



Full wwPDB EM Validation Report ⓘ

Jun 17, 2026 – 03:31 pm BST

PDB ID : 9QQQ / pdb_00009qqq
EMDB ID : EMD-53311
Title : Cryo-EM structure of SKM-70S ribosomal stalled complex in the major state (vacant A-site, canon)
Authors : Morici, M.; Corazza, M.; Safdari, H.A.; Wilson, D.N.
Deposited on : 2025-04-01
Resolution : 2.26 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

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:

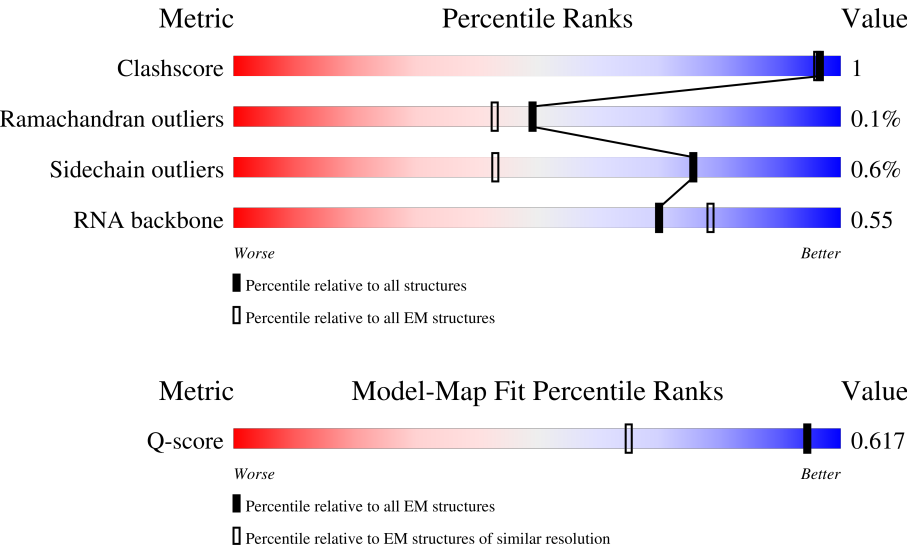
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 2.26 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	3535 (1.76 - 2.76)

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	V	470	19% 19% 81%
2	0	55	42% 89% 7%
3	1	46	93% ••

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Mol	Chain	Length	Quality of chain
4	2	65	
5	3	38	
6	4	70	
7	A	1541	
8	B	241	
9	C	233	
10	D	206	
11	E	167	
12	F	135	
13	G	179	
14	H	130	
15	I	130	
16	J	103	
17	K	129	
18	L	124	
19	M	118	
20	N	101	
21	O	89	
22	P	82	
23	Q	84	
24	R	75	
25	S	92	
26	T	87	
27	U	71	
28	X	136	

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Mol	Chain	Length	Quality of chain
29	Z	73	
30	a	2900	
31	b	120	
32	c	273	
33	d	209	
34	e	201	
35	f	179	
36	g	177	
37	h	149	
38	i	142	
39	j	123	
40	k	144	
41	l	136	
42	m	127	
43	n	117	
44	o	115	
45	p	118	
46	q	103	
47	r	110	
48	s	100	
49	t	104	
50	u	94	
51	v	85	
52	w	78	
53	x	63	

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Mol	Chain	Length	Quality of chain
54	y	59	61% 92% 5%
55	z	57	35% 91% 5%

2 Entry composition [i](#)

There are 59 unique types of molecules in this entry. The entry contains 148174 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 Small ribosomal subunit protein bS1.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	V	91	Total	C	N	O	0	0
			692	432	116	144		

- Molecule 2 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	0	51	Total	C	N	O	0	0
			417	269	76	72		

- Molecule 3 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1	45	Total	C	N	O	S	0	0
			367	222	88	55	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 5 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 6 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	58	Total	C	N	O	S	0	0
			464	289	87	82	6		

- Molecule 7 is a RNA chain called E. coli 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	1502	Total	C	N	O	P	0	0
			32256	14392	5930	10432	1502		

- Molecule 8 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	224	Total	C	N	O	S	0	0
			1753	1109	315	321	8		

- Molecule 9 is a protein called Small ribosomal subunit protein uS3.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS4.

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS5.

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

- Molecule 12 is a protein called Small ribosomal subunit protein bS6, fully modified isoform.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS7.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 15 is a protein called Small ribosomal subunit protein uS9.

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

- Molecule 16 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 17 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	116	Total	C	N	O	S	0	0
			866	534	169	160	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 18 is a protein called Small ribosomal subunit protein uS12.

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

- Molecule 19 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 20 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 21 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 22 is a protein called Small ribosomal subunit protein bS16.

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

- Molecule 23 is a protein called Small ribosomal subunit protein uS17.

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

- Molecule 24 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	65	Total	C	N	O	S	0	0
			535	339	100	95	1		

- Molecule 25 is a protein called Small ribosomal subunit protein uS19.

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

- Molecule 26 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	85	Total	C	N	O	S	0	0
			664	411	137	113	3		

- Molecule 27 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	70	Total	C	N	O	S	0	0
			589	366	125	97	1		

- Molecule 28 is a RNA chain called ermBL mRNA transcript.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	6	Total	C	N	O	P	0	0
			129	58	24	41	6		

- Molecule 29 is a RNA chain called P-site tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Z	73	Total	C	N	O	P	0	0
			1563	696	286	508	73		

- Molecule 30 is a RNA chain called E. coli 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	a	2751	Total	C	N	O	P	0	0
			59090	26366	10892	19081	2751		

- Molecule 31 is a RNA chain called E. coli 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	b	119	Total	C	N	O	P	0	0
			2549	1135	466	829	119		

- Molecule 32 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	c	270	Total	C	N	O	S	0	0
			2076	1285	422	362	7		

- Molecule 33 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	d	208	Total	C	N	O	S	0	0
			1560	977	287	292	4		

- Molecule 34 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	e	200	Total	C	N	O	S	0	0
			1546	971	282	288	5		

- Molecule 35 is a protein called Large ribosomal subunit protein uL5.

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

- Molecule 36 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	g	173	Total	C	N	O	S	0	0
			1295	814	237	242	2		

- Molecule 37 is a protein called Large ribosomal subunit protein bL9.

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

- Molecule 38 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	i	140	Total	C	N	O	S	0	0
			1112	703	210	196	3		

- Molecule 39 is a protein called Large ribosomal subunit protein uL14.

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

- Molecule 40 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 41 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 42 is a protein called Large ribosomal subunit protein bL17.

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

- Molecule 43 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	n	114	Total	C	N	O	S	0	0
			871	538	175	158			

- Molecule 44 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	o	113	Total	C	N	O	S	0	0
			908	570	177	160	1		

- Molecule 45 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 46 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	q	101	Total	C	N	O	S	0	0
			802	508	151	142	1		

- Molecule 47 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	r	108	Total	C	N	O	S	0	0
			837	522	161	151	3		

- Molecule 48 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	s	92	Total	C	N	O	S	0	0
			730	460	138	130	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	t	90	Total	C	N	O	S	0	0
			695	439	130	126			

- Molecule 50 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	u	92	Total	C	N	O	S	0	0
			739	471	135	131	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	v	83	Total	C	N	O	S	0	0
			618	383	125	109	1		

- Molecule 52 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	w	75	Total	C	N	O	S	0	0
			603	373	126	102	2		

- Molecule 53 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	x	57	Total	C	N	O	S	0	0
			468	288	91	88	1		

- Molecule 54 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	y	57	Total	C	N	O	S	0	0
			439	276	86	75	2		

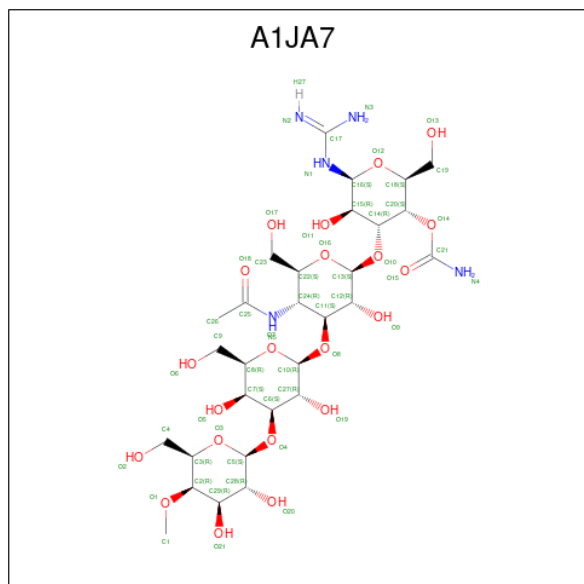
- Molecule 55 is a protein called Large ribosomal subunit protein bL32.

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

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	3	1	Total	Zn	0
			1	1	
56	4	1	Total	Zn	0
			1	1	

- Molecule 57 is [(2 {S},3 {S},4 {R},5 {R},6 {S})-4-[(2 {S},3 {R},4 {S},5 {R},6 {S})-5-acetamido-6-(hydroxymethyl)-4-[(2 {R},3 {R},4 {S},5 {S},6 {R})-6-(hydroxymethyl)-4-[(2 {S},3 {R},4 {R},5 {R},6 {R})-6-(hydroxymethyl)-5-methoxy-3,4-bis(oxidanyl)oxan-2-yl]oxy-3,5-bis(oxidanyl)oxan-2-yl]oxy-3-oxidanyl-oxan-2-yl]oxy-6-carbamimidamido-2-(hydroxymethyl)-5-oxidanyl-oxan-3-yl] carbamate (CCD ID: A1JA7) (formula: C₂₉H₅₁N₅O₂₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
57	A	1	Total	C	N	O	0
			55	29	5	21	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	A	104	Total	Mg	0
			104	104	

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Mol	Chain	Residues	Atoms		AltConf
58	Q	1	Total 1	Mg 1	0
58	a	200	Total 200	Mg 200	0
58	b	5	Total 5	Mg 5	0
58	c	1	Total 1	Mg 1	0
58	d	1	Total 1	Mg 1	0

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	0	9	Total 9	O 9	0
59	1	28	Total 28	O 28	0
59	2	27	Total 27	O 27	0
59	3	3	Total 3	O 3	0
59	4	5	Total 5	O 5	0
59	A	2813	Total 2813	O 2813	0
59	B	6	Total 6	O 6	0
59	C	47	Total 47	O 47	0
59	D	37	Total 37	O 37	0
59	E	20	Total 20	O 20	0
59	F	3	Total 3	O 3	0
59	G	11	Total 11	O 11	0
59	H	37	Total 37	O 37	0
59	I	30	Total 30	O 30	0

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Mol	Chain	Residues	Atoms		AltConf
59	J	23	Total 23	O 23	0
59	K	18	Total 18	O 18	0
59	L	37	Total 37	O 37	0
59	M	25	Total 25	O 25	0
59	N	38	Total 38	O 38	0
59	O	20	Total 20	O 20	0
59	P	18	Total 18	O 18	0
59	Q	8	Total 8	O 8	0
59	R	8	Total 8	O 8	0
59	S	17	Total 17	O 17	0
59	T	20	Total 20	O 20	0
59	U	10	Total 10	O 10	0
59	X	12	Total 12	O 12	0
59	Z	19	Total 19	O 19	0
59	a	4053	Total 4053	O 4053	0
59	b	154	Total 154	O 154	0
59	c	112	Total 112	O 112	0
59	d	45	Total 45	O 45	0
59	e	38	Total 38	O 38	0
59	f	31	Total 31	O 31	0
59	h	3	Total 3	O 3	0

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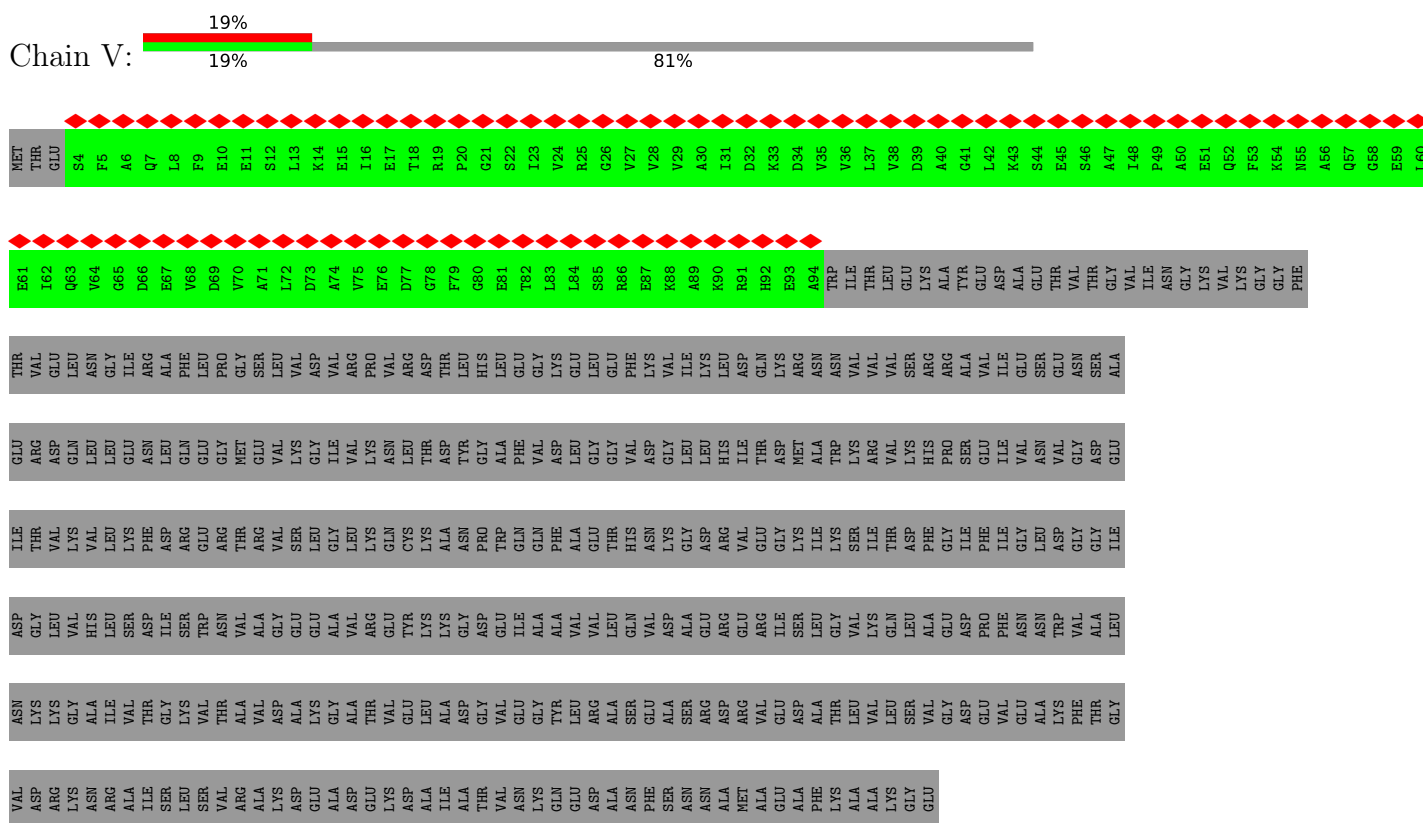
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Mol	Chain	Residues	Atoms		AltConf
59	i	14	Total 14	O 14	0
59	j	17	Total 17	O 17	0
59	k	49	Total 49	O 49	0
59	l	25	Total 25	O 25	0
59	m	31	Total 31	O 31	0
59	n	35	Total 35	O 35	0
59	o	17	Total 17	O 17	0
59	p	30	Total 30	O 30	0
59	q	19	Total 19	O 19	0
59	r	22	Total 22	O 22	0
59	s	7	Total 7	O 7	0
59	u	7	Total 7	O 7	0
59	v	13	Total 13	O 13	0
59	w	22	Total 22	O 22	0
59	x	2	Total 2	O 2	0
59	y	5	Total 5	O 5	0
59	z	28	Total 28	O 28	0

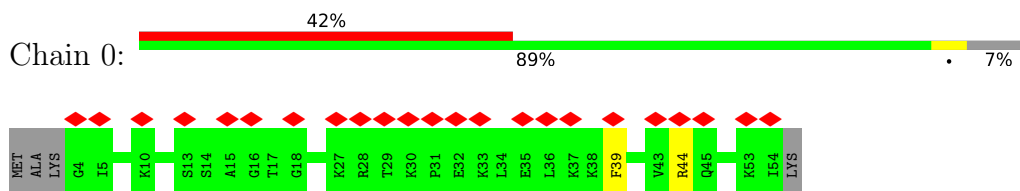
3 Residue-property plots

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: Small ribosomal subunit protein bS1



- Molecule 2: Large ribosomal subunit protein bL33

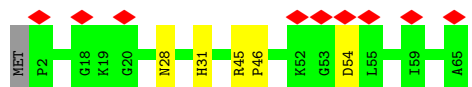
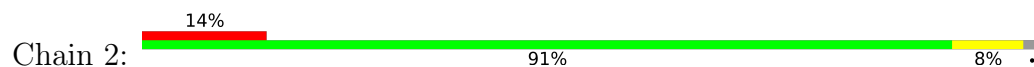


- Molecule 3: Large ribosomal subunit protein bL34

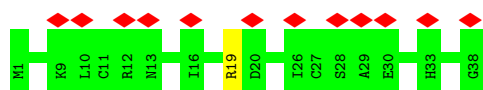




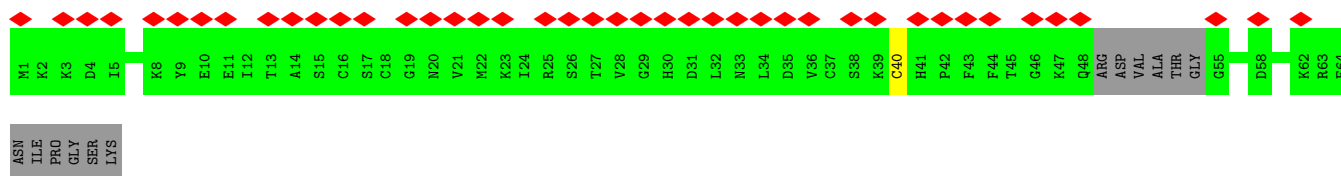
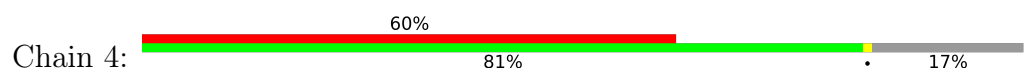
- Molecule 4: Large ribosomal subunit protein bL35



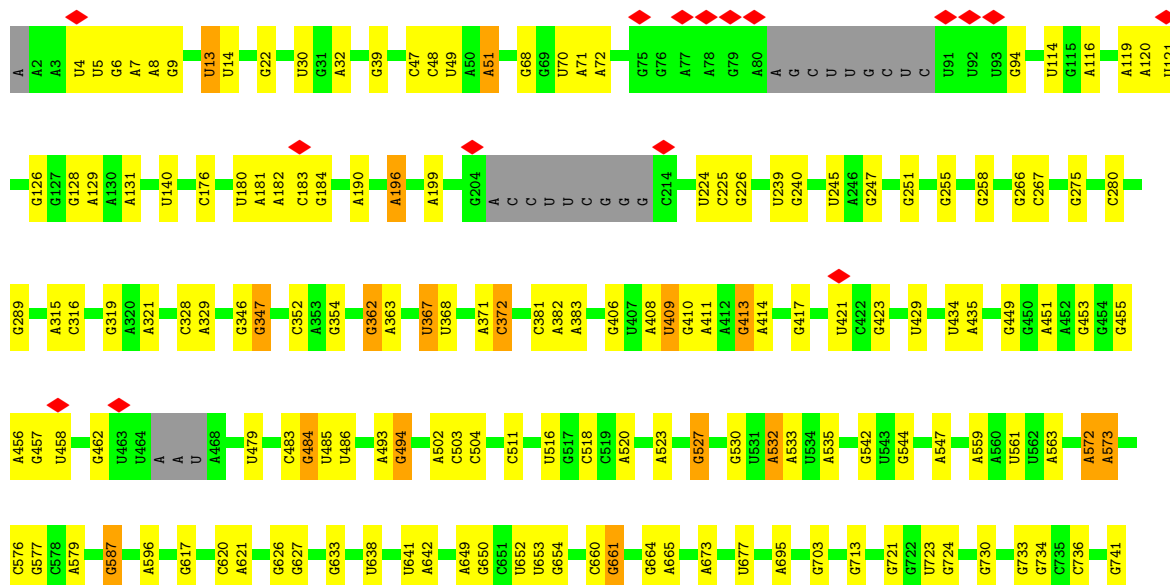
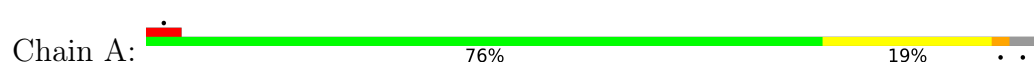
- Molecule 5: Large ribosomal subunit protein bL36A

