Full wwPDB EM Validation Report ⓘ

Oct 29, 2026 – 12:40 PM EDT

PDB ID	:	12DM / pdb_000012dm
EMDB ID	:	EMD-76336
Title	:	AHA hibernation factor bound to the 70S ribosome of Haloferax volcanii
Authors	:	Souza, D.P.; Davis, J.H.
Deposited on	:	2026-03-29
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

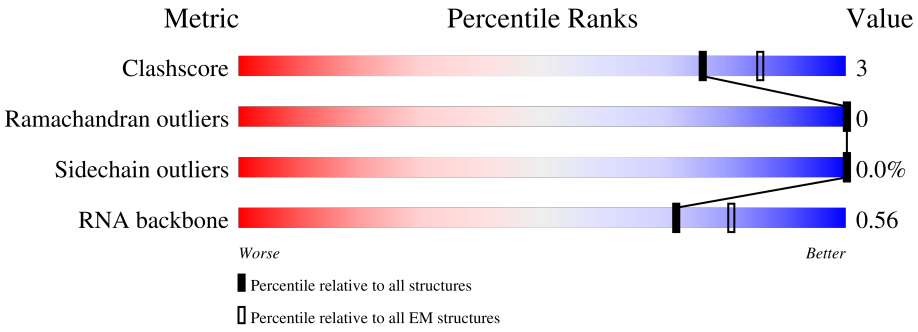
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

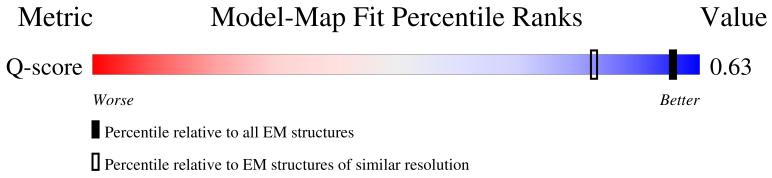
1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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





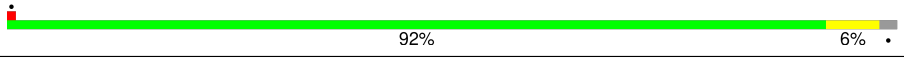
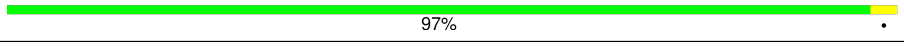
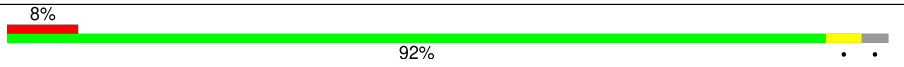
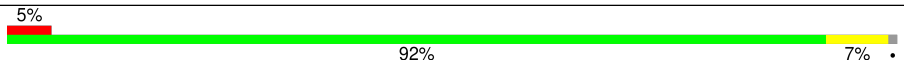
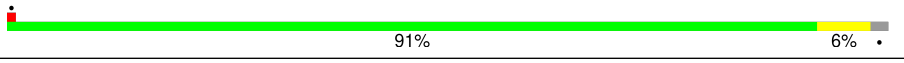
