



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 03:00 PM UTC

PDB ID : 7PWG / pdb_00007pwg
EMDB ID : EMD-13681
Title : Cryo-EM structure of large subunit of Giardia lamblia ribosome at 2.7 Å resolution
Authors : Hiregange, D.G.; Rivalta, A.; Bose, T.; Breiner-Goldstein, E.; Samiya, S.; Cimicata, G.; Kulakova, L.; Zimmerman, E.; Bashan, A.; Herzberg, O.; Yonath, A.
Deposited on : 2021-10-06
Resolution : 2.75 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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

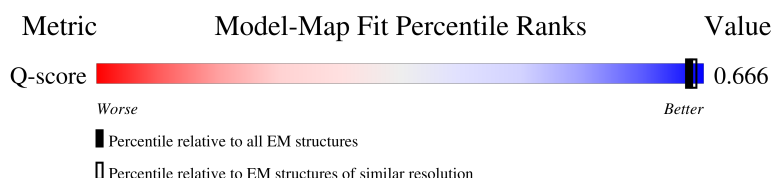
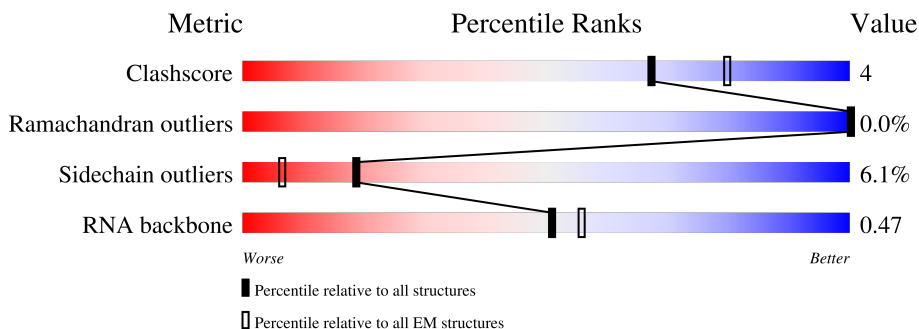
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.75 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	10570 (2.25 - 3.25)

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

Mol	Chain	Length	Quality of chain
1	1	2707	5% 66% 21% 9%
2	3	120	75% 17% 6%
3	4	139	12% 70% 26%

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Mol	Chain	Length	Quality of chain
4	A	251	
5	B	379	
6	C	316	
7	D	297	
8	F	235	
9	G	225	
10	H	185	
11	I	210	
12	J	173	
13	L	234	
14	M	131	
15	N	204	
16	O	197	
17	P	164	
18	Q	179	
19	R	196	
20	S	173	
21	T	159	
22	U	171	
23	V	142	
24	X	141	
25	Y	135	
26	Z	135	
27	a	149	
28	b	62	

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Mol	Chain	Length	Quality of chain
29	c	109	
30	d	106	
31	e	136	
32	f	123	
33	g	120	
34	h	124	
35	i	90	
36	j	89	
37	k	77	
38	l	51	
39	m	127	
40	o	106	
41	p	94	
42	w	76	
43	W	102	
44	E	3	

2 Entry composition

There are 48 unique types of molecules in this entry. The entry contains 109151 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 rRNA 28S.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	2450	Total	C	N	O	P	0	0
			52618	23393	9753	17022	2450		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	117	Total	C	N	O	P	0	0
			2501	1116	458	810	117		

- Molecule 3 is a RNA chain called rRNA 5.8S.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	138	Total	C	N	O	P	0	0
			2958	1315	553	952	138		

- Molecule 4 is a protein called Ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	249	Total	C	N	O	S	0	0
			1865	1152	382	319	12		

- Molecule 5 is a protein called Ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	378	Total	C	N	O	S	0	0
			2987	1886	566	514	21		

- Molecule 6 is a protein called Ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	314	Total	C	N	O	S	0	0
			2446	1539	474	424	9		

- Molecule 7 is a protein called Ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	266	Total	C	N	O	S	0	0
			2118	1342	392	376	8		

- Molecule 8 is a protein called Ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	214	Total	C	N	O	S	0	0
			1730	1100	315	310	5		

- Molecule 9 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	G	182	Total	C	N	O	S	0	0
			1450	923	264	257	6		

- Molecule 10 is a protein called Ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	184	Total	C	N	O	S	0	0
			1442	912	263	257	10		

- Molecule 11 is a protein called Ribosomal protein L10.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	200	Total	C	N	O	S	0	0
			1621	1019	321	273	8		

- Molecule 12 is a protein called Ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	164	Total	C	N	O	S	0	0
			1305	821	246	233	5		

- Molecule 13 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	189	Total	C	N	O	S	0	0
			1512	942	309	255	6		

- Molecule 14 is a protein called Ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	128	Total	C	N	O	S	0	0
			990	626	178	181	5		

- Molecule 15 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	204	Total	C	N	O	S	0	0
			1712	1083	358	265	6		

- Molecule 16 is a protein called Ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	195	Total	C	N	O	S	0	0
			1587	997	310	267	13		

- Molecule 17 is a protein called Ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	154	Total	C	N	O	S	0	0
			1235	781	239	211	4		

- Molecule 18 is a protein called Ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Q	178	Total	C	N	O	S	0	0
			1402	871	279	243	9		

- Molecule 19 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	R	177	Total	C	N	O	S	0	0
			1463	902	313	243	5		

- Molecule 20 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	173	Total	C	N	O	S	0	0
			1418	895	274	240	9		

- Molecule 21 is a protein called Ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	T	153	Total	C	N	O	S	0	0
			1226	766	252	201	7		

- Molecule 22 is a protein called Ribosomal protein eL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	98	Total	C	N	O	S	0	0
			802	513	138	149	2		

- Molecule 23 is a protein called Ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	139	Total	C	N	O	S	0	0
			1057	665	204	183	5		

- Molecule 24 is a protein called Ribosomal protein L23A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	116	Total	C	N	O	S	0	0
			936	601	169	163	3		

- Molecule 25 is a protein called Ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	133	Total	C	N	O	S	0	0
			1076	665	219	184	8		

- Molecule 26 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	129	Total	C	N	O	S	0	0
			980	623	179	173	5		

- Molecule 27 is a protein called Ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	148	Total	C	N	O	S	0	0
			1201	759	240	199	3		

- Molecule 28 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	56	Total	C	N	O	S	0	0
			463	280	104	77	2		

- Molecule 29 is a protein called Ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	101	Total	C	N	O	S	0	0
			756	475	133	144	4		

- Molecule 30 is a protein called Ribosomal protein L31B.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	94	Total	C	N	O	S	0	0
			748	479	148	121			

- Molecule 31 is a protein called Ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	126	Total	C	N	O	S	0	0
			1039	661	207	165	6		

- Molecule 32 is a protein called Ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	123	Total	C	N	O	S	0	0
			974	619	180	171	4		

- Molecule 33 is a protein called Ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	99	Total	C	N	O	S	0	0
			798	493	167	134	4		

- Molecule 34 is a protein called Ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	h	116	Total	C	N	O	S	0	0
			926	589	178	154	5		

- Molecule 35 is a protein called Ribosomal protein L36-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	i	85	Total	C	N	O	S	0	0
			691	438	138	111	4		

- Molecule 36 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	j	87	Total	C	N	O	S	0	0
			692	423	146	116	7		

- Molecule 37 is a protein called Ribosomal L38e.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	k	66	Total	C	N	O	S	0	0
			500	317	85	94	4		

- Molecule 38 is a protein called Ribosomal protein L39.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	l	50	Total	C	N	O	0	0
			434	278	91	65		

- Molecule 39 is a protein called Ubiquitin/Ribosomal protein L40e.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	m	51	Total	C	N	O	S	0	0
			421	257	88	69	7		

- Molecule 40 is a protein called Ribosomal protein L44.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	94	Total	C	N	O	S	0	0
			762	474	157	126	5		

- Molecule 41 is a protein called Ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	91	Total	C	N	O	S	0	0
			708	436	144	122	6		

- Molecule 42 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	w	14	Total	C	N	O	P	0	0
			299	133	56	96	14		

- Molecule 43 is a protein called Ribosomal protein L24A.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	W	65	Total	C	N	O	S	0	0
			540	343	110	85	2		

- Molecule 44 is a RNA chain called P-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	E	3	Total	C	N	O	P	0	0
			62	28	11	20	3		

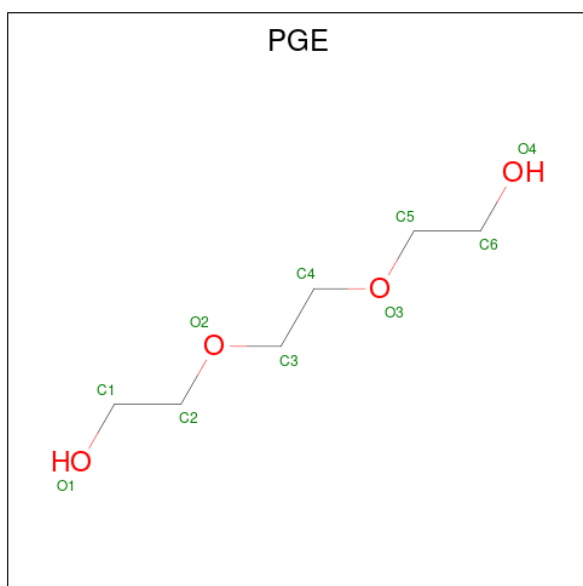
- Molecule 45 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
45	1	99	Total	Mg	0
			99	99	
45	4	5	Total	Mg	0
			5	5	
45	C	1	Total	Mg	0
			1	1	
45	F	1	Total	Mg	0
			1	1	
45	I	1	Total	Mg	0
			1	1	
45	P	1	Total	Mg	0
			1	1	
45	V	1	Total	Mg	0
			1	1	
45	a	1	Total	Mg	0
			1	1	
45	b	1	Total	Mg	0
			1	1	
45	o	1	Total	Mg	0
			1	1	

- Molecule 46 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
46	1	163	Total 163	K 163	0
46	3	1	Total 1	K 1	0
46	A	3	Total 3	K 3	0
46	B	3	Total 3	K 3	0
46	C	2	Total 2	K 2	0
46	I	1	Total 1	K 1	0
46	L	1	Total 1	K 1	0
46	N	2	Total 2	K 2	0
46	V	1	Total 1	K 1	0
46	a	1	Total 1	K 1	0
46	e	1	Total 1	K 1	0
46	j	1	Total 1	K 1	0
46	o	1	Total 1	K 1	0

- Molecule 47 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			AltConf
47	1	1	Total	C	O	0
			10	6	4	

- Molecule 48 is water.

Mol	Chain	Residues	Atoms			AltConf
48	1	3220	Total	O		0
			3220	3220		
48	3	71	Total	O		0
			71	71		
48	4	132	Total	O		0
			132	132		
48	A	54	Total	O		0
			54	54		
48	B	67	Total	O		0
			67	67		
48	C	57	Total	O		0
			57	57		
48	D	30	Total	O		0
			30	30		
48	F	23	Total	O		0
			23	23		
48	G	27	Total	O		0
			27	27		
48	H	15	Total	O		0
			15	15		
48	I	31	Total	O		0
			31	31		
48	J	19	Total	O		0
			19	19		
48	L	42	Total	O		0
			42	42		
48	M	7	Total	O		0
			7	7		
48	N	65	Total	O		0
			65	65		
48	O	35	Total	O		0
			35	35		
48	P	25	Total	O		0
			25	25		
48	Q	35	Total	O		0
			35	35		
48	R	19	Total	O		0
			19	19		

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Mol	Chain	Residues	Atoms		AltConf
48	S	27	Total 27	O 27	0
48	T	38	Total 38	O 38	0
48	U	9	Total 9	O 9	0
48	V	12	Total 12	O 12	0
48	X	30	Total 30	O 30	0
48	Y	18	Total 18	O 18	0
48	Z	23	Total 23	O 23	0
48	a	41	Total 41	O 41	0
48	b	19	Total 19	O 19	0
48	c	3	Total 3	O 3	0
48	d	12	Total 12	O 12	0
48	e	28	Total 28	O 28	0
48	f	15	Total 15	O 15	0
48	g	27	Total 27	O 27	0
48	h	14	Total 14	O 14	0
48	i	15	Total 15	O 15	0
48	j	28	Total 28	O 28	0
48	k	4	Total 4	O 4	0
48	l	7	Total 7	O 7	0
48	m	4	Total 4	O 4	0
48	o	15	Total 15	O 15	0

