



Full wwPDB EM Validation Report ⓘ

Jul 14, 2024 – 04:33 pm BST

PDB ID : 8BUU
EMDB ID : EMD-16246
Title : ARE-ABCF VmlR2 bound to a 70S ribosome
Authors : Crowe-McAuliffe, C.; Wilson, D.N.
Deposited on : 2022-11-30
Resolution : 2.90 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.dev92
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

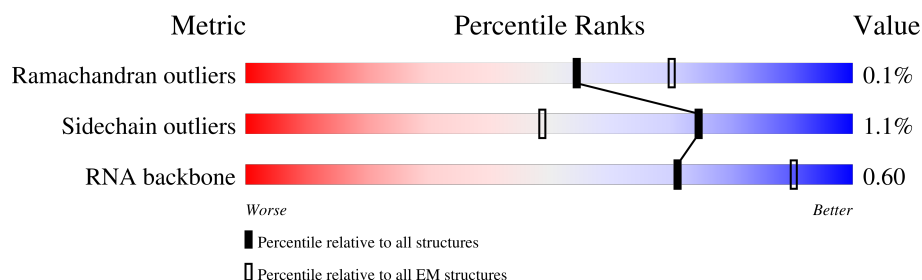
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A	2927	
2	B	119	
3	C	277	
4	D	209	
5	E	207	
6	F	179	
7	G	179	
8	J	145	

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Mol	Chain	Length	Quality of chain
9	K	122	
10	L	146	
11	M	144	
12	N	120	
13	O	120	
14	P	115	
15	Q	119	
16	R	102	
17	S	113	
18	T	95	
19	U	103	
20	V	77	
21	W	94	
22	X	62	
23	Y	66	
24	Z	59	
25	b	246	
26	u	15	
27	0	59	
28	1	49	
29	2	44	
30	3	66	
31	4	37	
32	f	95	
33	p	90	

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Mol	Chain	Length	Quality of chain
34	r	79	
35	t	88	
36	d	200	
37	e	166	
38	h	132	
39	a	1554	
40	k	131	
41	l	138	
42	o	89	
43	q	87	
44	c	218	
45	g	156	
46	i	130	
47	j	102	
48	m	121	
49	n	61	
50	s	92	
51	9	622	

2 Entry composition

There are 55 unique types of molecules in this entry. The entry contains 144765 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2852	Total	C	N	O	P	0	0
			61256	27328	11322	19755	2851		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	112	Total	C	N	O	P	0	0
			2392	1068	435	778	111		

- Molecule 3 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	273	Total	C	N	O	S	0	0
			2094	1302	412	374	6		

- Molecule 4 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	207	Total	C	N	O	S	0	0
			1575	988	290	292	5		

- Molecule 5 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	206	Total	C	N	O	S	0	0
			1567	983	290	292	2		

- Molecule 6 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	178	Total	C	N	O	S	0	0
			1405	893	245	260	7		

- Molecule 7 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	175	Total	C	N	O	S	0	0
			1342	835	248	257	2		

- Molecule 8 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	144	Total	C	N	O	S	0	0
			1142	720	211	206	5		

- Molecule 9 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	122	Total	C	N	O	S	0	0
			921	571	173	173	4		

- Molecule 10 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	146	Total	C	N	O	S	0	0
			1082	671	207	202	2		

- Molecule 11 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	135	Total	C	N	O	S	0	0
			1076	690	205	176	5		

- Molecule 12 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	N	119	Total	C	N	O	S	0	0
			954	583	186	181	4		

- Molecule 13 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	O	120	Total	C	N	O	S	0	0
			913	564	176	172	1		

- Molecule 14 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	P	115	Total	C	N	O	S	0	0
			945	600	185	159	1		

- Molecule 15 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Q	118	Total	C	N	O	S	0	0
			950	597	191	158	4		

- Molecule 16 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	102	Total	C	N	O	S	0	0
			795	506	140	148	1		

- Molecule 17 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	110	Total	C	N	O	S	0	0
			850	530	165	151	4		

- Molecule 18 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	91	Total	C	N	O	S	0	0
			733	458	135	137	3		

- Molecule 19 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	102	Total	C	N	O	S	0	0
			770	482	143	141	4		

- Molecule 20 is a RNA chain called tRNA-fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	73	Total	C	N	O	P	0	0
			1560	695	282	510	73		

- Molecule 21 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	W	79	Total	C	N	O		
			610	376	119	115	0	0

- Molecule 22 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	61	Total	C	N	O	S		
			468	289	98	79	2	0	0

- Molecule 23 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	66	Total	C	N	O	S		
			540	334	104	100	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	58	Total	C	N	O	S		
			456	281	89	85	1	0	0

- Molecule 25 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	226	Total	C	N	O	S		
			1818	1157	319	334	8	0	0

- Molecule 26 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	u	9	Total	C	N	O	P		
			199	88	39	63	9	0	0

- Molecule 27 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	0	52	Total	C	N	O	S		
			410	252	83	68	7	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	1	49	Total	C	N	O	S	0	0
			411	250	82	75	4		

- Molecule 29 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	2	44	Total	C	N	O	S	0	0
			368	222	89	55	2		

- Molecule 30 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	3	65	Total	C	N	O	S	0	0
			522	327	109	84	2		

- Molecule 31 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	4	37	Total	C	N	O	S	0	0
			297	186	60	46	5		

- Molecule 32 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	92	Total	C	N	O	S	0	0
			757	477	135	144	1		

- Molecule 33 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	p	87	Total	C	N	O	S	0	0
			691	439	127	123	2		

- Molecule 34 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	r	65	Total	C	N	O	S	0	0
			522	334	97	89	2		

- Molecule 35 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	t	86	Total	C	N	O	S	0	0
			658	402	134	121	1		

- Molecule 36 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	199	Total	C	N	O	S	0	0
			1604	1013	298	291	2		

- Molecule 37 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	e	163	Total	C	N	O	S	0	0
			1208	761	221	224	2		

- Molecule 38 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	131	Total	C	N	O	S	0	0
			1037	655	191	188	3		

- Molecule 39 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a	1538	Total	C	N	O	P	0	0
			32991	14713	6050	10690	1538		

- Molecule 40 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	k	115	Total	C	N	O	S	0	0
			847	520	166	159	2		

- Molecule 41 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	l	135	Total	C	N	O	S	0	0
			1047	650	210	185	2		

- Molecule 42 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	o	87	Total	C	N	O	S	0	0
			730	448	149	132	1		

- Molecule 43 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	q	82	Total	C	N	O	S	0	0
			676	427	126	121	2		

- Molecule 44 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	c	205	Total	C	N	O	S	0	0
			1611	1005	303	300	3		

- Molecule 45 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	g	155	Total	C	N	O	S	0	0
			1246	783	235	222	6		

- Molecule 46 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	i	128	Total	C	N	O	S	0	0
			994	615	198	180	1		

- Molecule 47 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	j	98	Total	C	N	O	S	0	0
			788	497	144	145	2		

- Molecule 48 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	m	115	Total	C	N	O		0	0
			920	565	189	166			

- Molecule 49 is a protein called 30S ribosomal protein S14.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	n	60	Total	C	N	O	S	0	0
			498	317	98	78	5		

- Molecule 50 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	s	83	Total	C	N	O	S	0	0
			668	429	122	115	2		

- Molecule 51 is a protein called ExpZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	9	573	Total	C	N	O	S	0	0
			4684	2963	831	878	12		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
9	147	GLN	GLU	engineered mutation	UNP W1SM44
9	459	GLN	GLU	engineered mutation	UNP W1SM44
9	579	GLY	-	expression tag	UNP W1SM44
9	580	GLY	-	expression tag	UNP W1SM44
9	581	HIS	-	expression tag	UNP W1SM44
9	582	HIS	-	expression tag	UNP W1SM44
9	583	HIS	-	expression tag	UNP W1SM44
9	584	HIS	-	expression tag	UNP W1SM44
9	585	HIS	-	expression tag	UNP W1SM44
9	586	HIS	-	expression tag	UNP W1SM44
9	587	ALA	-	expression tag	UNP W1SM44
9	588	LYS	-	expression tag	UNP W1SM44
9	589	GLY	-	expression tag	UNP W1SM44
9	590	GLY	-	expression tag	UNP W1SM44
9	591	GLU	-	expression tag	UNP W1SM44
9	592	ASN	-	expression tag	UNP W1SM44
9	593	LEU	-	expression tag	UNP W1SM44
9	594	TYR	-	expression tag	UNP W1SM44
9	595	PHE	-	expression tag	UNP W1SM44
9	596	GLN	-	expression tag	UNP W1SM44
9	597	GLY	-	expression tag	UNP W1SM44
9	598	VAL	-	expression tag	UNP W1SM44
9	599	ALA	-	expression tag	UNP W1SM44
9	600	ASP	-	expression tag	UNP W1SM44
9	601	TYR	-	expression tag	UNP W1SM44

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Chain	Residue	Modelled	Actual	Comment	Reference
9	602	LYS	-	expression tag	UNP W1SM44
9	603	ASP	-	expression tag	UNP W1SM44
9	604	HIS	-	expression tag	UNP W1SM44
9	605	ASP	-	expression tag	UNP W1SM44
9	606	GLY	-	expression tag	UNP W1SM44
9	607	ASP	-	expression tag	UNP W1SM44
9	608	TYR	-	expression tag	UNP W1SM44
9	609	LYS	-	expression tag	UNP W1SM44
9	610	ASP	-	expression tag	UNP W1SM44
9	611	HIS	-	expression tag	UNP W1SM44
9	612	ASP	-	expression tag	UNP W1SM44
9	613	ILE	-	expression tag	UNP W1SM44
9	614	ASP	-	expression tag	UNP W1SM44
9	615	TYR	-	expression tag	UNP W1SM44
9	616	LYS	-	expression tag	UNP W1SM44
9	617	ASP	-	expression tag	UNP W1SM44
9	618	ASP	-	expression tag	UNP W1SM44
9	619	ASP	-	expression tag	UNP W1SM44
9	620	ASP	-	expression tag	UNP W1SM44
9	621	LYS	-	expression tag	UNP W1SM44
9	622	GLY	-	expression tag	UNP W1SM44

- Molecule 52 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
52	A	14	Total K 14 14	0
52	U	1	Total K 1 1	0
52	a	1	Total K 1 1	0

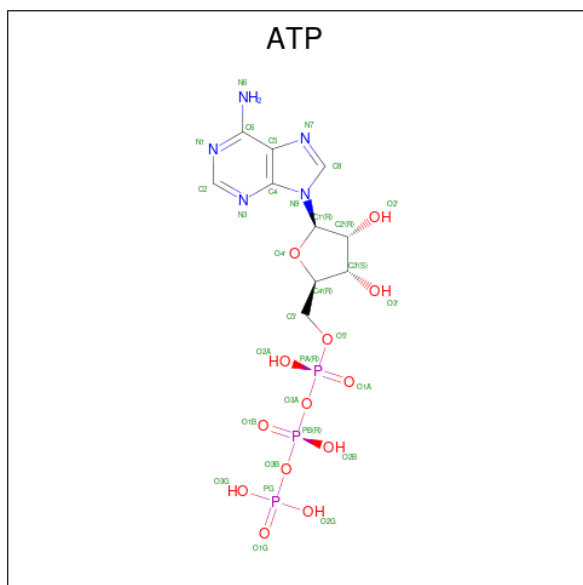
- Molecule 53 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
53	A	82	Total Mg 82 82	0
53	C	1	Total Mg 1 1	0
53	9	2	Total Mg 2 2	0

- Molecule 54 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
54	0	1	Total	Zn	0
			1	1	
54	1	1	Total	Zn	0
			1	1	
54	4	1	Total	Zn	0
			1	1	
54	n	1	Total	Zn	0
			1	1	

