



wwPDB EM Validation Summary Report ⓘ

Jun 23, 2026 – 02:11 PM JST

PDB ID : 8INE / pdb_00008ine
EMDB ID : EMD-35596
Title : human nuclear pre-60S ribosomal particle - State G'
Authors : Zhang, Y.; Gao, N.
Deposited on : 2023-03-09
Resolution : 3.20 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 : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

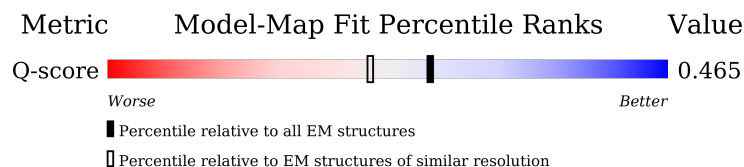
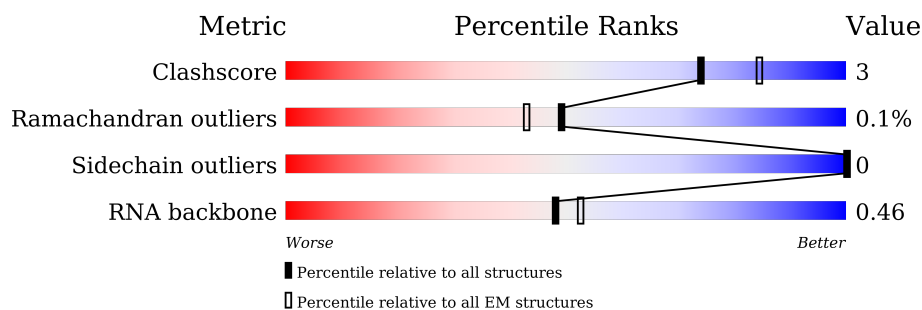
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	u	490	
2	t	293	
3	3	255	

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Mol	Chain	Length	Quality of chain
4	2	5054	
5	4	634	
6	5	120	
7	6	245	
8	7	163	
9	9	134	
10	B	403	
11	C	159	
12	D	427	
13	E	115	
14	F	117	
15	G	266	
16	H	123	
17	I	192	
18	K	105	
19	L	148	
20	M	97	
21	N	178	
22	O	70	
23	P	51	
24	Q	211	
25	S	215	
26	U	204	
27	V	203	
28	X	92	

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Mol	Chain	Length	Quality of chain
29	Y	184	
30	Z	188	
31	a	196	
32	b	176	
33	c	160	
34	d	128	
35	e	140	
36	g	156	
37	h	145	
38	i	136	
39	j	125	
40	k	135	
41	l	137	
42	m	257	
43	n	110	
44	o	288	
45	p	248	
46	r	297	
47	z	129	
48	A	731	
49	R	203	
50	J	239	
51	y	165	
52	v	588	
53	8	156	

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Mol	Chain	Length	Quality of chain
54	W	106	20% 87% 8% 5%
55	T	99	6% 40% 10% 49%
56	s	260	10% 7% 6% 87%
57	w	478	28% 46% 8% 46%
58	x	60	95% 70% 25% 5%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 159473 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Ribosomal L1 domain-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	u	239	Total	C	N	O	S	0	0
			1924	1232	338	348	6		

- Molecule 2 is a protein called MKI67 FHA domain-interacting nucleolar phosphoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	t	111	Total	C	N	O	S	0	0
			928	601	157	167	3		

- Molecule 3 is a protein called 60S ribosomal protein L7-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	230	Total	C	N	O	S	0	0
			1901	1229	358	310	4		

- Molecule 4 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	3537	Total	C	N	O	P	0	0
			75949	33873	13891	24649	3536		

- Molecule 5 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	611	Total	C	N	O	S	0	0
			5016	3151	918	920	27		

- Molecule 6 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	5	120	Total	C	N	O	P	0	0
			2558	1141	456	842	119		

- Molecule 7 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	244	Total	C	N	O	S	0	0
			1852	1149	318	372	13		

- Molecule 8 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	139	Total	C	N	O	S	0	0
			1184	754	229	191	10		

- Molecule 9 is a protein called Zinc finger protein 593.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	9	97	Total	C	N	O	S	0	0
			787	481	168	134	4		

- Molecule 10 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	402	Total	C	N	O	S	1	0
			3244	2065	609	556	14		

- Molecule 11 is a protein called 60S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	93	Total	C	N	O	S	0	0
			764	476	167	117	4		

- Molecule 12 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	358	Total	C	N	O	S	0	0
			2853	1797	570	473	13		

- Molecule 13 is a protein called 60S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	98	Total	C	N	O	S	0	0
			764	485	135	138	6		

- Molecule 14 is a protein called 60S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	113	Total	C	N	O	S	0	0
			897	560	185	146	6		

- Molecule 15 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	241	Total	C	N	O	S	1	0
			1935	1233	374	324	4		

- Molecule 16 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	122	Total	C	N	O	S	0	0
			1015	641	205	168	1		

- Molecule 17 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	190	Total	C	N	O	S	0	0
			1518	956	284	272	6		

- Molecule 18 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	K	102	Total	C	N	O	S	0	0
			832	521	177	129	5		

- Molecule 19 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	147	Total	C	N	O	S	0	0
			1162	736	237	186	3		

- Molecule 20 is a protein called 60S ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	M	86	Total	C	N	O	S	0	0
			705	434	155	111	5		

- Molecule 21 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	164	Total	C	N	O	S	0	0
			1310	830	243	232	5		

- Molecule 22 is a protein called 60S ribosomal protein L38.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	O	69	Total	C	N	O	S	0	0
			569	366	103	99	1		

- Molecule 23 is a protein called 60S ribosomal protein L39.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	50	Total	C	N	O	S	0	0
			444	281	98	64	1		

- Molecule 24 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	210	Total	C	N	O	S	0	0
			1701	1064	352	281	4		

- Molecule 25 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	135	Total	C	N	O	S	0	0
			1111	713	213	178	7		

- Molecule 26 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	203	Total	C	N	O	S	0	0
			1701	1072	359	266	4		

- Molecule 27 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	V	201	Total	C	N	O	S	0	0
			1650	1063	321	261	5		

- Molecule 28 is a protein called 60S ribosomal protein L37a.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	91	Total	C	N	O	S	0	0
			708	445	136	120	7		

- Molecule 29 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	167	Total	C	N	O	S	0	0
			1355	848	260	238	9		

- Molecule 30 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Z	187	Total	C	N	O	S	0	0
			1513	944	314	250	5		

- Molecule 31 is a protein called 60S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	a	148	Total	C	N	O	S	0	0
			1239	772	266	192	9		

- Molecule 32 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	b	176	Total	C	N	O	S	0	0
			1461	930	284	236	11		

- Molecule 33 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	c	155	Total	C	N	O	S	0	0
			1264	801	248	210	5		

- Molecule 34 is a protein called 60S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	d	104	Total	C	N	O	S	0	0
			850	542	149	157	2		

- Molecule 35 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	e	131	Total	C	N	O	S	0	0
			979	618	184	172	5		

- Molecule 36 is a protein called 60S ribosomal protein L23a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	143	Total	C	N	O	S	0	0
			1156	740	220	195	1		

- Molecule 37 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	h	134	Total	C	N	O	S	0	0
			1115	700	226	186	3		

- Molecule 38 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	135	Total	C	N	O	S	0	0
			1107	714	208	182	3		

- Molecule 39 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	j	111	Total	C	N	O	S	0	0
			918	578	178	160	2		

- Molecule 40 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	129	Total	C	N	O	S	0	0
			1064	673	220	166	5		

- Molecule 41 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	125	Total	C	N	O	S	0	0
			1002	622	207	168	5		

- Molecule 42 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	m	248	Total	C	N	O	S	0	0
			1898	1189	389	314	6		

- Molecule 43 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	109	Total	C	N	O	S	0	0
			876	555	174	144	3		

- Molecule 44 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	235	Total	C	N	O	S	0	0
			1897	1217	360	316	4		

- Molecule 45 is a protein called 60S ribosomal protein L7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	p	225	Total	C	N	O	S	1	0
			1878	1207	361	301	9		

- Molecule 46 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	284	Total	C	N	O	S	0	0
			2312	1463	420	415	14		

- Molecule 47 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	67	Total	C	N	O	S	0	0
			581	363	128	88	2		

- Molecule 48 is a protein called G Protein Nucleolar 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	A	333	Total	C	N	O	S	0	0
			2672	1710	457	497	8		

- Molecule 49 is a protein called Translation machinery-associated protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	R	153	Total	C	N	O	S	0	0
			1296	810	248	233	5		

- Molecule 50 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	J	223	Total	C	N	O	S	0	0
			1809	1140	309	349	11		

- Molecule 51 is a protein called 60S ribosomal protein L12.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	y	165	Total	C	N	O	S	0	0
			1250	779	232	234	5		

- Molecule 52 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	v	404	Total	C	N	O	S	0	0
			3317	2140	582	582	13		

- Molecule 53 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	8	155	Total	C	N	O	P	0	0
			3295	1472	583	1086	154		

- Molecule 54 is a protein called 60S ribosomal protein L36a.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	W	101	Total	C	N	O	S	0	0
			827	517	170	134	6		

- Molecule 55 is a protein called Leydig cell tumor 10 kDa protein homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	T	50	Total	C	N	O	S	0	0
			393	247	82	63	1		

- Molecule 56 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	s	35	Total	C	N	O	0	0
			316	196	68	52		

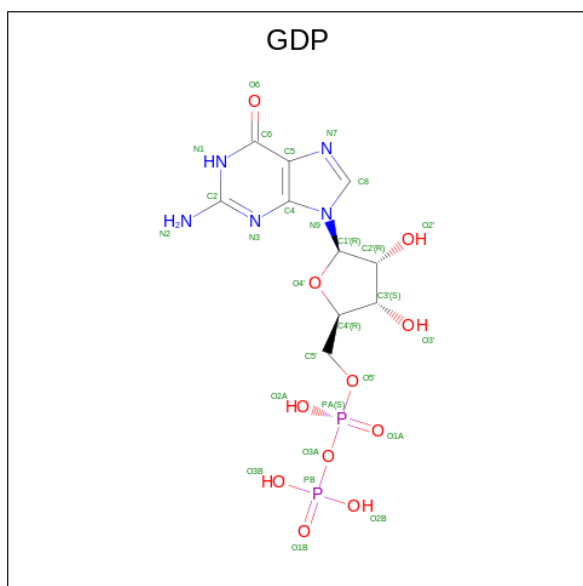
- Molecule 57 is a protein called Ribosome biogenesis protein NOP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	w	258	Total	C	N	O	S	0	0
			2137	1326	427	382	2		

- Molecule 58 is a RNA chain called Internal Transcribed Spacer 2.

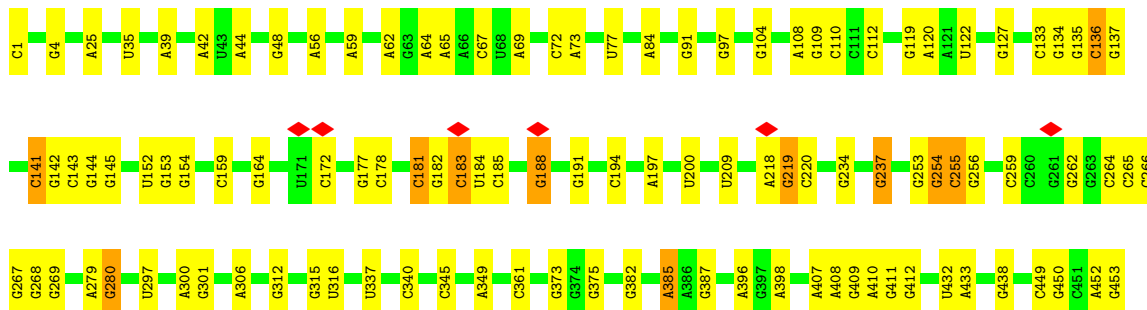
Mol	Chain	Residues	Atoms					AltConf	Trace
58	x	57	Total	C	N	O	P	0	0
			684	285	1	341	57		

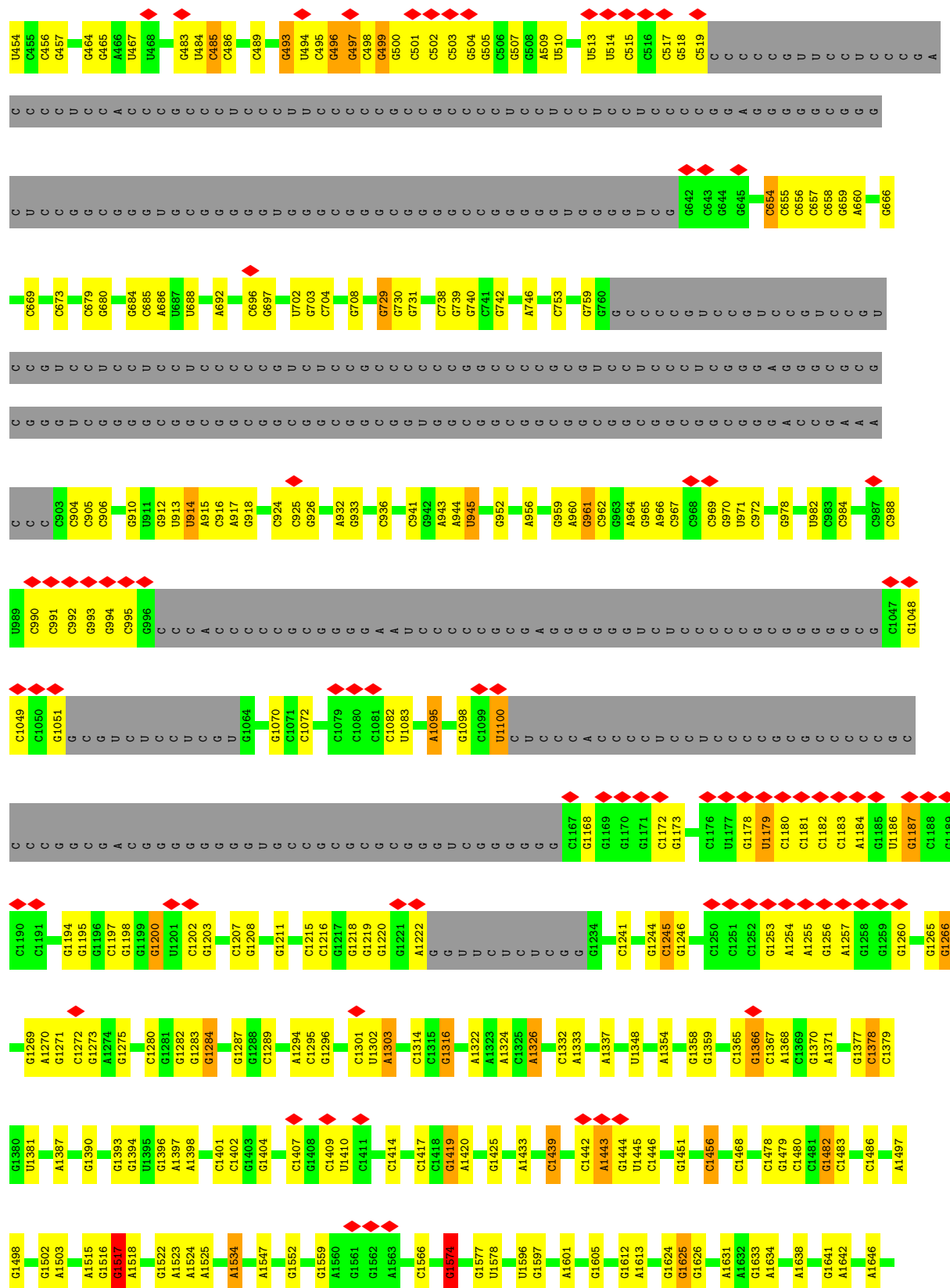
- Molecule 59 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



- Molecule 61 is POTASSIUM ION (CCD ID: K) (formula: K).