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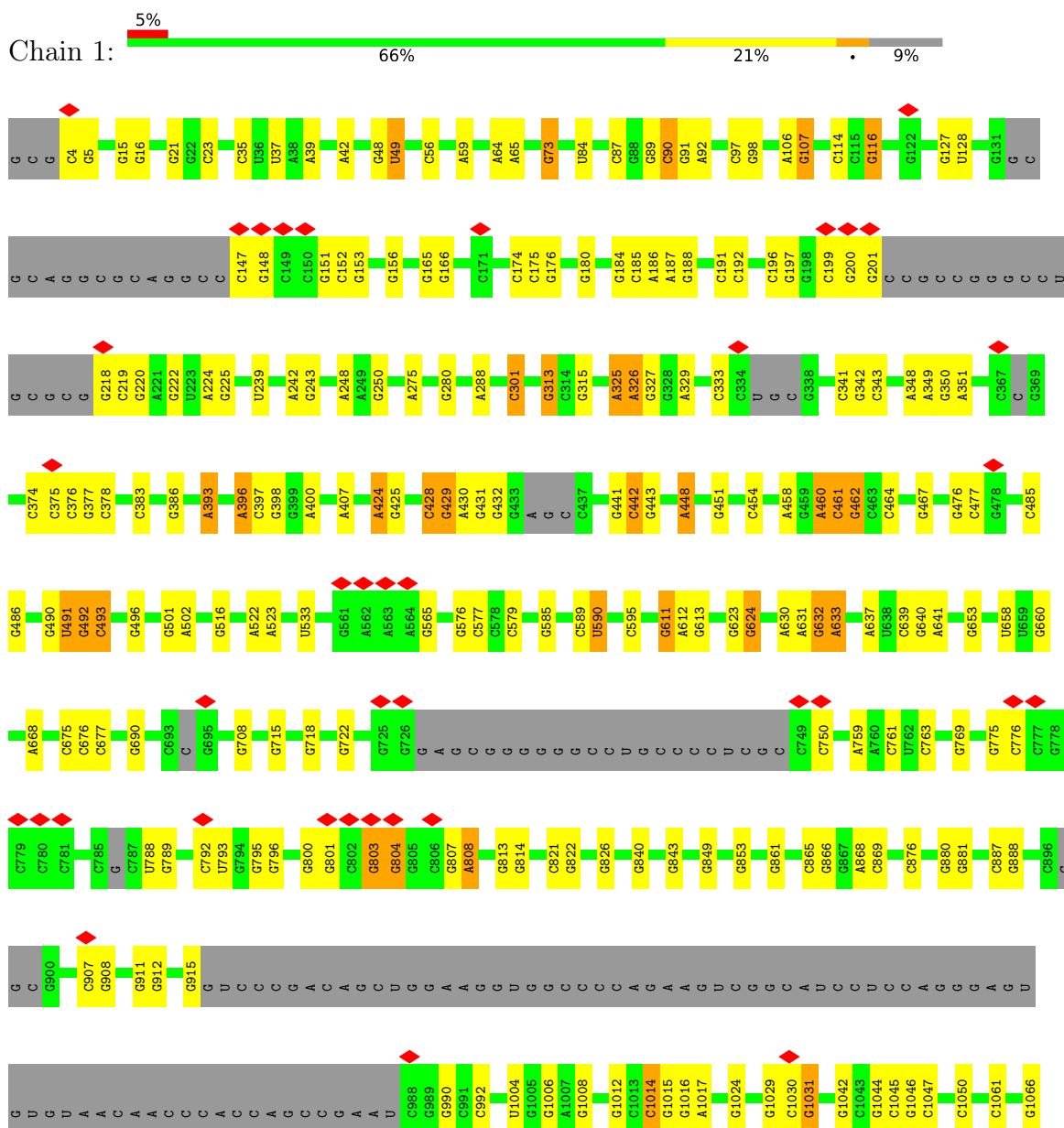
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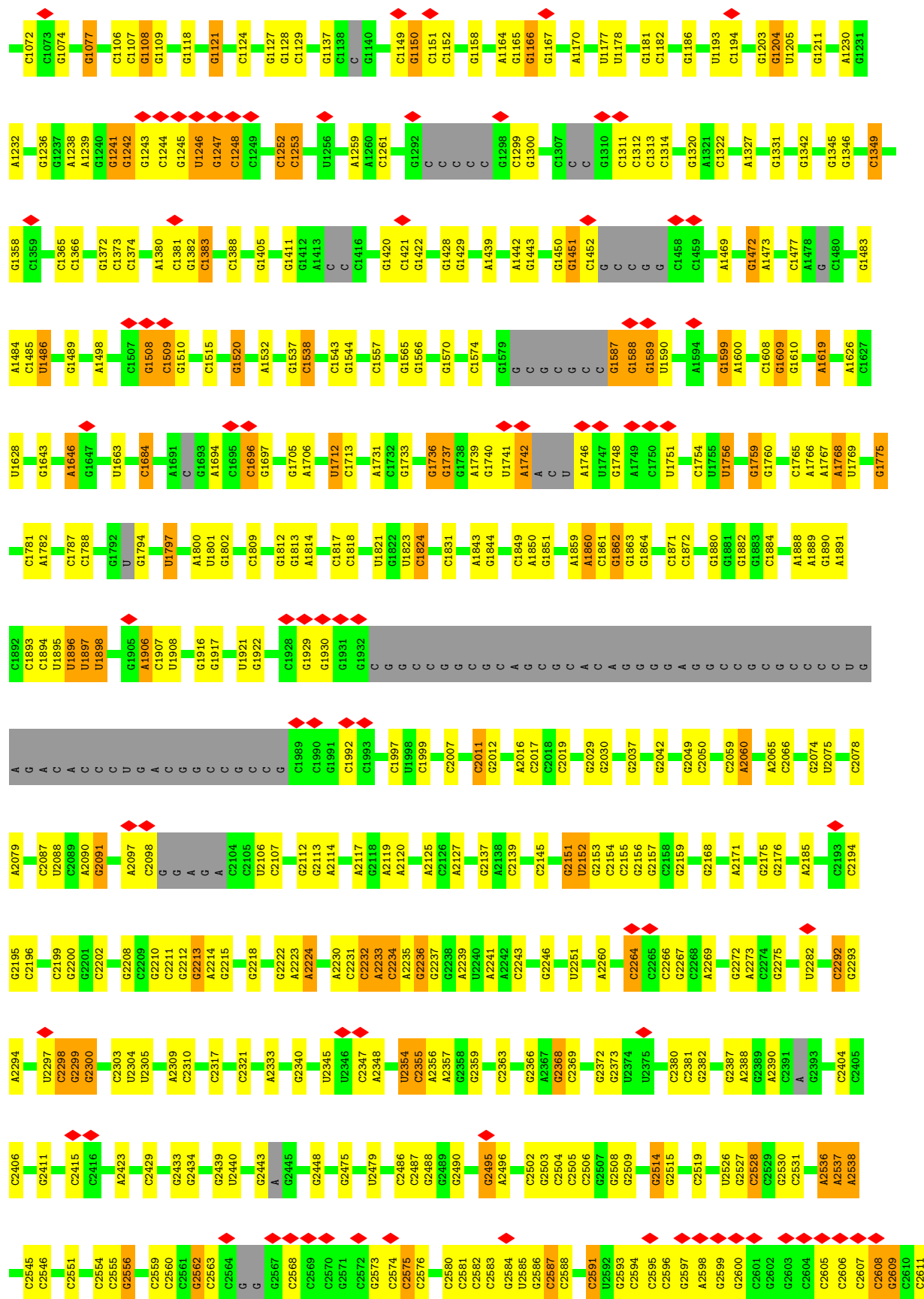
Mol	Chain	Residues	Atoms		AltConf
48	p	15	Total 15	O 15	0
48	w	6	Total 6	O 6	0
48	W	12	Total 12	O 12	0
48	E	1	Total 1	O 1	0

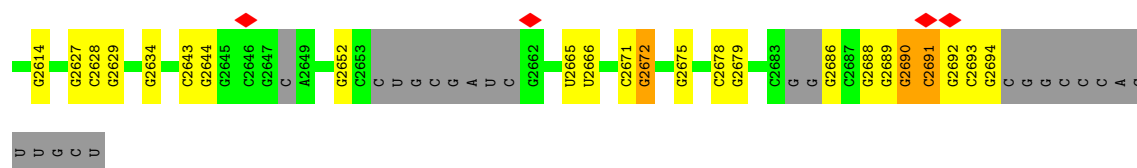
3 Residue-property plots

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: rRNA 28S

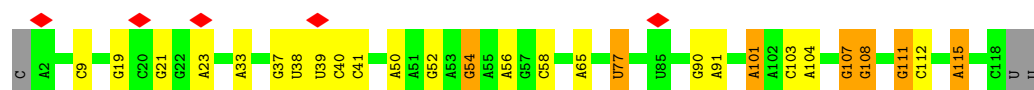






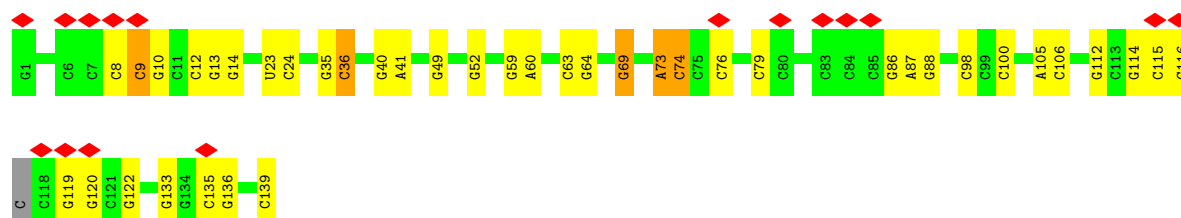
• Molecule 2: rRNA 5S

Chain 3: 75% 17% 6%



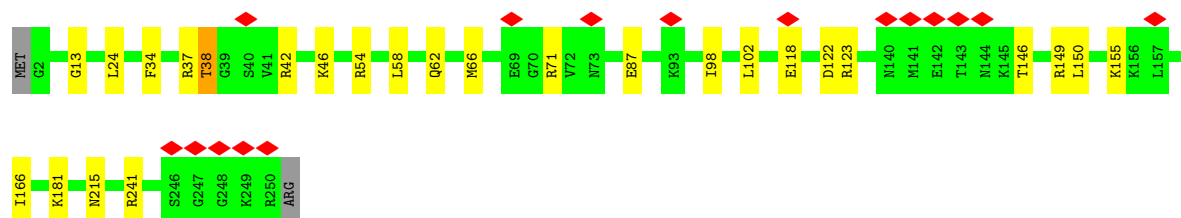
• Molecule 3: rRNA 5.8S

Chain 4: 12% 70% 26%



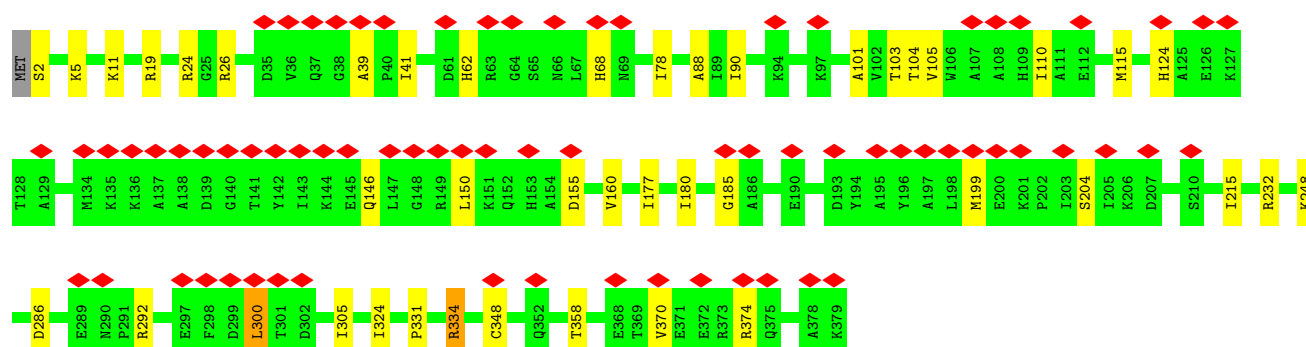
• Molecule 4: Ribosomal protein L2

Chain A: 6% 89% 10%

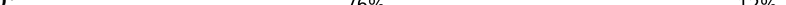


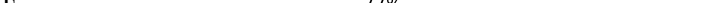
• Molecule 5: Ribosomal protein L3

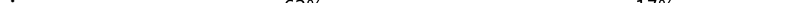
Chain B: 19% 88% 11%

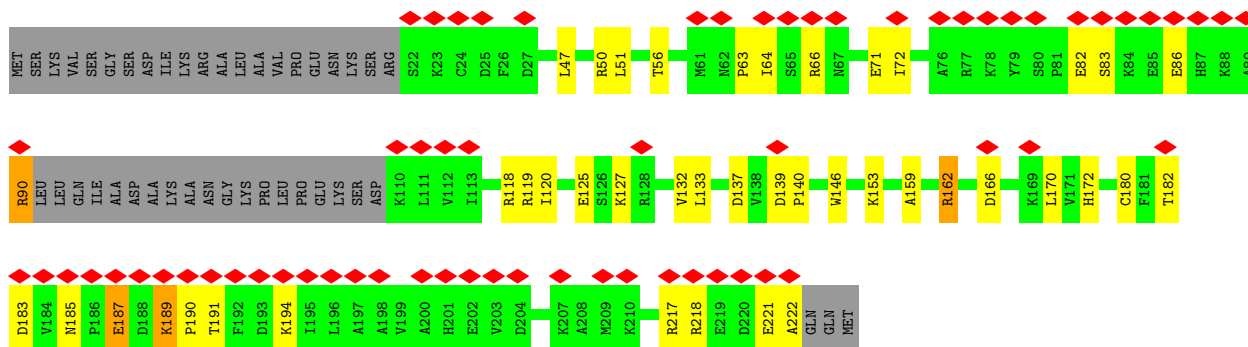


Chain C:  29% 82% 17%

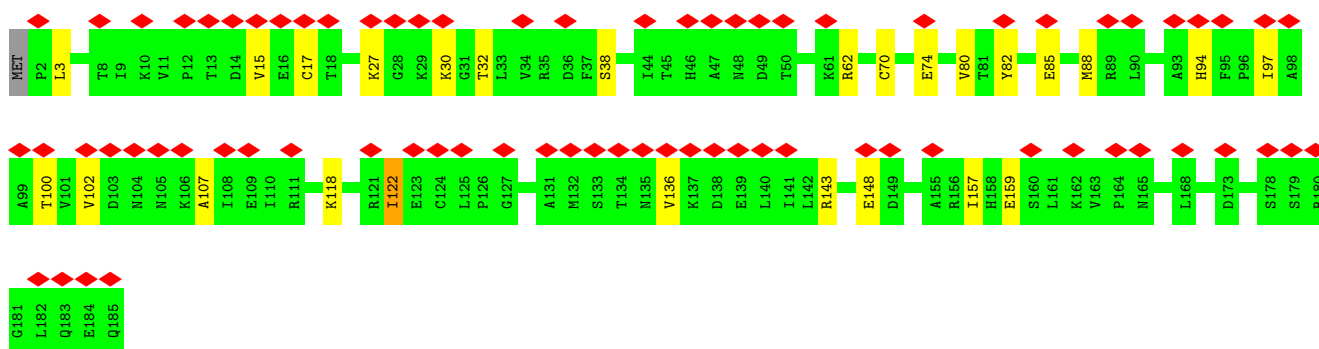
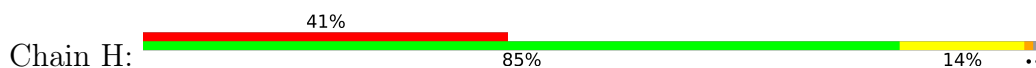
Chain D:  41% 76% 12% 10%

