



wwPDB EM Validation Summary Report ⓘ

Jun 24, 2026 – 05:14 AM EDT

PDB ID : 8G7R / pdb_00008g7r
EMDB ID : EMD-29821
Title : Structure of the Escherichia coli 70S ribosome in complex with A-site tR-NAIle(LAU) bound to the cognate AUA codon (Structure III)
Authors : Rybak, M.Y.; Gagnon, M.G.
Deposited on : 2023-02-16
Resolution : 2.80 Å(reported)
Based on initial model : 7K00

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:

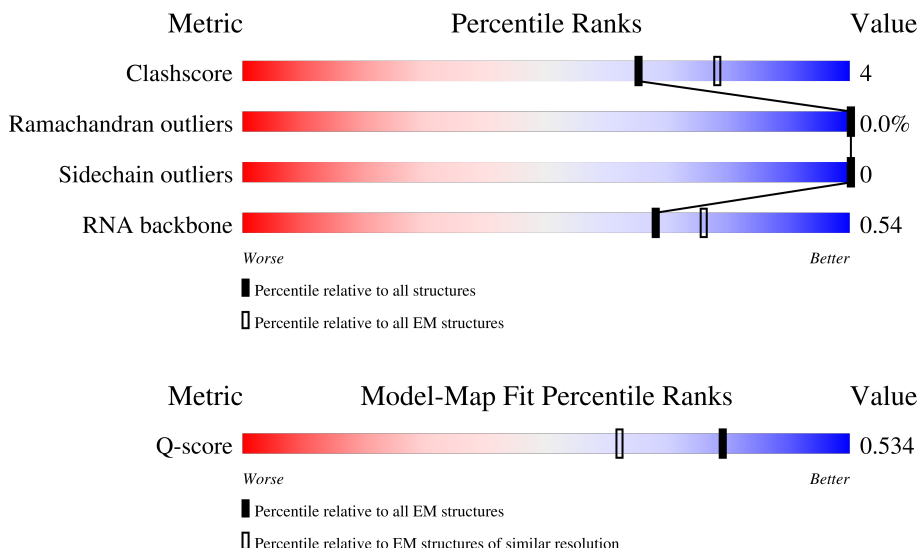
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	11806 (2.30 - 3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	a	1542	
2	b	241	
3	c	233	

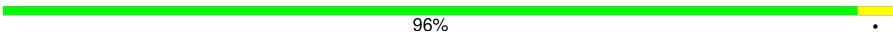
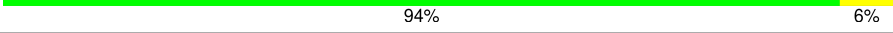
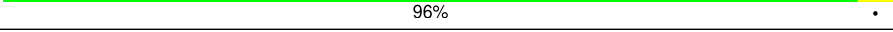
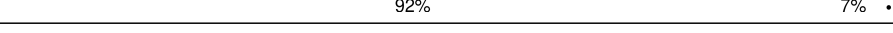
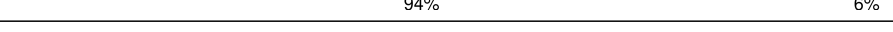
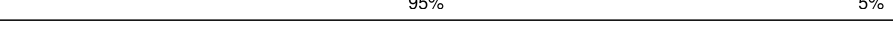
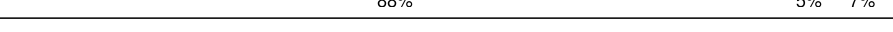
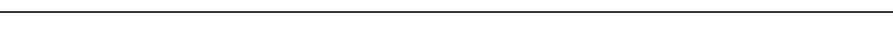
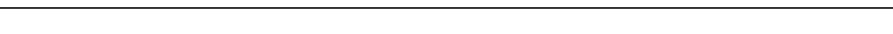
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Mol	Chain	Length	Quality of chain
4	d	206	
5	e	167	
6	f	131	
7	g	156	
8	h	130	
9	i	130	
10	j	103	
11	k	129	
12	l	124	
13	m	118	
14	n	101	
15	o	89	
16	p	82	
17	q	84	
18	r	75	
19	s	92	
20	t	87	
21	u	71	
22	w	76	
22	y	76	
23	x	77	
24	v	27	
25	A	2904	
26	B	120	
27	C	273	

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Mol	Chain	Length	Quality of chain
28	D	209	
29	E	201	
30	F	179	
31	G	177	
32	H	149	
33	L	142	
34	M	123	
35	N	144	
36	O	136	
37	P	127	
38	Q	117	
39	R	115	
40	S	118	
41	T	103	
42	U	110	
43	V	100	
44	W	104	
45	X	94	
46	Y	85	
47	Z	78	
48	1	63	
49	2	59	
50	3	70	
51	4	57	
52	5	55	

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Mol	Chain	Length	Quality of chain
53	6	46	 91%9%
54	7	65	 92%6% •
55	8	38	 82%18%

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 147376 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 16S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	1528	Total	C	N	O	P	0	0
			32803	14637	6019	10619	1528		

- Molecule 2 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	224	Total	C	N	O	S	0	0
			1754	1110	315	321	8		

- Molecule 3 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 4 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 5 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	156	Total	C	N	O	S	0	0
			1152	717	217	212	6		

- Molecule 6 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	103	Total	C	N	O	S	0	0
			839	530	151	151	7		

- Molecule 7 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	152	Total	C	N	O	S	0	0
			1191	741	230	216	4		

- Molecule 8 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 9 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	127	Total	C	N	O	S	0	0
			1022	634	206	179	3		

- Molecule 10 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 11 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	119	IAS	ASN	modified residue	UNP A0A0H3PWX2

- Molecule 12 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 13 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 14 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 15 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	o	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 16 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	p	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 17 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 18 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	r	54	Total	C	N	O	0	0
			446	283	85	78		

- Molecule 19 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	s	83	Total	C	N	O	S	0	0
			663	424	126	111	2		

- Molecule 20 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	t	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 21 is a protein called 30S ribosomal protein S21.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	u	55	Total	C	N	O	S	0	0
			460	287	95	77	1		

- Molecule 22 is a RNA chain called Isoleucine tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
22	w	76	Total	C	N	O	P	S	0	0
			1645	740	292	537	75	1		
22	y	76	Total	C	N	O	P	S	0	0
			1644	740	292	536	75	1		

- Molecule 23 is a RNA chain called P-site initiator tRNA.

Mol	Chain	Residues	Atoms						AltConf	Trace
23	x	76	Total	C	N	O	P	S	0	0
			1625	725	294	529	76	1		

- Molecule 24 is a RNA chain called M-I mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	v	11	Total	C	N	O	P	0	0
			239	108	49	71	11		

- Molecule 25 is a RNA chain called 23S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	A	2899	Total	C	N	O	P	0	0
			62252	27778	11456	20119	2899		

- Molecule 26 is a RNA chain called 5S Ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	B	120	Total	C	N	O	P	0	0
			2572	1145	470	837	120		

- Molecule 27 is a protein called 50S ribosomal protein L2.

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

- Molecule 28 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	D	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 29 is a protein called 50S ribosomal protein L4.

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

- Molecule 30 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	F	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 31 is a protein called 50S ribosomal protein L6.

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

- Molecule 32 is a protein called 50S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	H	41	Total	C	N	O	S	0	0
			303	194	54	54	1		

- Molecule 33 is a protein called 50S ribosomal protein L13.

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

- Molecule 34 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	M	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 35 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	N	144	Total	C	N	O	S	0	0
			1052	653	207	190	2		

- Molecule 36 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	O	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	82	MS6	MET	modified residue	UNP E6BI61

- Molecule 37 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	P	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 38 is a protein called 50S ribosomal protein L18.

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

- Molecule 39 is a protein called 50S ribosomal protein L19.

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

- Molecule 40 is a protein called 50S ribosomal protein L20.

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

- Molecule 41 is a protein called Ribosomal protein L21.

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

- Molecule 42 is a protein called 50S ribosomal protein L22.

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

- Molecule 43 is a protein called 50S ribosomal protein L23.

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

- Molecule 44 is a protein called 50S ribosomal protein L24.

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

- Molecule 45 is a protein called 50S ribosomal protein L25.

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

- Molecule 46 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Y	76	Total	C	N	O	S	0	0
			582	360	117	104	1		

- Molecule 47 is a protein called 50S ribosomal protein L28.

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

- Molecule 48 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	1	61	Total	C	N	O	S	0	0
			495	305	97	92	1		

- Molecule 49 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	2	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 50 is a protein called 50S ribosomal protein L31.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	3	60	Total	C	N	O	S	0	0
			468	290	87	85	6		

- Molecule 51 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	4	55	Total	C	N	O	S	0	0
			434	263	92	78	1		

- Molecule 52 is a protein called 50S ribosomal protein L33.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	5	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 53 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

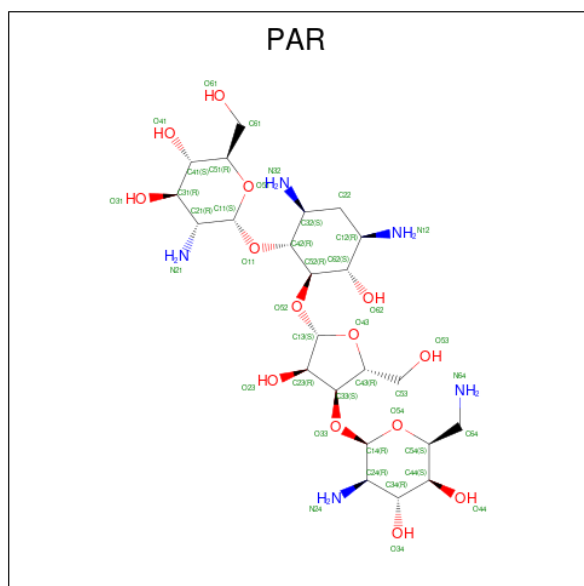
- Molecule 54 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	7	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 55 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	8	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 56 is PAROMOMYCIN (CCD ID: PAR) (formula: $C_{23}H_{45}N_5O_{14}$).



Mol	Chain	Residues	Atoms				AltConf
56	a	1	Total	C	N	O	0
			42	23	5	14	

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
57	a	91	Total	Mg	0
			91	91	
57	e	2	Total	Mg	0
			2	2	
57	l	1	Total	Mg	0
			1	1	
57	x	2	Total	Mg	0
			2	2	

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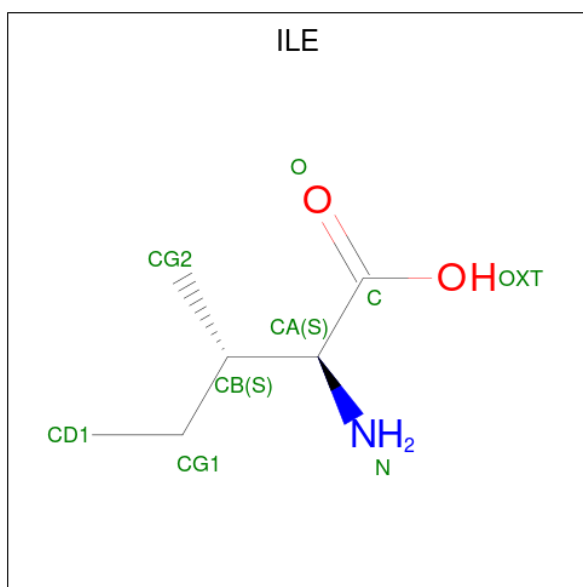
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Mol	Chain	Residues	Atoms		AltConf
57	v	2	Total 2	Mg 2	0
57	A	603	Total 603	Mg 603	0
57	B	6	Total 6	Mg 6	0
57	D	1	Total 1	Mg 1	0
57	E	2	Total 2	Mg 2	0
57	L	4	Total 4	Mg 4	0
57	N	2	Total 2	Mg 2	0
57	P	1	Total 1	Mg 1	0
57	R	1	Total 1	Mg 1	0
57	S	2	Total 2	Mg 2	0
57	U	1	Total 1	Mg 1	0
57	V	2	Total 2	Mg 2	0
57	Y	1	Total 1	Mg 1	0
57	4	7	Total 7	Mg 7	0
57	8	3	Total 3	Mg 3	0

- Molecule 58 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
58	a	1	Total 1	K 1	0
58	l	1	Total 1	K 1	0

- Molecule 59 is ISOLEUCINE (CCD ID: ILE) (formula: C₆H₁₃NO₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
59	y	1	Total	C	N	O	0
			8	6	1	1	

- Molecule 60 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
60	3	1	Total	Zn	0
			1	1	
60	8	1	Total	Zn	0
			1	1	

- Molecule 61 is water.

Mol	Chain	Residues	Atoms		AltConf
61	a	31	Total	O	0
			31	31	
61	k	1	Total	O	0
			1	1	
61	l	2	Total	O	0
			2	2	
61	w	1	Total	O	0
			1	1	
61	A	278	Total	O	0
			278	278	
61	B	3	Total	O	0
			3	3	