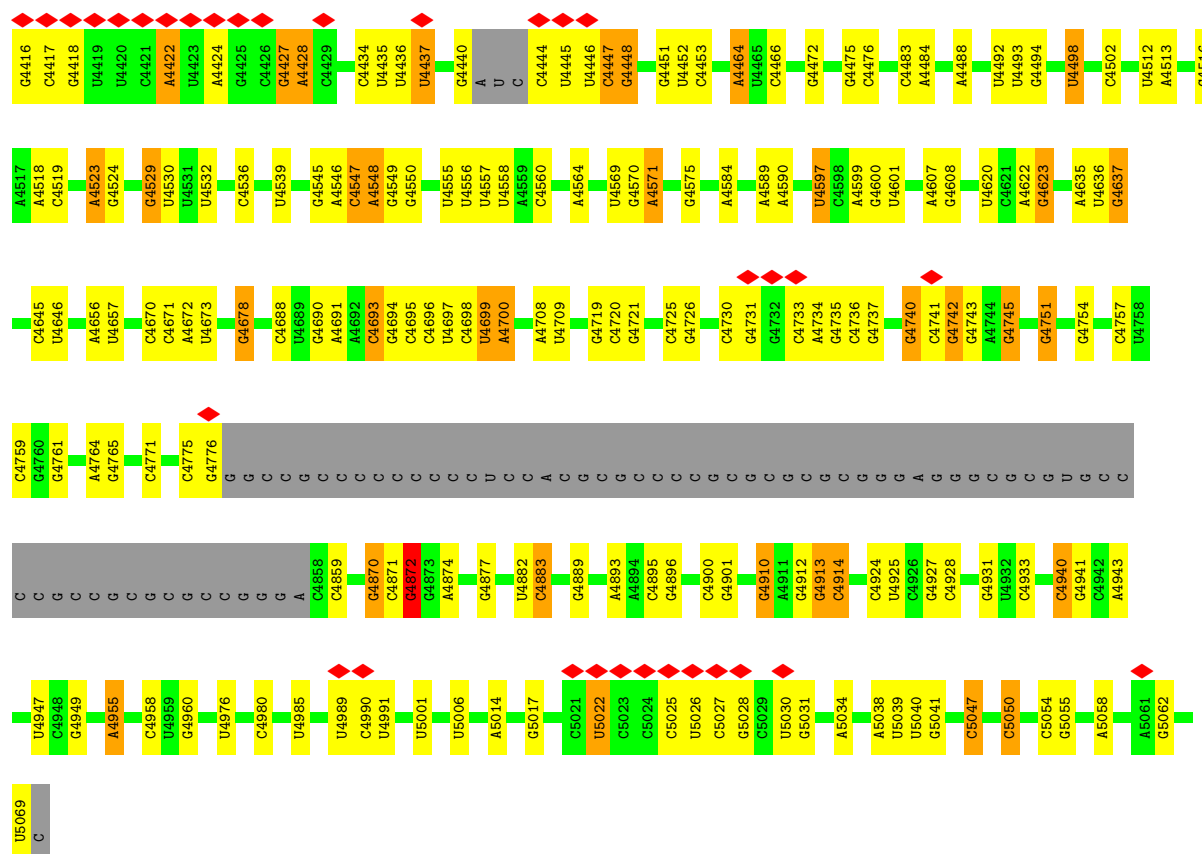
Mol	Chain	Residues	Atoms		AltConf
61	A	1	Total 1	K 1	0



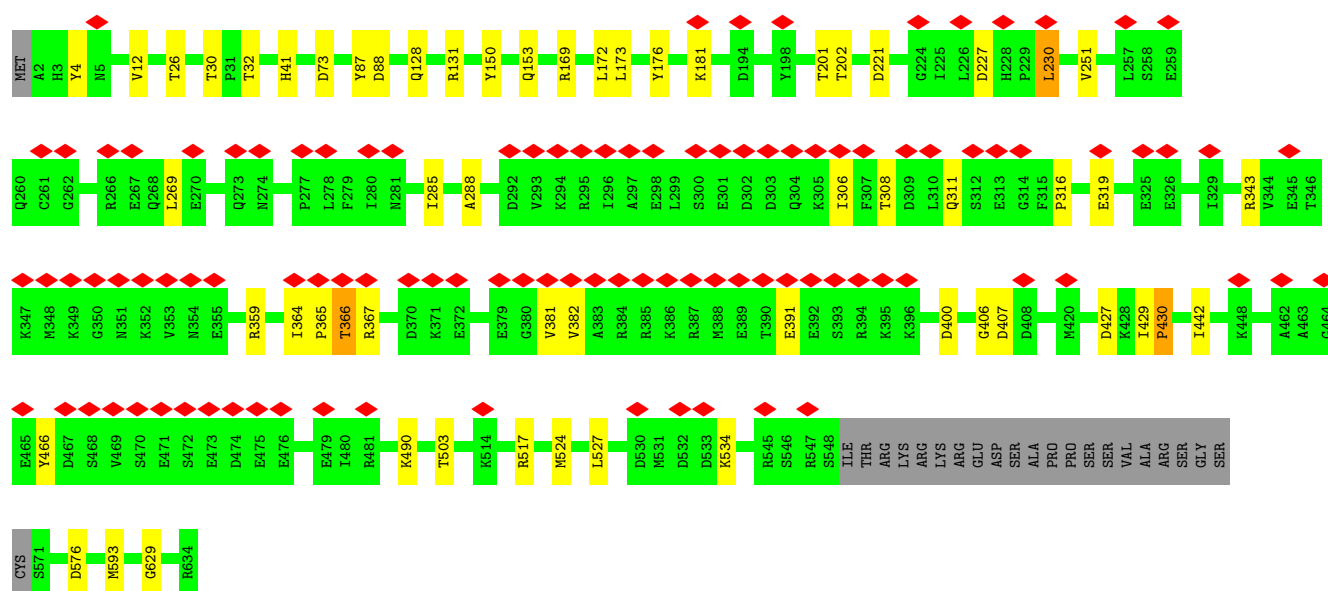
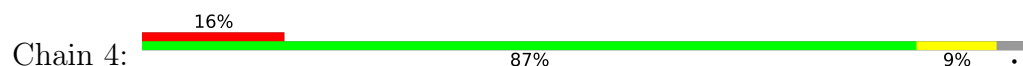




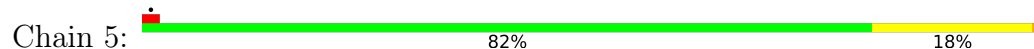


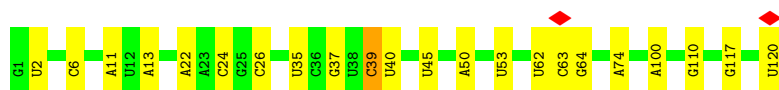


• Molecule 5: GTP-binding protein 4

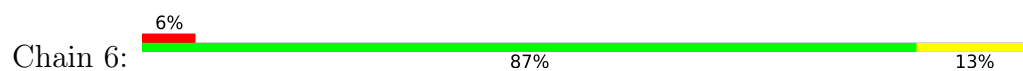


• Molecule 6: 5S rRNA

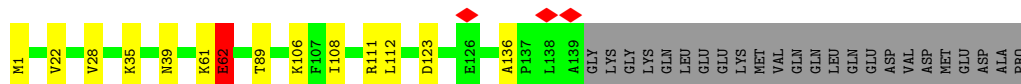
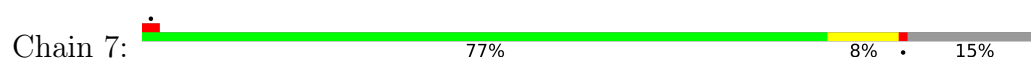




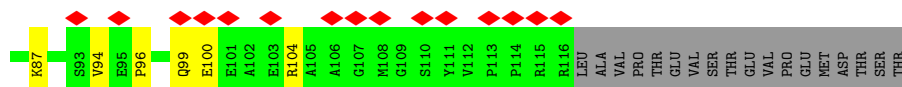
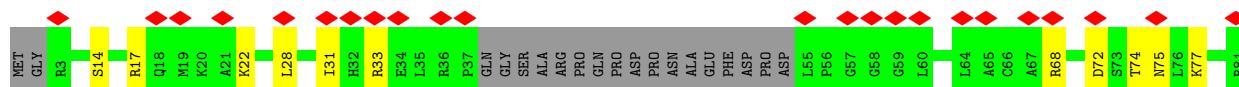
- Molecule 7: Eukaryotic translation initiation factor 6



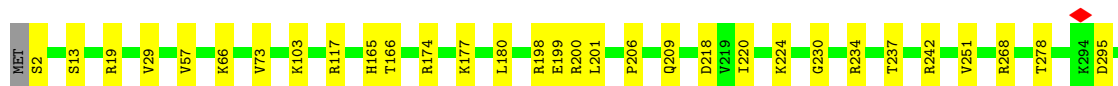
- Molecule 8: Probable ribosome biogenesis protein RLP24



- Molecule 9: Zinc finger protein 593



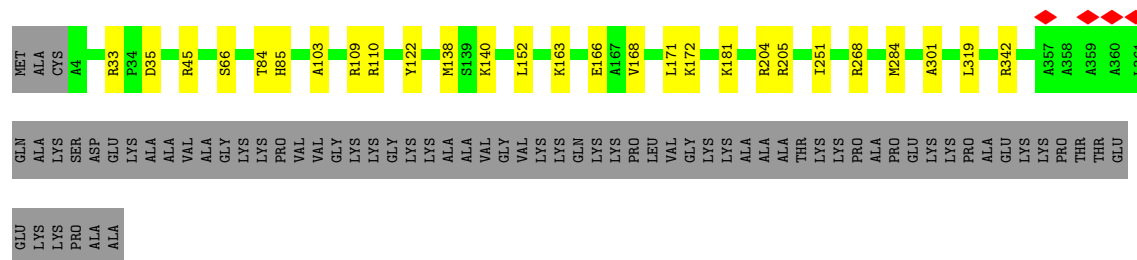
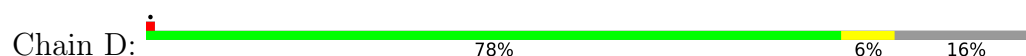
- Molecule 10: 60S ribosomal protein L3



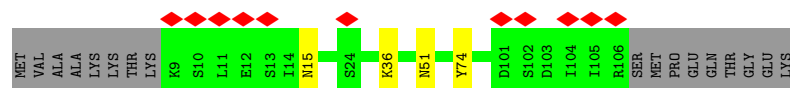
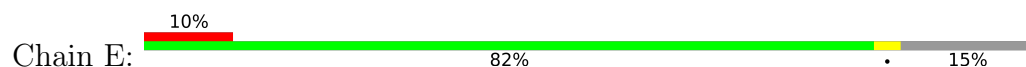
- Molecule 11: 60S ribosomal protein L29



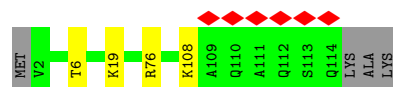
- Molecule 12: 60S ribosomal protein L4



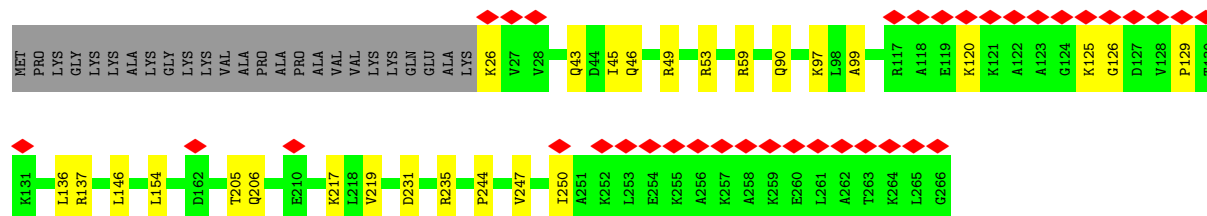
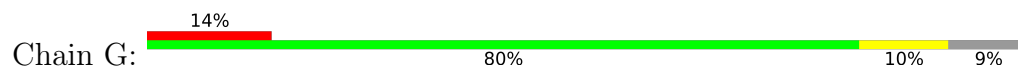
- Molecule 13: 60S ribosomal protein L30



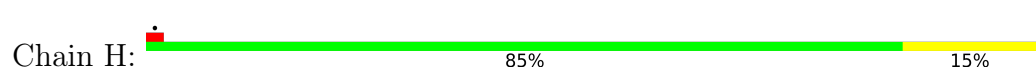
- Molecule 14: 60S ribosomal protein L34



- Molecule 15: 60S ribosomal protein L7a

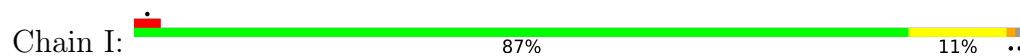


- Molecule 16: 60S ribosomal protein L35

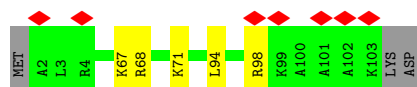




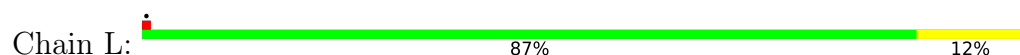
- Molecule 17: 60S ribosomal protein L9



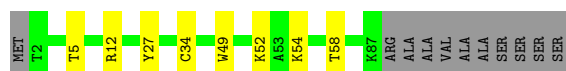
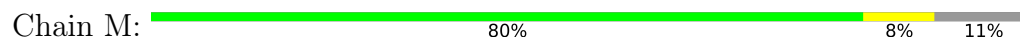
- Molecule 18: 60S ribosomal protein L36



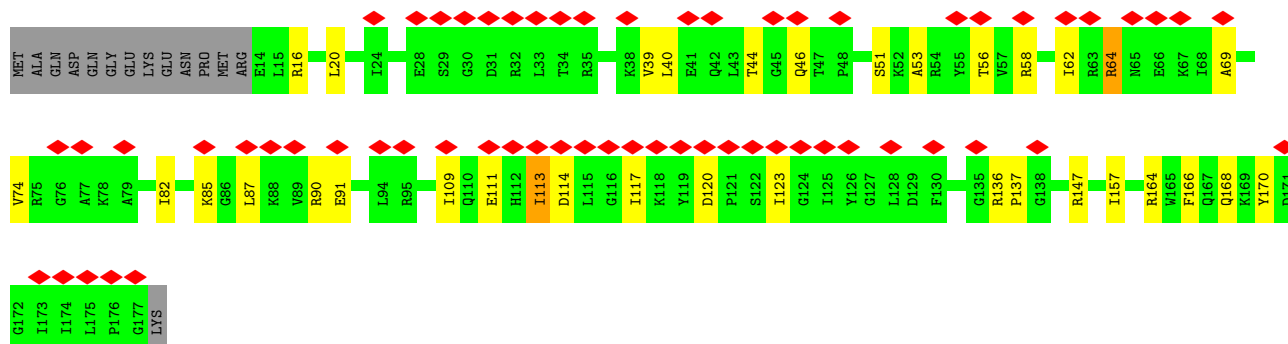
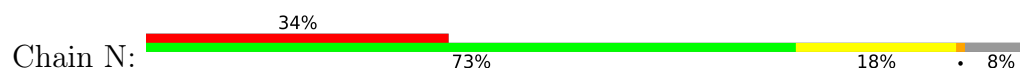
- Molecule 19: 60S ribosomal protein L27a



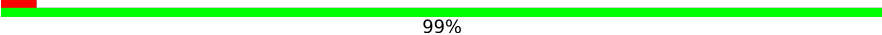
- Molecule 20: 60S ribosomal protein L37

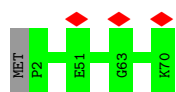


- Molecule 21: 60S ribosomal protein L11



- Molecule 22: 60S ribosomal protein L38

Chain O:  99%



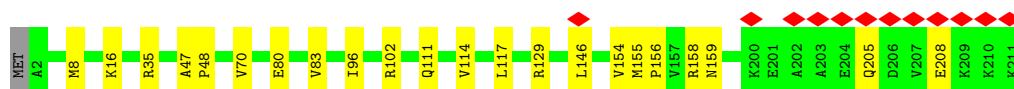
- Molecule 23: 60S ribosomal protein L39