Chain F:  29% 77% 13% 9%

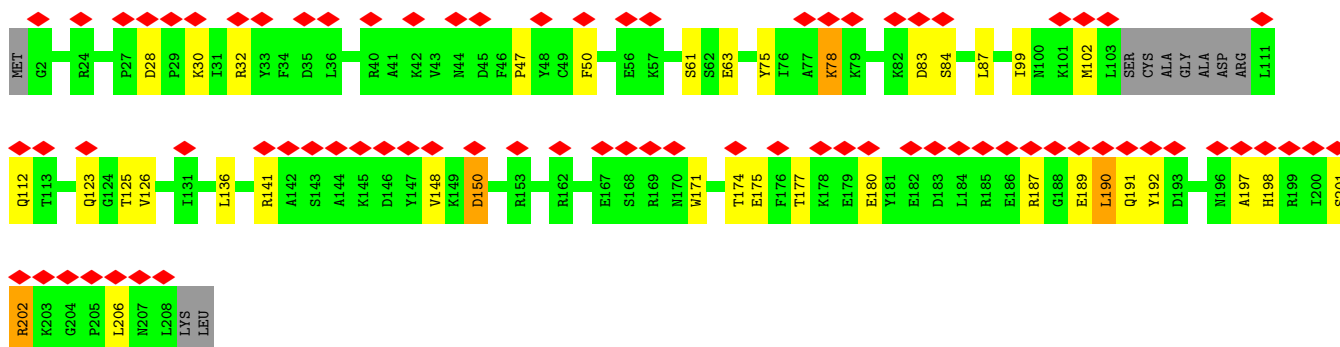
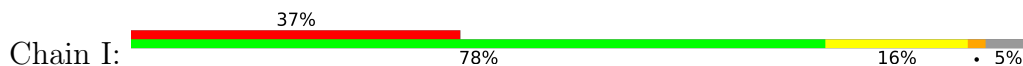
Chain G: 



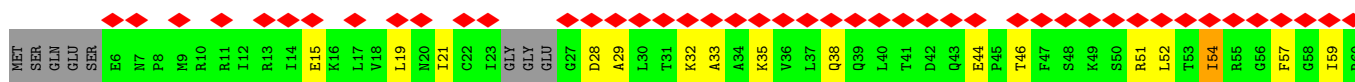
• Molecule 10: Ribosomal protein L6

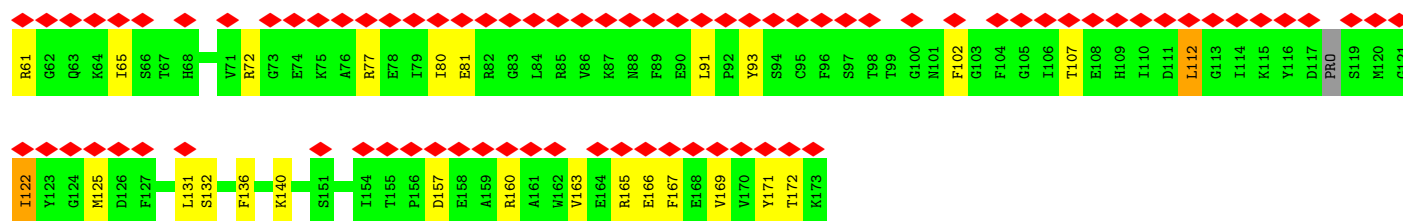


• Molecule 11: Ribosomal protein L10

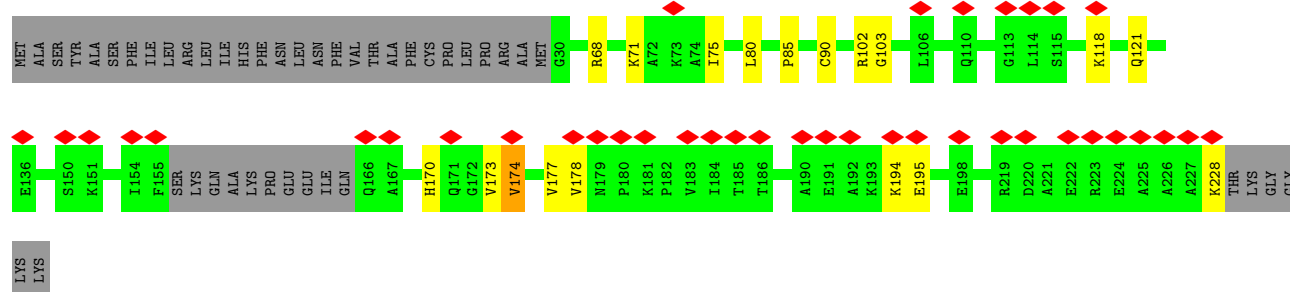
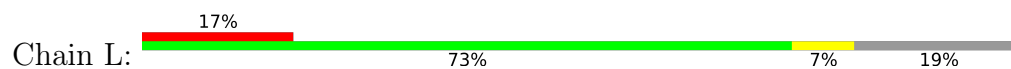


• Molecule 12: Ribosomal protein L11

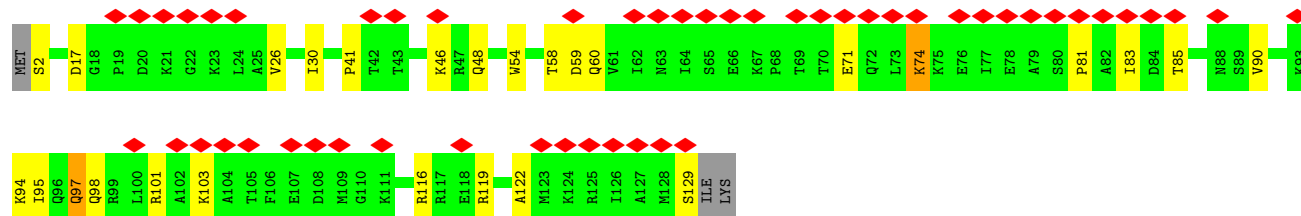
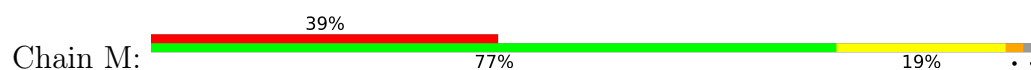




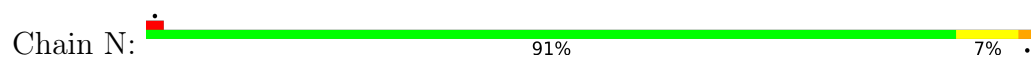
• Molecule 13: 60S ribosomal protein L13



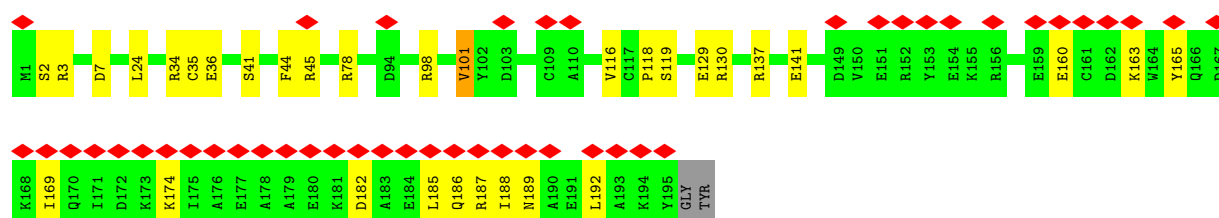
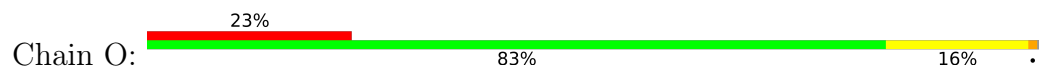
• Molecule 14: Ribosomal protein L14



• Molecule 15: Ribosomal protein L15

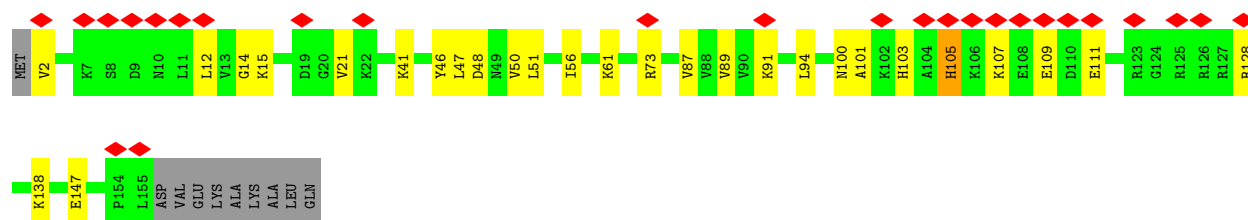


• Molecule 16: Ribosomal protein L13a



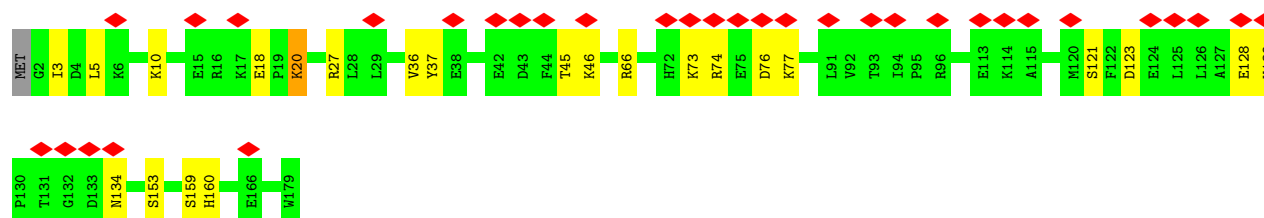
- Molecule 17: Ribosomal protein L17

Chain P: 



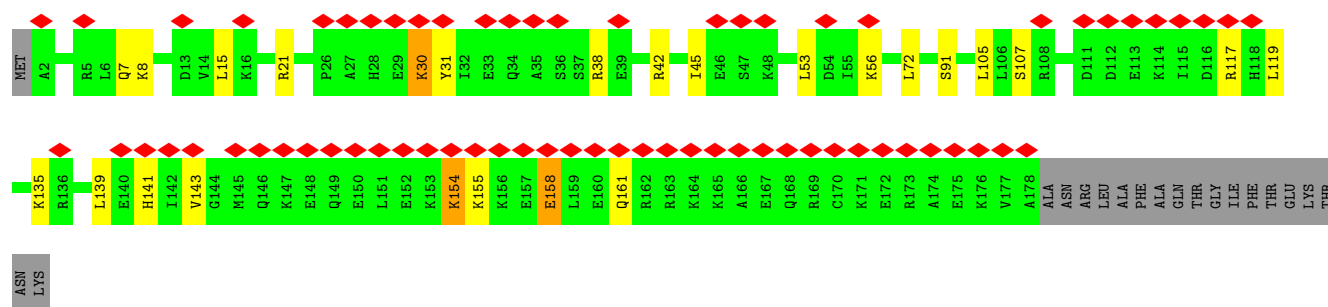
- Molecule 18: Ribosomal protein L18

Chain Q: 



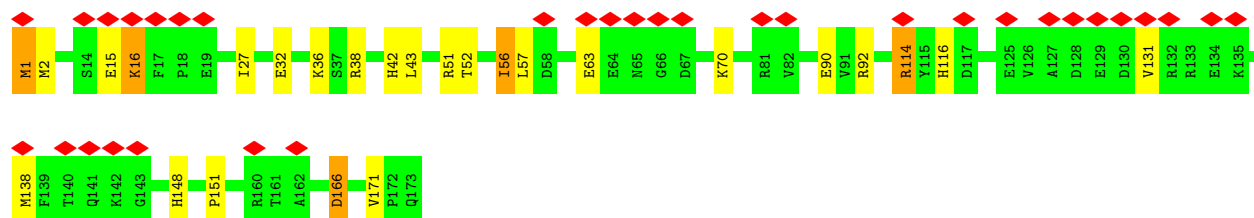
- Molecule 19: Ribosomal protein L19

Chain R: 



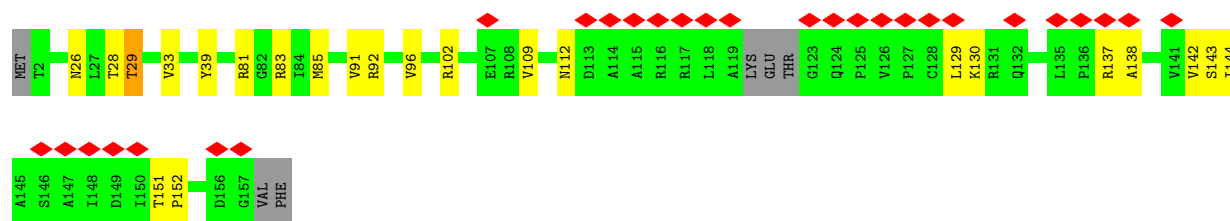
- Molecule 20: 60S ribosomal protein L18a

Chain S: 

