2	655	OMG	7	0
1	1	1526	OMG	2	0
1	1	955	A2M	2	0
2	2	554	OMC	3	0
2	2	443	OMC	7	0
2	2	571	OMG	1	0
2	2	1079	OMG	9	0
2	2	1398	OMC	4	0
2	2	1153	OMU	6	0
2	2	534	OMG	4	0
1	1	48	OMU	4	0
2	2	1078	OMU	11	0
2	2	1160	OMC	3	0
1	1	927	A2M	3	0
1	1	1628	OMG	1	0
1	1	847	OMU	3	0
2	2	1318	OMC	7	0
1	1	856	OMG	2	0
1	1	678	A2M	2	0
2	2	583	OMC	1	0
2	2	628	A2M	4	0
2	2	1254	OMG	10	0
2	2	527	A2M	13	0
2	2	1404	H2U	2	0
2	2	382	A2M	2	0
2	2	667	OMU	13	0
2	2	1249	OMC	1	0
1	1	959	OMG	9	0
2	2	591	A2M	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	681	A2M	2	0
2	2	1230	OMG	2	0
7	7	7	OMU	10	0
1	1	1542	OMG	2	0
1	1	1541	A2M	3	0
1	1	1529	OMC	6	0
2	2	572	A2M	2	0
1	1	845	OMU	2	0

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 109 ligands modelled in this entry, 109 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.

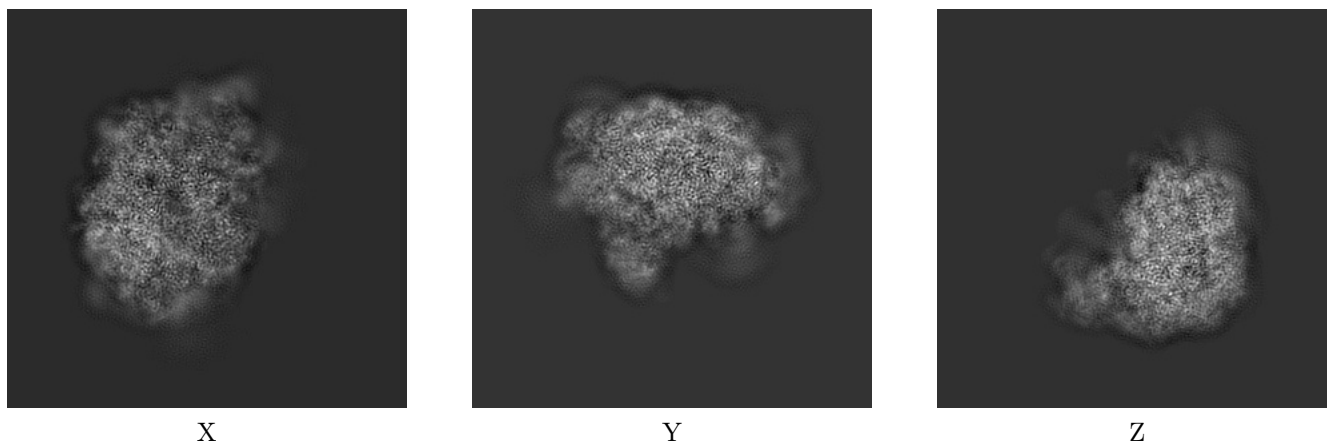
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6583. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