Chain P:  84% 14%



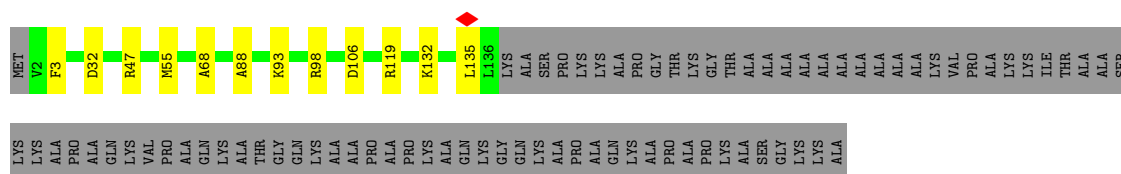
- Molecule 24: 60S ribosomal protein L13

Chain Q:  6% 89% 10%



- Molecule 25: 60S ribosomal protein L14

Chain S:  57% 6% 37%



- Molecule 26: 60S ribosomal protein L15

Chain U:  90% 10%



- Molecule 27: 60S ribosomal protein L13a

Chain V:  90% 9%

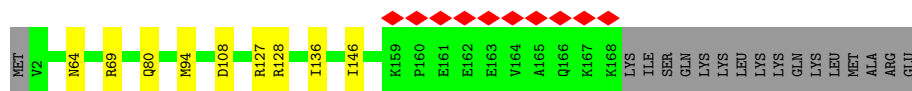
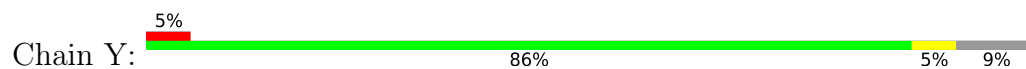


- Molecule 28: 60S ribosomal protein L37a

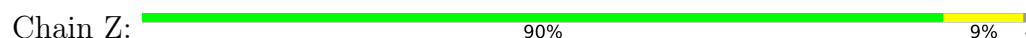
Chain X:  8% 88% 11%



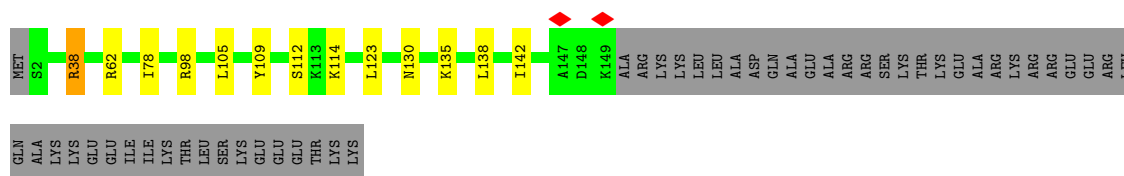
- Molecule 29: 60S ribosomal protein L17



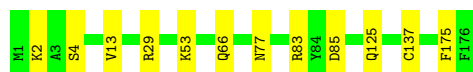
- Molecule 30: 60S ribosomal protein L18



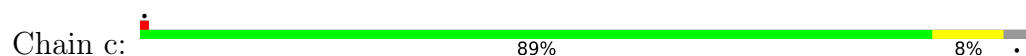
- Molecule 31: 60S ribosomal protein L19



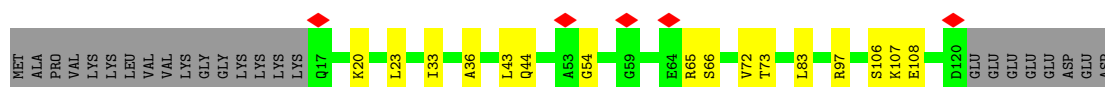
- Molecule 32: 60S ribosomal protein L18a



- Molecule 33: 60S ribosomal protein L21



- Molecule 34: 60S ribosomal protein L22



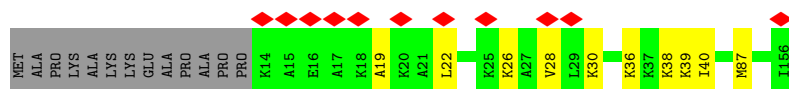
- Molecule 35: 60S ribosomal protein L23

Chain e: 



- Molecule 36: 60S ribosomal protein L23a

Chain g: 



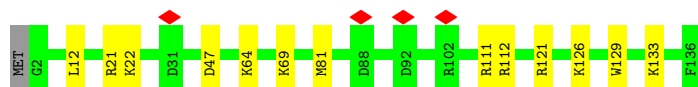
- Molecule 37: 60S ribosomal protein L26

Chain h: 



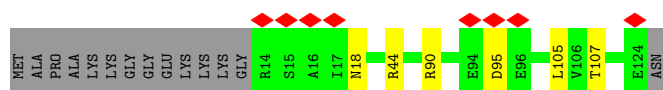
- Molecule 38: 60S ribosomal protein L27

Chain i: 

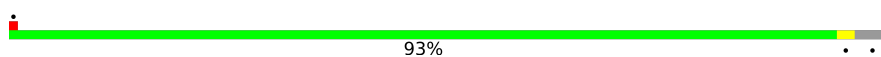


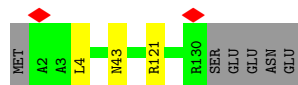
- Molecule 39: 60S ribosomal protein L31

Chain j: 



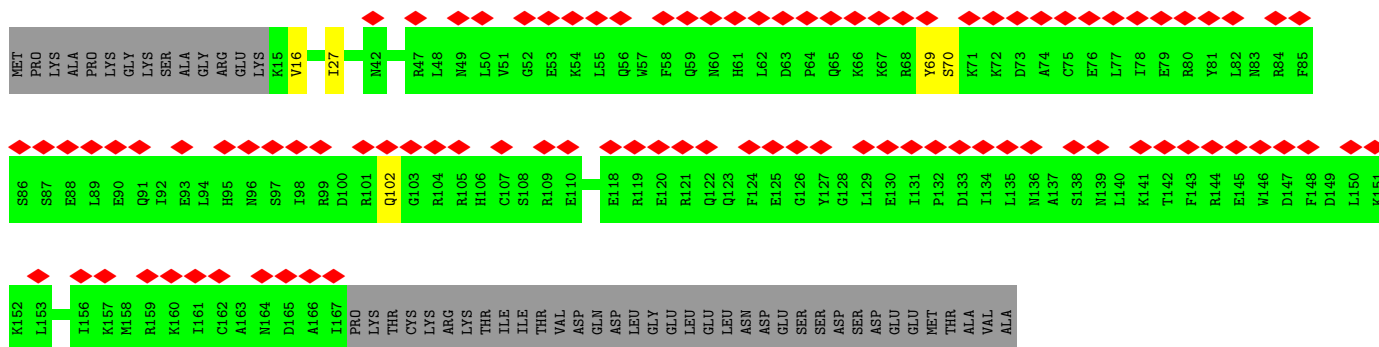
- Molecule 40: 60S ribosomal protein L32

Chain k: 

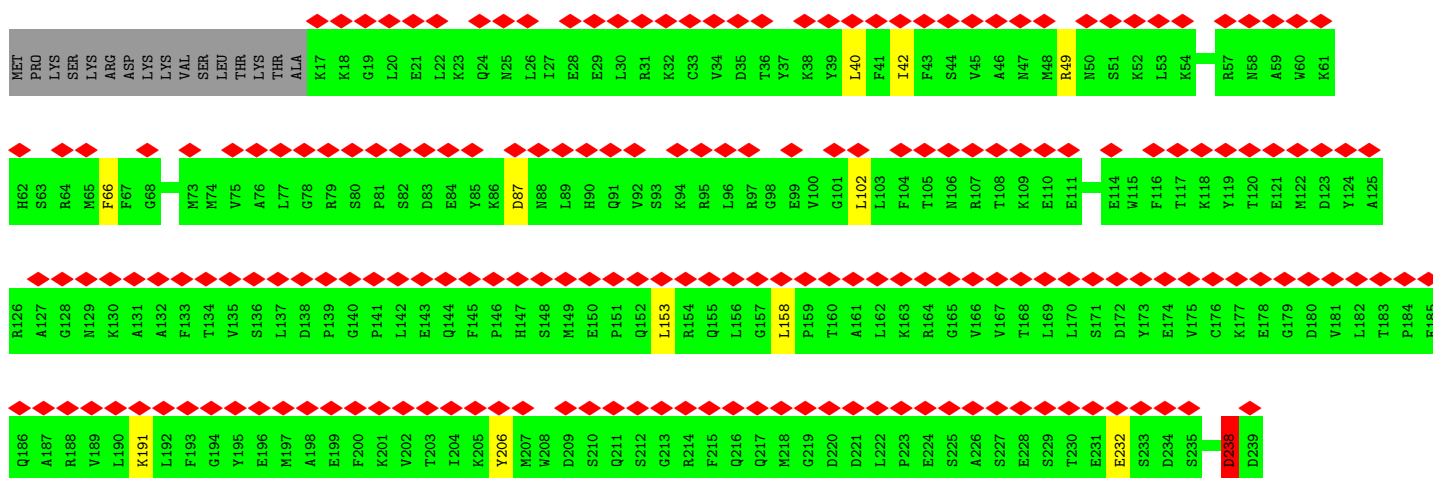
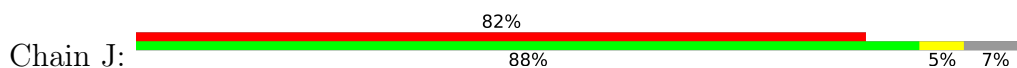


- Molecule 41: 60S ribosomal protein L28

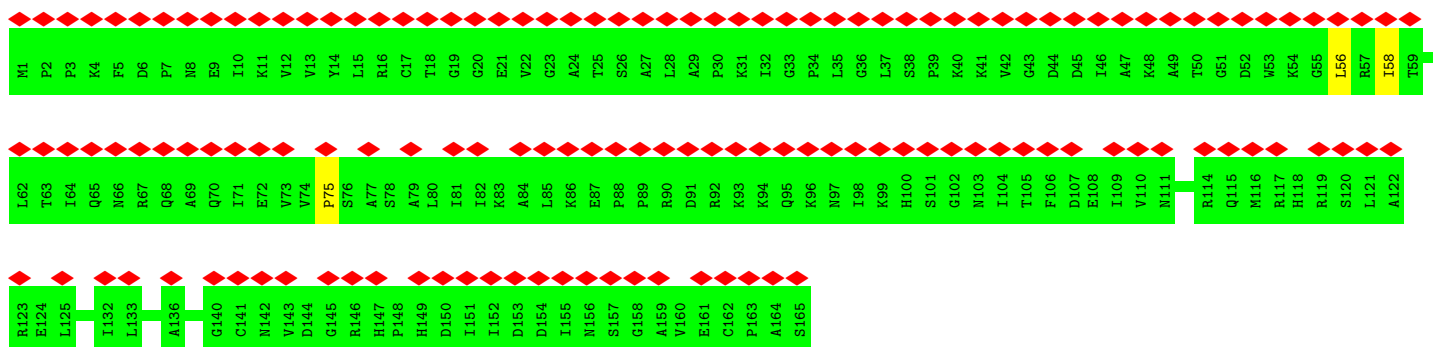
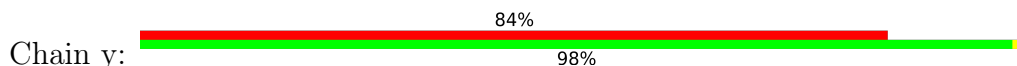
Chain l: 



- Molecule 50: mRNA turnover protein 4 homolog

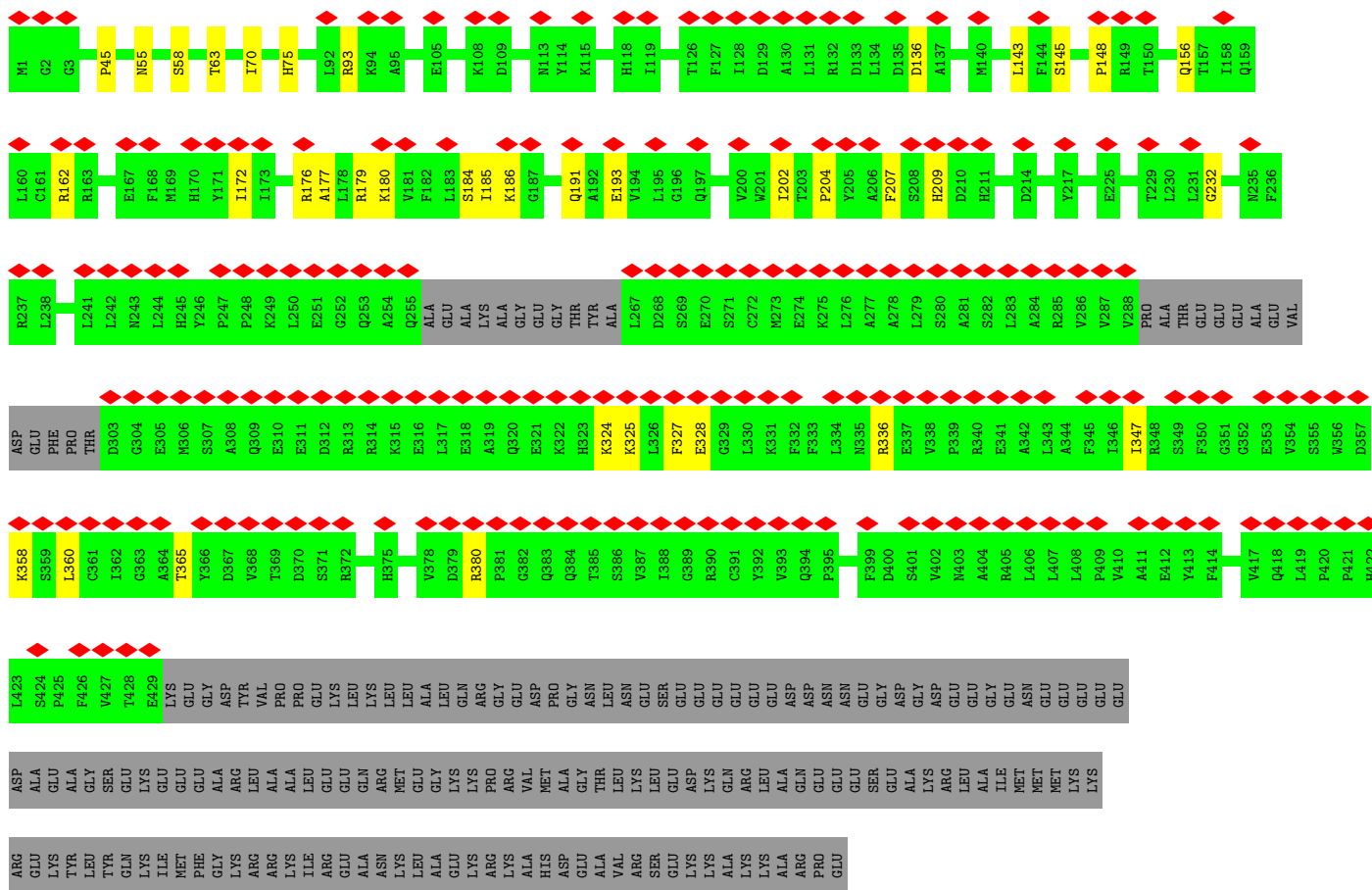


- Molecule 51: 60S ribosomal protein L12

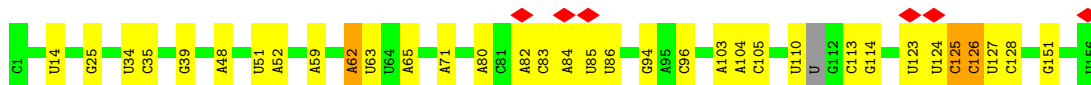
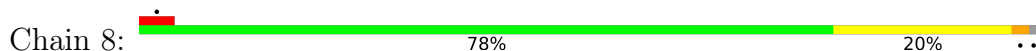


- Molecule 52: Pescadillo homolog

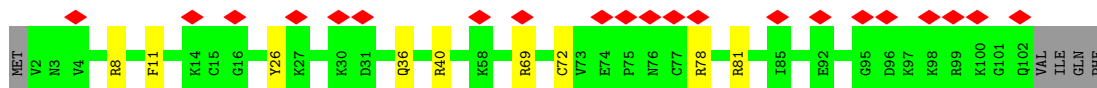
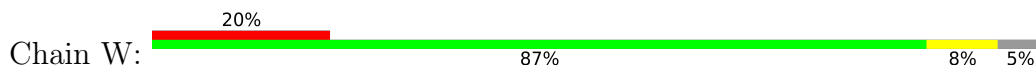