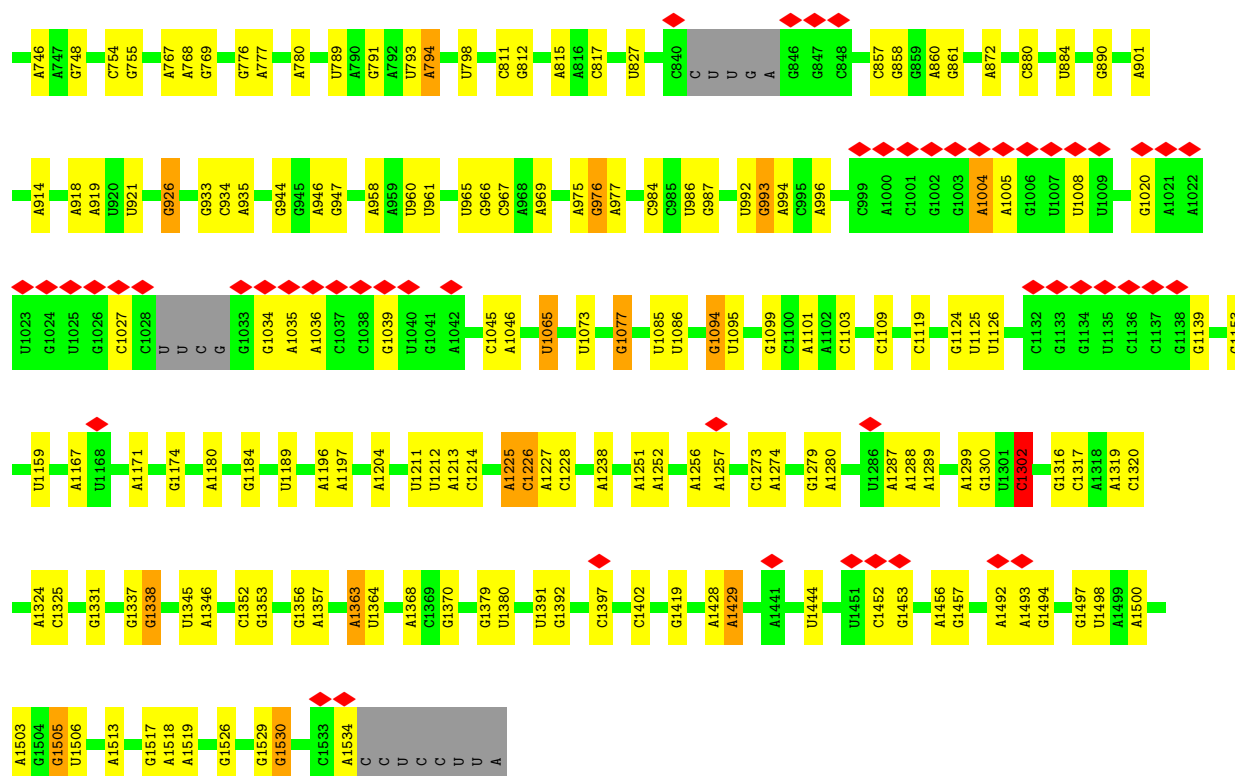


- Molecule 6: Large ribosomal subunit protein bL31

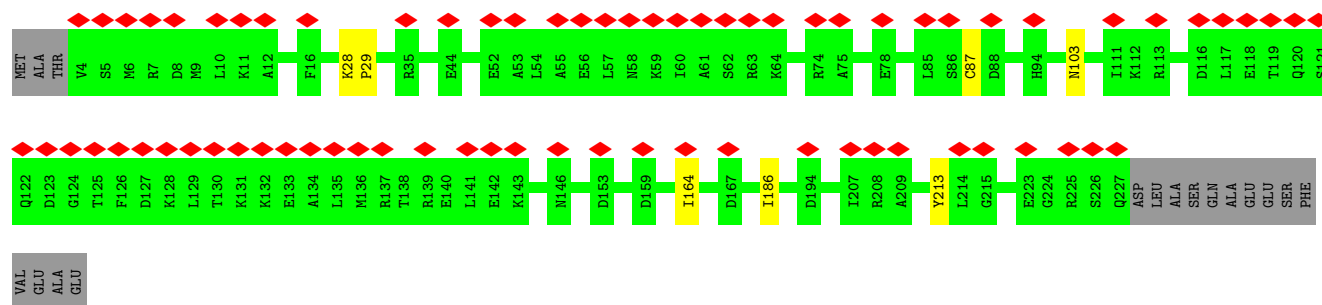
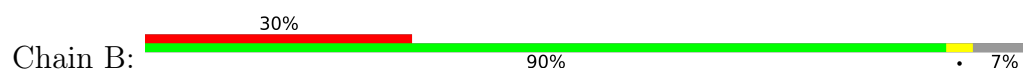


- Molecule 7: E. coli 16S rRNA

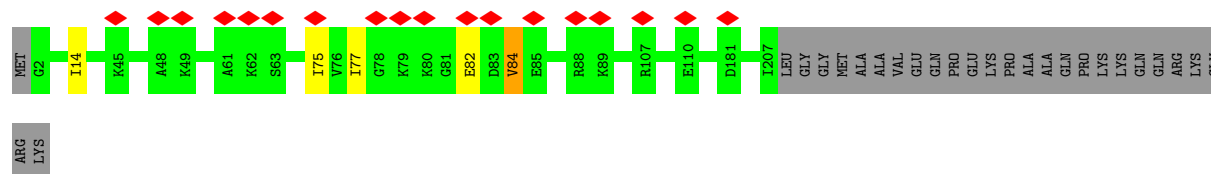
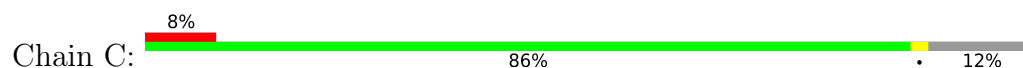




• Molecule 8: Small ribosomal subunit protein uS2

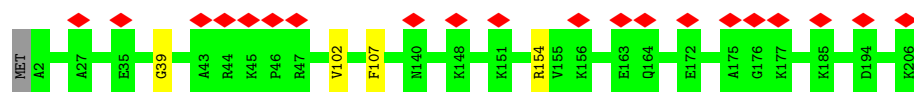


• Molecule 9: Small ribosomal subunit protein uS3

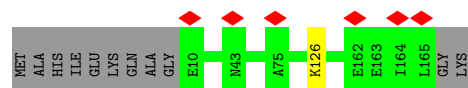
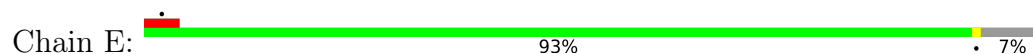


• Molecule 10: Small ribosomal subunit protein uS4

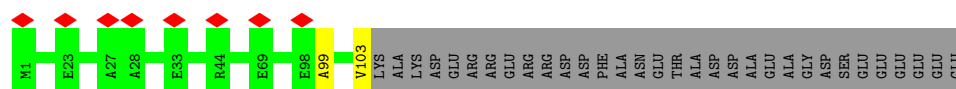
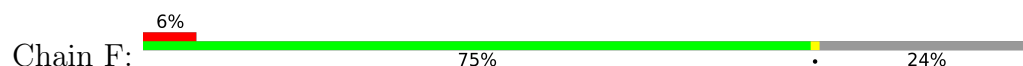




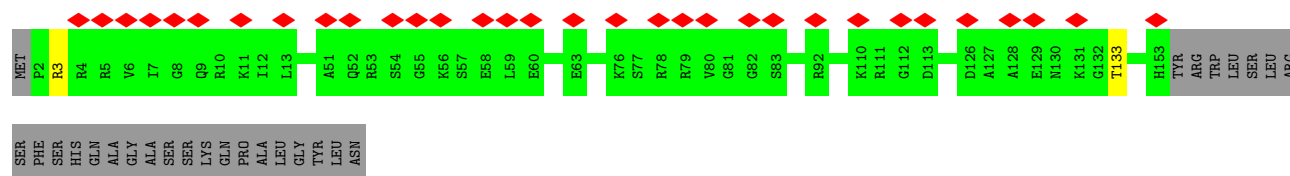
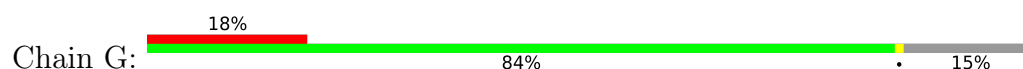
- Molecule 11: Small ribosomal subunit protein uS5



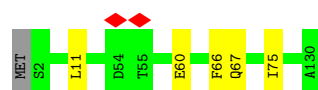
- Molecule 12: Small ribosomal subunit protein bS6, fully modified isoform



- Molecule 13: Small ribosomal subunit protein uS7



- Molecule 14: Small ribosomal subunit protein uS8

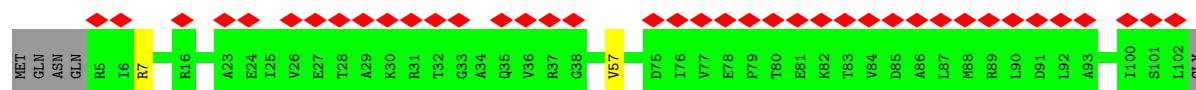


- Molecule 15: Small ribosomal subunit protein uS9



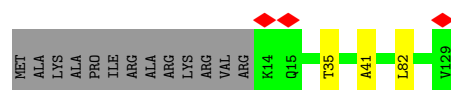
- Molecule 16: Small ribosomal subunit protein uS10





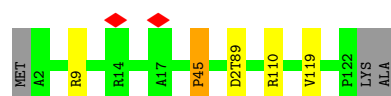
- Molecule 17: Small ribosomal subunit protein uS11

Chain K: 88% 10%



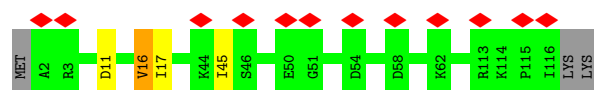
- Molecule 18: Small ribosomal subunit protein uS12

Chain L: 94% 10%



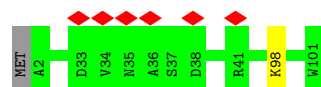
- Molecule 19: Small ribosomal subunit protein uS13

Chain M: 94% 10%



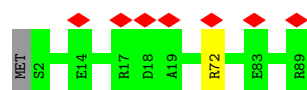
- Molecule 20: Small ribosomal subunit protein uS14

Chain N: 98% 6%



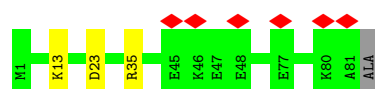
- Molecule 21: Small ribosomal subunit protein uS15

Chain O: 98% 8%

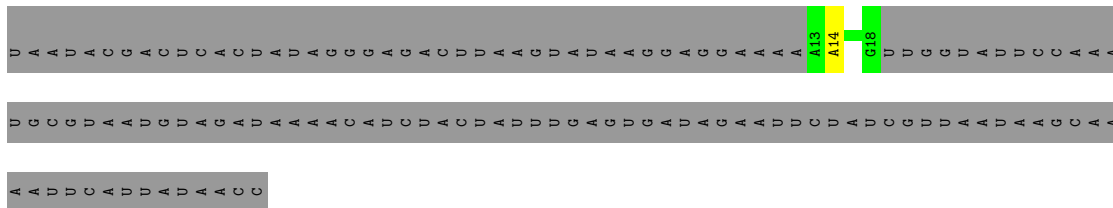
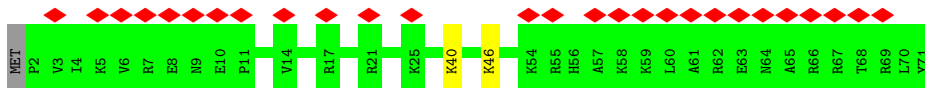
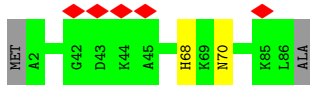
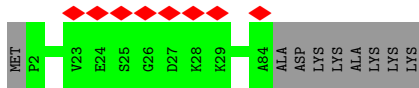
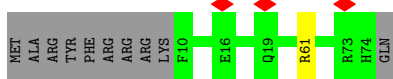
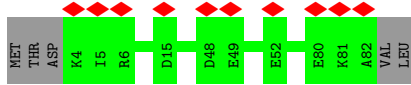


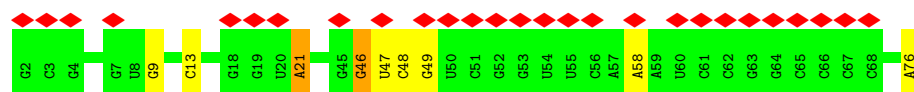
- Molecule 22: Small ribosomal subunit protein bS16

Chain P: 95% 7%



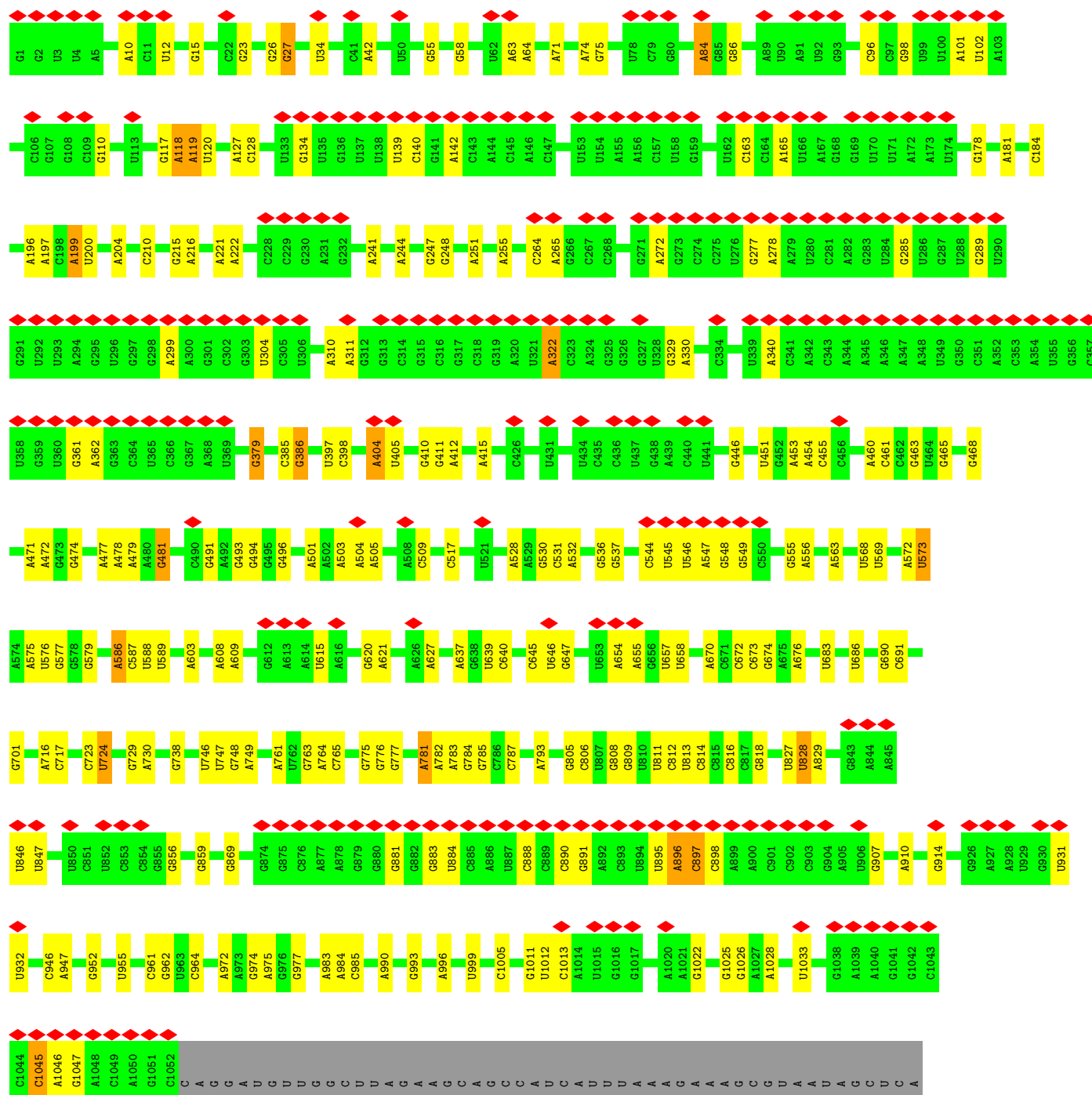
- Molecule 23: Small ribosomal subunit protein uS17



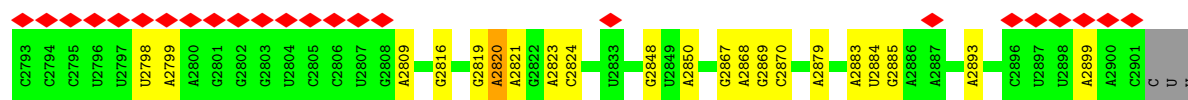


• Molecule 30: E. coli 23S rRNA

Chain a: 16% 74% 19% 5%

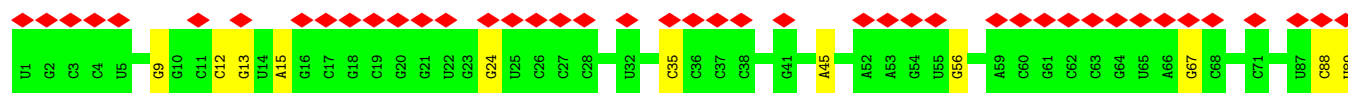






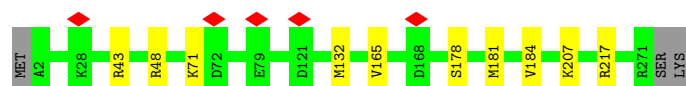
• Molecule 31: E. coli 5S rRNA

Chain b: 48% 87% 12% ..



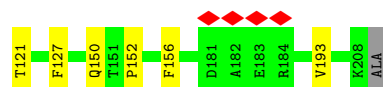
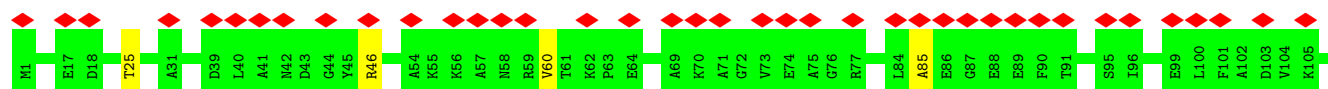
• Molecule 32: Large ribosomal subunit protein uL2

Chain c: 95% ..



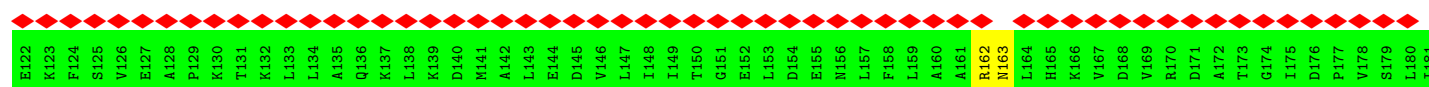
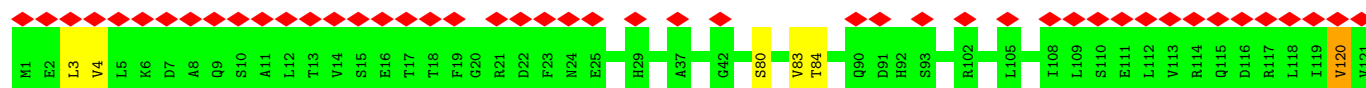
• Molecule 33: Large ribosomal subunit protein uL3

Chain d: 21% 95% 5%

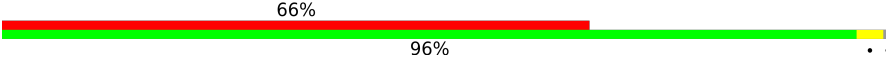


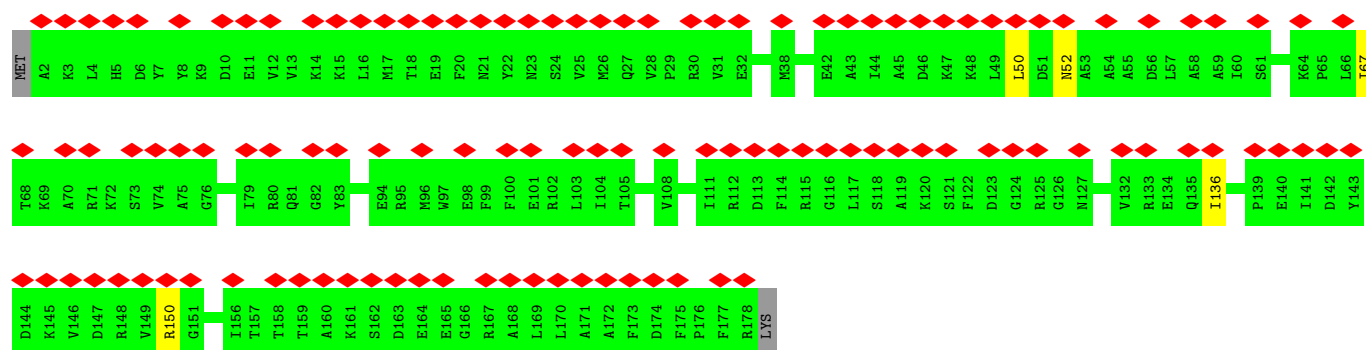
• Molecule 34: Large ribosomal subunit protein uL4

Chain e: 61% 96% .