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

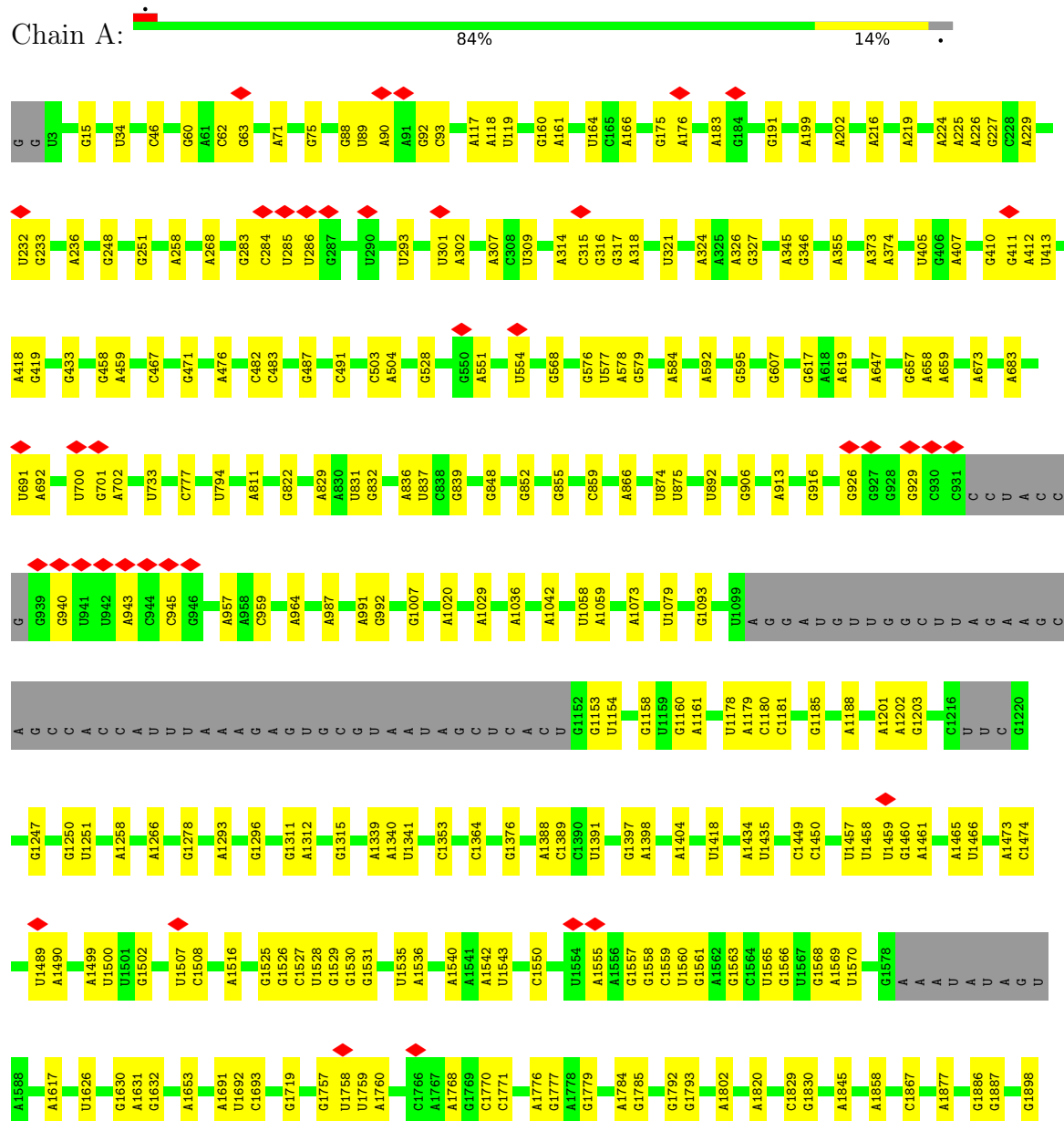


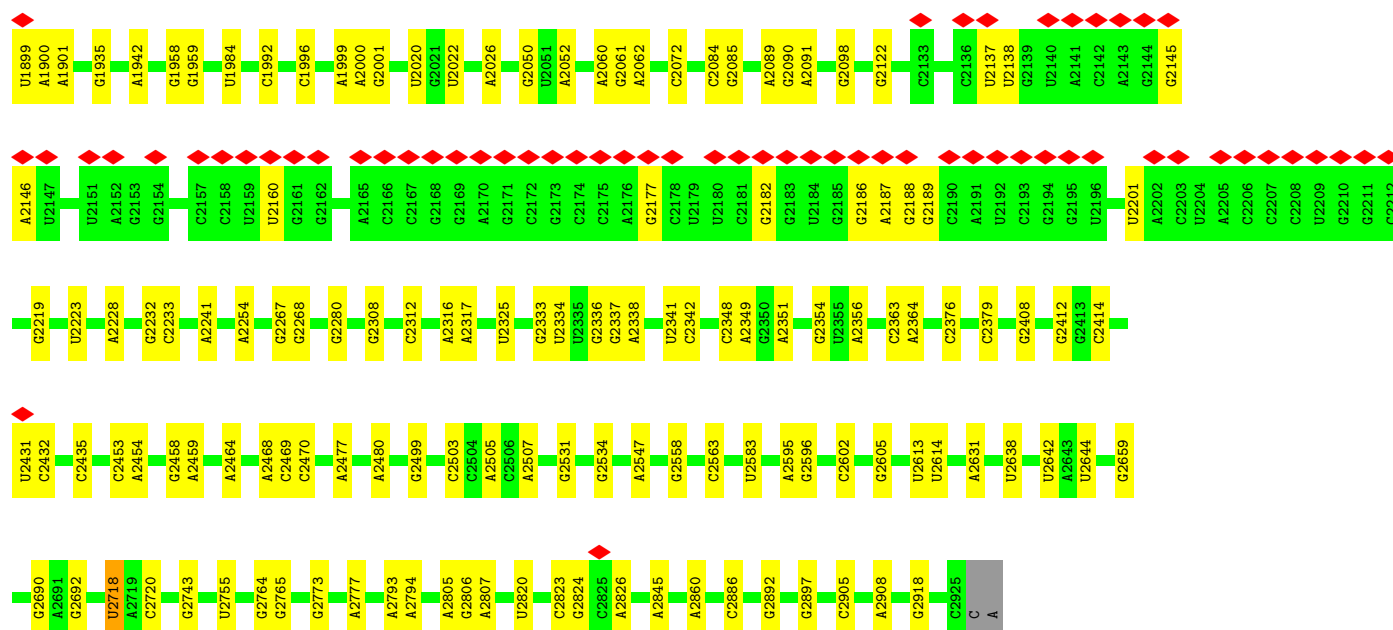
Mol	Chain	Residues	Atoms					AltConf
55	9	1	Total	C	N	O	P	0
			31	10	5	13	3	
55	9	1	Total	C	N	O	P	0
			31	10	5	13	3	

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.

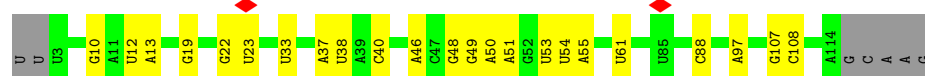
• Molecule 1: 23S rRNA





- Molecule 2: 5S rRNA

Chain B: 75% 19% 6%



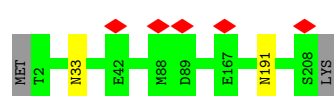
- Molecule 3: 50S ribosomal protein L2

Chain C: 97% 19% 6%



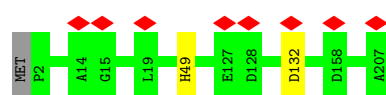
- Molecule 4: 50S ribosomal protein L3

Chain D: 98% 19% 6%

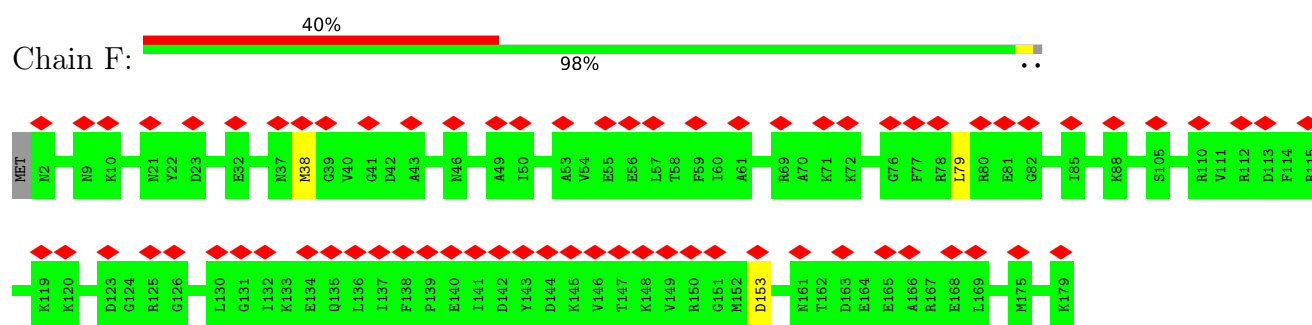


- Molecule 5: 50S ribosomal protein L4

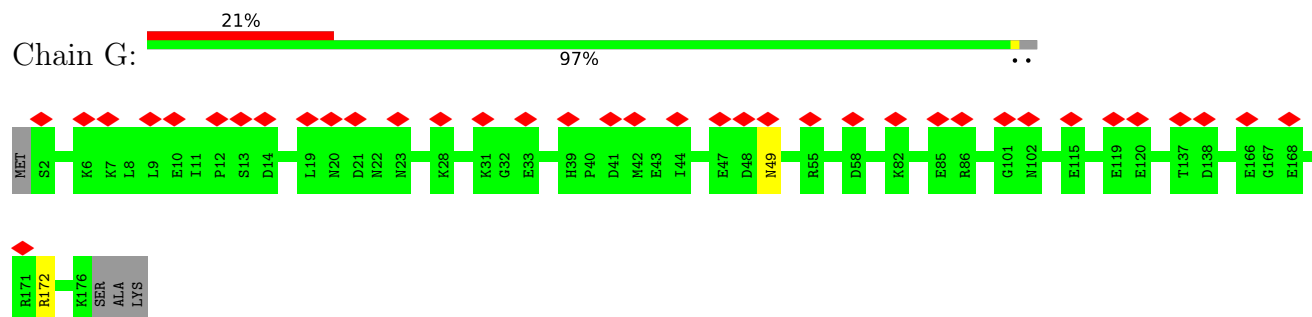
Chain E: 99% 19% 6%



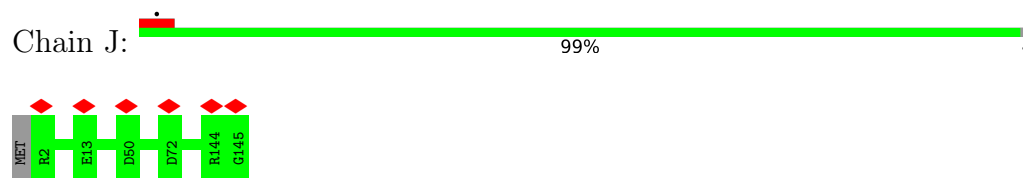
- Molecule 6: 50S ribosomal protein L5



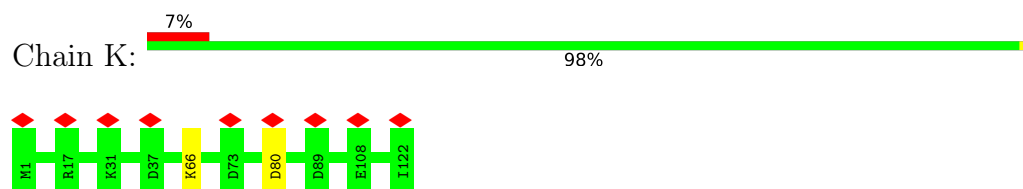
- Molecule 7: 50S ribosomal protein L6



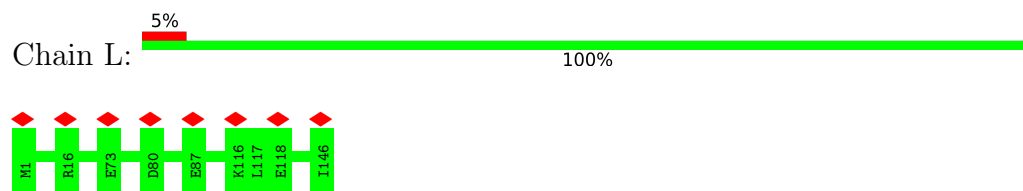
- Molecule 8: 50S ribosomal protein L13



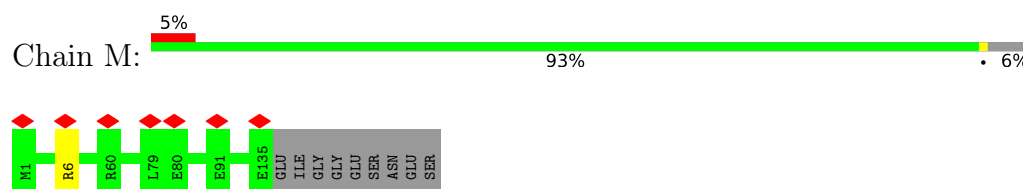
- Molecule 9: 50S ribosomal protein L14



- Molecule 10: 50S ribosomal protein L15

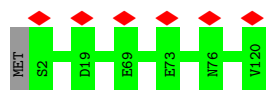


- Molecule 11: 50S ribosomal protein L16



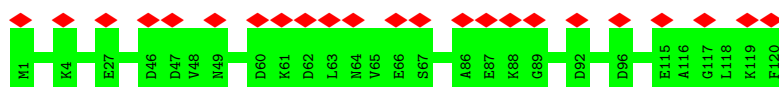
- Molecule 12: 50S ribosomal protein L17

Chain N:  5% 99%



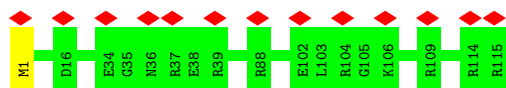
- Molecule 13: 50S ribosomal protein L18

Chain O:  19% 100%



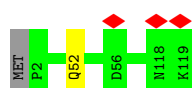
- Molecule 14: 50S ribosomal protein L19

Chain P:  11% 99%



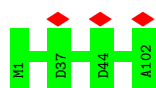
- Molecule 15: 50S ribosomal protein L20

Chain Q:  98%



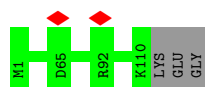
- Molecule 16: 50S ribosomal protein L21

Chain R:  100%



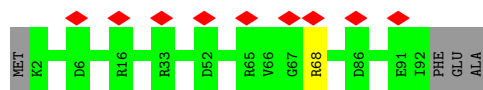
- Molecule 17: 50S ribosomal protein L22

Chain S:  97%

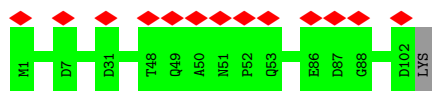


- Molecule 18: 50S ribosomal protein L23

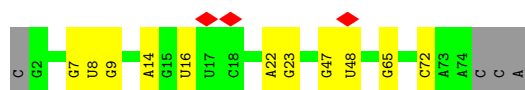
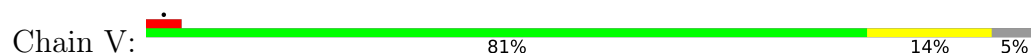
Chain T:  9% 95%



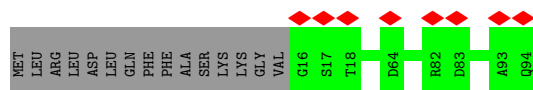
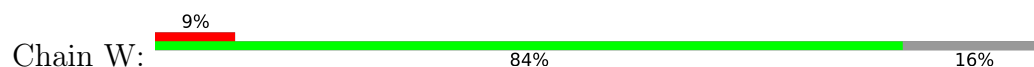
- Molecule 19: 50S ribosomal protein L24



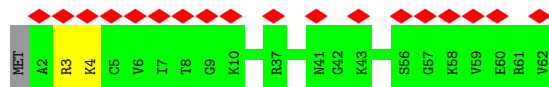
- Molecule 20: tRNA-fMet



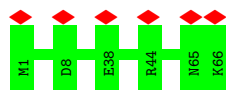
- Molecule 21: 50S ribosomal protein L27



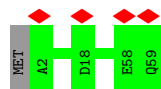
- Molecule 22: 50S ribosomal protein L28



