Full wwPDB EM Validation Report ⓘ

Apr 23, 2024 – 01:54 am BST

PDB ID	:	7NHL
EMDB ID	:	EMD-12332
Title	:	VgaA-LC, an antibiotic resistance ABCF, in complex with 70S ribosome from Staphylococcus aureus
Authors	:	Crowe-McAuliffe, C.; Murina, V.; Hauryliuk, V.; Wilson, D.N.
Deposited on	:	2021-02-10
Resolution	:	3.10 Å(reported)

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

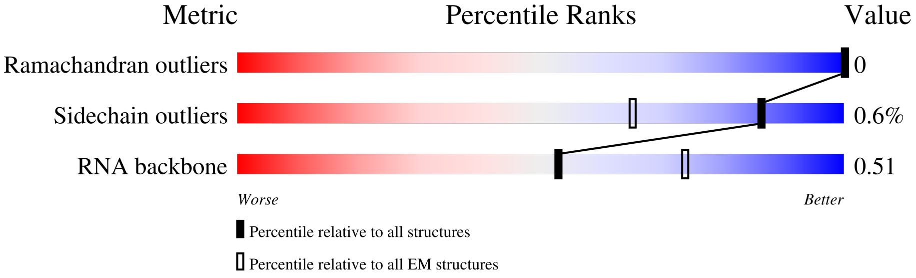
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

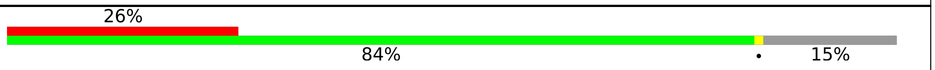
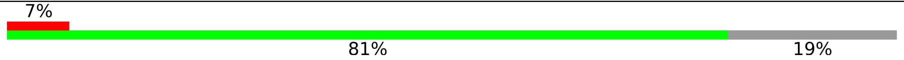
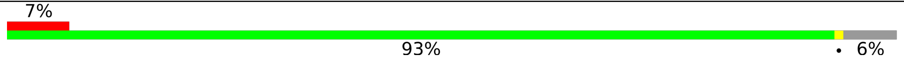
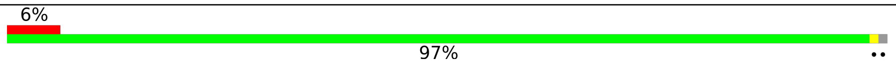
The reported resolution of this entry is 3.10 Å.

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 <=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	0	546	
2	D	76	
3	Z	94	
4	P	144	
5	A	2923	
6	a	1551	
7	B	115	
8	G	277	

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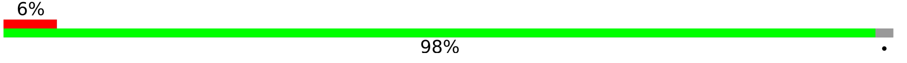
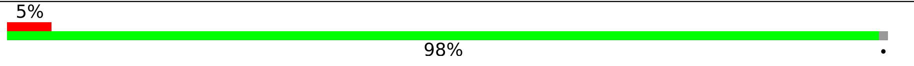
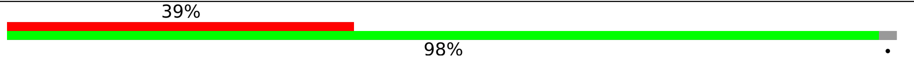
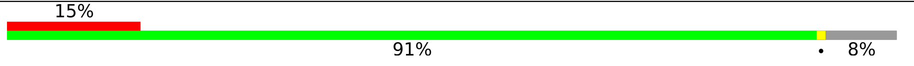
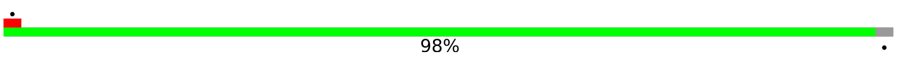
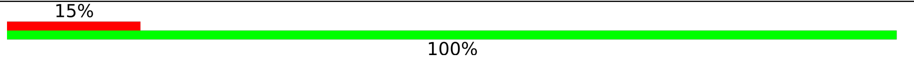
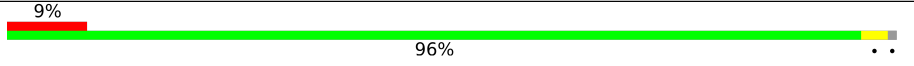
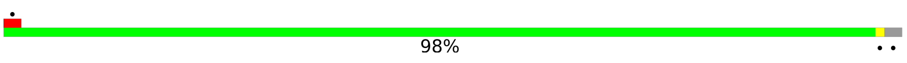
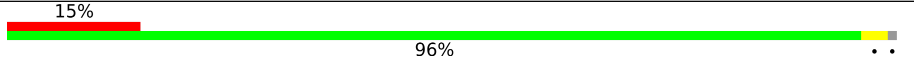
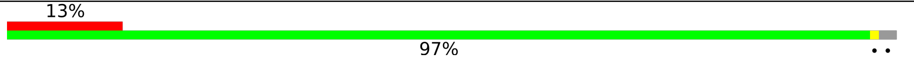
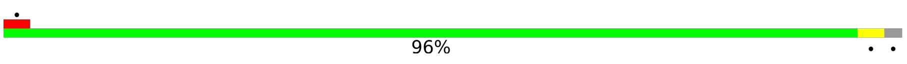
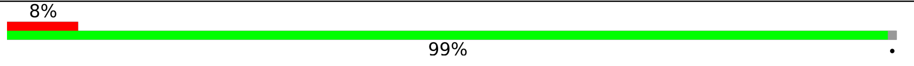
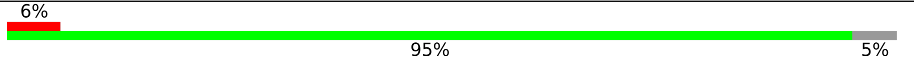
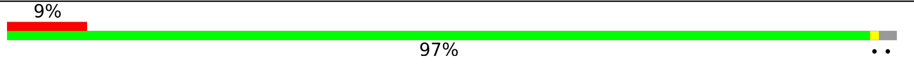
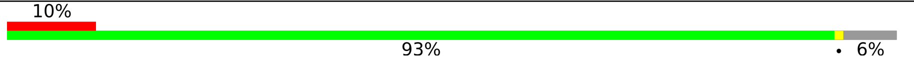
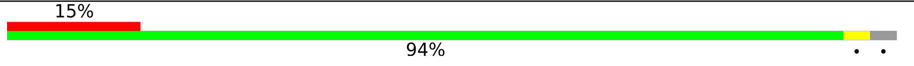
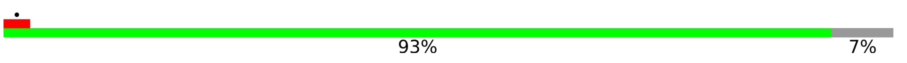
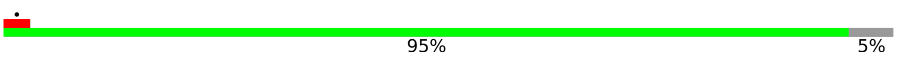
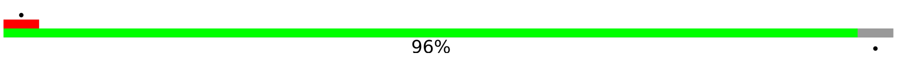
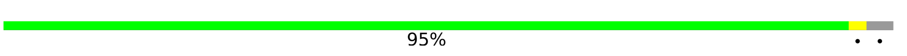
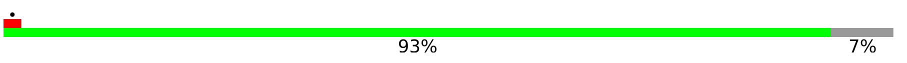
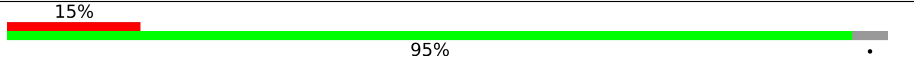
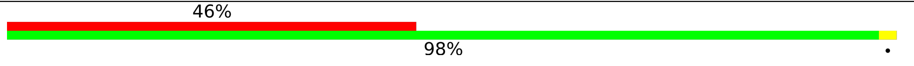
Mol	Chain	Length	Quality of chain
9	H	220	
10	I	207	
11	J	179	
12	K	178	
13	M	145	
14	N	122	
15	O	146	
16	Q	122	
17	R	119	
18	S	116	
19	T	118	
20	U	102	
21	V	117	
22	W	91	
23	X	105	
24	Y	217	
25	1	62	
26	2	69	
27	3	59	
28	6	49	
29	8	66	
30	7	45	
31	d	217	
32	e	200	
33	h	156	

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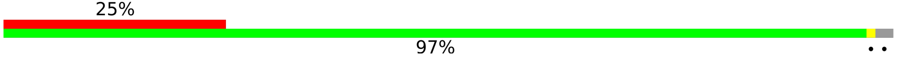
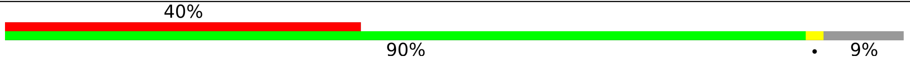
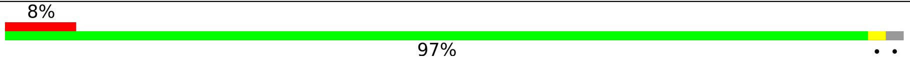
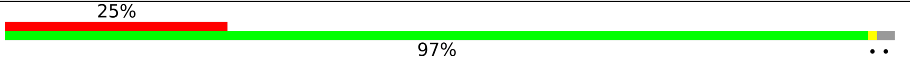
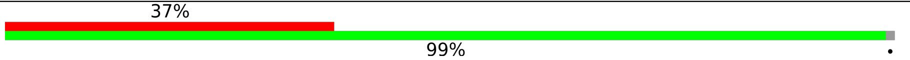
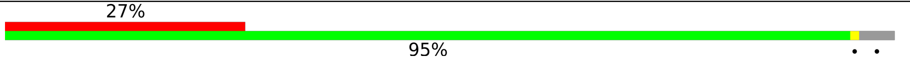
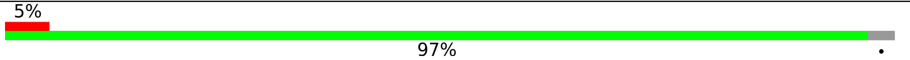
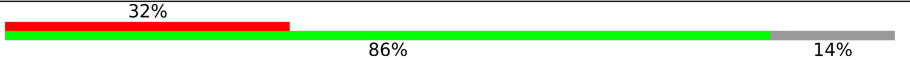
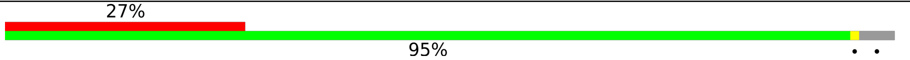
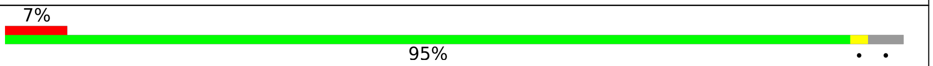
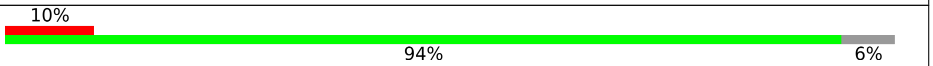
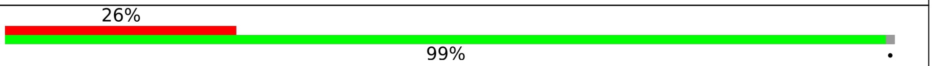
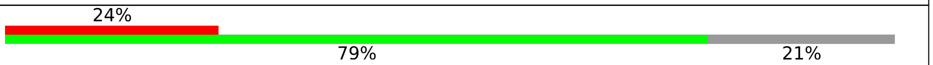
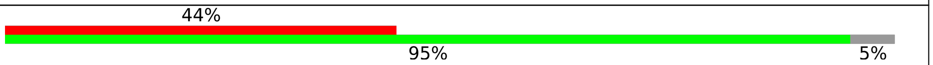
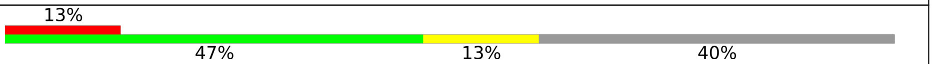
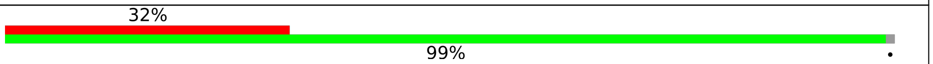
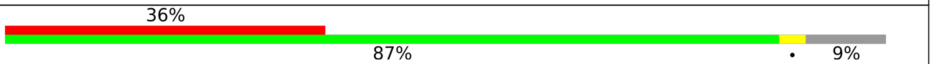
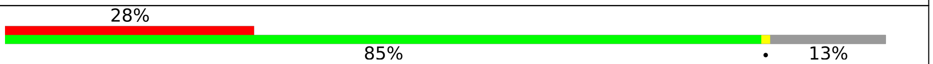
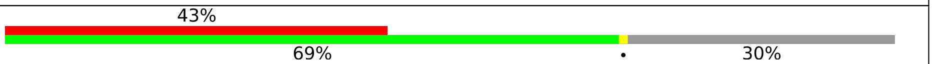
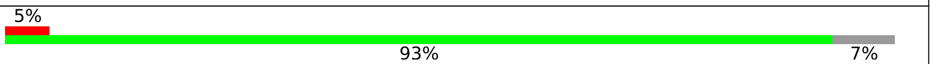
Mol	Chain	Length	Quality of chain
34	k	102	 25% 97%
35	l	129	 40% 90% 9%
36	o	60	 8% 97%
37	p	89	 25% 97%
38	q	91	 37% 99%
39	u	83	 27% 95%
40	9	37	 5% 97%
41	t	92	 32% 86% 14%
42	n	121	 27% 95%
43	j	132	 7% 95%
44	f	166	 10% 94% 6%
45	i	132	 26% 99%
46	s	80	 24% 79% 21%
47	g	98	 44% 95% 5%
48	b	15	 13% 47% 13% 40%
49	m	137	 32% 99%
50	r	87	 36% 87% 9%
51	c	255	 28% 85% 13%
52	4	84	 43% 69% 30%
53	5	57	 5% 93% 7%

2 Entry composition ⓘ

There are 57 unique types of molecules in this entry. The entry contains 145969 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 Lincosamide-streptogramin A resistance protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	0	465	3770	2397	659	707	7	0	0

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
0	105	GLN	GLU	engineered mutation	UNP A0SNL9
0	410	GLN	GLU	engineered mutation	UNP A0SNL9
0	523	GLY	-	expression tag	UNP A0SNL9
0	524	GLY	-	expression tag	UNP A0SNL9
0	525	ASP	-	expression tag	UNP A0SNL9
0	526	TYR	-	expression tag	UNP A0SNL9
0	527	LYS	-	expression tag	UNP A0SNL9
0	528	ASP	-	expression tag	UNP A0SNL9
0	529	HIS	-	expression tag	UNP A0SNL9
0	530	ASP	-	expression tag	UNP A0SNL9
0	531	GLY	-	expression tag	UNP A0SNL9
0	532	ASP	-	expression tag	UNP A0SNL9
0	533	TYR	-	expression tag	UNP A0SNL9
0	534	LYS	-	expression tag	UNP A0SNL9
0	535	ASP	-	expression tag	UNP A0SNL9
0	536	HIS	-	expression tag	UNP A0SNL9
0	537	ASP	-	expression tag	UNP A0SNL9
0	538	ILE	-	expression tag	UNP A0SNL9
0	539	ASP	-	expression tag	UNP A0SNL9
0	540	TYR	-	expression tag	UNP A0SNL9
0	541	LYS	-	expression tag	UNP A0SNL9
0	542	ASP	-	expression tag	UNP A0SNL9
0	543	ASP	-	expression tag	UNP A0SNL9
0	544	ASP	-	expression tag	UNP A0SNL9
0	545	ASP	-	expression tag	UNP A0SNL9
0	546	LYS	-	expression tag	UNP A0SNL9

- Molecule 2 is a RNA chain called P-tRNA fMet.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	D	73	1562	696	284	509	73	0	0

- Molecule 3 is a protein called 50S ribosomal protein L27.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	Z	76	585	361	114	110	0	0

- Molecule 4 is a protein called 50S ribosomal protein L16.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	P	135	1081	693	205	180	3	0	0

- Molecule 5 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
5	A	2914	62482	27895	11429	20244	2914	0	0

- Molecule 6 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	a	1538	32937	14706	6006	10687	1538	0	0

- Molecule 7 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	B	113	2408	1076	431	788	113	0	0

- Molecule 8 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	G	273	2085	1297	413	370	5	0	0

- Molecule 9 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	H	216	1637	1024	301	307	5	0	0

- Molecule 10 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	I	204	1564	981	286	295	2	0	0

- Molecule 11 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	J	175	1381	876	237	261	7	0	0

- Molecule 12 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	K	164	1284	799	232	250	3	0	0

- Molecule 13 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	M	142	1127	704	205	216	2	0	0

- Molecule 14 is a protein called 50S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	N	122	920	572	174	170	4	0	0

- Molecule 15 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	O	145	1090	674	214	201	1	0	0

- Molecule 16 is a protein called 50S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	120	Total	C	N	O	S	0	0
			952	584	182	185	1		

- Molecule 17 is a protein called 50S ribosomal protein L18.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	118	Total	C	N	O	0	0
			914	569	173	172		

- Molecule 18 is a protein called 50S ribosomal protein L19.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	S	114	Total	C	N	O	0	0
			922	580	185	157		

- Molecule 19 is a protein called 50S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	116	Total	C	N	O	S	0	0
			943	593	189	157	4		

- Molecule 20 is a protein called 50S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	101	Total	C	N	O	S	0	0
			793	503	141	148	1		

- Molecule 21 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	111	Total	C	N	O	S	0	0
			853	532	163	155	3		

- Molecule 22 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	89	Total	C	N	O	S	0	0
			725	457	130	134	4		

- Molecule 23 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X	99	761	480	140	139	2	0	0

- Molecule 24 is a protein called 50S ribosomal protein L25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	Y	94	738	471	131	134	2	0	0

- Molecule 25 is a protein called 50S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	1	60	474	293	103	77	1	0	0

- Molecule 26 is a protein called 50S ribosomal protein L29.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	2	64	527	324	99	104	0	0

- Molecule 27 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
27	3	56	436	271	82	83	0	0

- Molecule 28 is a protein called 50S ribosomal protein L33 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	6	47	389	232	79	74	4	0	0

- Molecule 29 is a protein called 50S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	8	64	521	324	113	82	2	0	0

- Molecule 30 is a protein called 50S ribosomal protein L34.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	7	42	360	220	88	51	1	0	0

- Molecule 31 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	208	1638	1032	306	298	2	0	0

- Molecule 32 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	e	199	1617	1020	302	293	2	0	0

- Molecule 33 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	h	138	1101	686	208	203	4	0	0

- Molecule 34 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
34	k	100	801	505	147	148	1	0	0

- Molecule 35 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	l	118	876	542	166	165	3	0	0

- Molecule 36 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	o	59	496	314	99	78	5	0	0

- Molecule 37 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	p	87	Total	C	N	O	S	0	0
			733	451	152	129	1		

- Molecule 38 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	q	90	Total	C	N	O	S	0	0
			712	448	132	131	1		

- Molecule 39 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	u	80	Total	C	N	O	S	0	0
			606	367	119	118	2		

- Molecule 40 is a protein called 50S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	9	36	Total	C	N	O	S	0	0
			292	184	59	44	5		

- Molecule 41 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	t	79	Total	C	N	O	S	0	0
			646	416	116	112	2		

- Molecule 42 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	116	Total	C	N	O	S	0	0
			922	566	183	172	1		

- Molecule 43 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	j	127	Total	C	N	O	S	0	0
			1008	624	201	182	1		

- Molecule 44 is a protein called 30S ribosomal protein S5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	f	156	1160	730	213	215	2	0	0

- Molecule 45 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	i	131	1032	652	183	193	4	0	0

- Molecule 46 is a protein called 30S ribosomal protein S18.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	s	63	516	330	96	87	3	0	0

- Molecule 47 is a protein called 30S ribosomal protein S6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	g	93	773	489	136	146	2	0	0

- Molecule 48 is a RNA chain called RNA (5’-R(P*GP*GP*AP*GP*GP*UP*AP*UP*G)-3’).

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

- Molecule 49 is a protein called 30S ribosomal protein S12.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	m	135	1058	658	214	184	2	0	0

- Molecule 50 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	r	79	651	413	116	121	1	0	0

- Molecule 51 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms	AltConf	Trace
51	c	221	Total C N O S 1781 1136 310 328 7	0	0

- Molecule 52 is a protein called 50S ribosomal protein L31 type B.

Mol	Chain	Residues	Atoms	AltConf	Trace
52	4	59	Total C N O S 486 310 88 87 1	0	0

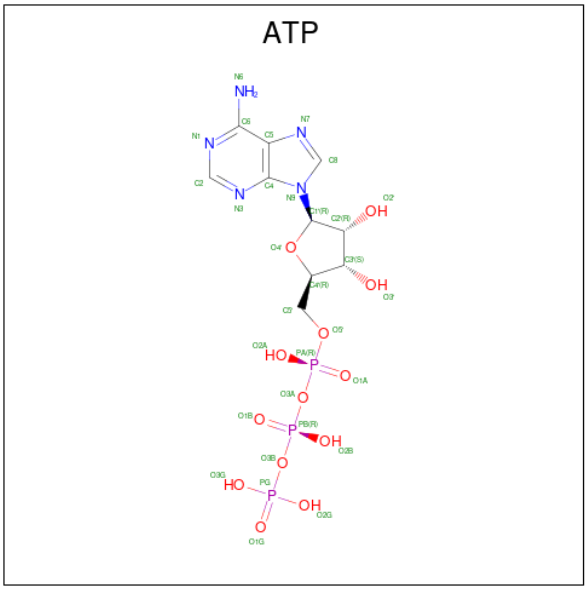
- Molecule 53 is a protein called 50S ribosomal protein L32.