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

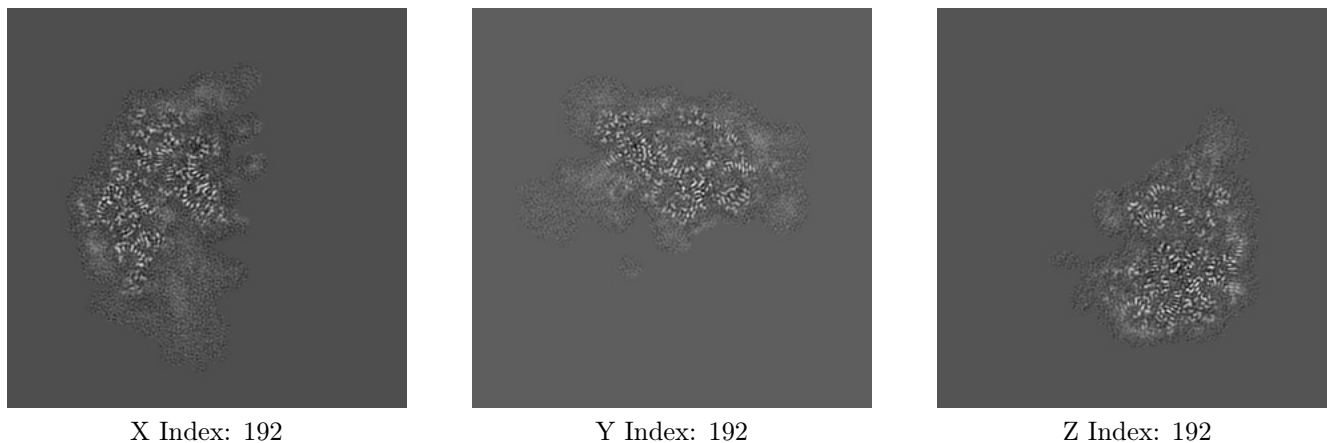
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

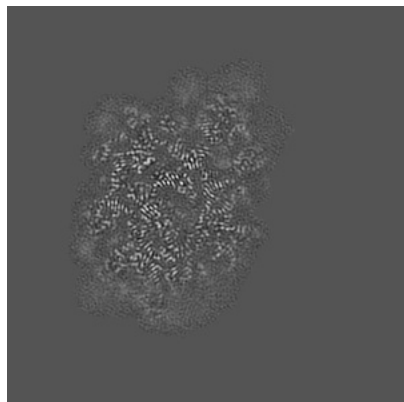
#### 6.2.1 Primary map



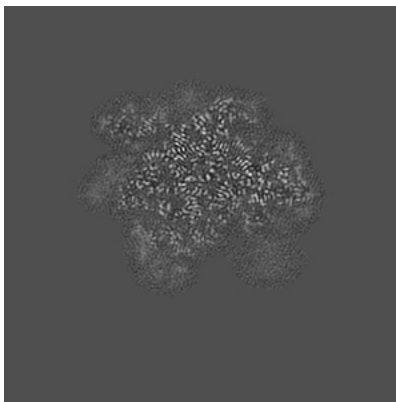
The images above show central slices of the map in three orthogonal directions.

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

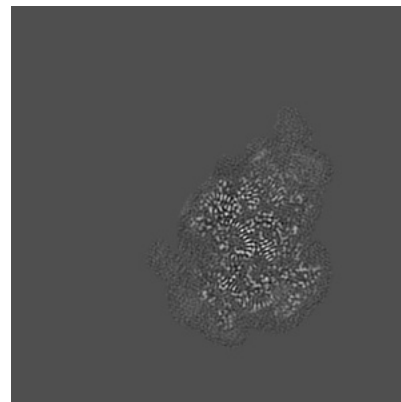
### 6.3.1 Primary map



X Index: 228



Y Index: 123

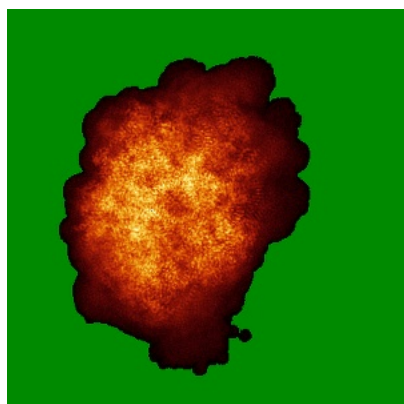


Z Index: 213

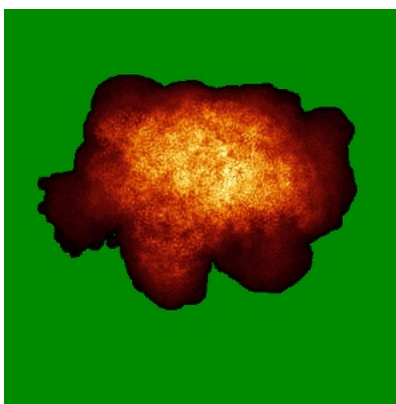
The images above show the largest variance slices of the map in three orthogonal directions.