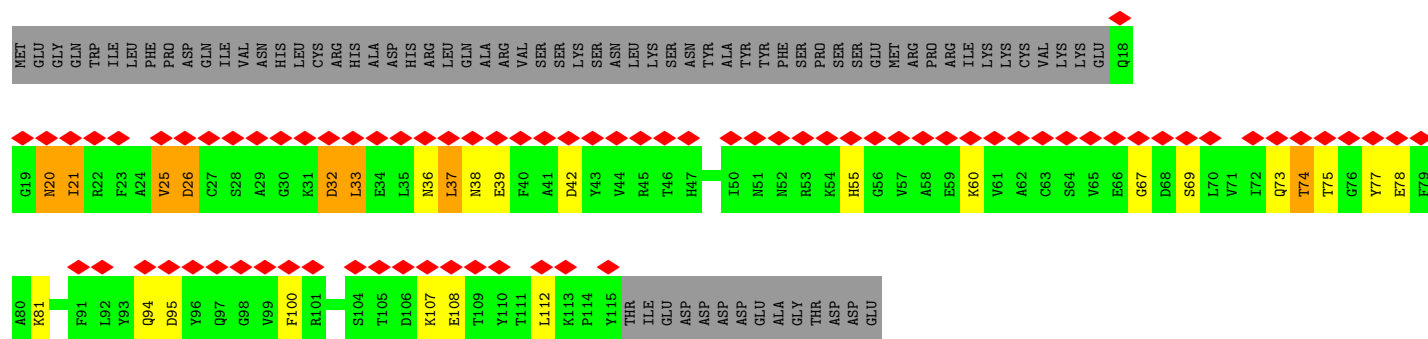


- Molecule 21: Ribosomal protein L21

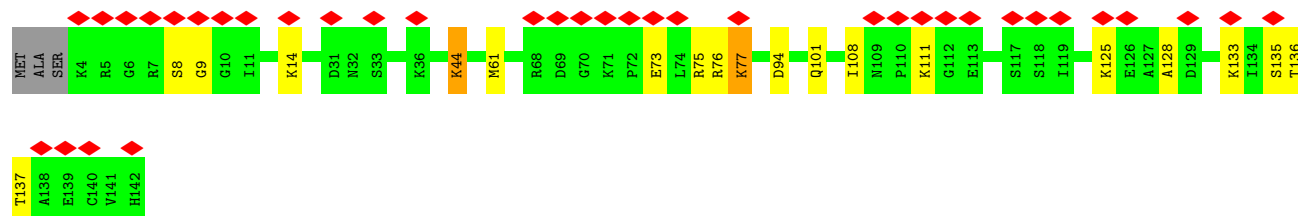
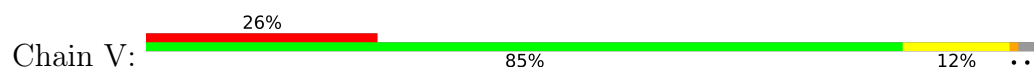
Chain T: 



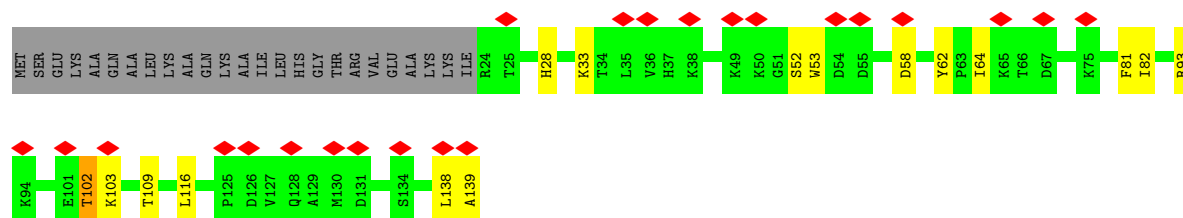
• Molecule 22: Ribosomal protein eL22



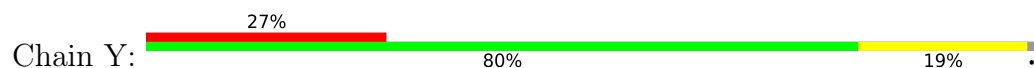
• Molecule 23: Ribosomal protein L23

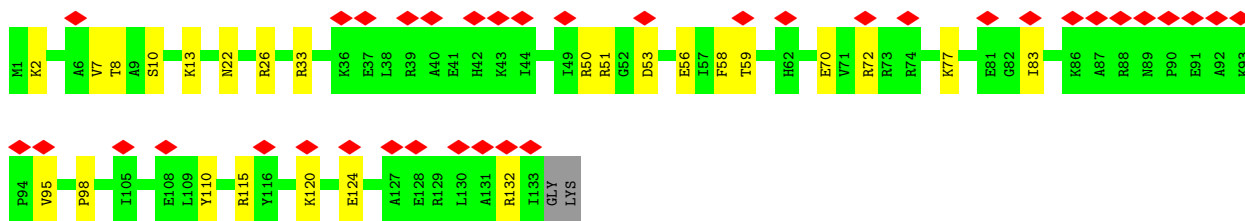


• Molecule 24: Ribosomal protein L23A

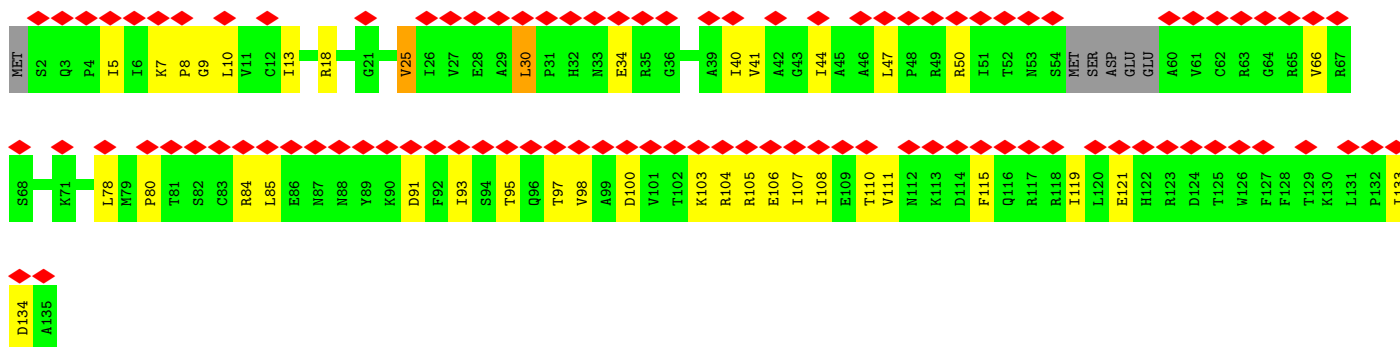
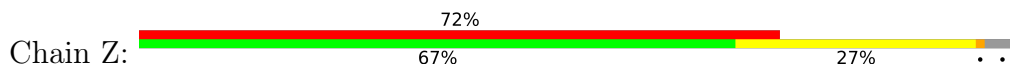


• Molecule 25: Ribosomal protein L26

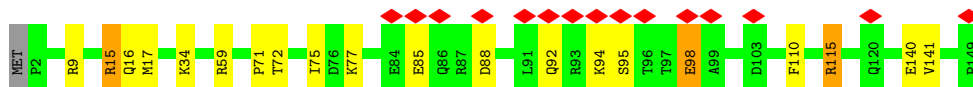
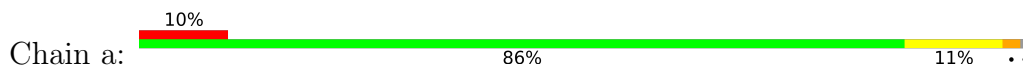




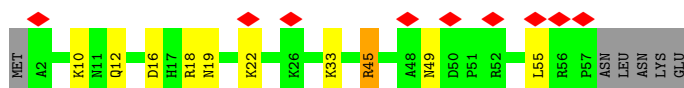
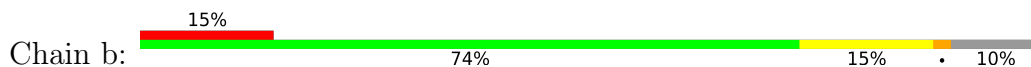
• Molecule 26: 60S ribosomal protein L27



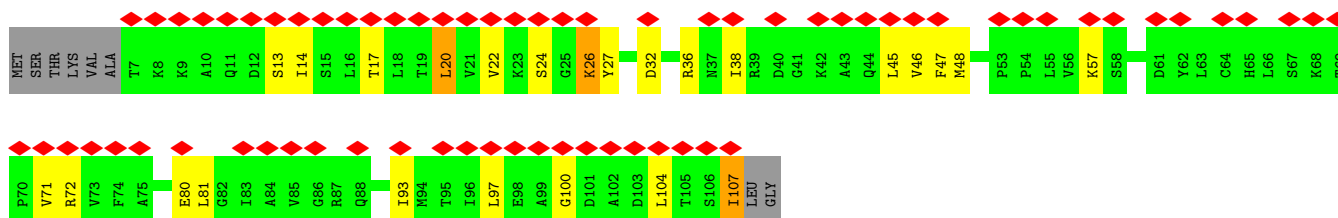
• Molecule 27: Ribosomal protein L27a



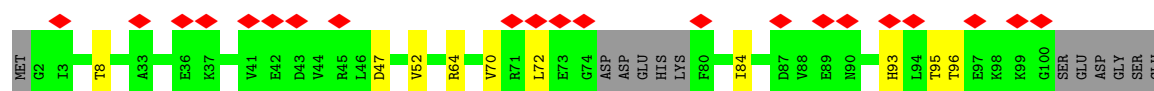
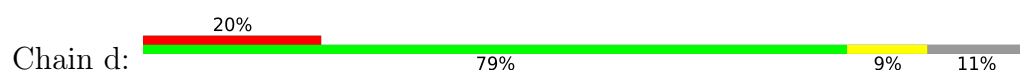
• Molecule 28: 60S ribosomal protein L29



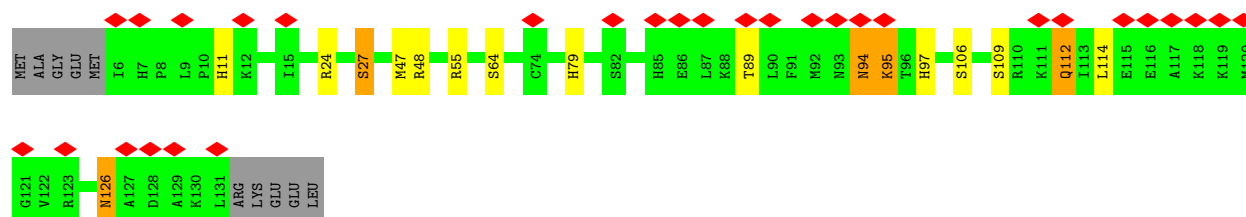
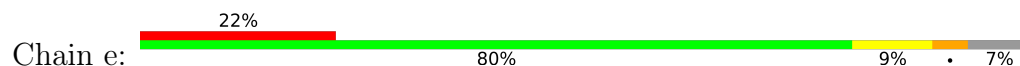
• Molecule 29: Ribosomal protein L30



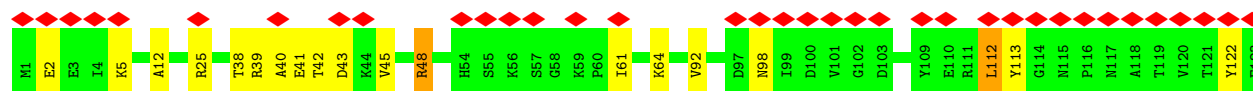
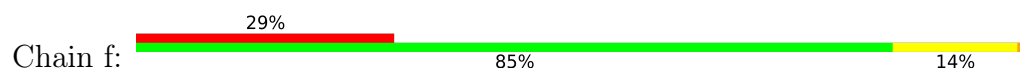
• Molecule 30: Ribosomal protein L31B



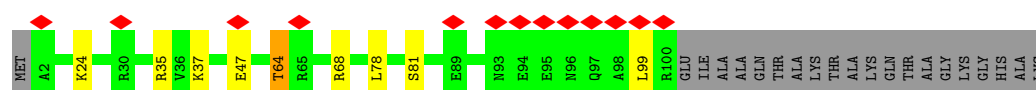
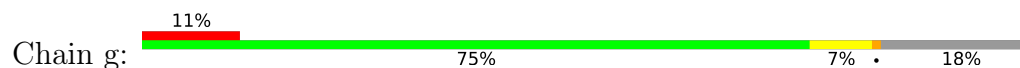
- Molecule 31: Ribosomal protein L32



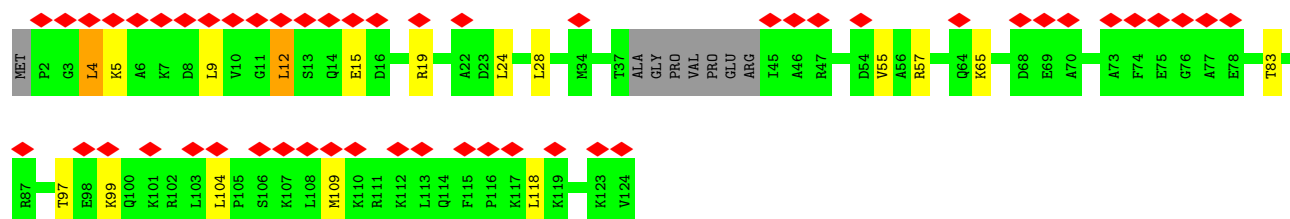
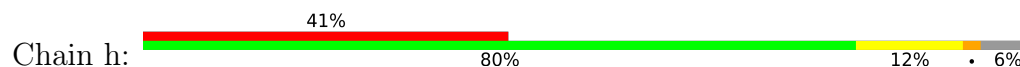
- Molecule 32: Ribosomal protein L35a



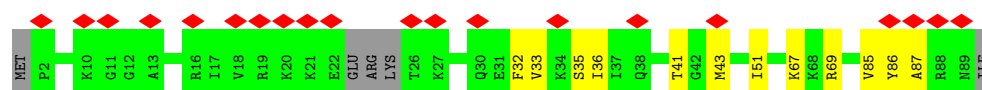
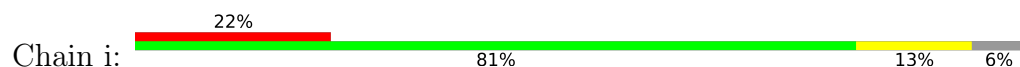
- Molecule 33: Ribosomal protein L34