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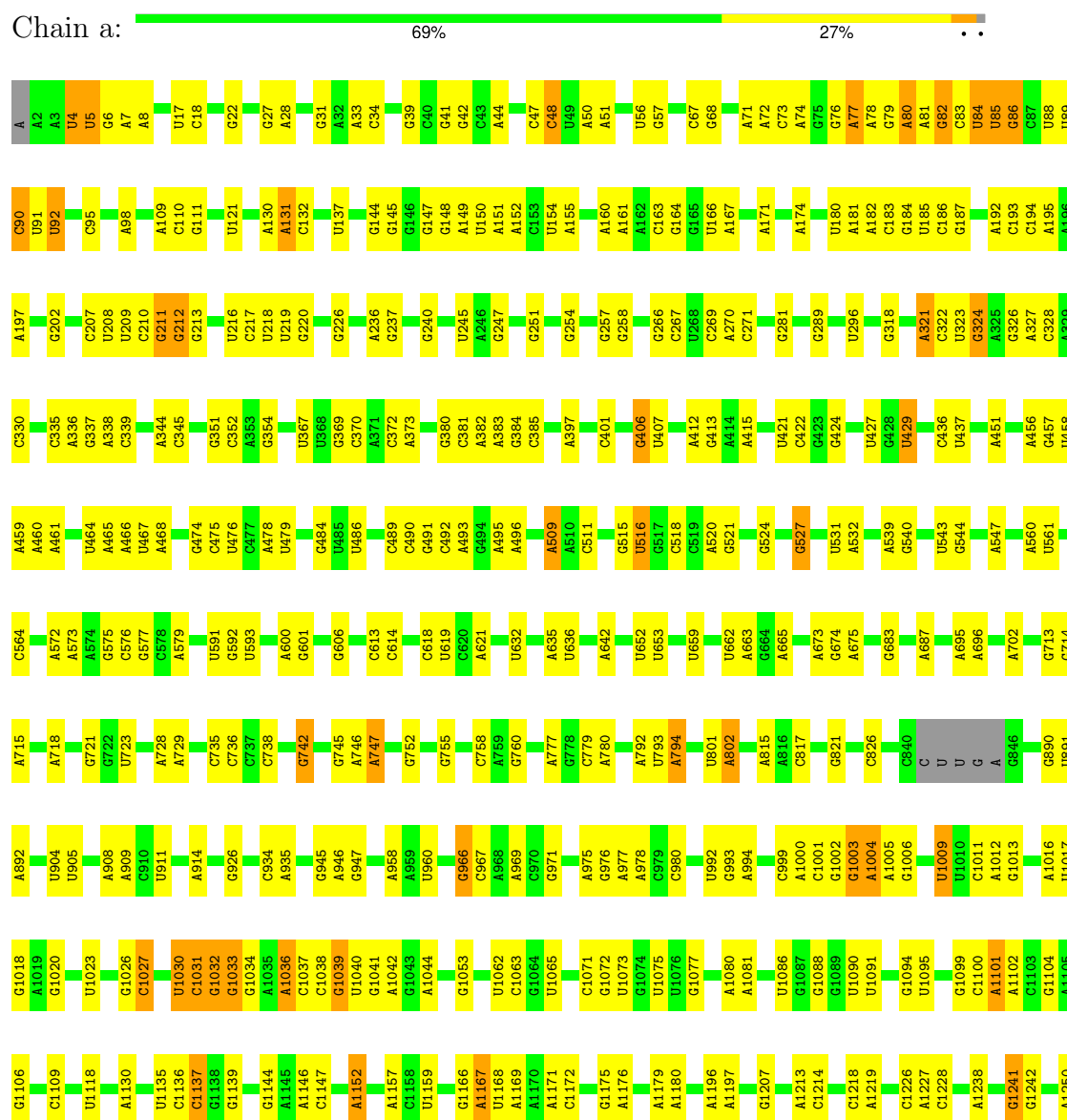
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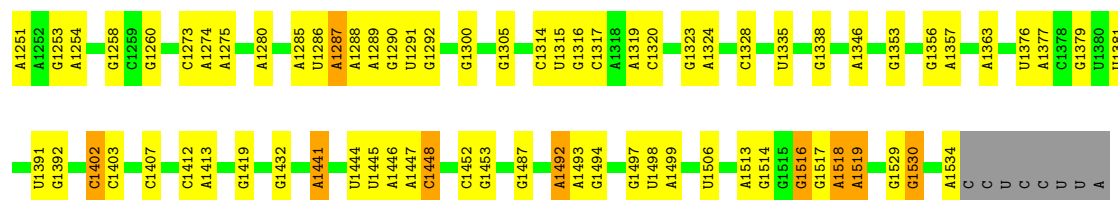
Mol	Chain	Residues	Atoms		AltConf
61	D	2	Total 2	O 2	0
61	L	2	Total 2	O 2	0
61	T	1	Total 1	O 1	0
61	U	2	Total 2	O 2	0
61	V	2	Total 2	O 2	0
61	Y	1	Total 1	O 1	0
61	Z	2	Total 2	O 2	0
61	4	3	Total 3	O 3	0

3 Residue-property plots

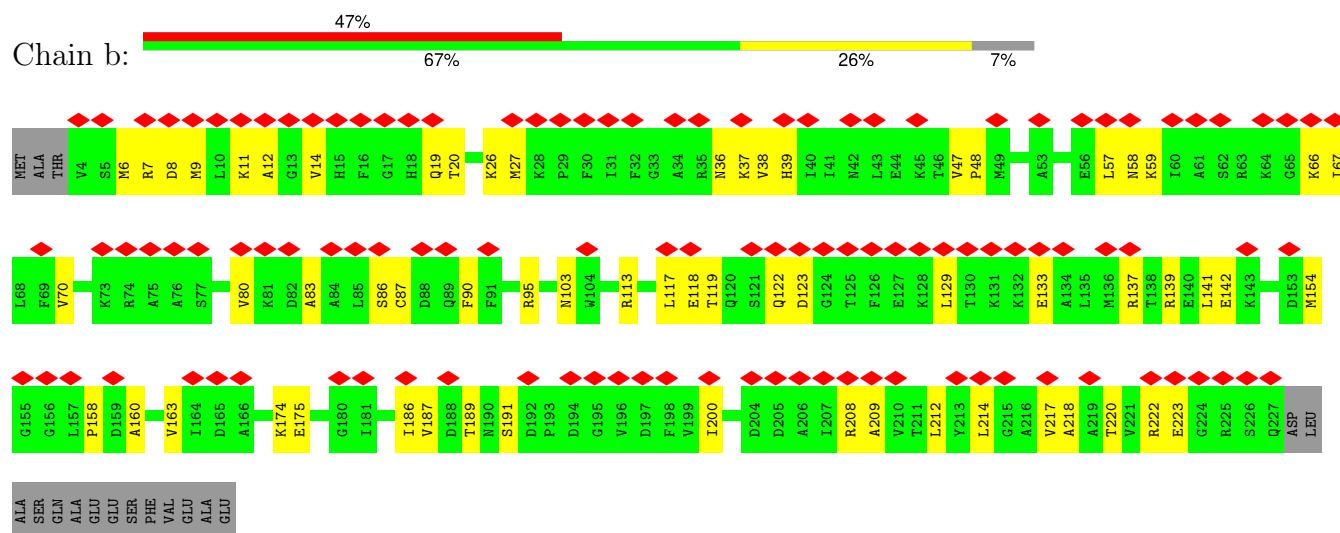
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 16S Ribosomal RNA

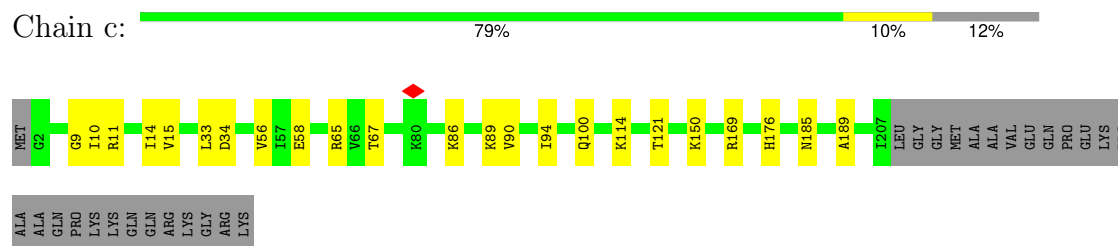




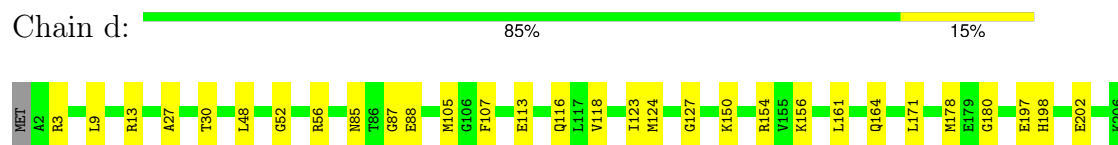
• Molecule 2: 30S ribosomal protein S2



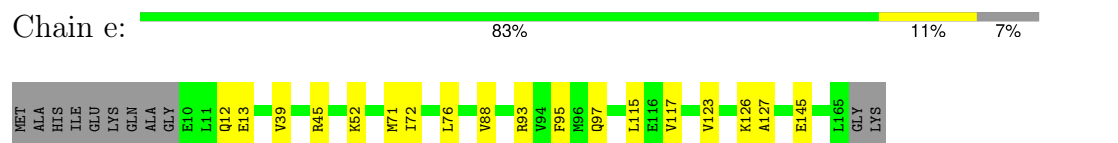
• Molecule 3: 30S ribosomal protein S3



• Molecule 4: 30S ribosomal protein S4

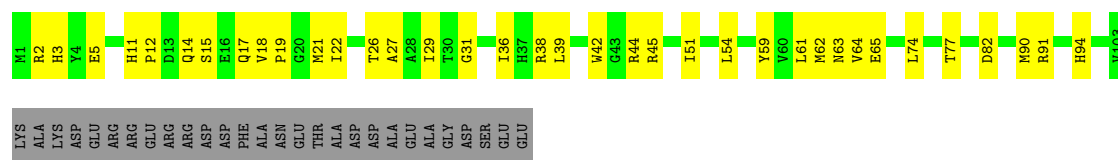


• Molecule 5: 30S ribosomal protein S5



• Molecule 6: 30S ribosomal protein S6

Chain f:  51% 27% 21%



- Molecule 7: 30S ribosomal protein S7

Chain g:  84% 13%



- Molecule 8: 30S ribosomal protein S8

Chain h:  91% 8%



- Molecule 9: 30S ribosomal protein S9

Chain i:  75% 23%



- Molecule 10: 30S ribosomal protein S10

Chain j:  71% 24% 5%



- Molecule 11: 30S ribosomal protein S11

Chain k:  71% 19% 9%



- Molecule 12: 30S ribosomal protein S12

Chain l:  91% 6%



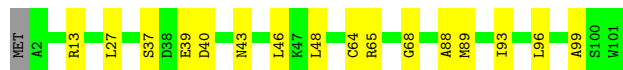
- Molecule 13: 30S ribosomal protein S13

Chain m:  81% 17%



- Molecule 14: 30S ribosomal protein S14

Chain n:  83% 16%



- Molecule 15: 30S ribosomal protein S15

Chain o:  89% 10%



- Molecule 16: 30S ribosomal protein S16

Chain p:  80% 18%



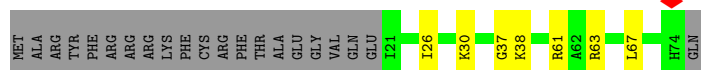
- Molecule 17: 30S ribosomal protein S17

Chain q:  81% 13% 6%



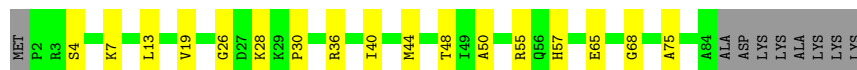
- Molecule 18: 30S ribosomal protein S18

Chain r:  63% 9% 28%

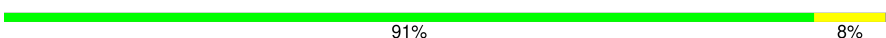


- Molecule 19: 30S ribosomal protein S19

Chain s:  72% 18% 10%



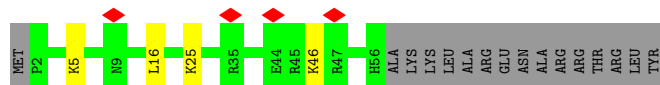
- Molecule 20: 30S ribosomal protein S20

Chain t:  91% 8%



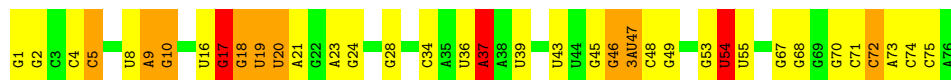
- Molecule 21: 30S ribosomal protein S21