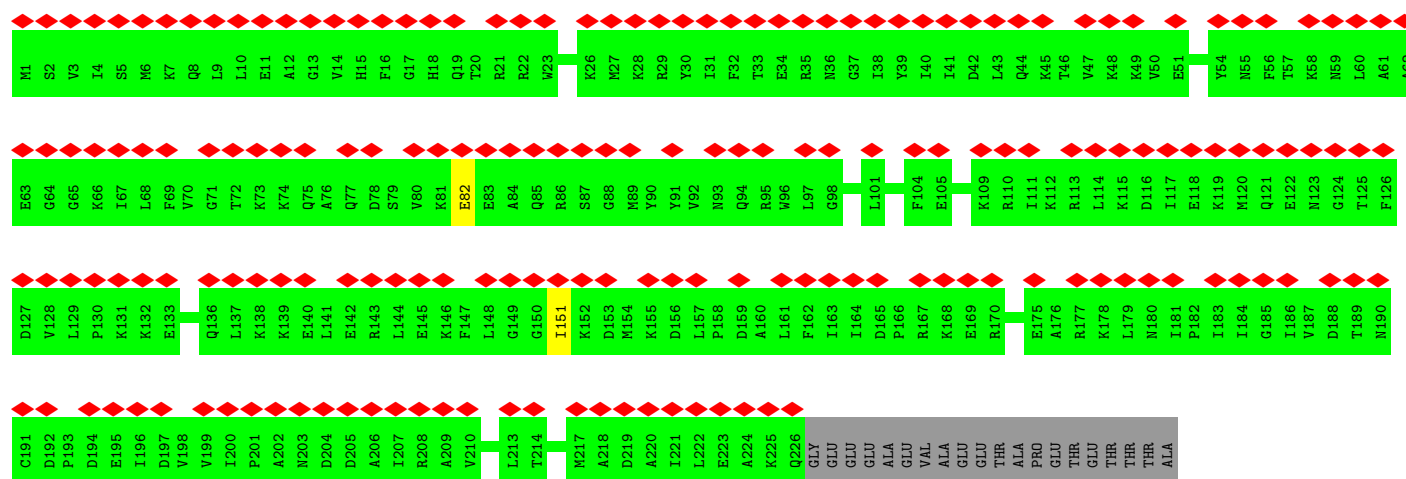
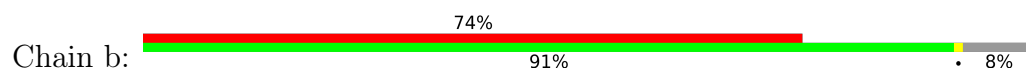
- Molecule 23: 50S ribosomal protein L29



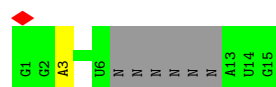
- Molecule 24: 50S ribosomal protein L30



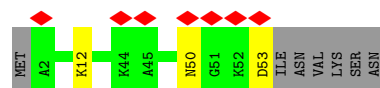
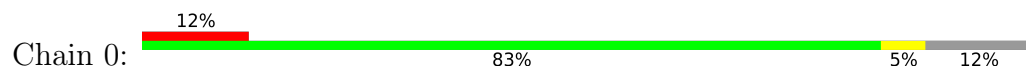
- Molecule 25: 30S ribosomal protein S2



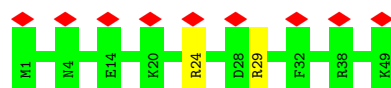
• Molecule 26: mRNA



• Molecule 27: 50S ribosomal protein L32



• Molecule 28: 50S ribosomal protein L33 1

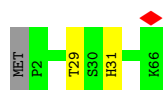


• Molecule 29: 50S ribosomal protein L34

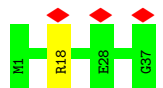


• Molecule 30: 50S ribosomal protein L35

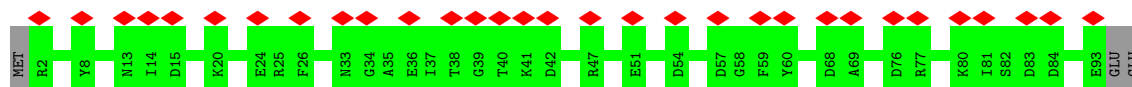




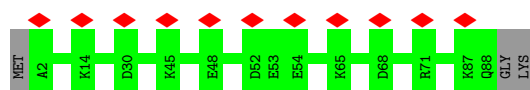
- Molecule 31: 50S ribosomal protein L36



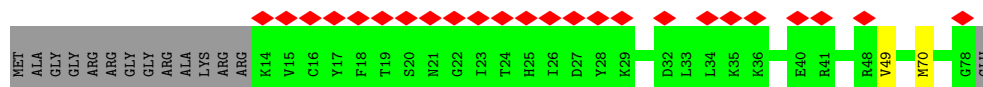
- Molecule 32: 30S ribosomal protein S6



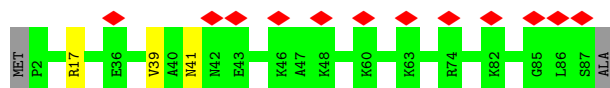
- Molecule 33: 30S ribosomal protein S16



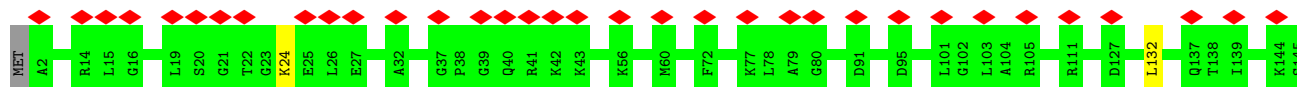
- Molecule 34: 30S ribosomal protein S18

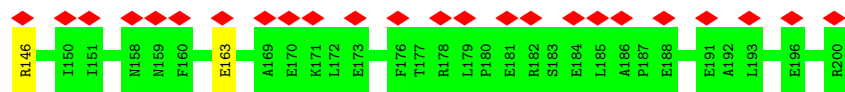


- Molecule 35: 30S ribosomal protein S20

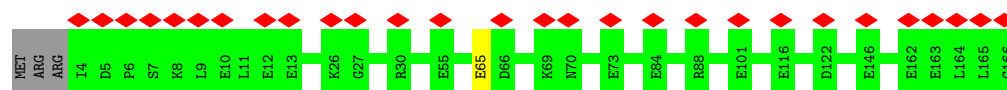


- Molecule 36: 30S ribosomal protein S4

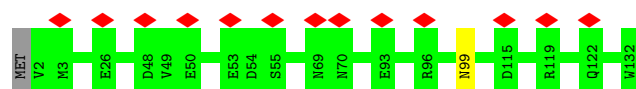




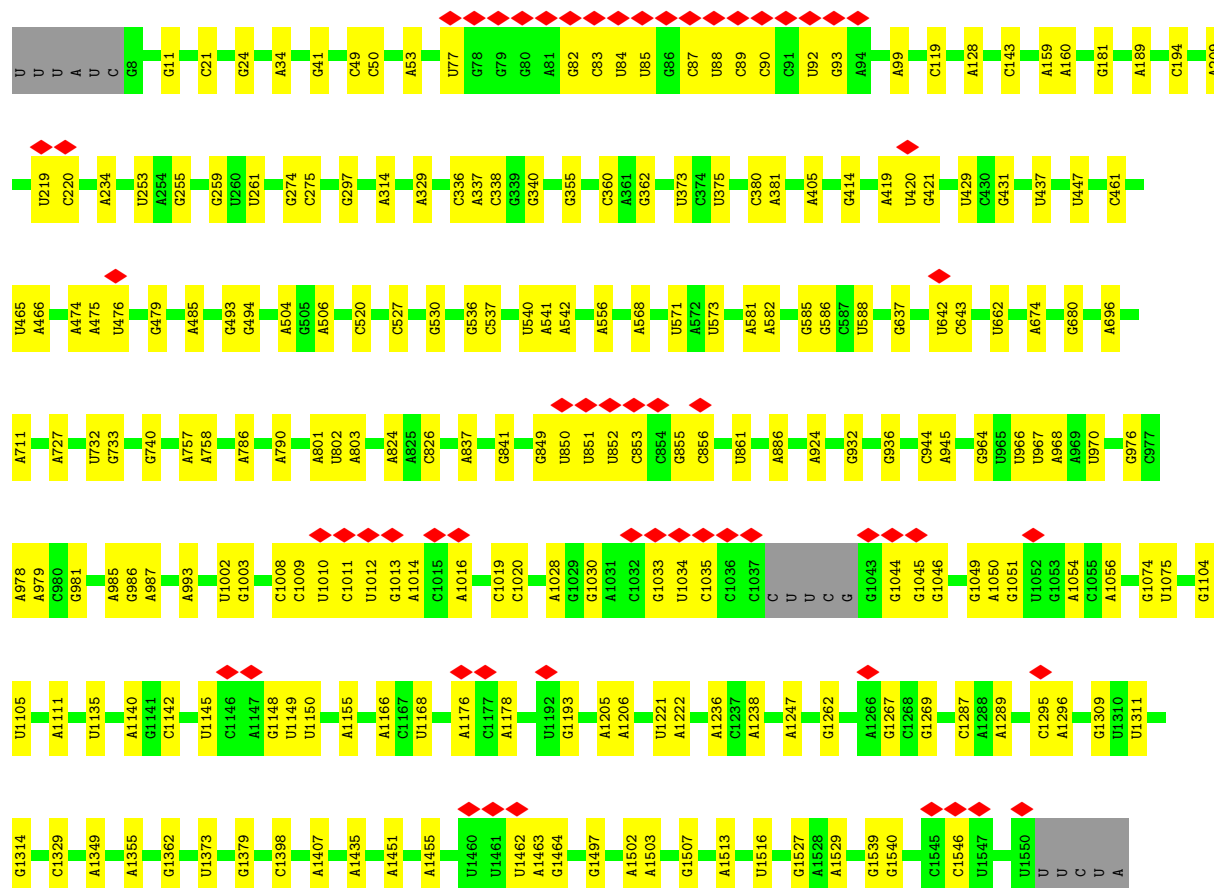
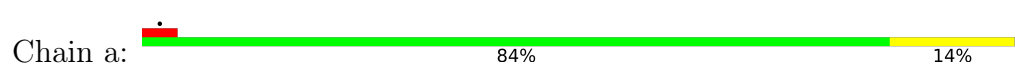
- Molecule 37: 30S ribosomal protein S5



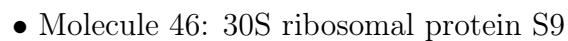
- Molecule 38: 30S ribosomal protein S8

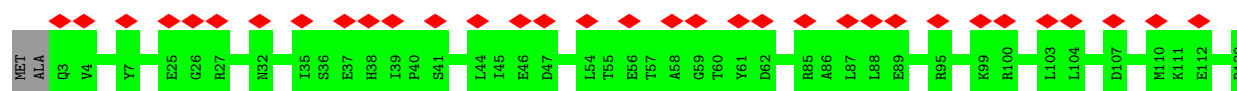


- Molecule 39: 16S rRNA

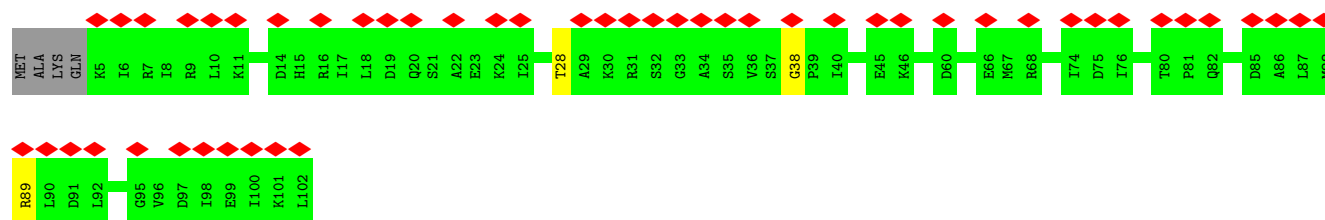
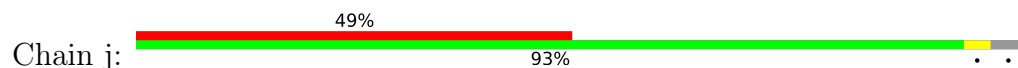


- Molecule 40: 30S ribosomal protein S11

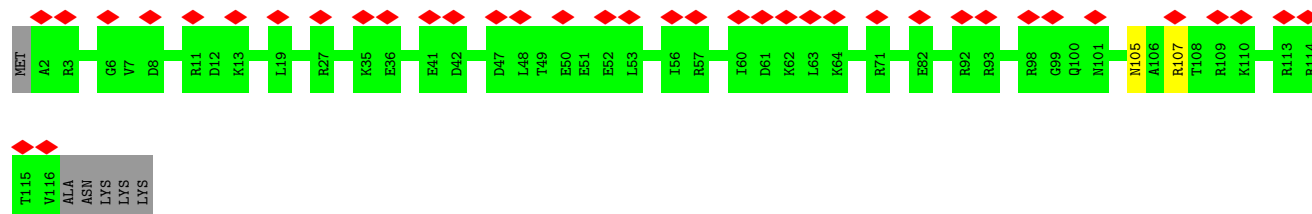




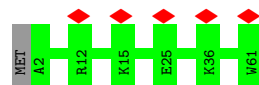
- Molecule 47: 30S ribosomal protein S10



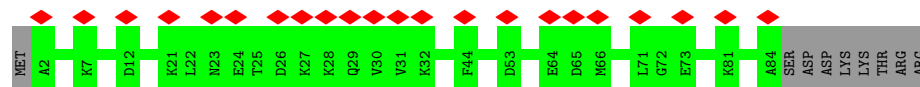
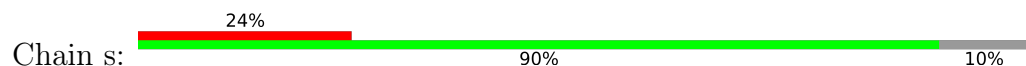
- Molecule 48: 30S ribosomal protein S13



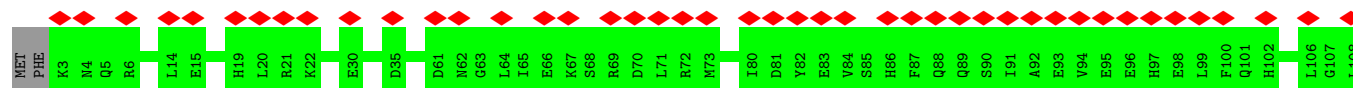
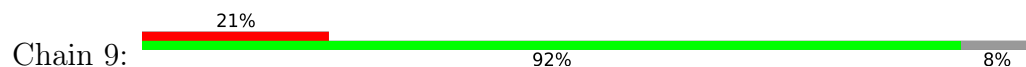
- Molecule 49: 30S ribosomal protein S14



- Molecule 50: 30S ribosomal protein S19



- Molecule 51: ExpZ



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	140804	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28.25	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.045	Depositor
Minimum map value	-0.019	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	319.8, 319.8, 319.8	wwPDB
Map dimensions	390, 390, 390	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82, 0.82, 0.82	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, OMG, ZN, K, PSU