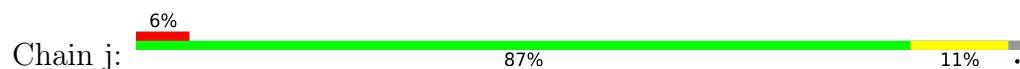
- Molecule 34: Ribosomal protein L29



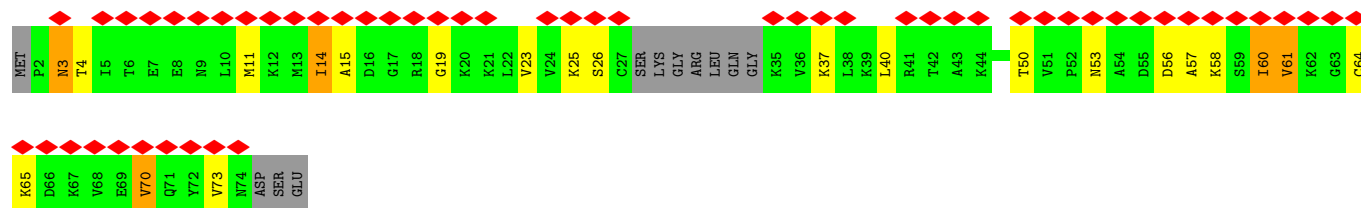
- Molecule 35: Ribosomal protein L36-1



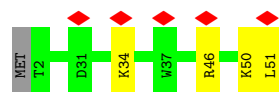
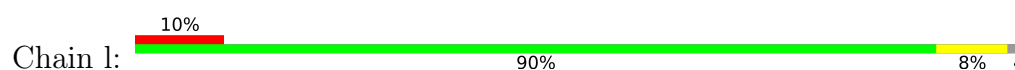
- Molecule 36: Ribosomal protein L37



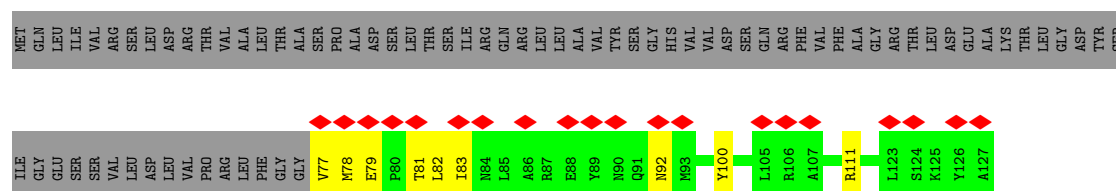
- Molecule 37: Ribosomal L38e



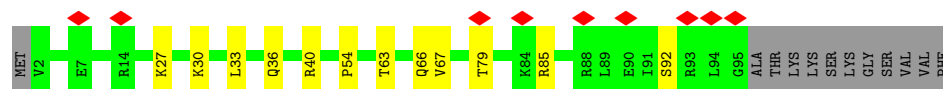
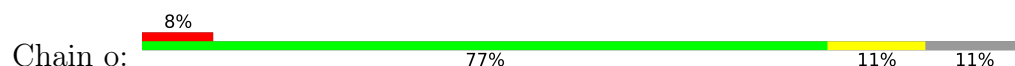
- Molecule 38: Ribosomal protein L39



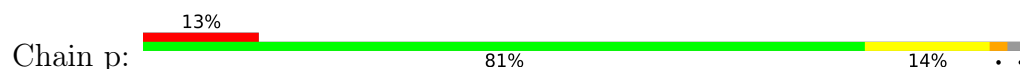
- Molecule 39: Ubiquitin/Ribosomal protein L40e



- Molecule 40: Ribosomal protein L44



- Molecule 41: Ribosomal protein L37a





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91058	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 ($e^-/\text{\AA}^2$)	1.0	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.246	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.034	Depositor
Map size ($\text{\AA}$)	374.0, 374.0, 374.0	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.85, 0.85, 0.85	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MC, A2M, MG, OMC, K, PGE, OMU, OMG

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	0.53	2/58200 (0.0%)	0.53	31/90778 (0.0%)
2	3	0.43	0/2797	0.45	0/4359
3	4	0.49	0/3277	0.47	0/5109
4	A	0.39	0/1898	0.54	0/2551
5	B	0.37	0/3058	0.49	0/4129
6	C	0.38	0/2498	0.55	0/3388
7	D	0.32	0/2160	0.51	0/2903
8	F	0.37	0/1760	0.51	0/2374
9	G	0.35	0/1476	0.49	0/1994
10	H	0.32	0/1469	0.49	0/1985
11	I	0.31	0/1657	0.46	0/2219
12	J	0.29	0/1325	0.46	0/1776
13	L	0.38	0/1533	0.51	0/2052
14	M	0.31	0/1002	0.42	0/1349
15	N	0.44	0/1755	0.56	0/2353
16	O	0.37	0/1618	0.47	0/2169
17	P	0.37	0/1261	0.52	0/1688
18	Q	0.36	0/1425	0.49	0/1907
19	R	0.33	0/1478	0.46	0/1954
20	S	0.37	0/1452	0.50	0/1955
21	T	0.37	0/1251	0.54	0/1682
22	U	0.30	0/818	0.45	0/1101
23	V	0.35	0/1077	0.49	0/1451
24	X	0.37	0/956	0.52	0/1293
25	Y	0.36	0/1091	0.50	0/1454
26	Z	0.31	0/997	0.49	0/1352
27	a	0.42	0/1231	0.58	0/1647
28	b	0.37	0/471	0.54	0/624
29	c	0.28	0/764	0.43	0/1033
30	d	0.37	0/760	0.46	0/1022
31	e	0.38	0/1063	0.55	0/1418
32	f	0.38	0/994	0.50	0/1338

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.35	0/813	0.51	0/1092
34	h	0.34	0/936	0.47	0/1247
35	i	0.35	0/700	0.48	0/927
36	j	0.41	0/708	0.52	0/941
37	k	0.27	0/503	0.43	0/675
38	l	0.36	0/445	0.51	0/594
39	m	0.33	0/426	0.46	0/568
40	o	0.38	0/773	0.52	0/1023
41	p	0.46	0/717	0.71	1/956 (0.1%)
42	w	0.40	0/332	0.46	0/511
43	W	0.36	0/551	0.46	0/738
44	E	0.28	0/68	0.38	0/103
All	All	0.46	2/111544 (0.0%)	0.52	32/163782 (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
4	A	0	1
7	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1768	A2M	O3'-P	5.17	1.61	1.56
1	1	49	OMU	O3'-P	5.12	1.61	1.56

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	2156	G	P-O3'-C3'	-7.87	108.39	120.20
1	1	2154	C	P-O3'-C3'	-7.43	109.05	120.20
1	1	1813	G	P-O3'-C3'	-7.28	109.28	120.20
1	1	2152	U	P-O3'-C3'	-6.91	109.83	120.20
1	1	2212	G	P-O3'-C3'	-6.82	109.97	120.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	13	GLY	Peptide
7	D	42	LYS	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	52618	0	26760	245	0
2	3	2501	0	1269	12	0
3	4	2958	0	1517	13	0
4	A	1865	0	1920	15	0
5	B	2987	0	3022	21	0
6	C	2446	0	2535	30	0
7	D	2118	0	2139	22	0
8	F	1730	0	1766	22	0
9	G	1450	0	1512	25	0
10	H	1442	0	1480	13	0
11	I	1621	0	1635	22	0
12	J	1305	0	1318	19	0
13	L	1512	0	1607	10	0
14	M	990	0	1022	18	0
15	N	1712	0	1790	16	0
16	O	1587	0	1634	22	0
17	P	1235	0	1265	13	0
18	Q	1402	0	1478	14	0
19	R	1463	0	1567	10	0
20	S	1418	0	1410	17	0
21	T	1226	0	1256	17	0
22	U	802	0	787	18	0
23	V	1057	0	1099	10	0
24	X	936	0	984	7	0
25	Y	1076	0	1140	13	0
26	Z	980	0	974	17	0
27	a	1201	0	1233	11	0
28	b	463	0	489	7	0
29	c	756	0	781	11	0
30	d	748	0	793	4	0
31	e	1039	0	1095	9	0
32	f	974	0	995	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	g	798	0	832	4	0
34	h	926	0	1011	9	0
35	i	691	0	748	5	0
36	j	692	0	680	7	0
37	k	500	0	524	10	0
38	l	434	0	468	1	0
39	m	421	0	441	5	0
40	o	762	0	805	6	0
41	p	708	0	745	9	0
42	w	299	0	156	2	0
43	W	540	0	575	4	0
44	E	62	0	34	0	0
45	1	99	0	0	1	0
45	4	5	0	0	0	0
45	C	1	0	0	0	0
45	F	1	0	0	0	0
45	I	1	0	0	0	0
45	P	1	0	0	0	0
45	V	1	0	0	0	0
45	a	1	0	0	0	0
45	b	1	0	0	0	0
45	o	1	0	0	0	0
46	1	163	0	0	1	0
46	3	1	0	0	0	0
46	A	3	0	0	0	0
46	B	3	0	0	0	0
46	C	2	0	0	0	0
46	I	1	0	0	0	0
46	L	1	0	0	0	0
46	N	2	0	0	0	0
46	V	1	0	0	0	0
46	a	1	0	0	0	0
46	e	1	0	0	0	0
46	j	1	0	0	0	0
46	o	1	0	0	0	0
47	1	10	0	14	0	0
48	1	3220	0	0	36	0
48	3	71	0	0	1	0
48	4	132	0	0	3	0
48	A	54	0	0	0	0
48	B	67	0	0	2	0
48	C	57	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	D	30	0	0	0	0
48	E	1	0	0	0	0
48	F	23	0	0	1	0
48	G	27	0	0	1	0
48	H	15	0	0	0	0
48	I	31	0	0	0	0
48	J	19	0	0	0	0
48	L	42	0	0	0	0
48	M	7	0	0	1	0
48	N	65	0	0	3	0
48	O	35	0	0	1	0
48	P	25	0	0	0	0
48	Q	35	0	0	0	0
48	R	19	0	0	0	0
48	S	27	0	0	0	0
48	T	38	0	0	0	0
48	U	9	0	0	1	0
48	V	12	0	0	0	0
48	W	12	0	0	0	0
48	X	30	0	0	0	0
48	Y	18	0	0	0	0
48	Z	23	0	0	0	0
48	a	41	0	0	0	0
48	b	19	0	0	0	0
48	c	3	0	0	0	0
48	d	12	0	0	1	0
48	e	28	0	0	0	0
48	f	15	0	0	0	0
48	g	27	0	0	0	0
48	h	14	0	0	1	0
48	i	15	0	0	0	0
48	j	28	0	0	2	0
48	k	4	0	0	0	0
48	l	7	0	0	0	0
48	m	4	0	0	1	0
48	o	15	0	0	0	0
48	p	15	0	0	0	0
48	w	6	0	0	0	0
All	All	109151	0	77305	673	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 4.

The worst 5 of 673 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:2011:C:OP1	4:A:37:ARG:NH1	2.05	0.88
1:1:2479:U:H3	1:1:2496:A:H61	1.27	0.81
1:1:329:A:N6	1:1:342:G:O2'	2.15	0.80
32:f:38:THR:HG22	32:f:40:ALA:H	1.48	0.78
1:1:451:G:N2	1:1:454:C:OP2	2.18	0.77