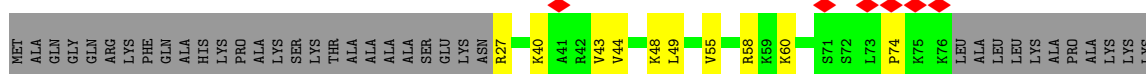
- Molecule 53: 5.8S rRNA



- Molecule 54: 60S ribosomal protein L36a



- Molecule 55: Leydig cell tumor 10 kDa protein homolog



N0	N1	N2	N3	N4	N	N6	N7	N8	N9	N10	N11	N12	N13	N14	N	N	N17	N18	N19	N20	N21	N22	N23	N24	N25	N26	N27	N28	N29	N30	N31	N32	N33	N34	N35	N36	N37	N38	N39	N40	N41	N42	N43	N44	N45	N46	N47	N48	N49	N50	N51	N52	N53	N54	N55	N56	N57	N58	N59
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25102	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 ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.206	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.032	Depositor
Map size (Å)	548.0, 548.0, 548.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.37, 1.37, 1.37	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: B8H, B8T, 6MZ, B8K, B9H, MG, 2MG, M7A, 5MU, P4U, UR3, B8Q, P7G, B9B, B8W, E6G, OMU, I4U, MHG, GDP, 5MC, OMG, BGH, A2M, E7G, OMC, 7MG, K, 1MA

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	u	0.27	0/1956	0.62	0/2631
2	t	0.30	0/955	0.81	2/1290 (0.2%)
3	3	0.33	0/1937	0.75	2/2595 (0.1%)
4	2	0.66	11/82935 (0.0%)	0.44	18/129293 (0.0%)
5	4	0.34	0/5099	0.83	14/6840 (0.2%)
6	5	0.23	0/2858	0.41	0/4455
7	6	0.29	0/1877	0.68	0/2554
8	7	0.33	0/1207	0.78	1/1600 (0.1%)
9	9	0.31	0/802	0.82	0/1069
10	B	0.28	0/3315	0.70	5/4435 (0.1%)
11	C	0.28	0/777	0.67	0/1026
12	D	0.28	0/2907	0.71	2/3905 (0.1%)
13	E	0.27	0/774	0.66	0/1038
14	F	0.26	0/907	0.62	0/1209
15	G	0.31	0/1971	0.69	2/2651 (0.1%)
16	H	0.31	0/1023	0.63	0/1351
17	I	0.33	0/1537	0.79	3/2066 (0.1%)
18	K	0.27	0/843	0.66	0/1115
19	L	0.23	0/1191	0.54	0/1591
20	M	0.28	0/720	0.65	0/952
21	N	0.33	0/1332	1.00	3/1782 (0.2%)
22	O	0.31	0/575	0.74	0/761
23	P	0.27	0/454	0.61	0/599
24	Q	0.32	0/1732	0.70	1/2315 (0.0%)
25	S	0.30	0/1133	0.67	2/1516 (0.1%)
26	U	0.26	0/1746	0.59	3/2338 (0.1%)
27	V	0.30	0/1682	0.62	1/2250 (0.0%)
28	X	0.28	0/718	0.59	0/953
29	Y	0.26	0/1383	0.58	0/1856
30	Z	0.25	0/1537	0.58	0/2052
31	a	0.30	0/1255	0.73	3/1662 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	b	0.26	0/1501	0.55	0/2013
33	c	0.26	0/1291	0.64	0/1725
34	d	0.40	0/864	1.01	9/1160 (0.8%)
35	e	0.26	0/993	0.67	2/1332 (0.2%)
36	g	0.29	0/1175	0.69	3/1572 (0.2%)
37	h	0.29	0/1132	0.69	0/1504
38	i	0.32	0/1130	0.68	0/1507
39	j	0.29	0/933	0.64	0/1256
40	k	0.30	0/1082	0.64	0/1443
41	l	0.26	0/1017	0.57	0/1364
42	m	0.26	0/1936	0.66	0/2596
43	n	0.30	0/895	0.76	4/1198 (0.3%)
44	o	0.30	0/1935	0.71	1/2596 (0.0%)
45	p	0.35	0/1916	0.71	4/2553 (0.2%)
46	r	0.30	0/2357	0.75	3/3158 (0.1%)
47	z	0.37	0/587	0.78	0/767
48	A	0.25	0/2733	0.55	0/3697
49	R	0.39	0/1317	0.82	0/1757
50	J	1.62	2/1844 (0.1%)	0.96	4/2476 (0.2%)
51	y	0.29	0/1269	0.74	1/1712 (0.1%)
52	v	0.26	0/3395	0.66	2/4578 (0.0%)
53	8	0.26	0/3656	0.44	1/5694 (0.0%)
54	W	0.26	0/840	0.63	0/1107
55	T	0.27	0/396	0.73	0/522
56	s	0.16	0/321	0.29	0/418
57	w	0.25	0/2169	0.66	2/2902 (0.1%)
All	All	0.54	13/167822 (0.0%)	0.57	98/244357 (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
8	7	0	1
24	Q	0	1
43	n	0	1
50	J	0	1
57	w	0	1
All	All	0	5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	1958	A	C6-N1	75.34	2.86	1.35
4	2	1958	A	N3-C4	75.29	2.85	1.34
4	2	1958	A	C2-N3	73.65	2.80	1.33
4	2	1958	A	N1-C2	72.48	2.79	1.34
4	2	1958	A	C5-C6	72.10	2.85	1.41

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	J	238	ASP	CA-CB-CG	25.38	137.98	112.60
50	J	238	ASP	CB-CA-C	15.18	135.18	110.29
50	J	238	ASP	N-CA-C	-8.66	96.00	109.25
5	4	503	THR	CA-C-N	8.26	136.57	121.70
5	4	503	THR	C-N-CA	8.26	136.57	121.70

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	7	123	ASP	Peptide
50	J	238	ASP	Peptide
24	Q	154	VAL	Peptide
43	n	106	TYR	Peptide
57	w	204	ARG	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	u	1924	0	2026	72	0
2	t	928	0	906	21	0
3	3	1901	0	2037	25	0
4	2	75949	0	38173	325	0
5	4	5016	0	5153	35	0
6	5	2558	0	1296	6	0
7	6	1852	0	1828	21	0
8	7	1184	0	1252	10	0
9	9	787	0	796	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	B	3244	0	3389	25	0
11	C	764	0	822	5	0
12	D	2853	0	3028	20	0
13	E	764	0	804	3	0
14	F	897	0	989	4	0
15	G	1935	0	2087	19	0
16	H	1015	0	1148	16	0
17	I	1518	0	1600	25	0
18	K	832	0	917	4	0
19	L	1162	0	1213	12	0
20	M	705	0	741	6	0
21	N	1310	0	1345	21	0
22	O	569	0	635	0	0
23	P	444	0	483	5	0
24	Q	1701	0	1818	16	0
25	S	1111	0	1174	8	0
26	U	1701	0	1749	12	0
27	V	1650	0	1794	12	0
28	X	708	0	760	7	0
29	Y	1355	0	1389	7	0
30	Z	1513	0	1628	13	0
31	a	1239	0	1363	10	0
32	b	1461	0	1502	9	0
33	c	1264	0	1337	11	0
34	d	850	0	868	7	0
35	e	979	0	1039	9	0
36	g	1156	0	1268	18	0
37	h	1115	0	1205	8	0
38	i	1107	0	1182	10	0
39	j	918	0	964	4	0
40	k	1064	0	1160	2	0
41	l	1002	0	1068	9	0
42	m	1898	0	1993	15	0
43	n	876	0	912	9	0
44	o	1897	0	2046	14	0
45	p	1878	0	2009	13	0
46	r	2312	0	2339	14	0
47	z	581	0	656	8	0
48	A	2672	0	2695	19	0
49	R	1296	0	1324	4	0
50	J	1809	0	1783	15	0
51	y	1250	0	1305	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	v	3317	0	3368	33	0
53	8	3295	0	1676	8	0
54	W	827	0	896	6	0
55	T	393	0	452	12	0
56	s	316	0	331	45	0
57	w	2137	0	2202	44	0
58	x	684	0	456	71	0
59	A	28	0	12	1	0
60	A	1	0	0	0	0
61	A	1	0	0	0	0
All	All	159473	0	122391	849	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 849 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)
4:2:4083:5MU:C5	4:2:4083:5MU:C4	1.79	1.70
4:2:4296:B8H:C5	4:2:4296:B8H:C4	1.82	1.57
4:2:1860:B8H:C5	4:2:1860:B8H:C4	1.82	1.51
1:u:256:GLU:OE1	58:x:47:N:C4'	1.78	1.31
1:u:171:ARG:HD2	58:x:26:N:OP1	1.31	1.29

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	u	237/490 (48%)	232 (98%)	5 (2%)	0	100	100
2	t	109/293 (37%)	103 (94%)	6 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	224/255 (88%)	215 (96%)	8 (4%)	1 (0%)	30	62
5	4	607/634 (96%)	556 (92%)	46 (8%)	5 (1%)	16	50
7	6	242/245 (99%)	226 (93%)	16 (7%)	0	100	100
8	7	137/163 (84%)	133 (97%)	3 (2%)	1 (1%)	18	52
9	9	93/134 (69%)	79 (85%)	13 (14%)	1 (1%)	11	43
10	B	401/403 (100%)	374 (93%)	27 (7%)	0	100	100
11	C	89/159 (56%)	85 (96%)	4 (4%)	0	100	100
12	D	356/427 (83%)	331 (93%)	25 (7%)	0	100	100
13	E	96/115 (84%)	91 (95%)	5 (5%)	0	100	100
14	F	111/117 (95%)	108 (97%)	3 (3%)	0	100	100
15	G	240/266 (90%)	230 (96%)	10 (4%)	0	100	100
16	H	120/123 (98%)	115 (96%)	5 (4%)	0	100	100
17	I	188/192 (98%)	181 (96%)	7 (4%)	0	100	100
18	K	100/105 (95%)	95 (95%)	5 (5%)	0	100	100
19	L	145/148 (98%)	136 (94%)	9 (6%)	0	100	100
20	M	84/97 (87%)	78 (93%)	6 (7%)	0	100	100
21	N	162/178 (91%)	139 (86%)	23 (14%)	0	100	100
22	O	67/70 (96%)	61 (91%)	6 (9%)	0	100	100
23	P	48/51 (94%)	47 (98%)	1 (2%)	0	100	100
24	Q	208/211 (99%)	191 (92%)	17 (8%)	0	100	100
25	S	133/215 (62%)	127 (96%)	6 (4%)	0	100	100
26	U	201/204 (98%)	192 (96%)	9 (4%)	0	100	100
27	V	199/203 (98%)	189 (95%)	10 (5%)	0	100	100
28	X	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
29	Y	165/184 (90%)	155 (94%)	10 (6%)	0	100	100
30	Z	185/188 (98%)	177 (96%)	8 (4%)	0	100	100
31	a	146/196 (74%)	142 (97%)	4 (3%)	0	100	100
32	b	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
33	c	153/160 (96%)	146 (95%)	7 (5%)	0	100	100
34	d	102/128 (80%)	94 (92%)	8 (8%)	0	100	100
35	e	129/140 (92%)	117 (91%)	12 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
36	g	141/156 (90%)	136 (96%)	4 (3%)	1 (1%)	18	52
37	h	132/145 (91%)	129 (98%)	3 (2%)	0	100	100
38	i	133/136 (98%)	126 (95%)	7 (5%)	0	100	100
39	j	109/125 (87%)	104 (95%)	5 (5%)	0	100	100
40	k	127/135 (94%)	122 (96%)	5 (4%)	0	100	100
41	l	123/137 (90%)	112 (91%)	11 (9%)	0	100	100
42	m	246/257 (96%)	226 (92%)	20 (8%)	0	100	100
43	n	107/110 (97%)	99 (92%)	7 (6%)	1 (1%)	14	47
44	o	231/288 (80%)	216 (94%)	15 (6%)	0	100	100
45	p	224/248 (90%)	214 (96%)	10 (4%)	0	100	100
46	r	282/297 (95%)	261 (93%)	21 (7%)	0	100	100
47	z	63/129 (49%)	60 (95%)	2 (3%)	1 (2%)	7	36
48	A	331/731 (45%)	324 (98%)	7 (2%)	0	100	100
49	R	151/203 (74%)	141 (93%)	10 (7%)	0	100	100
50	J	221/239 (92%)	209 (95%)	12 (5%)	0	100	100
51	y	163/165 (99%)	159 (98%)	4 (2%)	0	100	100
52	v	398/588 (68%)	386 (97%)	12 (3%)	0	100	100
54	W	99/106 (93%)	94 (95%)	5 (5%)	0	100	100
55	T	48/99 (48%)	46 (96%)	2 (4%)	0	100	100
56	s	33/260 (13%)	33 (100%)	0	0	100	100
57	w	254/478 (53%)	242 (95%)	11 (4%)	1 (0%)	30	62
All	All	9356/11794 (79%)	8840 (94%)	504 (5%)	12 (0%)	49	79

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
43	n	106	TYR
57	w	203	ASP
3	3	24	ASN
5	4	88	ASP
47	z	24	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	
1	u	222/437 (51%)	222 (100%)	0	100	100
2	t	103/274 (38%)	103 (100%)	0	100	100
3	3	207/228 (91%)	207 (100%)	0	100	100
5	4	554/574 (96%)	554 (100%)	0	100	100
7	6	212/213 (100%)	212 (100%)	0	100	100
8	7	128/149 (86%)	128 (100%)	0	100	100
9	9	81/114 (71%)	81 (100%)	0	100	100
10	B	349/349 (100%)	349 (100%)	0	100	100
11	C	78/126 (62%)	78 (100%)	0	100	100
12	D	298/348 (86%)	298 (100%)	0	100	100
13	E	83/97 (86%)	83 (100%)	0	100	100
14	F	97/100 (97%)	97 (100%)	0	100	100
15	G	204/223 (92%)	204 (100%)	0	100	100
16	H	109/110 (99%)	109 (100%)	0	100	100
17	I	169/171 (99%)	169 (100%)	0	100	100
18	K	86/89 (97%)	86 (100%)	0	100	100
19	L	120/121 (99%)	120 (100%)	0	100	100
20	M	73/80 (91%)	73 (100%)	0	100	100
21	N	137/149 (92%)	137 (100%)	0	100	100
22	O	64/65 (98%)	64 (100%)	0	100	100
23	P	47/48 (98%)	47 (100%)	0	100	100
24	Q	176/177 (99%)	176 (100%)	0	100	100
25	S	115/161 (71%)	115 (100%)	0	100	100
26	U	171/172 (99%)	171 (100%)	0	100	100
27	V	173/174 (99%)	173 (100%)	0	100	100
28	X	74/75 (99%)	74 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	Y	147/163 (90%)	147 (100%)	0	100	100
30	Z	164/165 (99%)	164 (100%)	0	100	100
31	a	133/175 (76%)	133 (100%)	0	100	100
32	b	157/157 (100%)	157 (100%)	0	100	100
33	c	136/140 (97%)	136 (100%)	0	100	100
34	d	94/115 (82%)	94 (100%)	0	100	100
35	e	101/107 (94%)	101 (100%)	0	100	100
36	g	124/133 (93%)	124 (100%)	0	100	100
37	h	124/135 (92%)	124 (100%)	0	100	100
38	i	117/118 (99%)	117 (100%)	0	100	100
39	j	101/110 (92%)	101 (100%)	0	100	100
40	k	115/121 (95%)	115 (100%)	0	100	100
41	l	109/121 (90%)	109 (100%)	0	100	100
42	m	190/199 (96%)	190 (100%)	0	100	100
43	n	88/89 (99%)	88 (100%)	0	100	100
44	o	208/252 (82%)	208 (100%)	0	100	100
45	p	195/215 (91%)	195 (100%)	0	100	100
46	r	240/250 (96%)	240 (100%)	0	100	100
47	z	61/115 (53%)	61 (100%)	0	100	100
48	A	296/654 (45%)	296 (100%)	0	100	100
49	R	141/184 (77%)	141 (100%)	0	100	100
50	J	199/214 (93%)	199 (100%)	0	100	100
51	y	137/137 (100%)	137 (100%)	0	100	100
52	v	359/509 (70%)	359 (100%)	0	100	100
54	W	89/94 (95%)	89 (100%)	0	100	100
55	T	43/76 (57%)	43 (100%)	0	100	100
56	s	32/228 (14%)	32 (100%)	0	100	100
57	w	222/402 (55%)	222 (100%)	0	100	100
All	All	8252/10202 (81%)	8252 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 75

such sidechains are listed below:

Mol	Chain	Res	Type
46	r	225	GLN
56	s	10	HIS
48	A	383	GLN
51	y	149	HIS
19	L	62	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
4	2	3519/5054 (69%)	821 (23%)	21 (0%)
53	8	153/156 (98%)	27 (17%)	2 (1%)
58	x	0/60	-	-
6	5	119/120 (99%)	15 (12%)	0
All	All	3791/5390 (70%)	863 (22%)	23 (0%)

5 of 863 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	2	25	A
4	2	39	A
4	2	42	A
4	2	44	A
4	2	48	G

5 of 23 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	2	3774	A
4	2	4547	C
4	2	4380	A
4	2	4555	U
4	2	2470	C

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

77 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
4	B8W	2	4185	4	23,26,27	2.75	6 (26%)	33,38,41	2.58	13 (39%)
4	OMG	2	4623	4	23,26,27	2.63	8 (34%)	33,38,41	2.76	11 (33%)
4	B8W	2	4472	4	23,26,27	2.75	5 (21%)	33,38,41	2.57	13 (39%)
4	P7G	2	1909	4	24,28,29	4.01	11 (45%)	27,41,44	1.60	3 (11%)
4	A2M	2	3867	4	22,25,26	3.17	9 (40%)	31,36,39	3.04	12 (38%)
4	OMG	2	4370	4	23,26,27	2.68	8 (34%)	33,38,41	2.75	9 (27%)
4	OMG	2	1883	4	23,26,27	2.71	8 (34%)	33,38,41	2.69	11 (33%)
4	OMC	2	3869	4	19,22,23	3.01	8 (42%)	26,31,34	0.90	2 (7%)
4	A2M	2	2401	4	22,25,26	3.21	10 (45%)	31,36,39	2.99	11 (35%)
4	A2M	2	3718	4	22,25,26	3.20	9 (40%)	31,36,39	2.81	10 (32%)
4	OMG	2	2050	4	23,26,27	2.59	9 (39%)	33,38,41	2.70	12 (36%)
4	M7A	2	4564	4	20,25,26	2.00	3 (15%)	28,37,40	3.91	6 (21%)
4	2MG	2	978	4	23,26,27	3.01	8 (34%)	32,38,41	2.19	9 (28%)
4	B8K	2	4690	4	24,28,29	3.37	11 (45%)	30,42,45	2.59	11 (36%)
4	A2M	2	1871	4	22,25,26	3.19	9 (40%)	31,36,39	3.06	11 (35%)
4	B9B	2	2754	4	25,28,29	1.72	6 (24%)	35,40,43	5.20	11 (31%)
4	7MG	2	1605	4	22,26,27	3.83	10 (45%)	29,39,42	1.98	7 (24%)
4	B9H	2	2786	4	20,25,26	3.22	5 (25%)	22,35,38	2.22	7 (31%)
4	OMC	2	2422	4	19,22,23	3.01	8 (42%)	26,31,34	1.06	2 (7%)
4	OMG	2	2773	4	23,26,27	2.70	8 (34%)	33,38,41	2.76	9 (27%)
4	A2M	2	2363	4	22,25,26	3.19	9 (40%)	31,36,39	2.99	11 (35%)
4	A2M	2	1326	4	22,25,26	3.14	9 (40%)	31,36,39	2.86	10 (32%)
4	2MG	2	4872	4	23,26,27	2.86	9 (39%)	32,38,41	2.33	9 (28%)
4	BGH	2	3899	4	25,29,30	4.60	17 (68%)	31,43,46	2.58	11 (35%)
4	OMC	2	2804	4	19,22,23	2.96	8 (42%)	26,31,34	1.33	3 (11%)
4	5MU	2	4083	4	19,22,23	7.28	8 (42%)	28,32,35	3.27	11 (39%)
4	2MG	2	1517	4	23,26,27	2.95	9 (39%)	32,38,41	2.24	9 (28%)
4	6MZ	2	4220	4	22,25,26	2.58	4 (18%)	30,36,39	3.35	10 (33%)
4	UR3	2	1866	4	19,22,23	2.94	6 (31%)	26,32,35	1.31	2 (7%)
4	B8Q	2	1456	4	17,22,23	2.97	5 (29%)	22,32,35	2.32	6 (27%)
4	B8H	2	1860	4	20,22,23	6.60	6 (30%)	21,32,35	2.32	5 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	E6G	2	4355	4	24,27,28	2.00	4 (16%)	34,39,42	2.79	15 (44%)
4	OMU	2	4620	4	19,22,23	2.93	8 (42%)	26,31,34	1.65	4 (15%)
4	OMG	2	4637	4	23,26,27	2.68	8 (34%)	33,38,41	2.77	10 (30%)
4	OMG	2	4196	4	23,26,27	2.75	8 (34%)	33,38,41	2.85	12 (36%)
4	7MG	2	4550	4	22,26,27	3.87	10 (45%)	29,39,42	1.98	9 (31%)
4	OMC	2	3887	4	19,22,23	3.05	8 (42%)	26,31,34	0.95	1 (3%)
4	B8T	2	4483	4	19,22,23	3.65	8 (42%)	26,31,34	1.37	4 (15%)
4	B8T	2	4671	4	19,22,23	3.60	8 (42%)	26,31,34	0.88	1 (3%)
53	OMU	8	14	4,53	19,22,23	2.90	8 (42%)	26,31,34	1.86	5 (19%)
4	A2M	2	398	4	22,25,26	3.21	9 (40%)	31,36,39	2.88	10 (32%)
4	P7G	2	3880	4	24,28,29	4.11	11 (45%)	27,41,44	1.42	3 (11%)
4	OMG	2	4494	4	23,26,27	2.69	8 (34%)	33,38,41	2.79	10 (30%)
4	B8H	2	4296	4	20,22,23	6.62	6 (30%)	21,32,35	2.35	5 (23%)
4	OMG	2	1625	4	23,26,27	2.72	8 (34%)	33,38,41	2.79	10 (30%)
4	A2M	2	1534	4	22,25,26	3.20	9 (40%)	31,36,39	3.05	10 (32%)
4	I4U	2	1659	4	21,24,25	3.57	9 (42%)	27,34,37	1.18	1 (3%)
4	P4U	2	1348	4	21,24,25	3.55	8 (38%)	27,33,36	1.04	1 (3%)
4	A2M	2	4523	4	22,25,26	3.17	9 (40%)	31,36,39	2.98	10 (32%)
4	UR3	2	4597	4	19,22,23	2.77	7 (36%)	26,32,35	2.03	5 (19%)
4	1MA	2	1322	4	21,25,26	3.03	5 (23%)	31,37,40	1.84	7 (22%)
4	B9B	2	237	4	25,28,29	1.78	6 (24%)	35,40,43	5.19	12 (34%)
4	OMG	2	2424	4	23,26,27	2.70	8 (34%)	33,38,41	2.84	10 (30%)
4	A2M	2	1524	4	22,25,26	3.19	9 (40%)	31,36,39	3.05	11 (35%)
4	B8K	2	3897	4	24,28,29	3.35	11 (45%)	30,42,45	2.48	11 (36%)
4	OMG	2	373	4	23,26,27	2.66	9 (39%)	33,38,41	2.66	13 (39%)
4	UR3	2	4530	4	19,22,23	2.90	6 (31%)	26,32,35	1.33	2 (7%)
4	OMG	2	1316	4	23,26,27	2.67	8 (34%)	33,38,41	2.74	12 (36%)
4	7MG	2	2522	4	22,26,27	3.71	10 (45%)	29,39,42	1.99	9 (31%)
4	OMC	2	2861	4	19,22,23	3.02	8 (42%)	26,31,34	1.18	3 (11%)
4	OMC	2	4536	4	19,22,23	3.01	8 (42%)	26,31,34	1.13	3 (11%)
4	MHG	2	4371	4	29,32,33	3.92	11 (37%)	34,46,49	2.35	13 (38%)
4	B8W	2	2380	4	23,26,27	2.73	5 (21%)	33,38,41	2.57	14 (42%)
4	2MG	2	729	4	23,26,27	2.92	7 (30%)	32,38,41	2.31	9 (28%)
4	A2M	2	4571	4	22,25,26	3.13	9 (40%)	31,36,39	2.99	10 (32%)
4	5MC	2	4335	4	18,22,23	3.58	7 (38%)	26,32,35	1.09	2 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	B9B	2	1574	4	25,28,29	1.71	6 (24%)	35,40,43	5.29	11 (31%)
4	OMG	2	2364	4	23,26,27	2.64	8 (34%)	33,38,41	2.73	11 (33%)
4	A2M	2	3723	4	22,25,26	3.20	10 (45%)	31,36,39	2.91	10 (32%)
4	OMG	2	1522	4	23,26,27	2.65	8 (34%)	33,38,41	2.75	12 (36%)
4	OMG	2	4870	4	23,26,27	2.72	8 (34%)	33,38,41	2.89	12 (36%)
4	E7G	2	1797	4	24,27,28	4.07	11 (45%)	30,40,43	2.26	9 (30%)
4	OMC	2	2365	4	19,22,23	2.94	8 (42%)	26,31,34	0.75	0
4	E7G	2	2297	4	24,27,28	3.95	11 (45%)	30,40,43	2.14	7 (23%)
4	OMU	2	4306	4	19,22,23	3.00	8 (42%)	26,31,34	1.70	5 (19%)
4	OMC	2	3701	4	19,22,23	3.01	8 (42%)	26,31,34	0.77	0
4	B8W	2	4529	4	23,26,27	2.77	5 (21%)	33,38,41	2.61	14 (42%)

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
4	B8W	2	4185	4	-	2/9/27/28	0/3/3/3
4	OMG	2	4623	4	-	0/9/27/28	0/3/3/3
4	B8W	2	4472	4	-	2/9/27/28	0/3/3/3
4	P7G	2	1909	4	-	3/10/40/41	0/3/3/3
4	A2M	2	3867	4	-	3/9/27/28	0/3/3/3
4	OMG	2	4370	4	-	0/9/27/28	0/3/3/3
4	OMG	2	1883	4	-	2/9/27/28	0/3/3/3
4	OMC	2	3869	4	-	7/9/27/28	0/2/2/2
4	A2M	2	2401	4	-	1/9/27/28	0/3/3/3
4	A2M	2	3718	4	-	0/9/27/28	0/3/3/3
4	OMG	2	2050	4	-	0/9/27/28	0/3/3/3
4	M7A	2	4564	4	-	0/7/37/38	0/3/3/3
4	2MG	2	978	4	-	0/9/27/28	0/3/3/3
4	B8K	2	4690	4	-	0/11/41/42	0/3/3/3
4	A2M	2	1871	4	-	0/9/27/28	0/3/3/3
4	B9B	2	2754	4	-	4/11/29/30	0/3/3/3
4	7MG	2	1605	4	-	0/7/37/38	0/3/3/3
4	B9H	2	2786	4	-	0/12/47/48	0/2/2/2
4	OMC	2	2422	4	-	1/9/27/28	0/2/2/2
4	OMG	2	2773	4	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	A2M	2	2363	4	-	0/9/27/28	0/3/3/3
4	A2M	2	1326	4	-	1/9/27/28	0/3/3/3
4	2MG	2	4872	4	-	2/9/27/28	0/3/3/3
4	BGH	2	3899	4	-	1/13/43/44	0/3/3/3
4	OMC	2	2804	4	-	0/9/27/28	0/2/2/2
4	5MU	2	4083	4	-	0/7/25/26	0/2/2/2
4	2MG	2	1517	4	-	3/9/27/28	0/3/3/3
4	6MZ	2	4220	4	-	2/9/27/28	0/3/3/3
4	UR3	2	1866	4	-	2/7/25/26	0/2/2/2
4	B8Q	2	1456	4	-	0/7/42/43	0/2/2/2
4	B8H	2	1860	4	-	2/7/25/26	0/2/2/2
4	E6G	2	4355	4	-	3/10/28/29	0/3/3/3
4	OMU	2	4620	4	-	0/9/27/28	0/2/2/2
4	OMG	2	4637	4	-	3/9/27/28	0/3/3/3
4	OMG	2	4196	4	-	2/9/27/28	0/3/3/3
4	7MG	2	4550	4	-	1/7/37/38	0/3/3/3
4	OMC	2	3887	4	-	1/9/27/28	0/2/2/2
4	B8T	2	4483	4	-	0/7/27/28	0/2/2/2
4	B8T	2	4671	4	-	0/7/27/28	0/2/2/2
53	OMU	8	14	4,53	-	1/9/27/28	0/2/2/2
4	A2M	2	398	4	-	2/9/27/28	0/3/3/3
4	P7G	2	3880	4	-	3/10/40/41	0/3/3/3
4	OMG	2	4494	4	-	1/9/27/28	0/3/3/3
4	B8H	2	4296	4	-	2/7/25/26	0/2/2/2
4	OMG	2	1625	4	-	3/9/27/28	0/3/3/3
4	A2M	2	1534	4	-	2/9/27/28	0/3/3/3
4	I4U	2	1659	4	-	1/9/29/30	0/2/2/2
4	P4U	2	1348	4	-	1/10/29/30	0/2/2/2
4	A2M	2	4523	4	-	5/9/27/28	0/3/3/3
4	UR3	2	4597	4	-	2/7/25/26	0/2/2/2
4	1MA	2	1322	4	-	0/7/25/26	0/3/3/3
4	B9B	2	237	4	-	6/11/29/30	0/3/3/3
4	OMG	2	2424	4	-	2/9/27/28	0/3/3/3
4	A2M	2	1524	4	-	3/9/27/28	0/3/3/3
4	B8K	2	3897	4	-	3/11/41/42	0/3/3/3
4	OMG	2	373	4	-	1/9/27/28	0/3/3/3
4	UR3	2	4530	4	-	0/7/25/26	0/2/2/2
4	OMG	2	1316	4	-	0/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	7MG	2	2522	4	-	0/7/37/38	0/3/3/3
4	OMC	2	2861	4	-	0/9/27/28	0/2/2/2
4	OMC	2	4536	4	-	0/9/27/28	0/2/2/2
4	MHG	2	4371	4	-	4/16/46/47	0/3/3/3
4	B8W	2	2380	4	-	2/9/27/28	0/3/3/3
4	2MG	2	729	4	-	2/9/27/28	0/3/3/3
4	A2M	2	4571	4	-	0/9/27/28	0/3/3/3
4	5MC	2	4335	4	-	0/7/25/26	0/2/2/2
4	B9B	2	1574	4	-	3/11/29/30	0/3/3/3
4	OMG	2	2364	4	-	3/9/27/28	0/3/3/3
4	A2M	2	3723	4	-	0/9/27/28	0/3/3/3
4	OMG	2	1522	4	-	0/9/27/28	0/3/3/3
4	OMG	2	4870	4	-	3/9/27/28	0/3/3/3
4	E7G	2	1797	4	-	2/9/39/40	0/3/3/3
4	OMC	2	2365	4	-	0/9/27/28	0/2/2/2
4	E7G	2	2297	4	-	1/9/39/40	0/3/3/3
4	OMU	2	4306	4	-	0/9/27/28	0/2/2/2
4	OMC	2	3701	4	-	7/9/27/28	0/2/2/2
4	B8W	2	4529	4	-	0/9/27/28	0/3/3/3

The worst 5 of 621 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	2	4083	5MU	C4-C5	20.58	1.79	1.44
4	2	4083	5MU	C6-N1	16.43	1.66	1.38
4	2	4296	B8H	C6-C5	-16.39	1.11	1.34
4	2	1860	B8H	C6-C5	-16.35	1.12	1.34
4	2	4296	B8H	C4-N3	-15.66	1.09	1.38

The worst 5 of 625 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	2	1574	B9B	O6-C6-C5	22.01	144.43	116.57
4	2	2754	B9B	O6-C6-C5	21.42	143.69	116.57
4	2	237	B9B	O6-C6-C5	21.15	143.35	116.57
4	2	1574	B9B	O6-C6-N1	-18.81	93.80	120.00
4	2	2754	B9B	O6-C6-N1	-18.34	94.46	120.00

There are no chirality outliers.