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

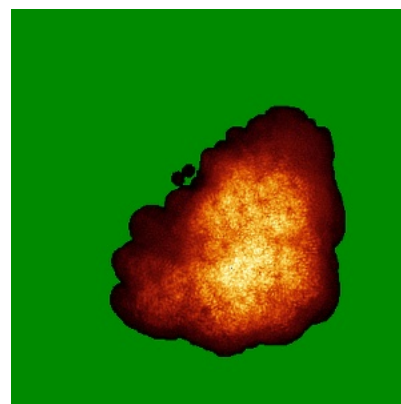
### 6.4.1 Primary map



X



Y



Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

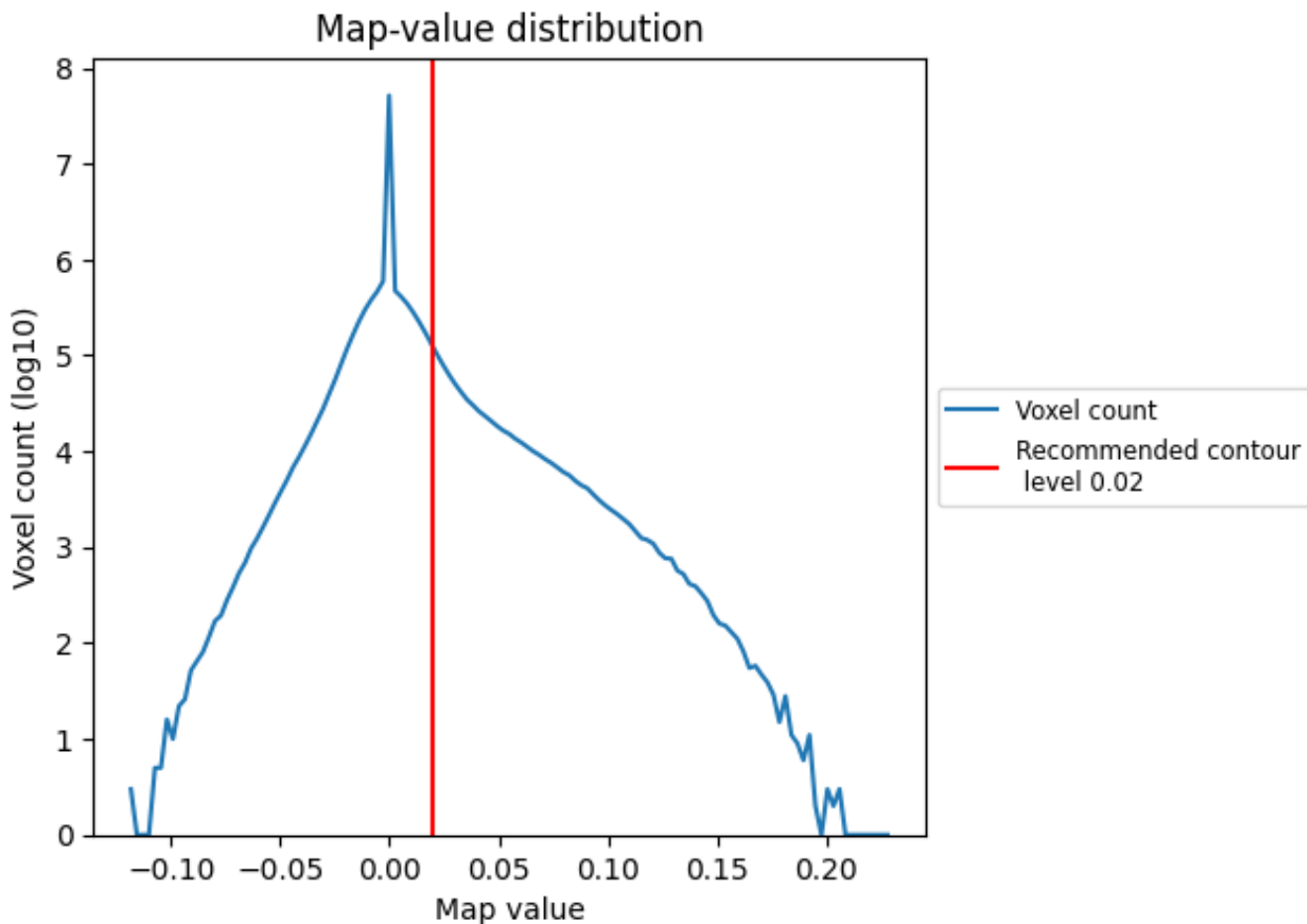
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