Chain u:  6% 72% 6% 23%



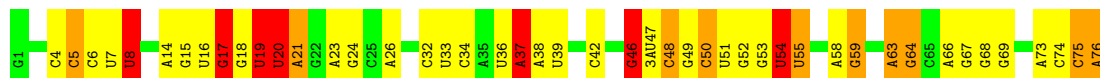
- Molecule 22: Isoleucine tRNA

Chain w:  51% 33% 12%



- Molecule 22: Isoleucine tRNA

Chain y:  39% 38% 13% 9%



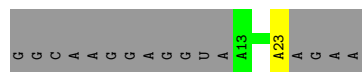
- Molecule 23: P-site initiator tRNA

Chain x:  66% 25% 8%



- Molecule 24: M-I mRNA

Chain v:  37% 59%

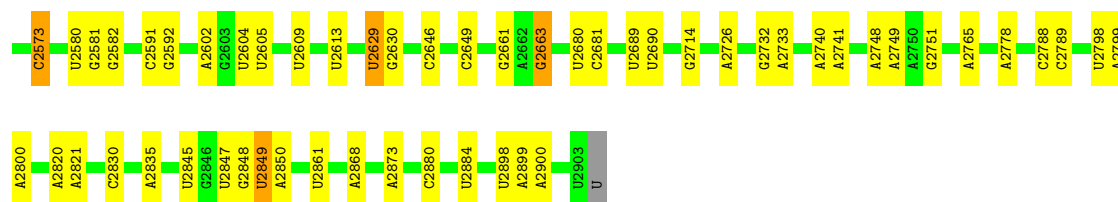


- Molecule 25: 23S Ribosomal RNA

Chain A:  77% 20%



G2429	A2430	U2441	G2445	A2448	U2449	U2457	G2458	A2459	A2469	G2470	A2471	G2472	U2473	A2474	G2475	A2476	U2477	A2478	C2498	C2499	G2502	A2503	G2504	U2505	U2506	C2507	U2514	C2515	A2518	U2519	C2520	G2529	G2532	A2547	U2548	U2552	G2553	U2554	U2555	G2556	G2557	C2558	A2566	G2567	C2568																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
C2261	A2268	G2271	G2272	A2273	A2278	C2283	G2286	A2287	A2288	U2291	U2292	U2305	U2306	U2307	U2308	U2309	G2308	U2312	A2322	G2325	G2326	A2327	A2328	U2329	G2330	A2333	U2334	A2335	G2345	C2350	C2361	G2383	U2384	C2385	U2402	A2406	G2410	U2420	A2425	A2426	U2427	G2428	C2429	U2430	U2431																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
U2151	C2152	C2153	A2154	U2155	G2156	A2157	A2158	C2159	C2160	C2161	G2162	A2163	C2164	C2165	U2166	A2169	A2170	A2171	U2172	U2173	C2174	C2175	A2176	C2177	A2178	C2179	U2182	A2183	U2184	U2185	U2186	U2187	U2188	U2189	A2190	A2191	U2192	A2198	G2204	A2211	A2225	U2238	G2239	A2240	U2241	U2242	U2243	U2244	U2245	A2246	A2247	G2250	C2251																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		
G2069	A2070	A2071	C2072	G2073	U2074	U2075	G2093	A2097	U2098	U2099	U2100	A2101	C2102	C2103	C2104	U2105	U2106	G2107	G2110	U2111	U2112	U2113	A2114	C2115	G2116	U2117	U2118	U2119	U2120	G2121	G2125	A2126	U2127	G2128	C2129	U2130	U2131	U2132	G2133	A2134	U2135	G2136	U2139	G2140	U2141	U2142	C2143	G2144	U2145	C2146	A2147	G2150																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			
3TD1915	A1916	U1917	A1918	A1919	U1923	U1929	G1930	A1937	A1938	U1939	U1955	C1962	C1963	U1964	C1967	U1970	U1971	U1972	U1973	U1991	G1992	U1993	C2006	A2013	C2023	A2030	G2032	A2031	G2033	U2034	G2035	C2036	C2043	A2052	C2055	G2056	A2059	A2060	G2061	A2062	C2063	C2064	C2065	C2066	U2067	C2068	C2069																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
A1745	A1746	U1747	G1756	C1764	A1773	G1776	U1782	A1783	A1784	C1795	G1799	C1800	A1801	A1802	A1803	A1808	A1809	A1810	C1816	G1826	A1829	G1835	A1847	A1848	A1853	A1854	U1855	G1856	G1857	A1858	U1864	A1872	G1873	A1889	A1890	G1906	U1911	A1912	A1913	G1914	G1915	U1916	U1917	U1918	U1919	U1920																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									
C1533	U1534	A1535	C1536	G1537	U1542	G1543	A1544	A1566	A1569	U1578	A1583	U1584	C1585	A1590	A1591	C1592	A1593	A1609	A1618	G1645	C1646	U1647	G1649	A1654	G1667	G1674	C1675	A1676	G1682	U1683	G1715	U1720	G1721	U1729	C1730	G1733	G1738	G1743	A1744	U1745	U1746	U1747	U1748	U1749																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
A1321	U1340	U1352	A1353	A1354	A1365	U1379	A1383	A1392	U1405	U1406	G1416	C1428	G1429	G1432	A1433	A1434	G1435	U1438	A1439	C1447	G1448	G1452	A1453	U1460	A1469	A1470	G1482	A1490	C1493	A1508	A1509	G1510	A1515	C1526	G1527	A1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																											
C1109	G1110	A1111	G1112	U1130	G1131	U1132	C1135	G1136	U1141	A1142	A1155	G1171	C1172	U	A	U	G1177	C1178	G1179	U1180	G1187	U1188	G1212	G1216	G1223	G1250	A1253	G1256	C1257	A1265	A1268	G1271	A1272	U1273	G1283	A1284	A1285	G1300	A1301	C1315	U1316	U1317	U1318	U1319	U1320																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
A1032	U1033	A1039	A1040	A1045	A1047	A1048	G1051	G1055	A1056	G1059	U1060	U1061	C915	G1062	G1063	U1064	U1065	U1066	A1067	G1068	A1069	A1070	G1071	C1072	A1073	C1075	C1076	A1077	U1078	C1079	A1080	U1081	A996	U1082	U1083	A1000	A1001	A1005	G1007	A1008	A1009	U1012	C1013	G1017	U1094	A1095	G1022	G856	G857	G1026	A1027	A1028	A1029	G1107	C1030	C1031	U1102	C1032	U1103	U1104	U1105	U1106	U1107	U1108	U1109	U1110	U1111	U1112	U1113	U1114	U1115	U1116	U1117	U1118	U1119	U1120	U1121	U1122	U1123	U1124	U1125	U1126	U1127	U1128	U1129	U1130	U1131	U1132	U1133	U1134	U1135	U1136	U1137	U1138	U1139	U1140	U1141	U1142	U1143	U1144	U1145	U1146	U1147	U1148	U1149	U1150	U1151	U1152	U1153	U1154	U1155	U1156	U1157	U1158	U1159	U1160	U1161	U1162	U1163	U1164	U1165	U1166	U1167	U1168	U1169	U1170	U1171	U1172	U1173	U1174	U1175	U1176	U1177	U1178	U1179	U1180	U1181	U1182	U1183	U1184	U1185	U1186	U1187	U1188	U1189	U1190	U1191	U1192	U1193	U1194	U1195	U1196	U1197	U1198	U1199	U1200	U1201	U1202	U1203	U1204	U1205	U1206	U1207	U1208	U1209	U1210	U1211	U1212	U1213	U1214	U1215	U1216	U1217	U1218	U1219	U1220	U1221	U1222	U1223	U1224	U1225	U1226	U1227	U1228	U1229	U1230	U1231	U1232	U1233	U1234	U1235	U1236	U1237	U1238	U1239	U1240	U1241	U1242	U1243	U1244	U1245	U1246	U1247	U1248	U1249	U1250	U1251	U1252	U1253	U1254	U1255	U1256	U1257	U1258	U1259	U1260	U1261	U1262	U1263	U1264	U1265	U1266	U1267	U1268	U1269	U1270	U1271	U1272	U1273	U1274	U1275	U1276	U1277	U1278	U1279	U1280	U1281	U1282	U1283	U1284	U1285	U1286	U1287	U1288	U1289	U1290	U1291	U1292	U1293	U1294	U1295	U1296	U1297	U1298	U1299	U1300	U1301	U1302	U1303	U1304	U1305	U1306	U1307	U1308	U1309	U1310	U1311	U1312	U1313	U1314	U1315	U1316	U1317	U1318	U1319	U1320	U1321	U1322	U1323	U1324	U1325	U1326	U1327	U1328	U1329	U1330	U1331	U1332	U1333	U1334	U1335	U1336	U1337	U1338	U1339	U1340	U1341	U1342	U1343	U1344	U1345	U1346	U1347	U1348	U1349	U1350	U1351	U1352	U1353	U1354	U1355	U1356	U1357	U1358	U1359	U1360	U1361	U1362	U1363	U1364	U1365	U1366	U1367	U1368	U1369	U1370	U1371	U1372	U1373	U1374	U1375	U1376	U1377	U1378	U1379	U1380	U1381	U1382	U1383	U1384	U1385	U1386	U1387	U1388	U1389	U1390	U1391	U1392	U1393	U1394	U1395	U1396	U1397	U1398	U1399	U1400	U1401	U1402	U1403	U1404	U1405	U1406	U1407	U1408	U1409	U1410	U1411	U1412	U1413	U1414	U1415	U1416	U1417	U1418	U1419	U1420	U1421	U1422	U1423	U1424	U1425	U1426	U1427	U1428	U1429	U1430	U1431	U1432	U1433	U1434	U1435	U1436	U1437	U1438	U1439	U1440	U1441	U1442	U1443	U1444	U1445	U1446	U1447	U1448	U1449	U1450	U1451	U1452	U1453	U1454	U1455	U1456	U1457	U1458	U1459	U1460	U1461	U1462	U1463	U1464	U1465	U1466	U1467	U1468	U1469	U1470	U1471	U1472	U1473	U1474	U1475	U1476	U1477	U1478	U1479	U1480	U1481	U1482	U1483	U1484	U1485	U1486	U1487	U1488	U1489	U1490	U1491	U1492	U1493	U1494	U1495	U1496	U1497	U1498	U1499	U1500	U1501	U1502	U1503	U1504	U1505	U1506	U1507	U1508	U1509	U1510	U1511	U1512	U1513	U1514	U1515	U1516	U1517	U1518	U1519	U1520	U1521	U1522	U1523	U1524	U1525	U1526	U1527	U1528	U1529	U1530	U1531	U1532	U1533	U1534	U1535	U1536	U1537	U1538	U1539	U1540	U1541	U1542	U1543	U1544	U1545	U1546	U1547	U1548	U1549	U1550	U1551	U1552	U1553	U1554	U1555	U1556	U1557	U1558	U1559	U1560	U1561	U1562	U1563	U1564	U1565	U1566	U1567	U1568	U1569	U1570	U1571	U1572	U1573	U1574	U1575	U1576	U1577	U1578	U1579	U1580	U1581	U1582	U1583	U1584	U1585	U1586	U1587	U1588	U1589	U1590	U1591	U1592	U1593	U1594	U1595	U1596	U1597	U1598	U1599	U1600	U1601	U1602	U1603	U1604	U1605	U1606	U1607	U1608	U1609	U1610	U1611	U1612	U1613	U1614	U1615	U1616	U1617	U1618	U1619	U1620	U1621	U1622	U1623	U1624	U1625	U1626	U1627	U1628	U1629	U1630	U1631	U1632	U1633	U1634	U1635	U1636	U1637	U1638	U1639	U1640	U1641	U1642	U1643	U1644	U1645	U1646	U1647	U1648	U1649	U1650	U1651	U1652	U1653	U1654	U1655	U1656	U1657	U1658	U1659	U1660	U1661	U1662	U1663	U1664	U1665	U1666	U1667	U1668	U1669	U1670	U1671	U1672	U1673	U1674	U1675	U1676	U1677	U1678	U1679	U1680	U1681	U1682	U1683	U1684	U1685	U1686	U1687	U1688	U1689	U1690	U1691	U1692	U1693	U1694	U1695	U1696	U1697	U1698	U1699	U1700	U1701	U1702	U1703	U1704	U1705	U1706	U1707	U1708	U1709	U1710	U1711	U1712	U1713	U1714	U1715	U1716	U1717	U1718	U1719	U1720	U1721	U1722	U1723	U1724	U1725	U1726	U1727	U1728	U1729	U1730	U1731	U1732	U1733	U1734	U1735	U1736	U1737	U1738	U1739	U1740	U1741	U1742	U1743	U1744	U1745	U1746	U1747	U1748	U1749	U1750	U1751	U1752	U1753	U1754	U1755	U1756	U1757	U1758	U1759	U1760	U1761	U1762	U1763	U1764	U1765	U1766	U1767	U1768	U1769	U1770	U1771	U1772	U1773	U1774	U1775	U1776	U1777	U1778	U1779	U1780	U1781	U1782	U1783	U1784	U1785	U1786	U1787	U1788	U1789	U1790	U1791	U1792	U1793	U1794	U1795	U1796	U1797	U1798	U1799	U1800	U1801	U1802	U1803	U1804	U1805	U1806	U1807	U1808	U1809	U1810	U1811	U1812	U1813	U1814	U1815	U1816	U1817	U1818	U1819	U1820	U1821	U1822	U1823	U1824	U1825	U1826	U1827	U1828	U1829	U1830	U1831	U1832	U1833	U1834	U1835	U1836	U1837	U1838	U1839	U1840	U1841	U1842	U1843	U1844	U1845	U1846	U1847	U1848	U1849	U1850	U1851	U1852	U1853	U1854	U1855	U1856	U1857	U1858	U1859	U1860	U1861	U1862	U1863	U1864	U1865	U1866	U1867	U1868	U1869	U1870	U1871	U1872	U1873	U1874	U1875	U1876	U1877	U1878	U1879	U1880	U1881	U1882	U1883</



- Molecule 26: 5S Ribosomal RNA

Chain B: 79% 18%



- Molecule 27: 50S ribosomal protein L2

Chain C: 92% 7%



- Molecule 28: 50S ribosomal protein L3

Chain D: 96%



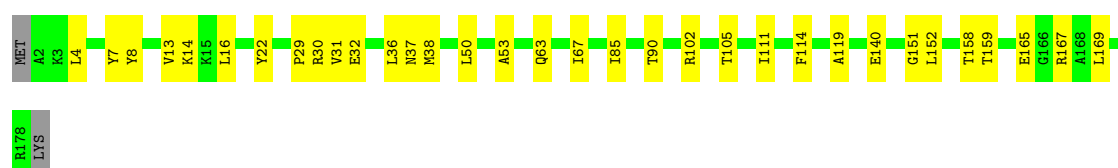
- Molecule 29: 50S ribosomal protein L4

Chain E: 89% 11%



- Molecule 30: 50S ribosomal protein L5

Chain F: 80% 18%

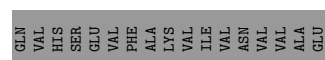
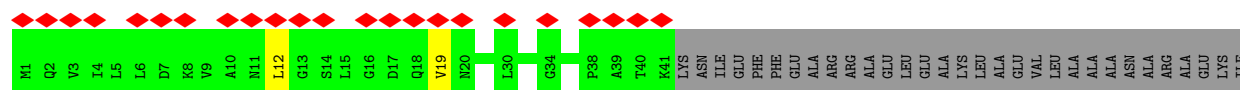


- Molecule 31: 50S ribosomal protein L6

Chain G: 90% 9%



- Molecule 32: 50S ribosomal protein L9



- Molecule 33: 50S ribosomal protein L13



- Molecule 34: 50S ribosomal protein L14



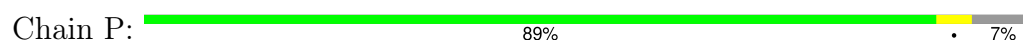
- Molecule 35: 50S ribosomal protein L15



- Molecule 36: 50S ribosomal protein L16



- Molecule 37: 50S ribosomal protein L17





- Molecule 38: 50S ribosomal protein L18

Chain Q: 90% 9%



- Molecule 39: 50S ribosomal protein L19

Chain R: 91% 8%



- Molecule 40: 50S ribosomal protein L20

Chain S: 92% 7%



- Molecule 41: Ribosomal protein L21

Chain T: 94% 6%



- Molecule 42: 50S ribosomal protein L22

Chain U: 95% 5%



- Molecule 43: 50S ribosomal protein L23

Chain V: 88% 5% 7%



- Molecule 44: 50S ribosomal protein L24

Chain W: 83% 15% 2%



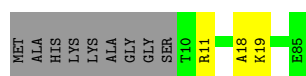
- Molecule 45: 50S ribosomal protein L25

Chain X: 91% 9%



- Molecule 46: 50S ribosomal protein L27

Chain Y: 86% 11%



- Molecule 47: 50S ribosomal protein L28

Chain Z: 94% 5%



- Molecule 48: 50S ribosomal protein L29

Chain 1: 94%



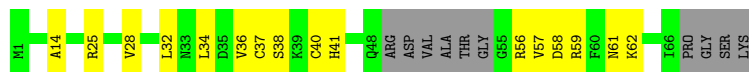
- Molecule 49: 50S ribosomal protein L30

Chain 2: 92% 7%



- Molecule 50: 50S ribosomal protein L31

Chain 3: 63% 23% 14%

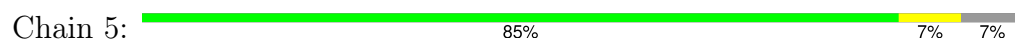


- Molecule 51: 50S ribosomal protein L32

Chain 4: 96%



- Molecule 52: 50S ribosomal protein L33



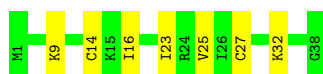
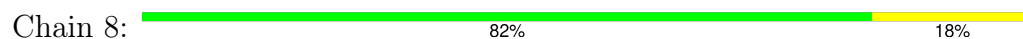
- Molecule 53: 50S ribosomal protein L34



- Molecule 54: 50S ribosomal protein L35



- Molecule 55: 50S ribosomal protein L36



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	466262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	96000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	1.865	Depositor
Minimum map value	-0.587	Depositor
Average map value	-0.003	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.12	Depositor
Map size ($\text{\AA}$)	440.32, 440.32, 440.32	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.86, 0.86, 0.86	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2MA, T6A, 1MG, MA6, IAS, 6MZ, M3X, MS6, PAR, 5MC, D2T, PSU, G7M, ZN, OMG, H2U, 3AU, K, 2MG, 4OC, OMC, 4D4, 3TD, UR3, OMU, 4SU, MEQ, MG, 5MU