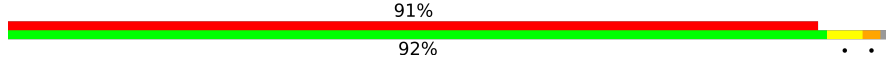


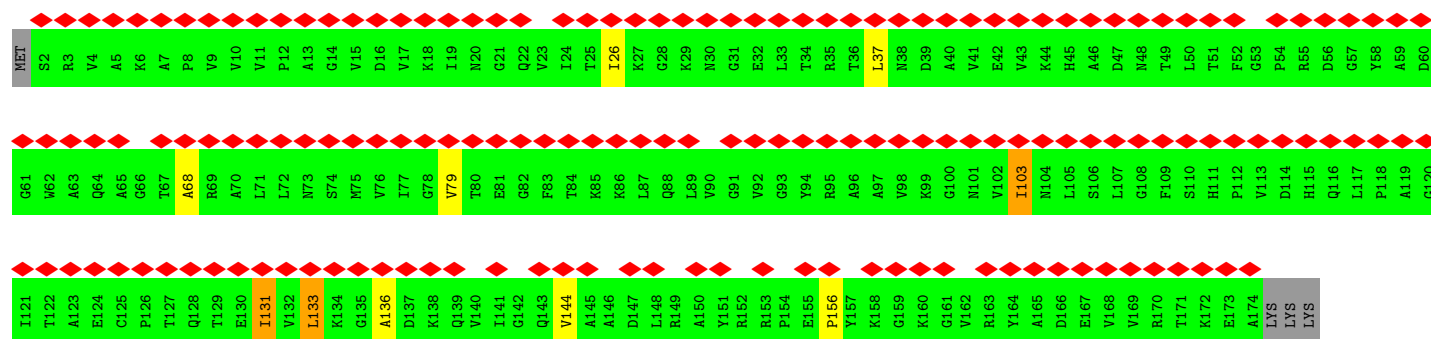
• Molecule 35: Large ribosomal subunit protein uL5

Chain f: 



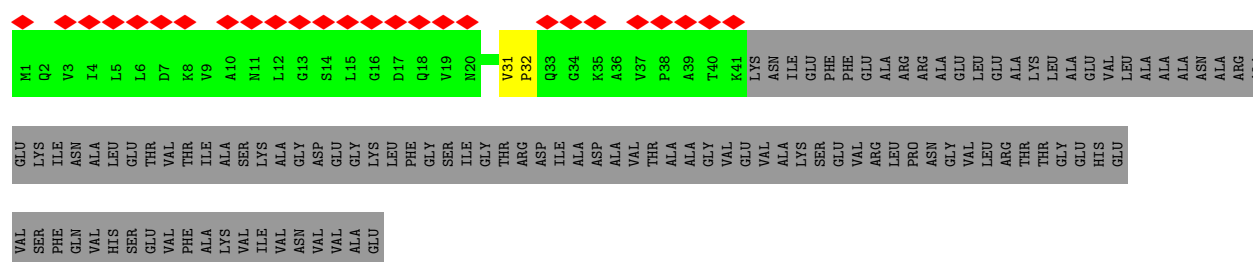
• Molecule 36: Large ribosomal subunit protein uL6

Chain g: 



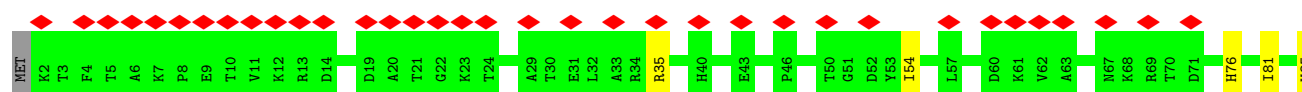
• Molecule 37: Large ribosomal subunit protein bL9

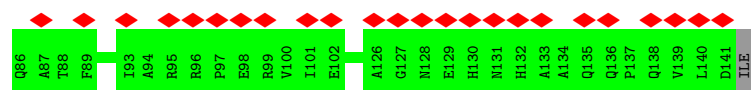
Chain h: 



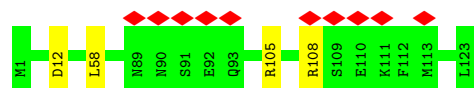
• Molecule 38: Large ribosomal subunit protein uL13

Chain i: 

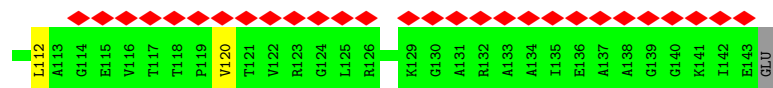
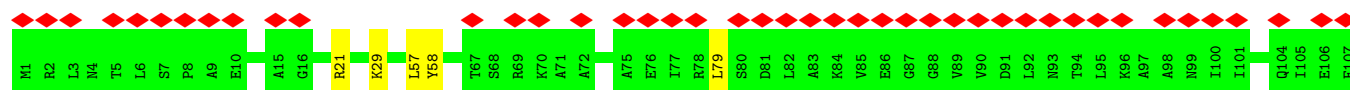
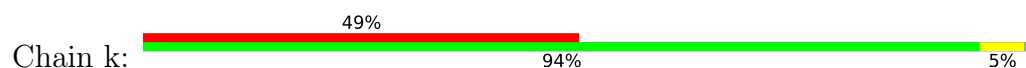




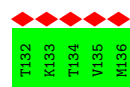
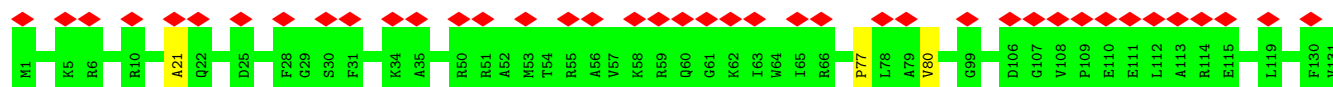
- Molecule 39: Large ribosomal subunit protein uL14



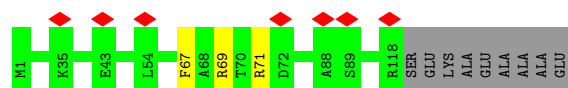
- Molecule 40: Large ribosomal subunit protein uL15



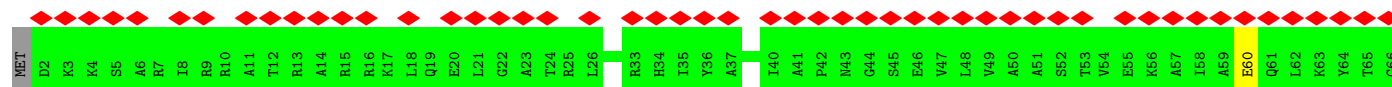
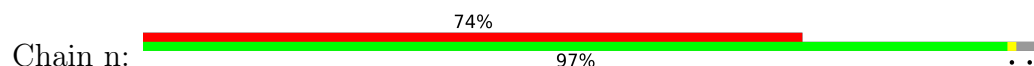
- Molecule 41: Large ribosomal subunit protein uL16

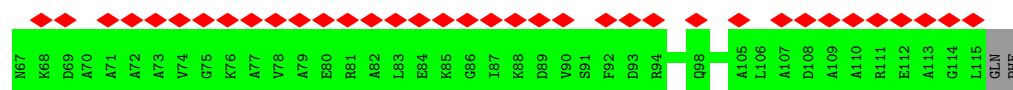


- Molecule 42: Large ribosomal subunit protein bL17

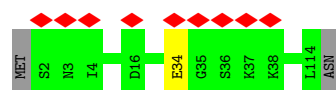


- Molecule 43: Large ribosomal subunit protein uL18

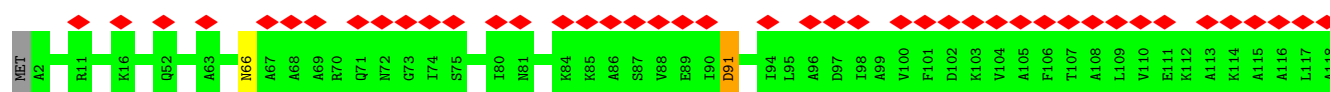




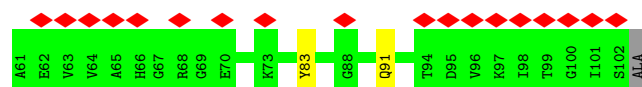
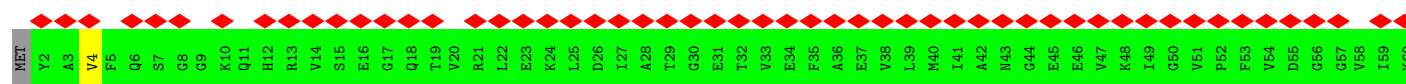
- Molecule 44: Large ribosomal subunit protein bL19



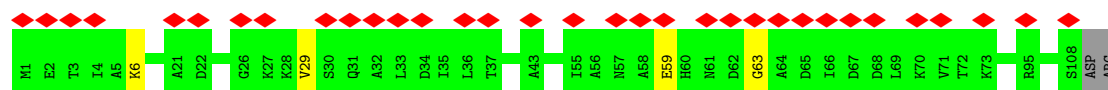
- Molecule 45: Large ribosomal subunit protein bL20



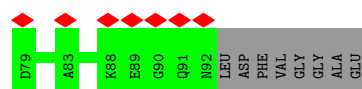
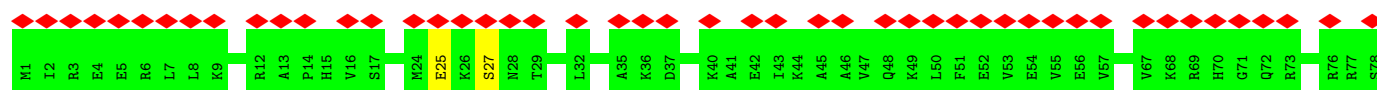
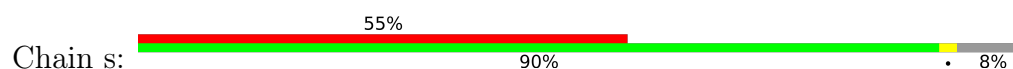
- Molecule 46: Large ribosomal subunit protein bL21



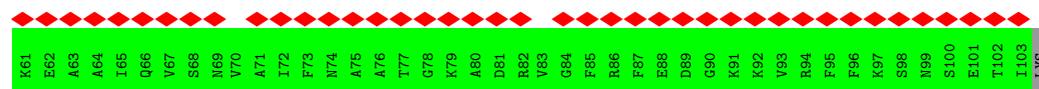
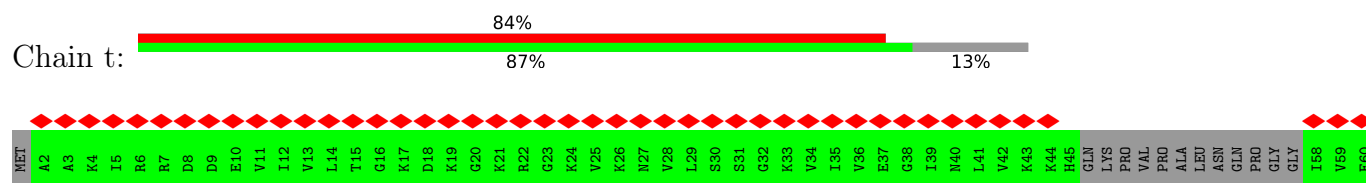
- Molecule 47: Large ribosomal subunit protein uL22



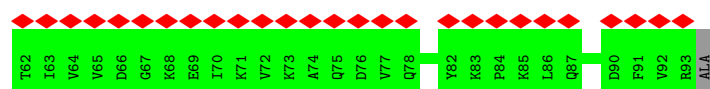
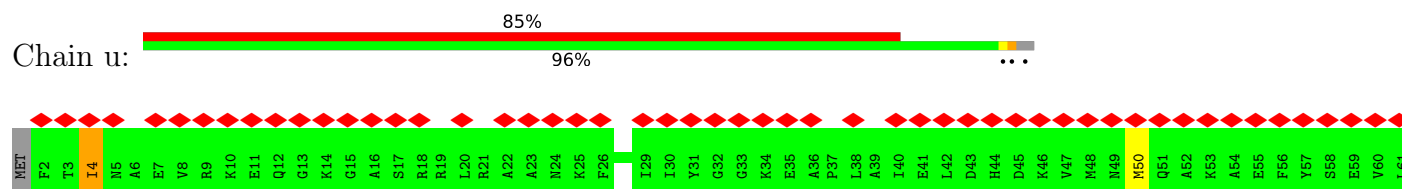
- Molecule 48: Large ribosomal subunit protein uL23



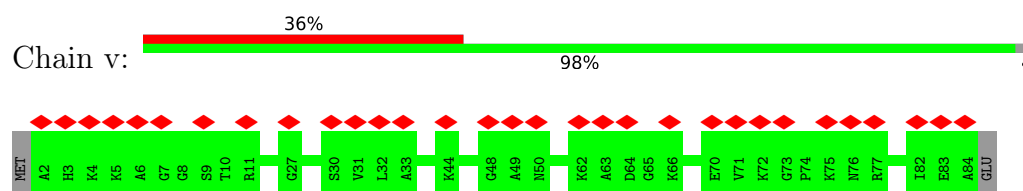
- Molecule 49: Large ribosomal subunit protein uL24



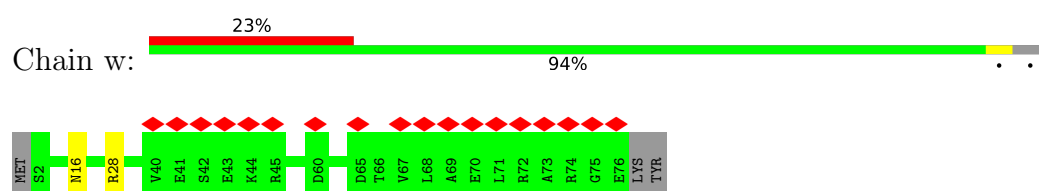
- Molecule 50: Large ribosomal subunit protein bL25



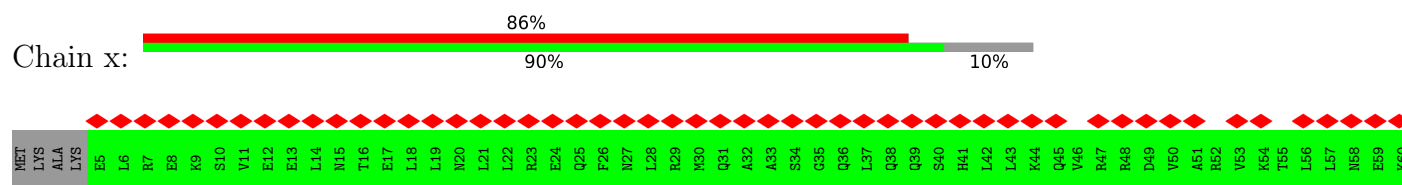
- Molecule 51: Large ribosomal subunit protein bL27



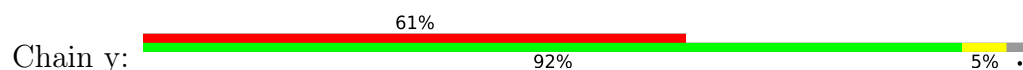
- Molecule 52: Large ribosomal subunit protein bL28

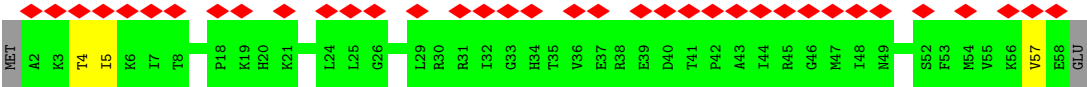


- Molecule 53: Large ribosomal subunit protein uL29

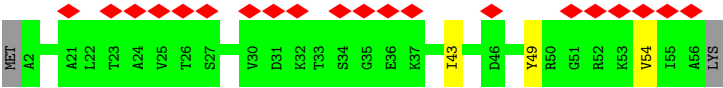
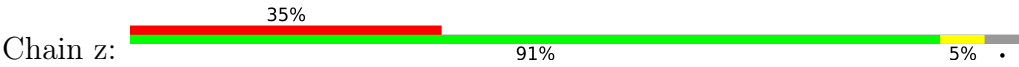


- Molecule 54: Large ribosomal subunit protein uL30





• Molecule 55: Large ribosomal subunit protein bL32



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	343986	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 ($e^-/\text{\AA}^2$)	1.14	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.200	Depositor
Minimum map value	-0.088	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	359.424, 359.424, 359.424	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1MG, UR3, OMU, MG, 2MG, 4OC, A1JA7, 5MU, OMG, 2MA, MA6, 6MZ, 5MC, OMC, MEQ, IAS, H2U, MS6, PSU, 3TD, 4D4, G7M, D2T

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	V	0.59	0/698	0.89	0/940
2	0	0.56	0/424	0.84	0/565
3	1	0.60	0/370	0.94	0/487
4	2	0.59	0/513	0.89	0/676
5	3	0.58	0/303	0.83	0/397
6	4	0.56	0/472	0.90	0/627
7	A	0.56	0/35864	0.99	84/55935 (0.2%)
8	B	0.58	0/1784	0.97	1/2403 (0.0%)
9	C	0.66	0/1651	0.89	1/2225 (0.0%)
10	D	0.62	0/1665	0.91	1/2227 (0.0%)
11	E	0.70	0/1165	0.90	0/1568
12	F	0.62	0/858	0.89	0/1160
13	G	0.61	0/1206	0.92	0/1617
14	H	0.69	0/989	0.91	0/1326
15	I	0.65	0/1034	0.92	0/1375
16	J	0.63	0/796	0.92	0/1077
17	K	0.68	0/873	0.84	0/1177
18	L	0.67	0/945	0.92	1/1268 (0.1%)
19	M	0.58	0/900	0.98	1/1204 (0.1%)
20	N	0.70	0/817	0.92	0/1088
21	O	0.72	0/722	0.90	0/964
22	P	0.73	0/653	0.92	1/877 (0.1%)
23	Q	0.60	0/650	0.84	0/871
24	R	0.67	0/544	0.92	0/731
25	S	0.66	0/680	0.90	0/915
26	T	0.70	0/670	0.95	0/888
27	U	0.62	0/597	1.01	0/792
28	X	0.70	0/144	0.97	0/222
29	Z	0.60	0/1746	0.89	0/2719
30	a	0.56	1/65607 (0.0%)	0.93	130/102345 (0.1%)
31	b	0.56	0/2850	0.86	1/4444 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	c	0.64	0/2115	0.88	0/2844
33	d	0.56	0/1570	0.89	1/2112 (0.0%)
34	e	0.55	0/1565	0.91	0/2106
35	f	0.55	0/1434	0.94	0/1926
36	g	0.58	0/1315	0.94	0/1783
37	h	0.59	0/306	0.94	0/413
38	i	0.55	0/1135	0.89	0/1530
39	j	0.60	0/955	0.92	1/1279 (0.1%)
40	k	0.57	0/1052	0.89	0/1401
41	l	0.53	0/1073	0.86	0/1433
42	m	0.58	0/958	0.94	0/1281
43	n	0.56	0/880	0.92	0/1181
44	o	0.60	0/920	0.84	0/1231
45	p	0.52	0/960	0.98	0/1278
46	q	0.56	0/815	0.82	0/1090
47	r	0.58	0/844	0.88	0/1131
48	s	0.55	0/736	0.88	0/983
49	t	0.55	0/699	0.85	0/928
50	u	0.55	0/752	0.86	0/1008
51	v	0.57	0/626	0.81	0/829
52	w	0.59	0/612	0.90	0/819
53	x	0.52	0/469	1.00	0/626
54	y	0.58	0/443	0.89	0/593
55	z	0.58	0/440	0.93	0/588
All	All	0.57	1/150864 (0.0%)	0.94	223/225503 (0.1%)

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
7	A	0	8
17	K	0	1
30	a	0	4
41	l	0	1
52	w	0	1
All	All	0	15

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2069	G7M	O3'-P	5.28	1.61	1.56