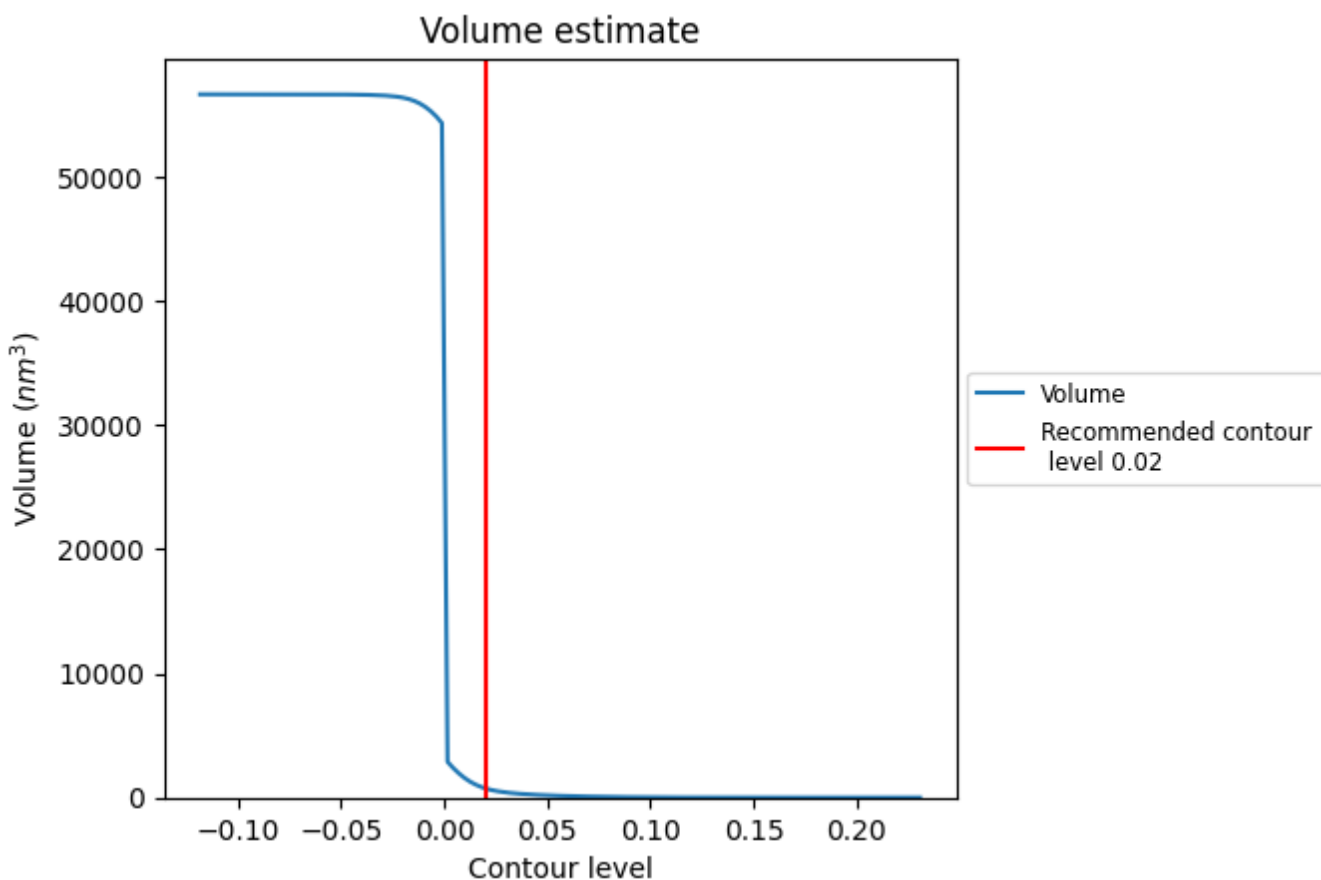
This section contains the results of statistical analysis of the map.