5 of 115 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
53	8	14	OMU	C1'-C2'-O2'-CM2
4	2	237	B9B	C5-C6-O6-C61
4	2	237	B9B	N1-C6-O6-C61
4	2	237	B9B	C3'-C4'-C5'-O5'
4	2	237	B9B	O4'-C4'-C5'-O5'

There are no ring outliers.

21 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	2	4185	B8W	1	0
4	2	4623	OMG	1	0
4	2	3718	A2M	1	0
4	2	2050	OMG	1	0
4	2	1871	A2M	1	0
4	2	2754	B9B	1	0
4	2	2773	OMG	1	0
4	2	2363	A2M	1	0
4	2	4872	2MG	1	0
4	2	4083	5MU	3	0
4	2	1517	2MG	1	0
4	2	1456	B8Q	1	0
4	2	1860	B8H	1	0
4	2	4296	B8H	1	0
4	2	1316	OMG	1	0
4	2	2522	7MG	1	0
4	2	729	2MG	1	0
4	2	4571	A2M	1	0
4	2	1574	B9B	1	0
4	2	2364	OMG	1	0
4	2	3723	A2M	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 2 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
59	GDP	A	801	61,60	28,30,30	1.27	3 (10%)	44,47,47	1.91	9 (20%)

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
59	GDP	A	801	61,60	-	2/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
59	A	801	GDP	C6-N1	-3.31	1.32	1.38
59	A	801	GDP	C5-N7	-2.51	1.34	1.39
59	A	801	GDP	C5-C4	2.34	1.45	1.38

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
59	A	801	GDP	C5-C4-N3	-6.17	118.45	128.46
59	A	801	GDP	C2-N3-C4	4.98	121.17	112.30
59	A	801	GDP	N9-C4-N3	4.62	135.22	125.94
59	A	801	GDP	PA-O3A-PB	-3.52	120.74	132.83
59	A	801	GDP	C6-C5-N7	3.09	136.00	130.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

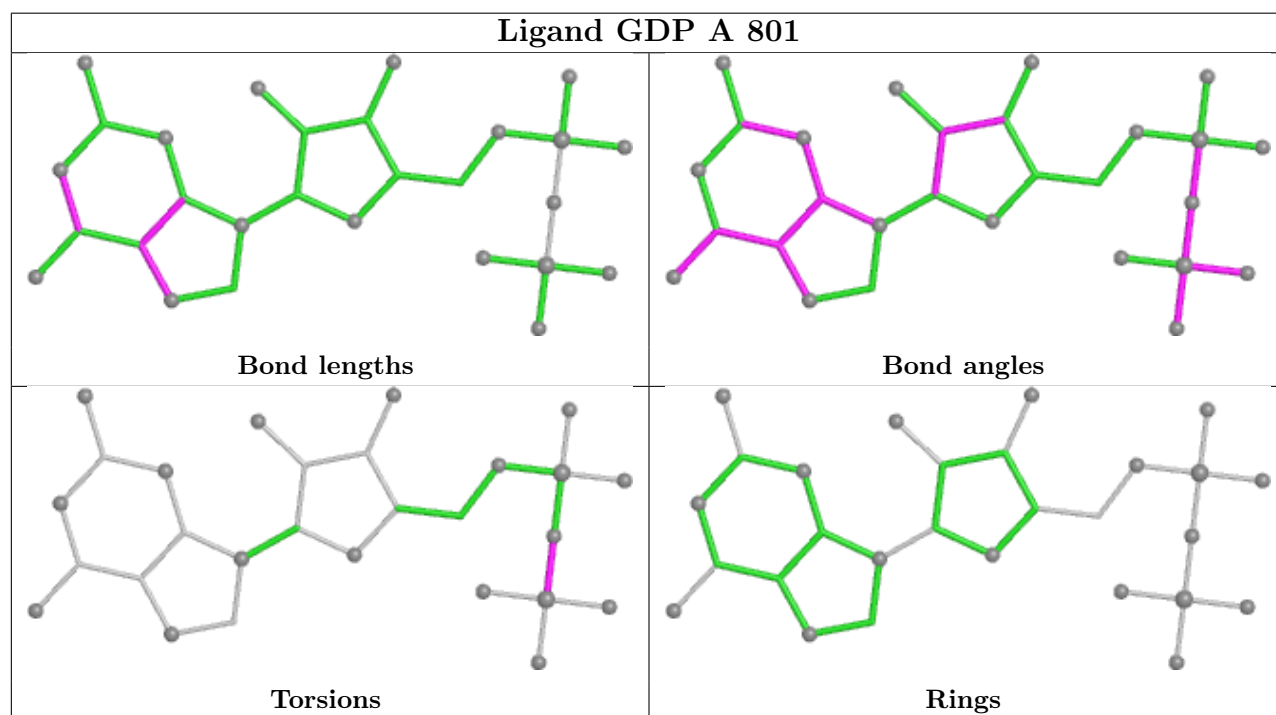
Mol	Chain	Res	Type	Atoms
59	A	801	GDP	PA-O3A-PB-O2B
59	A	801	GDP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
59	A	801	GDP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

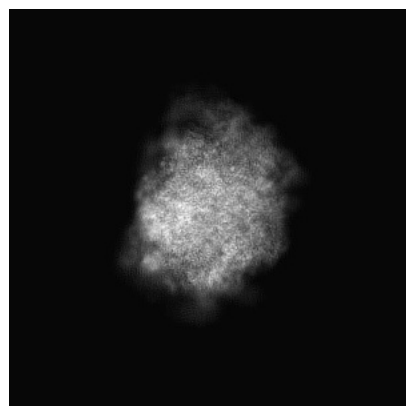
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35596. These allow visual inspection of the internal detail of the map and identification of artifacts.

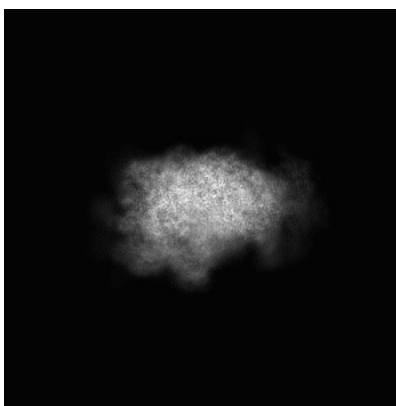
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

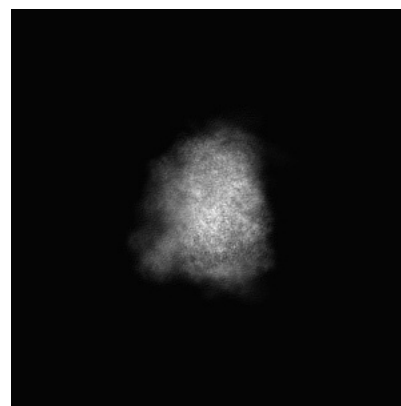
6.1.1 Primary map



X

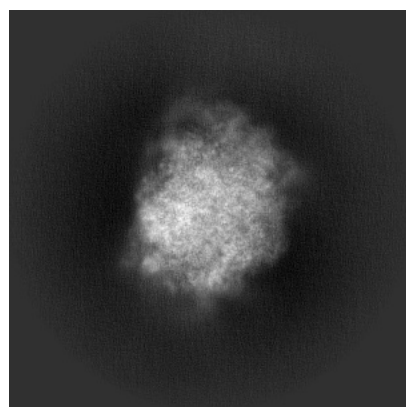


Y

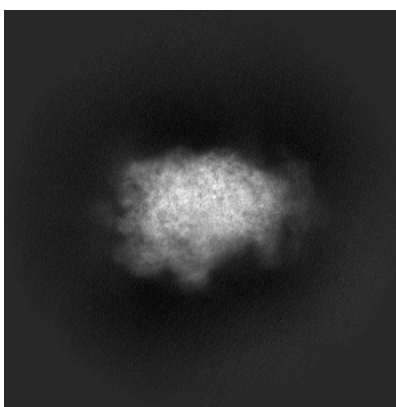


Z

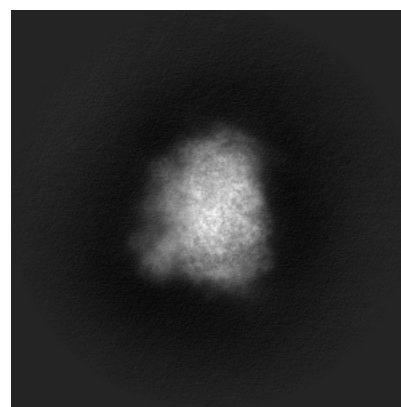
6.1.2 Raw map



X



Y

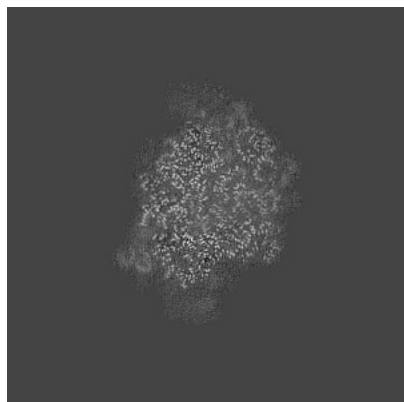


Z

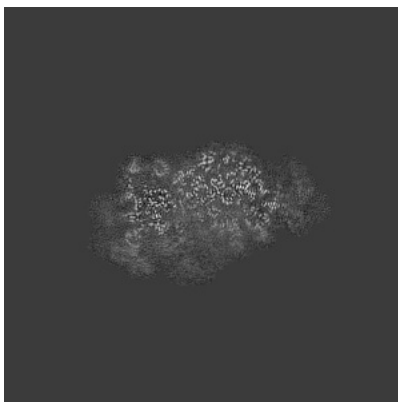
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

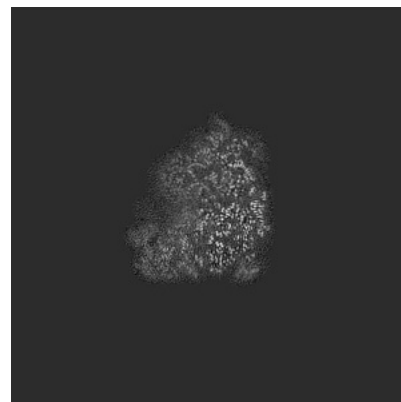
6.2.1 Primary map



X Index: 200

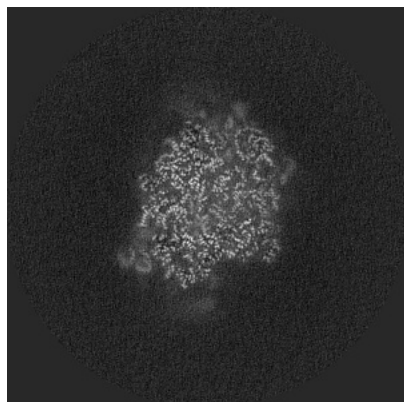


Y Index: 200

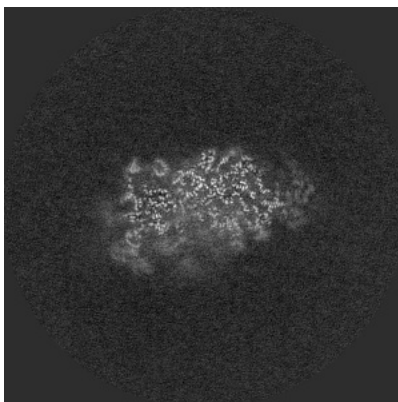


Z Index: 200

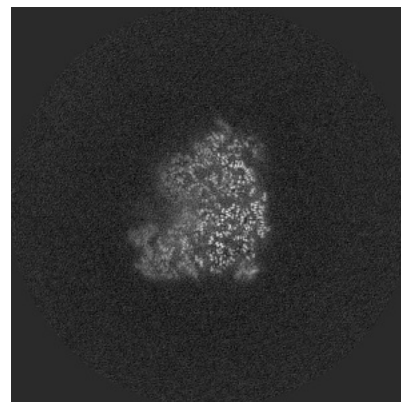
6.2.2 Raw map



X Index: 200



Y Index: 200

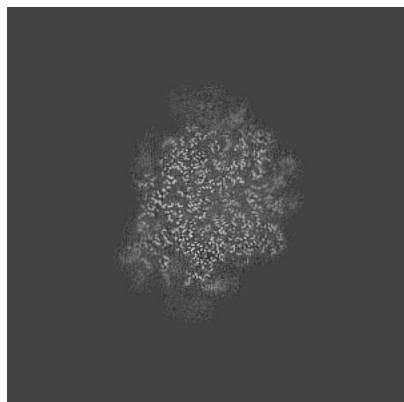


Z Index: 200

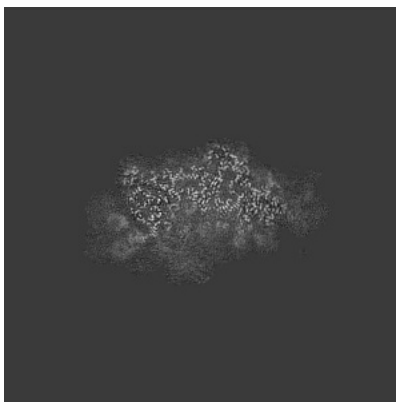
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

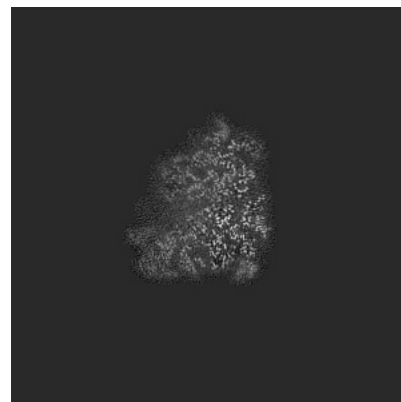
6.3.1 Primary map



X Index: 206

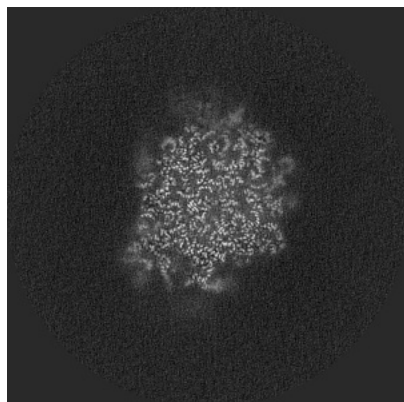


Y Index: 191

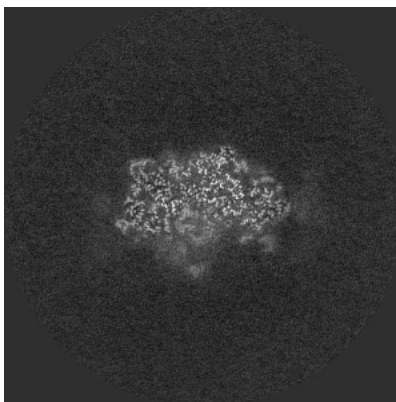


Z Index: 202

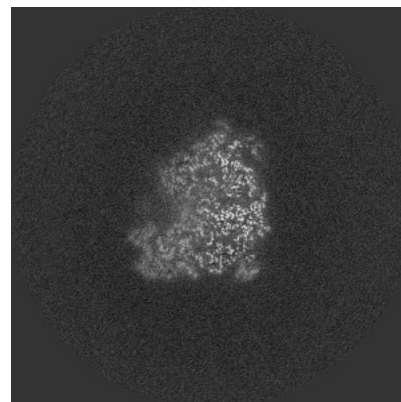
6.3.2 Raw map



X Index: 207



Y Index: 182

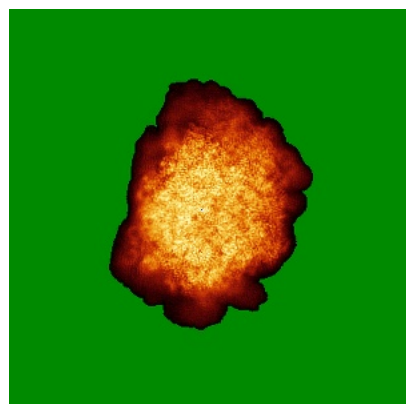


Z Index: 199

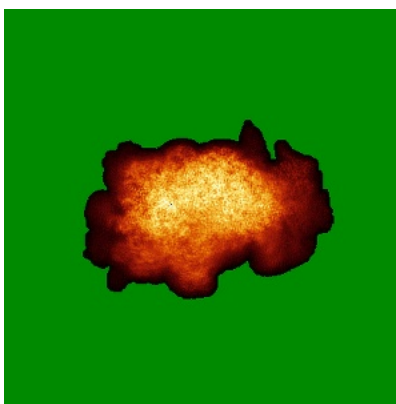
The images above show the largest variance slices of the map in three orthogonal directions.