Mol	Chain	Residues	Atoms	AltConf	Trace
53	5	53	Total C N O S 422 256 86 75 5	0	0

- Molecule 54 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
54	0	2	Total Mg 2 2	0
54	A	115	Total Mg 115 115	0
54	a	19	Total Mg 19 19	0
54	G	1	Total Mg 1 1	0
54	O	1	Total Mg 1 1	0

- Molecule 55 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 56 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
56	P	1	1	1	0
56	A	15	15	15	0
56	a	2	2	2	0

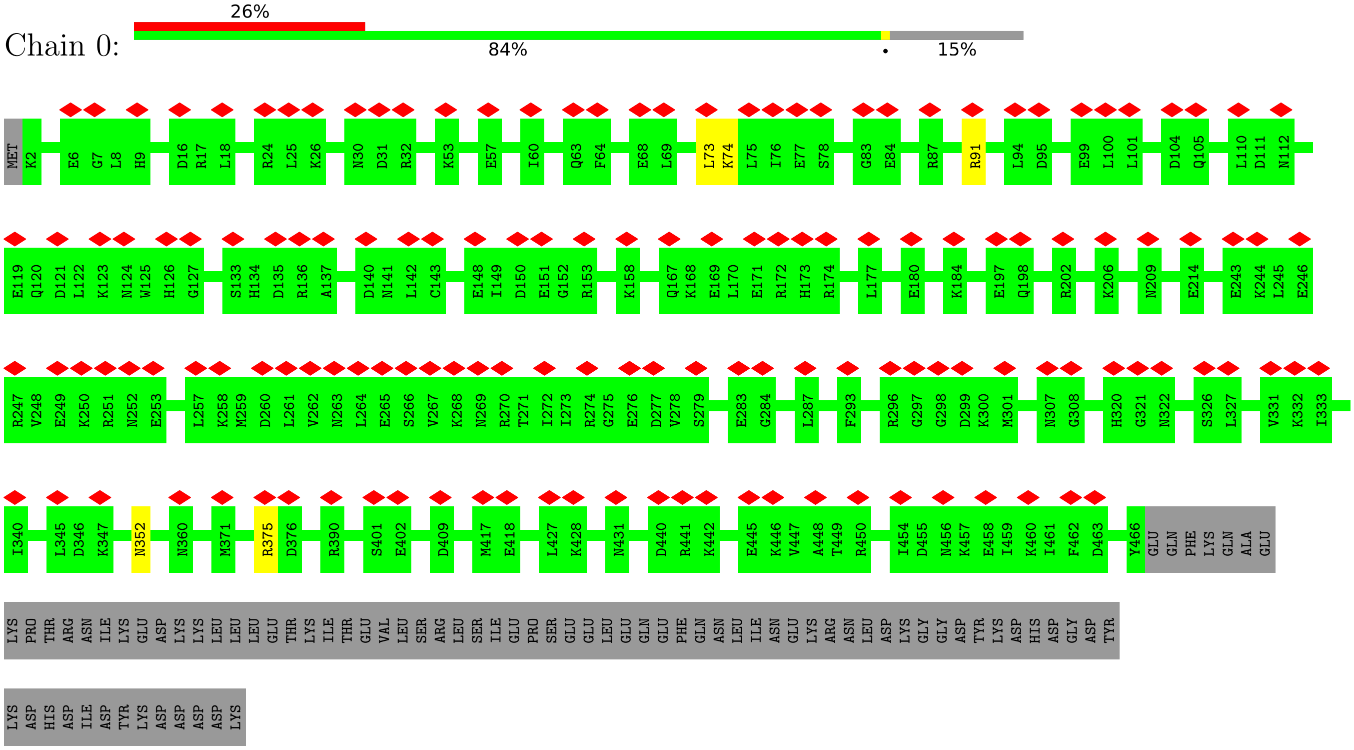
- Molecule 57 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
57	6	1	1	1	0
57	o	1	1	1	0
57	9	1	1	1	0
57	5	1	1	1	0

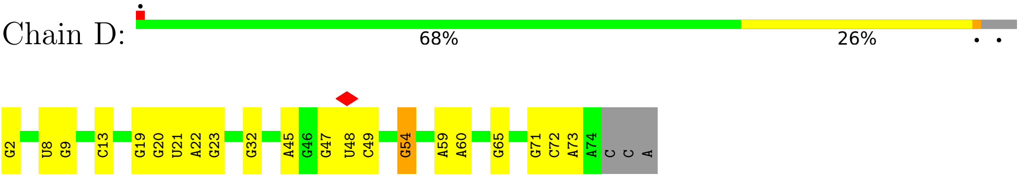
3 Residue-property plots (i)

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.

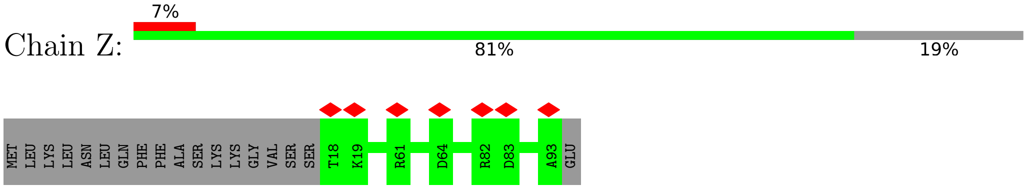
- Molecule 1: Lincosamide-streptogramin A resistance protein



- Molecule 2: P-tRNA fMet

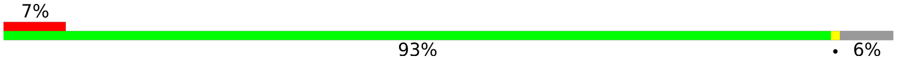


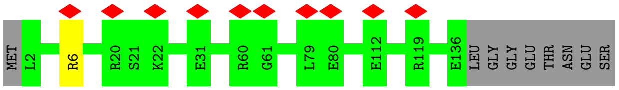
- Molecule 3: 50S ribosomal protein L27



- Molecule 4: 50S ribosomal protein L16

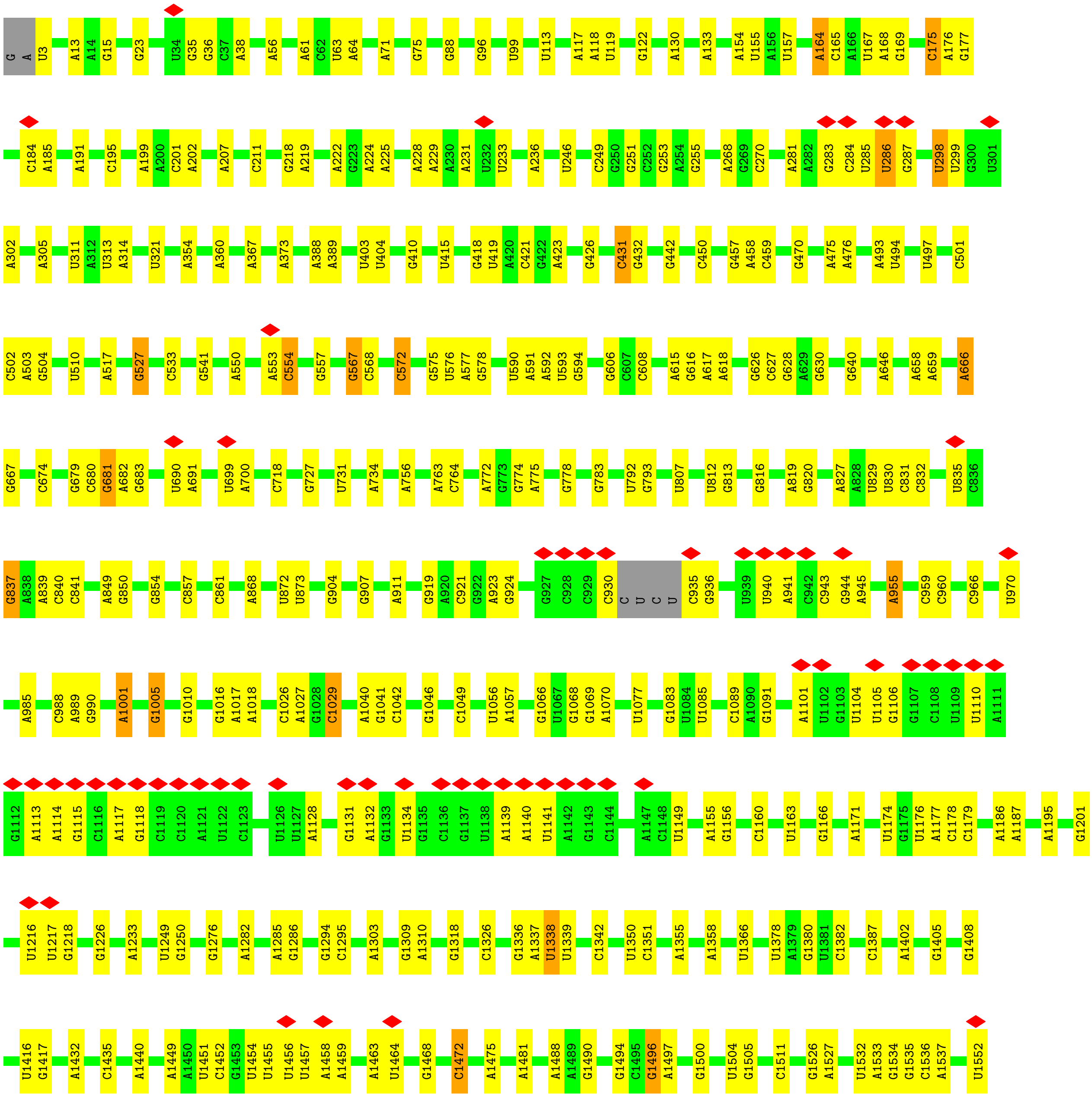
Chain P:

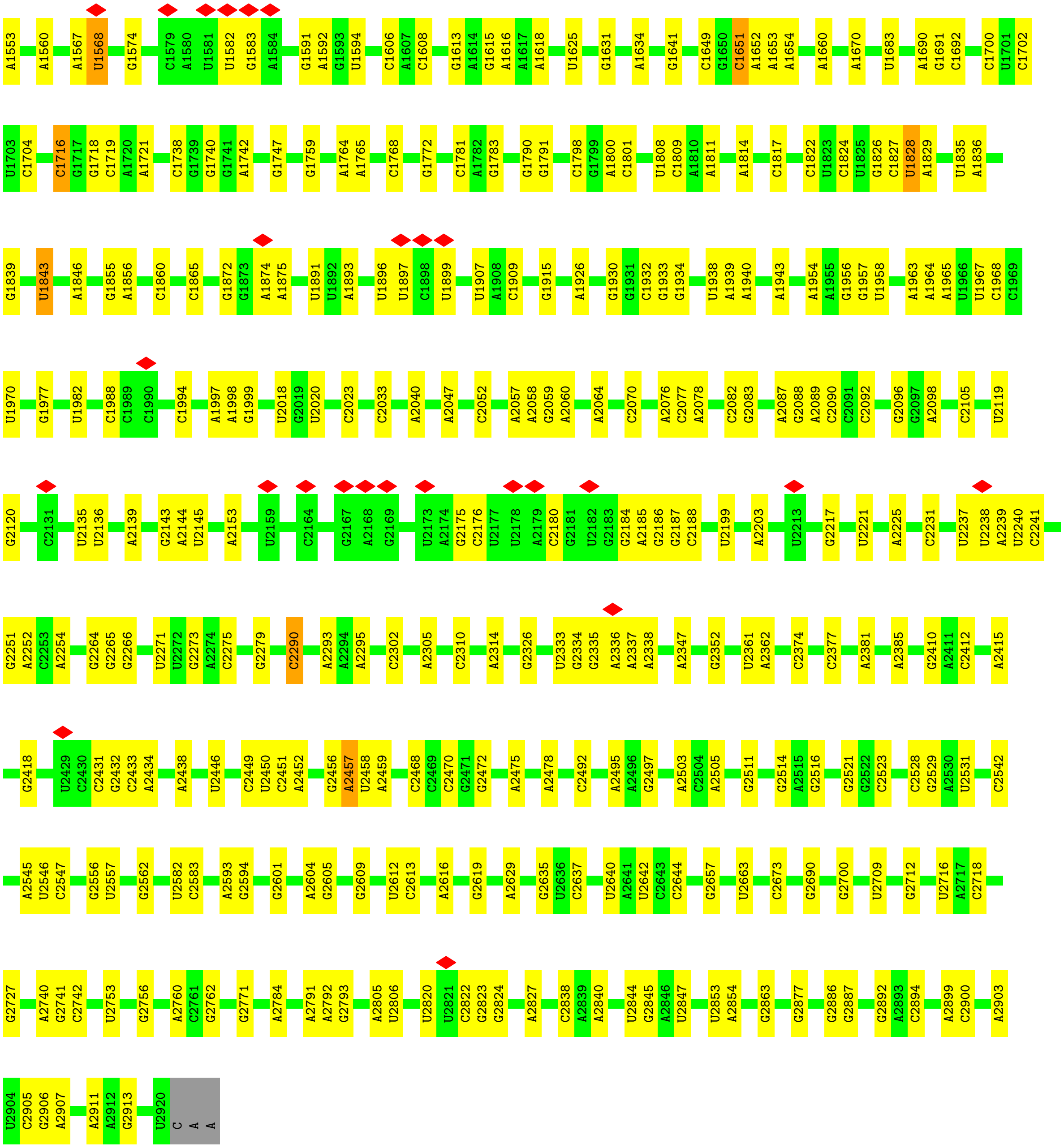




- Molecule 5: 23S rRNA

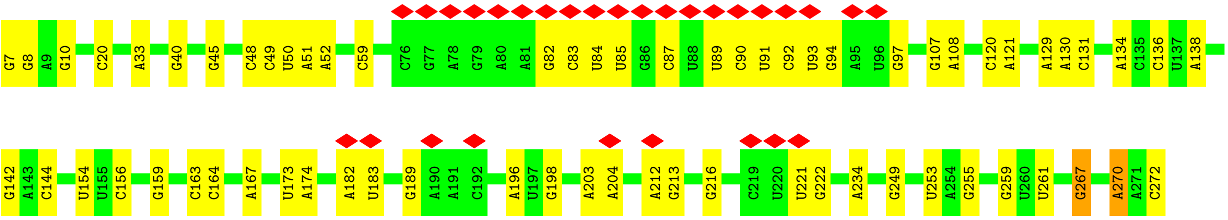
Chain A:

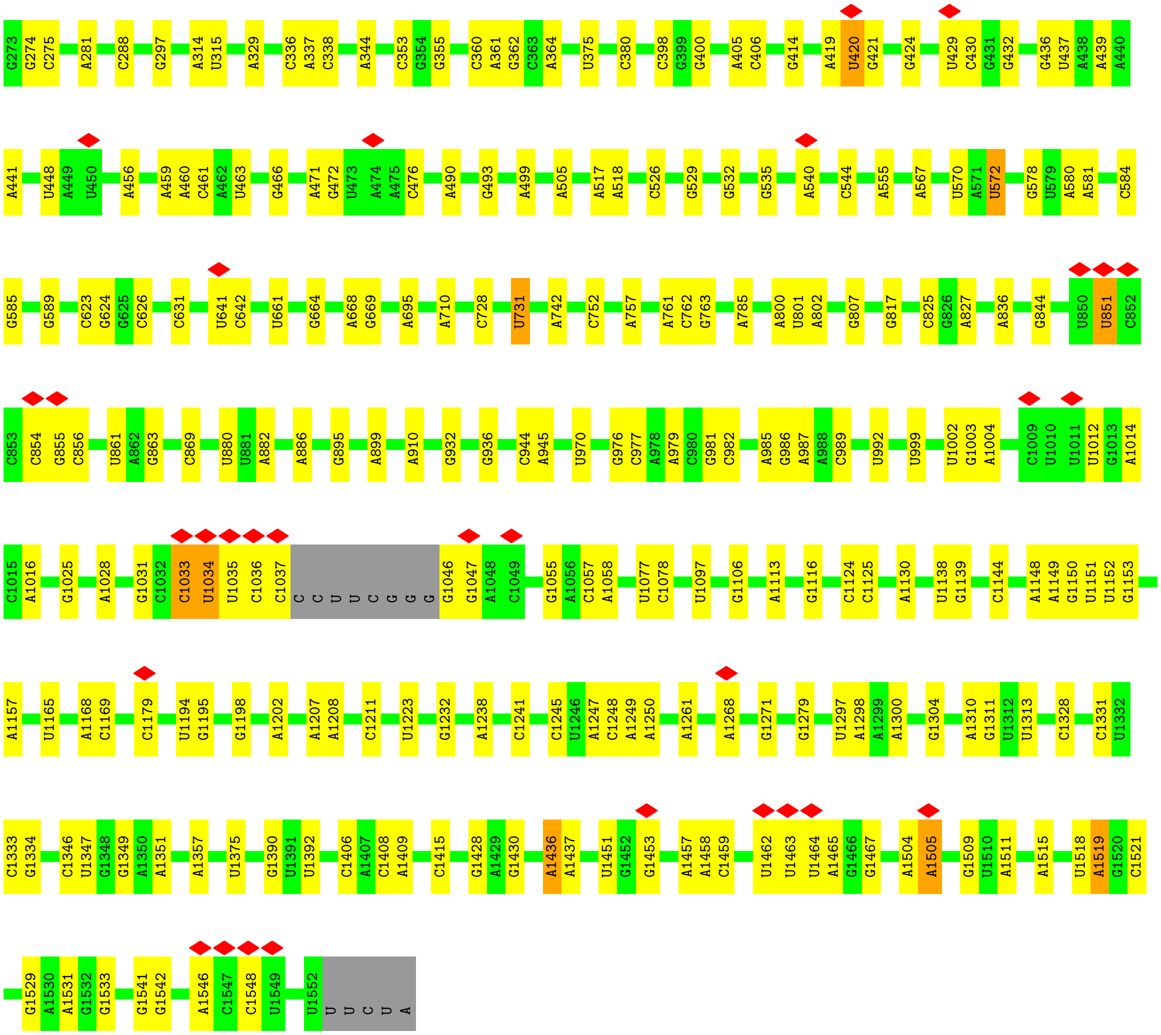




- Molecule 6: 16S rRNA

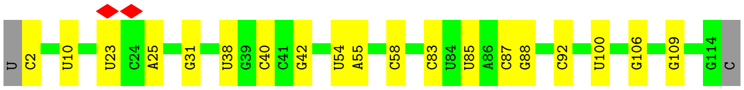
Chain a:





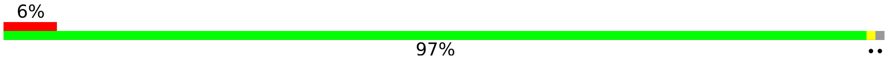
- Molecule 7: 5S rRNA

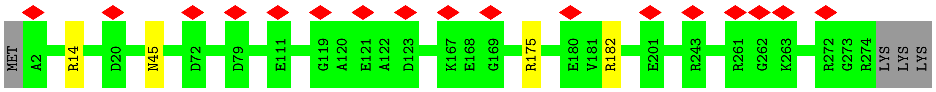
Chain B:



- Molecule 8: 50S ribosomal protein L2

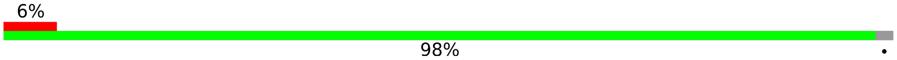
Chain G:

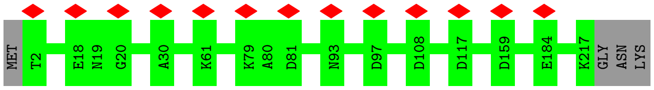




- Molecule 9: 50S ribosomal protein L3

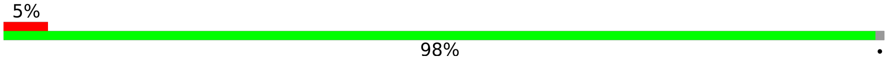
Chain H:

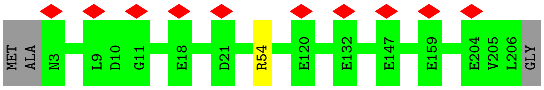




- Molecule 10: 50S ribosomal protein L4

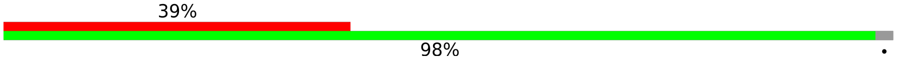
Chain I:

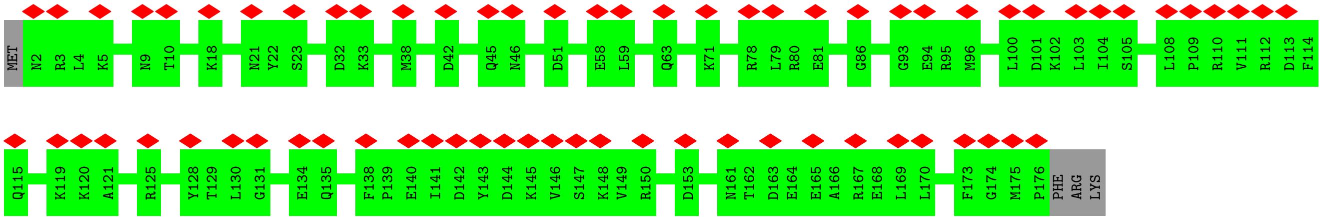




- Molecule 11: 50S ribosomal protein L5

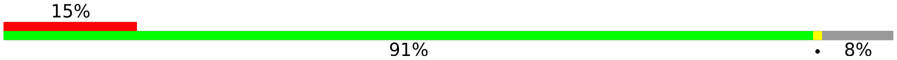
Chain J:

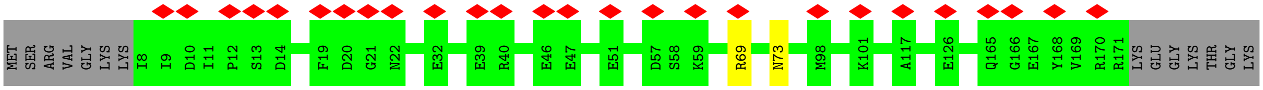




- Molecule 12: 50S ribosomal protein L6

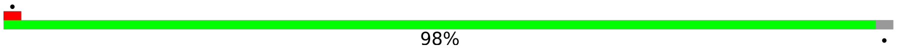
Chain K:

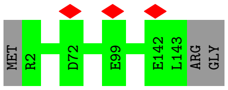




- Molecule 13: 50S ribosomal protein L13

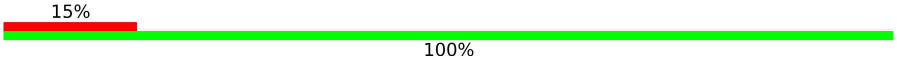
Chain M:

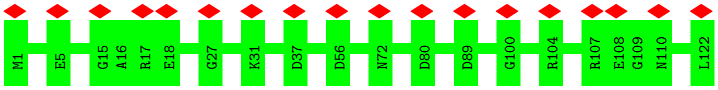




- Molecule 14: 50S ribosomal protein L14

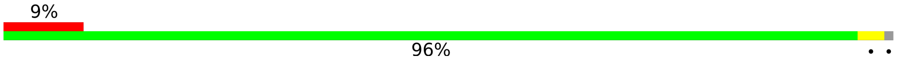
Chain N:





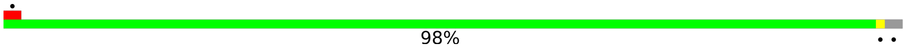
- Molecule 15: 50S ribosomal protein L15

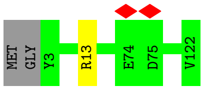
Chain O:



- Molecule 16: 50S ribosomal protein L17

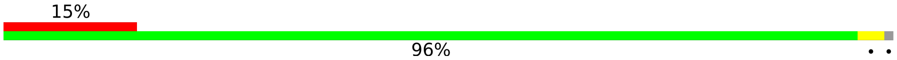
Chain Q:

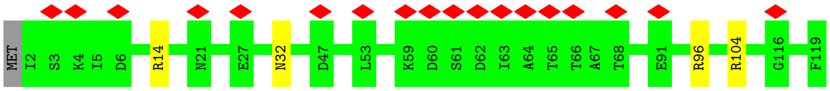




- Molecule 17: 50S ribosomal protein L18

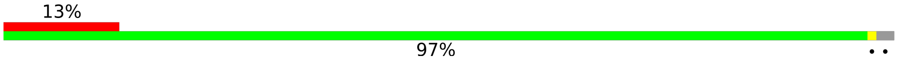
Chain R:

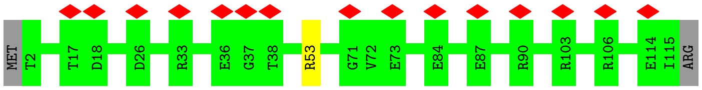




- Molecule 18: 50S ribosomal protein L19

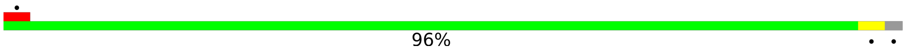
Chain S:

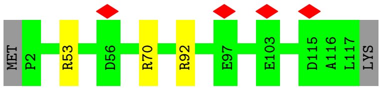




- Molecule 19: 50S ribosomal protein L20

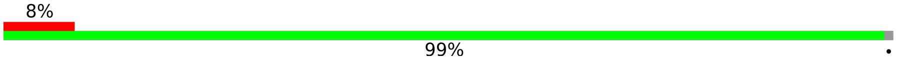
Chain T:

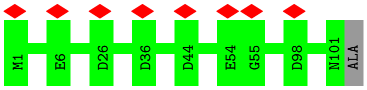




- Molecule 20: 50S ribosomal protein L21

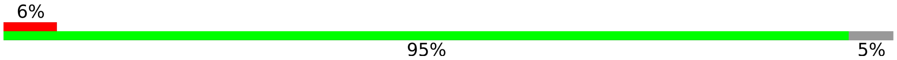
Chain U:

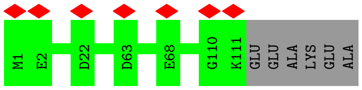




- Molecule 21: 50S ribosomal protein L22

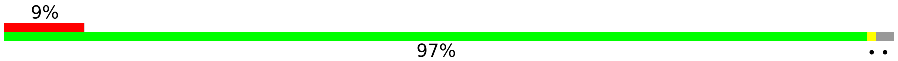
Chain V:

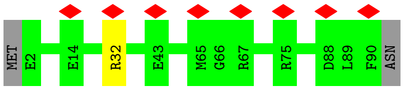




- Molecule 22: 50S ribosomal protein L23

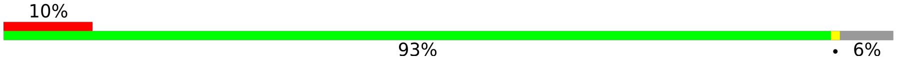
Chain W:

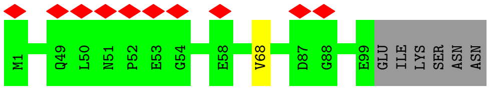




- Molecule 23: 50S ribosomal protein L24

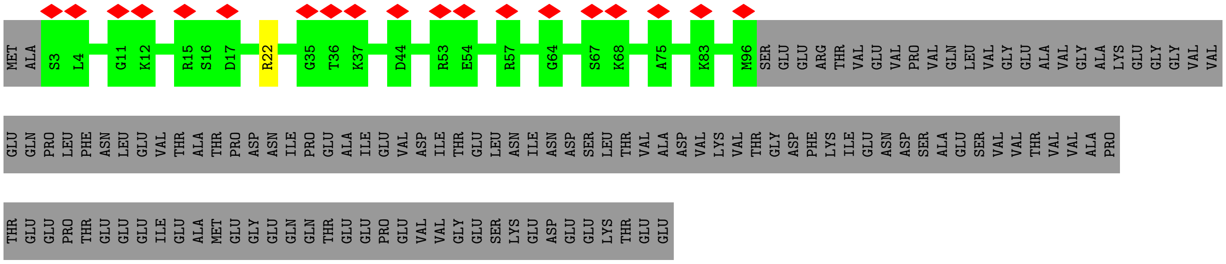
Chain X:





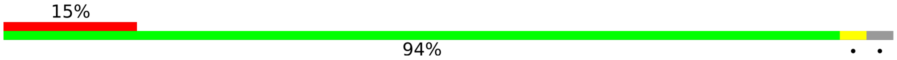
- Molecule 24: 50S ribosomal protein L25

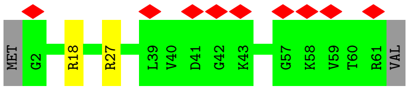
Chain Y:



- Molecule 25: 50S ribosomal protein L28

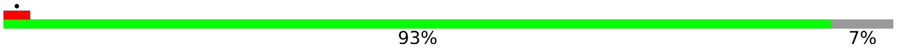
Chain 1:

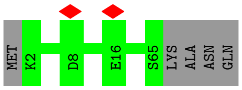




- Molecule 26: 50S ribosomal protein L29

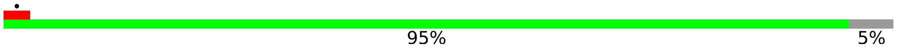
Chain 2:

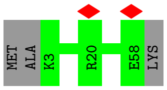




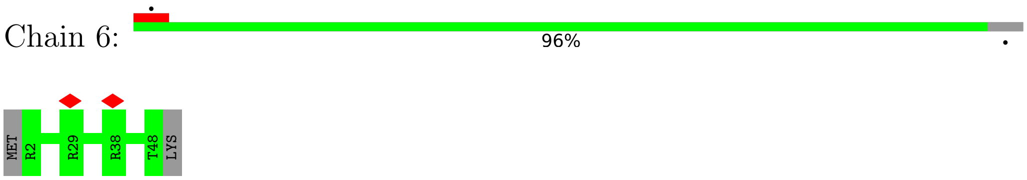
- Molecule 27: 50S ribosomal protein L30

Chain 3:

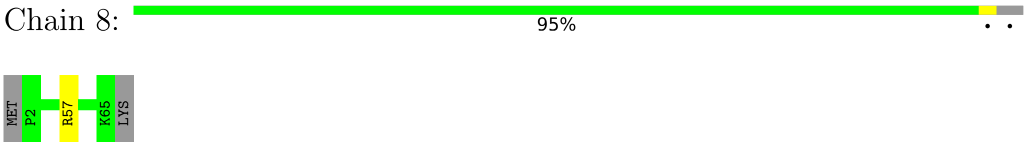




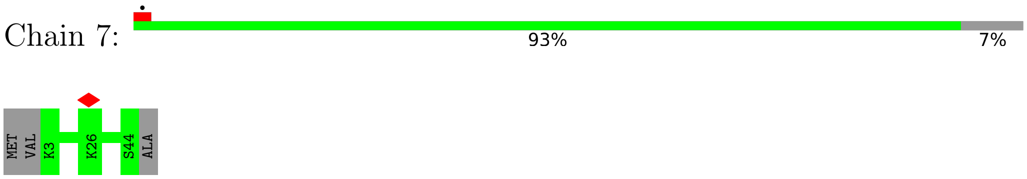
- Molecule 28: 50S ribosomal protein L33 2



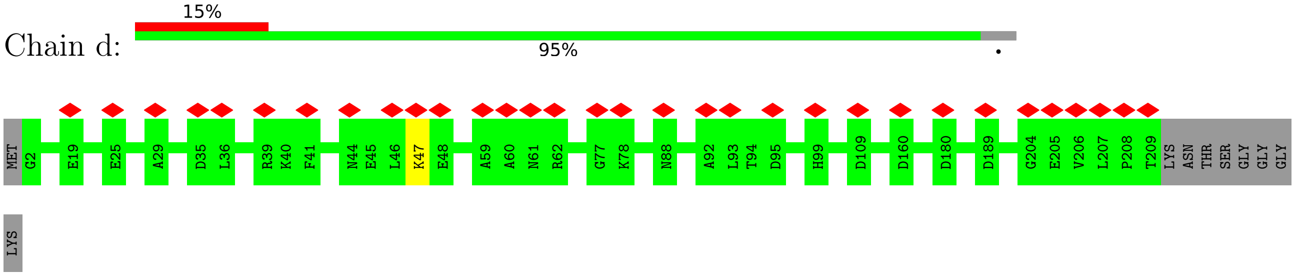
- Molecule 29: 50S ribosomal protein L35



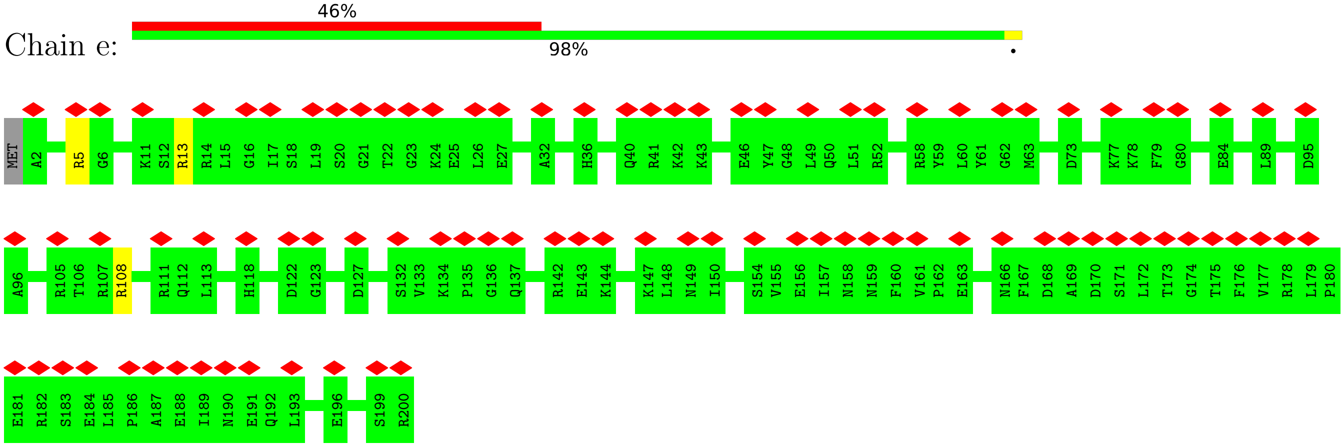
- Molecule 30: 50S ribosomal protein L34



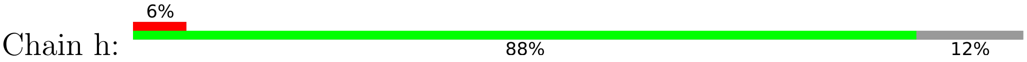
- Molecule 31: 30S ribosomal protein S3

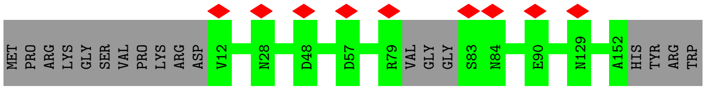


- Molecule 32: 30S ribosomal protein S4



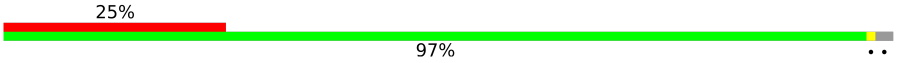
- Molecule 33: 30S ribosomal protein S7

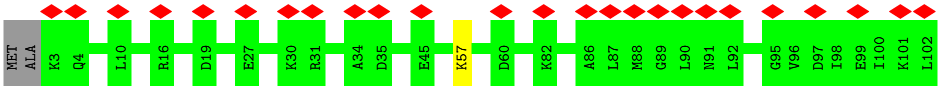




- Molecule 34: 30S ribosomal protein S10

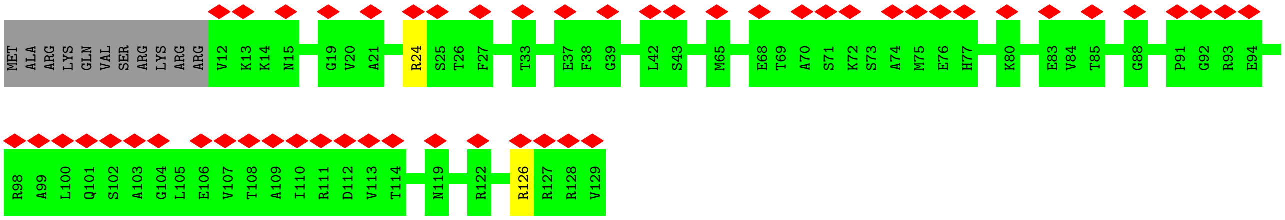
Chain k:





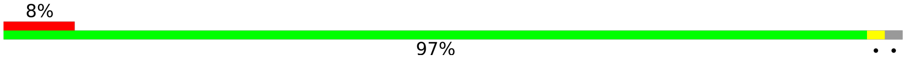
- Molecule 35: 30S ribosomal protein S11

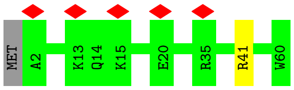
Chain l:



- Molecule 36: 30S ribosomal protein S14 type Z

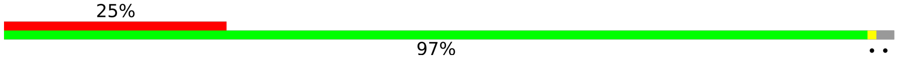
Chain o:

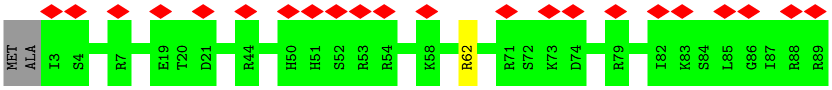




- Molecule 37: 30S ribosomal protein S15

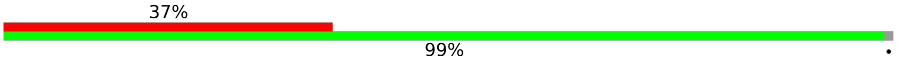
Chain p:

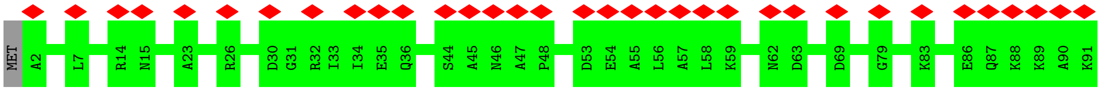




- Molecule 38: 30S ribosomal protein S16

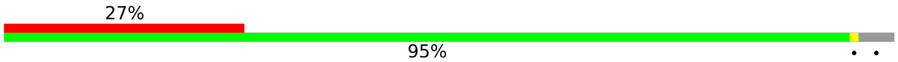
Chain q:

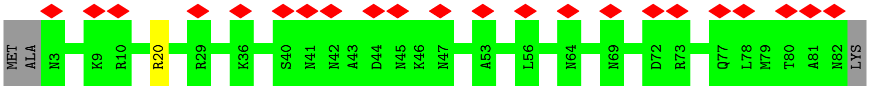




- Molecule 39: 30S ribosomal protein S20

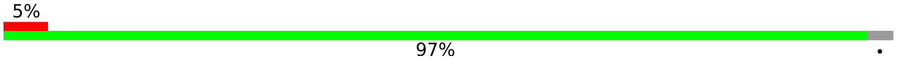
Chain u:

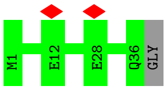




- Molecule 40: 50S ribosomal protein L36

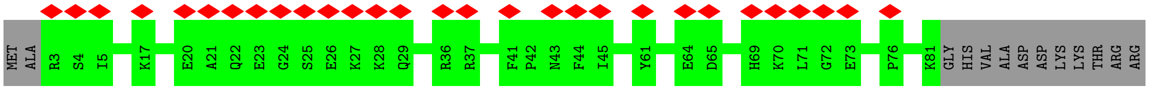
Chain 9:





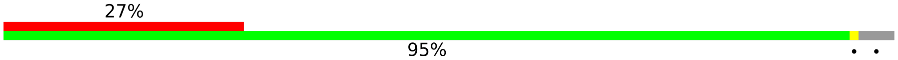
- Molecule 41: 30S ribosomal protein S19

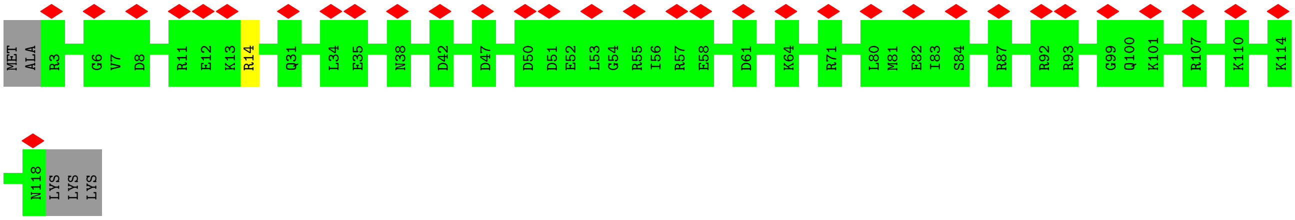
Chain t:



- Molecule 42: 30S ribosomal protein S13

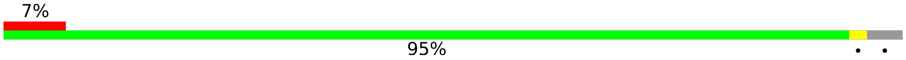
Chain n:

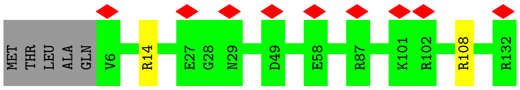




- Molecule 43: 30S ribosomal protein S9

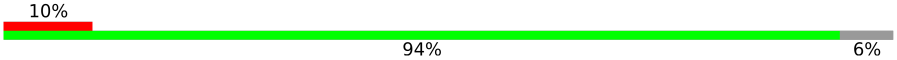
Chain j:

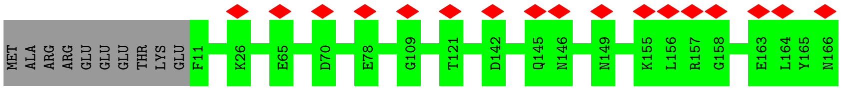




- Molecule 44: 30S ribosomal protein S5

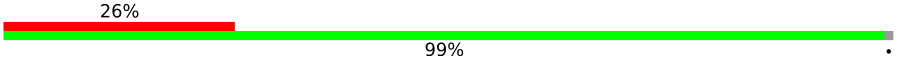
Chain f:

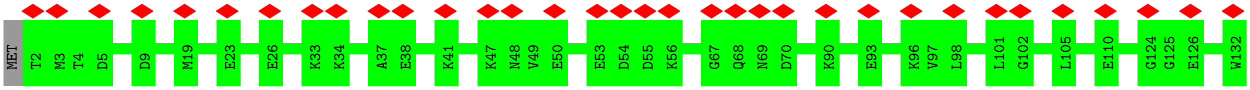




- Molecule 45: 30S ribosomal protein S8

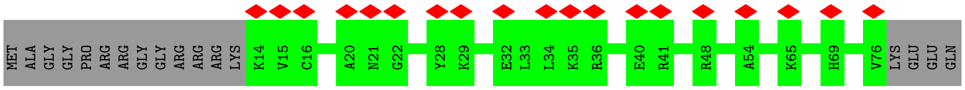
Chain i:





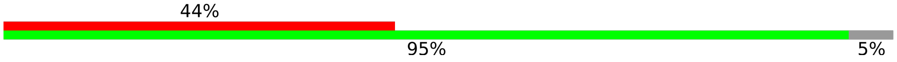
- Molecule 46: 30S ribosomal protein S18

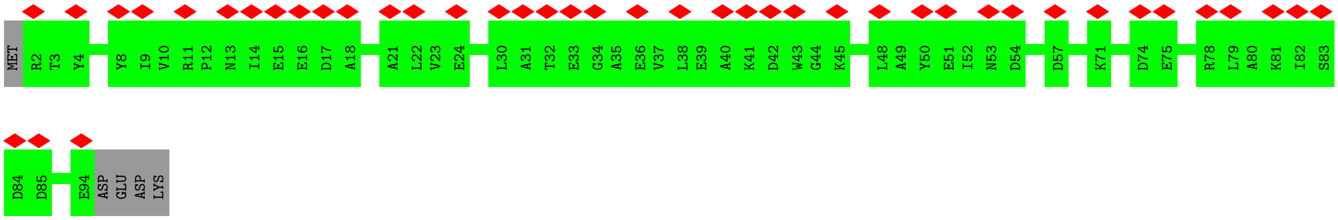
Chain s:



- Molecule 47: 30S ribosomal protein S6

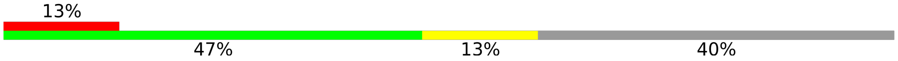
Chain g:





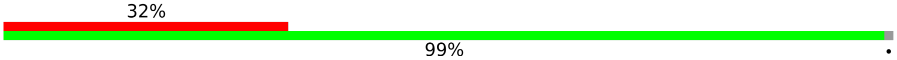
- Molecule 48: RNA (5'-R(P*GP*GP*AP*GP*GP*UP*AP*UP*G)-3')

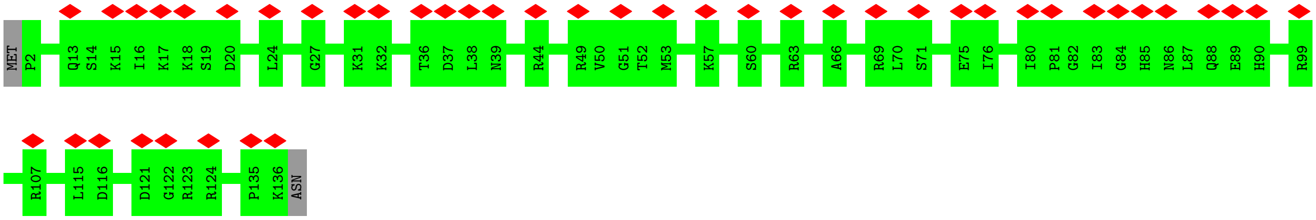
Chain b:



- Molecule 49: 30S ribosomal protein S12

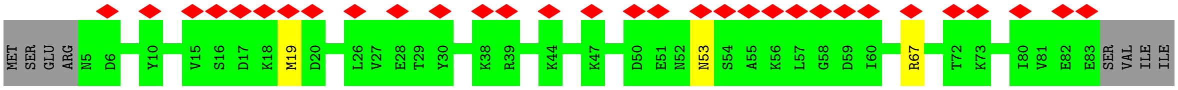
Chain m:





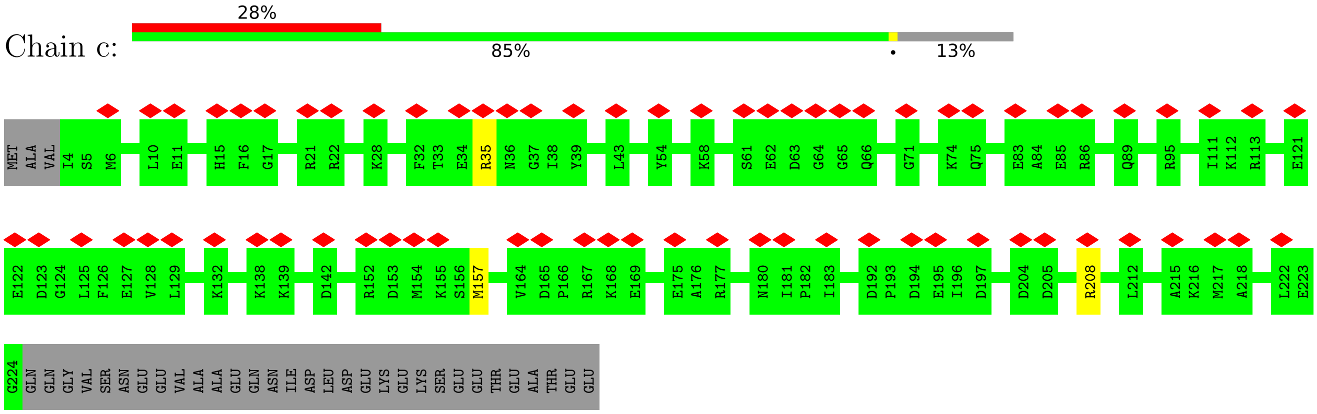
- Molecule 50: 30S ribosomal protein S17

Chain r:



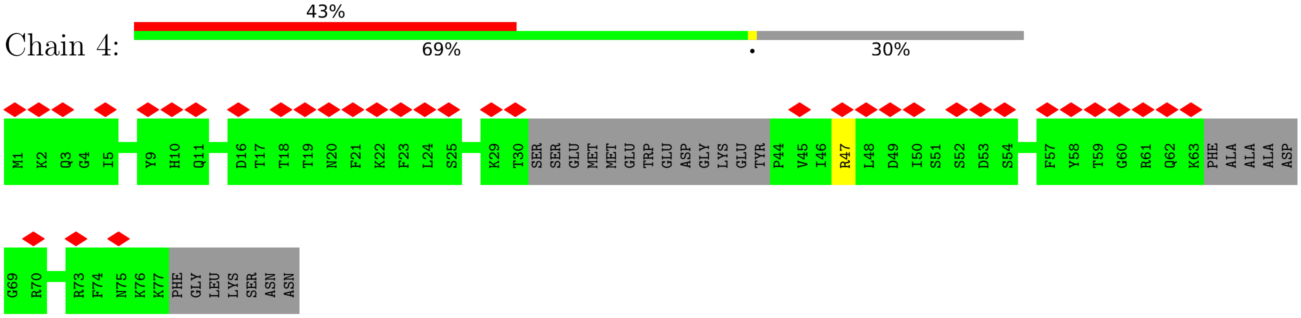
- Molecule 51: 30S ribosomal protein S2

Chain c:



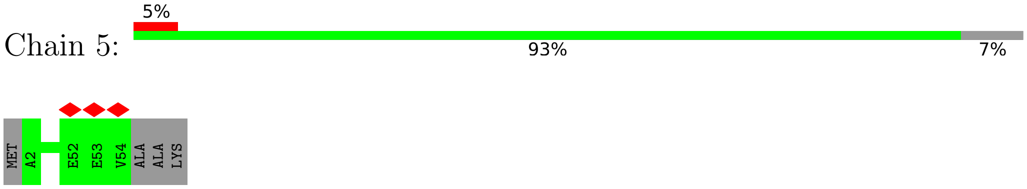
- Molecule 52: 50S ribosomal protein L31 type B

Chain 4:



- Molecule 53: 50S ribosomal protein L32

Chain 5:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61910	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 $(e^-/\text{Å}^2)$	26.3	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	0.031	Depositor
Minimum map value	-0.012	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.008	Depositor
Map size (Å)	366.432, 366.432, 366.432	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.041, 1.041, 1.041	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: K, ZN, ATP, MG

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	0	0.56	0/3827	0.70	1/5139 (0.0%)
2	D	1.01	0/1746	1.12	4/2721 (0.1%)
3	Z	0.81	0/591	0.75	0/785
4	P	0.80	0/1105	0.71	0/1483
5	A	1.32	33/69977 (0.0%)	1.21	177/109141 (0.2%)
6	a	0.94	0/36875	1.11	48/57502 (0.1%)
7	B	0.88	0/2692	1.09	3/4193 (0.1%)
8	G	0.82	0/2120	0.77	1/2847 (0.0%)
9	H	0.82	0/1661	0.70	0/2227
10	I	0.80	0/1587	0.73	1/2143 (0.0%)
11	J	0.49	0/1398	0.69	0/1877
12	K	0.53	0/1302	0.68	0/1757
13	M	0.77	0/1149	0.69	0/1549
14	N	0.76	0/927	0.87	0/1243
15	O	0.76	1/1104 (0.1%)	0.80	4/1471 (0.3%)
16	Q	0.70	0/956	0.80	1/1277 (0.1%)
17	R	0.54	0/923	0.73	3/1234 (0.2%)
18	S	0.74	0/934	0.79	0/1249
19	T	0.87	0/955	0.78	2/1265 (0.2%)
20	U	0.81	0/803	0.70	0/1073
21	V	0.77	0/861	0.78	0/1159
22	W	0.72	0/733	0.72	0/978
23	X	0.61	1/770 (0.1%)	0.70	0/1029
24	Y	0.55	0/746	0.72	1/1000 (0.1%)
25	1	0.63	0/480	0.84	2/639 (0.3%)
26	2	0.57	0/528	0.73	0/703
27	3	0.76	0/438	0.71	0/590
28	6	0.70	0/392	0.76	0/523
29	8	0.83	0/526	0.84	1/690 (0.1%)
30	7	0.94	0/364	0.91	0/474
31	d	0.57	0/1661	0.68	0/2233
32	e	0.50	0/1647	0.70	2/2211 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	h	0.49	0/1114	0.69	0/1498
34	k	0.54	0/813	0.74	0/1094
35	l	0.43	0/891	0.65	0/1203
36	o	0.67	0/506	0.67	0/671
37	p	0.47	0/742	0.75	2/989 (0.2%)
38	q	0.47	0/723	0.67	0/971
39	u	0.41	0/606	0.66	1/810 (0.1%)
40	9	0.80	0/295	0.77	0/388
41	t	0.49	0/663	0.64	0/889
42	n	0.49	0/929	0.72	1/1246 (0.1%)
43	j	0.56	0/1024	0.75	0/1374
44	f	0.64	0/1174	0.69	0/1583
45	i	0.50	0/1044	0.72	0/1401
46	s	0.52	0/525	0.65	0/704
47	g	0.44	0/784	0.69	0/1052
48	b	0.87	0/222	1.09	2/343 (0.6%)
49	m	0.56	0/1075	0.71	0/1439
50	r	0.51	0/659	0.65	0/881
51	c	0.44	0/1808	0.64	1/2426 (0.0%)
52	4	0.42	0/496	0.58	0/661
53	5	0.86	0/429	0.78	0/571
All	All	1.06	35/158300 (0.0%)	1.07	258/236599 (0.1%)

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2457	A	N9-C4	-8.62	1.32	1.37
5	A	1817	C	C4-C5	-6.14	1.38	1.43
5	A	2033	C	C4-C5	-5.91	1.38	1.43
5	A	674	C	N1-C6	-5.72	1.33	1.37
5	A	666	A	N9-C4	-5.59	1.34	1.37
5	A	840	C	C4-C5	-5.58	1.38	1.43
5	A	2092	C	C4-C5	-5.50	1.38	1.43
5	A	1817	C	N1-C6	-5.48	1.33	1.37
5	A	2092	C	N1-C6	-5.44	1.33	1.37
5	A	2528	C	C4-C5	-5.44	1.38	1.43
5	A	2616	A	N9-C4	-5.43	1.34	1.37
5	A	567	G	N9-C8	-5.35	1.34	1.37
15	O	19	VAL	CB-CG1	-5.34	1.41	1.52
5	A	2542	C	C4-C5	-5.33	1.38	1.43
5	A	831	C	N1-C6	-5.32	1.33	1.37
5	A	849	A	N9-C4	-5.31	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1351	C	C4-C5	-5.25	1.38	1.43
5	A	1822	C	N1-C6	-5.20	1.34	1.37
5	A	841	C	N1-C6	-5.19	1.34	1.37
5	A	1855	G	C6-N1	-5.19	1.35	1.39
5	A	1700	C	C4-C5	-5.18	1.38	1.43
5	A	2523	C	N1-C6	-5.18	1.34	1.37
5	A	201	C	C4-C5	-5.15	1.38	1.43
5	A	2470	C	N1-C6	-5.13	1.34	1.37
5	A	2457	A	N3-C4	-5.12	1.31	1.34
5	A	442	G	N9-C8	-5.10	1.34	1.37
5	A	1824	C	N1-C6	-5.07	1.34	1.37
5	A	628	G	N9-C4	-5.04	1.33	1.38
5	A	627	C	N1-C6	-5.04	1.34	1.37
5	A	195	C	C4-C5	-5.04	1.39	1.43
5	A	2290	C	C4-C5	-5.04	1.39	1.43
23	X	68	VAL	CB-CG1	-5.04	1.42	1.52
5	A	1295	C	C4-C5	-5.02	1.39	1.43
5	A	1702	C	C4-C5	-5.01	1.39	1.43
5	A	191	A	N9-C4	-5.01	1.34	1.37