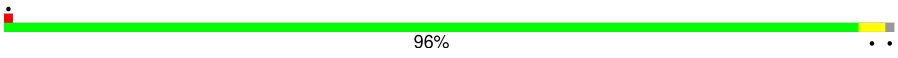
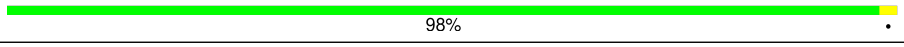
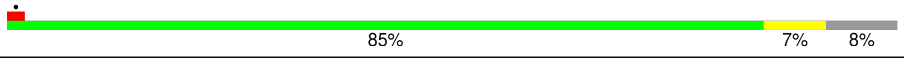
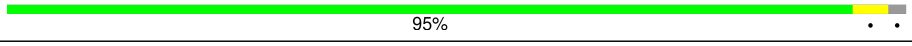
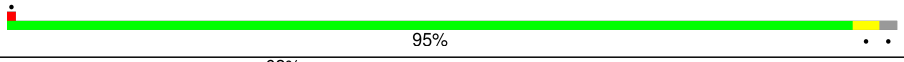
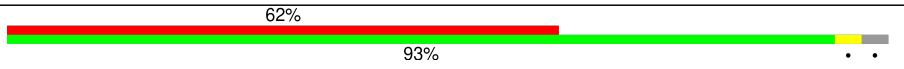
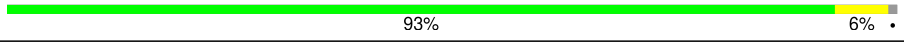
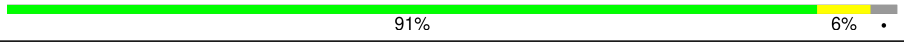
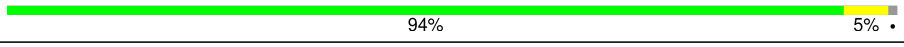
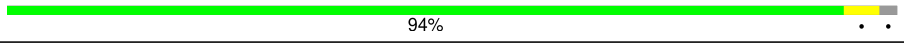
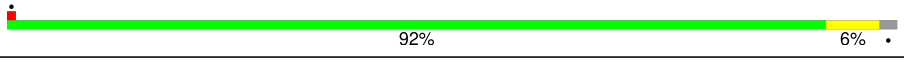
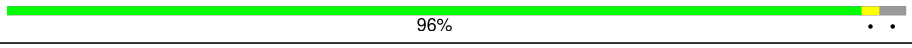
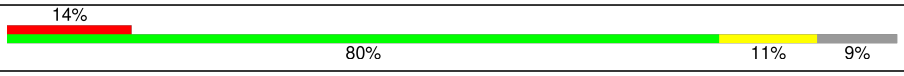
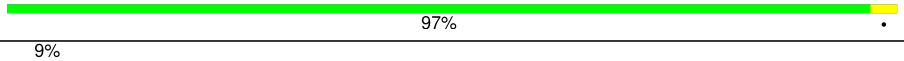
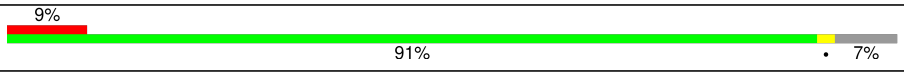
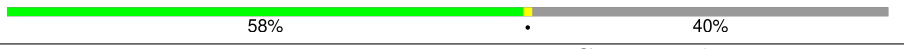
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	5628 (1.90 - 2.90)