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	367	U	O3'-P-O5'	-11.90	86.15	104.00
7	A	652	U	O3'-P-O5'	-9.17	90.24	104.00
7	A	413	G	C4'-C3'-O3'	8.88	122.72	109.40
7	A	493	A	O3'-P-O5'	-8.88	90.68	104.00
30	a	1185	G	O3'-P-O5'	-8.81	90.79	104.00
7	A	413	G	O3'-P-O5'	8.30	116.46	104.00
30	a	2519	U	O3'-P-O5'	-8.24	91.64	104.00
19	M	16	VAL	N-CA-CB	8.08	119.48	110.51
7	A	921	U	O3'-P-O5'	-8.05	91.92	104.00
7	A	746	A	O3'-P-O5'	-7.99	92.01	104.00
30	a	781	A	O3'-P-O5'	-7.93	92.10	104.00
30	a	1785	A	O3'-P-O5'	-7.89	92.17	104.00
30	a	1971	U	C4'-C3'-O3'	-7.83	101.25	113.00
30	a	972	A	O3'-P-O5'	-7.81	92.29	104.00
30	a	808	G	O3'-P-O5'	-7.63	92.55	104.00
7	A	316	C	O3'-P-O5'	-7.57	92.64	104.00
30	a	385	C	O3'-P-O5'	-7.54	92.69	104.00
7	A	703	G	O3'-P-O5'	-7.49	92.76	104.00
30	a	2222	C	O3'-P-O5'	-7.42	92.86	104.00
7	A	181	A	O3'-P-O5'	-7.37	92.95	104.00
30	a	672	C	O3'-P-O5'	-7.34	92.99	104.00
30	a	964	C	O3'-P-O5'	-7.34	92.99	104.00
30	a	1969	A	O3'-P-O5'	-7.31	93.04	104.00
30	a	990	A	O3'-P-O5'	-7.28	93.08	104.00
30	a	1847	A	O3'-P-O5'	-7.25	93.13	104.00
30	a	1981	A	C4'-C3'-O3'	-7.19	102.22	113.00
30	a	2718	G	O3'-P-O5'	-7.17	93.24	104.00
30	a	2050	C	O3'-P-O5'	-7.13	93.31	104.00
30	a	1974	C	O3'-P-O5'	-6.98	93.52	104.00
30	a	2581	G	O3'-P-O5'	-6.98	93.53	104.00
7	A	1363	A	O3'-P-O5'	-6.95	93.58	104.00
30	a	1810	A	O3'-P-O5'	-6.88	93.68	104.00
30	a	379	G	O3'-P-O5'	-6.88	93.69	104.00
30	a	2819	G	O3'-P-O5'	-6.86	93.71	104.00
7	A	434	U	O3'-P-O5'	-6.80	93.80	104.00
7	A	1444	U	O3'-P-O5'	-6.75	93.87	104.00
30	a	2726	A	O3'-P-O5'	-6.75	93.87	104.00
7	A	1180	A	O3'-P-O5'	-6.61	94.08	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	1293	C	O3'-P-O5'	-6.61	94.09	104.00
7	A	976	G	O3'-P-O5'	-6.60	94.10	104.00
30	a	2546	U	O3'-P-O5'	-6.60	94.10	104.00
7	A	1337	G	O3'-P-O5'	-6.57	94.14	104.00
30	a	204	A	O3'-P-O5'	-6.56	94.17	104.00
30	a	1895	C	O3'-P-O5'	-6.55	94.18	104.00
7	A	1352	C	O3'-P-O5'	-6.54	94.19	104.00
7	A	126	G	O3'-P-O5'	-6.51	94.24	104.00
30	a	1905	C	O3'-P-O5'	-6.48	94.28	104.00
30	a	1937	A	O3'-P-O5'	-6.46	94.30	104.00
30	a	2549	G	O3'-P-O5'	-6.46	94.31	104.00
7	A	409	U	O3'-P-O5'	-6.44	94.34	104.00
30	a	1992	G	O3'-P-O5'	-6.40	94.39	104.00
7	A	484	G	O3'-P-O5'	-6.37	94.45	104.00
30	a	1252	G	O3'-P-O5'	-6.36	94.46	104.00
30	a	410	G	O3'-P-O5'	-6.36	94.46	104.00
7	A	561	U	O3'-P-O5'	-6.36	94.46	104.00
18	L	45	PRO	N-CA-CB	-6.35	95.61	102.60
7	A	794	A	O3'-P-O5'	-6.35	94.47	104.00
30	a	763	G	O3'-P-O5'	-6.31	94.53	104.00
7	A	780	A	O3'-P-O5'	-6.28	94.58	104.00
7	A	530	G	O3'-P-O5'	-6.28	94.58	104.00
7	A	872	A	O3'-P-O5'	-6.25	94.63	104.00
7	A	435	A	O3'-P-O5'	-6.24	94.64	104.00
30	a	2685	G	O3'-P-O5'	-6.23	94.66	104.00
30	a	676	A	O3'-P-O5'	-6.21	94.68	104.00
30	a	184	C	O3'-P-O5'	-6.21	94.69	104.00
7	A	965	U	C3'-C2'-O2'	6.20	120.00	110.70
30	a	818	G	O3'-P-O5'	-6.16	94.77	104.00
30	a	2498	OMC	O3'-P-O5'	-6.12	94.81	104.00
30	a	2717	C	O3'-P-O5'	-6.11	94.83	104.00
7	A	347	G	O3'-P-O5'	-6.11	94.84	104.00
30	a	2094	A	O3'-P-O5'	-6.11	94.84	104.00
7	A	275	G	O3'-P-O5'	-6.09	94.86	104.00
39	j	12	ASP	CA-CB-CG	6.09	118.69	112.60
7	A	13	U	C1'-O4'-C4'	-6.09	103.61	109.70
7	A	532	A	O3'-P-O5'	-6.09	94.87	104.00
30	a	2824	C	O3'-P-O5'	-6.07	94.90	104.00
7	A	176	C	O3'-P-O5'	-6.06	94.92	104.00
30	a	787	C	O3'-P-O5'	-6.04	94.94	104.00
30	a	2620	C	O3'-P-O5'	-5.99	95.01	104.00
30	a	2550	G	O3'-P-O5'	-5.98	95.03	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	397	U	O3'-P-O5'	-5.95	95.07	104.00
30	a	1496	A	O3'-P-O5'	-5.94	95.09	104.00
7	A	455	G	O3'-P-O5'	-5.93	95.10	104.00
30	a	1757	A	C4'-C3'-O3'	-5.92	104.12	113.00
30	a	2493	U	O3'-P-O5'	-5.90	95.15	104.00
30	a	2452	C	O3'-P-O5'	-5.87	95.20	104.00
30	a	398	C	O3'-P-O5'	-5.84	95.24	104.00
30	a	2479	U	O3'-P-O5'	-5.84	95.24	104.00
33	d	60	VAL	N-CA-CB	5.82	116.87	110.53
30	a	2521	C	O3'-P-O5'	-5.81	95.28	104.00
7	A	798	U	O3'-P-O5'	-5.81	95.28	104.00
30	a	1379	U	O3'-P-O5'	-5.79	95.31	104.00
30	a	2198	A	O3'-P-O5'	-5.77	95.34	104.00
30	a	1959	G	O3'-P-O5'	-5.76	95.35	104.00
7	A	572	A	O3'-P-O5'	-5.76	95.37	104.00
30	a	2684	U	O3'-P-O5'	-5.75	95.38	104.00
30	a	277	G	C2'-C3'-O3'	-5.73	105.10	113.70
7	A	5	U	O3'-P-O5'	-5.73	95.41	104.00
7	A	239	U	C2'-C3'-O3'	-5.72	105.12	113.70
30	a	27	G	O3'-P-O5'	-5.72	95.42	104.00
30	a	199	A	O3'-P-O5'	-5.71	95.44	104.00
30	a	1373	A	O3'-P-O5'	-5.70	95.44	104.00
7	A	225	C	O3'-P-O5'	-5.69	95.47	104.00
30	a	1650	A	O3'-P-O5'	-5.68	95.47	104.00
7	A	1077	G	C1'-C2'-O2'	5.68	116.92	108.40
7	A	638	U	O3'-P-O5'	-5.67	95.50	104.00
30	a	2683	C	O3'-P-O5'	-5.67	95.50	104.00
7	A	563	A	C4'-C3'-O3'	-5.66	104.51	113.00
7	A	504	C	O3'-P-O5'	-5.65	95.52	104.00
7	A	1505	G	C2'-C3'-O3'	-5.64	105.24	113.70
30	a	1567	G	O3'-P-O5'	-5.63	95.55	104.00
30	a	1152	C	O3'-P-O5'	-5.62	95.57	104.00
30	a	241	A	O3'-P-O5'	-5.61	95.58	104.00
30	a	783	A	O3'-P-O5'	-5.61	95.59	104.00
30	a	977	G	O3'-P-O5'	-5.60	95.60	104.00
30	a	673	C	O3'-P-O5'	-5.59	95.62	104.00
7	A	1279	G	O3'-P-O5'	-5.58	95.63	104.00
7	A	901	A	O3'-P-O5'	-5.57	95.64	104.00
7	A	363	A	O3'-P-O5'	-5.57	95.65	104.00
30	a	2548	U	O3'-P-O5'	-5.56	95.66	104.00
30	a	1274	A	O3'-P-O5'	-5.54	95.70	104.00
7	A	1345	U	O3'-P-O5'	-5.53	95.70	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	493	A	C4'-C3'-O3'	-5.53	104.70	113.00
30	a	1378	A	O3'-P-O5'	-5.51	95.73	104.00
31	b	90	C	O3'-P-O5'	-5.51	95.73	104.00
30	a	576	U	O3'-P-O5'	-5.49	95.76	104.00
7	A	520	A	O3'-P-O5'	-5.49	95.76	104.00
9	C	14	ILE	N-CA-C	-5.49	106.84	111.56
30	a	64	A	O3'-P-O5'	-5.49	95.77	104.00
7	A	456	A	O3'-P-O5'	-5.48	95.78	104.00
30	a	2848	G	O3'-P-O5'	-5.47	95.80	104.00
30	a	1432	G	O3'-P-O5'	-5.45	95.83	104.00
7	A	140	U	O3'-P-O5'	-5.45	95.83	104.00
7	A	1103	C	O3'-P-O5'	-5.44	95.84	104.00
30	a	1237	A	O3'-P-O5'	-5.43	95.85	104.00
7	A	812	G	O3'-P-O5'	-5.43	95.86	104.00
30	a	210	C	O3'-P-O5'	-5.42	95.87	104.00
30	a	446	G	O3'-P-O5'	-5.42	95.88	104.00
30	a	999	U	O3'-P-O5'	-5.41	95.88	104.00
30	a	2054	A	O3'-P-O5'	-5.41	95.88	104.00
30	a	2572	A	O3'-P-O5'	-5.40	95.90	104.00
7	A	196	A	O3'-P-O5'	-5.39	95.91	104.00
7	A	695	A	C4'-C3'-O3'	-5.39	104.91	113.00
30	a	1906	G	O3'-P-O5'	-5.39	95.91	104.00
7	A	780	A	C4'-C3'-O3'	-5.38	104.93	113.00
30	a	1359	A	O3'-P-O5'	-5.37	95.94	104.00
30	a	1664	A	O3'-P-O5'	-5.37	95.95	104.00
7	A	190	A	O3'-P-O5'	-5.36	95.95	104.00
30	a	816	C	O3'-P-O5'	-5.36	95.96	104.00
30	a	2197	U	O3'-P-O5'	-5.36	95.96	104.00
7	A	129	A	O3'-P-O5'	-5.34	95.99	104.00
7	A	8	A	O3'-P-O5'	-5.33	96.00	104.00
7	A	730	G	O3'-P-O5'	-5.33	96.01	104.00
7	A	1153	G	O3'-P-O5'	-5.33	96.01	104.00
7	A	1380	U	O3'-P-O5'	-5.32	96.02	104.00
7	A	1065	U	O3'-P-O5'	-5.32	96.03	104.00
30	a	1349	C	O3'-P-O5'	-5.31	96.03	104.00
30	a	2679	A	O3'-P-O5'	-5.31	96.03	104.00
30	a	404	A	C2'-C3'-O3'	5.30	117.45	109.50
7	A	958	A	O3'-P-O5'	-5.29	96.06	104.00
30	a	2719	G	O3'-P-O5'	-5.29	96.06	104.00
30	a	2682	A	O3'-P-O5'	-5.29	96.07	104.00
30	a	701	G	O3'-P-O5'	-5.28	96.08	104.00
30	a	1613	G	O3'-P-O5'	-5.27	96.10	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	15	G	O3'-P-O5'	-5.27	96.10	104.00
30	a	674	G	O3'-P-O5'	-5.27	96.10	104.00
30	a	683	U	O3'-P-O5'	-5.27	96.10	104.00
30	a	1436	G	O3'-P-O5'	-5.27	96.10	104.00
7	A	1302	C	O3'-P-O5'	-5.25	96.12	104.00
30	a	716	A	O3'-P-O5'	-5.25	96.12	104.00
7	A	617	G	O3'-P-O5'	-5.25	96.13	104.00
30	a	1025	G	O3'-P-O5'	5.24	111.86	104.00
30	a	2622	U	O3'-P-O5'	-5.24	96.14	104.00
30	a	2543	G	O3'-P-O5'	-5.24	96.15	104.00
10	D	154	ARG	CB-CA-C	-5.23	102.05	110.74
30	a	2820	A	C2'-C3'-O3'	5.22	117.33	109.50
30	a	474	G	O3'-P-O5'	-5.22	96.17	104.00
7	A	255	G	O3'-P-O5'	-5.21	96.18	104.00
30	a	1553	A	O3'-P-O5'	-5.21	96.19	104.00
7	A	68	G	O3'-P-O5'	-5.21	96.19	104.00
7	A	346	G	C2'-C3'-O3'	-5.20	105.90	113.70
7	A	523	A	O3'-P-O5'	-5.20	96.20	104.00
7	A	627	G	O3'-P-O5'	-5.20	96.20	104.00
30	a	2235	G	O3'-P-O5'	-5.19	96.22	104.00
22	P	23	ASP	CA-CB-CG	5.18	117.78	112.60
30	a	1131	G	O3'-P-O5'	-5.18	96.23	104.00
30	a	1299	G	C2'-C3'-O3'	-5.17	105.94	113.70
7	A	224	U	O3'-P-O5'	-5.17	96.25	104.00
30	a	2809	A	O3'-P-O5'	-5.17	96.25	104.00
30	a	1367	A	O3'-P-O5'	-5.17	96.25	104.00
7	A	944	G	O3'-P-O5'	-5.16	96.26	104.00
7	A	1338	G	O3'-P-O5'	-5.15	96.27	104.00
30	a	1246	A	O3'-P-O5'	-5.14	96.28	104.00
30	a	1697	G	O3'-P-O5'	-5.13	96.31	104.00
7	A	523	A	C4'-C3'-O3'	-5.12	105.31	113.00
8	B	213	TYR	N-CA-CB	5.11	117.73	110.16
7	A	544	G	O3'-P-O5'	-5.10	96.35	104.00
30	a	1134	A	O3'-P-O5'	-5.10	96.34	104.00
30	a	1653	G	O3'-P-O5'	-5.10	96.35	104.00
30	a	2710	C	O3'-P-O5'	-5.10	96.35	104.00
30	a	2867	G	O3'-P-O5'	-5.10	96.36	104.00
30	a	761	A	C4'-C3'-O3'	-5.09	105.36	113.00
30	a	134	G	O3'-P-O5'	-5.09	96.37	104.00
30	a	2282	G	O3'-P-O5'	-5.08	96.37	104.00
30	a	2879	A	O3'-P-O5'	-5.08	96.37	104.00
7	A	315	A	O3'-P-O5'	-5.08	96.38	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	a	952	G	O3'-P-O5'	-5.08	96.38	104.00
7	A	811	C	C4'-C3'-O3'	-5.07	105.39	113.00
30	a	2766	A	O3'-P-O5'	-5.07	96.40	104.00
30	a	517	C	O3'-P-O5'	-5.06	96.41	104.00
30	a	748	G	C1'-O4'-C4'	-5.05	104.85	109.90
30	a	806	C	O3'-P-O5'	-5.05	96.42	104.00
7	A	30	U	O3'-P-O5'	-5.05	96.43	104.00
30	a	2453	A	O3'-P-O5'	-5.05	96.43	104.00
30	a	1261	C	O3'-P-O5'	-5.04	96.44	104.00
30	a	1643	G	O3'-P-O5'	-5.04	96.45	104.00
7	A	926	G	C4'-C3'-O3'	-5.03	105.45	113.00
7	A	494	G	O3'-P-O5'	-5.02	96.47	104.00
7	A	587	G	N9-C1'-C2'	-5.02	106.47	114.00
7	A	180	U	O3'-P-O5'	-5.02	96.47	104.00
30	a	2050	C	C4'-C3'-O3'	-5.02	105.48	113.00
30	a	2761	A	O3'-P-O5'	-5.01	96.48	104.00
7	A	449	G	O3'-P-O5'	-5.00	96.50	104.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A	1077	G	Sidechain
7	A	1094	G	Sidechain
7	A	1316	G	Sidechain
7	A	1331	G	Sidechain
7	A	362	G	Sidechain
7	A	573	A	Sidechain
7	A	587	G	Sidechain
7	A	673	A	Sidechain
17	K	82	LEU	Peptide
30	a	1631	G	Sidechain
30	a	1938	A	Sidechain
30	a	2595	G	Sidechain
30	a	463	G	Sidechain
41	l	21	ALA	Peptide
52	w	16	ASN	Peptide

5.2 Too-close contacts

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	V	692	0	687	0	0
2	0	417	0	451	1	0
3	1	367	0	405	2	0
4	2	504	0	572	2	0
5	3	302	0	340	1	0
6	4	464	0	461	0	0
7	A	32256	0	16253	47	0
8	B	1753	0	1780	3	0
9	C	1624	0	1696	1	0
10	D	1643	0	1707	2	0
11	E	1152	0	1196	1	0
12	F	839	0	833	1	0
13	G	1191	0	1245	1	0
14	H	979	0	1031	2	0
15	I	1022	0	1070	3	0
16	J	786	0	828	1	0
17	K	866	0	871	1	0
18	L	942	0	999	2	0
19	M	891	0	952	2	0
20	N	805	0	844	1	0
21	O	714	0	734	1	0
22	P	643	0	661	2	0
23	Q	641	0	682	0	0
24	R	535	0	552	1	0
25	S	663	0	688	0	0
26	T	664	0	714	1	0
27	U	589	0	629	2	0
28	X	129	0	65	1	0
29	Z	1563	0	794	1	0
30	a	59090	0	29746	92	0
31	b	2549	0	1291	0	0
32	c	2076	0	2149	6	0
33	d	1560	0	1613	5	0
34	e	1546	0	1614	3	0
35	f	1410	0	1444	2	0
36	g	1295	0	1332	4	0
37	h	303	0	327	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	i	1112	0	1139	3	0
39	j	946	0	1023	2	0
40	k	1043	0	1123	4	0
41	l	1075	0	1145	1	0
42	m	945	0	989	2	0
43	n	871	0	906	0	0
44	o	908	0	956	1	0
45	p	947	0	1019	2	0
46	q	802	0	822	2	0
47	r	837	0	905	2	0
48	s	730	0	796	0	0
49	t	695	0	743	0	0
50	u	739	0	763	1	0
51	v	618	0	636	0	0
52	w	603	0	630	1	0
53	x	468	0	492	0	0
54	y	439	0	482	1	0
55	z	434	0	445	2	0
56	3	1	0	0	0	0
56	4	1	0	0	0	0
57	A	55	0	0	0	0
58	A	104	0	0	0	0
58	Q	1	0	0	0	0
58	a	200	0	0	0	0
58	b	5	0	0	0	0
58	c	1	0	0	0	0
58	d	1	0	0	0	0
59	0	9	0	0	0	0
59	1	28	0	0	0	0
59	2	27	0	0	0	0
59	3	3	0	0	0	0
59	4	5	0	0	0	0
59	A	2813	0	0	0	0
59	B	6	0	0	0	0
59	C	47	0	0	0	0
59	D	37	0	0	0	0
59	E	20	0	0	0	0
59	F	3	0	0	0	0
59	G	11	0	0	0	0
59	H	37	0	0	0	0
59	I	30	0	0	0	0
59	J	23	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	K	18	0	0	0	0
59	L	37	0	0	0	0
59	M	25	0	0	0	0
59	N	38	0	0	0	0
59	O	20	0	0	0	0
59	P	18	0	0	0	0
59	Q	8	0	0	0	0
59	R	8	0	0	0	0
59	S	17	0	0	0	0
59	T	20	0	0	0	0
59	U	10	0	0	0	0
59	X	12	0	0	0	0
59	Z	19	0	0	0	0
59	a	4053	0	0	1	0
59	b	154	0	0	0	0
59	c	112	0	0	0	0
59	d	45	0	0	0	0
59	e	38	0	0	0	0
59	f	31	0	0	0	0
59	h	3	0	0	0	0
59	i	14	0	0	0	0
59	j	17	0	0	0	0
59	k	49	0	0	0	0
59	l	25	0	0	0	0
59	m	31	0	0	0	0
59	n	35	0	0	0	0
59	o	17	0	0	0	0
59	p	30	0	0	0	0
59	q	19	0	0	0	0
59	r	22	0	0	0	0
59	s	7	0	0	0	0
59	u	7	0	0	0	0
59	v	13	0	0	0	0
59	w	22	0	0	0	0
59	x	2	0	0	0	0
59	y	5	0	0	0	0
59	z	28	0	0	0	0
All	All	148174	0	94270	187	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 1.