### 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.

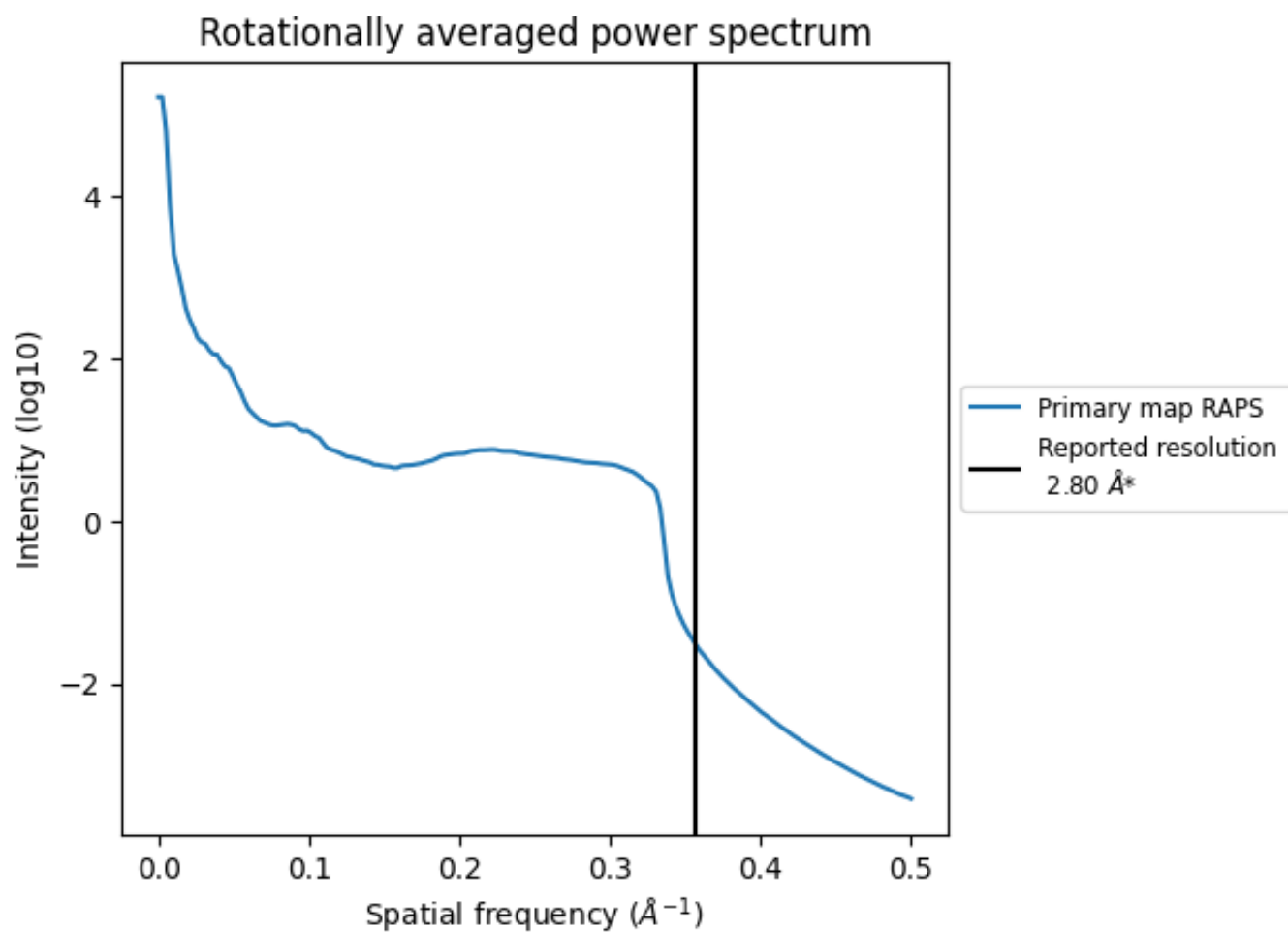
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 742  $\text{nm}^3$ ; this corresponds to an approximate mass of 670 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 0.357 Å<sup>-1</sup>