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.54	0/68565	0.73	0/106963
2	B	0.35	0/2675	0.70	0/4170
3	C	0.32	0/2131	0.57	0/2859
4	D	0.31	0/1597	0.54	0/2140
5	E	0.30	0/1586	0.52	0/2139
6	F	0.26	0/1424	0.51	0/1910
7	G	0.26	0/1360	0.53	0/1832
8	J	0.29	0/1165	0.51	0/1566
9	K	0.31	0/928	0.58	0/1245
10	L	0.30	0/1094	0.53	0/1457
11	M	0.30	0/1099	0.55	0/1468
12	N	0.29	0/961	0.57	0/1284
13	O	0.27	0/922	0.54	0/1236
14	P	0.31	0/958	0.60	0/1279
15	Q	0.31	0/962	0.53	0/1277
16	R	0.32	0/806	0.51	0/1080
17	S	0.29	0/859	0.58	0/1156
18	T	0.29	0/739	0.56	0/985
19	U	0.28	0/780	0.48	0/1043
20	V	0.33	0/1743	0.69	0/2716
21	W	0.30	0/618	0.59	0/821
22	X	0.28	0/472	0.57	0/627
23	Y	0.26	0/541	0.54	0/718
24	Z	0.27	0/458	0.54	0/613
25	b	0.26	0/1843	0.48	0/2472
26	u	0.33	0/222	0.62	0/343
27	o	0.33	0/417	0.62	0/552
28	1	0.28	0/416	0.60	0/551
29	2	0.31	0/371	0.69	0/483
30	3	0.28	0/529	0.54	0/691
31	4	0.31	0/300	0.52	0/393
32	f	0.27	0/768	0.51	0/1033

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	p	0.28	0/704	0.51	0/945
34	r	0.26	0/530	0.54	0/710
35	t	0.24	0/661	0.48	0/882
36	d	0.27	0/1635	0.53	0/2196
37	e	0.26	0/1220	0.52	0/1641
38	h	0.27	0/1049	0.54	0/1407
39	a	0.40	0/36936	0.70	0/57617
40	k	0.24	0/861	0.53	0/1164
41	l	0.29	0/1064	0.59	0/1428
42	o	0.24	0/738	0.54	0/985
43	q	0.27	0/684	0.53	0/913
44	c	0.26	0/1633	0.53	0/2197
45	g	0.26	0/1266	0.52	0/1699
46	i	0.26	0/1007	0.57	0/1351
47	j	0.26	0/800	0.53	0/1077
48	m	0.24	0/926	0.61	0/1238
49	n	0.30	0/508	0.55	0/672
50	s	0.27	0/685	0.49	0/920
51	9	0.27	0/4763	0.50	0/6394
All	All	0.44	0/156979	0.67	0/234538

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
3	C	0	1
31	4	0	1
43	q	0	1
51	9	0	2
All	All	0	5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
31	4	18	ARG	Sidechain
51	9	313	ARG	Sidechain

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Mol	Chain	Res	Type	Group
51	9	441	ARG	Sidechain
3	C	14	ARG	Sidechain
43	q	4	ARG	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	
3	C	271/277 (98%)	267 (98%)	3 (1%)	1 (0%)	34	66
4	D	205/209 (98%)	197 (96%)	8 (4%)	0	100	100
5	E	204/207 (99%)	200 (98%)	4 (2%)	0	100	100
6	F	176/179 (98%)	168 (96%)	8 (4%)	0	100	100
7	G	173/179 (97%)	160 (92%)	13 (8%)	0	100	100
8	J	142/145 (98%)	139 (98%)	3 (2%)	0	100	100
9	K	120/122 (98%)	117 (98%)	3 (2%)	0	100	100
10	L	144/146 (99%)	139 (96%)	5 (4%)	0	100	100
11	M	133/144 (92%)	131 (98%)	2 (2%)	0	100	100
12	N	117/120 (98%)	112 (96%)	5 (4%)	0	100	100
13	O	118/120 (98%)	112 (95%)	6 (5%)	0	100	100
14	P	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
15	Q	116/119 (98%)	115 (99%)	1 (1%)	0	100	100
16	R	100/102 (98%)	98 (98%)	2 (2%)	0	100	100
17	S	108/113 (96%)	107 (99%)	1 (1%)	0	100	100
18	T	89/95 (94%)	87 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	U	100/103 (97%)	97 (97%)	3 (3%)	0	100	100
21	W	77/94 (82%)	73 (95%)	4 (5%)	0	100	100
22	X	59/62 (95%)	56 (95%)	3 (5%)	0	100	100
23	Y	64/66 (97%)	63 (98%)	1 (2%)	0	100	100
24	Z	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
25	b	224/246 (91%)	218 (97%)	6 (3%)	0	100	100
27	0	50/59 (85%)	47 (94%)	3 (6%)	0	100	100
28	1	47/49 (96%)	46 (98%)	1 (2%)	0	100	100
29	2	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
30	3	63/66 (96%)	62 (98%)	1 (2%)	0	100	100
31	4	35/37 (95%)	35 (100%)	0	0	100	100
32	f	90/95 (95%)	85 (94%)	5 (6%)	0	100	100
33	p	85/90 (94%)	83 (98%)	2 (2%)	0	100	100
34	r	63/79 (80%)	62 (98%)	1 (2%)	0	100	100
35	t	84/88 (96%)	83 (99%)	1 (1%)	0	100	100
36	d	197/200 (98%)	187 (95%)	9 (5%)	1 (0%)	29	61
37	e	161/166 (97%)	158 (98%)	3 (2%)	0	100	100
38	h	129/132 (98%)	126 (98%)	3 (2%)	0	100	100
40	k	113/131 (86%)	109 (96%)	4 (4%)	0	100	100
41	l	133/138 (96%)	128 (96%)	5 (4%)	0	100	100
42	o	85/89 (96%)	84 (99%)	1 (1%)	0	100	100
43	q	80/87 (92%)	78 (98%)	2 (2%)	0	100	100
44	c	203/218 (93%)	195 (96%)	8 (4%)	0	100	100
45	g	153/156 (98%)	148 (97%)	5 (3%)	0	100	100
46	i	126/130 (97%)	121 (96%)	5 (4%)	0	100	100
47	j	96/102 (94%)	93 (97%)	2 (2%)	1 (1%)	15	45
48	m	113/121 (93%)	110 (97%)	2 (2%)	1 (1%)	17	48
49	n	58/61 (95%)	58 (100%)	0	0	100	100
50	s	81/92 (88%)	78 (96%)	3 (4%)	0	100	100
51	9	571/622 (92%)	549 (96%)	22 (4%)	0	100	100
All	All	5767/6074 (95%)	5586 (97%)	177 (3%)	4 (0%)	54	82

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
36	d	24	LYS
48	m	105	ASN
3	C	155	VAL
47	j	38	GLY

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	
3	C	221/225 (98%)	218 (99%)	3 (1%)	67	89
4	D	168/170 (99%)	166 (99%)	2 (1%)	71	91
5	E	169/170 (99%)	167 (99%)	2 (1%)	71	91
6	F	153/154 (99%)	150 (98%)	3 (2%)	55	82
7	G	148/151 (98%)	146 (99%)	2 (1%)	67	89
8	J	122/123 (99%)	122 (100%)	0	100	100
9	K	101/101 (100%)	99 (98%)	2 (2%)	55	82
10	L	110/110 (100%)	110 (100%)	0	100	100
11	M	109/116 (94%)	108 (99%)	1 (1%)	78	93
12	N	99/100 (99%)	99 (100%)	0	100	100
13	O	93/93 (100%)	93 (100%)	0	100	100
14	P	100/100 (100%)	99 (99%)	1 (1%)	76	92
15	Q	97/98 (99%)	96 (99%)	1 (1%)	76	92
16	R	84/84 (100%)	84 (100%)	0	100	100
17	S	91/93 (98%)	91 (100%)	0	100	100
18	T	82/85 (96%)	81 (99%)	1 (1%)	71	91
19	U	86/87 (99%)	86 (100%)	0	100	100
21	W	61/74 (82%)	61 (100%)	0	100	100
22	X	49/50 (98%)	47 (96%)	2 (4%)	30	64
23	Y	57/57 (100%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Z	52/53 (98%)	52 (100%)	0	100	100
25	b	197/212 (93%)	195 (99%)	2 (1%)	76	92
27	0	46/53 (87%)	43 (94%)	3 (6%)	17	45
28	1	47/47 (100%)	45 (96%)	2 (4%)	29	62
29	2	39/39 (100%)	39 (100%)	0	100	100
30	3	55/56 (98%)	53 (96%)	2 (4%)	35	69
31	4	35/35 (100%)	35 (100%)	0	100	100
32	f	81/84 (96%)	81 (100%)	0	100	100
33	p	74/76 (97%)	74 (100%)	0	100	100
34	r	56/64 (88%)	54 (96%)	2 (4%)	35	69
35	t	69/70 (99%)	66 (96%)	3 (4%)	29	62
36	d	172/173 (99%)	169 (98%)	3 (2%)	60	86
37	e	127/130 (98%)	126 (99%)	1 (1%)	81	94
38	h	111/112 (99%)	110 (99%)	1 (1%)	78	93
40	k	87/100 (87%)	85 (98%)	2 (2%)	50	80
41	l	114/116 (98%)	113 (99%)	1 (1%)	78	93
42	o	82/83 (99%)	82 (100%)	0	100	100
43	q	75/80 (94%)	74 (99%)	1 (1%)	69	90
44	c	167/178 (94%)	165 (99%)	2 (1%)	71	91
45	g	131/132 (99%)	129 (98%)	2 (2%)	65	87
46	i	101/102 (99%)	101 (100%)	0	100	100
47	j	89/92 (97%)	87 (98%)	2 (2%)	52	81
48	m	99/104 (95%)	98 (99%)	1 (1%)	76	92
49	n	53/54 (98%)	53 (100%)	0	100	100
50	s	72/81 (89%)	72 (100%)	0	100	100
51	9	519/558 (93%)	517 (100%)	2 (0%)	91	97
All	All	4950/5125 (97%)	4898 (99%)	52 (1%)	74	92

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	13	ARG
3	C	63	ARG

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Mol	Chain	Res	Type
3	C	100	GLU
4	D	33	ASN
4	D	191	ASN
5	E	49	HIS
5	E	132	ASP
6	F	38	MET
6	F	79	LEU
6	F	153	ASP
7	G	49	ASN
7	G	172	ARG
9	K	66	LYS
9	K	80	ASP
11	M	6	ARG
14	P	1	MET
15	Q	52	GLN
18	T	68	ARG
22	X	3	ARG
22	X	4	LYS
25	b	82	GLU
25	b	151	ILE
27	0	12	LYS
27	0	50	ASN
27	0	53	ASP
28	1	24	ARG
28	1	29	ARG
30	3	29	THR
30	3	31	HIS
34	r	49	VAL
34	r	70	MET
35	t	17	ARG
35	t	39	VAL
35	t	41	ASN
36	d	132	LEU
36	d	146	ARG
36	d	163	GLU
37	e	65	GLU
38	h	99	ASN
40	k	95	ARG
40	k	121	ASN
41	l	99	ARG
43	q	4	ARG
44	c	16	ARG

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Mol	Chain	Res	Type
44	c	189	ASP
45	g	75	VAL
45	g	153	HIS
47	j	28	THR
47	j	89	ARG
48	m	107	ARG
51	9	206	TYR
51	9	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	21	ASN
25	b	18	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	2847/2927 (97%)	389 (13%)	28 (0%)
2	B	111/119 (93%)	21 (18%)	3 (2%)
20	V	72/77 (93%)	11 (15%)	1 (1%)
26	u	7/15 (46%)	1 (14%)	0
39	a	1536/1554 (98%)	225 (14%)	0
All	All	4573/4692 (97%)	647 (14%)	32 (0%)

All (647) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	15	G
1	A	34	U
1	A	46	C
1	A	60	G
1	A	63	G
1	A	71	A
1	A	75	G
1	A	89	U
1	A	90	A
1	A	93	C
1	A	117	A
1	A	118	A

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Mol	Chain	Res	Type
1	A	119	U
1	A	161	A
1	A	164	U
1	A	166	A
1	A	175	G
1	A	176	A
1	A	183	A
1	A	191	G
1	A	199	A
1	A	202	A
1	A	216	A
1	A	219	A
1	A	224	A
1	A	225	A
1	A	226	A
1	A	227	G
1	A	229	A
1	A	232	U
1	A	233	G
1	A	236	A
1	A	248	G
1	A	251	G
1	A	258	A
1	A	268	A
1	A	283	G
1	A	284	C
1	A	285	U
1	A	286	U
1	A	293	U
1	A	301	U
1	A	302	A
1	A	307	A
1	A	309	U
1	A	314	A
1	A	315	C
1	A	316	G
1	A	317	G
1	A	318	A
1	A	321	U
1	A	324	A
1	A	327	G
1	A	345	A

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Mol	Chain	Res	Type
1	A	346	G
1	A	355	A
1	A	373	A
1	A	374	A
1	A	405	U
1	A	407	A
1	A	411	G
1	A	412	A
1	A	413	U
1	A	418	A
1	A	419	G
1	A	433	G
1	A	458	G
1	A	459	A
1	A	467	C
1	A	471	G
1	A	476	A
1	A	482	C
1	A	483	C
1	A	487	G
1	A	491	C
1	A	503	C
1	A	504	A
1	A	528	G
1	A	551	A
1	A	554	U
1	A	568	G
1	A	576	G
1	A	577	U
1	A	578	A
1	A	579	G
1	A	584	A
1	A	592	A
1	A	595	G
1	A	607	G
1	A	617	G
1	A	619	A
1	A	647	A
1	A	657	G
1	A	658	A
1	A	659	A
1	A	673	A

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Mol	Chain	Res	Type
1	A	683	A
1	A	691	U
1	A	692	A
1	A	700	U
1	A	701	G
1	A	702	A
1	A	733	U
1	A	777	C
1	A	794	U
1	A	811	A
1	A	822	G
1	A	829	A
1	A	831	U
1	A	832	G
1	A	836	A
1	A	837	U
1	A	839	G
1	A	852	G
1	A	859	C
1	A	866	A
1	A	874	U
1	A	875	U
1	A	892	U
1	A	906	G
1	A	913	A
1	A	916	G
1	A	926	G
1	A	929	G
1	A	940	G
1	A	943	A
1	A	945	C
1	A	957	A
1	A	959	C
1	A	964	A
1	A	987	A
1	A	991	A
1	A	992	G
1	A	1007	G
1	A	1020	A
1	A	1029	A
1	A	1036	A
1	A	1042	A

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Mol	Chain	Res	Type
1	A	1058	U
1	A	1059	A
1	A	1073	A
1	A	1079	U
1	A	1093	G
1	A	1153	G
1	A	1154	U
1	A	1158	G
1	A	1160	G
1	A	1161	A
1	A	1178	U
1	A	1179	A
1	A	1180	C
1	A	1181	C
1	A	1185	G
1	A	1188	A
1	A	1201	A
1	A	1202	A
1	A	1203	G
1	A	1247	G
1	A	1251	U
1	A	1258	A
1	A	1278	G
1	A	1293	A
1	A	1296	G
1	A	1311	G
1	A	1312	A
1	A	1315	G
1	A	1339	A
1	A	1340	A
1	A	1341	U
1	A	1353	C
1	A	1364	C
1	A	1376	G
1	A	1388	A
1	A	1389	C
1	A	1391	U
1	A	1398	A
1	A	1404	A
1	A	1418	U
1	A	1434	A
1	A	1435	U