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	2	122	80% 16%
2	4	76	11% 50% 38% 8%
3	0	380	91% 9%

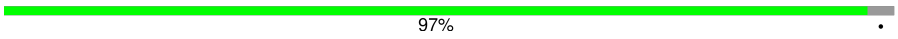
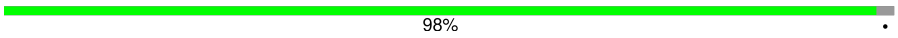
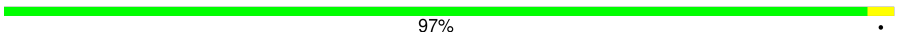
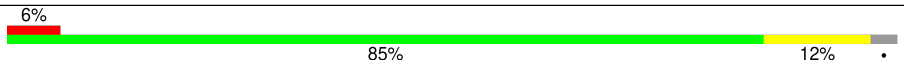
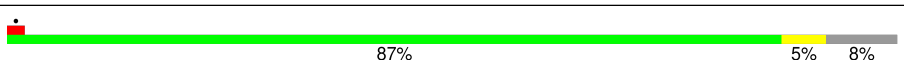
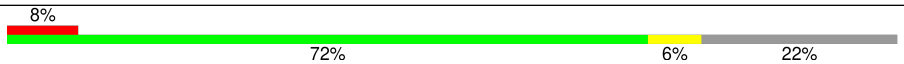
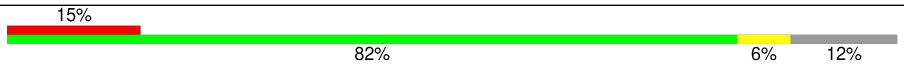
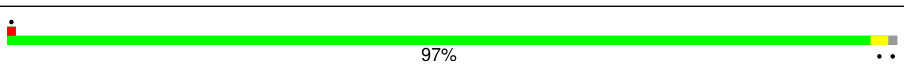
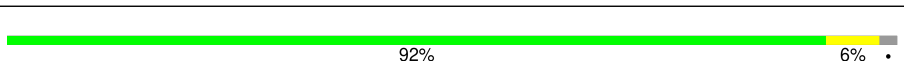
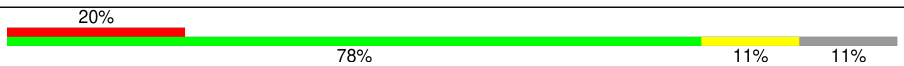
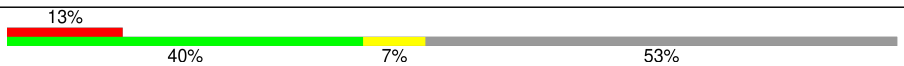
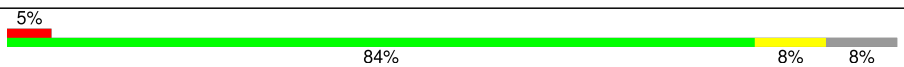
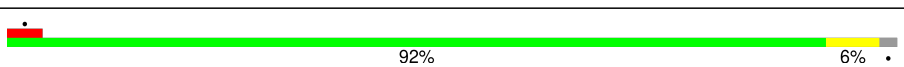
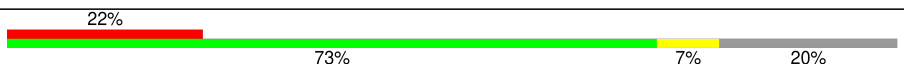
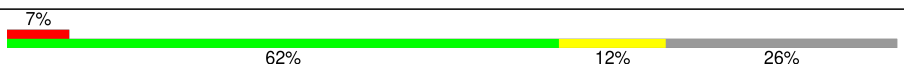
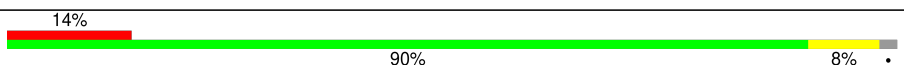
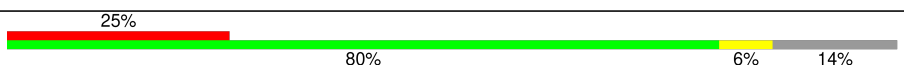
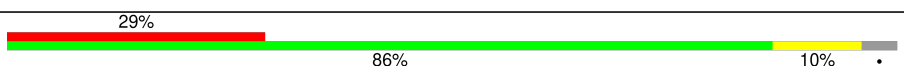
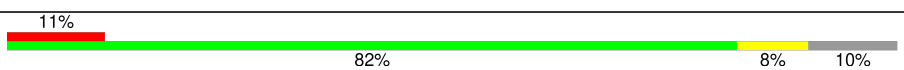
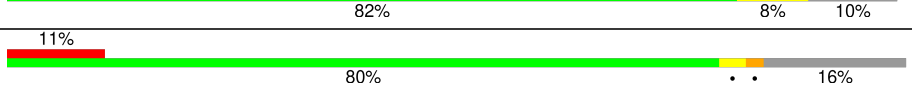
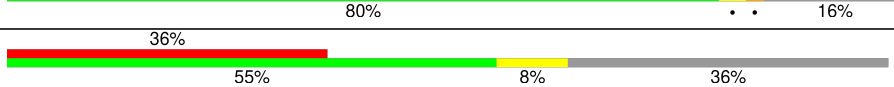
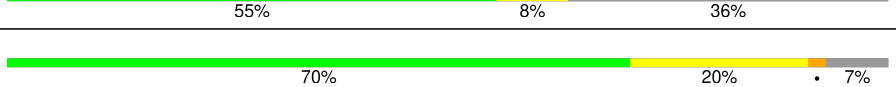
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Mol	Chain	Length	Quality of chain
4	3	1473	
5	A	241	
6	B	338	
7	C	248	
8	D	172	
9	E	178	
10	F	120	
11	H	176	
12	J	145	
13	K	132	
14	L	165	
15	M	196	
16	N	184	
17	O	58	
18	P	116	
19	Q	151	
20	R	96	
21	S	153	
22	T	83	
23	U	118	
24	V	66	
25	W	70	
26	X	154	
27	Y	92	
28	Z	235	