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	
4	A	247/251 (98%)	236 (96%)	11 (4%)	0	100	100
5	B	376/379 (99%)	366 (97%)	10 (3%)	0	100	100
6	C	312/316 (99%)	290 (93%)	22 (7%)	0	100	100
7	D	264/297 (89%)	245 (93%)	19 (7%)	0	100	100
8	F	212/235 (90%)	208 (98%)	4 (2%)	0	100	100
9	G	178/225 (79%)	169 (95%)	9 (5%)	0	100	100
10	H	182/185 (98%)	173 (95%)	9 (5%)	0	100	100
11	I	196/210 (93%)	186 (95%)	10 (5%)	0	100	100
12	J	158/173 (91%)	145 (92%)	13 (8%)	0	100	100
13	L	185/234 (79%)	179 (97%)	6 (3%)	0	100	100
14	M	126/131 (96%)	121 (96%)	5 (4%)	0	100	100
15	N	202/204 (99%)	192 (95%)	10 (5%)	0	100	100
16	O	193/197 (98%)	188 (97%)	5 (3%)	0	100	100
17	P	152/164 (93%)	143 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	Q	176/179 (98%)	170 (97%)	6 (3%)	0	100	100
19	R	175/196 (89%)	170 (97%)	5 (3%)	0	100	100
20	S	171/173 (99%)	166 (97%)	5 (3%)	0	100	100
21	T	149/159 (94%)	145 (97%)	4 (3%)	0	100	100
22	U	96/171 (56%)	90 (94%)	6 (6%)	0	100	100
23	V	137/142 (96%)	131 (96%)	6 (4%)	0	100	100
24	X	114/141 (81%)	107 (94%)	7 (6%)	0	100	100
25	Y	131/135 (97%)	126 (96%)	5 (4%)	0	100	100
26	Z	125/135 (93%)	113 (90%)	12 (10%)	0	100	100
27	a	146/149 (98%)	139 (95%)	7 (5%)	0	100	100
28	b	54/62 (87%)	54 (100%)	0	0	100	100
29	c	99/109 (91%)	95 (96%)	4 (4%)	0	100	100
30	d	90/106 (85%)	85 (94%)	5 (6%)	0	100	100
31	e	124/136 (91%)	117 (94%)	6 (5%)	1 (1%)	16	30
32	f	121/123 (98%)	117 (97%)	4 (3%)	0	100	100
33	g	97/120 (81%)	95 (98%)	2 (2%)	0	100	100
34	h	112/124 (90%)	109 (97%)	3 (3%)	0	100	100
35	i	81/90 (90%)	78 (96%)	3 (4%)	0	100	100
36	j	85/89 (96%)	82 (96%)	3 (4%)	0	100	100
37	k	62/77 (80%)	60 (97%)	2 (3%)	0	100	100
38	l	48/51 (94%)	45 (94%)	3 (6%)	0	100	100
39	m	49/127 (39%)	47 (96%)	2 (4%)	0	100	100
40	o	92/106 (87%)	90 (98%)	2 (2%)	0	100	100
41	p	89/94 (95%)	87 (98%)	2 (2%)	0	100	100
43	W	63/102 (62%)	61 (97%)	2 (3%)	0	100	100
All	All	5669/6297 (90%)	5420 (96%)	248 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
31	e	95	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	A	188/192 (98%)	184 (98%)	4 (2%)	47	67
5	B	312/313 (100%)	301 (96%)	11 (4%)	32	56
6	C	261/263 (99%)	246 (94%)	15 (6%)	18	35
7	D	211/242 (87%)	201 (95%)	10 (5%)	23	45
8	F	184/204 (90%)	177 (96%)	7 (4%)	29	52
9	G	160/198 (81%)	144 (90%)	16 (10%)	7	14
10	H	160/164 (98%)	151 (94%)	9 (6%)	19	36
11	I	166/177 (94%)	158 (95%)	8 (5%)	23	44
12	J	137/149 (92%)	121 (88%)	16 (12%)	5	9
13	L	159/197 (81%)	153 (96%)	6 (4%)	29	52
14	M	103/111 (93%)	95 (92%)	8 (8%)	11	21
15	N	174/175 (99%)	167 (96%)	7 (4%)	28	50
16	O	164/165 (99%)	159 (97%)	5 (3%)	36	60
17	P	130/139 (94%)	121 (93%)	9 (7%)	14	26
18	Q	154/155 (99%)	151 (98%)	3 (2%)	50	70
19	R	149/167 (89%)	136 (91%)	13 (9%)	9	18
20	S	147/154 (96%)	136 (92%)	11 (8%)	12	24
21	T	126/133 (95%)	121 (96%)	5 (4%)	28	50
22	U	85/153 (56%)	75 (88%)	10 (12%)	5	9
23	V	111/114 (97%)	104 (94%)	7 (6%)	16	30
24	X	104/123 (85%)	98 (94%)	6 (6%)	18	34
25	Y	114/115 (99%)	107 (94%)	7 (6%)	17	31
26	Z	101/119 (85%)	87 (86%)	14 (14%)	3	6
27	a	126/127 (99%)	115 (91%)	11 (9%)	9	18
28	b	51/57 (90%)	48 (94%)	3 (6%)	18	33
29	c	84/92 (91%)	72 (86%)	12 (14%)	3	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	d	77/92 (84%)	72 (94%)	5 (6%)	15	29
31	e	112/120 (93%)	104 (93%)	8 (7%)	13	25
32	f	102/103 (99%)	96 (94%)	6 (6%)	18	33
33	g	87/100 (87%)	84 (97%)	3 (3%)	32	57
34	h	98/107 (92%)	92 (94%)	6 (6%)	17	31
35	i	72/78 (92%)	68 (94%)	4 (6%)	19	36
36	j	70/74 (95%)	68 (97%)	2 (3%)	37	61
37	k	55/68 (81%)	47 (86%)	8 (14%)	3	5
38	l	46/48 (96%)	44 (96%)	2 (4%)	26	47
39	m	46/110 (42%)	44 (96%)	2 (4%)	26	47
40	o	81/93 (87%)	76 (94%)	5 (6%)	16	31
41	p	71/73 (97%)	63 (89%)	8 (11%)	5	11
43	W	58/92 (63%)	56 (97%)	2 (3%)	32	57
All	All	4836/5356 (90%)	4542 (94%)	294 (6%)	19	31

5 of 294 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
29	c	93	ILE
41	p	39	CYS
31	e	27	SER
34	h	83	THR
13	L	173	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
20	S	122	ASN
37	k	9	ASN
26	Z	112	ASN
43	W	25	HIS
34	h	90	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	2423/2707 (89%)	395 (16%)	20 (0%)
2	3	116/120 (96%)	17 (14%)	2 (1%)
3	4	136/139 (97%)	28 (20%)	1 (0%)
42	w	12/76 (15%)	5 (41%)	0
44	E	2/3 (66%)	1 (50%)	0
All	All	2689/3045 (88%)	446 (16%)	23 (0%)

5 of 446 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	21	G
1	1	39	A
1	1	42	A
1	1	48	G
1	1	56	C

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	1871	C
1	1	2354	U
1	1	2151	G
1	1	2530	G
1	1	675	C

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	1	393	1	22,25,26	1.35	3 (13%)	30,36,39	1.20	4 (13%)
1	OMG	1	1775	1	23,26,27	0.92	0	32,38,41	1.18	4 (12%)
1	OMG	1	2074	1	23,26,27	0.94	3 (13%)	32,38,41	1.00	2 (6%)
1	OMC	1	2380	1	19,22,23	0.88	1 (5%)	25,31,34	1.19	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	A2M	1	396	46,1	22,25,26	1.42	1 (4%)	30,36,39	0.90	1 (3%)
1	OMG	1	1882	1	23,26,27	1.23	3 (13%)	32,38,41	2.22	7 (21%)
1	OMU	1	1896	46,1	19,22,23	0.82	1 (5%)	25,31,34	1.04	2 (8%)
1	OMG	1	624	1	23,26,27	0.84	0	32,38,41	1.31	7 (21%)
1	OMG	1	1204	1	23,26,27	0.93	1 (4%)	32,38,41	1.48	6 (18%)
1	OMG	1	1520	1	23,26,27	0.87	0	32,38,41	1.19	5 (15%)
1	5MC	1	1765	1	19,22,23	1.54	5 (26%)	26,32,35	1.12	3 (11%)
1	OMC	1	1684	46,1	19,22,23	0.94	1 (5%)	25,31,34	1.25	4 (16%)
1	OMU	1	1897	46,1	19,22,23	0.82	0	25,31,34	0.97	1 (4%)
3	OMG	4	133	3,1	23,26,27	0.95	2 (8%)	32,38,41	0.99	1 (3%)
1	OMG	1	2042	44,1	23,26,27	0.93	1 (4%)	32,38,41	1.13	4 (12%)
1	OMU	1	49	46,1	19,22,23	0.91	1 (5%)	25,31,34	0.95	1 (4%)
1	OMC	1	1824	1	19,22,23	0.79	1 (5%)	25,31,34	1.26	4 (16%)
1	OMG	1	1121	45,1	23,26,27	0.89	1 (4%)	32,38,41	1.17	3 (9%)
1	OMU	1	1908	1	19,22,23	1.86	5 (26%)	25,31,34	1.38	4 (16%)
1	5MC	1	2292	46,1	19,22,23	1.79	7 (36%)	26,32,35	1.47	3 (11%)
1	A2M	1	523	1	22,25,26	1.38	3 (13%)	30,36,39	1.04	2 (6%)
1	A2M	1	1768	1	22,25,26	1.22	1 (4%)	30,36,39	1.63	4 (13%)
1	OMG	1	2237	46,1	23,26,27	0.81	0	32,38,41	1.13	3 (9%)
1	OMG	1	386	1	23,26,27	0.98	1 (4%)	32,38,41	1.20	3 (9%)
1	OMG	1	313	1	23,26,27	0.91	1 (4%)	32,38,41	1.16	3 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	A2M	1	393	1	-	2/9/27/28	0/3/3/3
1	OMG	1	1775	1	-	2/9/27/28	0/3/3/3
1	OMG	1	2074	1	-	1/9/27/28	0/3/3/3
1	OMC	1	2380	1	-	0/9/27/28	0/2/2/2
1	A2M	1	396	46,1	-	0/9/27/28	0/3/3/3
1	OMG	1	1882	1	-	3/9/27/28	0/3/3/3
1	OMU	1	1896	46,1	-	0/9/27/28	0/2/2/2
1	OMG	1	624	1	-	1/9/27/28	0/3/3/3
1	OMG	1	1204	1	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	1	1520	1	-	2/9/27/28	0/3/3/3
1	5MC	1	1765	1	-	0/7/25/26	0/2/2/2
1	OMC	1	1684	46,1	-	5/9/27/28	0/2/2/2
1	OMU	1	1897	46,1	-	0/9/27/28	0/2/2/2
3	OMG	4	133	3,1	-	1/9/27/28	0/3/3/3
1	OMG	1	2042	44,1	-	0/9/27/28	0/3/3/3
1	OMU	1	49	46,1	-	1/9/27/28	0/2/2/2
1	OMC	1	1824	1	-	1/9/27/28	0/2/2/2
1	OMG	1	1121	45,1	-	2/9/27/28	0/3/3/3
1	OMU	1	1908	1	-	2/9/27/28	0/2/2/2
1	5MC	1	2292	46,1	-	5/7/25/26	0/2/2/2
1	A2M	1	523	1	-	1/9/27/28	0/3/3/3
1	A2M	1	1768	1	-	3/9/27/28	0/3/3/3
1	OMG	1	2237	46,1	-	0/9/27/28	0/3/3/3
1	OMG	1	386	1	-	0/9/27/28	0/3/3/3
1	OMG	1	313	1	-	2/9/27/28	0/3/3/3

The worst 5 of 43 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	1	1908	OMU	O5'-C5'	-5.36	1.28	1.44
1	1	393	A2M	O5'-C5'	-4.19	1.32	1.44
1	1	396	A2M	O5'-C5'	-4.07	1.32	1.44
1	1	2292	5MC	C2-N1	4.04	1.48	1.40
1	1	1768	A2M	O5'-C5'	-3.89	1.32	1.44

The worst 5 of 85 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	1882	OMG	C5-C4-N3	-6.39	118.22	128.39
1	1	1882	OMG	C2-N3-C4	5.25	121.33	112.30
1	1	1768	A2M	C2'-C1'-N9	-4.80	105.86	113.75
1	1	1882	OMG	N9-C4-N3	4.67	135.30	125.95
1	1	1882	OMG	C2'-C1'-N9	-4.45	105.80	114.24

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	4	133	OMG	C1'-C2'-O2'-CM2

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Mol	Chain	Res	Type	Atoms
1	1	49	OMU	C1'-C2'-O2'-CM2
1	1	313	OMG	O4'-C4'-C5'-O5'
1	1	624	OMG	C1'-C2'-O2'-CM2
1	1	1684	OMC	C2'-C1'-N1-C6

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1	393	A2M	1	0
1	1	1896	OMU	2	0
1	1	624	OMG	1	0
1	1	1684	OMC	1	0
1	1	1897	OMU	1	0
1	1	49	OMU	1	0
1	1	1824	OMC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 294 ligands modelled in this entry, 293 are monoatomic - leaving 1 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	PGE	1	3063	46	9,9,9	0.29	0	8,8,8	0.35	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	PGE	1	3063	46	-	4/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
47	1	3063	PGE	O3-C5-C6-O4
47	1	3063	PGE	C6-C5-O3-C4
47	1	3063	PGE	O1-C1-C2-O2
47	1	3063	PGE	O2-C3-C4-O3

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.

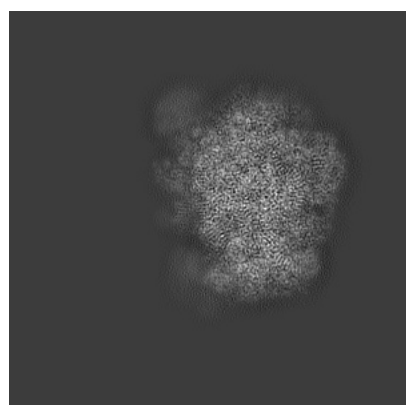
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13681. These allow visual inspection of the internal detail of the map and identification of artifacts.

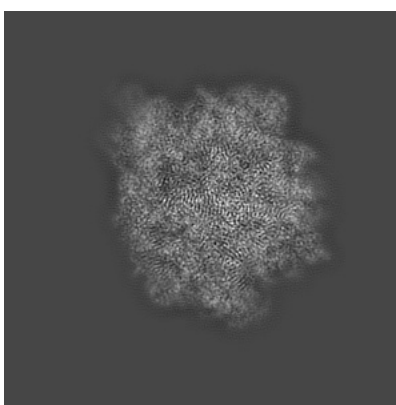
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

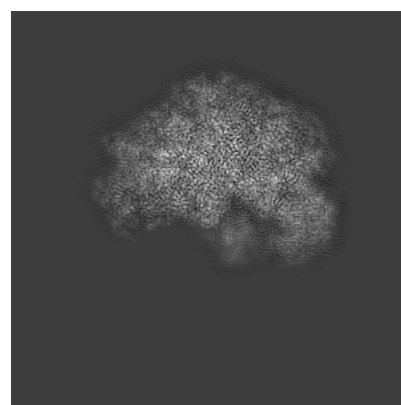
6.1.1 Primary map



X



Y

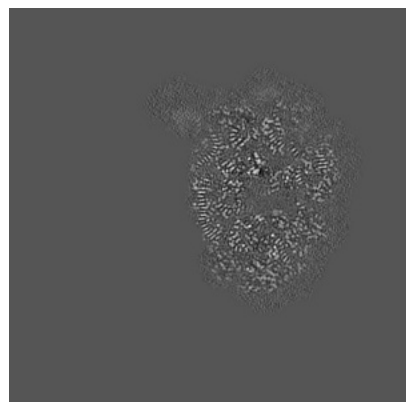


Z

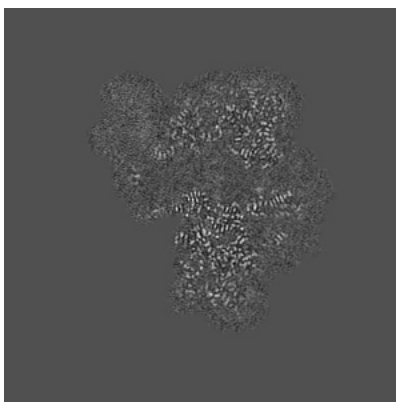
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