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Mol	Chain	Res	Type
1	A	1449	C
1	A	1450	C
1	A	1457	U
1	A	1458	U
1	A	1459	U
1	A	1460	G
1	A	1461	A
1	A	1465	A
1	A	1466	U
1	A	1473	A
1	A	1474	C
1	A	1489	U
1	A	1490	A
1	A	1499	A
1	A	1500	U
1	A	1502	G
1	A	1507	U
1	A	1508	C
1	A	1516	A
1	A	1525	G
1	A	1526	G
1	A	1527	C
1	A	1528	U
1	A	1529	G
1	A	1531	G
1	A	1536	A
1	A	1540	A
1	A	1542	A
1	A	1543	U
1	A	1550	C
1	A	1555	A
1	A	1557	G
1	A	1558	G
1	A	1559	C
1	A	1560	U
1	A	1561	G
1	A	1563	G
1	A	1566	G
1	A	1568	G
1	A	1569	A
1	A	1570	U
1	A	1617	A

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Mol	Chain	Res	Type
1	A	1626	U
1	A	1630	G
1	A	1631	A
1	A	1632	G
1	A	1653	A
1	A	1691	A
1	A	1692	U
1	A	1693	C
1	A	1719	G
1	A	1757	G
1	A	1758	U
1	A	1759	U
1	A	1760	A
1	A	1768	A
1	A	1770	C
1	A	1771	C
1	A	1776	A
1	A	1777	G
1	A	1779	G
1	A	1785	G
1	A	1792	G
1	A	1793	G
1	A	1802	A
1	A	1820	A
1	A	1829	C
1	A	1830	G
1	A	1845	A
1	A	1858	A
1	A	1867	C
1	A	1877	A
1	A	1886	G
1	A	1887	G
1	A	1898	G
1	A	1899	U
1	A	1900	A
1	A	1901	A
1	A	1935	G
1	A	1942	A
1	A	1958	G
1	A	1959	G
1	A	1984	U
1	A	1992	C

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Mol	Chain	Res	Type
1	A	1996	C
1	A	1999	A
1	A	2000	A
1	A	2001	G
1	A	2020	U
1	A	2022	U
1	A	2026	A
1	A	2050	G
1	A	2052	A
1	A	2060	A
1	A	2061	G
1	A	2062	A
1	A	2072	C
1	A	2084	C
1	A	2085	G
1	A	2089	A
1	A	2090	G
1	A	2091	A
1	A	2098	G
1	A	2122	G
1	A	2137	U
1	A	2138	U
1	A	2145	G
1	A	2146	A
1	A	2160	U
1	A	2177	G
1	A	2182	G
1	A	2186	G
1	A	2187	A
1	A	2188	G
1	A	2189	G
1	A	2201	U
1	A	2219	G
1	A	2223	U
1	A	2228	A
1	A	2232	G
1	A	2233	C
1	A	2241	A
1	A	2254	A
1	A	2267	G
1	A	2268	G
1	A	2308	G

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Mol	Chain	Res	Type
1	A	2312	C
1	A	2316	A
1	A	2317	A
1	A	2325	U
1	A	2333	G
1	A	2334	U
1	A	2336	G
1	A	2337	G
1	A	2338	A
1	A	2341	U
1	A	2342	C
1	A	2348	C
1	A	2349	A
1	A	2351	A
1	A	2354	G
1	A	2356	A
1	A	2363	C
1	A	2364	A
1	A	2376	C
1	A	2379	C
1	A	2408	G
1	A	2412	G
1	A	2414	C
1	A	2431	U
1	A	2432	C
1	A	2435	C
1	A	2453	C
1	A	2454	A
1	A	2458	G
1	A	2459	A
1	A	2464	A
1	A	2468	A
1	A	2469	C
1	A	2470	C
1	A	2477	A
1	A	2480	A
1	A	2499	G
1	A	2503	C
1	A	2505	A
1	A	2507	A
1	A	2531	G
1	A	2534	G

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Mol	Chain	Res	Type
1	A	2547	A
1	A	2558	G
1	A	2563	C
1	A	2583	U
1	A	2595	A
1	A	2596	G
1	A	2602	C
1	A	2605	G
1	A	2613	U
1	A	2614	U
1	A	2631	A
1	A	2638	U
1	A	2642	U
1	A	2644	U
1	A	2659	G
1	A	2690	G
1	A	2692	G
1	A	2718	PSU
1	A	2720	C
1	A	2743	G
1	A	2755	U
1	A	2764	G
1	A	2765	G
1	A	2773	G
1	A	2777	A
1	A	2793	A
1	A	2794	A
1	A	2806	G
1	A	2807	A
1	A	2820	U
1	A	2823	C
1	A	2824	G
1	A	2826	A
1	A	2845	A
1	A	2860	A
1	A	2886	C
1	A	2892	G
1	A	2897	G
1	A	2905	C
1	A	2908	A
1	A	2918	G
2	B	10	G

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Mol	Chain	Res	Type
2	B	12	U
2	B	13	A
2	B	19	G
2	B	22	G
2	B	23	U
2	B	33	U
2	B	38	U
2	B	40	C
2	B	46	A
2	B	49	G
2	B	50	A
2	B	51	A
2	B	53	U
2	B	54	U
2	B	55	A
2	B	61	U
2	B	88	C
2	B	97	A
2	B	107	G
2	B	108	C
20	V	7	G
20	V	8	U
20	V	9	G
20	V	14	A
20	V	16	U
20	V	22	A
20	V	23	G
20	V	47	G
20	V	48	U
20	V	65	G
20	V	72	C
26	u	3	A
39	a	11	G
39	a	21	C
39	a	24	G
39	a	34	A
39	a	41	G
39	a	49	C
39	a	50	C
39	a	53	A
39	a	77	U
39	a	82	G

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Mol	Chain	Res	Type
39	a	83	C
39	a	84	U
39	a	85	U
39	a	87	C
39	a	88	U
39	a	89	C
39	a	90	C
39	a	92	U
39	a	93	G
39	a	99	A
39	a	119	C
39	a	128	A
39	a	143	C
39	a	159	A
39	a	160	A
39	a	181	G
39	a	189	A
39	a	194	C
39	a	209	A
39	a	219	U
39	a	220	C
39	a	234	A
39	a	253	U
39	a	255	G
39	a	259	G
39	a	261	U
39	a	274	G
39	a	275	C
39	a	297	G
39	a	314	A
39	a	329	A
39	a	336	C
39	a	337	A
39	a	338	C
39	a	340	G
39	a	355	G
39	a	360	C
39	a	362	G
39	a	373	U
39	a	375	U
39	a	380	C
39	a	381	A

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Mol	Chain	Res	Type
39	a	405	A
39	a	414	G
39	a	419	A
39	a	420	U
39	a	421	G
39	a	429	U
39	a	431	G
39	a	437	U
39	a	447	U
39	a	461	C
39	a	465	U
39	a	466	A
39	a	474	A
39	a	475	A
39	a	476	U
39	a	479	G
39	a	485	A
39	a	493	G
39	a	494	G
39	a	504	A
39	a	506	A
39	a	520	C
39	a	527	C
39	a	530	G
39	a	536	G
39	a	537	C
39	a	540	U
39	a	541	A
39	a	542	A
39	a	556	A
39	a	568	A
39	a	571	U
39	a	573	U
39	a	581	A
39	a	582	A
39	a	585	G
39	a	586	G
39	a	588	U
39	a	637	G
39	a	642	U
39	a	643	C
39	a	662	U

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Mol	Chain	Res	Type
39	a	674	A
39	a	680	G
39	a	696	A
39	a	711	A
39	a	727	A
39	a	732	U
39	a	733	G
39	a	740	G
39	a	757	A
39	a	758	A
39	a	786	A
39	a	790	A
39	a	801	A
39	a	802	U
39	a	803	A
39	a	824	A
39	a	826	C
39	a	837	A
39	a	841	G
39	a	849	G
39	a	850	U
39	a	851	U
39	a	852	U
39	a	853	C
39	a	855	G
39	a	856	C
39	a	861	U
39	a	886	A
39	a	924	A
39	a	932	G
39	a	936	G
39	a	944	C
39	a	945	A
39	a	964	G
39	a	966	U
39	a	967	U
39	a	968	A
39	a	970	U
39	a	976	G
39	a	978	A
39	a	979	A
39	a	981	G

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Mol	Chain	Res	Type
39	a	985	A
39	a	986	G
39	a	987	A
39	a	993	A
39	a	1002	U
39	a	1003	G
39	a	1008	C
39	a	1009	C
39	a	1010	U
39	a	1011	C
39	a	1012	U
39	a	1013	G
39	a	1014	A
39	a	1016	A
39	a	1019	C
39	a	1020	C
39	a	1028	A
39	a	1030	G
39	a	1033	G
39	a	1034	U
39	a	1035	C
39	a	1044	G
39	a	1045	G
39	a	1046	G
39	a	1049	G
39	a	1050	A
39	a	1051	G
39	a	1054	A
39	a	1056	A
39	a	1074	G
39	a	1075	U
39	a	1104	G
39	a	1105	U
39	a	1111	A
39	a	1135	U
39	a	1140	A
39	a	1142	C
39	a	1145	U
39	a	1148	G
39	a	1149	U
39	a	1150	U
39	a	1155	A

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Mol	Chain	Res	Type
39	a	1166	A
39	a	1168	U
39	a	1176	A
39	a	1178	A
39	a	1193	G
39	a	1205	A
39	a	1206	A
39	a	1221	U
39	a	1222	A
39	a	1236	A
39	a	1238	A
39	a	1247	A
39	a	1262	G
39	a	1267	G
39	a	1269	G
39	a	1287	C
39	a	1289	A
39	a	1295	C
39	a	1296	A
39	a	1309	G
39	a	1311	U
39	a	1314	G
39	a	1329	C
39	a	1349	A
39	a	1355	A
39	a	1362	G
39	a	1373	U
39	a	1379	G
39	a	1398	C
39	a	1407	A
39	a	1435	A
39	a	1451	A
39	a	1455	A
39	a	1462	U
39	a	1463	A
39	a	1464	G
39	a	1497	G
39	a	1502	A
39	a	1503	A
39	a	1507	G
39	a	1513	A
39	a	1516	U

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Mol	Chain	Res	Type
39	a	1527	G
39	a	1529	A
39	a	1539	G
39	a	1540	G
39	a	1546	C

All (32) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	62	C
1	A	88	G
1	A	92	G
1	A	160	G
1	A	226	A
1	A	314	A
1	A	326	A
1	A	410	G
1	A	831	U
1	A	848	G
1	A	855	G
1	A	1202	A
1	A	1203	G
1	A	1250	G
1	A	1266	A
1	A	1339	A
1	A	1397	G
1	A	1507	U
1	A	1525	G
1	A	1528	U
1	A	1530	G
1	A	1535	U
1	A	1565	U
1	A	1784	A
1	A	2137	U
1	A	2337	G
1	A	2468	A
1	A	2805	A
2	B	37	A
2	B	48	G
2	B	49	G
20	V	22	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PSU	A	2718	1	18,21,22	0.98	1 (5%)	22,30,33	1.66	4 (18%)
1	OMG	A	2280	53,1	18,26,27	1.19	2 (11%)	19,38,41	0.89	1 (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
1	PSU	A	2718	1	-	2/7/25/26	0/2/2/2
1	OMG	A	2280	53,1	-	0/5/27/28	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2718	PSU	C6-C5	3.10	1.38	1.35
1	A	2280	OMG	C8-N7	-3.08	1.29	1.35
1	A	2280	OMG	C5-C6	-2.49	1.42	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2718	PSU	C4-N3-C2	-4.50	119.86	126.34
1	A	2718	PSU	N1-C2-N3	4.41	120.13	115.13
1	A	2280	OMG	O6-C6-C5	2.68	129.60	124.37
1	A	2718	PSU	O2-C2-N1	-2.32	120.24	122.79
1	A	2718	PSU	C6-N1-C2	-2.06	120.58	122.68

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	2718	PSU	O4'-C4'-C5'-O5'
1	A	2718	PSU	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 107 ligands modelled in this entry, 105 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
55	ATP	9	702	53	26,33,33	0.65	0	31,52,52	1.07	2 (6%)
55	ATP	9	701	53	26,33,33	0.63	0	31,52,52	1.05	2 (6%)

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
55	ATP	9	702	53	-	7/18/38/38	0/3/3/3
55	ATP	9	701	53	-	3/18/38/38	0/3/3/3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
55	9	701	ATP	C5-C6-N6	2.30	123.84	120.35
55	9	702	ATP	C5-C6-N6	2.26	123.79	120.35
55	9	702	ATP	PB-O3B-PG	2.02	139.77	132.83
55	9	701	ATP	O2'-C2'-C3'	-2.00	105.35	111.82

There are no chirality outliers.