All (187) 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)
7:A:664:G:H22	7:A:741:G:H1	1.38	0.70
30:a:568:U:H1'	30:a:2030:6MZ:H9C1	1.78	0.66
3:l:12:ARG:NH2	30:a:465:G:OP1	2.29	0.64
30:a:453:A:OP1	59:a:4601:HOH:O	2.15	0.63
30:a:811:U:H2'	40:k:21:ARG:HA	1.83	0.59
30:a:12:U:H2'	30:a:12:U:O2	2.02	0.58
30:a:1939:5MU:OP1	30:a:2604:PSU:O2'	2.21	0.58
30:a:1799:G:N7	32:c:178:SER:OG	2.35	0.58
7:A:677:U:H3	7:A:713:G:H22	1.50	0.58
7:A:754:C:OP1	21:O:72:ARG:NH2	2.38	0.57
30:a:1853:A:N1	30:a:2087:G:H1'	2.20	0.57
7:A:371:A:H2'	7:A:372:C:O4'	2.04	0.56
7:A:769:G:H4'	7:A:1513:A:H4'	1.89	0.55
7:A:1302:C:C5	19:M:17:ILE:HG13	2.42	0.55
30:a:896:A:H3'	30:a:897:C:H4'	1.90	0.54
30:a:1434:A:H2'	30:a:1435:G:C8	2.42	0.54
37:h:31:VAL:HB	37:h:32:PRO:HD3	1.90	0.54
30:a:579:G:O2'	30:a:2019:A:OP1	2.28	0.52
7:A:381:C:O4'	7:A:381:C:O2	2.27	0.52
7:A:626:G:OP1	22:P:35:ARG:NH1	2.43	0.52
30:a:1434:A:H2'	30:a:1435:G:H8	1.75	0.52
30:a:717:C:O2	30:a:717:C:O4'	2.28	0.52
47:r:59:GLU:HA	47:r:63:GLY:O	2.10	0.52
7:A:1391:U:H2'	7:A:1392:G:C8	2.46	0.51
30:a:2395:C:H2'	30:a:2396:G:O4'	2.12	0.50
30:a:1182:G:H2'	30:a:1183:U:O4'	2.12	0.50
7:A:986:U:H2'	7:A:987:G:O4'	2.12	0.50
30:a:2014:A:H2'	30:a:2015:A:C8	2.46	0.49
7:A:660:C:H2'	7:A:661:G:O4'	2.12	0.49
7:A:1402:4OC:O2	7:A:1500:A:N1	2.46	0.49
7:A:1073:U:O2'	8:B:103:ASN:ND2	2.45	0.49
33:d:156:PHE:CE1	38:i:81:ILE:HD13	2.48	0.49
40:k:79:LEU:HD11	40:k:112:LEU:HD12	1.94	0.49
8:B:164:ILE:O	8:B:186:ILE:HB	2.13	0.49
7:A:1119:C:OP1	15:I:85:ARG:NH2	2.46	0.49
30:a:1378:A:O2'	30:a:1380:G:N7	2.46	0.49
42:m:67:PHE:O	42:m:71:ARG:HD2	2.13	0.48
15:I:52:LEU:HD11	15:I:63:LEU:HD11	1.95	0.48
7:A:1251:A:H2'	7:A:1252:A:O4'	2.14	0.47
30:a:793:A:OP2	30:a:2071:A:O2'	2.28	0.47
35:f:50:LEU:HD11	35:f:67:ILE:HD12	1.96	0.47
4:2:54:ASP:HB3	40:k:57:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:1125:G:C6	30:a:1126:A:N6	2.83	0.47
30:a:1266:G:O2'	30:a:2012:G:O6	2.30	0.47
7:A:1086:U:H3	7:A:1099:G:H22	1.62	0.47
30:a:657:U:H2'	30:a:658:U:C6	2.49	0.47
39:j:108:ARG:HH22	44:o:34:GLU:HA	1.80	0.47
19:M:11:ASP:HA	19:M:45:ILE:HB	1.96	0.47
30:a:1668:A:O2'	30:a:1674:G:N7	2.47	0.47
35:f:52:ASN:HB2	35:f:150:ARG:HH22	1.80	0.47
30:a:1932:A:H2'	30:a:1933:G:O4'	2.15	0.47
7:A:1126:U:P	16:J:7:ARG:HH22	2.38	0.47
30:a:608:A:H2'	30:a:609:A:C8	2.50	0.47
30:a:2063:C:O2	30:a:2450:A:N1	2.48	0.46
30:a:118:A:N3	30:a:178:G:H1'	2.30	0.46
30:a:1357:C:H2'	30:a:1358:G:O4'	2.15	0.46
30:a:1778:U:H2'	30:a:1784:A:N6	2.30	0.46
39:j:105:ARG:O	39:j:108:ARG:HG2	2.15	0.46
26:T:68:HIS:HD2	26:T:70:ASN:H	1.63	0.46
34:e:3:LEU:HB3	34:e:120:VAL:HG11	1.97	0.46
7:A:502:A:H2'	7:A:503:C:O4'	2.16	0.46
30:a:299:A:N1	30:a:322:A:O2'	2.46	0.46
30:a:2291:U:H2'	30:a:2292:U:C6	2.52	0.45
50:u:4:ILE:HG22	50:u:50:MET:HE1	1.98	0.45
30:a:569:U:H1'	30:a:947:A:O4'	2.17	0.45
30:a:588:U:H2'	30:a:589:U:C6	2.51	0.45
41:l:77:PRO:HG2	41:l:80:VAL:HG21	1.98	0.45
30:a:127:A:H5''	30:a:128:C:C6	2.51	0.45
30:a:723:C:H2'	30:a:724:U:O4'	2.16	0.45
30:a:2243:U:H2'	30:a:2244:U:C6	2.51	0.45
32:c:43:ARG:HA	32:c:48:ARG:O	2.15	0.45
30:a:586:A:N1	30:a:809:G:O2'	2.45	0.45
36:g:26:ILE:HG22	36:g:79:VAL:HG21	1.97	0.45
30:a:572:A:C2	30:a:2033:A:C2	3.05	0.45
30:a:1790:C:H2'	30:a:1791:A:C5	2.52	0.45
36:g:133:LEU:HD11	36:g:144:VAL:HG11	1.98	0.45
30:a:1197:G:H2'	30:a:1198:U:C6	2.52	0.45
30:a:2680:U:O2'	30:a:2681:C:H5'	2.17	0.44
30:a:572:A:H5''	30:a:573:U:OP2	2.18	0.44
30:a:2273:A:H2'	30:a:2274:A:C8	2.51	0.44
7:A:1324:A:H2'	7:A:1325:C:O4'	2.17	0.44
33:d:121:THR:HB	33:d:127:PHE:CD2	2.53	0.44
34:e:83:VAL:O	34:e:84:THR:C	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:X:14:A:H8	28:X:14:A:O5'	2.00	0.44
7:A:1530:G:N7	27:U:46:LYS:NZ	2.64	0.44
30:a:1433:A:H2'	30:a:1434:A:O4'	2.17	0.44
4:2:45:ARG:N	4:2:46:PRO:HD2	2.33	0.44
14:H:66:PHE:CD2	14:H:67:GLN:HG2	2.53	0.44
30:a:251:A:OP1	40:k:58:TYR:OH	2.31	0.44
55:z:43:ILE:HG22	55:z:49:TYR:HB2	2.00	0.44
5:3:19:ARG:NE	30:a:2756:U:OP2	2.50	0.44
7:A:736:C:OP1	24:R:61:ARG:NH1	2.43	0.43
30:a:1187:G:H5''	46:q:83:TYR:CE1	2.52	0.43
38:i:76:HIS:CE1	38:i:85:LYS:HB2	2.52	0.43
7:A:767:A:H2'	7:A:768:A:O4'	2.18	0.43
9:C:77:ILE:HA	9:C:84:VAL:HG23	2.00	0.43
7:A:542:G:H5'	10:D:39:GLY:HA3	2.00	0.43
30:a:477:A:H2'	30:a:478:A:C8	2.54	0.43
30:a:494:G:H4'	47:r:6:LYS:HB2	1.99	0.43
30:a:84:A:N1	30:a:98:G:O2'	2.47	0.43
30:a:828:U:H2'	30:a:829:A:C8	2.53	0.43
2:0:39:PHE:CZ	2:0:44:ARG:HA	2.53	0.43
30:a:26:G:C6	30:a:27:G:N1	2.87	0.43
30:a:479:A:N3	30:a:481:G:H5''	2.34	0.43
30:a:781:A:P	32:c:217:ARG:HH22	2.42	0.43
7:A:860:A:H2'	7:A:861:G:O4'	2.19	0.43
7:A:1189:U:OP1	20:N:98:LYS:NZ	2.52	0.43
8:B:28:LYS:N	8:B:29:PRO:CD	2.81	0.42
7:A:946:A:H2'	7:A:947:G:C8	2.54	0.42
7:A:1288:A:H2'	7:A:1289:A:O4'	2.19	0.42
30:a:1045:C:O2	30:a:1045:C:O4'	2.37	0.42
54:y:5:ILE:HG23	54:y:57:VAL:HG13	2.01	0.42
45:p:91:ASP:OD1	45:p:91:ASP:C	2.63	0.42
7:A:1273:C:H2'	7:A:1274:A:O4'	2.19	0.42
12:F:99:ALA:HB1	12:F:103:VAL:HG23	2.02	0.42
30:a:2038:G:H2'	30:a:2039:U:O4'	2.18	0.42
30:a:2522:U:O2'	30:a:2647:U:OP1	2.37	0.42
7:A:483:C:O2	22:P:13:LYS:NZ	2.53	0.42
30:a:55:G:O2'	30:a:127:A:N1	2.48	0.42
33:d:25:THR:HG21	33:d:193:VAL:HG22	2.01	0.42
3:1:39:ARG:NH2	30:a:468:G:N7	2.54	0.42
7:A:527:G7M:O2'	7:A:535:A:N1	2.47	0.42
30:a:577:G:O2'	30:a:1254:A:OP1	2.36	0.42
30:a:244:A:C2	30:a:255:A:C4	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:2591:C:H2'	30:a:2592:G:C8	2.55	0.42
30:a:2816:G:N3	30:a:2883:A:O2'	2.47	0.42
38:i:35:ARG:HB2	38:i:54:ILE:HD11	2.02	0.42
7:A:880:C:OP1	18:L:9:ARG:NH1	2.53	0.42
14:H:11:LEU:HD22	14:H:75:ILE:HD11	2.01	0.42
30:a:1370:C:H2'	30:a:1371:G:O4'	2.20	0.42
32:c:132:MET:HE1	32:c:184:VAL:HG21	2.02	0.42
7:A:1428:A:H2'	7:A:1429:A:O4'	2.20	0.41
30:a:117:G:C6	30:a:119:A:C6	3.08	0.41
30:a:2032:G:O2'	33:d:150:MEQ:OE1	2.32	0.41
55:z:49:TYR:HB3	55:z:54:VAL:HG11	2.01	0.41
7:A:49:U:O2	7:A:362:G:H1'	2.19	0.41
7:A:1004:A:H2'	7:A:1005:A:O4'	2.20	0.41
7:A:51:A:N7	7:A:114:U:O2'	2.53	0.41
15:I:21:ILE:HG12	15:I:63:LEU:HD22	2.02	0.41
30:a:639:U:H2'	30:a:640:C:C6	2.56	0.41
30:a:729:G:C6	32:c:207:LYS:HB2	2.55	0.41
30:a:813:U:H2'	30:a:814:C:C6	2.56	0.41
7:A:9:G:OP2	11:E:126:LYS:NZ	2.51	0.41
7:A:408:A:H2'	7:A:409:U:O4'	2.21	0.41
30:a:536:G:C6	30:a:537:G:C4	3.07	0.41
30:a:1141:U:H4'	30:a:1142:A:O4'	2.21	0.41
30:a:1881:C:H2'	30:a:1882:U:O4'	2.20	0.41
32:c:165:VAL:HG11	32:c:181:MET:HE1	2.03	0.41
30:a:493:G:H2'	30:a:494:G:O4'	2.20	0.41
30:a:1028:A:N6	30:a:1125:G:H2'	2.36	0.41
17:K:35:THR:HG22	17:K:41:ALA:HA	2.03	0.41
7:A:1356:G:H2'	7:A:1357:A:C8	2.55	0.41
30:a:415:A:C2	30:a:2409:G:C2	3.09	0.41
30:a:2400:G:N2	30:a:2417:C:C2	2.88	0.41
42:m:69:ARG:O	42:m:71:ARG:N	2.51	0.41
7:A:993:G:N3	7:A:993:G:H2'	2.36	0.41
7:A:1456:A:H2'	7:A:1457:G:O4'	2.21	0.41
10:D:102:VAL:HG13	10:D:107:PHE:HB2	2.02	0.41
30:a:471:A:H2'	30:a:472:A:O4'	2.21	0.41
30:a:690:G:H2'	30:a:691:C:O4'	2.21	0.41
30:a:340:A:O2'	34:e:162:ARG:NH1	2.54	0.41
30:a:993:G:N3	46:q:91:GLN:NE2	2.69	0.41
30:a:1604:C:O2'	30:a:1610:A:N1	2.51	0.41
36:g:37:LEU:HD13	36:g:68:ALA:HB1	2.03	0.41
18:L:110:ARG:HB3	18:L:119:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:a:460:A:H2'	30:a:461:C:O4'	2.21	0.40
30:a:1011:G:OP2	45:p:66:ASN:ND2	2.48	0.40
30:a:1365:A:O5'	52:w:28:ARG:NH2	2.39	0.40
30:a:1930:G:O2'	30:a:1968:G:O6	2.38	0.40
30:a:2850:A:N7	30:a:2868:A:O2'	2.47	0.40
29:Z:21:A:H61	29:Z:46:G:H2'	1.85	0.40
30:a:2579:C:H6	30:a:2579:C:O5'	2.05	0.40
30:a:2627:G:N2	30:a:2777:G:OP2	2.52	0.40
33:d:46:ARG:NH1	33:d:85:ALA:O	2.55	0.40
7:A:382:A:H2'	7:A:383:A:C8	2.56	0.40
7:A:918:A:H2'	7:A:919:A:O4'	2.21	0.40
7:A:933:G:OP2	13:G:3:ARG:HB2	2.21	0.40
7:A:1225:A:H2'	7:A:1226:C:C5	2.56	0.40
30:a:247:G:H4'	30:a:386:G:C5	2.56	0.40
30:a:379:G:O2'	30:a:2232:C:OP1	2.34	0.40
30:a:1197:G:H2'	30:a:1198:U:H6	1.87	0.40
30:a:2869:G:H2'	30:a:2870:C:O4'	2.22	0.40
36:g:103:ILE:HD12	36:g:131:ILE:HG21	2.04	0.40
7:A:620:C:H2'	7:A:621:A:O4'	2.21	0.40
7:A:789:U:O2'	7:A:791:G:N7	2.44	0.40
7:A:1526:G:N7	27:U:40:LYS:NZ	2.68	0.40
30:a:2520:C:C6	30:a:2567:G:H1'	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	V	89/470 (19%)	81 (91%)	8 (9%)	0	100	100
2	0	49/55 (89%)	48 (98%)	1 (2%)	0	100	100
3	1	43/46 (94%)	43 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	2	62/65 (95%)	58 (94%)	3 (5%)	1 (2%)	7	4
5	3	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
6	4	54/70 (77%)	46 (85%)	7 (13%)	1 (2%)	6	3
8	B	222/241 (92%)	216 (97%)	6 (3%)	0	100	100
9	C	204/233 (88%)	196 (96%)	8 (4%)	0	100	100
10	D	203/206 (98%)	199 (98%)	4 (2%)	0	100	100
11	E	154/167 (92%)	150 (97%)	4 (3%)	0	100	100
12	F	101/135 (75%)	100 (99%)	1 (1%)	0	100	100
13	G	150/179 (84%)	147 (98%)	3 (2%)	0	100	100
14	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
15	I	125/130 (96%)	119 (95%)	6 (5%)	0	100	100
16	J	96/103 (93%)	93 (97%)	2 (2%)	1 (1%)	12	10
17	K	112/129 (87%)	110 (98%)	2 (2%)	0	100	100
18	L	118/124 (95%)	112 (95%)	6 (5%)	0	100	100
19	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
20	N	98/101 (97%)	98 (100%)	0	0	100	100
21	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
22	P	79/82 (96%)	74 (94%)	5 (6%)	0	100	100
23	Q	77/84 (92%)	74 (96%)	3 (4%)	0	100	100
24	R	63/75 (84%)	63 (100%)	0	0	100	100
25	S	81/92 (88%)	80 (99%)	1 (1%)	0	100	100
26	T	83/87 (95%)	83 (100%)	0	0	100	100
27	U	68/71 (96%)	65 (96%)	3 (4%)	0	100	100
32	c	268/273 (98%)	257 (96%)	11 (4%)	0	100	100
33	d	205/209 (98%)	194 (95%)	11 (5%)	0	100	100
34	e	198/201 (98%)	187 (94%)	11 (6%)	0	100	100
35	f	175/179 (98%)	165 (94%)	10 (6%)	0	100	100
36	g	171/177 (97%)	149 (87%)	21 (12%)	1 (1%)	21	21
37	h	39/149 (26%)	34 (87%)	5 (13%)	0	100	100
38	i	138/142 (97%)	133 (96%)	5 (4%)	0	100	100
39	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
40	k	141/144 (98%)	130 (92%)	10 (7%)	1 (1%)	18	17
41	l	132/136 (97%)	126 (96%)	6 (4%)	0	100	100
42	m	116/127 (91%)	105 (90%)	11 (10%)	0	100	100
43	n	112/117 (96%)	104 (93%)	8 (7%)	0	100	100
44	o	111/115 (96%)	107 (96%)	4 (4%)	0	100	100
45	p	115/118 (98%)	110 (96%)	5 (4%)	0	100	100
46	q	99/103 (96%)	91 (92%)	8 (8%)	0	100	100
47	r	106/110 (96%)	101 (95%)	5 (5%)	0	100	100
48	s	90/100 (90%)	77 (86%)	12 (13%)	1 (1%)	11	8
49	t	86/104 (83%)	82 (95%)	4 (5%)	0	100	100
50	u	90/94 (96%)	84 (93%)	6 (7%)	0	100	100
51	v	81/85 (95%)	79 (98%)	2 (2%)	0	100	100
52	w	73/78 (94%)	70 (96%)	3 (4%)	0	100	100
53	x	55/63 (87%)	52 (94%)	3 (6%)	0	100	100
54	y	55/59 (93%)	52 (94%)	3 (6%)	0	100	100
55	z	53/57 (93%)	49 (92%)	4 (8%)	0	100	100
All	All	5523/6383 (86%)	5260 (95%)	257 (5%)	6 (0%)	49	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	4	40	CYS
16	J	57	VAL
48	s	27	SER
4	2	28	ASN
36	g	136	ALA
40	k	29	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	V	74/384 (19%)	74 (100%)	0	100	100
2	0	46/49 (94%)	46 (100%)	0	100	100
3	1	37/38 (97%)	37 (100%)	0	100	100
4	2	51/52 (98%)	50 (98%)	1 (2%)	48	59
5	3	34/34 (100%)	34 (100%)	0	100	100
6	4	53/62 (86%)	53 (100%)	0	100	100
8	B	186/199 (94%)	185 (100%)	1 (0%)	81	87
9	C	170/190 (90%)	167 (98%)	3 (2%)	51	63
10	D	172/173 (99%)	172 (100%)	0	100	100
11	E	119/126 (94%)	119 (100%)	0	100	100
12	F	90/116 (78%)	90 (100%)	0	100	100
13	G	125/147 (85%)	124 (99%)	1 (1%)	73	80
14	H	104/105 (99%)	103 (99%)	1 (1%)	68	77
15	I	105/107 (98%)	105 (100%)	0	100	100
16	J	86/90 (96%)	86 (100%)	0	100	100
17	K	88/98 (90%)	88 (100%)	0	100	100
18	L	101/103 (98%)	100 (99%)	1 (1%)	68	77
19	M	93/96 (97%)	92 (99%)	1 (1%)	65	75
20	N	83/84 (99%)	83 (100%)	0	100	100
21	O	76/77 (99%)	76 (100%)	0	100	100
22	P	65/65 (100%)	65 (100%)	0	100	100
23	Q	73/78 (94%)	73 (100%)	0	100	100
24	R	56/65 (86%)	56 (100%)	0	100	100
25	S	72/79 (91%)	72 (100%)	0	100	100
26	T	65/66 (98%)	65 (100%)	0	100	100
27	U	60/61 (98%)	60 (100%)	0	100	100
32	c	215/218 (99%)	214 (100%)	1 (0%)	81	87
33	d	163/163 (100%)	162 (99%)	1 (1%)	78	84
34	e	165/165 (100%)	161 (98%)	4 (2%)	43	54
35	f	148/150 (99%)	147 (99%)	1 (1%)	76	82
36	g	134/138 (97%)	130 (97%)	4 (3%)	36	45
37	h	32/114 (28%)	32 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	i	114/116 (98%)	114 (100%)	0	100	100
39	j	104/104 (100%)	103 (99%)	1 (1%)	68	77
40	k	102/103 (99%)	101 (99%)	1 (1%)	68	77
41	l	107/107 (100%)	107 (100%)	0	100	100
42	m	98/103 (95%)	98 (100%)	0	100	100
43	n	84/87 (97%)	83 (99%)	1 (1%)	63	74
44	o	98/100 (98%)	98 (100%)	0	100	100
45	p	89/90 (99%)	88 (99%)	1 (1%)	65	75
46	q	83/84 (99%)	82 (99%)	1 (1%)	63	74
47	r	91/93 (98%)	90 (99%)	1 (1%)	65	75
48	s	79/84 (94%)	78 (99%)	1 (1%)	61	72
49	t	74/85 (87%)	74 (100%)	0	100	100
50	u	77/78 (99%)	76 (99%)	1 (1%)	61	72
51	v	60/63 (95%)	60 (100%)	0	100	100
52	w	65/68 (96%)	65 (100%)	0	100	100
53	x	52/55 (94%)	52 (100%)	0	100	100
54	y	47/49 (96%)	46 (98%)	1 (2%)	47	58
55	z	46/48 (96%)	46 (100%)	0	100	100
All	All	4611/5209 (88%)	4582 (99%)	29 (1%)	76	84

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	2	31	HIS
8	B	87	CYS
9	C	75	ILE
9	C	82	GLU
9	C	84	VAL
13	G	133	THR
14	H	60	GLU
18	L	45	PRO
19	M	16	VAL
32	c	71	LYS
33	d	152	PRO
34	e	4	VAL
34	e	80	SER

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Mol	Chain	Res	Type
34	e	120	VAL
34	e	163	ASN
35	f	136	ILE
36	g	103	ILE
36	g	131	ILE
36	g	133	LEU
36	g	156	PRO
39	j	58	LEU
40	k	120	VAL
43	n	60	GLU
45	p	91	ASP
46	q	4	VAL
47	r	29	VAL
48	s	25	GLU
50	u	4	ILE
54	y	4	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
6	4	20	ASN
8	B	58	ASN
8	B	89	GLN
8	B	103	ASN
9	C	100	GLN
9	C	140	ASN
10	D	40	GLN
11	E	82	GLN
11	E	132	ASN
11	E	148	ASN
12	F	46	GLN
12	F	55	HIS
13	G	68	ASN
14	H	4	GLN
14	H	21	ASN
15	I	25	ASN
15	I	31	ASN
15	I	110	GLN
16	J	58	ASN
17	K	118	HIS
18	L	112	GLN
20	N	66	GLN

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Mol	Chain	Res	Type
22	P	59	HIS
23	Q	51	ASN
25	S	14	HIS
25	S	52	HIS
25	S	83	HIS
26	T	13	GLN
26	T	20	HIS
26	T	84	ASN
27	U	56	HIS
32	c	115	GLN
32	c	197	ASN
33	d	148	GLN
34	e	136	GLN
34	e	163	ASN
35	f	21	ASN
36	g	20	ASN
36	g	88	GLN
36	g	115	HIS
38	i	58	ASN
38	i	80	HIS
39	j	5	GLN
39	j	9	ASN
41	l	13	HIS
41	l	60	GLN
41	l	97	GLN
42	m	9	GLN
43	n	29	HIS
43	n	98	GLN
44	o	12	GLN
45	p	52	GLN
45	p	71	GLN
45	p	81	ASN
52	w	32	ASN
53	x	31	GLN
53	x	36	GLN
54	y	9	GLN
55	z	6	ASN

5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
28	X	5/136 (3%)	0	0
29	Z	71/73 (97%)	9 (12%)	2 (2%)
30	a	2747/2900 (94%)	345 (12%)	0
31	b	118/120 (98%)	15 (12%)	0
7	A	1496/1541 (97%)	173 (11%)	36 (2%)
All	All	4437/4770 (93%)	542 (12%)	38 (0%)

All (542) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	A	4	U
7	A	6	G
7	A	7	A
7	A	13	U
7	A	14	U
7	A	22	G
7	A	32	A
7	A	39	G
7	A	47	C
7	A	48	C
7	A	51	A
7	A	71	A
7	A	72	A
7	A	94	G
7	A	116	A
7	A	119	A
7	A	120	A
7	A	121	U
7	A	128	G
7	A	131	A
7	A	182	A
7	A	183	C
7	A	184	G
7	A	226	G
7	A	240	G
7	A	245	U
7	A	247	G
7	A	251	G
7	A	258	G
7	A	266	G
7	A	267	C

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Mol	Chain	Res	Type
7	A	280	C
7	A	289	G
7	A	319	G
7	A	321	A
7	A	328	C
7	A	329	A
7	A	347	G
7	A	352	C
7	A	354	G
7	A	367	U
7	A	368	U
7	A	372	C
7	A	406	G
7	A	410	G
7	A	411	A
7	A	413	G
7	A	414	A
7	A	417	G
7	A	421	U
7	A	423	G
7	A	429	U
7	A	451	A
7	A	453	G
7	A	457	G
7	A	458	U
7	A	462	G
7	A	479	U
7	A	484	G
7	A	485	U
7	A	486	U
7	A	494	G
7	A	511	C
7	A	518	C
7	A	532	A
7	A	533	A
7	A	547	A
7	A	559	A
7	A	572	A
7	A	573	A
7	A	576	C
7	A	577	G
7	A	579	A

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Mol	Chain	Res	Type
7	A	596	A
7	A	633	G
7	A	642	A
7	A	649	A
7	A	650	G
7	A	653	U
7	A	654	G
7	A	661	G
7	A	665	A
7	A	721	G
7	A	723	U
7	A	724	G
7	A	734	G
7	A	748	G
7	A	755	G
7	A	777	A
7	A	793	U
7	A	794	A
7	A	815	A
7	A	817	C
7	A	857	C
7	A	890	G
7	A	914	A
7	A	926	G
7	A	934	C
7	A	935	A
7	A	960	U
7	A	961	U
7	A	966	2MG
7	A	969	A
7	A	975	A
7	A	976	G
7	A	977	A
7	A	984	C
7	A	993	G
7	A	994	A
7	A	996	A
7	A	1004	A
7	A	1008	U
7	A	1020	G
7	A	1027	C
7	A	1034	G

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Mol	Chain	Res	Type
7	A	1036	A
7	A	1039	G
7	A	1065	U
7	A	1085	U
7	A	1094	G
7	A	1095	U
7	A	1101	A
7	A	1124	G
7	A	1125	U
7	A	1139	G
7	A	1159	U
7	A	1167	A
7	A	1171	A
7	A	1174	G
7	A	1184	G
7	A	1196	A
7	A	1197	A
7	A	1212	U
7	A	1213	A
7	A	1214	C
7	A	1225	A
7	A	1226	C
7	A	1227	A
7	A	1228	C
7	A	1238	A
7	A	1256	A
7	A	1257	A
7	A	1280	A
7	A	1287	A
7	A	1299	A
7	A	1300	G
7	A	1302	C
7	A	1317	C
7	A	1319	A
7	A	1320	C
7	A	1338	G
7	A	1346	A
7	A	1353	G
7	A	1363	A
7	A	1364	U
7	A	1368	A
7	A	1370	G

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Mol	Chain	Res	Type
7	A	1379	G
7	A	1397	C
7	A	1419	G
7	A	1429	A
7	A	1453	G
7	A	1492	A
7	A	1493	A
7	A	1494	G
7	A	1497	G
7	A	1503	A
7	A	1505	G
7	A	1506	U
7	A	1517	G
7	A	1529	G
7	A	1530	G
7	A	1534	A
29	Z	9	G
29	Z	13	C
29	Z	21	A
29	Z	46	G
29	Z	47	U
29	Z	48	C
29	Z	49	G
29	Z	58	A
29	Z	76	A
30	a	10	A
30	a	23	G
30	a	34	U
30	a	42	A
30	a	58	G
30	a	63	A
30	a	71	A
30	a	74	A
30	a	75	G
30	a	84	A
30	a	86	G
30	a	96	C
30	a	101	A
30	a	102	U
30	a	110	G
30	a	118	A
30	a	119	A

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Mol	Chain	Res	Type
30	a	120	U
30	a	139	U
30	a	140	C
30	a	142	A
30	a	163	C
30	a	165	A
30	a	181	A
30	a	196	A
30	a	197	A
30	a	199	A
30	a	200	U
30	a	215	G
30	a	216	A
30	a	221	A
30	a	222	A
30	a	248	G
30	a	264	C
30	a	265	A
30	a	272	A
30	a	278	A
30	a	285	G
30	a	289	G
30	a	304	U
30	a	310	A
30	a	311	A
30	a	322	A
30	a	329	G
30	a	330	A
30	a	361	G
30	a	362	A
30	a	386	G
30	a	404	A
30	a	405	U
30	a	411	G
30	a	412	A
30	a	451	U
30	a	454	A
30	a	455	C
30	a	481	G
30	a	491	G
30	a	496	G
30	a	501	A