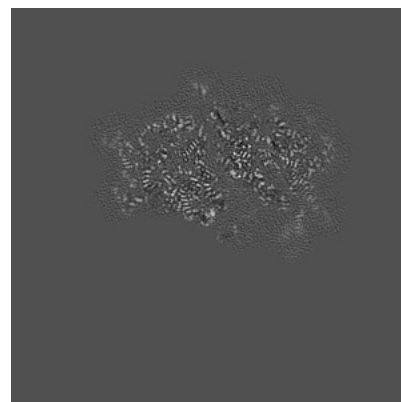
6.2.1 Primary map



X Index: 220



Y Index: 220

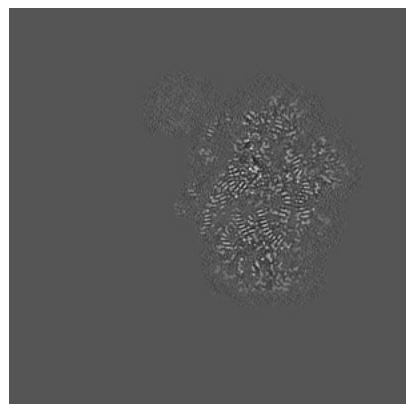


Z Index: 220

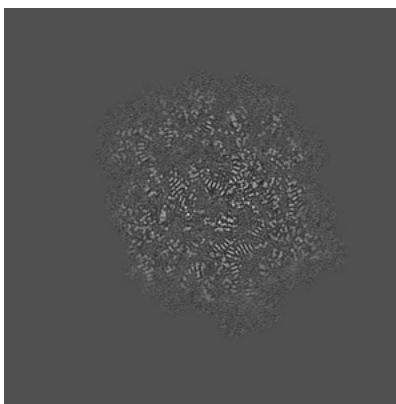
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

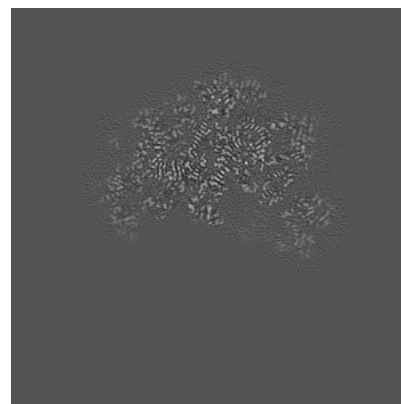
6.3.1 Primary map



X Index: 230



Y Index: 264

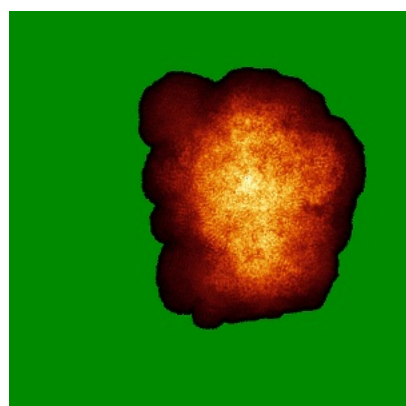


Z Index: 245

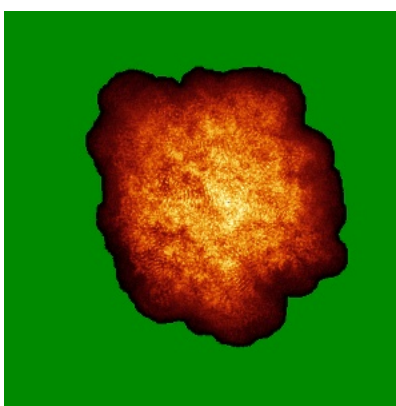
The images above show the largest variance slices of the map in three orthogonal directions.

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

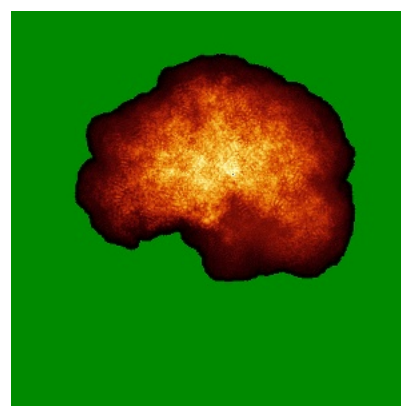
6.4.1 Primary map



X



Y

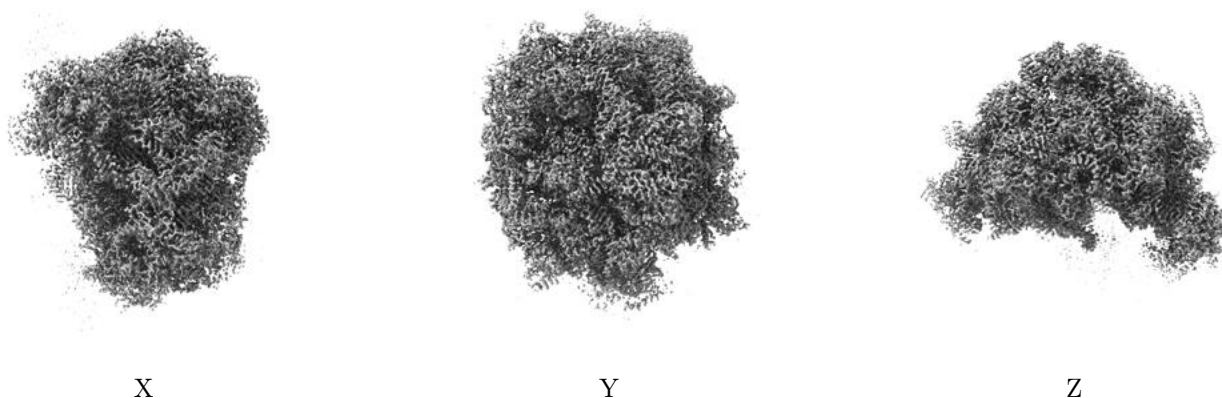


Z

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 0.034. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

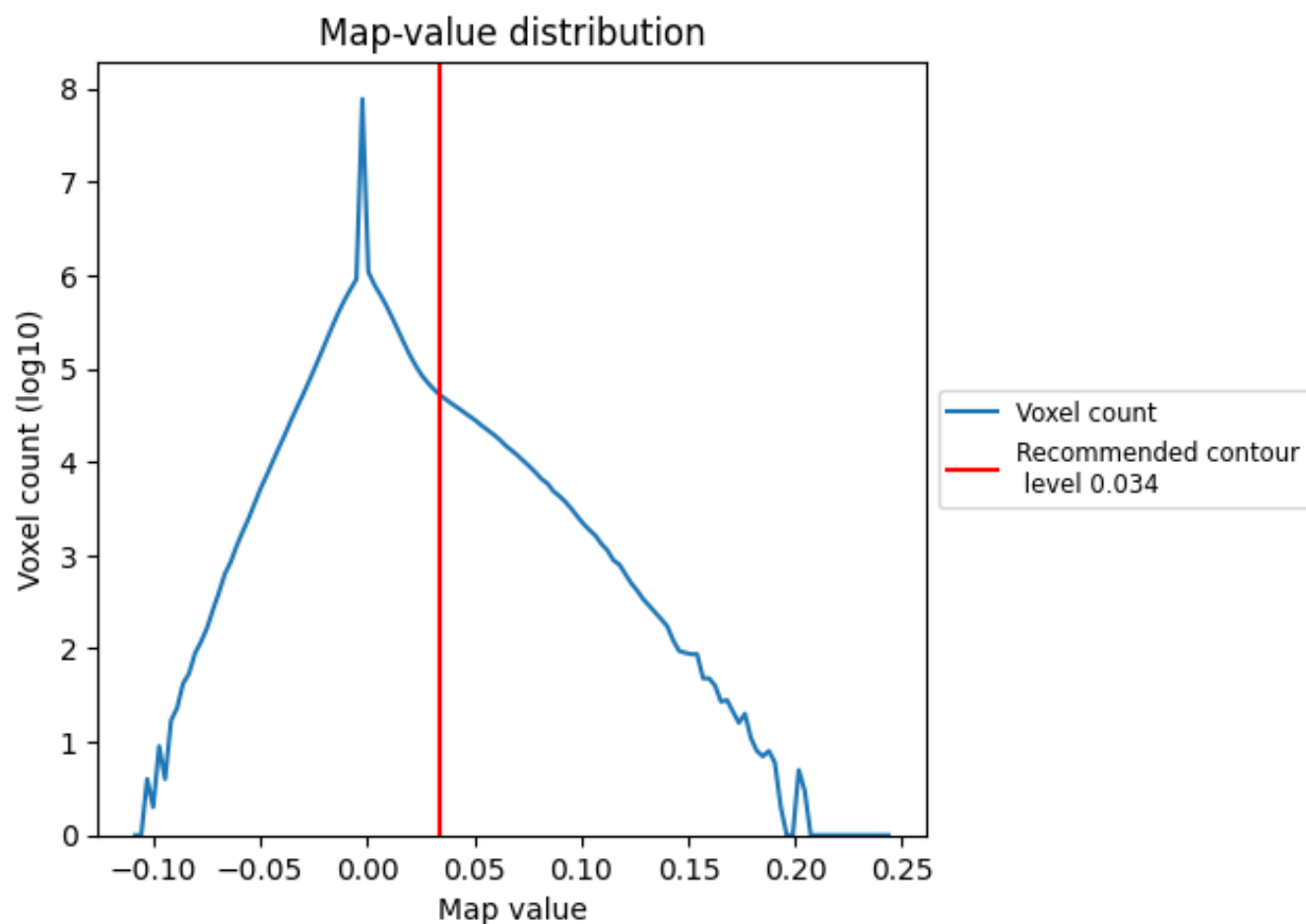
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

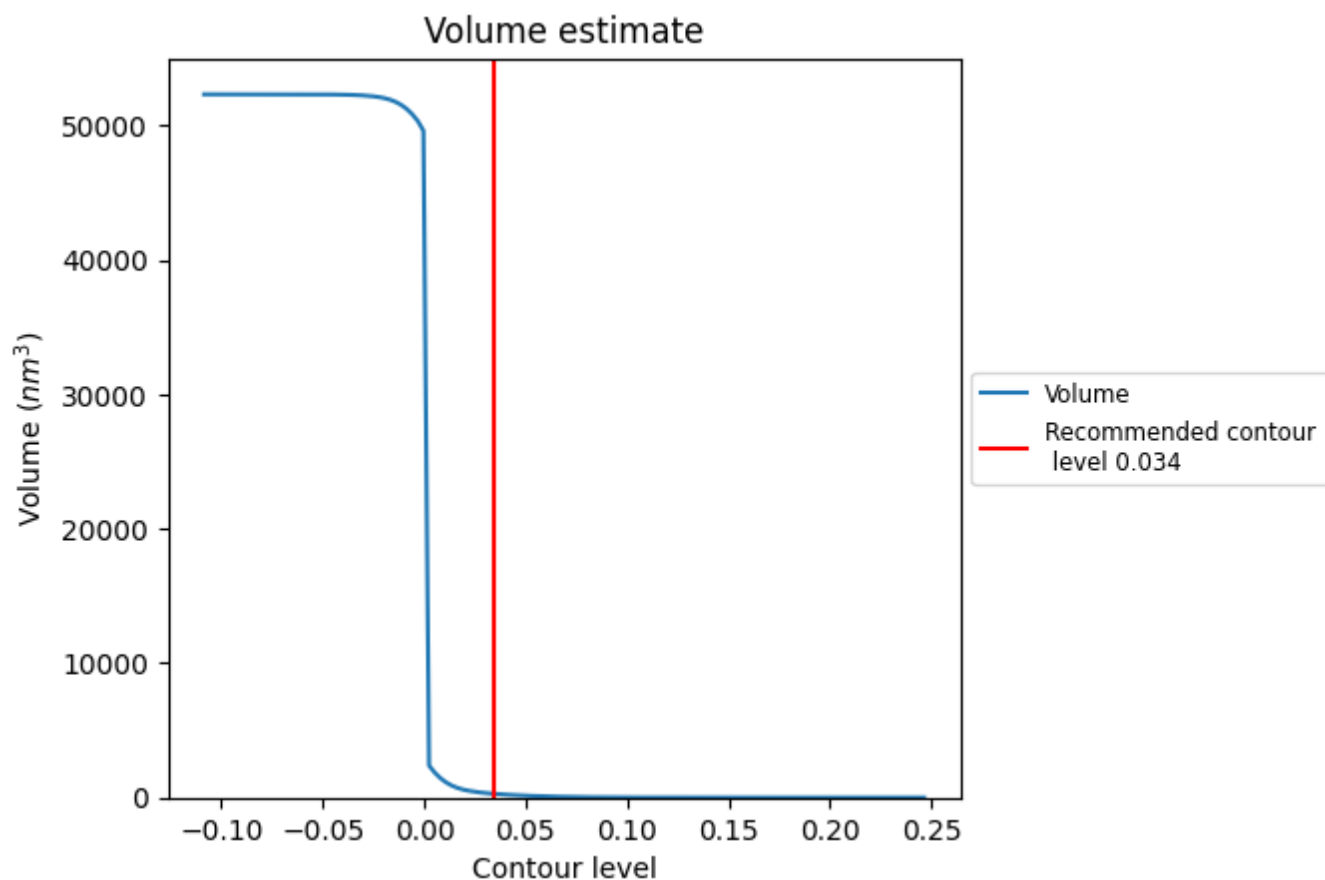
This section contains the results of statistical analysis of the map.

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.