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

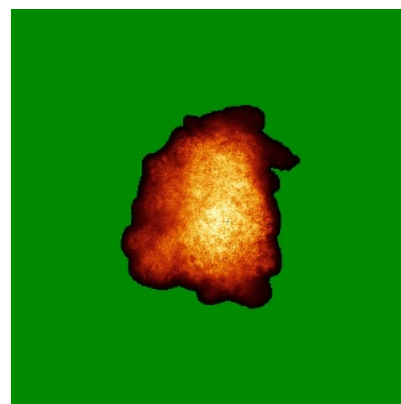
6.4.1 Primary map



X

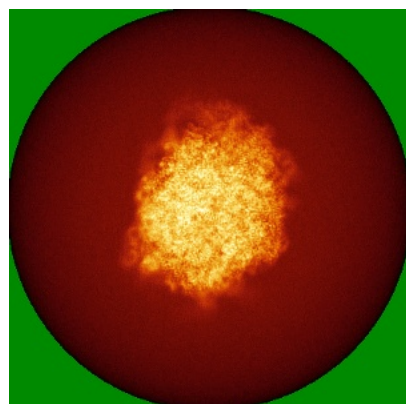


Y

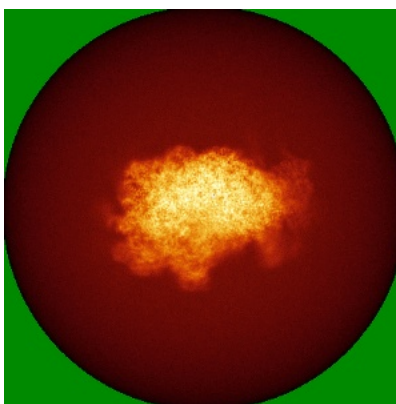


Z

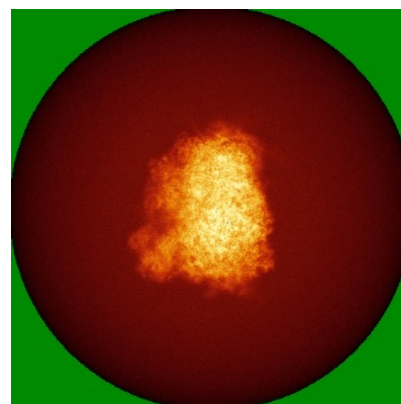
6.4.2 Raw map



X



Y

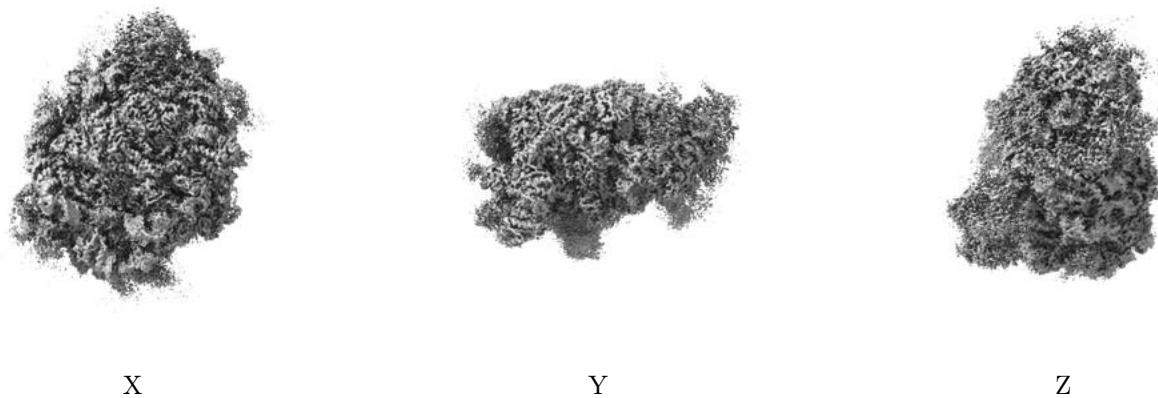


Z

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

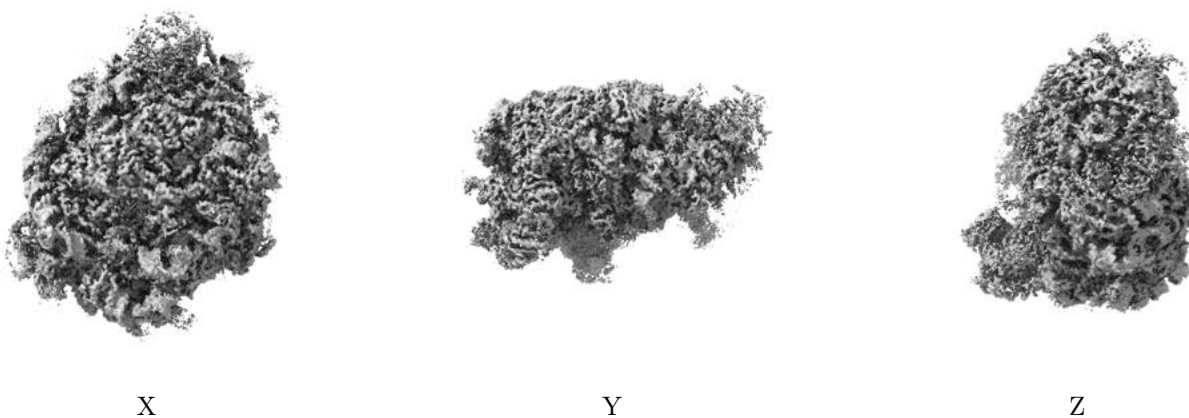
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.032. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

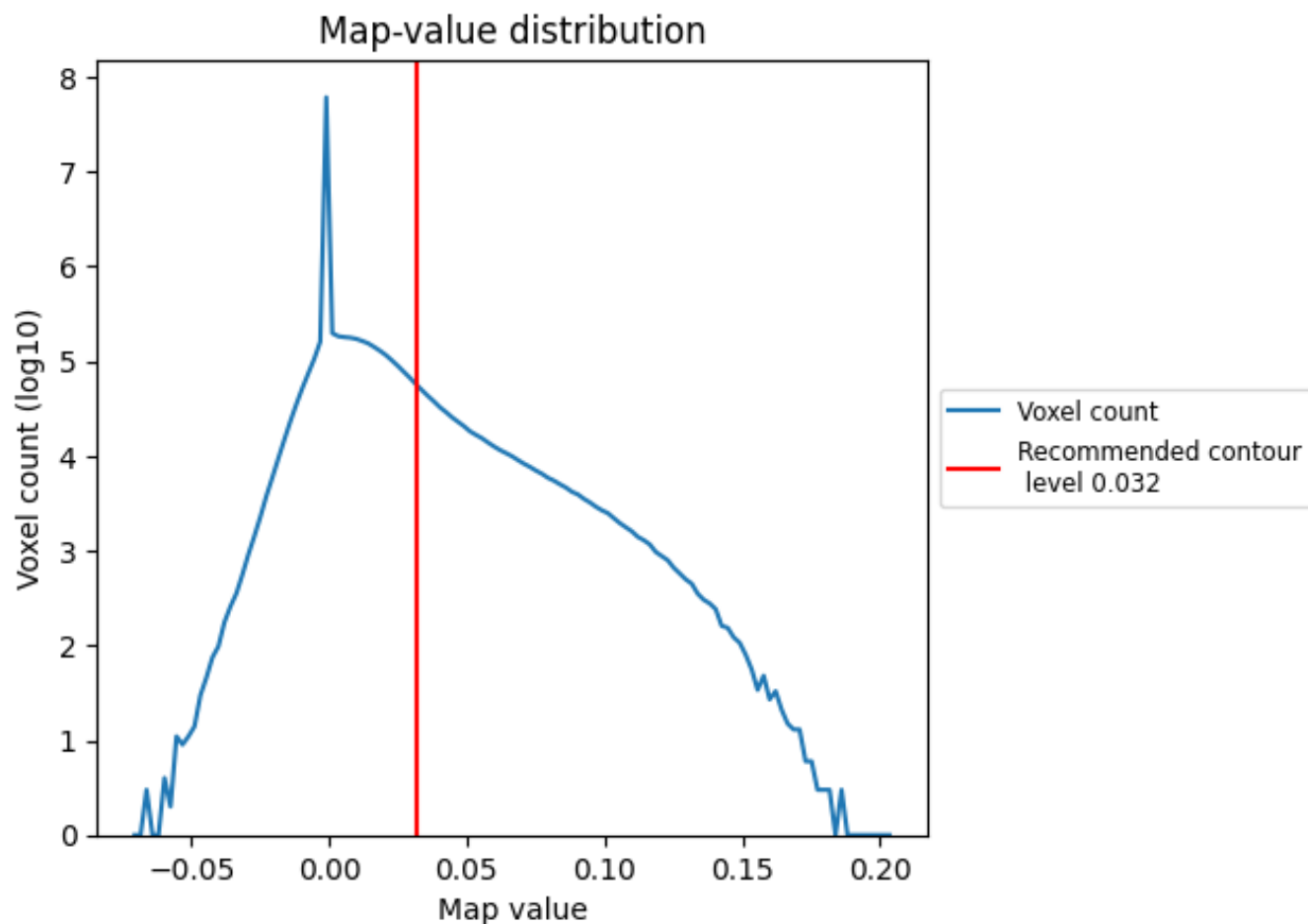
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

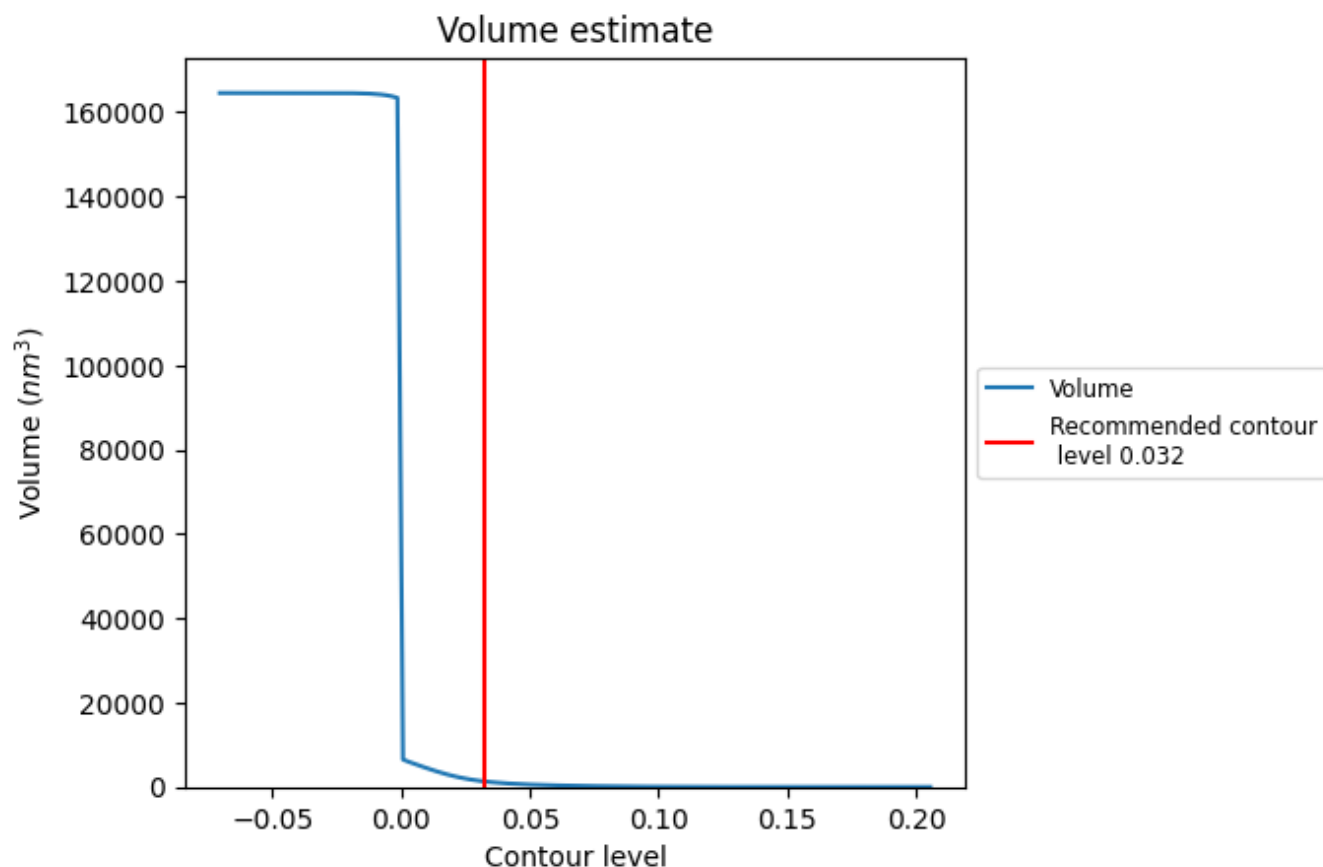
This section contains the results of statistical analysis of the map.

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.

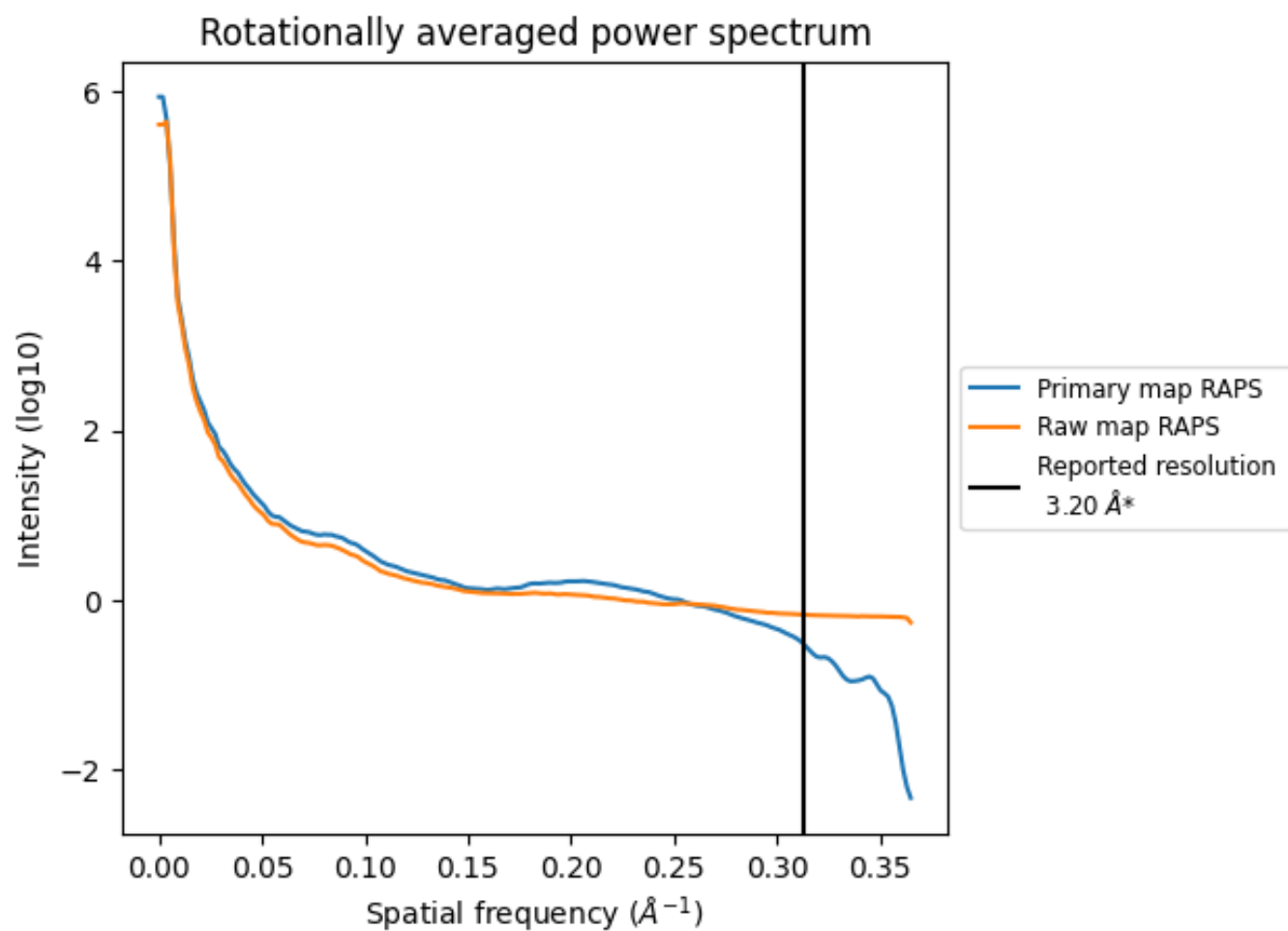
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1336 nm^3 ; this corresponds to an approximate mass of 1207 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 ⓘ