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	a	0.16	0/36450	0.28	0/56856
2	b	0.13	0/1785	0.39	0/2404
3	c	0.14	0/1651	0.32	0/2225
4	d	0.12	0/1665	0.28	0/2227
5	e	0.15	0/1165	0.33	0/1568
6	f	0.13	0/858	0.35	0/1160
7	g	0.14	0/1206	0.33	0/1617
8	h	0.15	0/989	0.30	0/1326
9	i	0.12	0/1034	0.28	0/1375
10	j	0.12	0/796	0.34	0/1077
11	k	0.14	0/884	0.29	0/1191
12	l	0.16	0/945	0.36	0/1268
13	m	0.12	0/900	0.32	0/1204
14	n	0.11	0/817	0.25	0/1088
15	o	0.15	0/722	0.29	0/964
16	p	0.14	0/653	0.39	0/877
17	q	0.15	0/650	0.33	0/871
18	r	0.12	0/453	0.25	0/609
19	s	0.11	0/680	0.26	0/915
20	t	0.16	0/676	0.35	0/895
21	u	0.10	0/467	0.23	0/620
22	w	0.21	0/1550	0.28	0/2411
22	y	0.31	2/1549 (0.1%)	0.31	0/2408
23	x	0.18	0/1725	0.26	0/2689
24	v	0.16	0/269	0.27	0/417
25	A	0.23	1/69147 (0.0%)	0.33	0/107869
26	B	0.18	0/2876	0.31	0/4483
27	C	0.19	0/2121	0.32	0/2852
28	D	0.22	0/1576	0.35	0/2119
29	E	0.16	0/1571	0.31	0/2113
30	F	0.12	0/1434	0.29	0/1926

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
31	G	0.14	0/1343	0.30	0/1816
32	H	0.11	0/306	0.34	0/413
33	L	0.20	0/1152	0.32	0/1551
34	M	0.20	0/955	0.36	0/1279
35	N	0.18	0/1061	0.29	0/1412
36	O	0.20	0/1073	0.32	0/1433
37	P	0.21	0/958	0.33	0/1281
38	Q	0.15	0/902	0.32	0/1209
39	R	0.18	0/929	0.28	0/1242
40	S	0.22	0/960	0.28	0/1278
41	T	0.19	0/829	0.34	0/1107
42	U	0.19	0/864	0.29	0/1156
43	V	0.16	0/744	0.31	0/994
44	W	0.19	0/787	0.51	2/1051 (0.2%)
45	X	0.18	0/766	0.29	0/1025
46	Y	0.18	0/589	0.40	0/779
47	Z	0.19	0/635	0.31	0/848
48	1	0.15	0/496	0.24	0/660
49	2	0.18	0/453	0.32	0/605
50	3	0.10	0/475	0.30	0/633
51	4	0.20	0/440	0.33	0/588
52	5	0.16	0/424	0.33	0/565
53	6	0.22	0/380	0.30	0/498
54	7	0.21	0/513	0.32	0/676
55	8	0.22	0/303	0.40	0/397
All	All	0.20	3/157601 (0.0%)	0.31	2/236120 (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
36	O	0	1
54	7	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	y	76	A	C6-N6	7.01	1.48	1.33
22	y	37	T6A	O3'-P	5.03	1.61	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	2552	OMU	O3'-P	5.02	1.61	1.56

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	W	98	SER	CA-C-N	6.47	133.90	121.54
44	W	98	SER	C-N-CA	6.47	133.90	121.54

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
54	7	30	ARG	Peptide
36	O	81	4D4	Mainchain

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	a	32803	0	16528	247	0
2	b	1754	0	1782	43	0
3	c	1624	0	1696	15	0
4	d	1643	0	1707	23	0
5	e	1152	0	1196	10	0
6	f	839	0	833	29	0
7	g	1191	0	1244	15	0
8	h	979	0	1031	8	0
9	i	1022	0	1070	23	0
10	j	786	0	828	14	0
11	k	877	0	884	14	0
12	l	942	0	999	5	0
13	m	891	0	952	14	0
14	n	805	0	844	11	0
15	o	714	0	734	7	0
16	p	643	0	661	10	0
17	q	641	0	682	7	0
18	r	446	0	472	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	s	663	0	688	11	0
20	t	670	0	719	5	0
21	u	460	0	486	4	0
22	w	1645	0	834	14	0
22	y	1644	0	833	42	0
23	x	1625	0	829	13	0
24	v	239	0	120	0	0
25	A	62252	0	31333	274	0
26	B	2572	0	1301	11	0
27	C	2082	0	2154	17	0
28	D	1566	0	1618	6	0
29	E	1552	0	1619	14	0
30	F	1410	0	1444	20	0
31	G	1323	0	1371	10	0
32	H	303	0	327	2	0
33	L	1129	0	1162	7	0
34	M	946	0	1023	9	0
35	N	1052	0	1127	8	0
36	O	1075	0	1146	3	0
37	P	945	0	989	4	0
38	Q	892	0	923	7	0
39	R	917	0	962	8	0
40	S	947	0	1019	8	0
41	T	816	0	839	4	0
42	U	857	0	922	3	0
43	V	738	0	807	4	0
44	W	779	0	831	8	0
45	X	753	0	780	5	0
46	Y	582	0	599	3	0
47	Z	625	0	652	3	0
48	1	495	0	526	1	0
49	2	449	0	488	2	0
50	3	468	0	460	12	0
51	4	434	0	445	0	0
52	5	417	0	451	3	0
53	6	377	0	418	2	0
54	7	504	0	572	2	0
55	8	302	0	340	5	0
56	a	42	0	45	0	0
57	4	7	0	0	0	0
57	8	3	0	0	0	0
57	A	603	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	B	6	0	0	0	0
57	D	1	0	0	0	0
57	E	2	0	0	0	0
57	L	4	0	0	0	0
57	N	2	0	0	0	0
57	P	1	0	0	0	0
57	R	1	0	0	0	0
57	S	2	0	0	0	0
57	U	1	0	0	0	0
57	V	2	0	0	0	0
57	Y	1	0	0	0	0
57	a	91	0	0	0	0
57	e	2	0	0	0	0
57	l	1	0	0	0	0
57	v	2	0	0	0	0
57	x	2	0	0	0	0
58	a	1	0	0	0	0
58	l	1	0	0	0	0
59	y	8	0	10	0	0
60	3	1	0	0	0	0
60	8	1	0	0	0	0
61	4	3	0	0	0	0
61	A	278	0	0	2	0
61	B	3	0	0	0	0
61	D	2	0	0	0	0
61	L	2	0	0	0	0
61	T	1	0	0	0	0
61	U	2	0	0	0	0
61	V	2	0	0	0	0
61	Y	1	0	0	0	0
61	Z	2	0	0	0	0
61	a	31	0	0	0	0
61	k	1	0	0	0	0
61	l	2	0	0	0	0
61	w	1	0	0	0	0
All	All	147376	0	97355	943	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 943 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)
25:A:1093:G:N2	25:A:1098:A:H62	1.38	1.19
25:A:1093:G:H21	25:A:1098:A:N6	1.43	1.17
1:a:1088:G:N2	1:a:1167:A:H61	1.49	1.07
1:a:1088:G:H21	1:a:1167:A:N6	1.53	1.05
22:y:15:G:N2	22:y:48:C:H42	1.61	0.98

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	b	222/241 (92%)	203 (91%)	19 (9%)	0	100	100
3	c	204/233 (88%)	192 (94%)	12 (6%)	0	100	100
4	d	203/206 (98%)	198 (98%)	5 (2%)	0	100	100
5	e	154/167 (92%)	149 (97%)	5 (3%)	0	100	100
6	f	101/131 (77%)	95 (94%)	6 (6%)	0	100	100
7	g	150/156 (96%)	142 (95%)	8 (5%)	0	100	100
8	h	127/130 (98%)	124 (98%)	3 (2%)	0	100	100
9	i	125/130 (96%)	122 (98%)	3 (2%)	0	100	100
10	j	96/103 (93%)	90 (94%)	5 (5%)	1 (1%)	12	38
11	k	113/129 (88%)	106 (94%)	7 (6%)	0	100	100
12	l	118/124 (95%)	114 (97%)	4 (3%)	0	100	100
13	m	113/118 (96%)	108 (96%)	5 (4%)	0	100	100
14	n	98/101 (97%)	98 (100%)	0	0	100	100
15	o	86/89 (97%)	83 (96%)	3 (4%)	0	100	100
16	p	79/82 (96%)	72 (91%)	7 (9%)	0	100	100
17	q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	r	52/75 (69%)	48 (92%)	4 (8%)	0	100	100
19	s	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
20	t	84/87 (97%)	81 (96%)	3 (4%)	0	100	100
21	u	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
27	C	269/273 (98%)	259 (96%)	10 (4%)	0	100	100
28	D	206/209 (99%)	198 (96%)	8 (4%)	0	100	100
29	E	199/201 (99%)	189 (95%)	10 (5%)	0	100	100
30	F	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
31	G	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
32	H	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
33	L	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
34	M	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
35	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
36	O	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
37	P	116/127 (91%)	114 (98%)	2 (2%)	0	100	100
38	Q	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
39	R	112/115 (97%)	109 (97%)	3 (3%)	0	100	100
40	S	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
41	T	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
42	U	108/110 (98%)	107 (99%)	1 (1%)	0	100	100
43	V	91/100 (91%)	82 (90%)	9 (10%)	0	100	100
44	W	100/104 (96%)	94 (94%)	5 (5%)	1 (1%)	12	38
45	X	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
46	Y	74/85 (87%)	73 (99%)	1 (1%)	0	100	100
47	Z	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
48	1	59/63 (94%)	57 (97%)	2 (3%)	0	100	100
49	2	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
50	3	56/70 (80%)	51 (91%)	5 (9%)	0	100	100
51	4	53/57 (93%)	53 (100%)	0	0	100	100
52	5	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
53	6	44/46 (96%)	43 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	7	62/65 (95%)	57 (92%)	5 (8%)	0	100	100
55	8	36/38 (95%)	36 (100%)	0	0	100	100
All	All	5446/5886 (92%)	5223 (96%)	221 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
10	j	57	VAL
44	W	99	ASN

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	
2	b	186/199 (94%)	186 (100%)	0	100	100
3	c	170/190 (90%)	170 (100%)	0	100	100
4	d	172/173 (99%)	172 (100%)	0	100	100
5	e	119/126 (94%)	119 (100%)	0	100	100
6	f	90/112 (80%)	90 (100%)	0	100	100
7	g	125/129 (97%)	125 (100%)	0	100	100
8	h	104/105 (99%)	104 (100%)	0	100	100
9	i	105/107 (98%)	105 (100%)	0	100	100
10	j	86/90 (96%)	86 (100%)	0	100	100
11	k	89/98 (91%)	89 (100%)	0	100	100
12	l	101/103 (98%)	101 (100%)	0	100	100
13	m	93/96 (97%)	93 (100%)	0	100	100
14	n	83/84 (99%)	83 (100%)	0	100	100
15	o	76/77 (99%)	76 (100%)	0	100	100
16	p	65/65 (100%)	65 (100%)	0	100	100
17	q	73/78 (94%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	r	47/65 (72%)	47 (100%)	0	100	100
19	s	72/79 (91%)	72 (100%)	0	100	100
20	t	65/66 (98%)	65 (100%)	0	100	100
21	u	48/61 (79%)	48 (100%)	0	100	100
27	C	216/218 (99%)	216 (100%)	0	100	100
28	D	163/163 (100%)	163 (100%)	0	100	100
29	E	165/165 (100%)	165 (100%)	0	100	100
30	F	148/150 (99%)	148 (100%)	0	100	100
31	G	137/138 (99%)	137 (100%)	0	100	100
32	H	32/114 (28%)	32 (100%)	0	100	100
33	L	116/116 (100%)	116 (100%)	0	100	100
34	M	104/104 (100%)	104 (100%)	0	100	100
35	N	103/103 (100%)	103 (100%)	0	100	100
36	O	107/107 (100%)	107 (100%)	0	100	100
37	P	98/103 (95%)	98 (100%)	0	100	100
38	Q	86/87 (99%)	86 (100%)	0	100	100
39	R	99/100 (99%)	99 (100%)	0	100	100
40	S	89/90 (99%)	89 (100%)	0	100	100
41	T	84/84 (100%)	84 (100%)	0	100	100
42	U	93/93 (100%)	93 (100%)	0	100	100
43	V	80/84 (95%)	80 (100%)	0	100	100
44	W	83/85 (98%)	83 (100%)	0	100	100
45	X	78/78 (100%)	78 (100%)	0	100	100
46	Y	58/63 (92%)	58 (100%)	0	100	100
47	Z	67/68 (98%)	67 (100%)	0	100	100
48	1	54/55 (98%)	54 (100%)	0	100	100
49	2	48/49 (98%)	48 (100%)	0	100	100
50	3	53/62 (86%)	53 (100%)	0	100	100
51	4	46/48 (96%)	46 (100%)	0	100	100
52	5	46/49 (94%)	46 (100%)	0	100	100
53	6	38/38 (100%)	38 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
54	7	51/52 (98%)	51 (100%)	0	100	100
55	8	34/34 (100%)	34 (100%)	0	100	100
All	All	4545/4803 (95%)	4545 (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 54 such sidechains are listed below:

Mol	Chain	Res	Type
27	C	134	ASN
29	E	165	HIS
44	W	45	HIS
27	C	232	HIS
28	D	49	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	a	1526/1542 (98%)	193 (12%)	0
22	w	75/76 (98%)	20 (26%)	0
22	y	75/76 (98%)	22 (29%)	0
23	x	75/77 (97%)	9 (12%)	0
24	v	10/27 (37%)	1 (10%)	0
25	A	2897/2904 (99%)	366 (12%)	13 (0%)
26	B	119/120 (99%)	15 (12%)	2 (1%)
All	All	4777/4822 (99%)	626 (13%)	15 (0%)

5 of 626 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	a	4	U
1	a	5	U
1	a	6	G
1	a	7	A
1	a	8	A

5 of 15 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
25	A	1583	A

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Mol	Chain	Res	Type
26	B	3	C
25	A	2097	A
26	B	66	A
25	A	2473	U