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Mol	Chain	Res	Type
30	a	503	A
30	a	504	A
30	a	505	A
30	a	509	C
30	a	528	A
30	a	530	G
30	a	531	C
30	a	532	A
30	a	544	C
30	a	545	U
30	a	546	U
30	a	547	A
30	a	548	G
30	a	549	G
30	a	555	G
30	a	556	A
30	a	563	A
30	a	573	U
30	a	575	A
30	a	586	A
30	a	587	C
30	a	603	A
30	a	615	U
30	a	620	G
30	a	621	A
30	a	627	A
30	a	637	A
30	a	645	C
30	a	646	U
30	a	647	G
30	a	654	A
30	a	655	A
30	a	670	A
30	a	686	U
30	a	724	U
30	a	730	A
30	a	738	G
30	a	747	5MU
30	a	749	A
30	a	764	A
30	a	765	C
30	a	775	G

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Mol	Chain	Res	Type
30	a	776	G
30	a	777	G
30	a	782	A
30	a	784	G
30	a	785	G
30	a	805	G
30	a	812	C
30	a	827	U
30	a	828	U
30	a	846	U
30	a	847	U
30	a	856	G
30	a	859	G
30	a	869	G
30	a	881	G
30	a	883	G
30	a	884	U
30	a	888	C
30	a	890	C
30	a	891	G
30	a	895	U
30	a	896	A
30	a	897	C
30	a	898	C
30	a	907	G
30	a	910	A
30	a	914	G
30	a	931	U
30	a	932	U
30	a	946	C
30	a	961	C
30	a	962	G
30	a	974	G
30	a	975	A
30	a	983	A
30	a	984	A
30	a	985	C
30	a	996	A
30	a	1005	C
30	a	1012	U
30	a	1013	C
30	a	1022	G

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Mol	Chain	Res	Type
30	a	1026	G
30	a	1033	U
30	a	1045	C
30	a	1046	A
30	a	1047	G
30	a	1109	C
30	a	1110	G
30	a	1111	A
30	a	1112	G
30	a	1115	G
30	a	1116	G
30	a	1122	G
30	a	1128	G
30	a	1129	A
30	a	1130	U
30	a	1132	U
30	a	1133	A
30	a	1134	A
30	a	1135	C
30	a	1142	A
30	a	1143	A
30	a	1156	A
30	a	1171	G
30	a	1227	G
30	a	1248	G
30	a	1253	A
30	a	1256	G
30	a	1271	G
30	a	1272	A
30	a	1273	U
30	a	1284	A
30	a	1286	A
30	a	1287	A
30	a	1300	G
30	a	1301	A
30	a	1302	A
30	a	1352	U
30	a	1359	A
30	a	1365	A
30	a	1379	U
30	a	1383	A
30	a	1403	A

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Mol	Chain	Res	Type
30	a	1416	G
30	a	1417	C
30	a	1427	A
30	a	1428	C
30	a	1452	G
30	a	1453	A
30	a	1455	G
30	a	1460	U
30	a	1482	G
30	a	1493	C
30	a	1509	A
30	a	1510	G
30	a	1515	A
30	a	1533	C
30	a	1534	U
30	a	1535	A
30	a	1536	C
30	a	1537	G
30	a	1566	A
30	a	1569	A
30	a	1578	U
30	a	1583	A
30	a	1584	U
30	a	1585	C
30	a	1608	A
30	a	1609	A
30	a	1616	A
30	a	1647	U
30	a	1648	U
30	a	1649	G
30	a	1674	G
30	a	1715	G
30	a	1729	U
30	a	1730	C
30	a	1732	C
30	a	1733	G
30	a	1738	G
30	a	1750	G
30	a	1764	C
30	a	1773	A
30	a	1782	U
30	a	1783	A

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Mol	Chain	Res	Type
30	a	1800	C
30	a	1801	A
30	a	1807	G
30	a	1808	A
30	a	1816	C
30	a	1829	A
30	a	1848	A
30	a	1858	A
30	a	1870	C
30	a	1871	A
30	a	1872	A
30	a	1873	G
30	a	1906	G
30	a	1907	G
30	a	1913	A
30	a	1914	C
30	a	1929	G
30	a	1930	G
30	a	1937	A
30	a	1938	A
30	a	1955	U
30	a	1965	C
30	a	1967	C
30	a	1970	A
30	a	1971	U
30	a	1972	G
30	a	1982	U
30	a	1991	U
30	a	1993	U
30	a	2020	A
30	a	2023	C
30	a	2031	A
30	a	2033	A
30	a	2043	C
30	a	2055	C
30	a	2056	G
30	a	2060	A
30	a	2061	G
30	a	2062	A
30	a	2069	G7M
30	a	2198	A
30	a	2204	G

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Mol	Chain	Res	Type
30	a	2211	A
30	a	2212	A
30	a	2225	A
30	a	2238	G
30	a	2239	G
30	a	2268	A
30	a	2282	G
30	a	2283	C
30	a	2287	A
30	a	2288	A
30	a	2305	U
30	a	2308	G
30	a	2312	U
30	a	2319	G
30	a	2322	A
30	a	2324	U
30	a	2325	G
30	a	2333	A
30	a	2335	A
30	a	2347	C
30	a	2350	C
30	a	2361	G
30	a	2383	G
30	a	2385	C
30	a	2396	G
30	a	2402	U
30	a	2406	A
30	a	2424	C
30	a	2425	A
30	a	2429	G
30	a	2435	A
30	a	2441	U
30	a	2447	G
30	a	2448	A
30	a	2476	A
30	a	2478	A
30	a	2491	U
30	a	2492	U
30	a	2502	G
30	a	2505	G
30	a	2518	A
30	a	2525	G

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Mol	Chain	Res	Type
30	a	2529	G
30	a	2547	A
30	a	2554	U
30	a	2566	A
30	a	2567	G
30	a	2573	C
30	a	2575	C
30	a	2602	A
30	a	2609	U
30	a	2613	U
30	a	2629	U
30	a	2630	G
30	a	2663	G
30	a	2682	A
30	a	2689	U
30	a	2690	U
30	a	2714	G
30	a	2726	A
30	a	2744	G
30	a	2748	A
30	a	2757	A
30	a	2765	A
30	a	2778	A
30	a	2780	G
30	a	2791	G
30	a	2798	U
30	a	2799	A
30	a	2820	A
30	a	2821	A
30	a	2823	A
30	a	2884	U
30	a	2885	G
30	a	2893	A
30	a	2899	A
31	b	9	G
31	b	12	C
31	b	13	G
31	b	15	A
31	b	24	G
31	b	35	C
31	b	45	A
31	b	56	G

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Mol	Chain	Res	Type
31	b	67	G
31	b	88	C
31	b	89	U
31	b	90	C
31	b	99	A
31	b	102	G
31	b	109	A

All (38) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
7	A	13	U
7	A	70	U
7	A	119	A
7	A	183	C
7	A	196	A
7	A	199	A
7	A	413	G
7	A	484	G
7	A	485	U
7	A	532	A
7	A	547	A
7	A	641	U
7	A	653	U
7	A	733	G
7	A	776	G
7	A	793	U
7	A	827	U
7	A	858	G
7	A	884	U
7	A	992	U
7	A	993	G
7	A	1035	A
7	A	1045	C
7	A	1046	A
7	A	1109	C
7	A	1124	G
7	A	1139	G
7	A	1204	A
7	A	1211	U
7	A	1212	U
7	A	1213	A

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Mol	Chain	Res	Type
7	A	1225	A
7	A	1319	A
7	A	1320	C
7	A	1452	C
7	A	1505	G
29	Z	46	G
29	Z	48	C

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

39 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	$\# Z > 2$
7	MA6	A	1518	7	23,26,27	0.46	0	34,38,41	0.71	1 (2%)
7	PSU	A	516	58,7	18,21,22	1.08	2 (11%)	22,30,33	0.65	0
7	2MG	A	1516	7	23,26,27	0.43	0	32,38,41	0.54	0
7	MA6	A	1519	7	23,26,27	0.68	1 (4%)	34,38,41	0.89	2 (5%)
7	4OC	A	1402	7	20,23,24	0.39	0	26,32,35	0.62	0
18	D2T	L	89	18	7,9,10	1.10	1 (14%)	6,11,13	1.74	3 (50%)
30	2MA	a	2503	58,30	22,25,26	1.04	3 (13%)	33,37,40	1.14	3 (9%)
41	4D4	l	81	41	9,11,12	0.62	0	8,13,15	0.55	0
30	H2U	a	2449	30	18,21,22	0.61	0	21,30,33	0.76	0
30	1MG	a	745	30	22,26,27	0.63	0	33,39,42	0.54	0
30	5MU	a	747	30	19,22,23	0.31	0	28,32,35	0.38	0
30	PSU	a	2605	30	18,21,22	0.99	1 (5%)	22,30,33	0.84	0
30	6MZ	a	2030	30	22,25,26	0.58	0	30,36,39	0.62	0
30	PSU	a	2604	30	18,21,22	0.96	1 (5%)	22,30,33	0.90	1 (4%)
30	6MZ	a	1618	30	22,25,26	0.45	0	30,36,39	0.61	0
30	2MG	a	1835	30	23,26,27	0.38	0	32,38,41	0.51	0
30	3TD	a	1915	30	18,22,23	1.01	1 (5%)	22,32,35	0.66	0
30	PSU	a	1911	30	18,21,22	0.82	1 (5%)	22,30,33	0.62	0
30	PSU	a	746	58,30	18,21,22	0.96	1 (5%)	22,30,33	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	IAS	K	119	17	6,7,8	0.96	0	6,8,10	0.93	0
30	PSU	a	2457	30	18,21,22	0.94	1 (5%)	22,30,33	0.63	0
30	2MG	a	2445	30	23,26,27	0.58	0	32,38,41	0.51	0
7	5MC	A	967	7	18,22,23	0.42	0	26,32,35	0.79	2 (7%)
30	PSU	a	955	30	18,21,22	0.84	1 (5%)	22,30,33	0.69	0
30	5MC	a	1962	30	18,22,23	0.40	0	26,32,35	0.60	0
41	MS6	l	82	41	5,7,8	0.29	0	2,7,9	0.22	0
7	UR3	A	1498	7	19,22,23	0.44	0	26,32,35	0.68	1 (3%)
7	G7M	A	527	7	23,26,27	0.71	1 (4%)	35,39,42	0.67	1 (2%)
30	OMU	a	2552	30	19,22,23	0.33	0	26,31,34	0.49	0
30	G7M	a	2069	30	23,26,27	0.60	1 (4%)	35,39,42	0.71	0
7	5MC	A	1407	7	18,22,23	0.40	0	26,32,35	0.73	0
30	5MU	a	1939	30	19,22,23	0.48	0	28,32,35	0.40	0
30	OMG	a	2251	29,30	23,26,27	0.31	0	33,38,41	0.45	0
30	PSU	a	1917	30	18,21,22	0.91	1 (5%)	22,30,33	0.67	0
30	PSU	a	2504	30	18,21,22	0.96	1 (5%)	22,30,33	0.75	0
30	PSU	a	2580	58,30	18,21,22	1.10	1 (5%)	22,30,33	0.77	1 (4%)
33	MEQ	d	150	33	8,9,10	0.56	0	5,10,12	0.95	0
30	OMC	a	2498	58,30	19,22,23	0.50	0	26,31,34	0.52	0
7	2MG	A	966	7	23,26,27	0.46	0	32,38,41	0.46	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
7	MA6	A	1518	7	-	0/11/29/30	0/3/3/3
7	PSU	A	516	58,7	-	0/7/25/26	0/2/2/2
7	2MG	A	1516	7	-	0/9/27/28	0/3/3/3
7	MA6	A	1519	7	-	2/11/29/30	0/3/3/3
7	4OC	A	1402	7	-	0/9/29/30	0/2/2/2
18	D2T	L	89	18	-	5/7/12/14	-
30	2MA	a	2503	58,30	-	2/7/25/26	0/3/3/3
41	4D4	l	81	41	-	1/11/12/14	-
30	H2U	a	2449	30	-	0/7/38/39	0/2/2/2
30	1MG	a	745	30	-	0/7/25/26	0/3/3/3
30	5MU	a	747	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2605	30	-	0/7/25/26	0/2/2/2
30	6MZ	a	2030	30	-	2/9/27/28	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	PSU	a	2604	30	-	0/7/25/26	0/2/2/2
30	6MZ	a	1618	30	-	0/9/27/28	0/3/3/3
30	2MG	a	1835	30	-	0/9/27/28	0/3/3/3
30	3TD	a	1915	30	-	0/7/25/26	0/2/2/2
30	PSU	a	1911	30	-	0/7/25/26	0/2/2/2
30	PSU	a	746	58,30	-	3/7/25/26	0/2/2/2
17	IAS	K	119	17	-	0/7/7/8	-
30	PSU	a	2457	30	-	0/7/25/26	0/2/2/2
30	2MG	a	2445	30	-	0/9/27/28	0/3/3/3
7	5MC	A	967	7	-	0/7/25/26	0/2/2/2
30	PSU	a	955	30	-	0/7/25/26	0/2/2/2
30	5MC	a	1962	30	-	0/7/25/26	0/2/2/2
41	MS6	l	82	41	-	1/4/6/8	-
7	UR3	A	1498	7	-	0/7/25/26	0/2/2/2
7	G7M	A	527	7	-	1/7/25/26	0/3/3/3
30	OMU	a	2552	30	-	0/9/27/28	0/2/2/2
30	G7M	a	2069	30	-	1/7/25/26	0/3/3/3
7	5MC	A	1407	7	-	0/7/25/26	0/2/2/2
30	5MU	a	1939	30	-	0/7/25/26	0/2/2/2
30	OMG	a	2251	29,30	-	0/9/27/28	0/3/3/3
30	PSU	a	1917	30	-	0/7/25/26	0/2/2/2
30	PSU	a	2504	30	-	2/7/25/26	0/2/2/2
30	PSU	a	2580	58,30	-	0/7/25/26	0/2/2/2
33	MEQ	d	150	33	-	3/8/9/11	-
30	OMC	a	2498	58,30	-	0/9/27/28	0/2/2/2
7	2MG	A	966	7	-	0/9/27/28	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2580	PSU	C6-C5	4.25	1.40	1.35
30	a	1915	3TD	C6-C5	3.87	1.39	1.35
30	a	2504	PSU	C6-C5	3.66	1.39	1.35
30	a	746	PSU	C6-C5	3.58	1.39	1.35
30	a	2457	PSU	C6-C5	3.57	1.39	1.35
30	a	2604	PSU	C6-C5	3.26	1.39	1.35
30	a	1917	PSU	C6-C5	3.24	1.39	1.35
30	a	2605	PSU	C6-C5	3.11	1.38	1.35
7	A	516	PSU	C6-C5	2.92	1.38	1.35
30	a	1911	PSU	C6-C5	2.88	1.38	1.35
30	a	955	PSU	C6-C5	2.80	1.38	1.35
7	A	516	PSU	C4-C5	-2.57	1.36	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a	2503	2MA	C6-N6	-2.55	1.27	1.34
7	A	1519	MA6	O5'-C5'	-2.33	1.39	1.44
7	A	527	G7M	C8-N7	2.26	1.37	1.33
30	a	2503	2MA	C2-N1	2.12	1.37	1.34
18	L	89	D2T	OD2-CG	-2.11	1.23	1.30
30	a	2069	G7M	C8-N7	2.04	1.36	1.33
30	a	2503	2MA	C2-N3	2.04	1.37	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1519	MA6	C2-N1-C6	3.12	119.13	111.75
30	a	2503	2MA	C5-C4-N3	-3.03	123.78	127.19
7	A	1518	MA6	C2-N1-C6	2.91	118.62	111.75
30	a	2503	2MA	CM2-C2-N1	2.50	121.06	117.15
7	A	967	5MC	O3'-C3'-C4'	-2.40	104.11	111.05
30	a	2503	2MA	N3-C2-N1	-2.36	121.39	125.72
7	A	1519	MA6	C2'-C3'-C4'	-2.31	98.15	102.64
18	L	89	D2T	OD1-CG-CB	-2.23	117.77	122.44
18	L	89	D2T	OD2-CG-CB	2.23	117.96	113.15
30	a	2604	PSU	C2'-C3'-C4'	-2.22	98.33	102.64
18	L	89	D2T	O-C-CA	-2.21	119.00	124.78
7	A	1498	UR3	C6-N1-C2	-2.16	119.85	121.79
30	a	2580	PSU	C3'-C2'-C1'	2.11	104.10	101.64
7	A	967	5MC	O3'-C3'-C2'	2.09	118.57	111.82
7	A	527	G7M	N9-C8-N7	-2.00	107.26	112.21

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	L	89	D2T	CG-CB-SB-CB1
18	L	89	D2T	CA-CB-CG-OD1
18	L	89	D2T	CA-CB-CG-OD2
30	a	746	PSU	C2'-C1'-C5-C4
30	a	746	PSU	C2'-C1'-C5-C6
30	a	746	PSU	O4'-C1'-C5-C6
30	a	2030	6MZ	O4'-C4'-C5'-O5'
30	a	2030	6MZ	C3'-C4'-C5'-O5'
33	d	150	MEQ	OE1-CD-CG-CB
33	d	150	MEQ	NE2-CD-CG-CB
7	A	1519	MA6	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
33	d	150	MEQ	OE1-CD-NE2-CE
30	a	2504	PSU	O4'-C4'-C5'-O5'
7	A	527	G7M	C3'-C4'-C5'-O5'
30	a	2069	G7M	O4'-C4'-C5'-O5'
7	A	1519	MA6	C3'-C4'-C5'-O5'
18	L	89	D2T	CA-CB-SB-CB1
18	L	89	D2T	SB-CB-CG-OD2
30	a	2504	PSU	C3'-C4'-C5'-O5'
41	l	82	MS6	CB-CG-SD-CE
30	a	2503	2MA	O4'-C1'-N9-C8
30	a	2503	2MA	O4'-C4'-C5'-O5'
41	l	81	4D4	O-C-CA-CB

There are no ring outliers.

6 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1402	4OC	1	0
30	a	2030	6MZ	1	0
30	a	2604	PSU	1	0
7	A	527	G7M	1	0
30	a	1939	5MU	1	0
33	d	150	MEQ	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 315 ligands modelled in this entry, 314 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
57	A1JA7	A	1601	-	58,58,58	0.57	0	79,84,84	1.10	4 (5%)

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
57	A1JA7	A	1601	-	-	7/34/114/114	0/4/4/4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	A	1601	A1JA7	O12-C16-N1	4.38	115.88	108.01
57	A	1601	A1JA7	C18-O12-C16	-3.01	108.44	112.52
57	A	1601	A1JA7	O14-C20-C18	-2.94	102.32	108.22
57	A	1601	A1JA7	C11-C24-N5	-2.48	106.79	110.91

There are no chirality outliers.

All (7) torsion outliers are listed below:

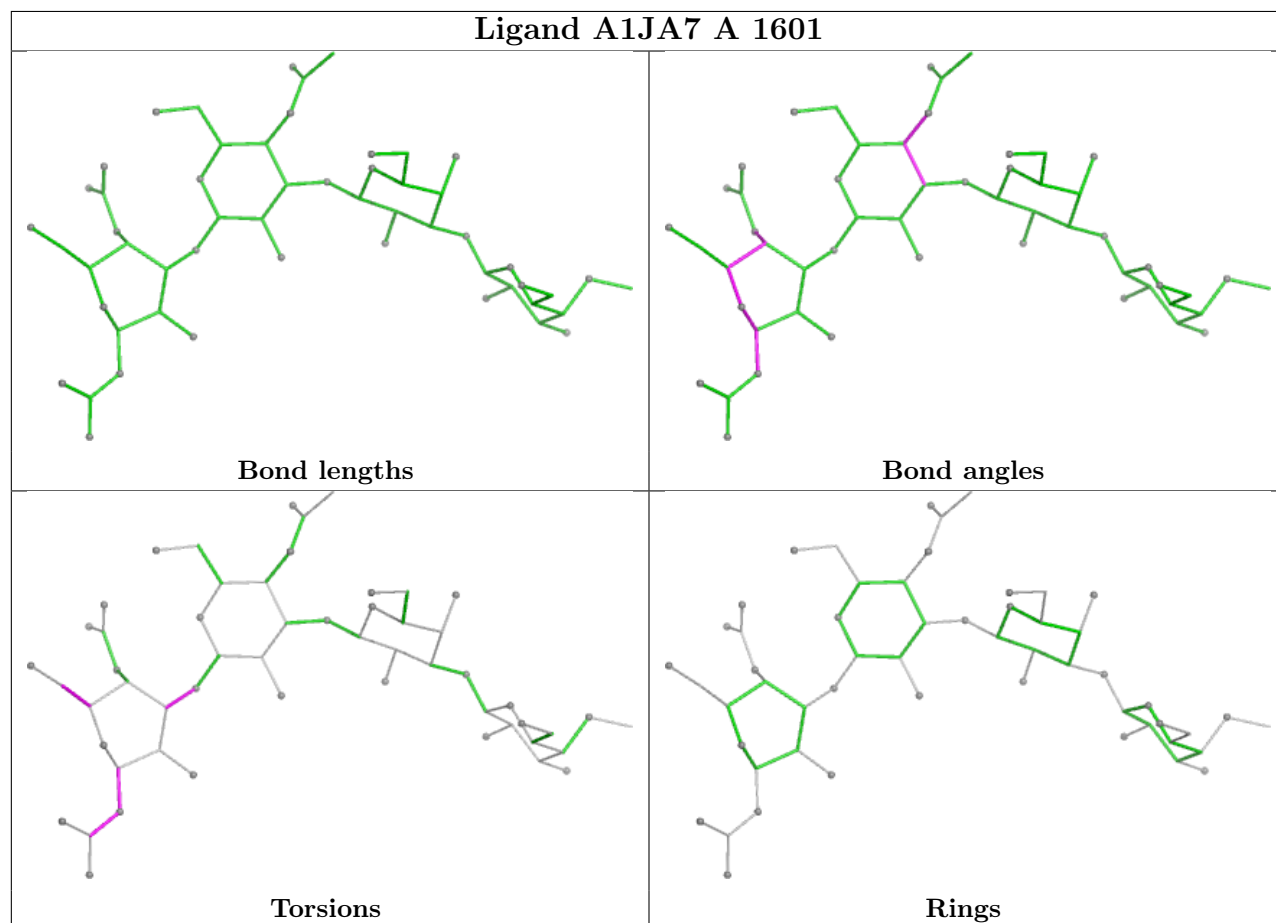
Mol	Chain	Res	Type	Atoms
57	A	1601	A1JA7	O12-C16-N1-C17
57	A	1601	A1JA7	O12-C18-C19-O13
57	A	1601	A1JA7	C20-C18-C19-O13
57	A	1601	A1JA7	C20-C14-O10-C13
57	A	1601	A1JA7	C15-C14-O10-C13
57	A	1601	A1JA7	N2-C17-N1-C16
57	A	1601	A1JA7	N3-C17-N1-C16

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
30	a	1
29	Z	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	a	1172:C	O3'	1177:G	P	16.00
1	Z	15:G	O3'	18:G	P	9.28

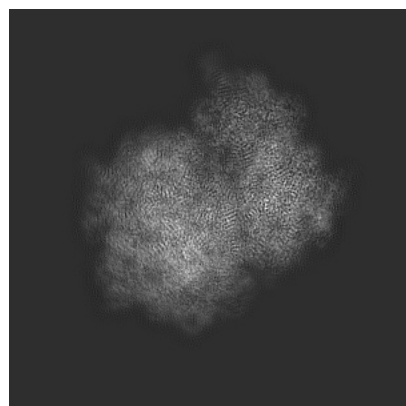
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53311. These allow visual inspection of the internal detail of the map and identification of artifacts.