All (258) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2528	C	C5-C4-N4	-10.31	112.98	120.20
5	A	1351	C	C6-N1-C2	-8.91	116.74	120.30
5	A	608	C	C5-C4-N4	-8.67	114.13	120.20
5	A	2271	U	N3-C4-O4	8.66	125.46	119.40
5	A	1817	C	C5-C4-N4	-8.33	114.37	120.20
5	A	1351	C	C2-N1-C1’	8.22	127.84	118.80
6	a	1033	C	C2-N1-C1’	8.21	127.83	118.80
6	a	1033	C	N1-C2-O2	8.08	123.75	118.90
6	a	827	A	N1-C6-N6	7.65	123.19	118.60
6	a	762	C	C2-N1-C1’	7.62	127.19	118.80
5	A	2271	U	C5-C4-O4	-7.54	121.38	125.90
6	a	7	G	OP1-P-OP2	-7.52	108.32	119.60
5	A	1716	C	C5-C4-N4	-7.30	115.09	120.20
6	a	1046	G	OP1-P-OP2	-7.29	108.66	119.60
5	A	2457	A	N3-C4-N9	-7.25	121.60	127.40
48	b	1	G	OP1-P-OP2	-7.25	108.73	119.60
6	a	827	A	C5-C6-N6	-7.14	117.98	123.70
5	A	666	A	N1-C6-N6	7.02	122.81	118.60
5	A	1843	U	N3-C2-O2	-6.94	117.34	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1932	C	N1-C2-O2	6.94	123.06	118.90
6	a	989	C	C6-N1-C2	-6.93	117.53	120.30
5	A	2613	C	C5-C4-N4	-6.91	115.37	120.20
15	O	71	ARG	NE-CZ-NH2	-6.90	116.85	120.30
6	a	752	C	N1-C2-O2	6.86	123.02	118.90
5	A	2052	C	C6-N1-C2	-6.85	117.56	120.30
6	a	398	C	C6-N1-C2	-6.84	117.56	120.30
7	B	2	C	OP1-P-OP2	-6.77	109.45	119.60
5	A	2583	C	C5-C4-N4	-6.77	115.46	120.20
5	A	2604	A	N9-C4-C5	-6.70	103.12	105.80
5	A	935	C	OP1-P-OP2	-6.67	109.60	119.60
6	a	731	U	N1-C2-O2	6.65	127.45	122.80
5	A	1826	G	N3-C4-N9	-6.63	122.02	126.00
2	D	65	G	N3-C2-N2	6.62	124.53	119.90
5	A	2740	A	N1-C6-N6	6.61	122.57	118.60
5	A	1843	U	N1-C2-O2	6.61	127.43	122.80
5	A	3	U	OP1-P-OP2	-6.60	109.70	119.60
5	A	431	C	N1-C2-O2	6.59	122.86	118.90
5	A	527	G	O4'-C1'-N9	6.57	113.46	108.20
5	A	1350	U	C2-N1-C1'	6.56	125.58	117.70
5	A	2528	C	N3-C4-N4	6.51	122.56	118.00
16	Q	13	ARG	NE-CZ-NH1	6.51	123.56	120.30
5	A	2275	C	N1-C2-O2	6.51	122.81	118.90
5	A	861	C	N1-C2-O2	6.50	122.80	118.90
25	1	18	ARG	NE-CZ-NH2	6.48	123.54	120.30
2	D	2	G	OP1-P-OP2	-6.48	109.88	119.60
5	A	1201	G	C4-N9-C1'	6.44	134.88	126.50
5	A	2457	A	N3-C4-C5	6.39	131.28	126.80
5	A	2528	C	N3-C4-C5	6.37	124.45	121.90
5	A	2302	C	N1-C2-O2	6.35	122.71	118.90
6	a	398	C	C5-C6-N1	6.30	124.15	121.00
5	A	628	G	C2-N3-C4	-6.28	108.76	111.90
29	8	57	ARG	NE-CZ-NH1	6.27	123.43	120.30
5	A	666	A	C5-N7-C8	-6.20	100.80	103.90
24	Y	22	ARG	NE-CZ-NH1	6.20	123.40	120.30
6	a	315	U	N3-C2-O2	-6.18	117.87	122.20
6	a	762	C	C6-N1-C1'	-6.18	113.38	120.80
6	a	851	U	N3-C2-O2	-6.17	117.88	122.20
5	A	840	C	N1-C2-O2	6.16	122.60	118.90
5	A	1828	U	N3-C2-O2	-6.15	117.89	122.20
5	A	1475	A	C4-C5-N7	6.15	113.78	110.70
5	A	1068	G	C6-C5-N7	-6.13	126.72	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2431	C	C5-C4-N4	-6.13	115.91	120.20
5	A	1201	G	C8-N9-C1'	-6.09	119.08	127.00
5	A	2457	A	C2-N3-C4	-6.09	107.55	110.60
5	A	837	G	N9-C4-C5	6.09	107.83	105.40
5	A	195	C	C5-C4-N4	-6.07	115.95	120.20
5	A	211	C	C5-C4-N4	-6.06	115.96	120.20
6	a	1415	C	C2-N1-C1'	6.05	125.45	118.80
5	A	1201	G	C4-C5-N7	6.05	113.22	110.80
5	A	421	C	N1-C2-O2	6.05	122.53	118.90
5	A	1475	A	N9-C4-C5	-6.04	103.38	105.80
6	a	1033	C	C6-N1-C1'	-6.04	113.55	120.80
5	A	1700	C	C5-C4-N4	-6.02	115.98	120.20
5	A	222	A	OP1-P-OP2	-6.01	110.59	119.60
5	A	175	C	N1-C2-O2	6.00	122.50	118.90
5	A	533	C	N1-C2-O2	5.99	122.49	118.90
5	A	1435	C	N1-C2-O2	5.98	122.49	118.90
6	a	851	U	C6-N1-C2	-5.96	117.43	121.00
6	a	544	C	C5-C4-N4	-5.95	116.03	120.20
5	A	2583	C	N3-C4-N4	5.94	122.16	118.00
48	b	13	A	OP1-P-OP2	-5.93	110.71	119.60
6	a	1033	C	N3-C2-O2	-5.92	117.76	121.90
5	A	1171	A	N1-C6-N6	5.91	122.14	118.60
5	A	778	G	C2-N3-C4	-5.90	108.95	111.90
5	A	608	C	N3-C4-N4	5.90	122.13	118.00
5	A	1915	G	C2-N3-C4	-5.90	108.95	111.90
37	p	62	ARG	NE-CZ-NH1	5.89	123.25	120.30
5	A	1201	G	C6-C5-N7	-5.89	126.87	130.40
17	R	96	ARG	NE-CZ-NH1	5.88	123.24	120.30
6	a	203	A	N1-C6-N6	5.88	122.13	118.60
32	e	108	ARG	NE-CZ-NH1	5.87	123.24	120.30
5	A	1828	U	N1-C2-O2	5.87	126.91	122.80
5	A	2612	U	C2-N1-C1'	5.85	124.72	117.70
5	A	305	A	C5-C6-N6	-5.85	119.02	123.70
5	A	1326	C	C5-C4-N4	-5.83	116.12	120.20
6	a	731	U	N3-C2-O2	-5.81	118.13	122.20
5	A	1496	G	C4-N9-C1'	-5.79	118.97	126.50
5	A	1187	A	N1-C6-N6	5.79	122.07	118.60
5	A	2542	C	N1-C2-O2	5.78	122.37	118.90
6	a	1415	C	N1-C2-O2	5.77	122.36	118.90
5	A	1700	C	N1-C2-O2	5.77	122.36	118.90
5	A	1817	C	N3-C4-C5	5.77	124.21	121.90
6	a	1533	G	OP1-P-OP2	-5.76	110.96	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	C	C6-N1-C2	-5.75	118.00	120.30
6	a	800	A	O4'-C1'-N9	5.75	112.80	108.20
39	u	20	ARG	NE-CZ-NH1	5.75	123.17	120.30
5	A	567	G	N7-C8-N9	5.74	115.97	113.10
5	A	1226	G	C2-N3-C4	-5.72	109.04	111.90
5	A	2077	C	N1-C2-O2	5.71	122.32	118.90
5	A	2516	G	C6-C5-N7	-5.69	126.99	130.40
5	A	2451	C	C5-C4-N4	-5.68	116.22	120.20
17	R	104	ARG	NE-CZ-NH2	-5.68	117.46	120.30
5	A	1828	U	C5-C6-N1	5.65	125.53	122.70
5	A	2105	C	N1-C2-O2	5.65	122.29	118.90
5	A	554	C	N1-C2-O2	5.64	122.29	118.90
5	A	1016	G	C8-N9-C4	-5.64	104.15	106.40
19	T	53	ARG	NE-CZ-NH1	5.63	123.12	120.30
5	A	572	C	C5-C4-N4	-5.62	116.26	120.20
5	A	1010	G	C2-N3-C4	-5.62	109.09	111.90
5	A	839	A	C5-N7-C8	-5.61	101.10	103.90
5	A	1801	C	C6-N1-C2	-5.61	118.06	120.30
5	A	666	A	C2-N3-C4	-5.60	107.80	110.60
5	A	2033	C	C5-C4-N4	-5.58	116.29	120.20
5	A	1233	A	N9-C4-C5	-5.58	103.57	105.80
6	a	1245	C	N1-C2-O2	5.58	122.25	118.90
5	A	175	C	C2-N1-C1'	5.57	124.93	118.80
5	A	567	G	C4-N9-C1'	5.57	133.74	126.50
6	a	420	U	C2-N1-C1'	5.57	124.38	117.70
15	O	21	ARG	NE-CZ-NH2	5.56	123.08	120.30
5	A	1380	G	C4-N9-C1'	5.55	133.72	126.50
5	A	1351	C	C5-C6-N1	5.54	123.77	121.00
5	A	2619	G	N7-C8-N9	5.53	115.87	113.10
5	A	2064	A	C5-C6-N1	5.53	120.47	117.70
6	a	270	A	N1-C6-N6	5.53	121.92	118.60
5	A	2516	G	C4-C5-N7	5.53	113.01	110.80
5	A	1615	G	N3-C2-N2	-5.52	116.04	119.90
5	A	2090	C	C6-N1-C2	-5.52	118.09	120.30
5	A	1338	U	C5-C6-N1	5.51	125.46	122.70
5	A	1351	C	N1-C2-O2	5.51	122.21	118.90
5	A	1408	G	C2-N3-C4	-5.51	109.15	111.90
5	A	249	C	C5-C4-N4	-5.50	116.35	120.20
7	B	58	C	C6-N1-C2	-5.50	118.10	120.30
5	A	1651	C	OP2-P-O3'	5.49	117.28	105.20
6	a	1505	A	C2-N3-C4	5.48	113.34	110.60
5	A	1475	A	C5-C6-N6	-5.47	119.33	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	868	A	N9-C4-C5	-5.46	103.62	105.80
19	T	70	ARG	NE-CZ-NH2	-5.45	117.58	120.30
2	D	65	G	N1-C2-N2	-5.45	111.30	116.20
5	A	557	G	O4'-C1'-N9	5.43	112.54	108.20
5	A	568	C	C5-C4-N4	-5.43	116.40	120.20
5	A	1475	A	C5-N7-C8	-5.43	101.19	103.90
5	A	1001	A	N1-C6-N6	5.42	121.85	118.60
5	A	246	U	C5-C6-N1	5.42	125.41	122.70
5	A	2644	C	N3-C4-N4	5.42	121.80	118.00
5	A	2613	C	N3-C4-N4	5.42	121.79	118.00
5	A	1649	C	C5-C4-N4	-5.41	116.41	120.20
15	O	60	ARG	NE-CZ-NH1	5.40	123.00	120.30
6	a	572	U	N1-C2-O2	5.39	126.57	122.80
5	A	2290	C	C6-N1-C2	-5.39	118.14	120.30
5	A	2742	C	N1-C2-O2	5.38	122.13	118.90
5	A	680	C	C5-C4-N4	-5.38	116.44	120.20
5	A	966	C	N1-C2-O2	5.38	122.12	118.90
5	A	1702	C	C6-N1-C2	-5.37	118.15	120.30
5	A	988	C	N3-C4-C5	5.37	124.05	121.90
5	A	1932	C	C2-N1-C1'	5.36	124.70	118.80
5	A	832	C	N3-C4-C5	5.35	124.04	121.90
5	A	1472	C	C6-N1-C2	-5.34	118.16	120.30
6	a	827	A	C4-C5-N7	5.34	113.37	110.70
5	A	1716	C	N3-C4-C5	5.32	124.03	121.90
5	A	56	A	C5-N7-C8	-5.32	101.24	103.90
5	A	812	U	C5-C6-N1	5.32	125.36	122.70
42	n	14	ARG	NE-CZ-NH1	5.32	122.96	120.30
10	I	54	ARG	NE-CZ-NH1	-5.31	117.64	120.30
5	A	861	C	C5-C4-N4	-5.31	116.48	120.20
6	a	731	U	C2-N1-C1'	5.31	124.07	117.70
5	A	2528	C	C2-N3-C4	-5.30	117.25	119.90
5	A	286	U	C6-N1-C2	-5.30	117.82	121.00
6	a	1034	U	C6-N1-C1'	5.29	128.61	121.20
5	A	2635	G	C2-N3-C4	-5.29	109.25	111.90
5	A	504	G	N3-C2-N2	-5.28	116.20	119.90
6	a	1408	C	C6-N1-C2	-5.28	118.19	120.30
5	A	2673	C	C5-C4-N4	-5.28	116.50	120.20
5	A	1828	U	C6-N1-C2	-5.27	117.83	121.00
6	a	267	G	C4-C5-N7	5.27	112.91	110.80
5	A	2457	A	C4-C5-C6	-5.26	114.37	117.00
5	A	774	G	N3-C4-N9	-5.26	122.84	126.00
6	a	272	C	C6-N1-C2	-5.26	118.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2264	G	C2-N3-C4	-5.25	109.27	111.90
1	0	91	ARG	NE-CZ-NH2	5.25	122.92	120.30
5	A	1828	U	P-O3'-C3'	5.24	125.99	119.70
6	a	752	C	N3-C2-O2	-5.24	118.23	121.90
6	a	315	U	N1-C2-O2	5.24	126.47	122.80
6	a	851	U	C5-C6-N1	5.23	125.32	122.70
5	A	1649	C	N3-C4-N4	5.23	121.66	118.00
7	B	92	C	C5-C4-N4	-5.23	116.54	120.20
5	A	1417	G	C6-C5-N7	-5.23	127.27	130.40
15	O	79	LEU	CA-CB-CG	5.22	127.31	115.30
5	A	681	G	N1-C2-N2	-5.21	111.51	116.20
5	A	1042	C	N1-C2-O2	5.21	122.03	118.90
5	A	2188	C	N3-C2-O2	-5.21	118.26	121.90
5	A	1001	A	C5-C6-N6	-5.20	119.54	123.70
5	A	734	A	C5-C6-N1	5.20	120.30	117.70
5	A	1568	U	C2-N1-C1'	5.19	123.93	117.70
5	A	1977	G	N3-C2-N2	-5.18	116.27	119.90
5	A	837	G	C8-N9-C4	-5.18	104.33	106.40
25	1	18	ARG	NE-CZ-NH1	-5.18	117.71	120.30
6	a	1519	A	C5-C6-N1	5.18	120.29	117.70
5	A	2740	A	C5-C6-N6	-5.17	119.56	123.70
6	a	572	U	N3-C2-O2	-5.17	118.58	122.20
5	A	2431	C	N3-C4-N4	5.17	121.62	118.00
5	A	164	A	O4'-C1'-N9	5.17	112.33	108.20
5	A	2052	C	C2-N1-C1'	5.17	124.49	118.80
5	A	286	U	C2-N1-C1'	5.17	123.90	117.70
6	a	752	C	C2-N1-C1'	5.16	124.48	118.80
5	A	1029	C	N1-C2-O2	5.16	122.00	118.90
6	a	1415	C	C6-N1-C2	-5.16	118.24	120.30
5	A	2644	C	C5-C4-N4	-5.16	116.59	120.20
6	a	1436	A	O4'-C1'-N9	5.15	112.32	108.20
6	a	1428	G	N1-C2-N2	-5.15	111.57	116.20
5	A	38	A	C5-C6-N1	5.14	120.27	117.70
17	R	14	ARG	NE-CZ-NH1	5.14	122.87	120.30
5	A	955	A	N1-C6-N6	-5.13	115.52	118.60
5	A	1798	C	N1-C2-O2	5.13	121.98	118.90
5	A	421	C	C2-N1-C1'	5.12	124.44	118.80
5	A	2434	A	N9-C4-C5	-5.12	103.75	105.80
2	D	54	G	N3-C4-N9	5.10	129.06	126.00
5	A	772	A	C5-N7-C8	-5.10	101.35	103.90
5	A	2098	A	C5-N7-C8	-5.09	101.35	103.90
5	A	1336	G	N3-C4-C5	5.09	131.15	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1704	C	C5-C4-N4	-5.08	116.64	120.20
51	c	35	ARG	NE-CZ-NH1	5.08	122.84	120.30
6	a	267	G	C6-C5-N7	-5.08	127.35	130.40
6	a	1241	C	C5-C4-N4	-5.08	116.65	120.20
6	a	20	C	C6-N1-C2	-5.07	118.27	120.30
5	A	718	C	C5-C4-N4	-5.07	116.65	120.20
32	e	13	ARG	NE-CZ-NH1	5.07	122.83	120.30
5	A	1615	G	N3-C4-N9	-5.07	122.96	126.00
5	A	1814	A	C4-C5-N7	5.07	113.23	110.70
5	A	628	G	N3-C4-N9	-5.07	122.96	126.00
8	G	175	ARG	NE-CZ-NH1	5.06	122.83	120.30
5	A	423	A	C5-N7-C8	-5.06	101.37	103.90
5	A	1171	A	C5-N7-C8	-5.06	101.37	103.90
5	A	2047	A	C5-C6-N1	5.05	120.23	117.70
5	A	718	C	N3-C4-N4	5.04	121.53	118.00
5	A	907	G	C6-C5-N7	-5.04	127.38	130.40
5	A	113	U	N3-C4-O4	5.04	122.92	119.40
37	p	62	ARG	NE-CZ-NH2	-5.03	117.79	120.30
5	A	195	C	N3-C4-N4	5.02	121.52	118.00
5	A	1932	C	N3-C2-O2	-5.02	118.39	121.90
5	A	681	G	N3-C2-N2	5.01	123.41	119.90
5	A	1005	G	N3-C4-N9	-5.01	122.99	126.00
5	A	1201	G	N9-C4-C5	-5.01	103.39	105.40
5	A	298	U	P-O3'-C3'	5.01	125.71	119.70
5	A	1380	G	C8-N9-C1'	-5.01	120.49	127.00
5	A	2105	C	C2-N1-C1'	5.01	124.31	118.80
5	A	1338	U	C6-N1-C2	-5.01	118.00	121.00
5	A	1608	C	N1-C2-O2	5.01	121.90	118.90
5	A	2279	G	N3-C2-N2	-5.01	116.39	119.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	463/546 (85%)	420 (91%)	43 (9%)	0	100	100
3	Z	74/94 (79%)	68 (92%)	6 (8%)	0	100	100
4	P	133/144 (92%)	120 (90%)	13 (10%)	0	100	100
8	G	271/277 (98%)	245 (90%)	26 (10%)	0	100	100
9	H	214/220 (97%)	193 (90%)	21 (10%)	0	100	100
10	I	202/207 (98%)	180 (89%)	22 (11%)	0	100	100
11	J	173/179 (97%)	150 (87%)	23 (13%)	0	100	100
12	K	162/178 (91%)	155 (96%)	7 (4%)	0	100	100
13	M	140/145 (97%)	131 (94%)	9 (6%)	0	100	100
14	N	120/122 (98%)	107 (89%)	13 (11%)	0	100	100
15	O	143/146 (98%)	131 (92%)	12 (8%)	0	100	100
16	Q	118/122 (97%)	112 (95%)	6 (5%)	0	100	100
17	R	116/119 (98%)	105 (90%)	11 (10%)	0	100	100
18	S	112/116 (97%)	96 (86%)	16 (14%)	0	100	100
19	T	114/118 (97%)	107 (94%)	7 (6%)	0	100	100
20	U	99/102 (97%)	89 (90%)	10 (10%)	0	100	100
21	V	109/117 (93%)	106 (97%)	3 (3%)	0	100	100
22	W	87/91 (96%)	78 (90%)	9 (10%)	0	100	100
23	X	97/105 (92%)	92 (95%)	5 (5%)	0	100	100
24	Y	92/217 (42%)	81 (88%)	11 (12%)	0	100	100
25	1	58/62 (94%)	51 (88%)	7 (12%)	0	100	100
26	2	62/69 (90%)	57 (92%)	5 (8%)	0	100	100
27	3	54/59 (92%)	51 (94%)	3 (6%)	0	100	100
28	6	45/49 (92%)	38 (84%)	7 (16%)	0	100	100
29	8	62/66 (94%)	56 (90%)	6 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	7	40/45 (89%)	39 (98%)	1 (2%)	0	100	100
31	d	206/217 (95%)	185 (90%)	21 (10%)	0	100	100
32	e	197/200 (98%)	173 (88%)	24 (12%)	0	100	100
33	h	134/156 (86%)	121 (90%)	13 (10%)	0	100	100
34	k	98/102 (96%)	85 (87%)	13 (13%)	0	100	100
35	l	116/129 (90%)	107 (92%)	9 (8%)	0	100	100
36	o	57/60 (95%)	54 (95%)	3 (5%)	0	100	100
37	p	85/89 (96%)	80 (94%)	5 (6%)	0	100	100
38	q	88/91 (97%)	79 (90%)	9 (10%)	0	100	100
39	u	78/83 (94%)	73 (94%)	5 (6%)	0	100	100
40	9	34/37 (92%)	30 (88%)	4 (12%)	0	100	100
41	t	77/92 (84%)	69 (90%)	8 (10%)	0	100	100
42	n	114/121 (94%)	96 (84%)	18 (16%)	0	100	100
43	j	125/132 (95%)	118 (94%)	7 (6%)	0	100	100
44	f	154/166 (93%)	142 (92%)	12 (8%)	0	100	100
45	i	129/132 (98%)	117 (91%)	12 (9%)	0	100	100
46	s	61/80 (76%)	54 (88%)	7 (12%)	0	100	100
47	g	91/98 (93%)	79 (87%)	12 (13%)	0	100	100
49	m	133/137 (97%)	111 (84%)	22 (16%)	0	100	100
50	r	77/87 (88%)	67 (87%)	10 (13%)	0	100	100
51	c	219/255 (86%)	199 (91%)	20 (9%)	0	100	100
52	4	53/84 (63%)	47 (89%)	6 (11%)	0	100	100
53	5	51/57 (90%)	46 (90%)	5 (10%)	0	100	100
All	All	5737/6320 (91%)	5190 (90%)	547 (10%)	0	100	100

There are no Ramachandran outliers to report.

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	0	423/500 (85%)	419 (99%)	4 (1%)	78	91
3	Z	59/75 (79%)	59 (100%)	0	100	100
4	P	112/119 (94%)	111 (99%)	1 (1%)	78	91
8	G	220/224 (98%)	217 (99%)	3 (1%)	67	86
9	H	174/177 (98%)	174 (100%)	0	100	100
10	I	168/169 (99%)	168 (100%)	0	100	100
11	J	154/158 (98%)	154 (100%)	0	100	100
12	K	144/155 (93%)	142 (99%)	2 (1%)	67	86
13	M	121/123 (98%)	121 (100%)	0	100	100
14	N	100/100 (100%)	100 (100%)	0	100	100
15	O	111/112 (99%)	111 (100%)	0	100	100
16	Q	101/102 (99%)	101 (100%)	0	100	100
17	R	94/95 (99%)	93 (99%)	1 (1%)	73	89
18	S	100/102 (98%)	99 (99%)	1 (1%)	76	90
19	T	96/98 (98%)	95 (99%)	1 (1%)	76	90
20	U	86/86 (100%)	86 (100%)	0	100	100
21	V	90/94 (96%)	90 (100%)	0	100	100
22	W	80/82 (98%)	79 (99%)	1 (1%)	69	87
23	X	84/90 (93%)	84 (100%)	0	100	100
24	Y	83/190 (44%)	83 (100%)	0	100	100
25	1	50/52 (96%)	49 (98%)	1 (2%)	55	80
26	2	58/62 (94%)	58 (100%)	0	100	100
27	3	51/53 (96%)	51 (100%)	0	100	100
28	6	45/47 (96%)	45 (100%)	0	100	100
29	8	55/57 (96%)	55 (100%)	0	100	100
30	7	38/40 (95%)	38 (100%)	0	100	100
31	d	169/175 (97%)	168 (99%)	1 (1%)	86	94
32	e	174/175 (99%)	173 (99%)	1 (1%)	86	94
33	h	117/132 (89%)	117 (100%)	0	100	100
34	k	90/91 (99%)	89 (99%)	1 (1%)	73	89
35	l	94/104 (90%)	92 (98%)	2 (2%)	53	79
36	o	52/53 (98%)	51 (98%)	1 (2%)	57	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	p	80/81 (99%)	80 (100%)	0	100	100
38	q	76/77 (99%)	76 (100%)	0	100	100
39	u	67/69 (97%)	67 (100%)	0	100	100
40	9	35/35 (100%)	35 (100%)	0	100	100
41	t	70/80 (88%)	70 (100%)	0	100	100
42	n	100/104 (96%)	100 (100%)	0	100	100
43	j	105/109 (96%)	103 (98%)	2 (2%)	57	81
44	f	122/131 (93%)	122 (100%)	0	100	100
45	i	112/113 (99%)	112 (100%)	0	100	100
46	s	56/68 (82%)	56 (100%)	0	100	100
47	g	81/86 (94%)	81 (100%)	0	100	100
49	m	117/119 (98%)	117 (100%)	0	100	100
50	r	74/82 (90%)	71 (96%)	3 (4%)	30	64
51	c	192/221 (87%)	190 (99%)	2 (1%)	76	90
52	4	55/75 (73%)	54 (98%)	1 (2%)	59	82
53	5	48/50 (96%)	48 (100%)	0	100	100
All	All	4983/5392 (92%)	4954 (99%)	29 (1%)	86	94

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

Mol	Chain	Res	Type
1	0	73	LEU
1	0	74	LYS
1	0	352	ASN
1	0	375	ARG
4	P	6	ARG
8	G	14	ARG
8	G	45	ASN
8	G	182	ARG
12	K	69	ARG
12	K	73	ASN
17	R	32	ASN
18	S	53	ARG
19	T	92	ARG
22	W	32	ARG
25	1	27	ARG

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Mol	Chain	Res	Type
31	d	47	LYS
32	e	5	ARG
34	k	57	LYS
35	l	24	ARG
35	l	126	ARG
36	o	41	ARG
43	j	14	ARG
43	j	108	ARG
50	r	19	MET
50	r	53	ASN
50	r	67	ARG
51	c	157	MET
51	c	208	ARG
52	4	47	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	0	66	HIS
9	H	200	ASN
34	k	56	HIS
52	4	6	HIS
53	5	14	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	D	72/76 (94%)	19 (26%)	1 (1%)
48	b	7/15 (46%)	0	0
5	A	2912/2923 (99%)	532 (18%)	15 (0%)
6	a	1536/1551 (99%)	288 (18%)	0
7	B	112/115 (97%)	16 (14%)	0
All	All	4639/4680 (99%)	855 (18%)	16 (0%)

All (855) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	D	8	U
2	D	9	G
2	D	13	C

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Mol	Chain	Res	Type
2	D	19	G
2	D	20	G
2	D	21	U
2	D	22	A
2	D	23	G
2	D	32	G
2	D	45	A
2	D	47	G
2	D	48	U
2	D	49	C
2	D	54	G
2	D	59	A
2	D	60	A
2	D	71	G
2	D	72	C
2	D	73	A
5	A	13	A
5	A	15	G
5	A	23	G
5	A	35	G
5	A	36	G
5	A	61	A
5	A	63	U
5	A	64	A
5	A	71	A
5	A	75	G
5	A	88	G
5	A	96	G
5	A	99	U
5	A	117	A
5	A	118	A
5	A	119	U
5	A	122	G
5	A	130	A
5	A	133	A
5	A	154	A
5	A	155	U
5	A	157	U
5	A	164	A
5	A	165	C
5	A	167	U
5	A	168	A

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Mol	Chain	Res	Type
5	A	169	G
5	A	175	C
5	A	176	A
5	A	177	G
5	A	184	C
5	A	185	A
5	A	199	A
5	A	202	A
5	A	207	A
5	A	218	G
5	A	219	A
5	A	224	A
5	A	225	A
5	A	228	A
5	A	229	A
5	A	231	A
5	A	233	U
5	A	236	A
5	A	251	G
5	A	253	G
5	A	255	G
5	A	268	A
5	A	270	C
5	A	281	A
5	A	283	G
5	A	284	C
5	A	285	U
5	A	286	U
5	A	287	G
5	A	299	U
5	A	302	A
5	A	311	U
5	A	313	U
5	A	314	A
5	A	321	U
5	A	354	A
5	A	360	A
5	A	367	A
5	A	373	A
5	A	388	A
5	A	389	A
5	A	403	U