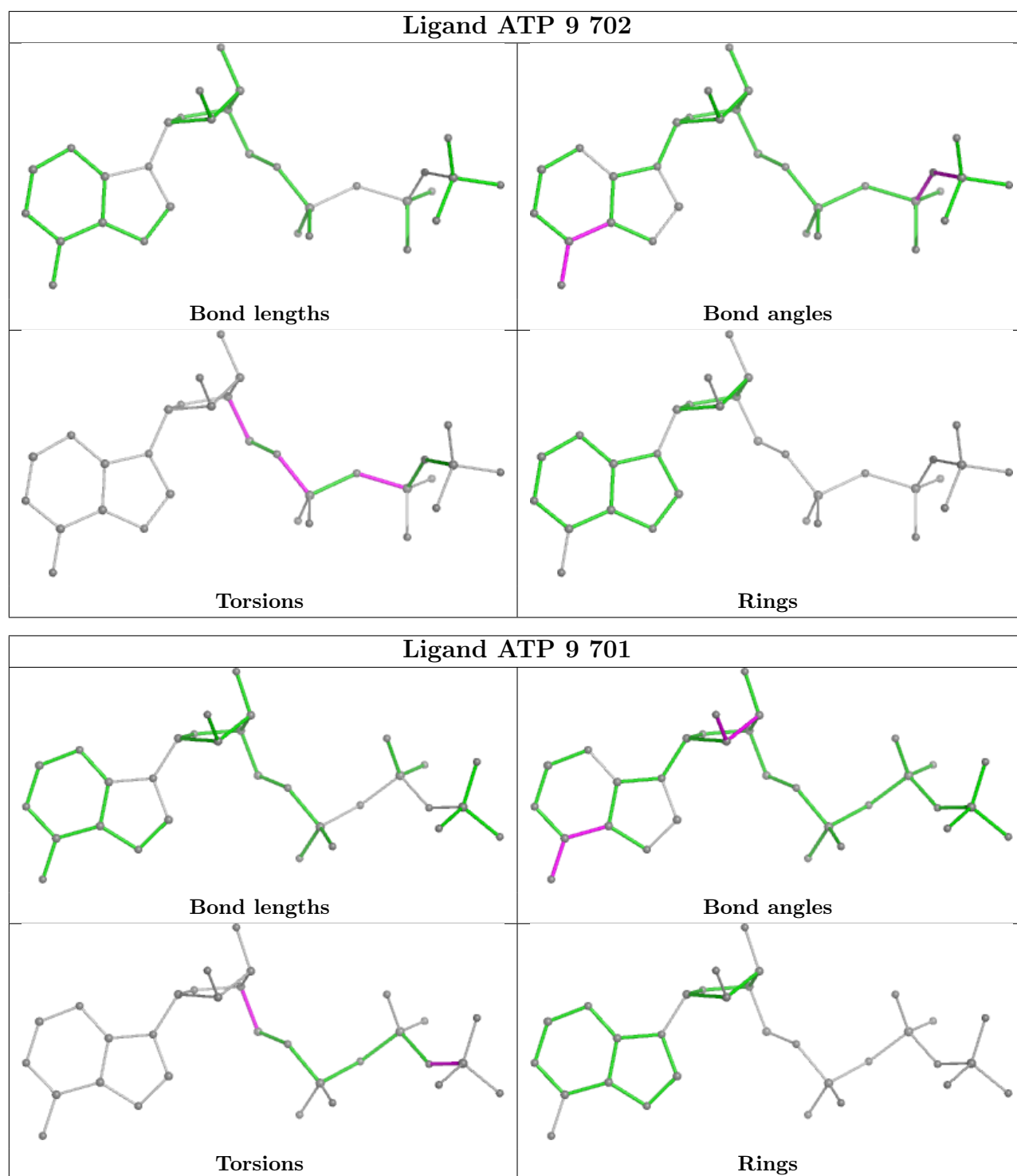
All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	9	701	ATP	PB-O3B-PG-O2G
55	9	701	ATP	O4'-C4'-C5'-O5'
55	9	702	ATP	C5'-O5'-PA-O2A
55	9	701	ATP	C3'-C4'-C5'-O5'
55	9	702	ATP	C3'-C4'-C5'-O5'
55	9	702	ATP	O4'-C4'-C5'-O5'
55	9	702	ATP	C5'-O5'-PA-O3A
55	9	702	ATP	PA-O3A-PB-O2B
55	9	702	ATP	C5'-O5'-PA-O1A
55	9	702	ATP	PA-O3A-PB-O1B

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

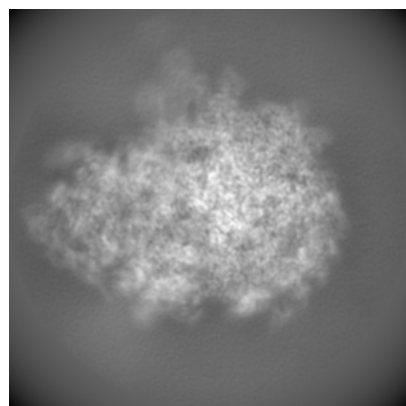
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-16246. These allow visual inspection of the internal detail of the map and identification of artifacts.

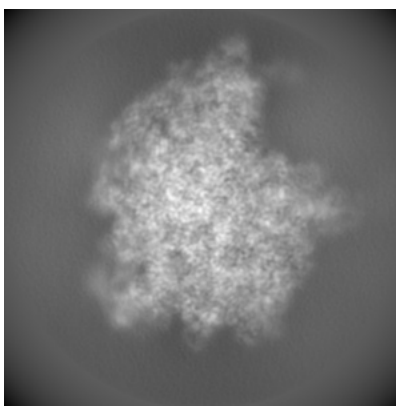
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

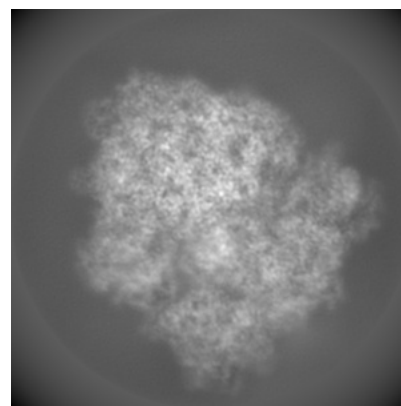
6.1.1 Primary map



X

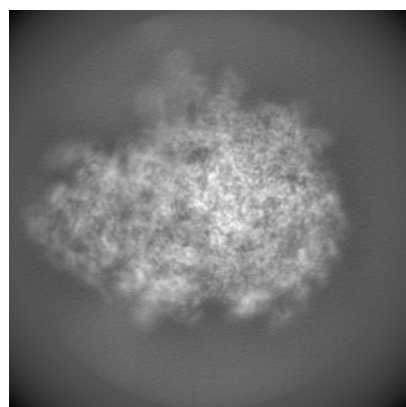


Y

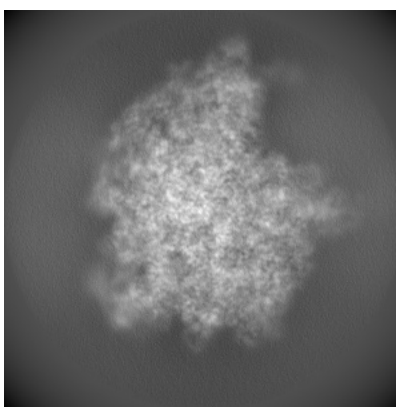


Z

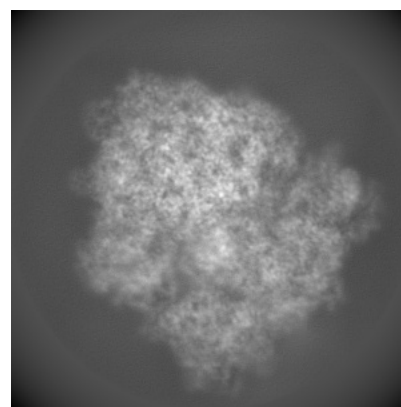
6.1.2 Raw map



X



Y

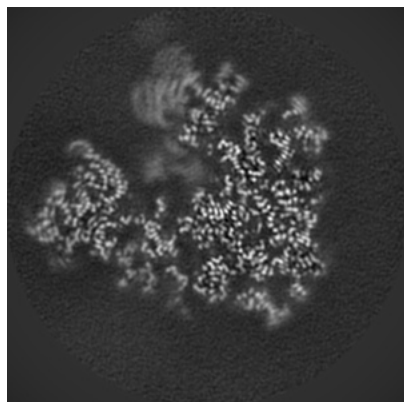


Z

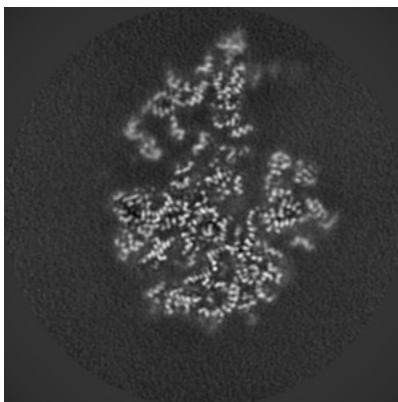
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

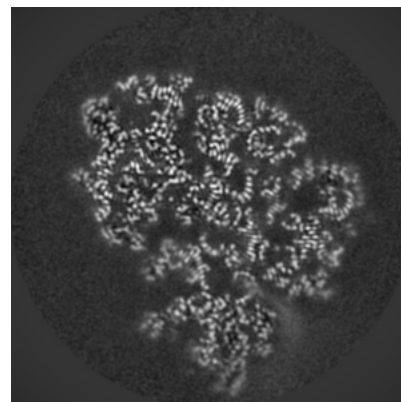
6.2.1 Primary map



X Index: 195

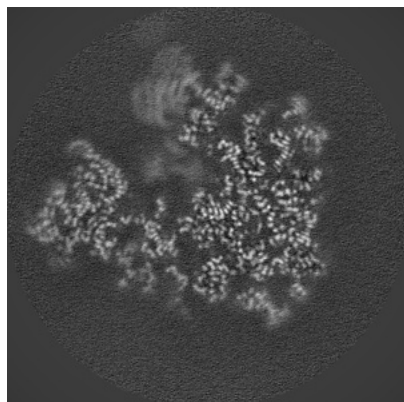


Y Index: 195

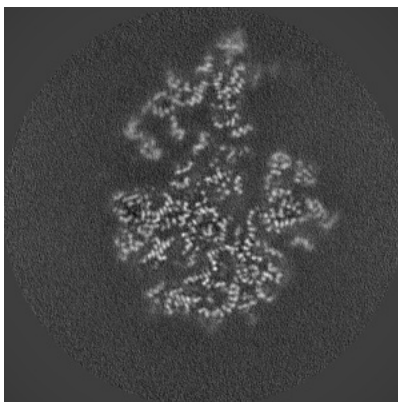


Z Index: 195

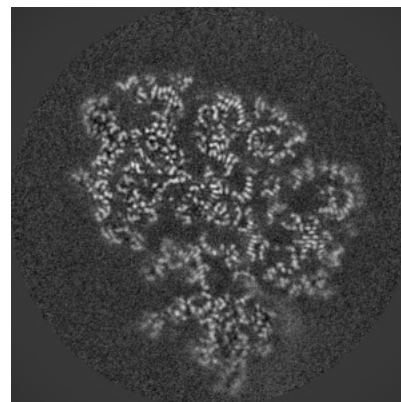
6.2.2 Raw map



X Index: 195



Y Index: 195

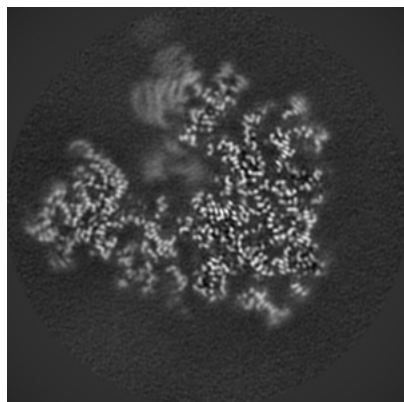


Z Index: 195

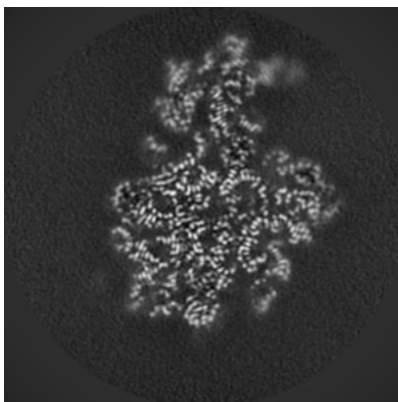
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

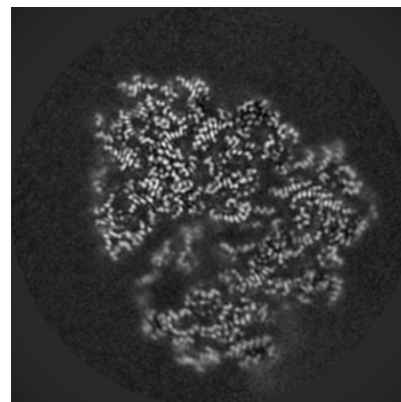
6.3.1 Primary map



X Index: 194

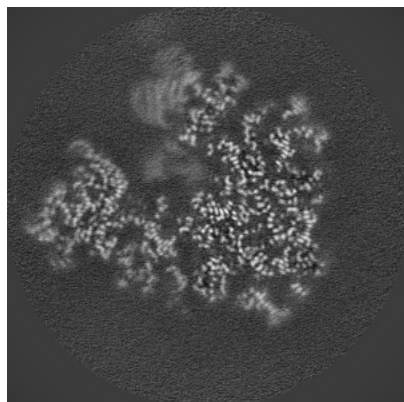


Y Index: 205

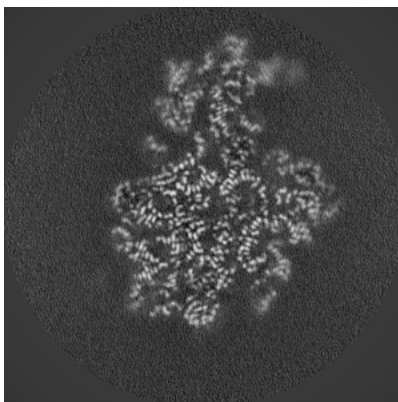


Z Index: 208

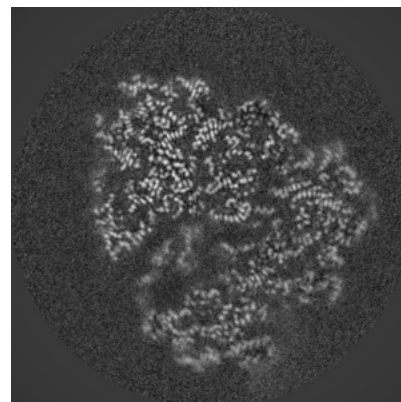
6.3.2 Raw map



X Index: 194



Y Index: 205



Z Index: 208

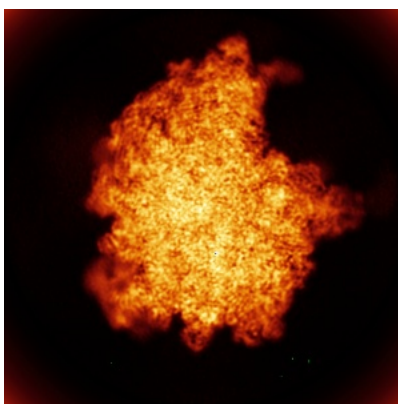
The images above show the largest variance slices of the map in three orthogonal directions.