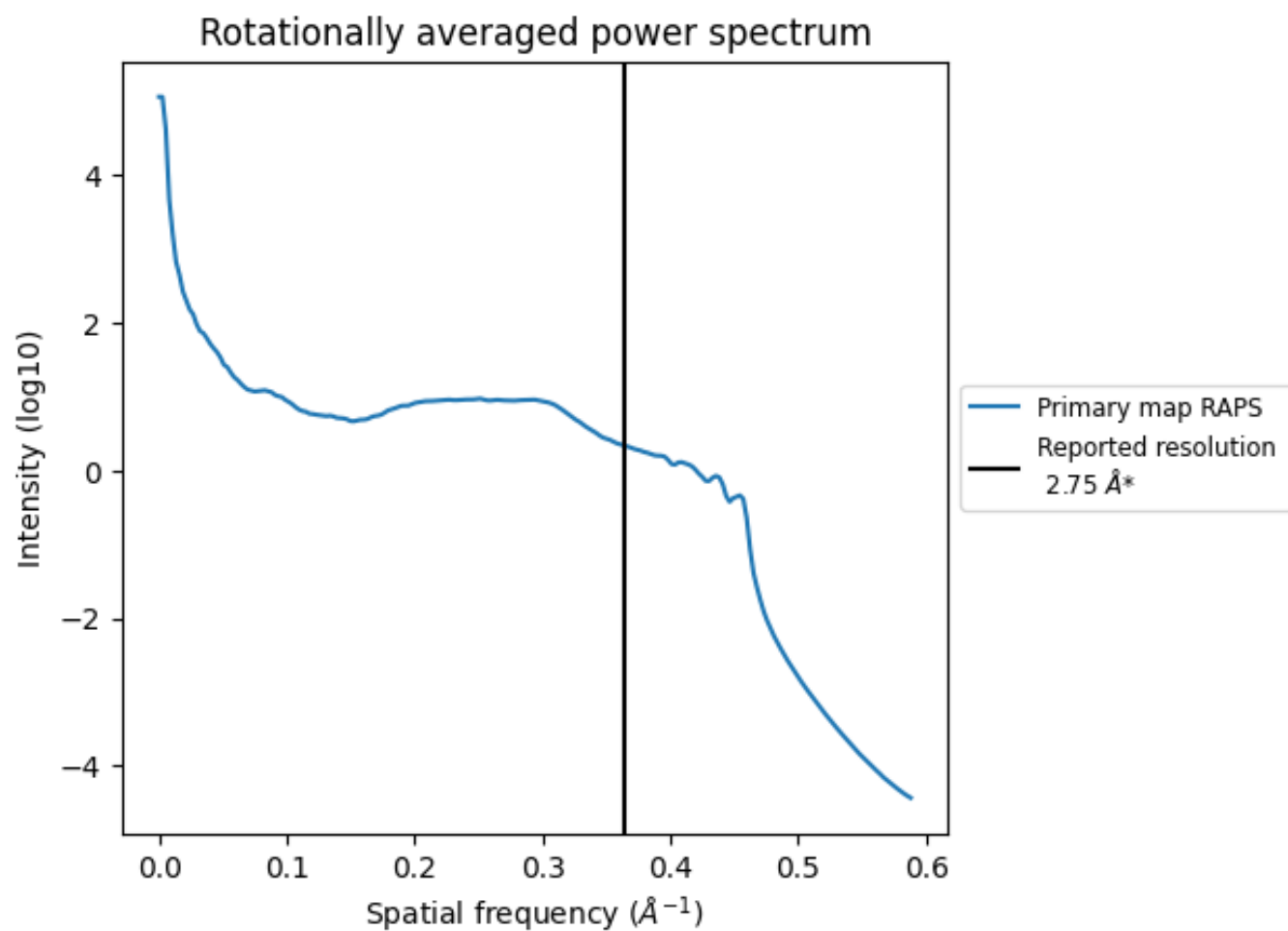
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 286 nm³; this corresponds to an approximate mass of 258 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.364 Å⁻¹

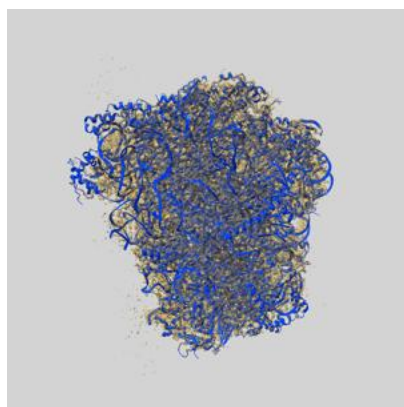
8 Fourier-Shell correlation

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

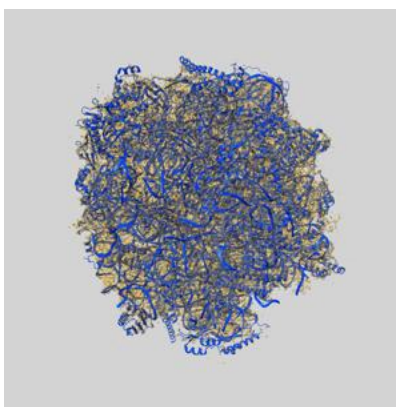
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13681 and PDB model 7PWG. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

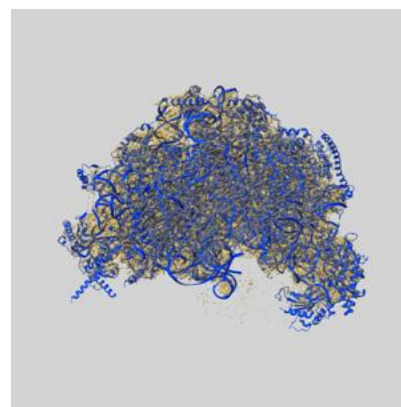
9.1 Map-model overlay [i](#)



X



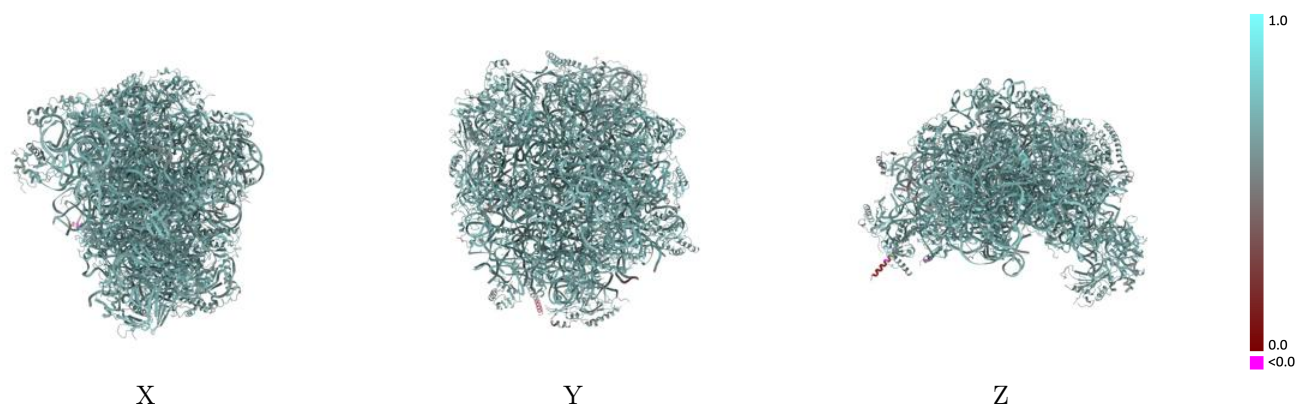
Y



Z

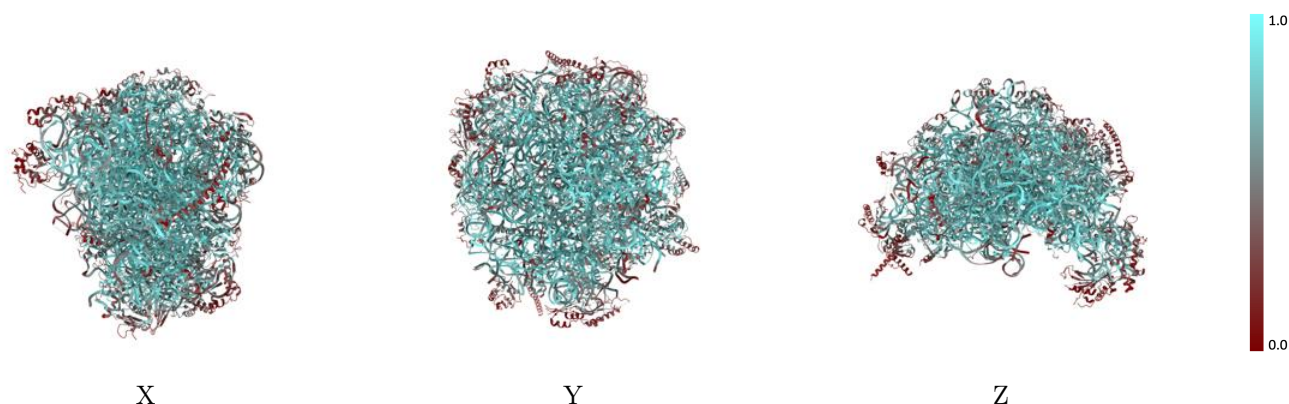
The images above show the 3D surface view of the map at the recommended contour level 0.034 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



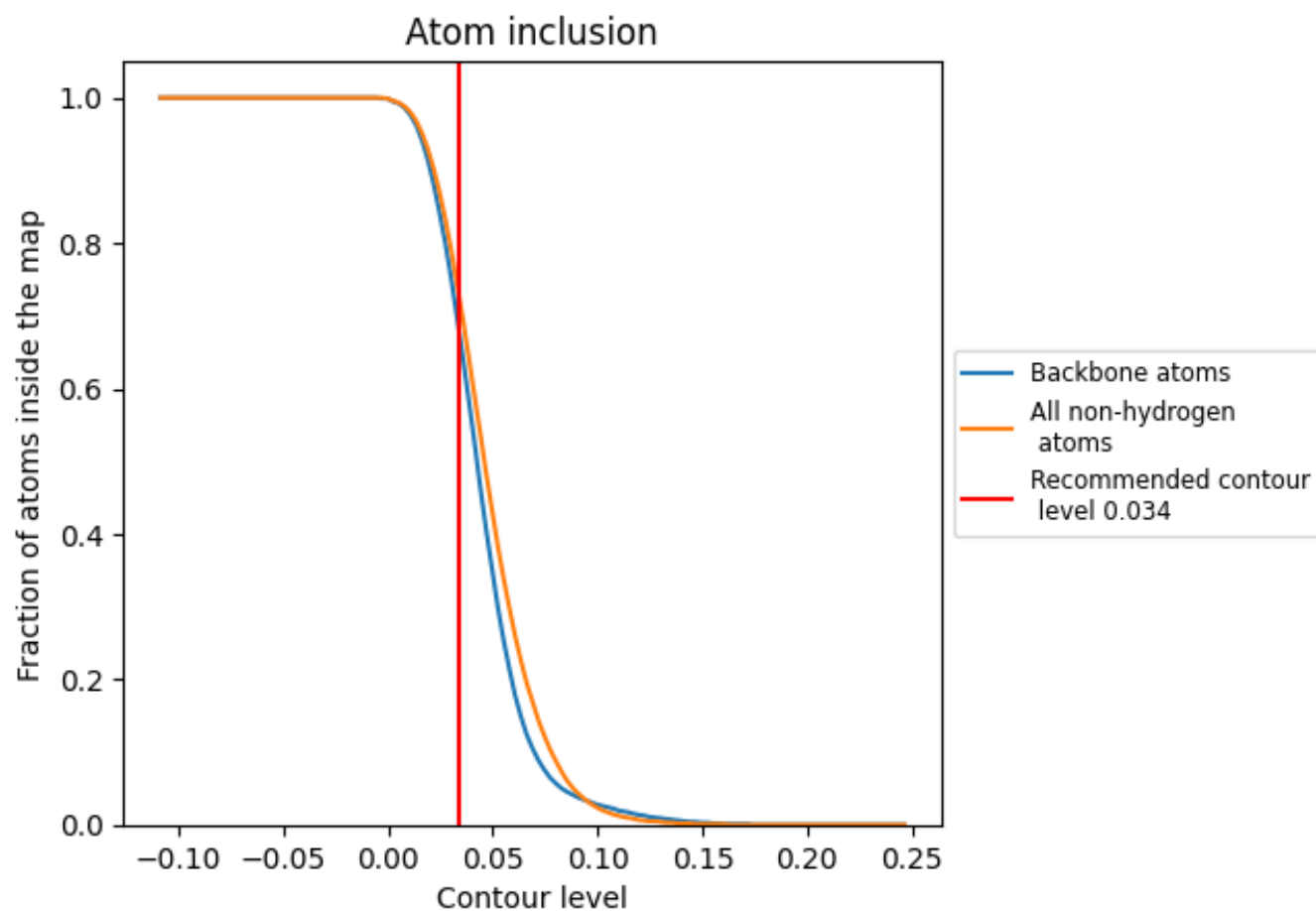
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.034).

9.4 Atom inclusion ⓘ



At the recommended contour level, 68% of all backbone atoms, 73% 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 (0.034) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7270	 0.6660
1	 0.8370	 0.6760
3	 0.7150	 0.6500
4	 0.7810	 0.6650
A	 0.7840	 0.6970
B	 0.6880	 0.6730
C	 0.6300	 0.6560
D	 0.4610	 0.6330
E	 0.1770	 0.5740
F	 0.6040	 0.6590
G	 0.5300	 0.6420
H	 0.4830	 0.6410
I	 0.5320	 0.6550
J	 0.2450	 0.5980
L	 0.6500	 0.6670
M	 0.4950	 0.6390
N	 0.8660	 0.7030
O	 0.6440	 0.6580
P	 0.7040	 0.6700
Q	 0.6250	 0.6670
R	 0.5390	 0.5930
S	 0.6700	 0.6630
T	 0.7160	 0.6760
U	 0.2330	 0.5810
V	 0.6100	 0.6690
W	 0.6340	 0.6420
X	 0.6440	 0.6640
Y	 0.5730	 0.6510
Z	 0.2840	 0.5950
a	 0.7840	 0.6840
b	 0.6970	 0.6770
c	 0.3150	 0.6240
d	 0.6270	 0.6640
e	 0.6330	 0.6580
f	 0.5940	 0.6510



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Chain	Atom inclusion	Q-score
g	 0.7080	 0.6770
h	 0.5240	 0.6440
i	 0.5850	 0.6520
j	 0.8390	 0.7020
k	 0.2210	 0.5850
l	 0.7310	 0.6830
m	 0.5070	 0.6540
o	 0.7380	 0.6870
p	 0.6910	 0.6770
w	 0.3310	 0.6040