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Mol	Chain	Res	Type
5	A	404	U
5	A	410	G
5	A	415	U
5	A	418	G
5	A	419	U
5	A	426	G
5	A	431	C
5	A	432	G
5	A	450	C
5	A	457	G
5	A	458	A
5	A	459	C
5	A	470	G
5	A	476	A
5	A	493	A
5	A	494	U
5	A	497	U
5	A	502	C
5	A	503	A
5	A	510	U
5	A	527	G
5	A	541	G
5	A	550	A
5	A	553	A
5	A	554	C
5	A	567	G
5	A	572	C
5	A	575	G
5	A	576	U
5	A	577	A
5	A	578	G
5	A	590	U
5	A	591	A
5	A	592	A
5	A	593	U
5	A	594	G
5	A	606	G
5	A	615	A
5	A	616	G
5	A	617	A
5	A	618	A
5	A	626	G

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Mol	Chain	Res	Type
5	A	630	G
5	A	646	A
5	A	658	A
5	A	659	A
5	A	666	A
5	A	667	G
5	A	679	G
5	A	681	G
5	A	682	A
5	A	683	G
5	A	690	U
5	A	691	A
5	A	699	U
5	A	700	A
5	A	727	G
5	A	731	U
5	A	763	A
5	A	764	C
5	A	775	A
5	A	783	G
5	A	792	U
5	A	793	G
5	A	807	U
5	A	813	G
5	A	816	G
5	A	819	A
5	A	820	G
5	A	827	A
5	A	829	U
5	A	830	U
5	A	835	U
5	A	837	G
5	A	850	G
5	A	854	G
5	A	857	C
5	A	872	U
5	A	873	U
5	A	904	G
5	A	911	A
5	A	919	G
5	A	921	C
5	A	923	A

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Mol	Chain	Res	Type
5	A	924	G
5	A	930	C
5	A	936	G
5	A	940	U
5	A	941	A
5	A	943	C
5	A	944	G
5	A	945	A
5	A	955	A
5	A	959	C
5	A	960	C
5	A	970	U
5	A	985	A
5	A	989	A
5	A	990	G
5	A	1001	A
5	A	1005	G
5	A	1017	A
5	A	1018	A
5	A	1026	C
5	A	1027	A
5	A	1029	C
5	A	1040	A
5	A	1041	G
5	A	1049	C
5	A	1056	U
5	A	1057	A
5	A	1066	G
5	A	1069	G
5	A	1070	A
5	A	1077	U
5	A	1083	G
5	A	1085	U
5	A	1089	C
5	A	1091	G
5	A	1101	A
5	A	1104	U
5	A	1105	U
5	A	1106	G
5	A	1110	U
5	A	1113	A
5	A	1114	A

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Mol	Chain	Res	Type
5	A	1115	G
5	A	1117	A
5	A	1118	G
5	A	1128	A
5	A	1131	G
5	A	1132	A
5	A	1134	U
5	A	1139	A
5	A	1140	A
5	A	1141	U
5	A	1149	U
5	A	1155	A
5	A	1156	G
5	A	1160	C
5	A	1163	U
5	A	1166	G
5	A	1174	U
5	A	1176	U
5	A	1177	A
5	A	1178	C
5	A	1179	C
5	A	1186	A
5	A	1195	A
5	A	1216	U
5	A	1217	U
5	A	1218	G
5	A	1249	U
5	A	1250	G
5	A	1276	G
5	A	1282	A
5	A	1285	A
5	A	1286	G
5	A	1294	G
5	A	1303	A
5	A	1309	G
5	A	1310	A
5	A	1318	G
5	A	1337	A
5	A	1338	U
5	A	1339	U
5	A	1342	C
5	A	1355	A

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Mol	Chain	Res	Type
5	A	1358	A
5	A	1366	U
5	A	1378	U
5	A	1382	C
5	A	1387	C
5	A	1402	A
5	A	1405	G
5	A	1416	U
5	A	1432	A
5	A	1440	A
5	A	1449	A
5	A	1451	U
5	A	1452	C
5	A	1454	U
5	A	1455	U
5	A	1456	U
5	A	1457	U
5	A	1458	A
5	A	1459	A
5	A	1463	A
5	A	1464	U
5	A	1468	G
5	A	1472	C
5	A	1481	A
5	A	1488	A
5	A	1490	G
5	A	1494	G
5	A	1496	G
5	A	1497	A
5	A	1500	G
5	A	1504	U
5	A	1505	G
5	A	1511	C
5	A	1526	G
5	A	1527	A
5	A	1532	U
5	A	1533	A
5	A	1534	G
5	A	1535	G
5	A	1536	C
5	A	1537	A
5	A	1552	U

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Mol	Chain	Res	Type
5	A	1553	A
5	A	1560	A
5	A	1567	A
5	A	1568	U
5	A	1574	G
5	A	1582	U
5	A	1583	G
5	A	1591	G
5	A	1592	A
5	A	1594	U
5	A	1606	C
5	A	1613	G
5	A	1616	A
5	A	1618	A
5	A	1625	U
5	A	1631	G
5	A	1634	A
5	A	1641	G
5	A	1651	C
5	A	1652	A
5	A	1653	A
5	A	1654	A
5	A	1660	A
5	A	1670	A
5	A	1683	U
5	A	1690	A
5	A	1691	G
5	A	1692	C
5	A	1716	C
5	A	1718	G
5	A	1719	C
5	A	1721	A
5	A	1738	C
5	A	1740	G
5	A	1742	A
5	A	1747	G
5	A	1759	G
5	A	1764	A
5	A	1765	A
5	A	1768	C
5	A	1772	G
5	A	1781	C

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Mol	Chain	Res	Type
5	A	1783	G
5	A	1790	G
5	A	1791	G
5	A	1800	A
5	A	1808	U
5	A	1809	C
5	A	1811	A
5	A	1827	C
5	A	1828	U
5	A	1829	A
5	A	1835	U
5	A	1836	A
5	A	1839	G
5	A	1843	U
5	A	1846	A
5	A	1856	A
5	A	1860	C
5	A	1865	C
5	A	1872	G
5	A	1875	A
5	A	1891	U
5	A	1893	A
5	A	1896	U
5	A	1897	U
5	A	1899	U
5	A	1907	U
5	A	1909	C
5	A	1926	A
5	A	1930	G
5	A	1933	G
5	A	1934	G
5	A	1939	A
5	A	1940	A
5	A	1943	A
5	A	1954	A
5	A	1956	G
5	A	1957	G
5	A	1958	U
5	A	1963	A
5	A	1964	A
5	A	1965	A
5	A	1967	U

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Mol	Chain	Res	Type
5	A	1968	C
5	A	1970	U
5	A	1982	U
5	A	1988	C
5	A	1994	C
5	A	1997	A
5	A	1998	A
5	A	1999	G
5	A	2018	U
5	A	2020	U
5	A	2023	C
5	A	2040	A
5	A	2057	A
5	A	2058	A
5	A	2059	G
5	A	2060	A
5	A	2070	C
5	A	2076	A
5	A	2078	A
5	A	2082	C
5	A	2083	G
5	A	2087	A
5	A	2088	G
5	A	2089	A
5	A	2096	G
5	A	2119	U
5	A	2120	G
5	A	2135	U
5	A	2136	U
5	A	2139	A
5	A	2143	G
5	A	2144	A
5	A	2145	U
5	A	2153	A
5	A	2175	G
5	A	2176	C
5	A	2180	C
5	A	2184	G
5	A	2185	A
5	A	2186	G
5	A	2187	G
5	A	2199	U

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Mol	Chain	Res	Type
5	A	2203	A
5	A	2217	G
5	A	2221	U
5	A	2225	A
5	A	2231	C
5	A	2237	U
5	A	2238	U
5	A	2239	A
5	A	2240	U
5	A	2241	C
5	A	2251	G
5	A	2252	A
5	A	2254	A
5	A	2265	G
5	A	2266	G
5	A	2273	G
5	A	2290	C
5	A	2293	A
5	A	2295	A
5	A	2305	A
5	A	2310	C
5	A	2314	A
5	A	2326	G
5	A	2333	U
5	A	2334	G
5	A	2335	G
5	A	2336	A
5	A	2337	A
5	A	2338	A
5	A	2347	A
5	A	2352	G
5	A	2361	U
5	A	2362	A
5	A	2374	C
5	A	2377	C
5	A	2381	A
5	A	2385	A
5	A	2410	G
5	A	2412	C
5	A	2415	A
5	A	2418	G
5	A	2433	C

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Mol	Chain	Res	Type
5	A	2438	A
5	A	2446	U
5	A	2449	C
5	A	2450	U
5	A	2452	A
5	A	2456	G
5	A	2457	A
5	A	2458	U
5	A	2459	A
5	A	2468	C
5	A	2472	G
5	A	2475	A
5	A	2478	A
5	A	2492	C
5	A	2495	A
5	A	2497	G
5	A	2503	A
5	A	2505	A
5	A	2511	G
5	A	2514	G
5	A	2521	G
5	A	2529	G
5	A	2531	U
5	A	2545	A
5	A	2546	U
5	A	2547	C
5	A	2556	G
5	A	2557	U
5	A	2562	G
5	A	2582	U
5	A	2593	A
5	A	2594	G
5	A	2601	G
5	A	2605	G
5	A	2609	G
5	A	2629	A
5	A	2637	C
5	A	2640	U
5	A	2642	U
5	A	2657	G
5	A	2663	U
5	A	2690	G

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Mol	Chain	Res	Type
5	A	2700	G
5	A	2709	U
5	A	2712	G
5	A	2716	U
5	A	2718	C
5	A	2727	G
5	A	2741	G
5	A	2753	U
5	A	2756	G
5	A	2760	A
5	A	2762	G
5	A	2771	G
5	A	2784	A
5	A	2791	A
5	A	2792	A
5	A	2793	G
5	A	2805	A
5	A	2806	U
5	A	2820	U
5	A	2822	C
5	A	2823	G
5	A	2824	G
5	A	2827	A
5	A	2838	C
5	A	2840	A
5	A	2844	U
5	A	2845	G
5	A	2847	U
5	A	2853	U
5	A	2854	A
5	A	2863	G
5	A	2877	G
5	A	2886	G
5	A	2887	G
5	A	2892	G
5	A	2894	C
5	A	2899	A
5	A	2900	C
5	A	2903	A
5	A	2905	C
5	A	2906	G
5	A	2907	A

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Mol	Chain	Res	Type
5	A	2911	A
5	A	2913	G
6	a	8	G
6	a	10	G
6	a	33	A
6	a	40	G
6	a	45	G
6	a	48	C
6	a	49	C
6	a	50	U
6	a	51	A
6	a	52	A
6	a	59	C
6	a	82	G
6	a	83	C
6	a	84	U
6	a	85	U
6	a	87	C
6	a	89	U
6	a	90	C
6	a	91	U
6	a	92	C
6	a	93	U
6	a	94	G
6	a	97	G
6	a	107	G
6	a	108	A
6	a	120	C
6	a	121	A
6	a	129	A
6	a	130	A
6	a	131	C
6	a	134	A
6	a	136	C
6	a	138	A
6	a	142	G
6	a	144	C
6	a	154	U
6	a	156	C
6	a	159	G
6	a	163	C
6	a	164	C

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Mol	Chain	Res	Type
6	a	167	A
6	a	173	U
6	a	174	A
6	a	182	A
6	a	183	U
6	a	189	G
6	a	196	A
6	a	198	G
6	a	204	A
6	a	212	A
6	a	213	G
6	a	216	G
6	a	221	U
6	a	222	G
6	a	234	A
6	a	249	G
6	a	253	U
6	a	255	G
6	a	259	G
6	a	261	U
6	a	267	G
6	a	270	A
6	a	274	G
6	a	275	C
6	a	281	A
6	a	288	C
6	a	297	G
6	a	314	A
6	a	329	A
6	a	336	C
6	a	337	A
6	a	338	C
6	a	344	A
6	a	353	C
6	a	355	G
6	a	360	C
6	a	361	A
6	a	362	G
6	a	364	A
6	a	375	U
6	a	380	C
6	a	400	G

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Mol	Chain	Res	Type
6	a	405	A
6	a	406	C
6	a	414	G
6	a	419	A
6	a	420	U
6	a	421	G
6	a	424	G
6	a	429	U
6	a	430	C
6	a	432	G
6	a	436	G
6	a	437	U
6	a	439	A
6	a	441	A
6	a	448	U
6	a	456	A
6	a	459	A
6	a	460	A
6	a	461	C
6	a	463	U
6	a	466	G
6	a	471	A
6	a	472	G
6	a	476	C
6	a	490	A
6	a	493	G
6	a	499	A
6	a	505	A
6	a	517	A
6	a	518	A
6	a	526	C
6	a	529	G
6	a	532	G
6	a	535	G
6	a	540	A
6	a	555	A
6	a	567	A
6	a	570	U
6	a	572	U
6	a	578	G
6	a	580	A
6	a	581	A

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Mol	Chain	Res	Type
6	a	584	C
6	a	585	G
6	a	589	G
6	a	623	C
6	a	624	G
6	a	626	C
6	a	631	C
6	a	641	U
6	a	642	C
6	a	661	U
6	a	664	G
6	a	668	A
6	a	669	G
6	a	695	A
6	a	710	A
6	a	728	C
6	a	731	U
6	a	742	A
6	a	757	A
6	a	761	A
6	a	763	G
6	a	785	A
6	a	801	U
6	a	802	A
6	a	807	G
6	a	817	G
6	a	825	C
6	a	836	A
6	a	844	G
6	a	851	U
6	a	854	C
6	a	855	G
6	a	856	C
6	a	861	U
6	a	863	G
6	a	869	C
6	a	880	U
6	a	882	A
6	a	886	A
6	a	895	G
6	a	899	A
6	a	910	A

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Mol	Chain	Res	Type
6	a	932	G
6	a	936	G
6	a	944	C
6	a	945	A
6	a	970	U
6	a	976	G
6	a	977	C
6	a	979	A
6	a	981	G
6	a	982	C
6	a	985	A
6	a	986	G
6	a	987	A
6	a	992	U
6	a	999	U
6	a	1002	U
6	a	1003	G
6	a	1004	A
6	a	1012	U
6	a	1014	A
6	a	1016	A
6	a	1025	G
6	a	1028	A
6	a	1031	G
6	a	1033	C
6	a	1034	U
6	a	1035	U
6	a	1036	C
6	a	1037	C
6	a	1047	G
6	a	1055	G
6	a	1057	C
6	a	1058	A
6	a	1077	U
6	a	1078	C
6	a	1097	U
6	a	1106	G
6	a	1113	A
6	a	1116	G
6	a	1124	C
6	a	1125	C
6	a	1130	A

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Mol	Chain	Res	Type
6	a	1138	U
6	a	1139	G
6	a	1144	C
6	a	1148	A
6	a	1149	A
6	a	1150	G
6	a	1151	U
6	a	1152	U
6	a	1153	G
6	a	1157	A
6	a	1165	U
6	a	1168	A
6	a	1169	C
6	a	1179	C
6	a	1194	U
6	a	1195	G
6	a	1198	G
6	a	1202	A
6	a	1207	A
6	a	1208	A
6	a	1211	C
6	a	1223	U
6	a	1232	G
6	a	1238	A
6	a	1247	A
6	a	1248	C
6	a	1249	A
6	a	1250	A
6	a	1261	A
6	a	1268	A
6	a	1271	G
6	a	1279	G
6	a	1297	U
6	a	1298	A
6	a	1300	A
6	a	1304	G
6	a	1310	A
6	a	1311	G
6	a	1313	U
6	a	1328	C
6	a	1331	C
6	a	1333	C

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Mol	Chain	Res	Type
6	a	1334	G
6	a	1346	C
6	a	1347	U
6	a	1349	G
6	a	1351	A
6	a	1357	A
6	a	1375	U
6	a	1390	G
6	a	1392	U
6	a	1406	C
6	a	1409	A
6	a	1430	G
6	a	1436	A
6	a	1437	A
6	a	1451	U
6	a	1453	G
6	a	1457	A
6	a	1458	A
6	a	1459	C
6	a	1462	U
6	a	1463	U
6	a	1464	U
6	a	1465	A
6	a	1467	G
6	a	1504	A
6	a	1505	A
6	a	1509	G
6	a	1511	A
6	a	1515	A
6	a	1518	U
6	a	1519	A
6	a	1521	C
6	a	1529	G
6	a	1531	A
6	a	1541	G
6	a	1542	G
6	a	1546	A
6	a	1548	C
7	B	10	U
7	B	23	U
7	B	25	A
7	B	31	G

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Mol	Chain	Res	Type
7	B	38	U
7	B	40	C
7	B	42	G
7	B	54	U
7	B	55	A
7	B	83	C
7	B	85	U
7	B	87	C
7	B	88	G
7	B	100	U
7	B	106	G
7	B	109	G

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	D	22	A
5	A	298	U
5	A	475	A
5	A	517	A
5	A	640	G
5	A	756	A
5	A	1046	G
5	A	1310	A
5	A	1457	U
5	A	1651	C
5	A	1828	U
5	A	1874	A
5	A	1938	U
5	A	2135	U
5	A	2239	A
5	A	2432	G

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 162 ligands modelled in this entry, 160 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	0	603	54	26,33,33	0.69	0	31,52,52	1.09	3 (9%)
55	ATP	0	604	54	26,33,33	0.64	0	31,52,52	1.09	1 (3%)

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	0	603	54	-	5/18/38/38	0/3/3/3
55	ATP	0	604	54	-	8/18/38/38	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(^{o})	Ideal(^{o})
55	0	604	ATP	C5-C6-N6	2.32	123.88	120.35
55	0	603	ATP	O2'-C2'-C3'	-2.23	104.61	111.82
55	0	603	ATP	C5-C6-N6	2.16	123.63	120.35
55	0	603	ATP	O3'-C3'-C2'	-2.02	105.29	111.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
55	0	603	ATP	C5'-O5'-PA-O1A
55	0	604	ATP	PB-O3B-PG-O2G
55	0	604	ATP	C5'-O5'-PA-O3A
55	0	603	ATP	O4'-C4'-C5'-O5'

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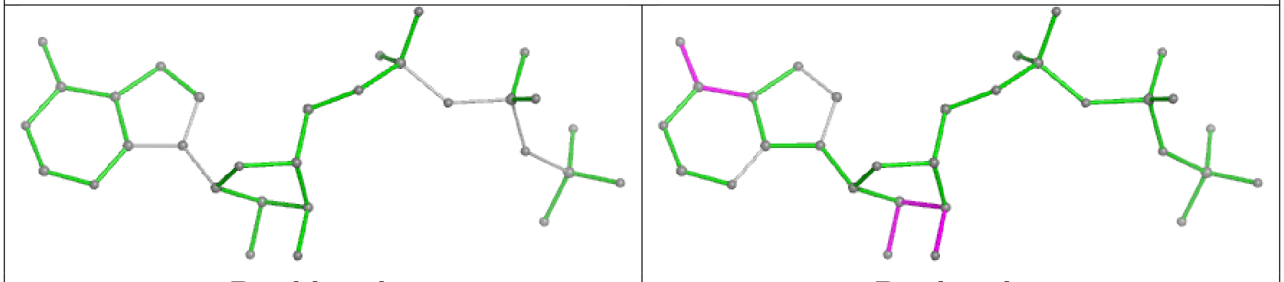
Mol	Chain	Res	Type	Atoms
55	0	603	ATP	C3'-C4'-C5'-O5'
55	0	604	ATP	O4'-C4'-C5'-O5'
55	0	603	ATP	C5'-O5'-PA-O2A
55	0	604	ATP	C5'-O5'-PA-O1A
55	0	604	ATP	PG-O3B-PB-O1B
55	0	604	ATP	PG-O3B-PB-O2B
55	0	604	ATP	PA-O3A-PB-O2B
55	0	604	ATP	PB-O3B-PG-O1G
55	0	603	ATP	C5'-O5'-PA-O3A

There are no ring outliers.

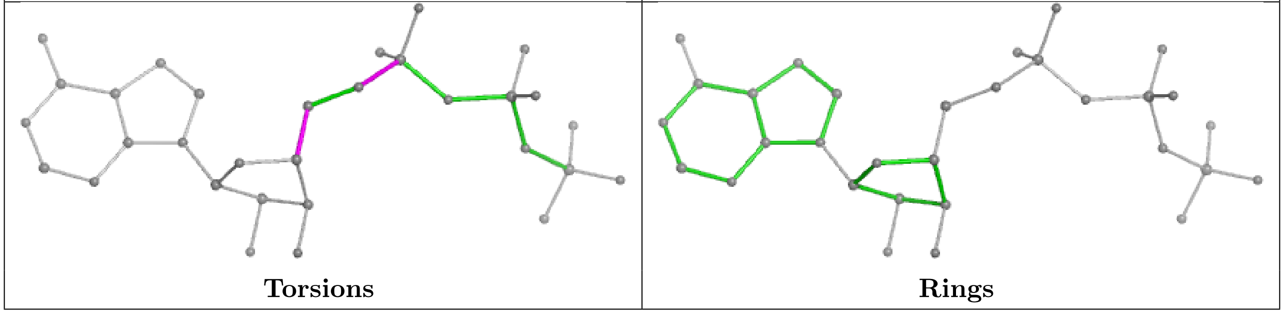
No monomer is involved in short contacts.

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 then 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.