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

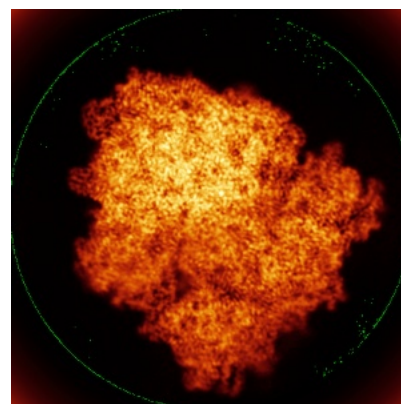
6.4.1 Primary map



X

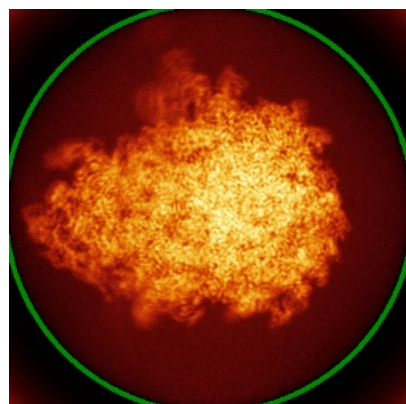


Y

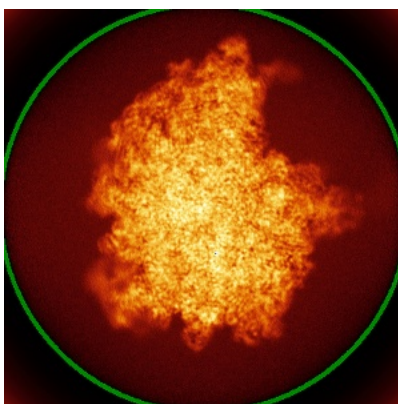


Z

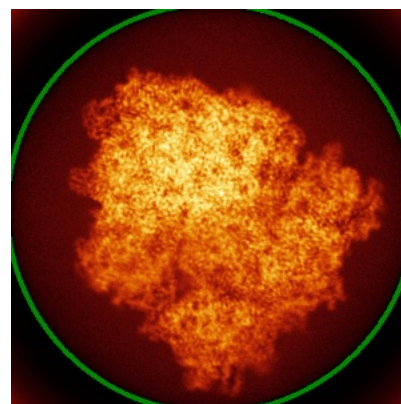
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

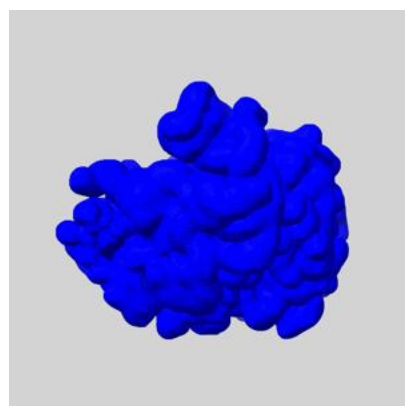
6.6 Mask visualisation [i](#)

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

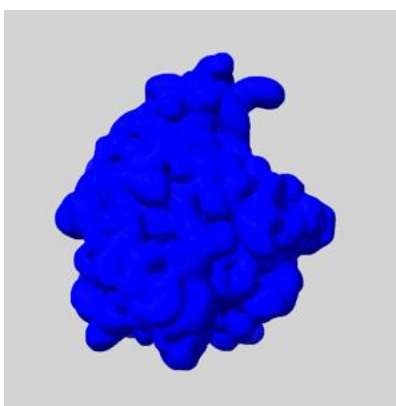
A mask typically either:

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

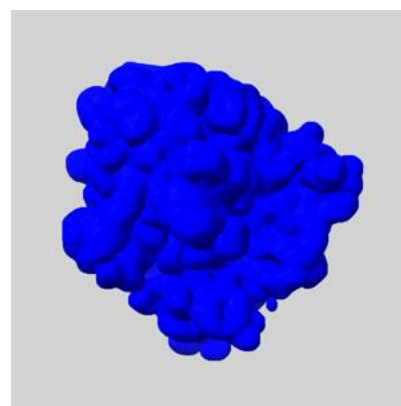
6.6.1 emd_16246_msk_1.map [i](#)



X



Y

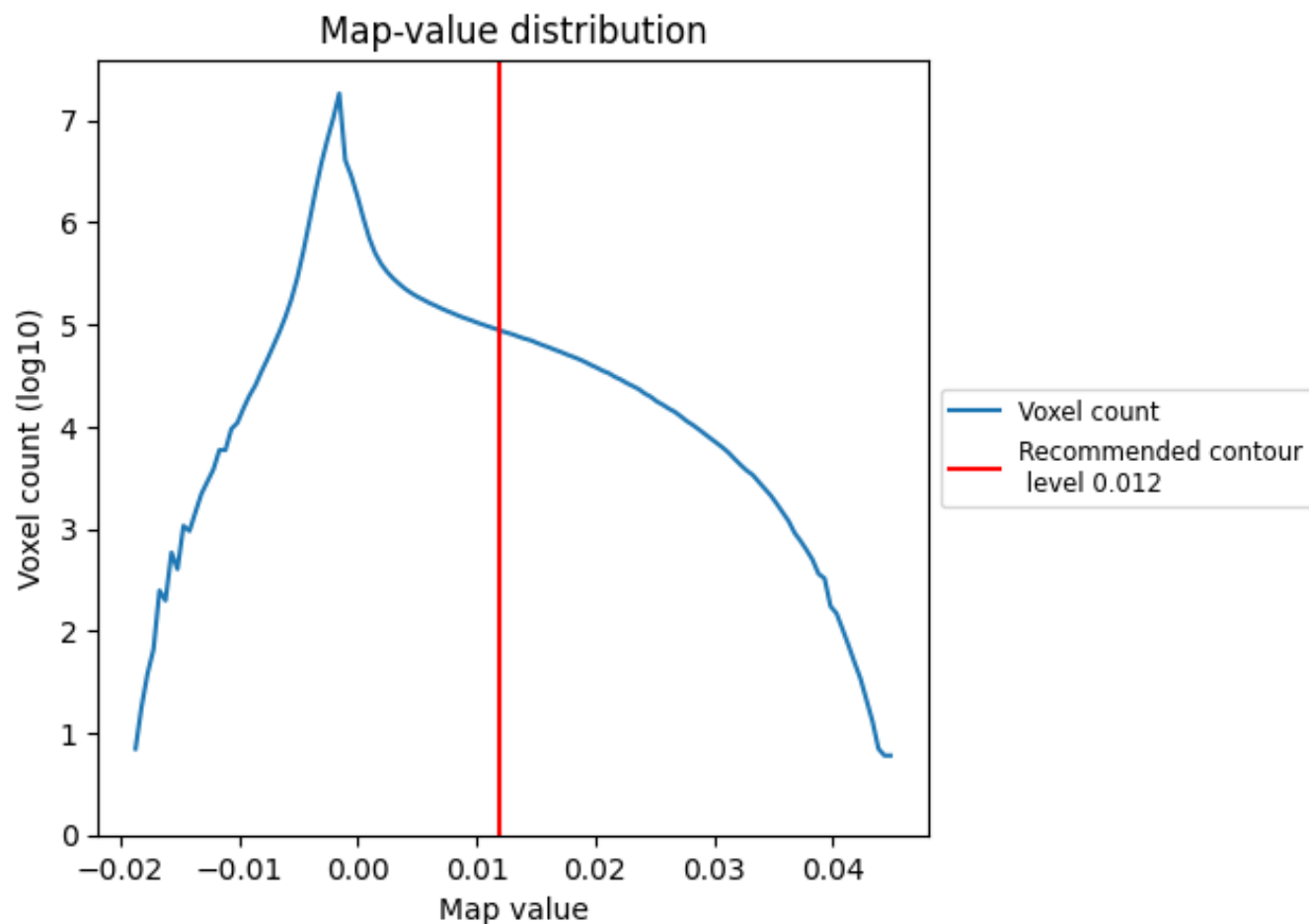


Z

7 Map analysis [i](#)

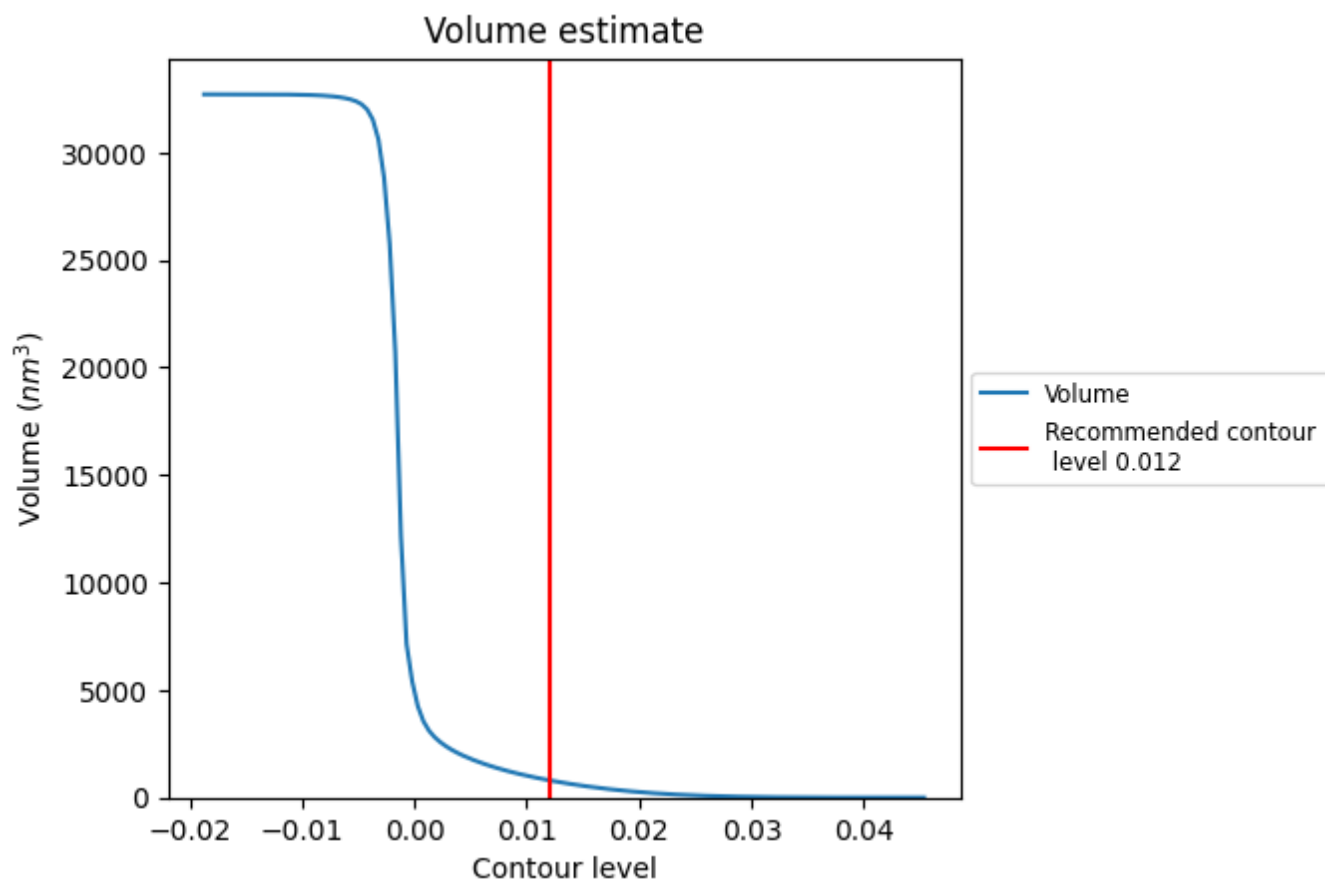
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

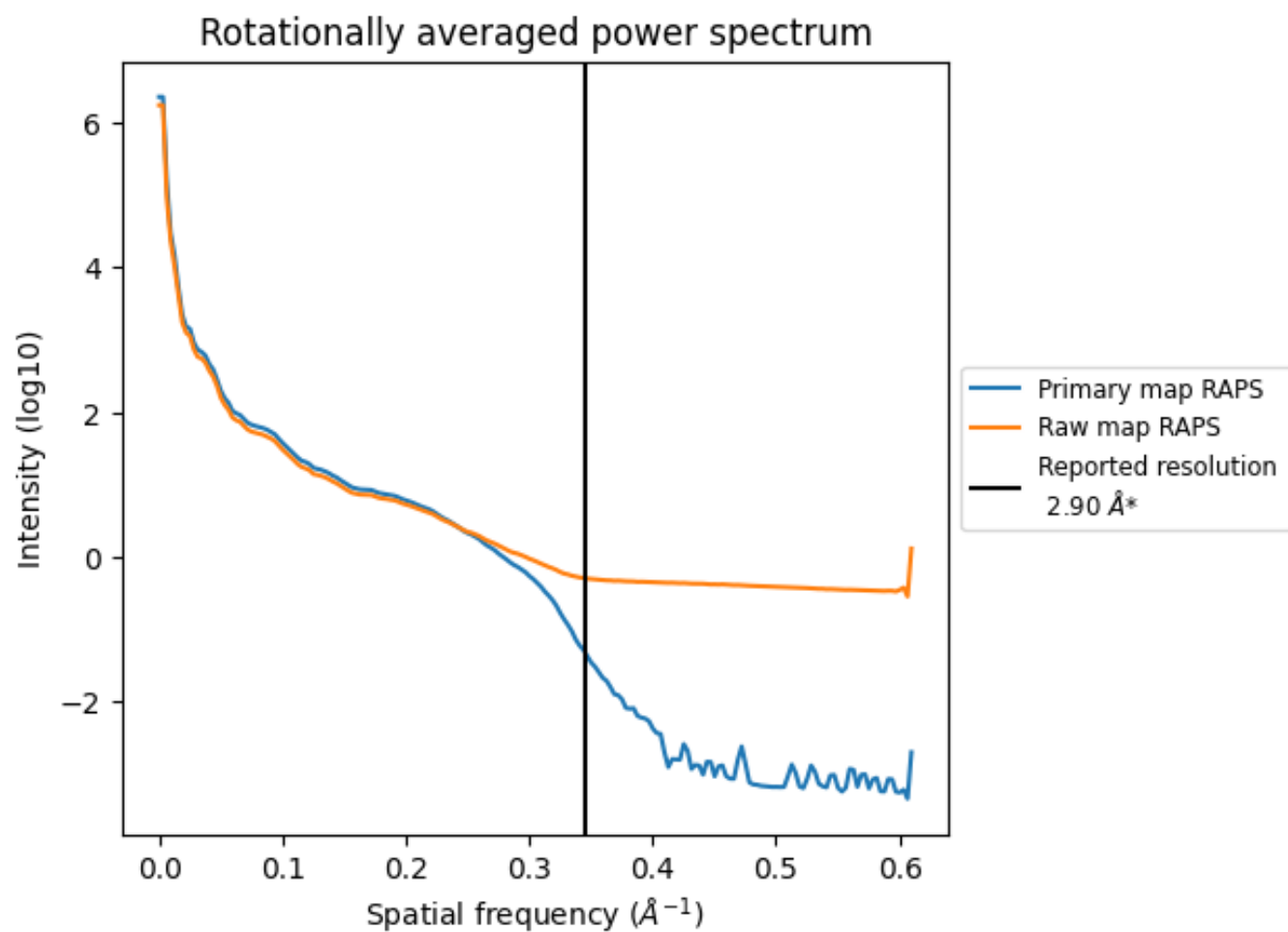
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 805 nm³; this corresponds to an approximate mass of 727 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 ⓘ