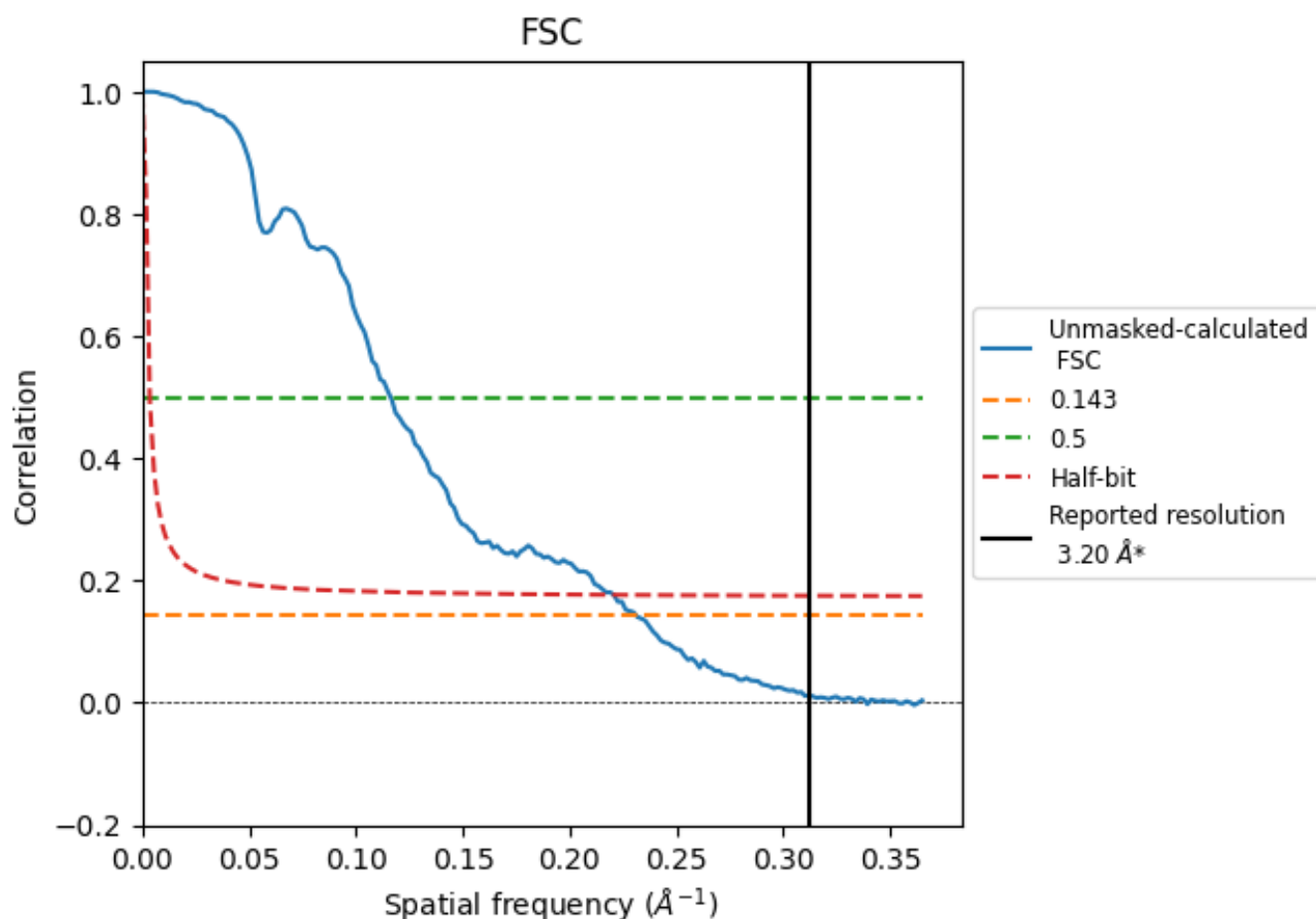


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

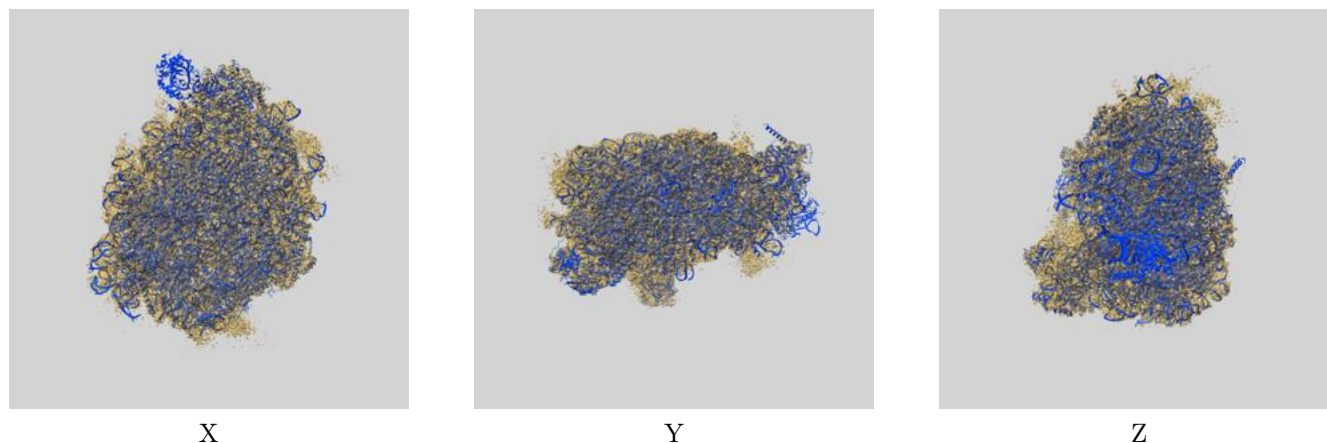
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.33	8.61	4.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.33 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

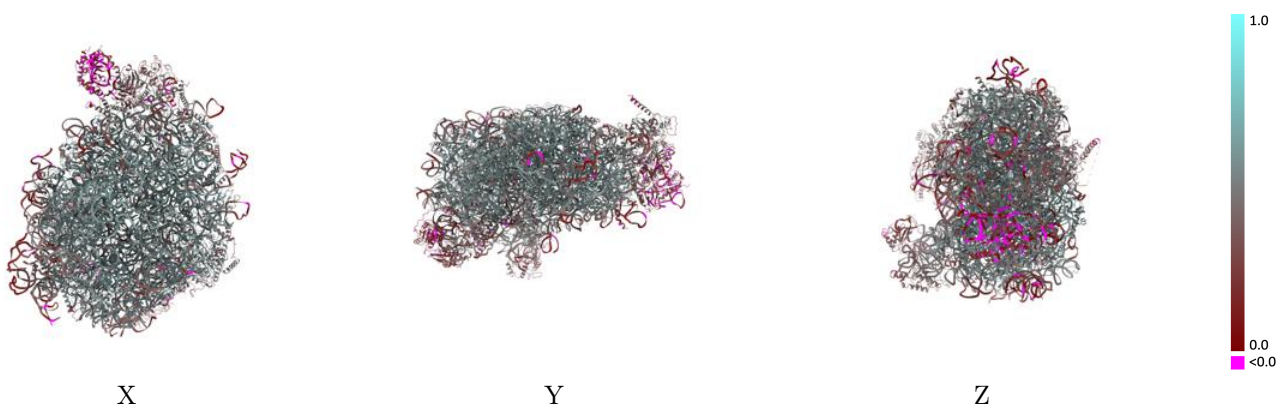
This section contains information regarding the fit between EMDB map EMD-35596 and PDB model 8INE. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



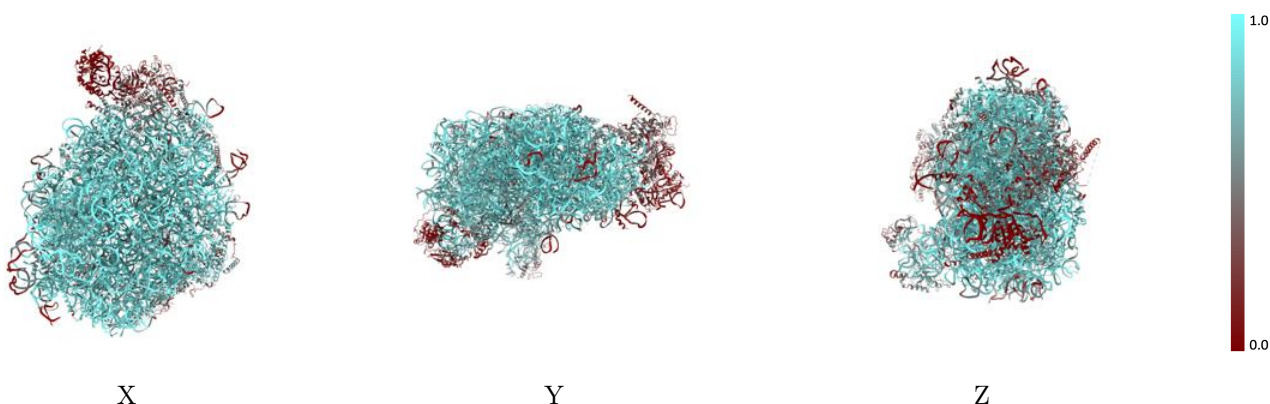
The images above show the 3D surface view of the map at the recommended contour level 0.032 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



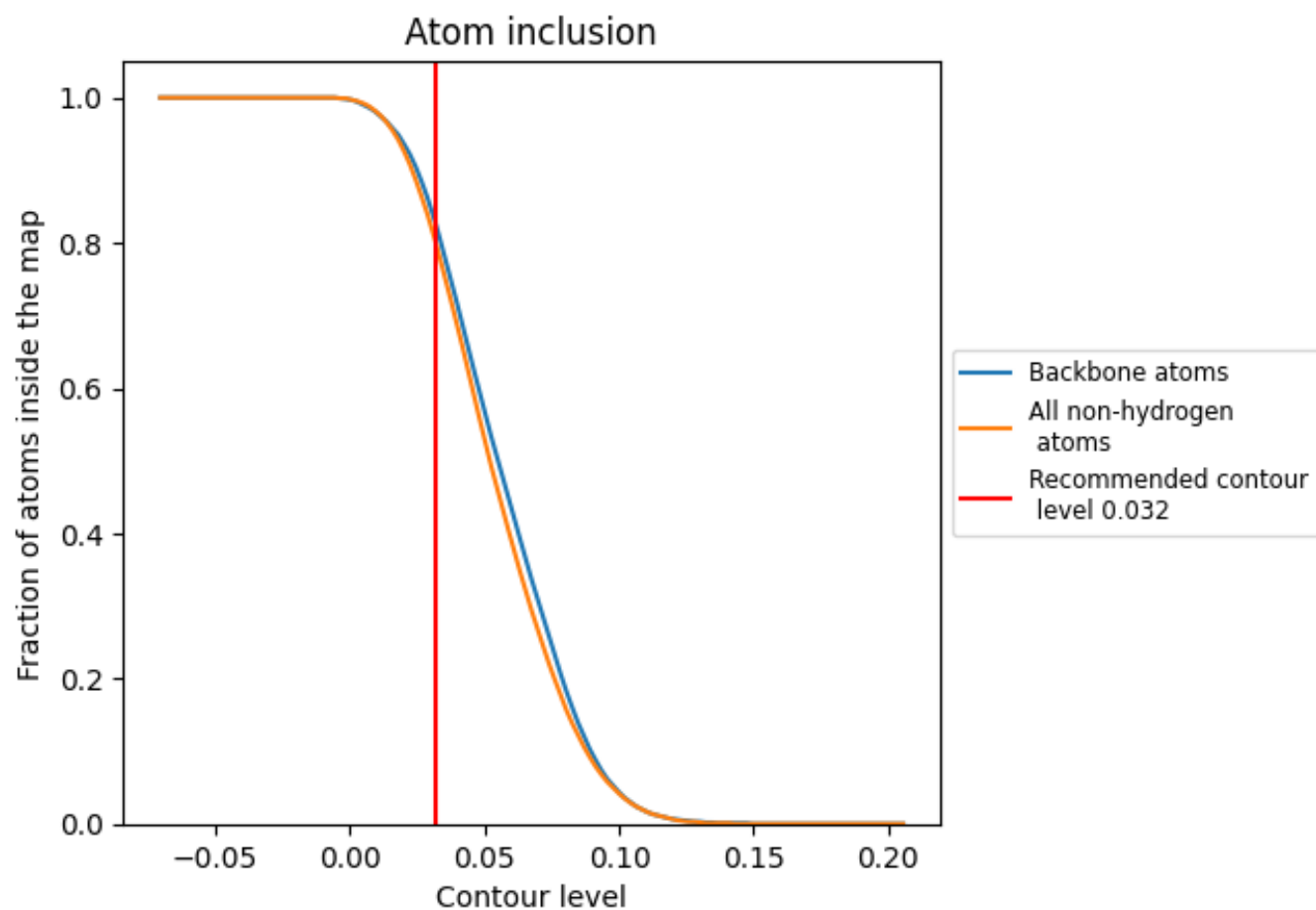
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.032).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 80% 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 (0.032) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7990	 0.4650
2	 0.8880	 0.4730
3	 0.2700	 0.3550
4	 0.6610	 0.4320
5	 0.8920	 0.4310
6	 0.7360	 0.4760
7	 0.7960	 0.5070
8	 0.9500	 0.5390
9	 0.5240	 0.4330
A	 0.5900	 0.4300
B	 0.8980	 0.5460
C	 0.7540	 0.4210
D	 0.9320	 0.5500
E	 0.7200	 0.4710
F	 0.8720	 0.5320
G	 0.7270	 0.4600
H	 0.8750	 0.5320
I	 0.8280	 0.5090
J	 0.1720	 0.1510
K	 0.8570	 0.5060
L	 0.9360	 0.5530
M	 0.9610	 0.5670
N	 0.4950	 0.2850
O	 0.7720	 0.4920
P	 0.9720	 0.5740
Q	 0.8450	 0.5170
R	 0.3670	 0.3580
S	 0.9080	 0.5380
T	 0.6580	 0.3820
U	 0.9590	 0.5650
V	 0.9320	 0.5610
W	 0.6090	 0.4630
X	 0.7760	 0.4970
Y	 0.8680	 0.5330
Z	 0.9410	 0.5630



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Chain	Atom inclusion	Q-score
a	 0.8820	 0.5190
b	 0.9480	 0.5700
c	 0.8590	 0.4840
d	 0.7850	 0.4840
e	 0.8820	 0.5270
g	 0.8310	 0.5110
h	 0.8870	 0.5420
i	 0.8320	 0.5070
j	 0.8370	 0.5130
k	 0.9530	 0.5640
l	 0.9210	 0.5480
m	 0.8580	 0.5210
n	 0.9600	 0.5760
o	 0.7880	 0.4690
p	 0.9150	 0.5380
r	 0.6050	 0.3620
s	 0.2630	 0.2070
t	 0.1190	 0.2320
u	 0.0000	 0.0970
v	 0.4290	 0.4110
w	 0.4130	 0.4110
x	 0.0040	 0.0100
y	 0.1650	 0.2130
z	 0.6370	 0.4350