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

66 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	UR3	a	1498	1	19,22,23	0.96	0	26,32,35	1.82	3 (11%)
1	4OC	a	1402	1,57	20,23,24	0.74	0	25,32,35	1.00	1 (4%)
1	2MG	a	966	1	23,26,27	1.25	4 (17%)	33,38,41	2.23	8 (24%)
22	3AU	w	47	22	24,28,29	2.70	9 (37%)	30,40,43	1.37	4 (13%)
1	PSU	a	516	1	18,21,22	1.41	4 (22%)	21,30,33	2.07	4 (19%)
1	G7M	a	527	1	23,26,27	1.57	3 (13%)	34,39,42	1.76	5 (14%)
22	H2U	y	19	22	18,21,22	1.02	2 (11%)	19,30,33	0.81	1 (5%)
1	5MC	a	967	1	19,22,23	1.54	3 (15%)	26,32,35	1.14	2 (7%)
22	PSU	y	39	22	18,21,22	1.46	3 (16%)	21,30,33	1.79	3 (14%)
25	2MG	A	1835	25	23,26,27	1.26	3 (13%)	33,38,41	2.20	7 (21%)
25	PSU	A	1917	25	18,21,22	1.40	3 (16%)	21,30,33	2.03	3 (14%)
23	5MC	x	32	23	19,22,23	1.42	3 (15%)	26,32,35	1.31	4 (15%)
25	PSU	A	1911	25	18,21,22	1.42	3 (16%)	21,30,33	2.13	4 (19%)
25	PSU	A	2604	25	18,21,22	1.43	3 (16%)	21,30,33	2.17	4 (19%)
11	IAS	k	119	11	6,7,8	0.95	0	3,8,10	1.46	1 (33%)
25	G7M	A	2069	25,57	23,26,27	1.58	3 (13%)	34,39,42	1.75	5 (14%)
25	PSU	A	2504	25	18,21,22	1.37	2 (11%)	21,30,33	2.00	3 (14%)
25	6MZ	A	1618	25	22,25,26	1.40	5 (22%)	29,36,39	2.20	9 (31%)
1	2MG	a	1516	1	23,26,27	1.26	3 (13%)	33,38,41	2.24	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
36	4D4	O	81	36	9,11,12	2.60	3 (33%)	7,13,15	0.98	0
22	PSU	w	39	22	18,21,22	1.36	2 (11%)	21,30,33	2.07	3 (14%)
1	5MC	a	1407	1	19,22,23	1.54	3 (15%)	26,32,35	1.17	3 (11%)
25	H2U	A	2449	25	18,21,22	1.16	2 (11%)	19,30,33	0.78	0
25	3TD	A	1915	25	19,22,23	4.18	7 (36%)	23,32,35	1.79	3 (13%)
22	OMG	w	17	22	23,26,27	1.18	3 (13%)	32,38,41	1.95	6 (18%)
22	PSU	y	55	22	18,21,22	1.35	2 (11%)	21,30,33	2.04	3 (14%)
25	PSU	A	955	25	18,21,22	1.46	3 (16%)	21,30,33	2.15	4 (19%)
22	4SU	w	8	22	18,21,22	1.84	4 (22%)	25,30,33	2.26	4 (16%)
22	5MU	w	54	22	19,22,23	1.42	6 (31%)	27,32,35	2.23	6 (22%)
23	4SU	x	8	23	18,21,22	1.83	4 (22%)	25,30,33	2.24	5 (20%)
1	MA6	a	1519	1	23,26,27	1.45	5 (21%)	33,38,41	2.50	14 (42%)
22	4SU	y	8	22	18,21,22	1.87	4 (22%)	25,30,33	2.38	5 (20%)
22	5MU	y	54	22	19,22,23	1.43	5 (26%)	27,32,35	2.13	8 (29%)
22	H2U	w	20	22	18,21,22	1.03	2 (11%)	19,30,33	0.86	1 (5%)
22	T6A	y	37	22	31,34,35	1.41	4 (12%)	43,49,52	1.98	10 (23%)
25	PSU	A	2580	25	18,21,22	1.43	5 (27%)	21,30,33	2.21	4 (19%)
22	G7M	y	46	22	23,26,27	1.53	3 (13%)	34,39,42	1.71	5 (14%)
22	OMG	y	17	22	23,26,27	1.18	3 (13%)	32,38,41	2.01	6 (18%)
25	5MC	A	1962	25	19,22,23	1.45	3 (15%)	26,32,35	1.09	2 (7%)
25	2MG	A	2445	25,57	23,26,27	1.29	3 (13%)	33,38,41	2.22	5 (15%)
25	OMG	A	2251	23,25,57	23,26,27	1.21	3 (13%)	32,38,41	2.08	7 (21%)
22	M3X	y	34	22	24,30,31	2.23	3 (12%)	24,41,44	0.99	2 (8%)
12	D2T	l	89	12	8,9,10	1.75	1 (12%)	6,11,13	2.48	2 (33%)
22	H2U	w	19	22	18,21,22	1.02	2 (11%)	19,30,33	0.82	1 (5%)
22	G7M	w	46	22	23,26,27	1.53	3 (13%)	34,39,42	1.74	5 (14%)
25	5MU	A	747	25	19,22,23	1.43	6 (31%)	27,32,35	2.08	6 (22%)
25	PSU	A	2457	25	18,21,22	1.43	4 (22%)	21,30,33	2.16	5 (23%)
25	2MA	A	2503	25,57	22,25,26	1.46	5 (22%)	32,37,40	2.27	9 (28%)
22	T6A	w	37	22	31,34,35	1.41	6 (19%)	43,49,52	1.90	11 (25%)
25	PSU	A	2605	25	18,21,22	1.43	4 (22%)	21,30,33	2.09	4 (19%)
25	PSU	A	746	25	18,21,22	1.44	5 (27%)	21,30,33	2.17	5 (23%)
1	MA6	a	1518	1	23,26,27	1.44	3 (13%)	33,38,41	2.48	13 (39%)
22	M3X	w	34	22,24	24,30,31	2.19	4 (16%)	24,41,44	1.00	2 (8%)
25	1MG	A	745	25	23,26,27	1.15	3 (13%)	33,39,42	1.74	5 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	OMU	A	2552	25,57	19,22,23	1.31	3 (15%)	25,31,34	1.88	5 (20%)
25	OMC	A	2498	25,57	19,22,23	0.82	0	25,31,34	0.98	1 (4%)
22	H2U	y	20	22	18,21,22	0.98	2 (11%)	19,30,33	0.86	1 (5%)
23	5MU	x	54	23	19,22,23	1.39	6 (31%)	27,32,35	2.10	6 (22%)
23	PSU	x	55	23	18,21,22	1.39	2 (11%)	21,30,33	2.06	3 (14%)
22	PSU	w	55	22	18,21,22	1.38	3 (16%)	21,30,33	2.07	4 (19%)
22	3AU	y	47	22	24,28,29	2.72	9 (37%)	30,40,43	1.40	5 (16%)
1	2MG	a	1207	1	23,26,27	1.27	4 (17%)	33,38,41	2.19	6 (18%)
25	6MZ	A	2030	25	22,25,26	1.43	5 (22%)	29,36,39	2.23	10 (34%)
36	MS6	O	82	36	5,7,8	0.54	0	2,7,9	1.23	0
25	5MU	A	1939	25	19,22,23	1.39	4 (21%)	27,32,35	2.12	6 (22%)
28	MEQ	D	150	28	8,9,10	0.52	0	5,10,12	0.33	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
1	UR3	a	1498	1	-	0/7/25/26	0/2/2/2
1	4OC	a	1402	1,57	-	2/9/29/30	0/2/2/2
1	2MG	a	966	1	-	0/9/27/28	0/3/3/3
22	3AU	w	47	22	-	4/16/34/35	0/2/2/2
1	PSU	a	516	1	-	0/7/25/26	0/2/2/2
1	G7M	a	527	1	-	2/7/25/26	0/3/3/3
22	H2U	y	19	22	-	3/7/38/39	0/2/2/2
1	5MC	a	967	1	-	0/7/25/26	0/2/2/2
22	PSU	y	39	22	-	3/7/25/26	0/2/2/2
25	2MG	A	1835	25	-	0/9/27/28	0/3/3/3
25	PSU	A	1917	25	-	2/7/25/26	0/2/2/2
23	5MC	x	32	23	-	1/7/25/26	0/2/2/2
25	PSU	A	1911	25	-	0/7/25/26	0/2/2/2
25	PSU	A	2604	25	-	0/7/25/26	0/2/2/2
11	IAS	k	119	11	-	0/7/7/8	-
25	G7M	A	2069	25,57	-	1/7/25/26	0/3/3/3
25	PSU	A	2504	25	-	2/7/25/26	0/2/2/2
25	6MZ	A	1618	25	-	0/9/27/28	0/3/3/3
1	2MG	a	1516	1	-	0/9/27/28	0/3/3/3
36	4D4	O	81	36	-	0/11/12/14	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	w	39	22	-	2/7/25/26	0/2/2/2
1	5MC	a	1407	1	-	0/7/25/26	0/2/2/2
25	H2U	A	2449	25	-	0/7/38/39	0/2/2/2
25	3TD	A	1915	25	-	0/7/25/26	0/2/2/2
22	OMG	w	17	22	-	0/9/27/28	0/3/3/3
22	PSU	y	55	22	-	0/7/25/26	0/2/2/2
25	PSU	A	955	25	-	0/7/25/26	0/2/2/2
22	4SU	w	8	22	-	0/7/25/26	0/2/2/2
22	5MU	w	54	22	-	0/7/25/26	0/2/2/2
23	4SU	x	8	23	-	0/7/25/26	0/2/2/2
1	MA6	a	1519	1	-	5/11/29/30	0/3/3/3
22	4SU	y	8	22	-	1/7/25/26	0/2/2/2
22	5MU	y	54	22	-	1/7/25/26	0/2/2/2
22	H2U	w	20	22	-	1/7/38/39	0/2/2/2
22	T6A	y	37	22	-	9/23/41/42	0/3/3/3
25	PSU	A	2580	25	-	0/7/25/26	0/2/2/2
22	G7M	y	46	22	-	2/7/25/26	0/3/3/3
22	OMG	y	17	22	-	0/9/27/28	0/3/3/3
25	5MC	A	1962	25	-	0/7/25/26	0/2/2/2
25	2MG	A	2445	25,57	-	0/9/27/28	0/3/3/3
25	OMG	A	2251	23,25,57	-	0/9/27/28	0/3/3/3
22	M3X	y	34	22	-	6/17/37/38	0/2/2/2
12	D2T	l	89	12	-	2/7/12/14	-
22	H2U	w	19	22	-	3/7/38/39	0/2/2/2
22	G7M	w	46	22	-	0/7/25/26	0/3/3/3
25	5MU	A	747	25	-	2/7/25/26	0/2/2/2
25	PSU	A	2457	25	-	0/7/25/26	0/2/2/2
25	2MA	A	2503	25,57	-	2/7/25/26	0/3/3/3
22	T6A	w	37	22	-	2/23/41/42	0/3/3/3
25	PSU	A	2605	25	-	0/7/25/26	0/2/2/2
25	PSU	A	746	25	-	1/7/25/26	0/2/2/2
1	MA6	a	1518	1	-	2/11/29/30	0/3/3/3
22	M3X	w	34	22,24	-	10/17/37/38	0/2/2/2
25	1MG	A	745	25	-	0/7/25/26	0/3/3/3
25	OMU	A	2552	25,57	-	2/9/27/28	0/2/2/2
25	OMC	A	2498	25,57	-	3/9/27/28	0/2/2/2
22	H2U	y	20	22	-	3/7/38/39	0/2/2/2
23	5MU	x	54	23	-	0/7/25/26	0/2/2/2
23	PSU	x	55	23	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	PSU	w	55	22	-	0/7/25/26	0/2/2/2
22	3AU	y	47	22	-	4/16/34/35	0/2/2/2
1	2MG	a	1207	1	-	0/9/27/28	0/3/3/3
25	6MZ	A	2030	25	-	2/9/27/28	0/3/3/3
36	MS6	O	82	36	-	2/4/6/8	-
25	5MU	A	1939	25	-	0/7/25/26	0/2/2/2
28	MEQ	D	150	28	-	3/8/9/11	-

The worst 5 of 222 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	1915	3TD	C6-C5	12.32	1.48	1.35
25	A	1915	3TD	C2-N1	9.73	1.49	1.37
22	y	34	M3X	C2-N2	8.86	1.47	1.34
22	w	34	M3X	C2-N2	8.53	1.47	1.34
22	y	47	3AU	C2-N1	6.50	1.47	1.38

The worst 5 of 299 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	2503	2MA	C5-C4-N3	-7.85	118.91	127.18
1	a	1498	UR3	C4-N3-C2	-7.27	118.73	124.58
25	A	2445	2MG	C2-N3-C4	7.27	121.09	112.00
1	a	1516	2MG	C2-N3-C4	7.25	121.06	112.00
25	A	1835	2MG	C2-N3-C4	7.21	121.02	112.00

There are no chirality outliers.

5 of 90 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	a	527	G7M	O4'-C4'-C5'-O5'
1	a	1518	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C9
1	a	1519	MA6	C5-C6-N6-C10
1	a	1519	MA6	N1-C6-N6-C9

There are no ring outliers.

21 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	a	1402	4OC	1	0
1	a	516	PSU	1	0
22	y	19	H2U	1	0
1	a	1516	2MG	1	0
25	A	1915	3TD	1	0
22	w	17	OMG	1	0
22	y	55	PSU	2	0
22	w	54	5MU	1	0
1	a	1519	MA6	1	0
22	y	8	4SU	2	0
22	y	54	5MU	2	0
22	y	37	T6A	5	0
22	y	46	G7M	1	0
22	y	17	OMG	2	0
22	w	37	T6A	2	0
1	a	1518	MA6	1	0
25	A	2498	OMC	1	0
22	y	20	H2U	1	0
23	x	54	5MU	1	0
23	x	55	PSU	1	0
25	A	2030	6MZ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 740 ligands modelled in this entry, 738 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
59	ILE	y	101	-	6,7,8	0.55	0	4,8,10	1.10	0
56	PAR	a	1601	-	44,45,45	3.17	12 (27%)	63,67,67	1.08	3 (4%)

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	ILE	y	101	-	-	1/7/8/10	-
56	PAR	a	1601	-	-	5/18/94/94	0/4/4/4

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	a	1601	PAR	C23-C33	-12.11	1.26	1.53
56	a	1601	PAR	C13-C23	10.88	1.66	1.52
56	a	1601	PAR	O43-C13	-7.07	1.29	1.41
56	a	1601	PAR	O43-C43	4.67	1.55	1.45
56	a	1601	PAR	C31-C21	-4.14	1.48	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	a	1601	PAR	C14-O33-C33	-2.97	110.94	117.98
56	a	1601	PAR	O11-C42-C32	-2.14	104.07	109.18
56	a	1601	PAR	C13-O52-C52	-2.13	112.92	117.98