Ligand ATP 0 603

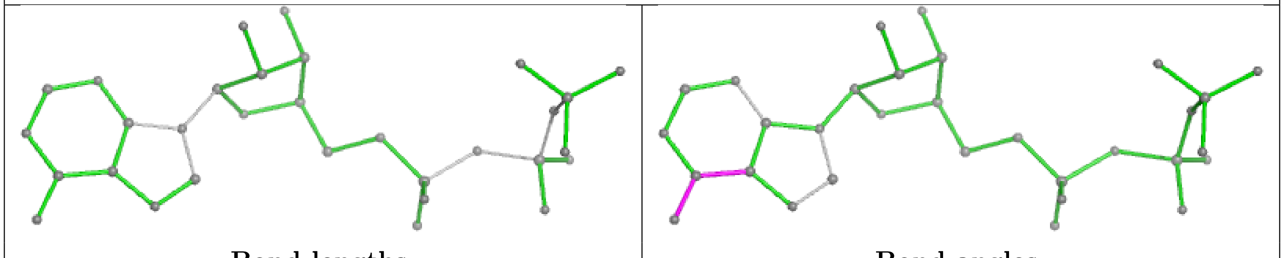


Bond lengths **Bond angles**



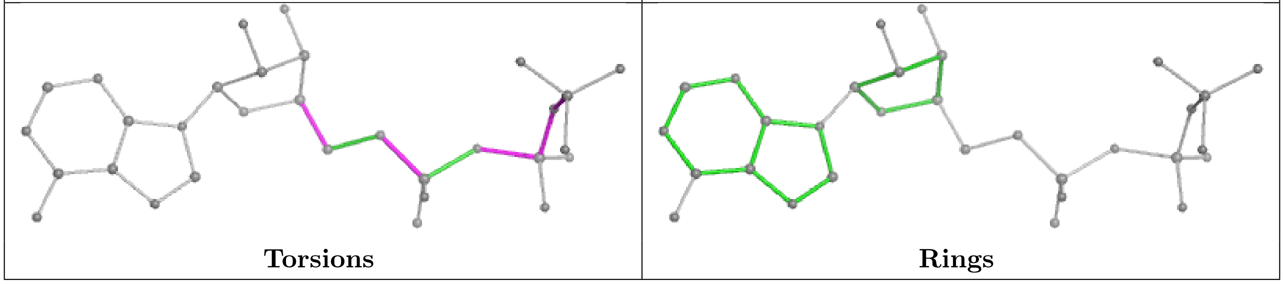
Torsions **Rings**

Ligand ATP 0 604



Bond lengths

Bond angles



Torsions

Rings

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.

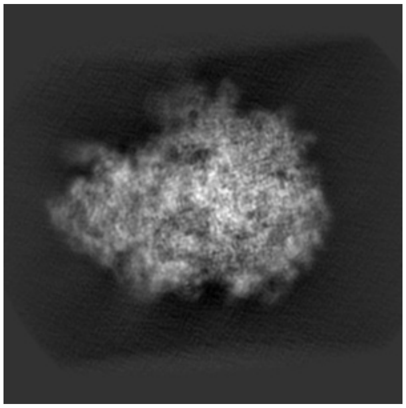
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-12332. These allow visual inspection of the internal detail of the map and identification of artifacts.

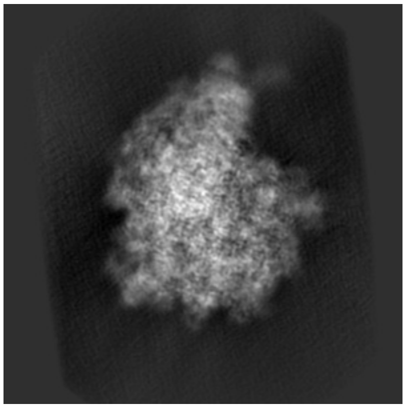
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

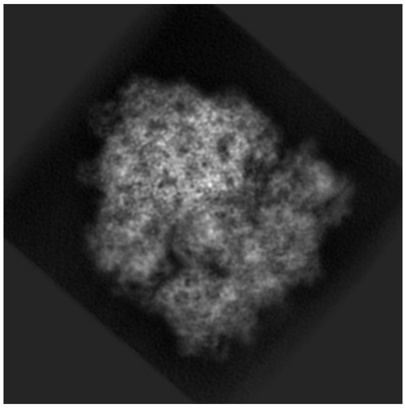
6.1.1 Primary map



X

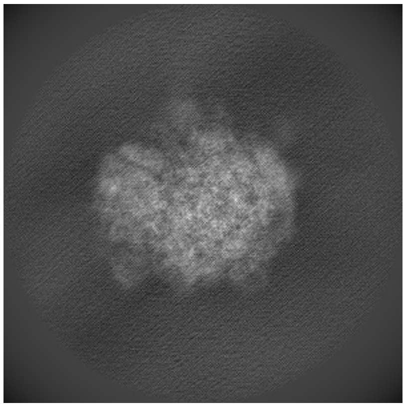


Y

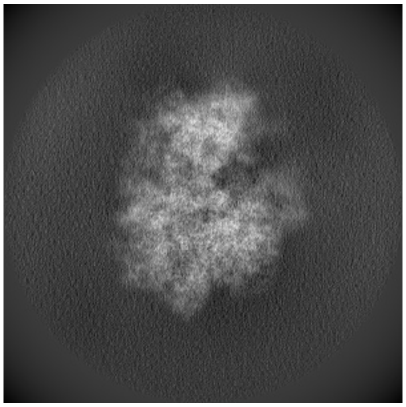


Z

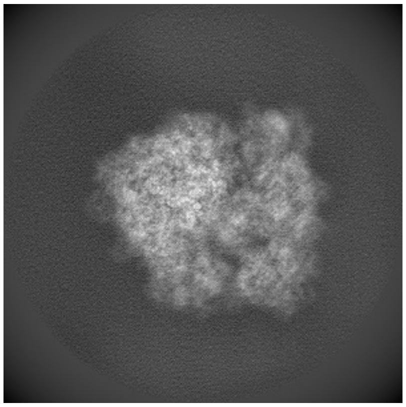
6.1.2 Raw map



X



Y

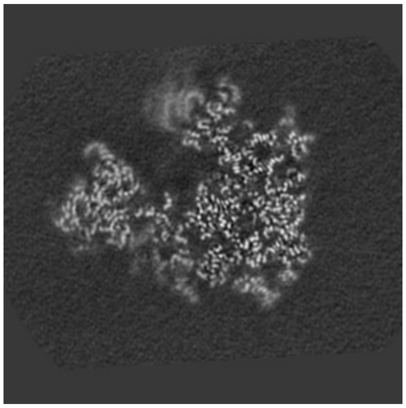


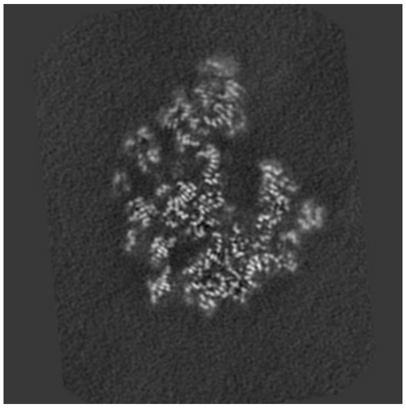
Z

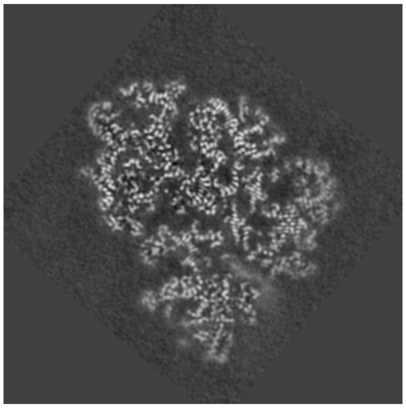
The images above show the map projected in three orthogonal directions.

6.2 Central slices ⓘ

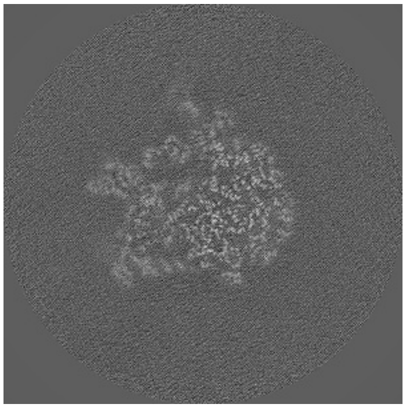
6.2.1 Primary map

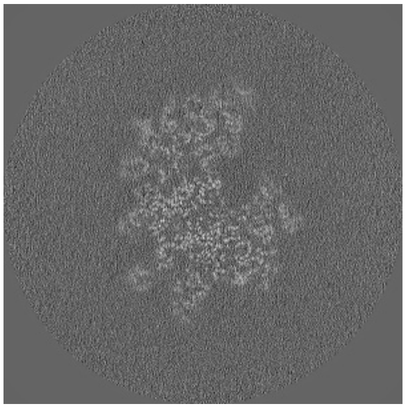

X Index: 176

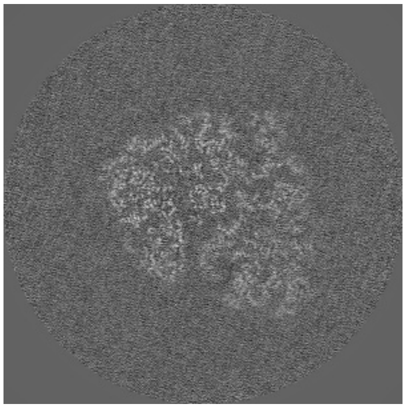

Y Index: 176


Z Index: 176

6.2.2 Raw map


X Index: 255

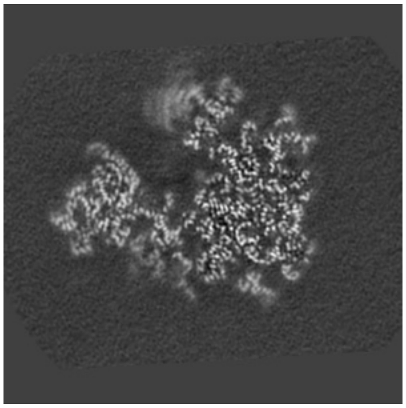

Y Index: 255


Z Index: 255

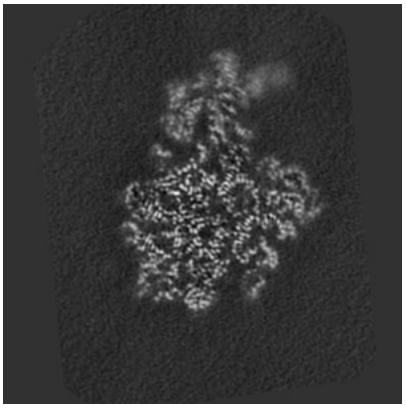
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices

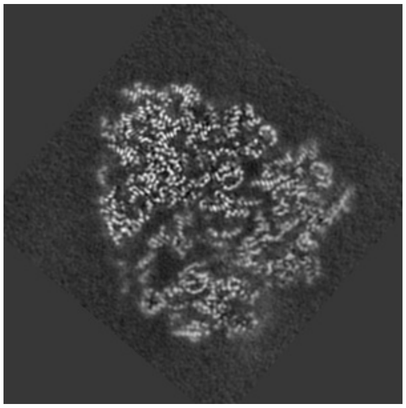
6.3.1 Primary map



X Index: 173

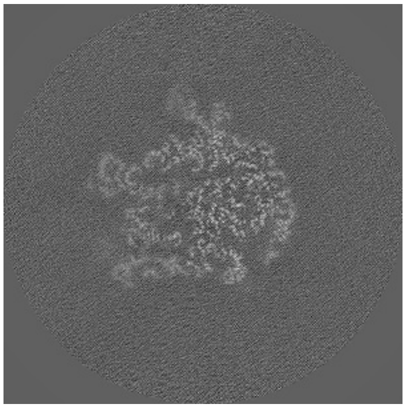


Y Index: 189

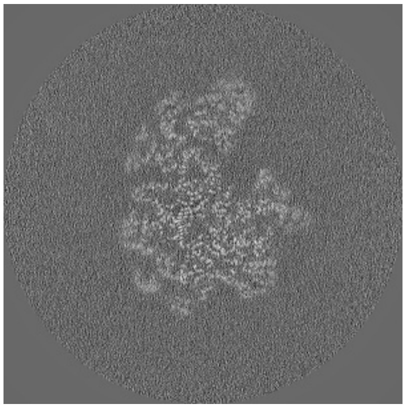


Z Index: 186

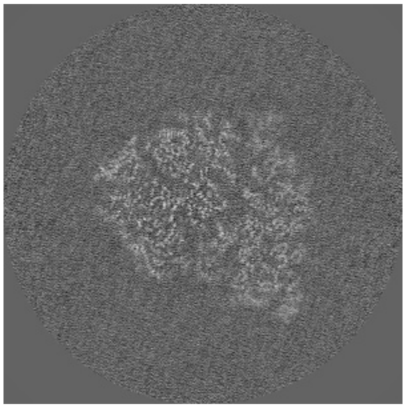
6.3.2 Raw map



X Index: 249



Y Index: 268

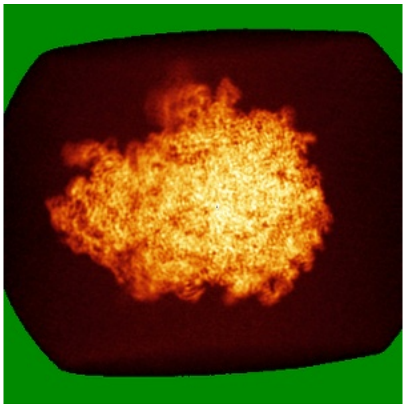


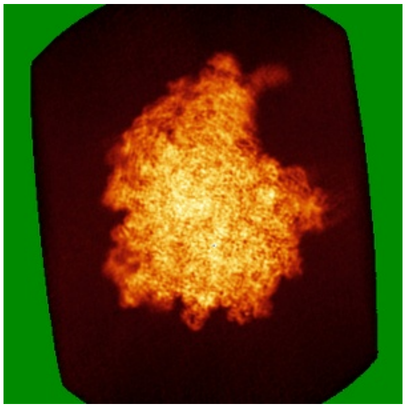
Z Index: 249

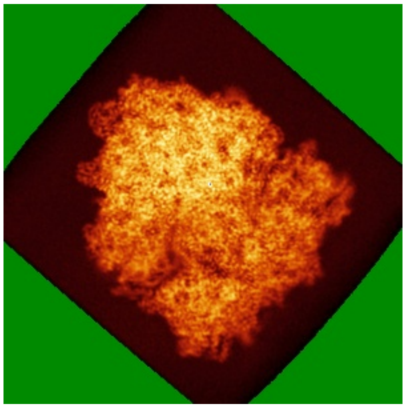
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color)

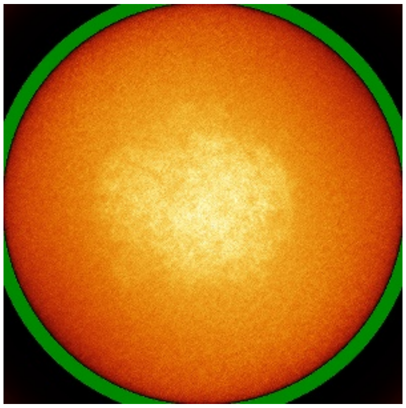
6.4.1 Primary map

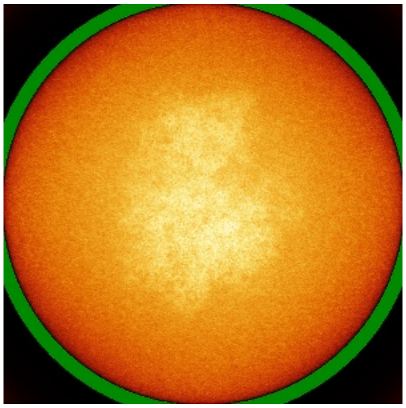

X

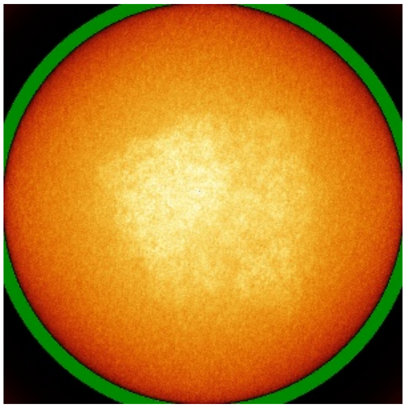

Y


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.

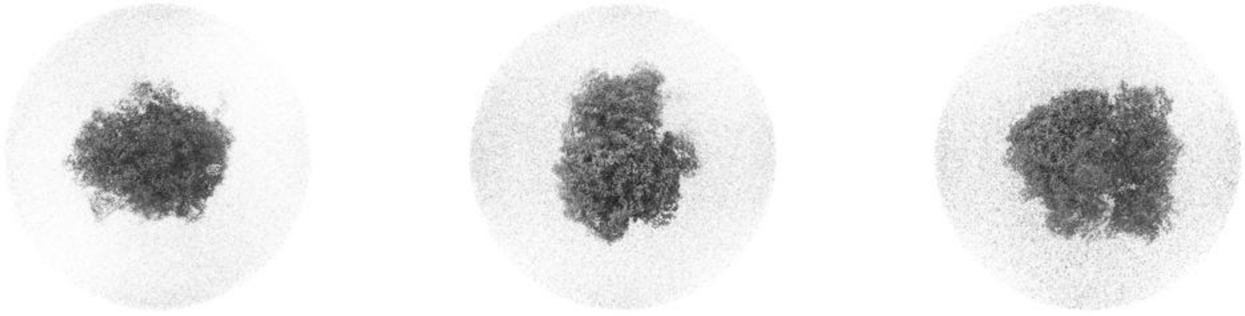
6.5 Orthogonal surface views

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.008. 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.