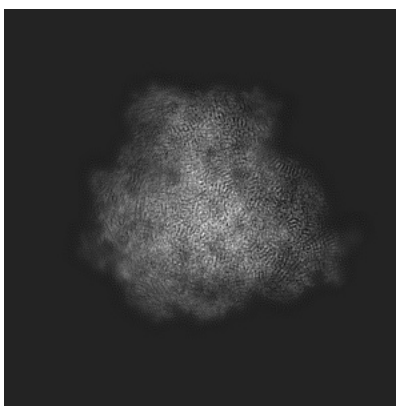
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

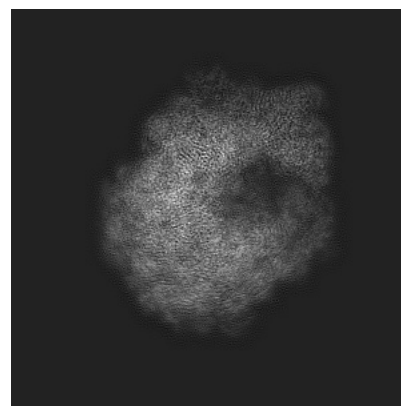
6.1.1 Primary map



X

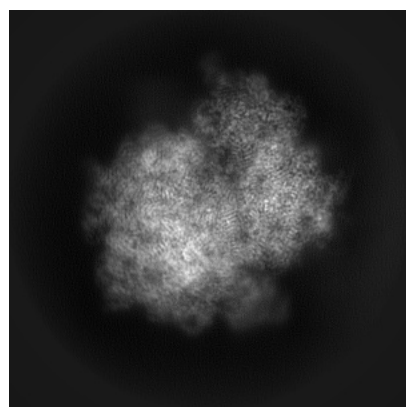


Y

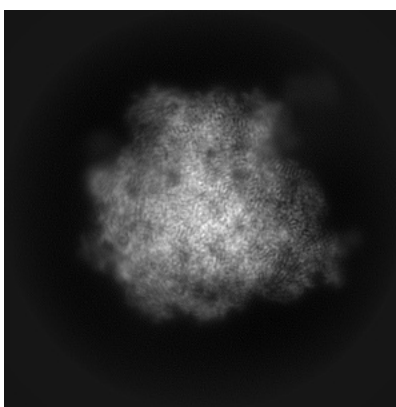


Z

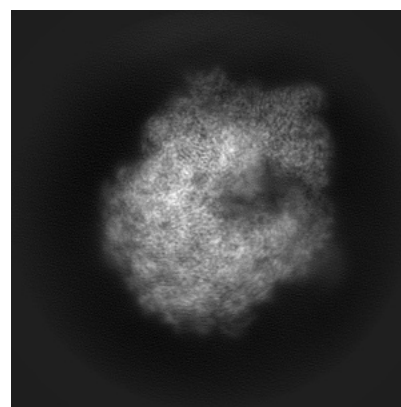
6.1.2 Raw map



X



Y

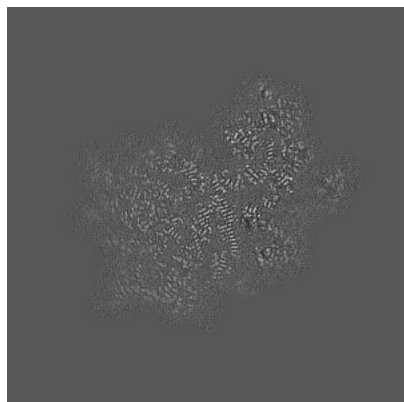


Z

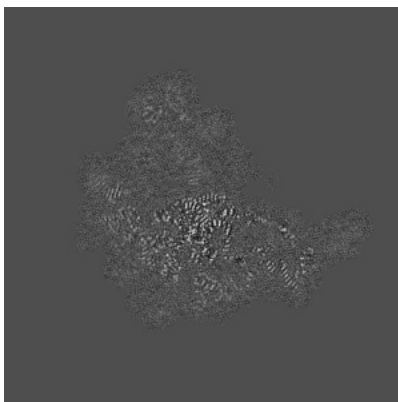
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

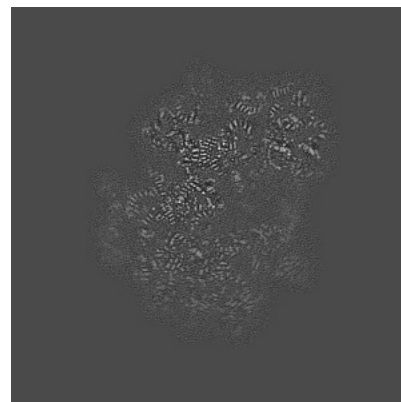
6.2.1 Primary map



X Index: 216

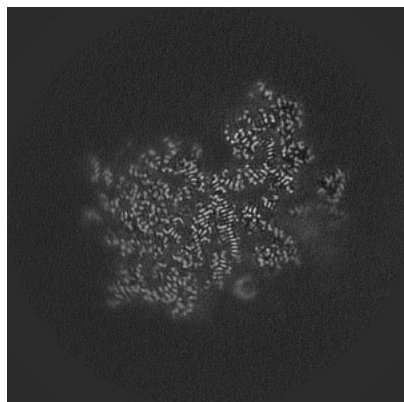


Y Index: 216

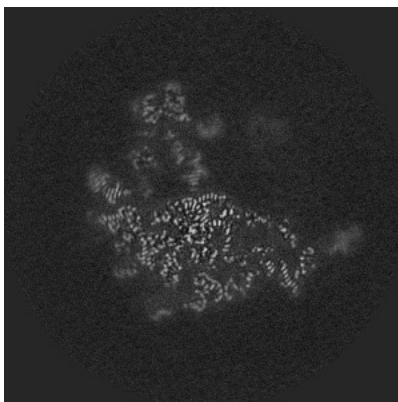


Z Index: 216

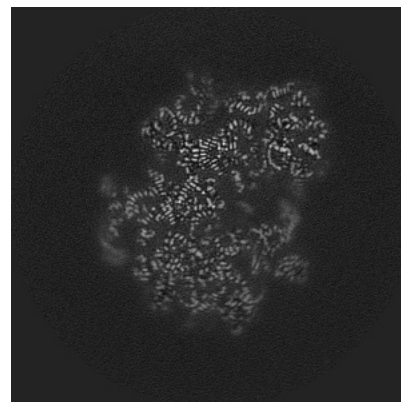
6.2.2 Raw map



X Index: 216



Y Index: 216

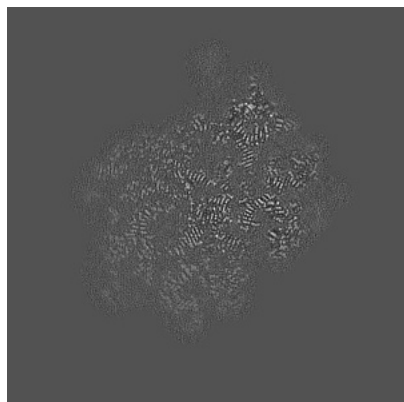


Z Index: 216

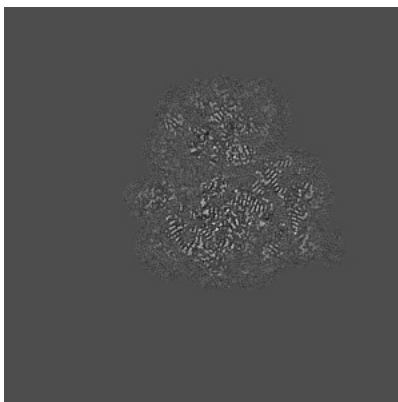
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

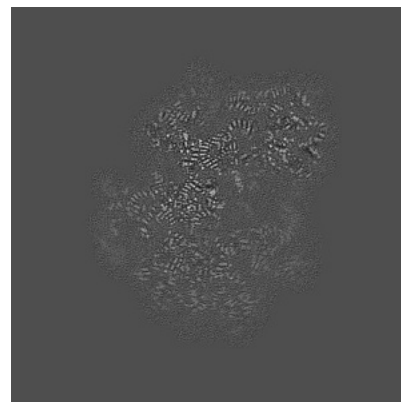
6.3.1 Primary map



X Index: 187

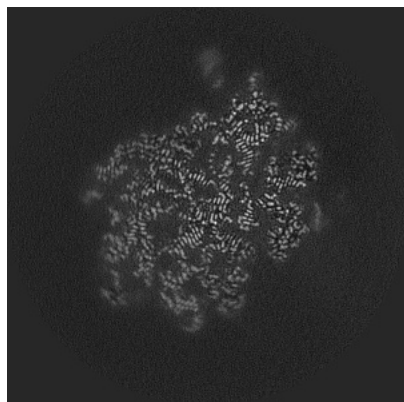


Y Index: 285

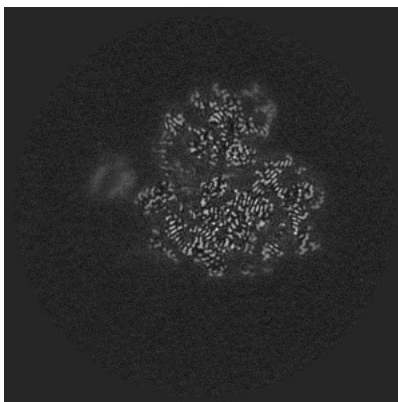


Z Index: 215

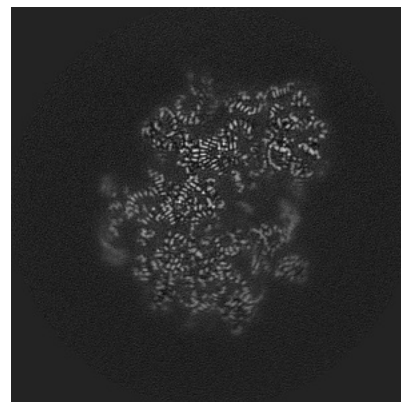
6.3.2 Raw map



X Index: 186



Y Index: 285

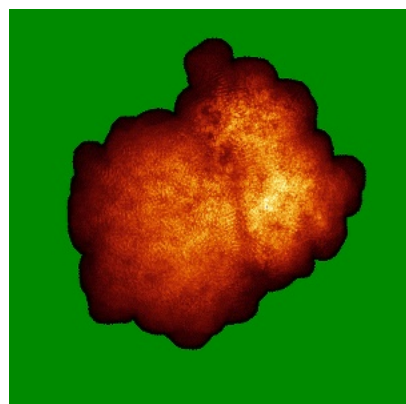


Z Index: 216

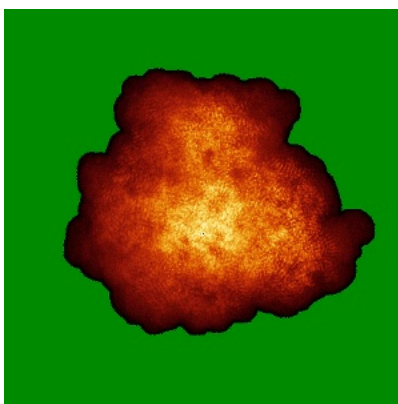
The images above show the largest variance slices of the map in three orthogonal directions.

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

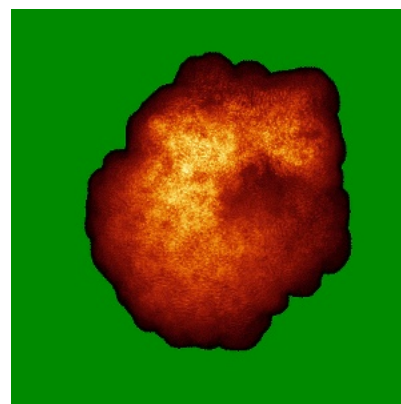
6.4.1 Primary map



X

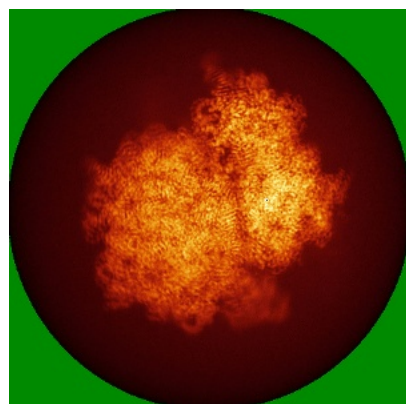


Y

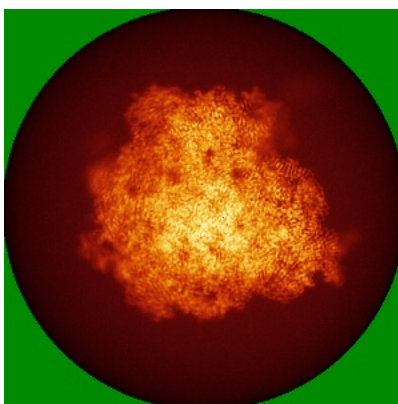


Z

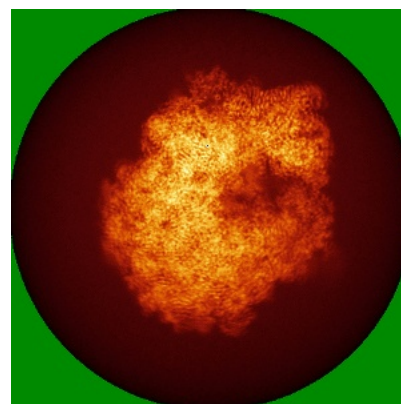
6.4.2 Raw map



X



Y



Z

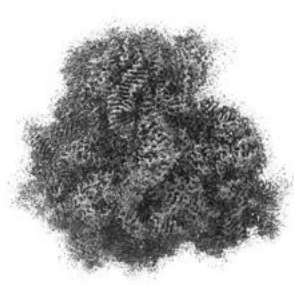
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



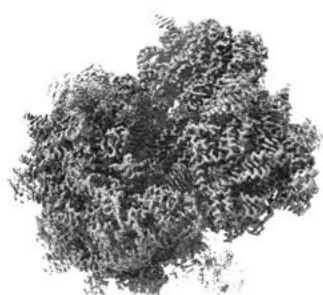
Y



Z

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

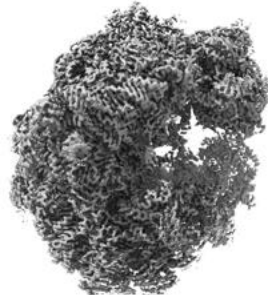
6.5.2 Raw map



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.

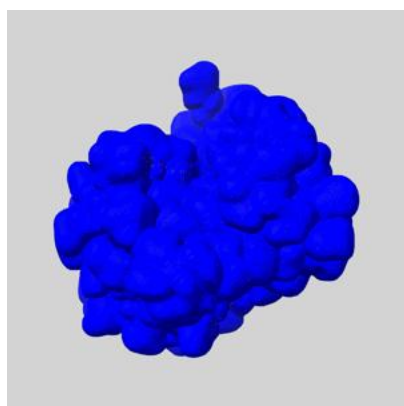
6.6 Mask visualisation [i](#)

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

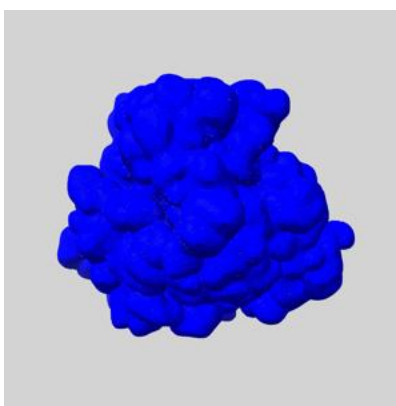
A mask typically either:

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

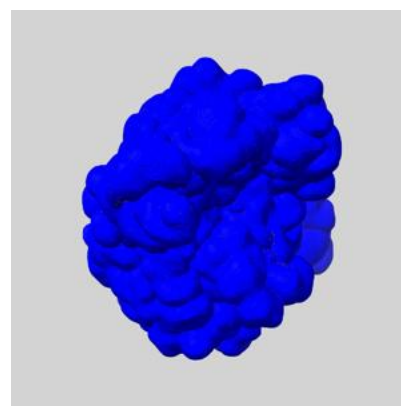
6.6.1 emd_53311_msk_1.map [i](#)



X

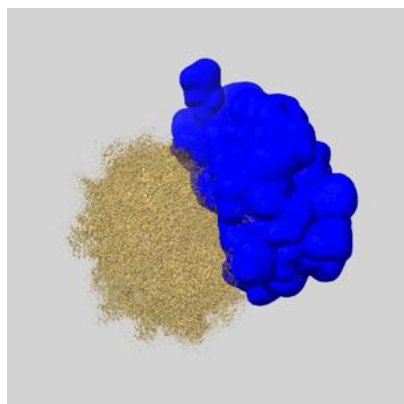


Y

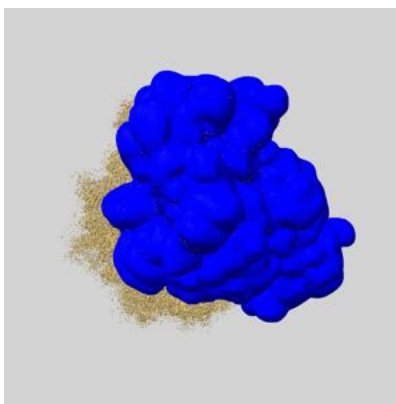


Z

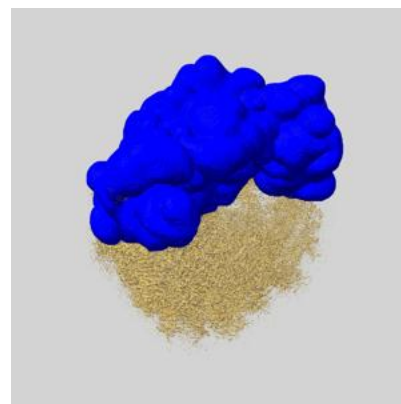
6.6.2 emd_53311_msk_2.map [i](#)