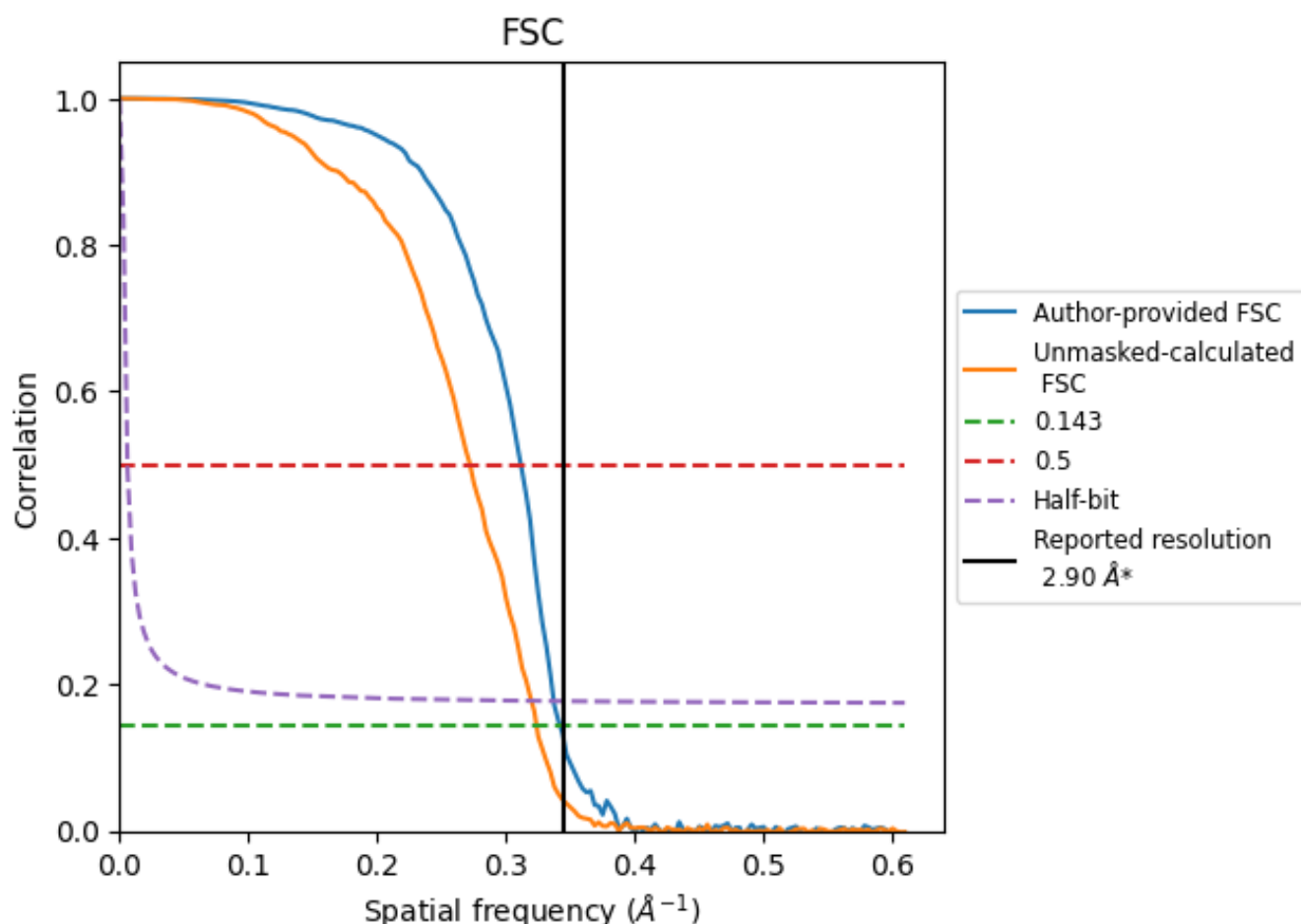


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 0.345 \AA^{-1}

8.2 Resolution estimates [i](#)

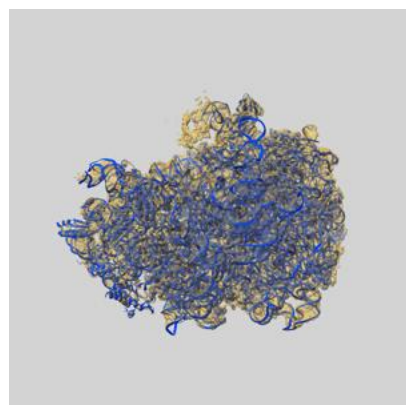
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	2.92	3.21	2.96
Unmasked-calculated*	3.09	3.67	3.13

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

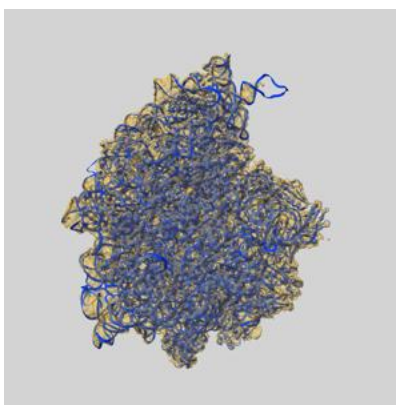
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-16246 and PDB model 8BUU. Per-residue inclusion information can be found in section [3](#) on page [15](#).

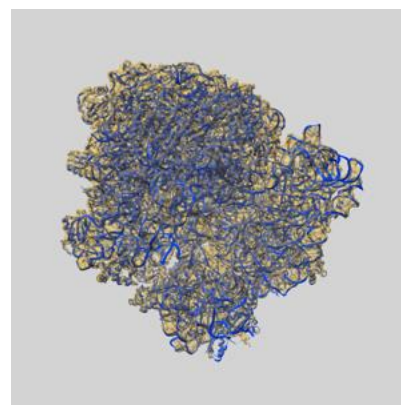
9.1 Map-model overlay [i](#)



X



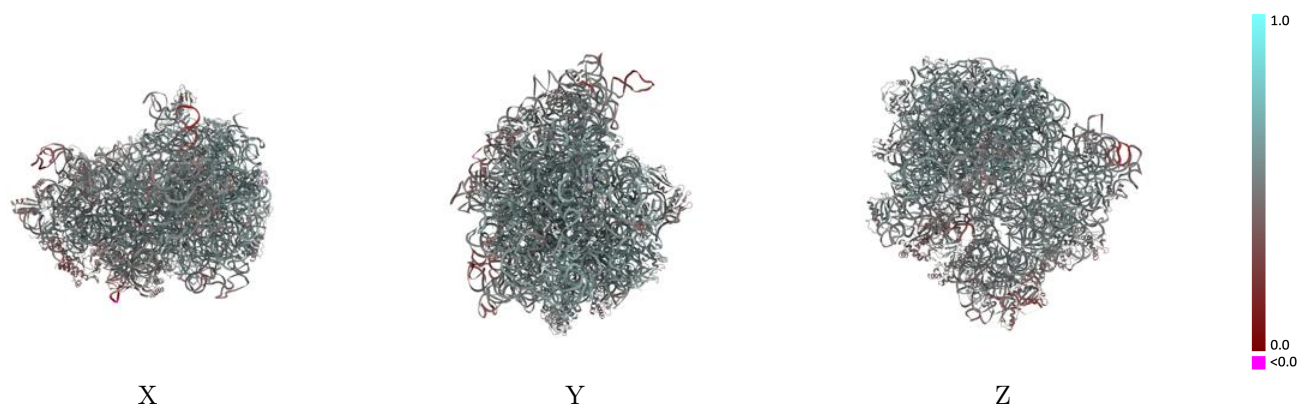
Y



Z

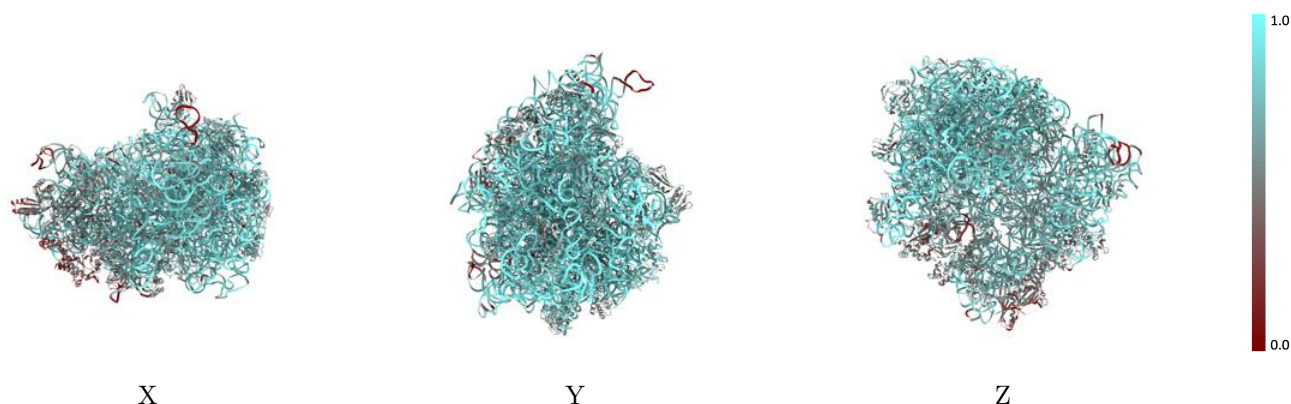
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



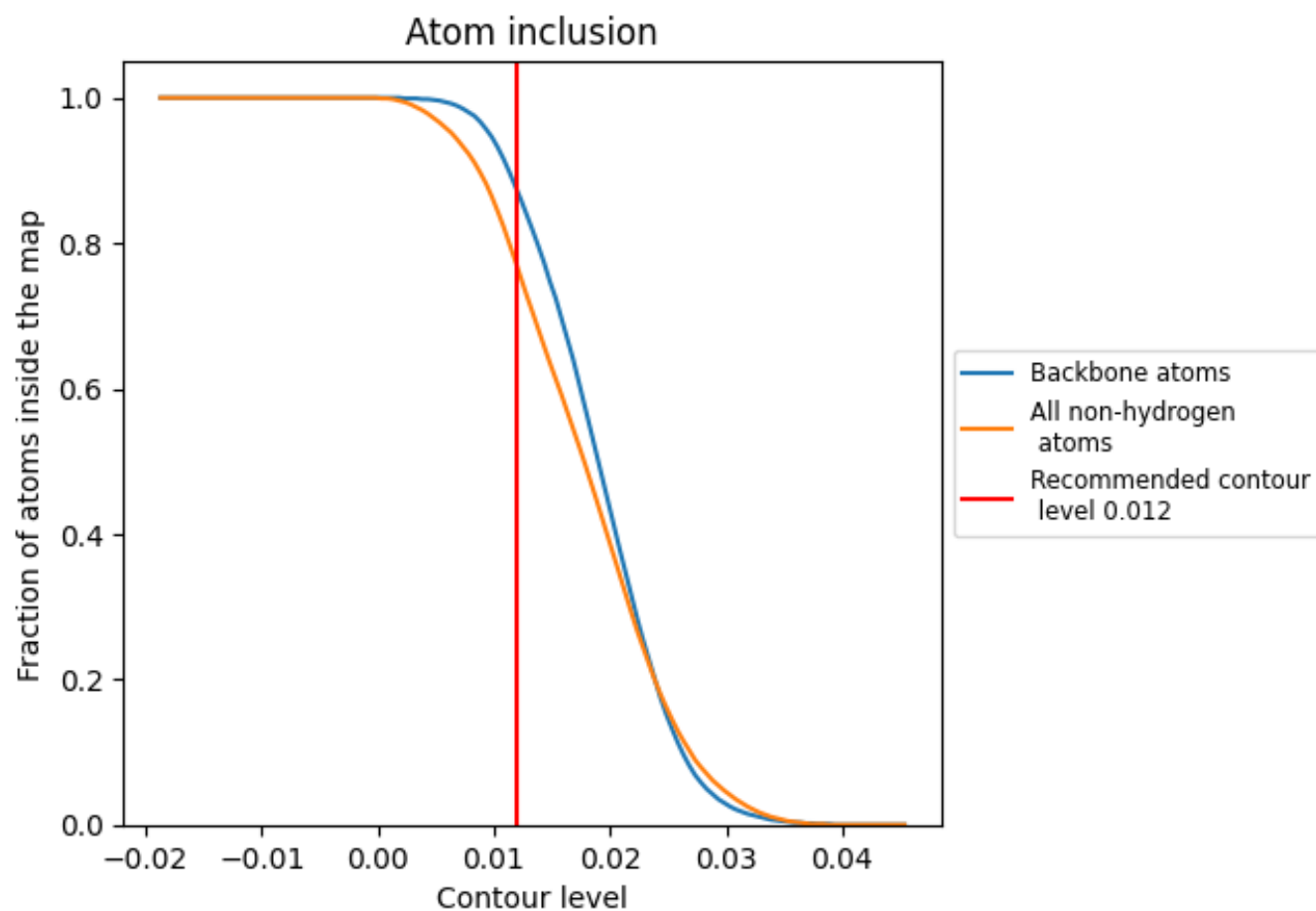
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.012).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ



































The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7680	 0.5140
0	 0.6760	 0.5010
1	 0.5650	 0.5280
2	 0.7600	 0.5670
3	 0.7050	 0.5600
4	 0.6850	 0.5440
9	 0.5270	 0.4710
A	 0.8770	 0.5330
B	 0.8600	 0.5030
C	 0.7190	 0.5560
D	 0.7180	 0.5550
E	 0.6920	 0.5310
F	 0.4210	 0.4170
G	 0.5430	 0.4620
J	 0.7250	 0.5460
K	 0.6440	 0.5540
L	 0.6610	 0.5360
M	 0.6910	 0.5360
N	 0.7070	 0.5370
O	 0.5640	 0.4650
P	 0.6580	 0.5370
Q	 0.7700	 0.5510
R	 0.7210	 0.5470
S	 0.6900	 0.5500
T	 0.6320	 0.5240
U	 0.5750	 0.5160
V	 0.7900	 0.4900
W	 0.6910	 0.5460
X	 0.5200	 0.5050
Y	 0.6240	 0.4700
Z	 0.6590	 0.5320
a	 0.8120	 0.5020
b	 0.2720	 0.3970
c	 0.4880	 0.4710
d	 0.4820	 0.4520



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
e	 0.5360	 0.4980
f	 0.4660	 0.4190
g	 0.5680	 0.4860
h	 0.5910	 0.4970
i	 0.5080	 0.4840
j	 0.3950	 0.4630
k	 0.5580	 0.4700
l	 0.6290	 0.5460
m	 0.4980	 0.4580
n	 0.5930	 0.5110
o	 0.5920	 0.4580
p	 0.5800	 0.4980
q	 0.5560	 0.5120
r	 0.4410	 0.4250
s	 0.4930	 0.4700
t	 0.5630	 0.4710
u	 0.6830	 0.4500