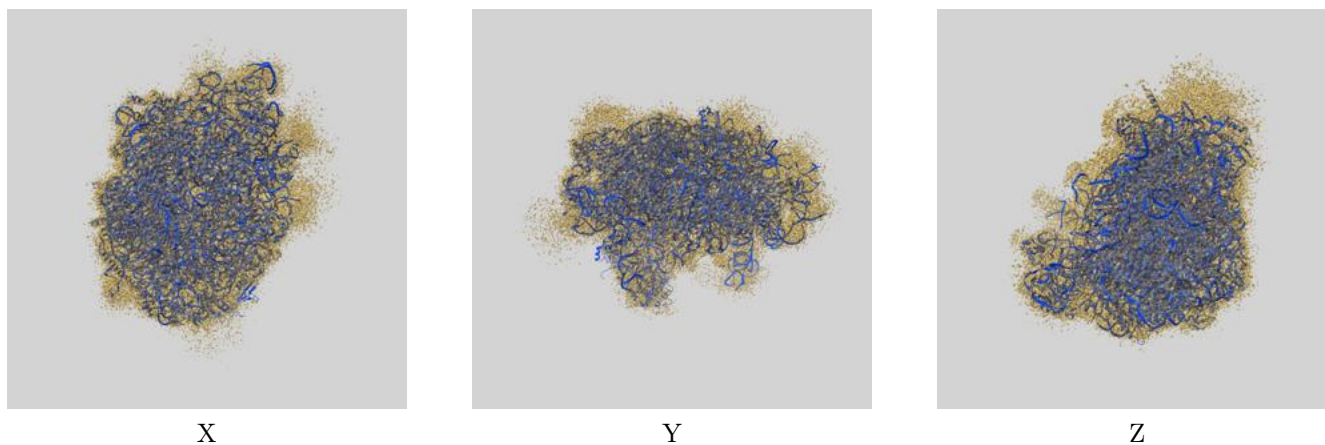
## 8 Fourier-Shell correlation

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

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

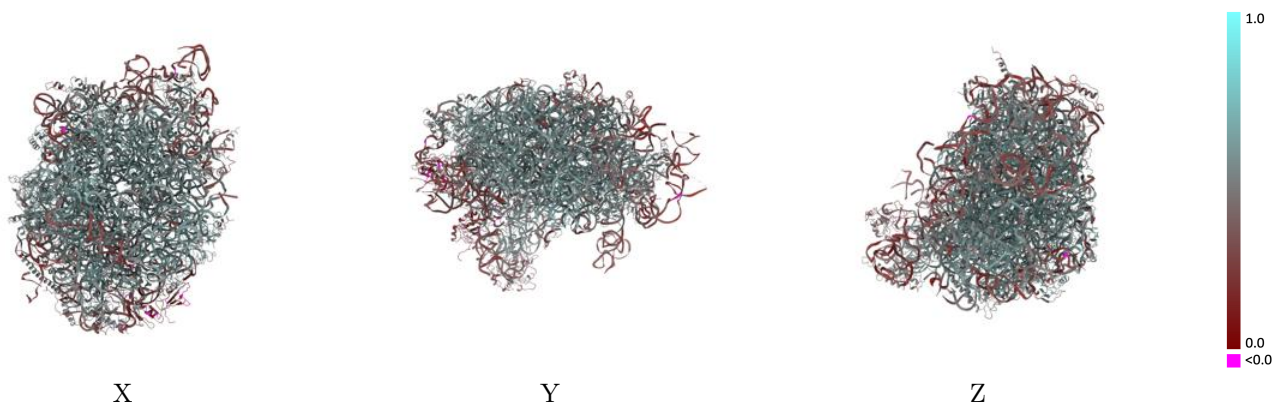
This section contains information regarding the fit between EMDB map EMD-6583 and PDB model 3JCS. Per-residue inclusion information can be found in section 3 on page 15.