X



Y

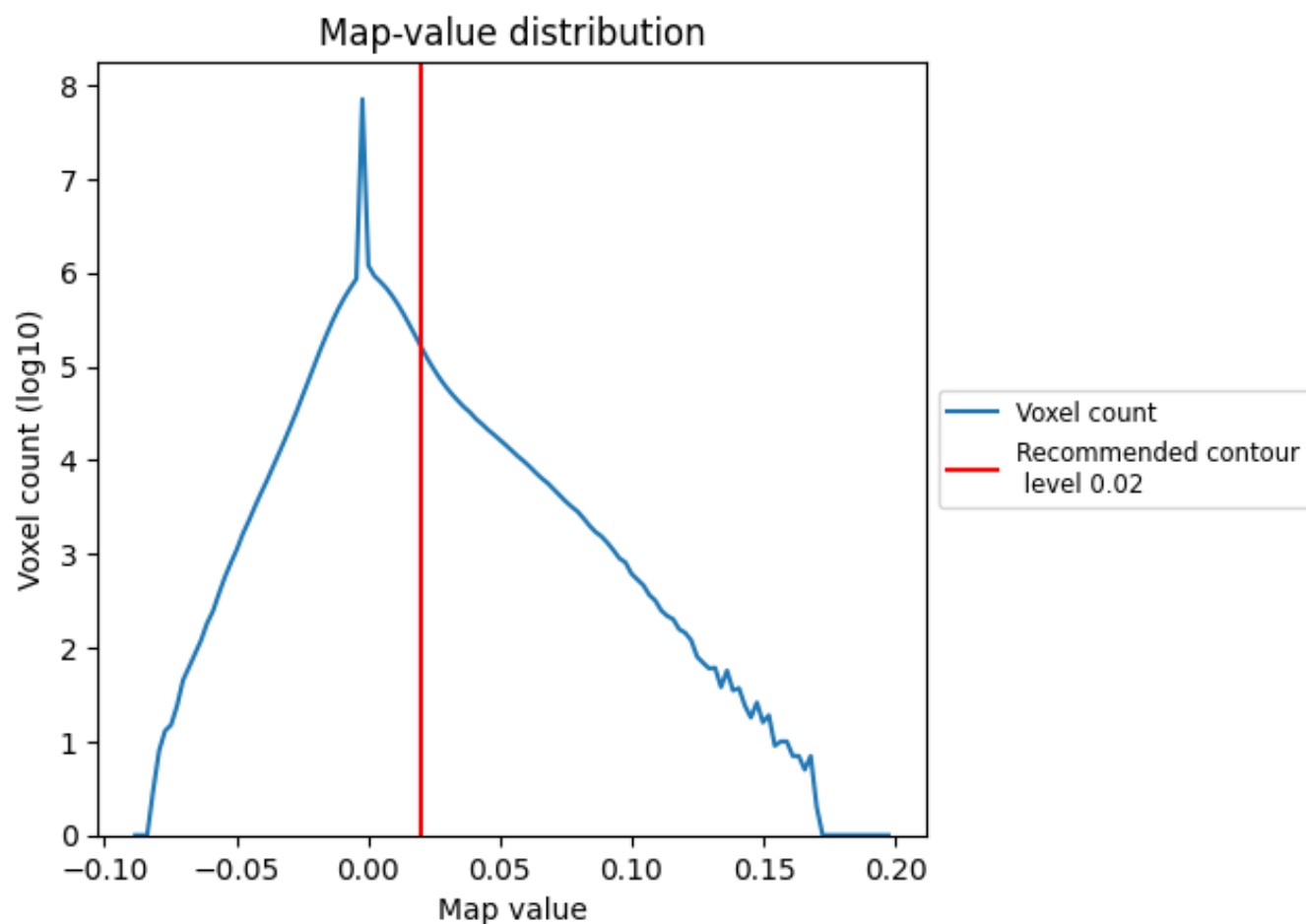


Z

7 Map analysis [i](#)

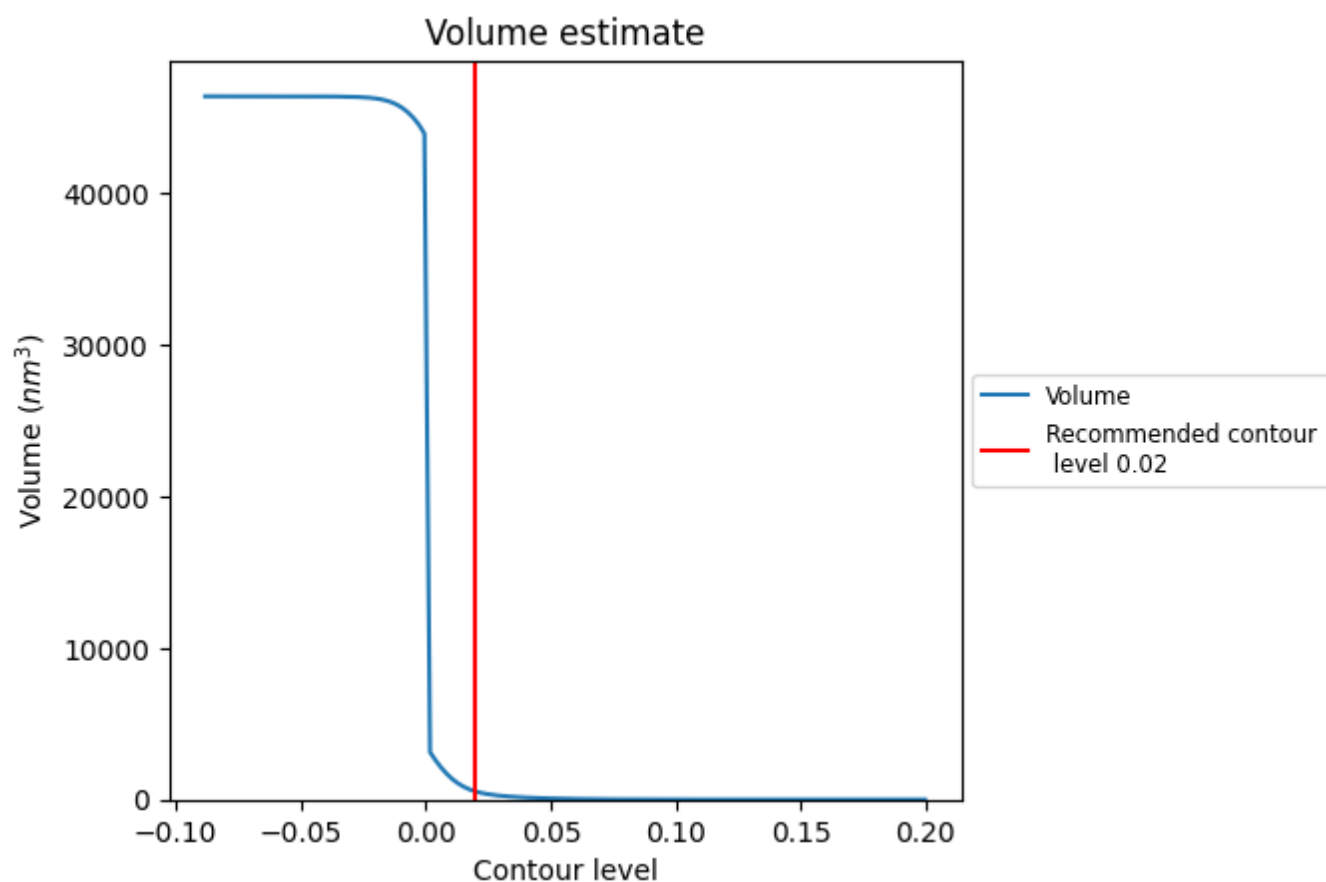
This section contains the results of statistical analysis of the map.

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.

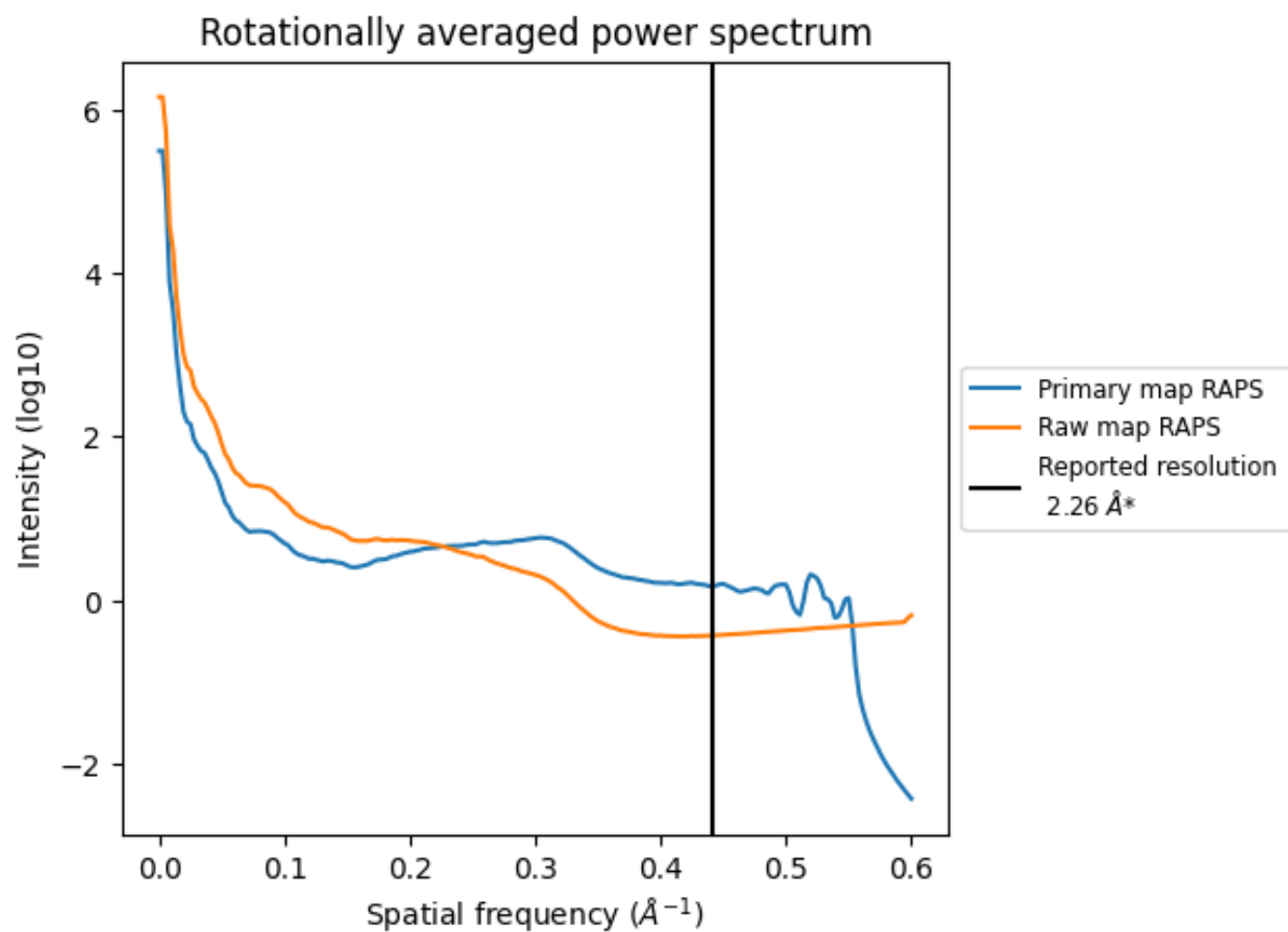
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 532 nm^3 ; this corresponds to an approximate mass of 481 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 ⓘ

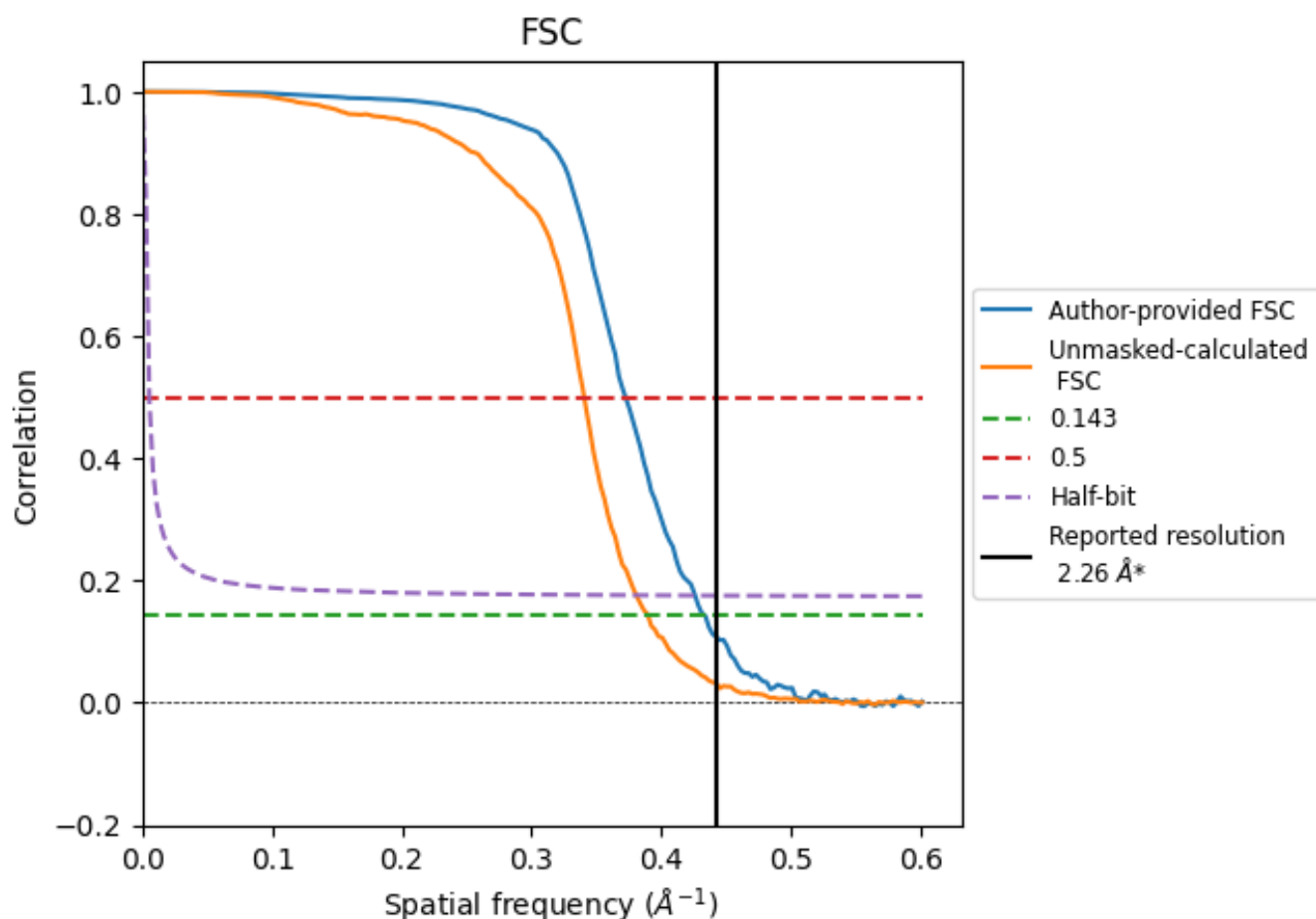


*Reported resolution corresponds to spatial frequency of 0.442 Å⁻¹

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 0.442 $\text{\AA}^{-1}$

8.2 Resolution estimates

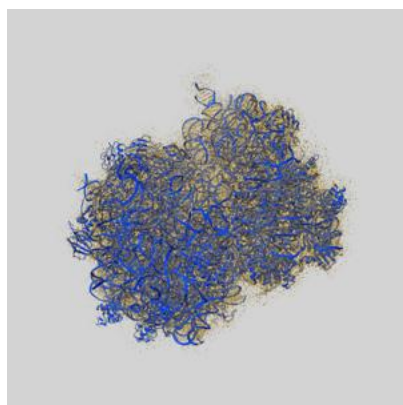
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.26	-	-
Author-provided FSC curve	2.31	2.69	2.35
Unmasked-calculated*	2.57	2.94	2.63

*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 2.57 differs from the reported value 2.26 by more than 10 %

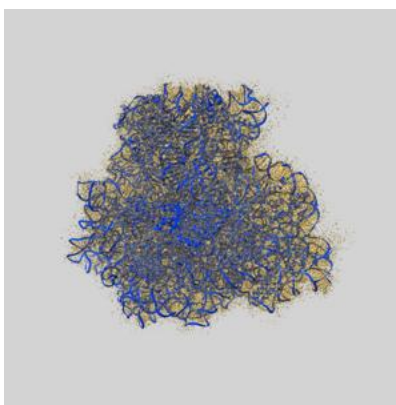
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53311 and PDB model 9QQQ. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

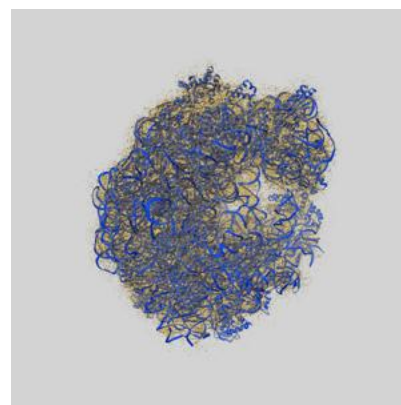
9.1 Map-model overlay [i](#)



X



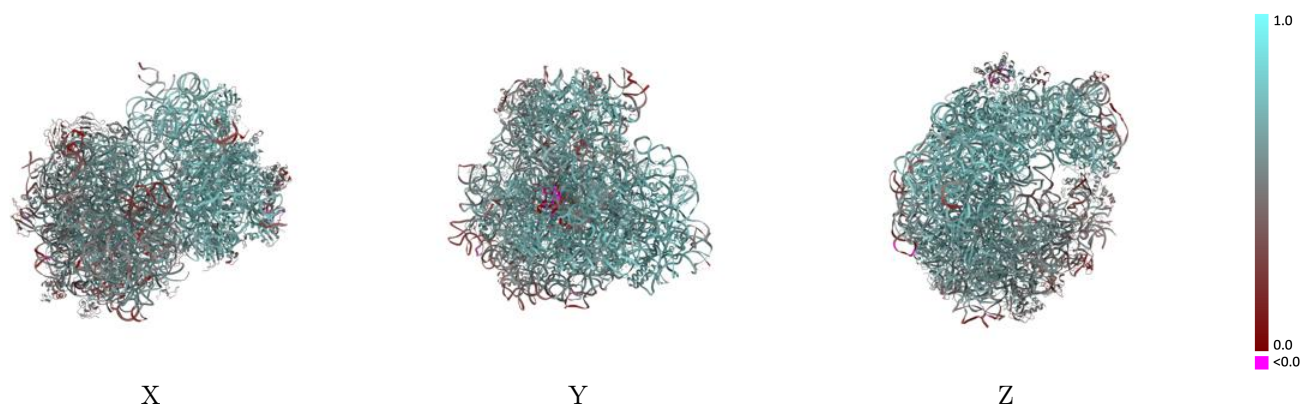
Y



Z

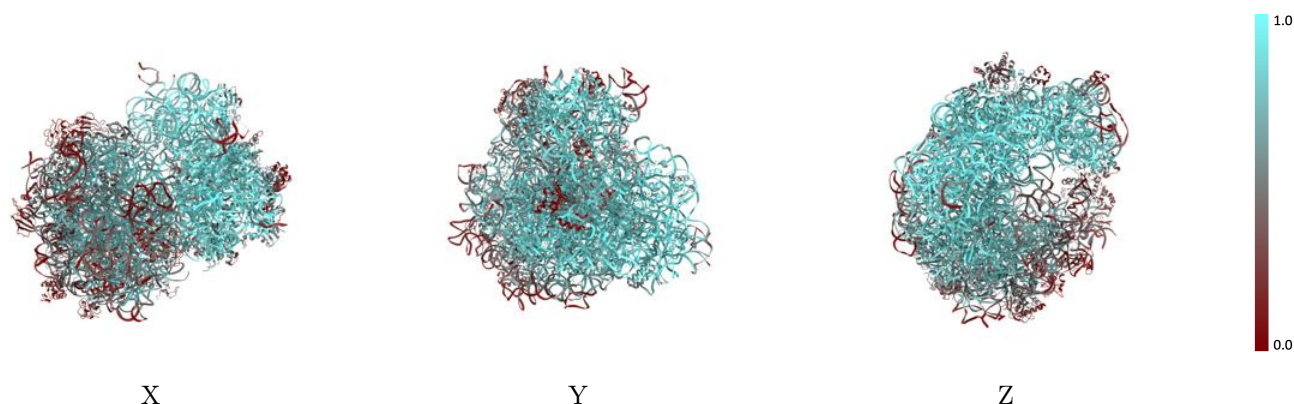
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



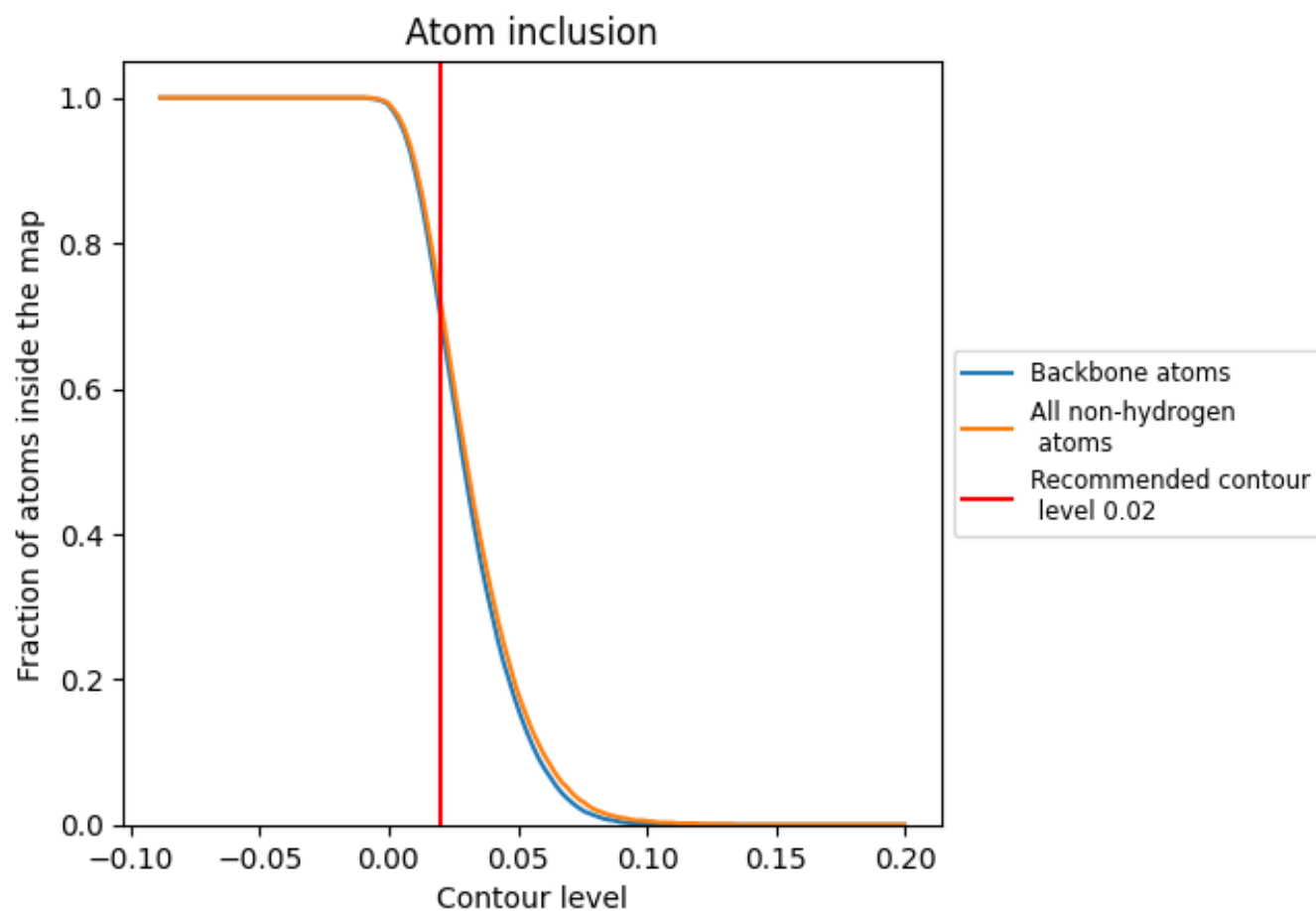
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 70% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7220	 0.6170
0	 0.4670	 0.5450
1	 0.8960	 0.6950
2	 0.7110	 0.6310
3	 0.5080	 0.5430
4	 0.3090	 0.4490
A	 0.9080	 0.6990
B	 0.5830	 0.5670
C	 0.7880	 0.6530
D	 0.8150	 0.6650
E	 0.8630	 0.6910
F	 0.7530	 0.6350
G	 0.6760	 0.5980
H	 0.8800	 0.7070
I	 0.7960	 0.6550
J	 0.5930	 0.5670
K	 0.8580	 0.6910
L	 0.9030	 0.7170
M	 0.7530	 0.6400
N	 0.8760	 0.6880
O	 0.8380	 0.6820
P	 0.8890	 0.7110
Q	 0.7730	 0.6450
R	 0.8520	 0.6880
S	 0.7970	 0.6540
T	 0.8600	 0.7010
U	 0.5420	 0.5230
V	 0.0280	 0.1360
X	 0.8450	 0.6550
Z	 0.5400	 0.5100
a	 0.7190	 0.6040
b	 0.4400	 0.4830
c	 0.8750	 0.7120
d	 0.6730	 0.6280
e	 0.3450	 0.4930



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f	 0.3440	 0.4710
g	 0.1760	 0.3990
h	 0.3870	 0.4980
i	 0.4960	 0.5440
j	 0.8140	 0.6820
k	 0.4690	 0.5490
l	 0.5450	 0.5580
m	 0.7550	 0.6530
n	 0.2730	 0.4360
o	 0.7790	 0.6650
p	 0.5560	 0.5790
q	 0.3080	 0.4660
r	 0.5600	 0.5850
s	 0.3740	 0.4810
t	 0.1390	 0.4070
u	 0.2130	 0.4330
v	 0.4920	 0.5530
w	 0.6210	 0.5940
x	 0.1510	 0.3820
y	 0.3770	 0.4870
z	 0.5930	 0.5830