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Mol	Chain	Length	Quality of chain
29	a	58	
30	b	50	
31	c	89	
32	d	93	
33	e	220	
34	f	175	
35	g	247	
36	h	133	
37	i	204	
38	j	130	
39	k	125	
40	l	132	
41	m	102	
42	n	130	
43	o	142	
44	p	167	
45	q	58	
46	r	155	
47	s	114	
48	t	140	
49	u	151	
50	v	101	
51	w	64	
52	x	74	
53	1	2915	

2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 142666 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	2	120	2552	1139	455	838	120	0	0

- Molecule 2 is a RNA chain called E-site tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	4	70	1500	668	278	484	70	0	0

- Molecule 3 is a protein called CBS domain protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	0	378	2969	1834	535	591	9	0	0

- Molecule 4 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	3	1372	29421	13118	5403	9528	1372	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	236	1769	1091	352	321	5	0	0

- Molecule 6 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	337	2607	1614	482	501	10	0	0

- Molecule 7 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	C	218	Total	C	N	O	0	0
			1680	1033	309	338		

- Molecule 8 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	166	Total	C	N	O	S	0	0
			1298	804	229	262	3		

- Molecule 9 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	174	Total	C	N	O	S	0	0
			1352	836	231	282	3		

- Molecule 10 is a protein called Large ribosomal subunit protein eL8.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	119	Total	C	N	O	S	0	0
			879	545	141	192	1		

- Molecule 11 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	172	Total	C	N	O	S	0	0
			1358	843	251	256	8		

- Molecule 12 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	144	Total	C	N	O	S	0	0
			1116	694	200	218	4		

- Molecule 13 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	132	Total	C	N	O	S	0	0
			995	611	188	191	5		

- Molecule 14 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	152	Total 1153	C 695	N 226	O 232	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein eL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	193	Total 1569	C 958	N 335	O 275	S 1	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	181	Total 1400	C 872	N 258	O 269	S 1	0	0

- Molecule 17 is a protein called Large ribosomal subunit protein eL20.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	O	56	Total 434	C 271	N 77	O 86	0	0

- Molecule 18 is a protein called Large ribosomal subunit protein eL18.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	115	Total 888	C 543	N 168	O 177	0	0

- Molecule 19 is a protein called Large ribosomal subunit protein eL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Q	146	Total 1177	C 710	N 241	O 225	S 1	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein eL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	95	Total 738	C 452	N 150	O 135	S 1	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	150	Total	C	N	O	S	0	0
			1165	723	214	224	4		

- Molecule 22 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	81	Total	C	N	O	S	0	0
			639	394	110	132	3		

- Molecule 23 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	U	115	Total	C	N	O	0	0
			914	552	172	190		

- Molecule 24 is a protein called Large ribosomal subunit protein eL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	V	57	Total	C	N	O	S	0	0
			459	283	81	93	2		

- Molecule 25 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	W	64	Total	C	N	O	S	0	0
			488	299	84	104	1		

- Molecule 26 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	X	154	Total	C	N	O	S	0	0
			1201	733	216	248	4		

- Molecule 27 is a protein called Large ribosomal subunit protein eL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Y	86	Total	C	N	O	S	0	0
			692	428	133	130	1		

- Molecule 28 is a protein called Large ribosomal subunit protein eL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Z	140	Total	C	N	O	S	0	0
			1117	683	224	209	1		

- Molecule 29 is a protein called Large ribosomal subunit protein eL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	56	Total	C	N	O	S	0	0
			430	261	88	77	4		

- Molecule 30 is a protein called Large ribosomal subunit protein eL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	b	49	Total	C	N	O	S	0	0
			416	253	89	72	2		

- Molecule 31 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	c	78	Total	C	N	O	S	0	0
			608	368	123	116	1		

- Molecule 32 is a protein called Large ribosomal subunit protein eL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	93	Total	C	N	O	S	0	0
			748	459	153	128	8		

- Molecule 33 is a protein called Small ribosomal subunit protein eS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	e	174	Total	C	N	O	S	0	0
			1398	875	249	273	1		

- Molecule 34 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	169	Total	C	N	O	S	0	0
			1367	838	256	271	2		

- Molecule 35 is a protein called Small ribosomal subunit protein eS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	228	Total	C	N	O	S	0	0
			1745	1094	297	353	1		

- Molecule 36 is a protein called Small ribosomal subunit protein eS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	h	104	Total	C	N	O	S	0	0
			784	480	140	162	2		