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

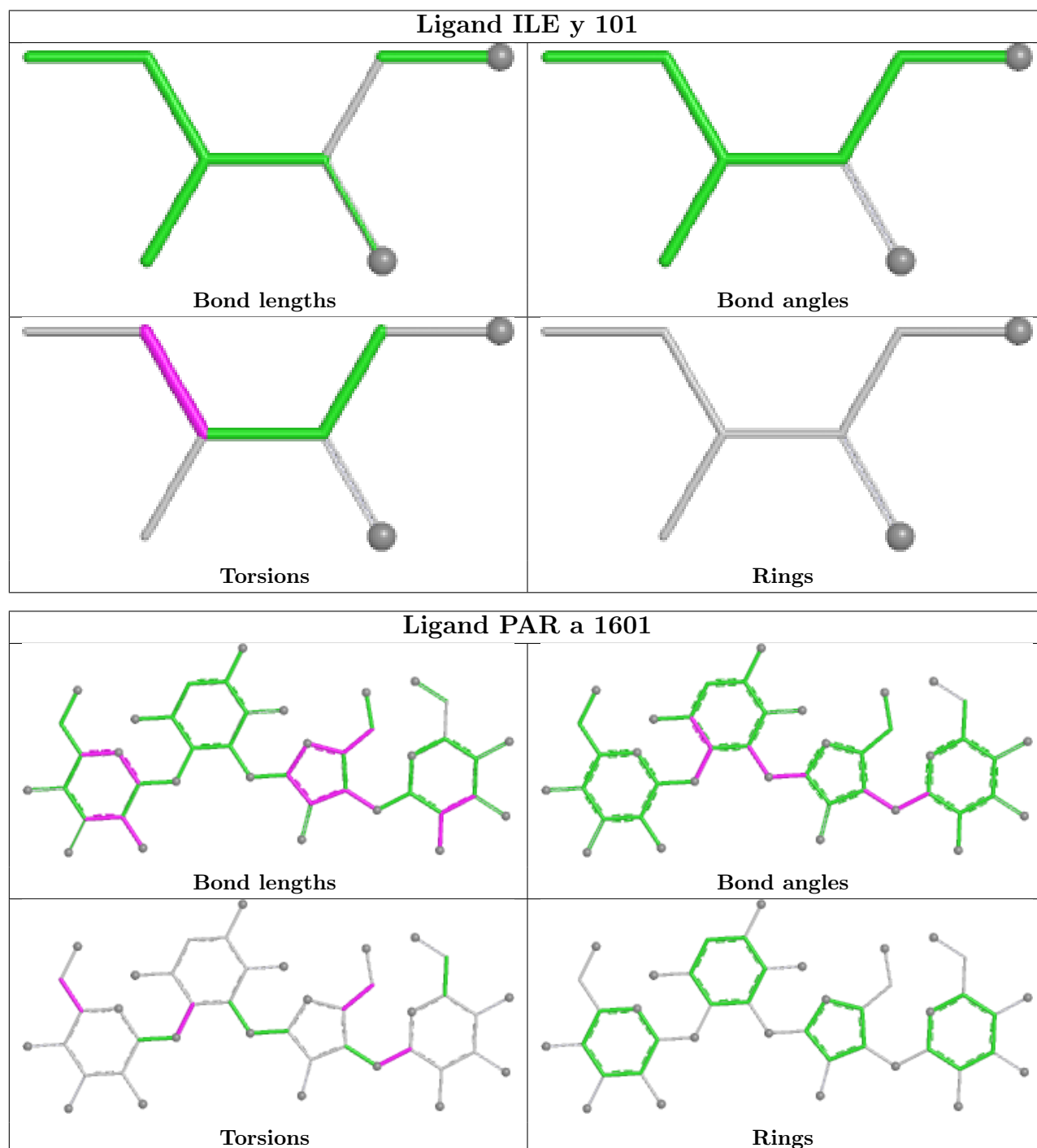
Mol	Chain	Res	Type	Atoms
56	a	1601	PAR	O43-C43-C53-O53
56	a	1601	PAR	C33-C43-C53-O53
56	a	1601	PAR	O51-C51-C61-O61
56	a	1601	PAR	O54-C14-O33-C33
56	a	1601	PAR	C52-C42-O11-C11

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

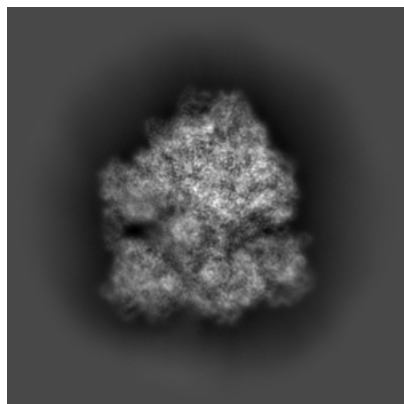
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-29821. These allow visual inspection of the internal detail of the map and identification of artifacts.

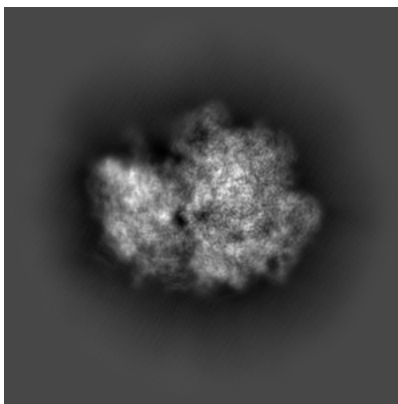
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

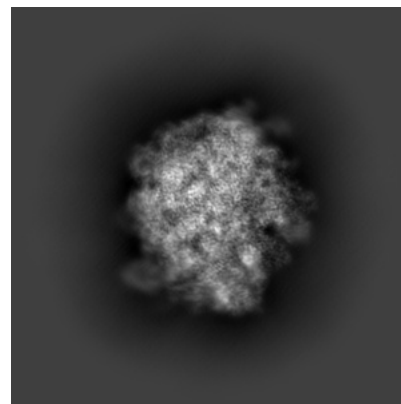
6.1.1 Primary map



X

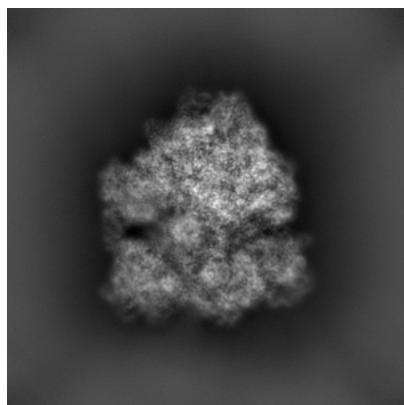


Y

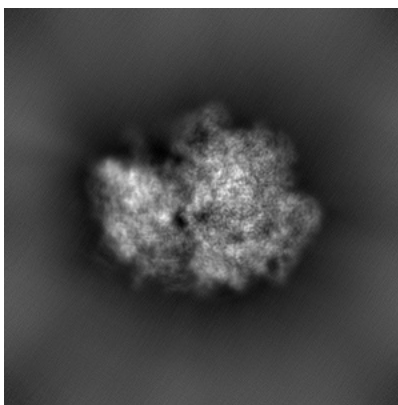


Z

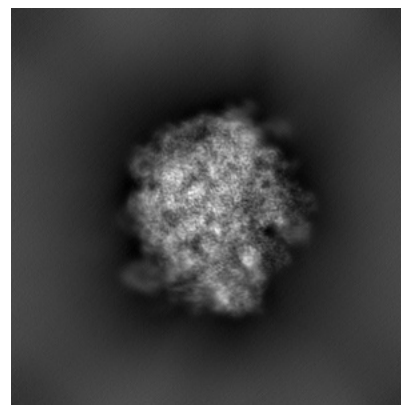
6.1.2 Raw map



X



Y

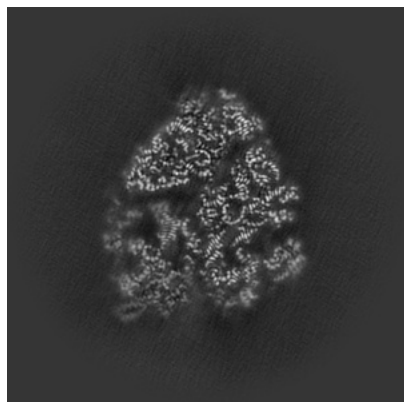


Z

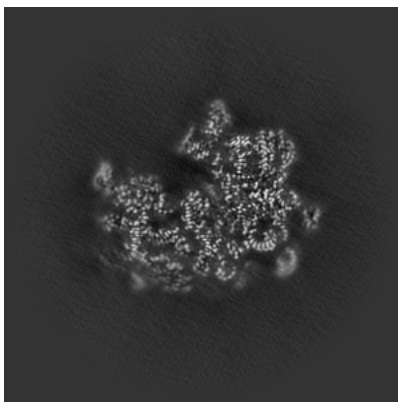
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

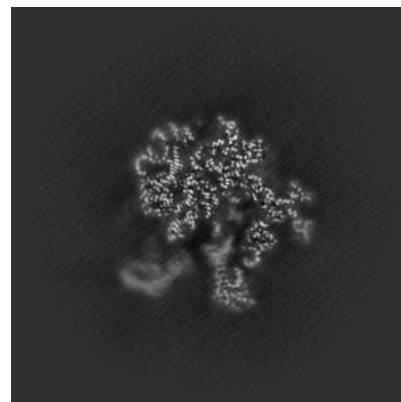
6.2.1 Primary map



X Index: 256

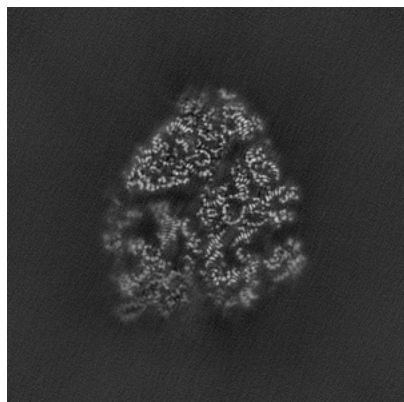


Y Index: 256

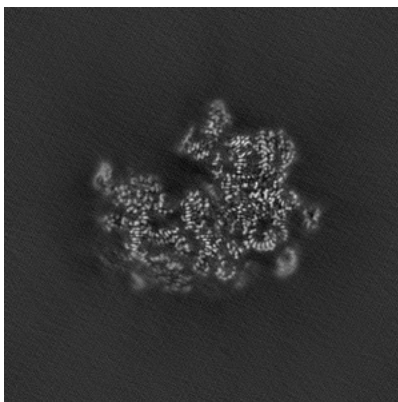


Z Index: 256

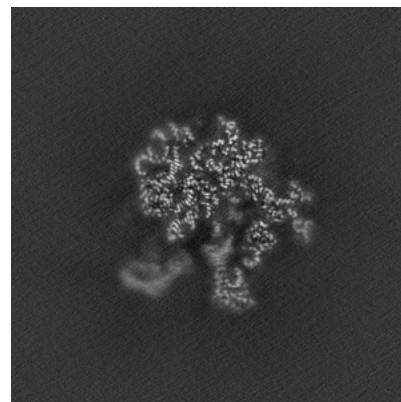
6.2.2 Raw map



X Index: 256



Y Index: 256

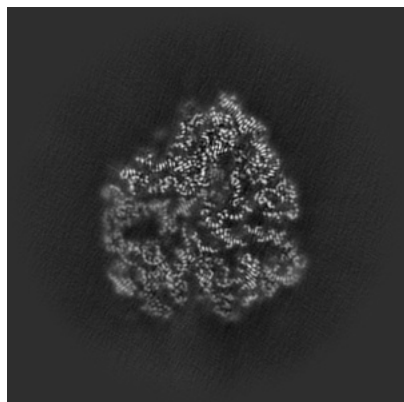


Z Index: 256

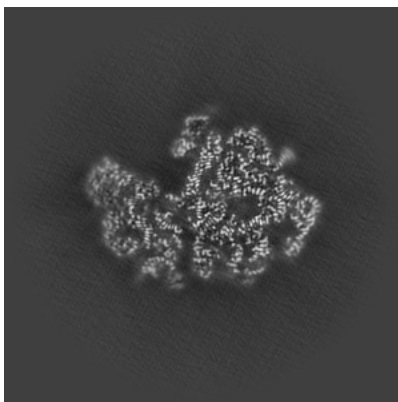
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

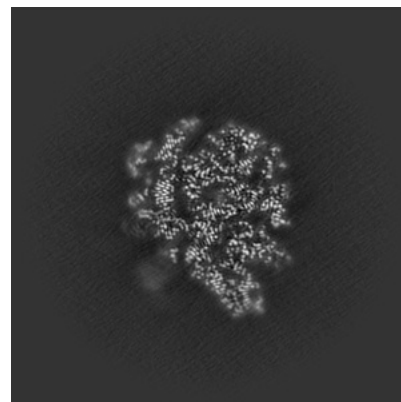
6.3.1 Primary map



X Index: 265

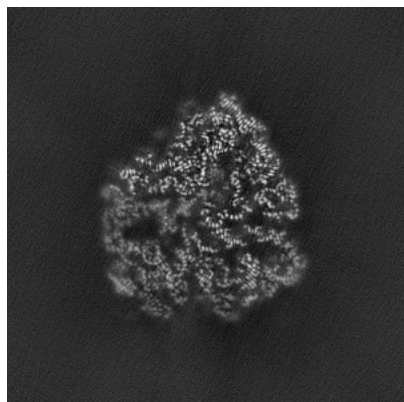


Y Index: 278

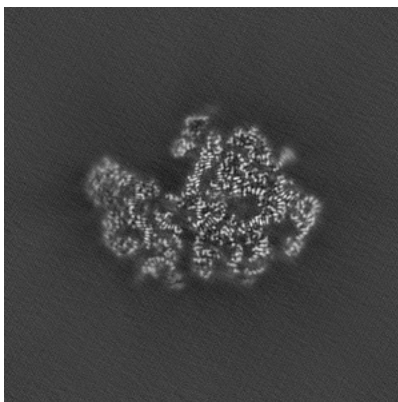


Z Index: 299

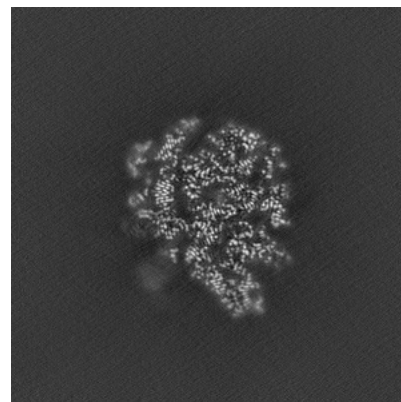
6.3.2 Raw map



X Index: 265



Y Index: 278

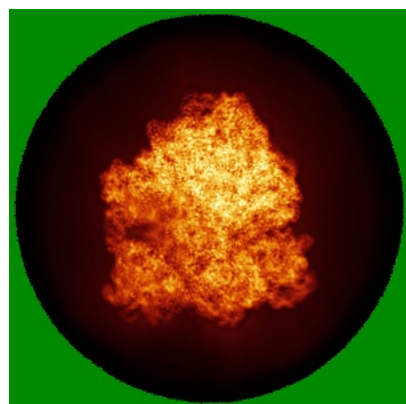


Z Index: 299

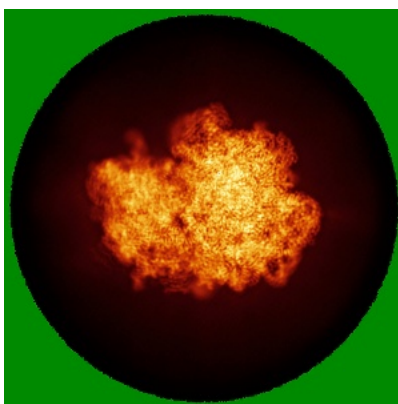
The images above show the largest variance slices of the map in three orthogonal directions.