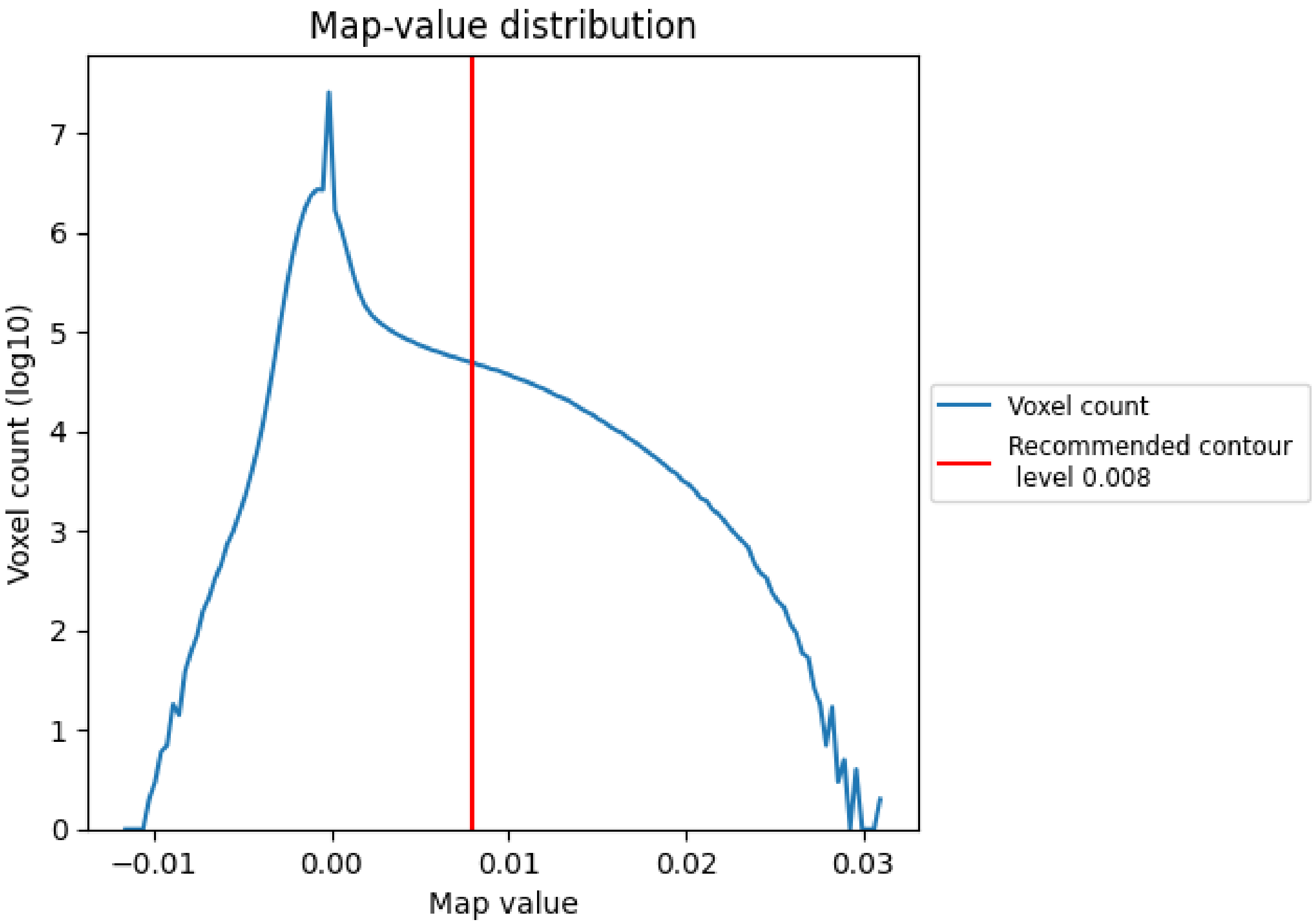
6.6 Mask visualisation

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

7 Map analysis ⓘ

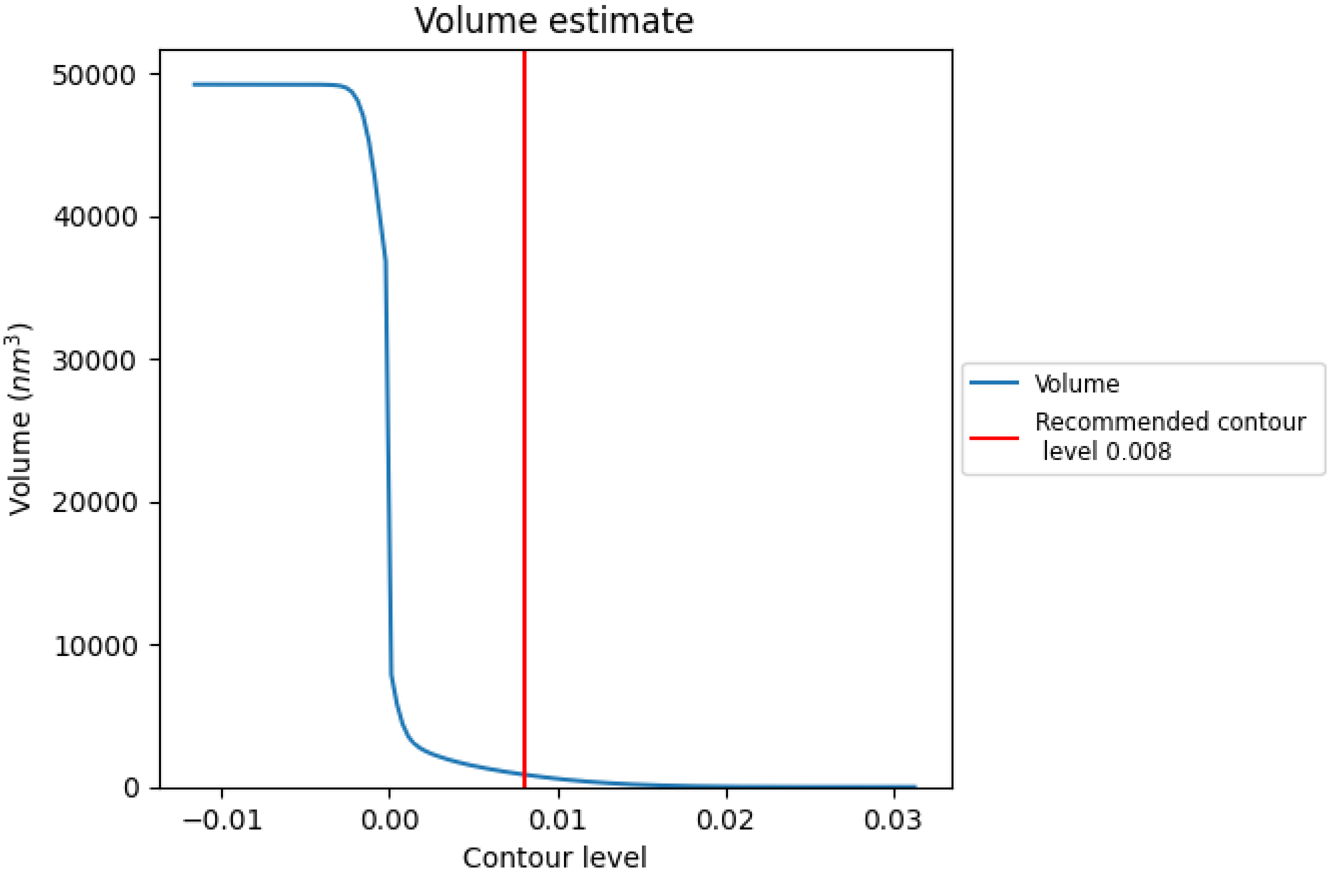
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

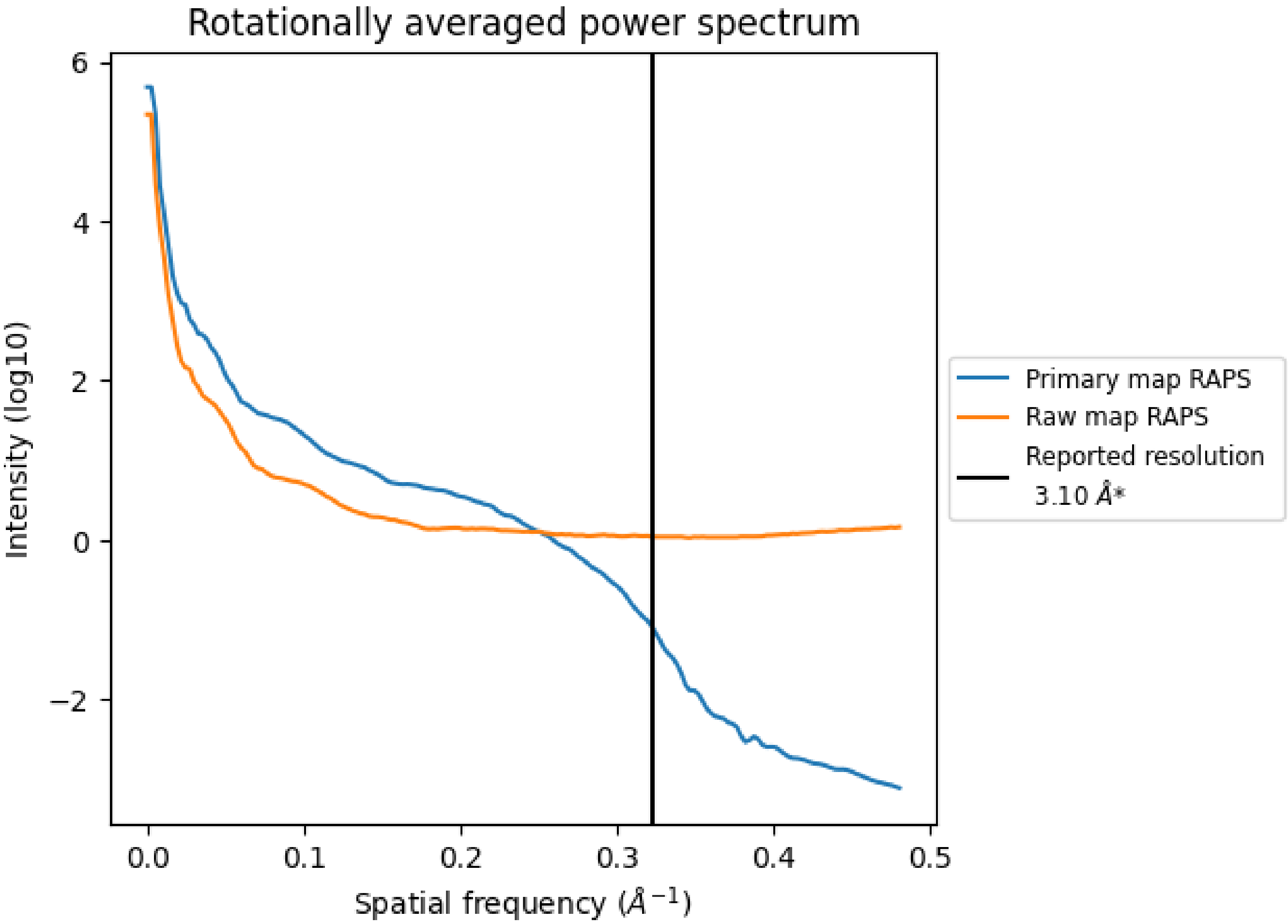
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 865 nm^3; this corresponds to an approximate mass of 782 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 ⓘ

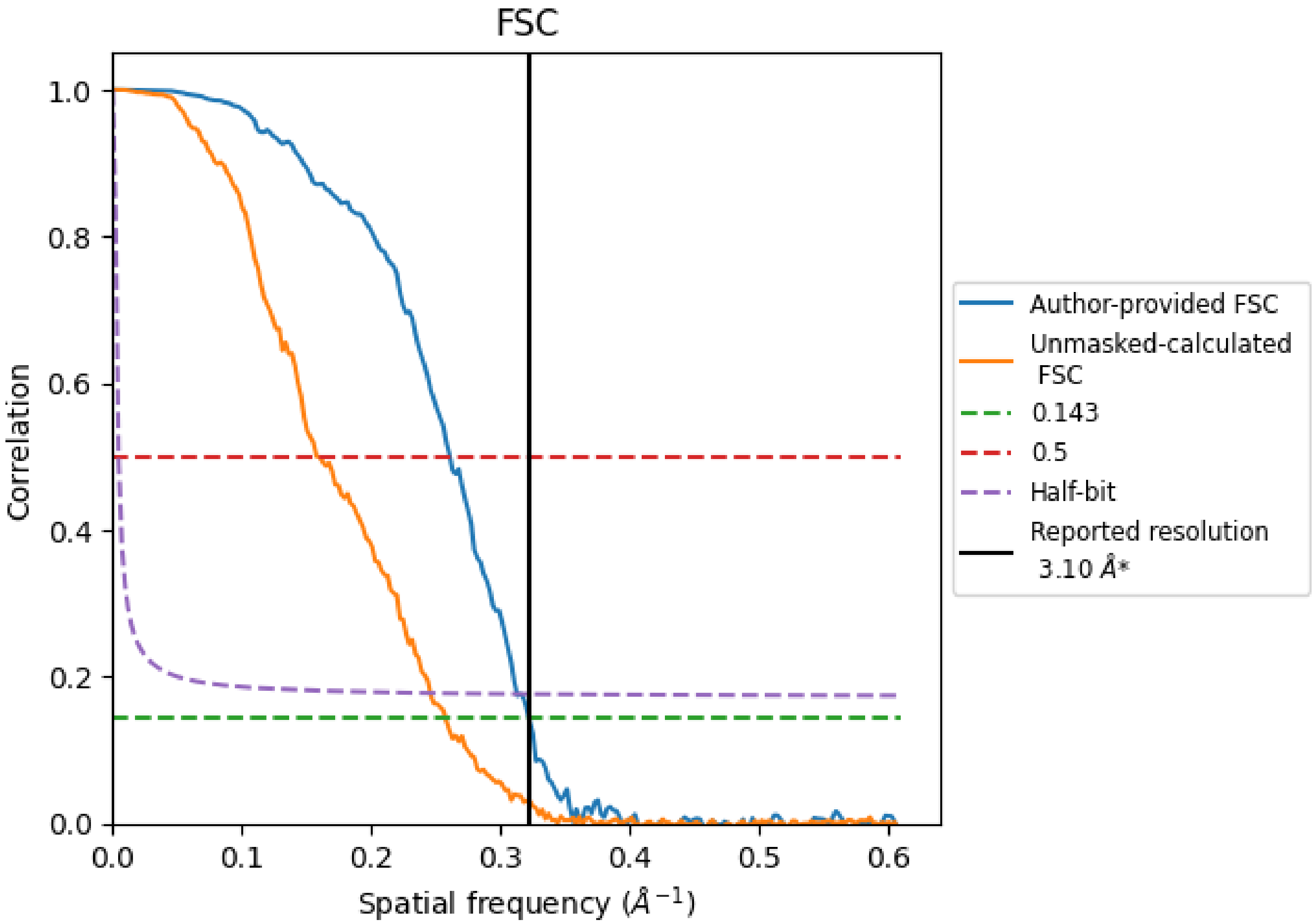


*Reported resolution corresponds to spatial frequency of 0.323 $\AA^{-1}$

8 Fourier-Shell correlation ⓘ

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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates ⓘ

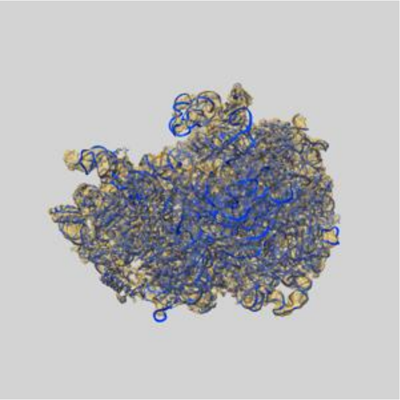
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.10	3.83	3.20
Unmasked-calculated*	3.88	6.34	4.07

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.88 differs from the reported value 3.1 by more than 10 %

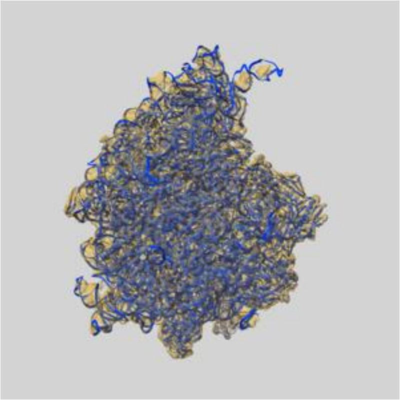
9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-12332 and PDB model 7NHL. Per-residue inclusion information can be found in section 3 on page 15.

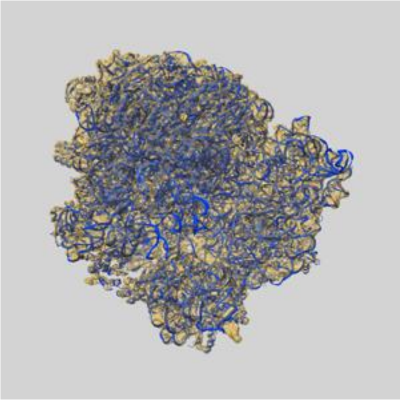
9.1 Map-model overlay ⓘ



X



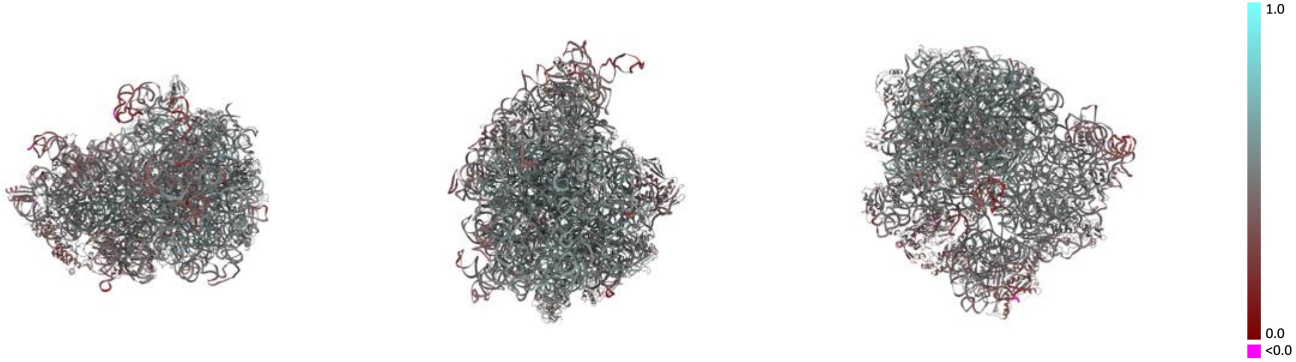
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.008 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.

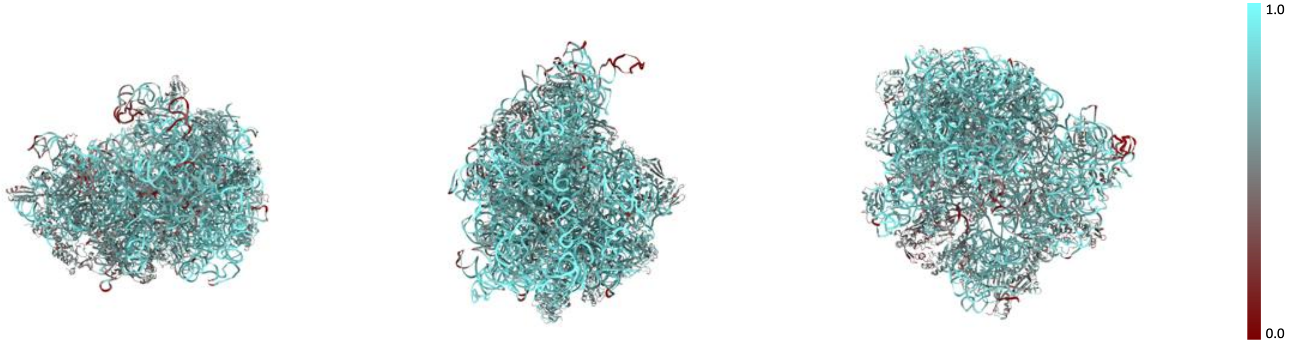
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

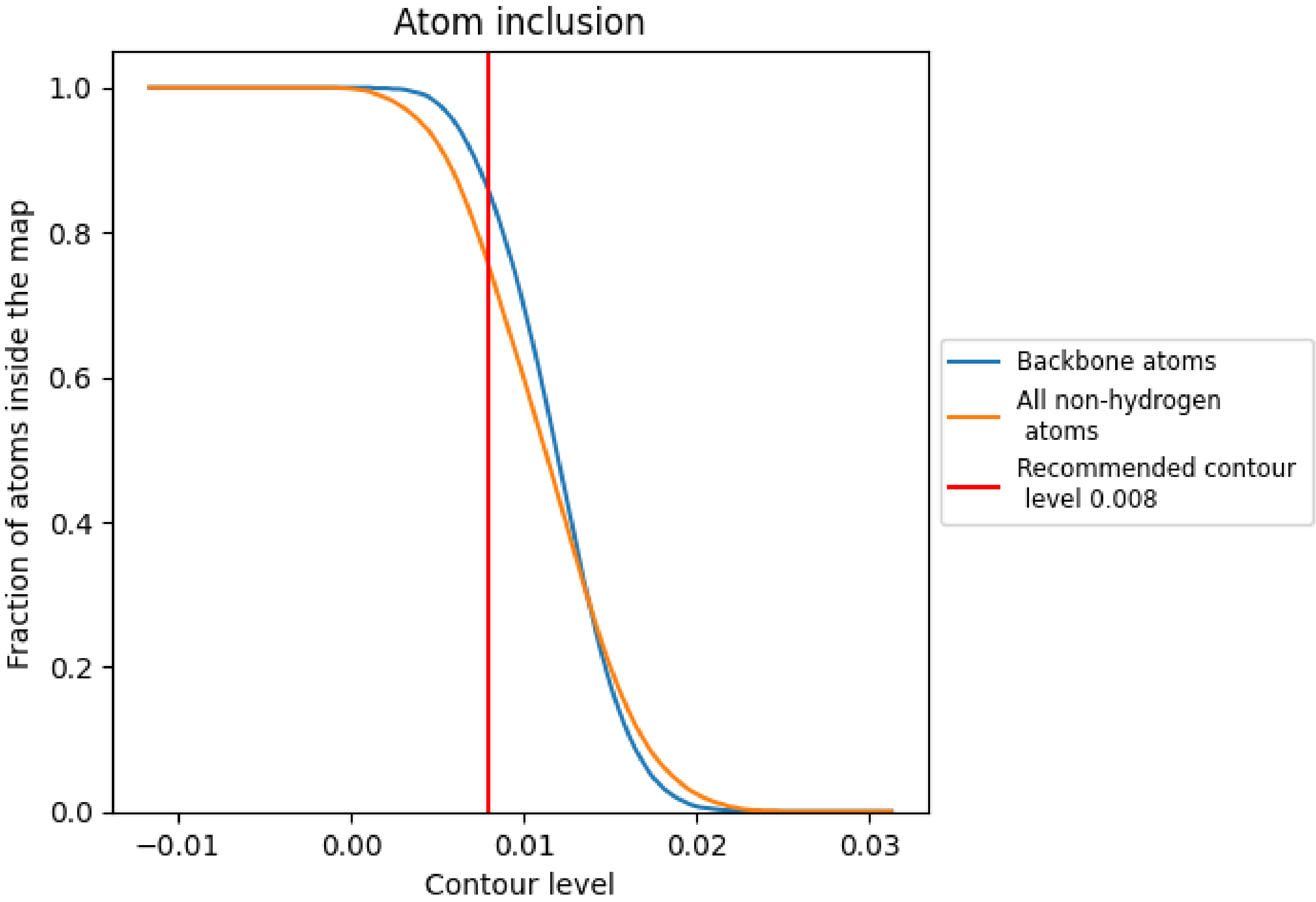
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.008).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7530	0.4760
0	0.4910	0.4250
1	0.5720	0.4960
2	0.6480	0.4410
3	0.6350	0.4720
4	0.3360	0.3180
5	0.6920	0.5010
6	0.6680	0.4730
7	0.7080	0.5400
8	0.6690	0.5280
9	0.6720	0.5070
A	0.8530	0.5040
B	0.8400	0.4520
D	0.7730	0.4950
G	0.6530	0.5140
H	0.6600	0.5050
I	0.6530	0.4850
J	0.4500	0.3630
K	0.5590	0.4100
M	0.6580	0.4900
N	0.5690	0.5020
O	0.6550	0.5010
P	0.6330	0.4980
Q	0.6570	0.4820
R	0.5860	0.4210
S	0.5900	0.4790
T	0.6860	0.4860
U	0.6540	0.4980
V	0.6640	0.5110
W	0.6380	0.4950
X	0.5800	0.4610
Y	0.5520	0.4350
Z	0.6520	0.5060
a	0.8090	0.4640
b	0.6480	0.4650

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Chain	Atom inclusion	Q-score
c	0.4800	0.3840
d	0.5820	0.4200
e	0.4530	0.4120
f	0.5940	0.4640
g	0.4340	0.3820
h	0.6230	0.4040
i	0.5150	0.4280
j	0.6290	0.4420
k	0.5310	0.4020
l	0.4120	0.3920
m	0.5010	0.4560
n	0.5100	0.3990
o	0.6240	0.4510
p	0.5210	0.3910
q	0.4730	0.4030
r	0.4700	0.4350
s	0.4900	0.4130
t	0.4690	0.4020
u	0.5050	0.3850