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



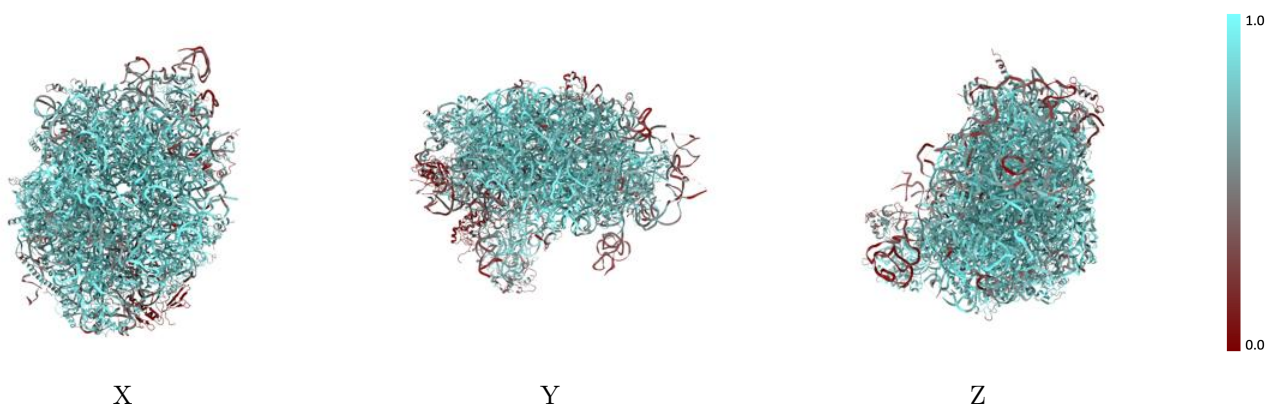
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