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

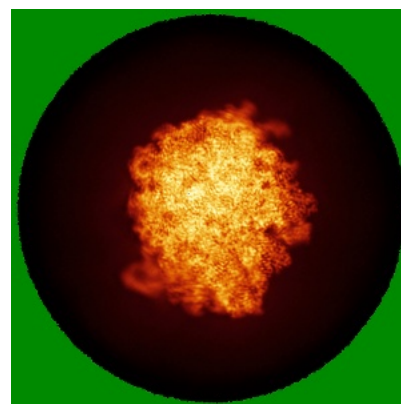
6.4.1 Primary map



X



Y

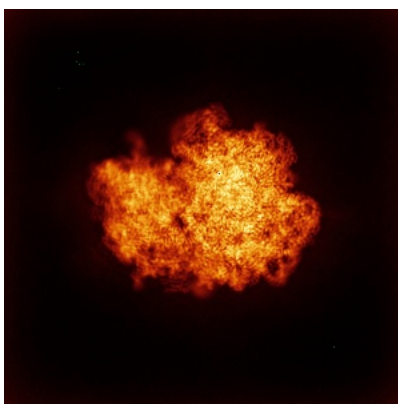


Z

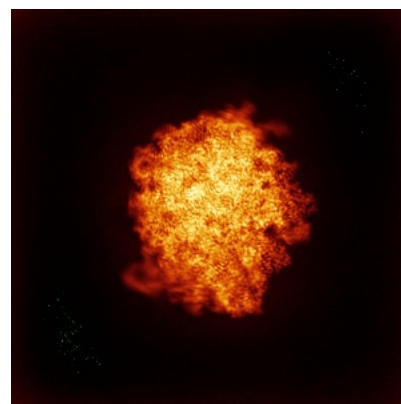
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



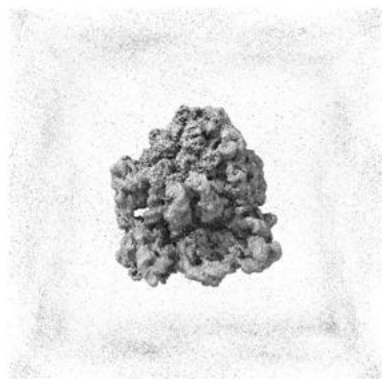
Y



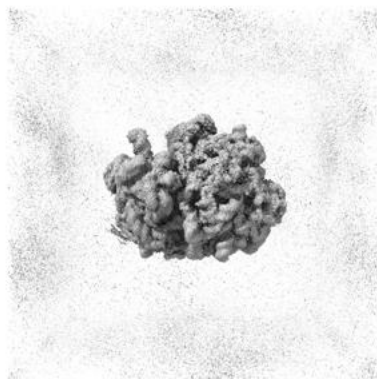
Z

The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

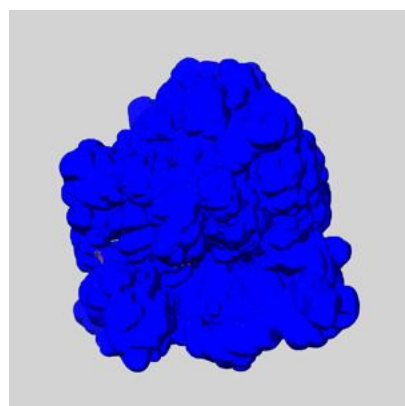
6.6 Mask visualisation [i](#)

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

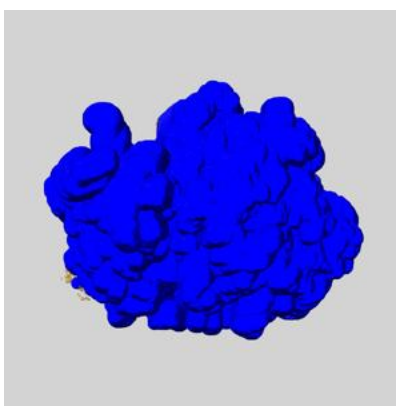
A mask typically either:

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

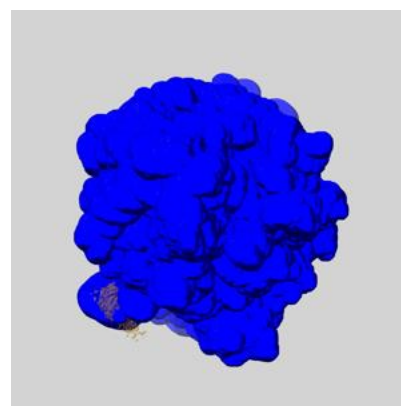
6.6.1 emd_29821_msk_1.map [i](#)



X



Y

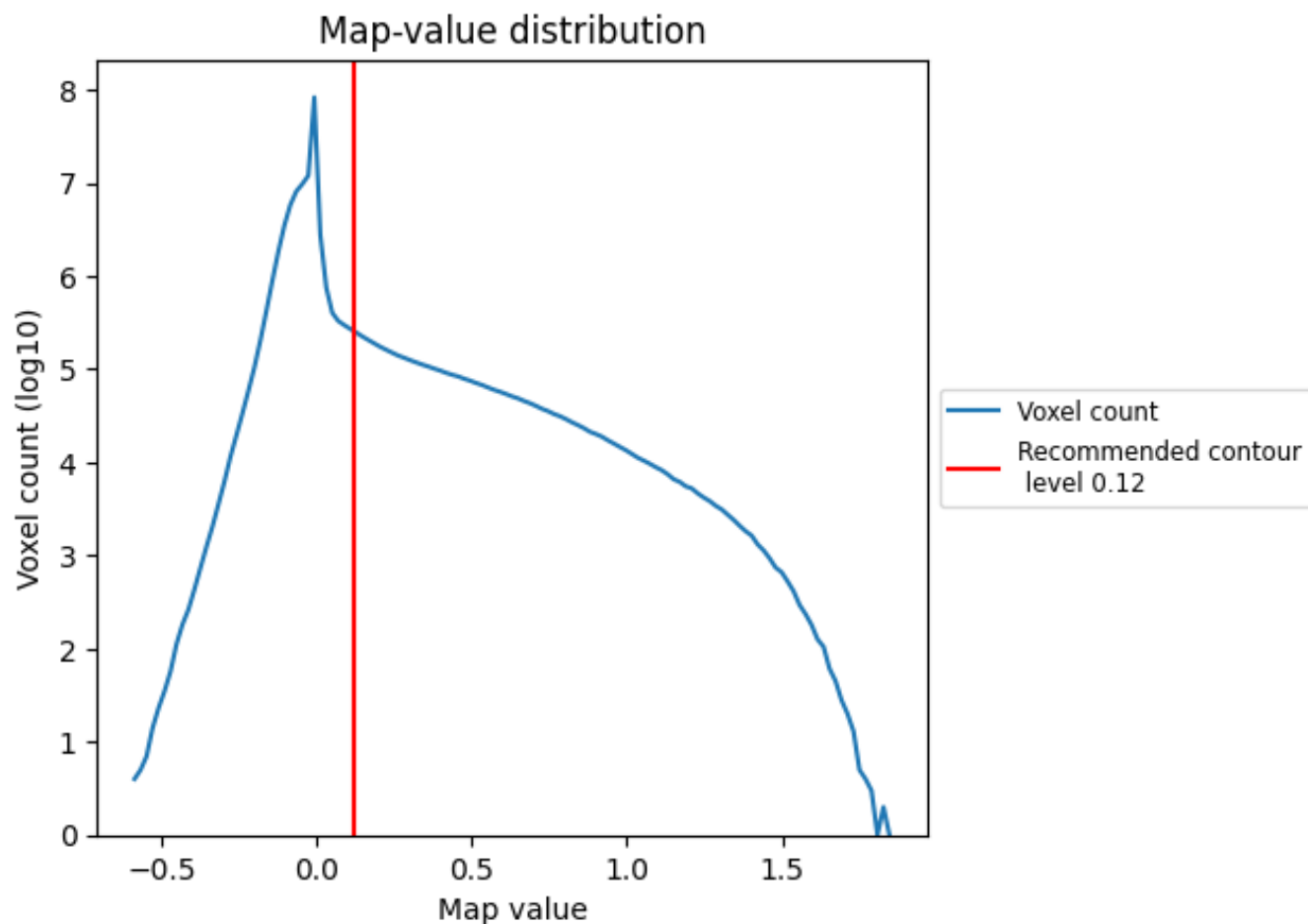


Z

7 Map analysis [i](#)

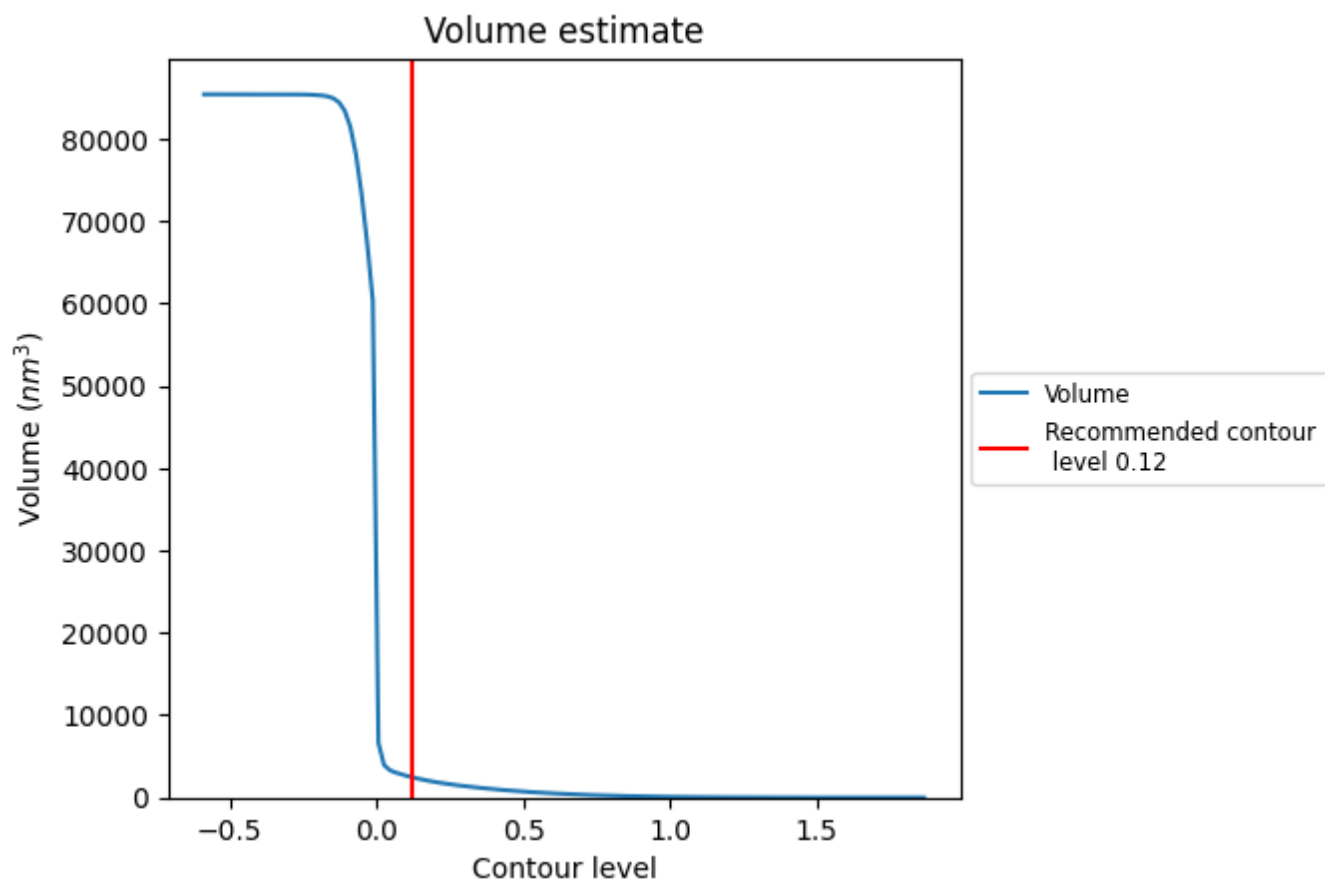
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

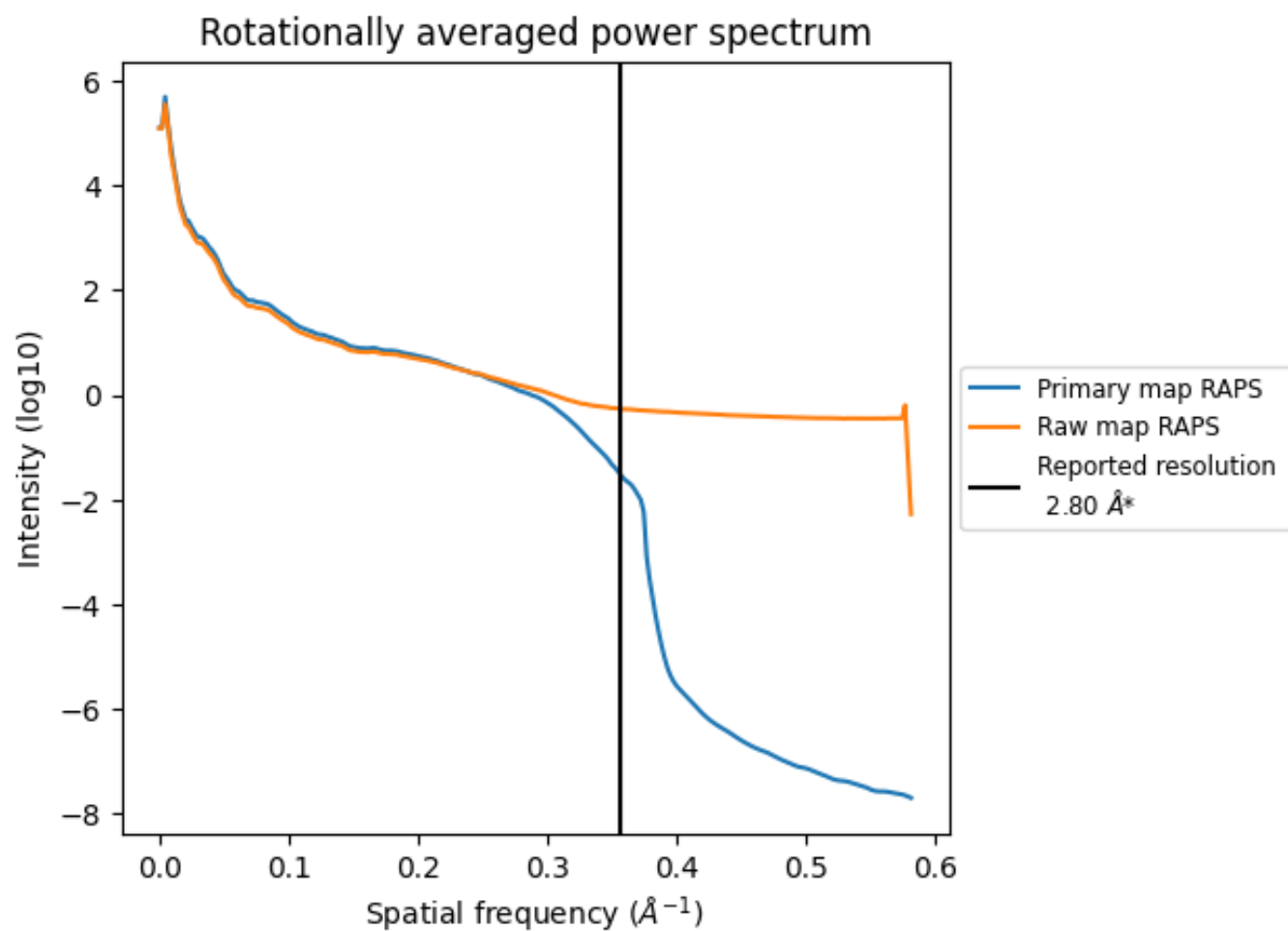
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2483 nm³; this corresponds to an approximate mass of 2243 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 ⓘ

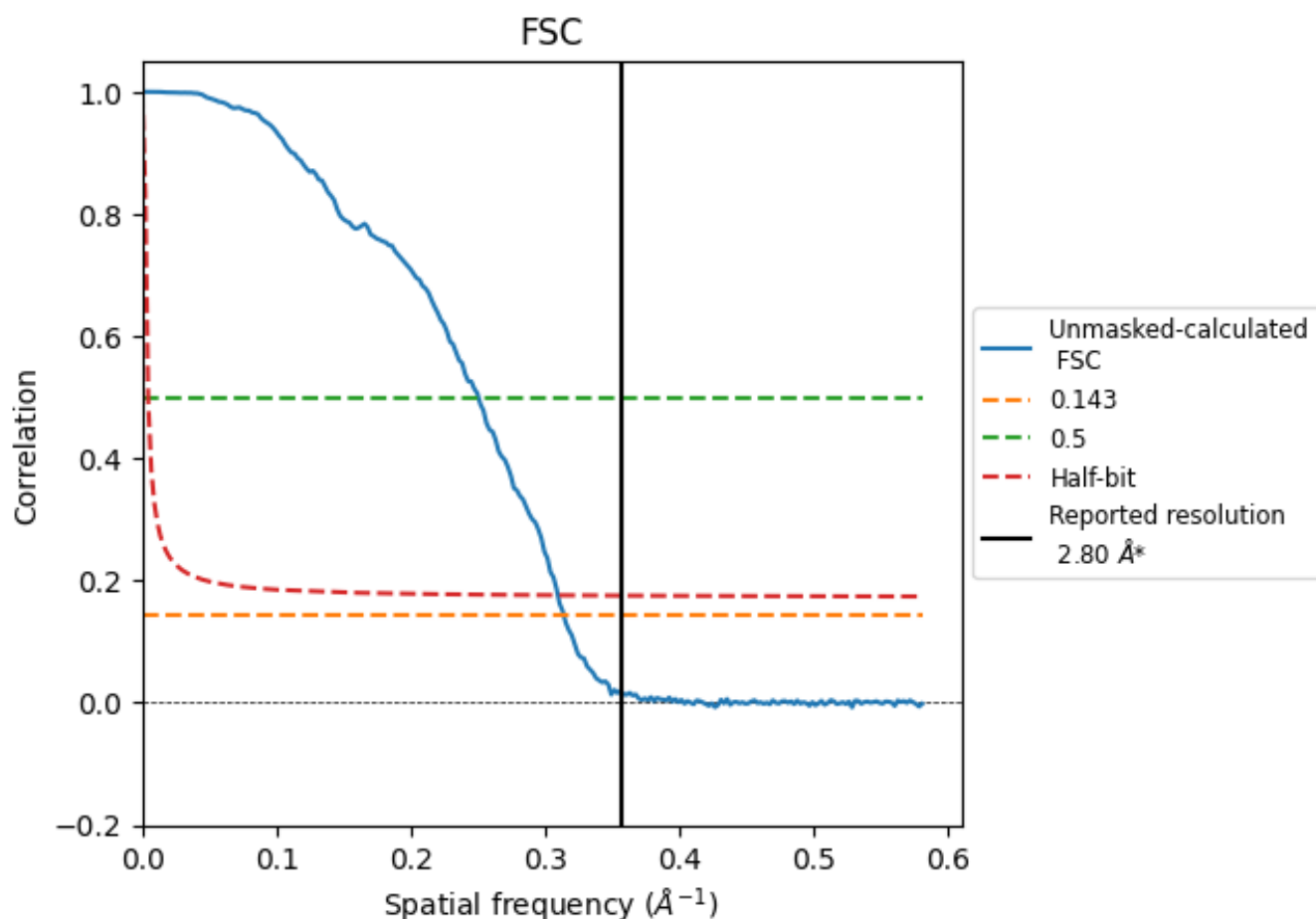


*Reported resolution corresponds to spatial frequency of 0.357 $\text{\AA}^{-1}$

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 0.357 Å⁻¹

8.2 Resolution estimates [i](#)

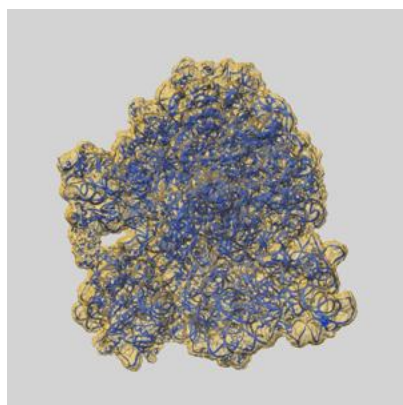
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.18	3.99	3.23

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.18 differs from the reported value 2.8 by more than 10 %

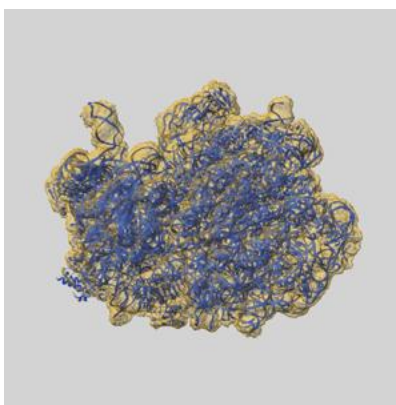
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-29821 and PDB model 8G7R. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

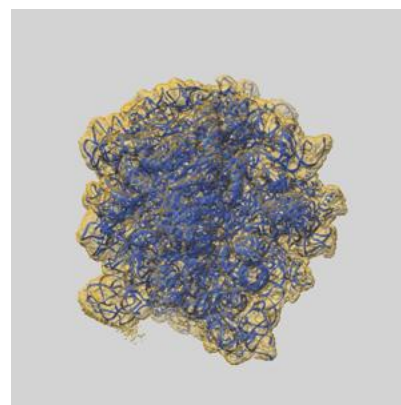
9.1 Map-model overlay [i](#)



X



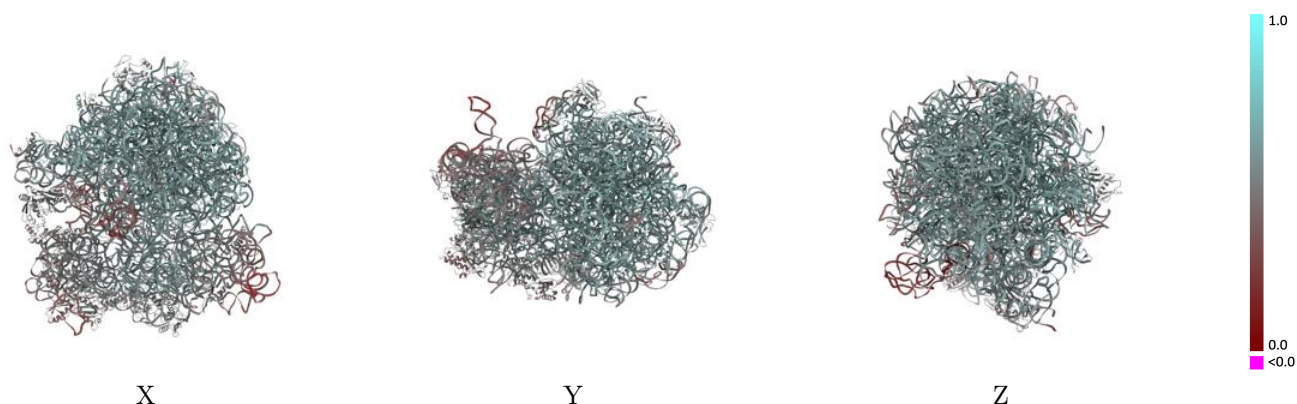
Y



Z

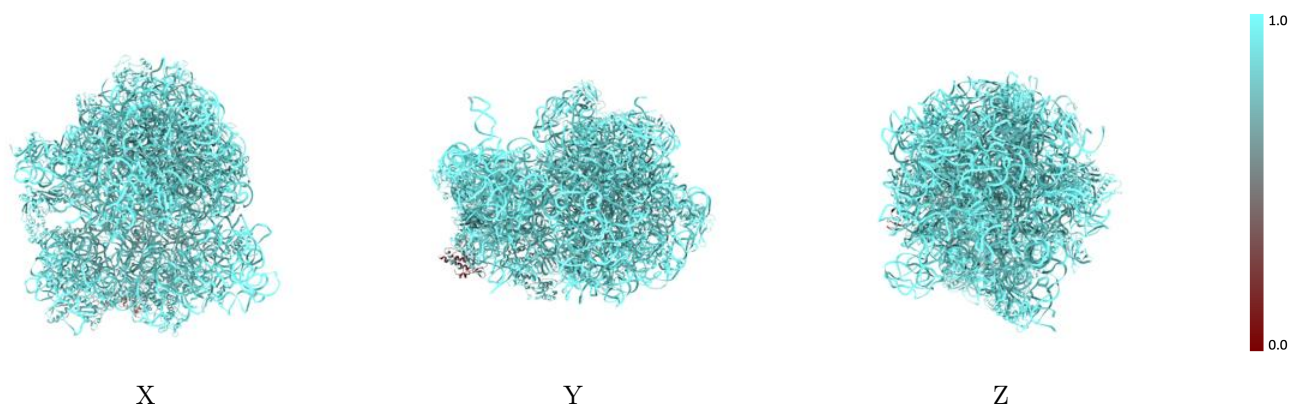
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



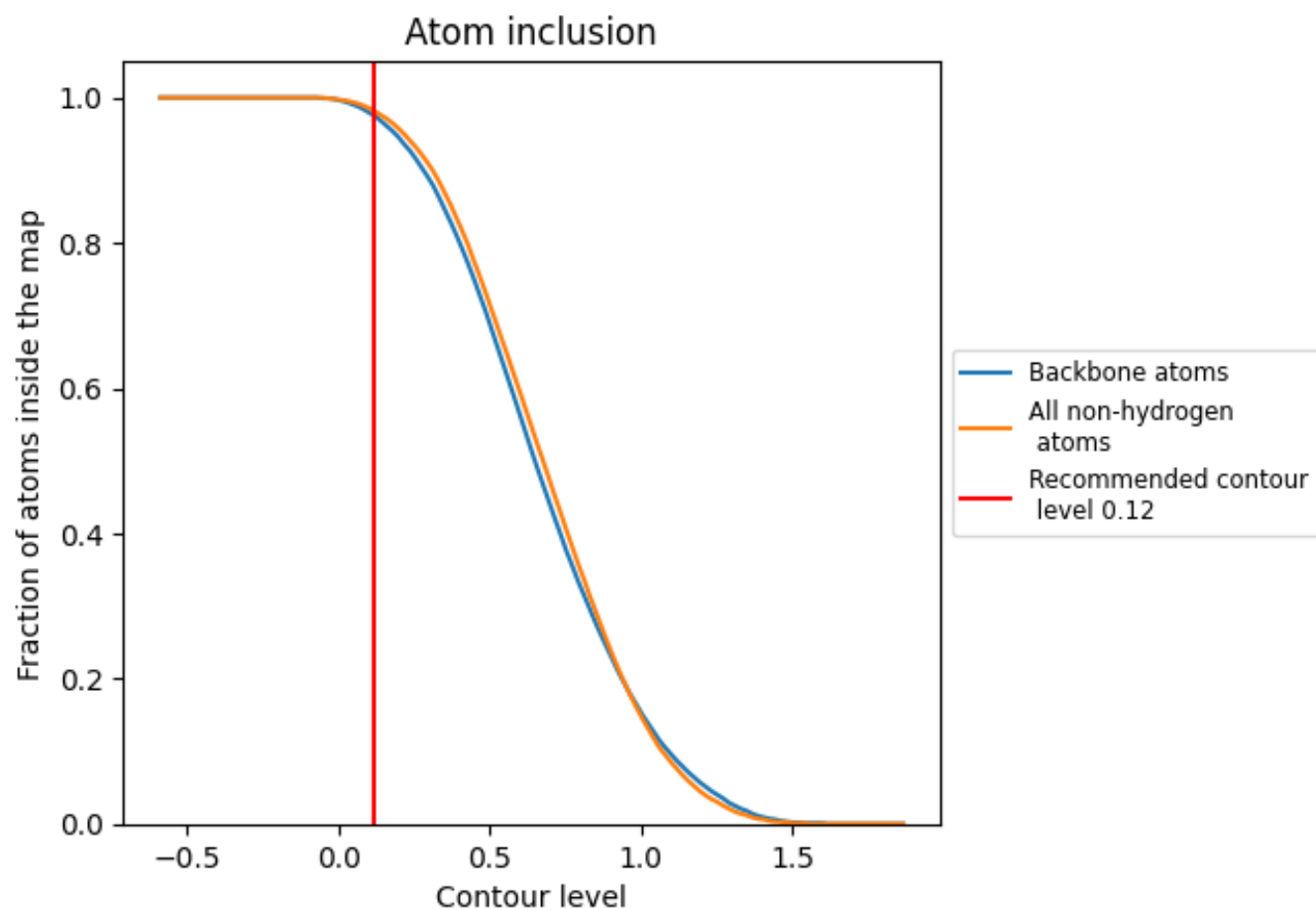
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9820	 0.5340
1	 0.9900	 0.5200
2	 0.9860	 0.5690
3	 0.9570	 0.4440
4	 0.9950	 0.5910
5	 0.9780	 0.5640
6	 0.9830	 0.6030
7	 0.9880	 0.6040
8	 0.9900	 0.5770
A	 0.9990	 0.5640
B	 0.9980	 0.5310
C	 0.9480	 0.5780
D	 0.9960	 0.5880
E	 0.9720	 0.5420
F	 0.9860	 0.4840
G	 0.9820	 0.5160
H	 0.4100	 0.3960
L	 0.9950	 0.5880
M	 0.9880	 0.5880
N	 0.9880	 0.5790
O	 0.9820	 0.5900
P	 0.9980	 0.6020
Q	 0.9940	 0.5280
R	 0.9850	 0.5780
S	 0.9960	 0.5960
T	 0.9770	 0.5710
U	 0.9890	 0.5760
V	 0.9780	 0.5490
W	 0.9940	 0.5310
X	 0.9840	 0.5550
Y	 0.9810	 0.5840
Z	 0.9850	 0.5780
a	 0.9980	 0.5050
b	 0.4140	 0.3940
c	 0.9350	 0.5040



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Chain	Atom inclusion	Q-score
d	 0.9650	 0.4770
e	 0.9810	 0.5340
f	 0.9070	 0.4430
g	 0.9710	 0.4350
h	 0.9810	 0.5200
i	 0.9840	 0.4610
j	 0.8870	 0.4450
k	 0.9750	 0.4900
l	 0.9800	 0.5600
m	 0.9830	 0.4720
n	 0.9740	 0.4910
o	 0.9810	 0.4790
p	 0.9840	 0.4920
q	 0.9840	 0.5050
r	 0.9180	 0.4850
s	 0.9910	 0.4720
t	 0.9880	 0.4500
u	 0.7180	 0.4540
v	 1.0000	 0.5510
w	 0.9760	 0.4850
x	 0.9930	 0.4960
y	 0.9550	 0.2960