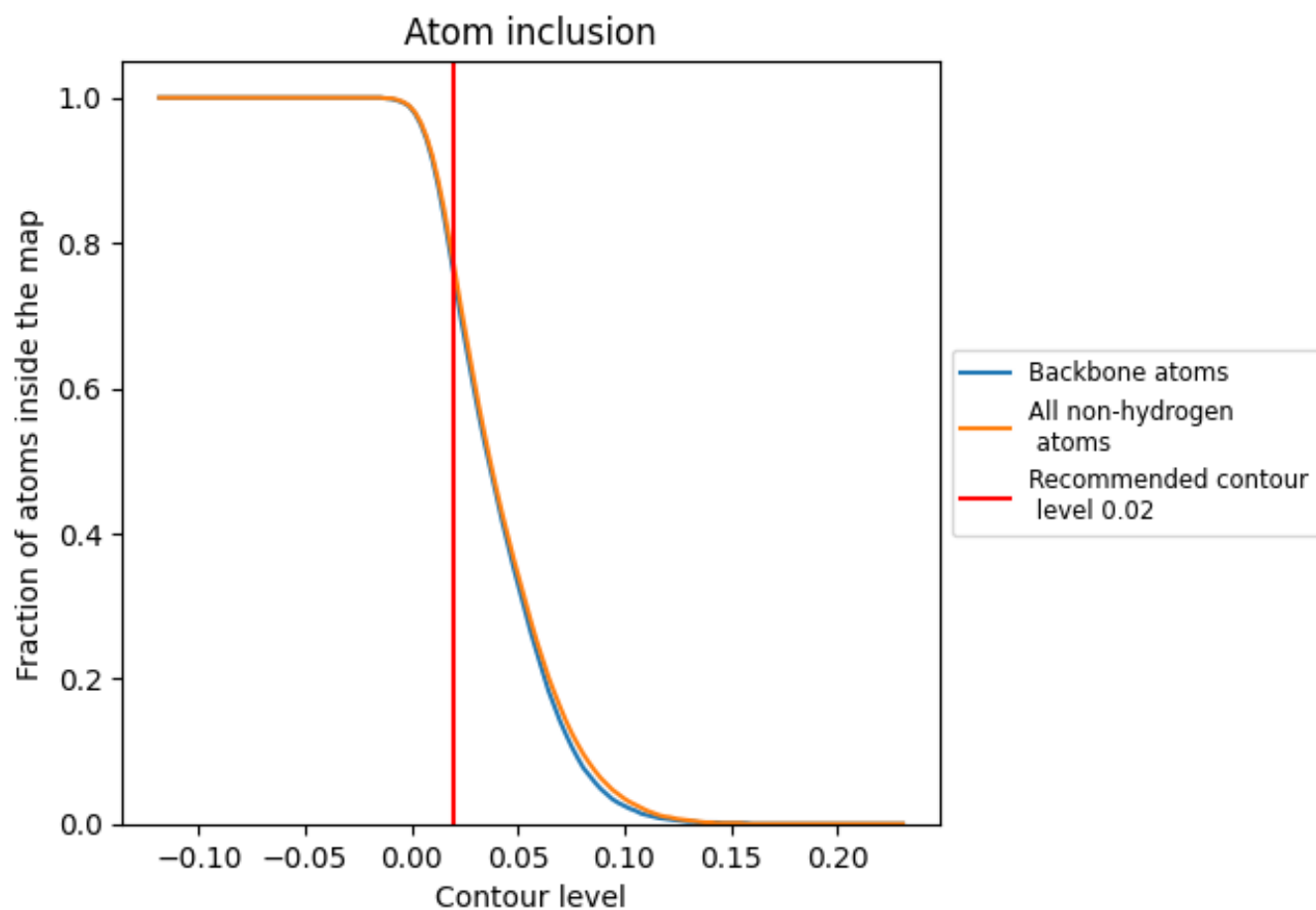
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.4990
1	 0.8180	 0.5060
2	 0.7560	 0.4850
3	 0.6910	 0.4460
4	 0.7950	 0.4970
5	 0.8880	 0.5440
6	 0.6720	 0.3910
7	 0.8930	 0.5550
8	 0.8060	 0.4420
A	 0.8580	 0.5770
B	 0.8240	 0.5530
C	 0.8480	 0.5580
D	 0.4590	 0.3530
E	 0.1210	 0.2290
F	 0.8040	 0.5200
G	 0.7570	 0.5140
H	 0.7840	 0.5300
I	 0.8460	 0.5620
J	 0.8230	 0.5510
K	 0.7090	 0.4450
L	 0.8400	 0.5570
M	 0.8660	 0.5820
N	 0.0710	 0.2100
O	 0.7580	 0.4740
P	 0.8270	 0.5570
Q	 0.7300	 0.5080
R	 0.8150	 0.5220
S	 0.7310	 0.5060
T	 0.8350	 0.5590
U	 0.4480	 0.3960
V	 0.8280	 0.5500
W	 0.8310	 0.5460
X	 0.7290	 0.5210
Y	 0.7680	 0.4950
Z	 0.6280	 0.4930



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Chain	Atom inclusion	Q-score
a	 0.8040	 0.5310
b	 0.8320	 0.5530
c	 0.8070	 0.5410
d	 0.6440	 0.4540
e	 0.7910	 0.5220
f	 0.8240	 0.5580
g	 0.8670	 0.5780
h	 0.7500	 0.5290
i	 0.7340	 0.5140
j	 0.8740	 0.5930
k	 0.5530	 0.4250
l	 0.8280	 0.5680
m	 0.7580	 0.5320
n	 0.6650	 0.4980