- Molecule 37 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	i	180	Total	C	N	O	S	0	0
			1410	877	249	280	4		

- Molecule 38 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	j	129	Total	C	N	O	S	0	0
			991	627	165	197	2		

- Molecule 39 is a protein called Small ribosomal subunit protein eS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	k	122	Total	C	N	O	S	0	0
			932	557	194	180	1		

- Molecule 40 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	l	117	Total	C	N	O	S	0	0
			907	560	176	168	3		

- Molecule 41 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	m	48	Total	C	N	O	S	0	0
			383	240	69	73	1		

- Molecule 42 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	n	120	Total	C	N	O	S	0	0
			864	530	166	166	2		

- Molecule 43 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	o	139	Total	C	N	O	S	0	0
			1058	652	205	197	4		

- Molecule 44 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	p	134	Total	C	N	O	S	0	0
			1076	658	208	206	4		

- Molecule 45 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	q	43	Total	C	N	O	S	0	0
			363	219	76	63	5		

- Molecule 46 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	r	152	Total	C	N	O	S	0	0
			1202	731	221	247	3		

- Molecule 47 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	s	109	Total	C	N	O	S	0	0
			853	539	141	168	5		

- Molecule 48 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	t	120	Total	C	N	O	S	0	0
			971	609	170	189	3		

- Molecule 49 is a protein called Small ribosomal subunit protein eS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	u	145	Total	C	N	O	S	0	0
			1126	696	200	228	2		

- Molecule 50 is a protein called Small ribosomal subunit protein eS24.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	v	91	Total	C	N	O	S	0	0
			741	458	130	149	4		

- Molecule 51 is a protein called Small ribosomal subunit protein eS27.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	w	54	Total	C	N	O	S	0	0
			385	236	63	82	4		

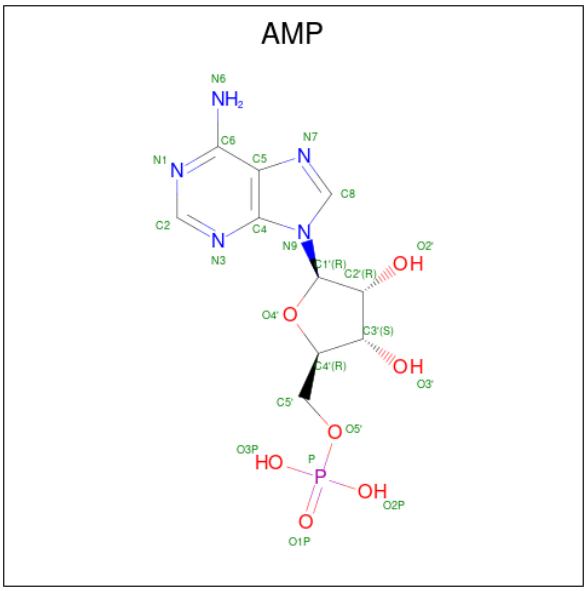
- Molecule 52 is a protein called Small ribosomal subunit protein eS28.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	x	47	Total	C	N	O	S	0	0
			361	223	69	66	3		

- Molecule 53 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	1	2704	Total	C	N	O	P	0	0
			57971	25869	10673	18725	2704		

- Molecule 54 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
54	0	1	Total	C	N	O	P	0
			23	10	5	7	1	
54	0	1	Total	C	N	O	P	0
			23	10	5	7	1	

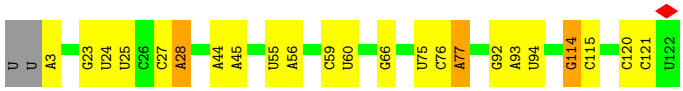
3 Residue-property plots (i)

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: 5S rRNA

Chain 2:

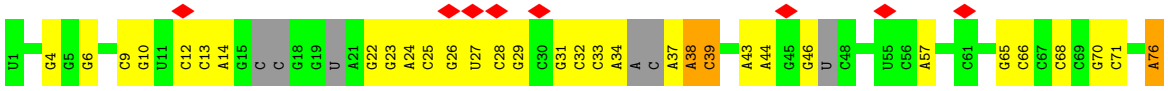




• Molecule 2: E-site tRNA

Chain 4:

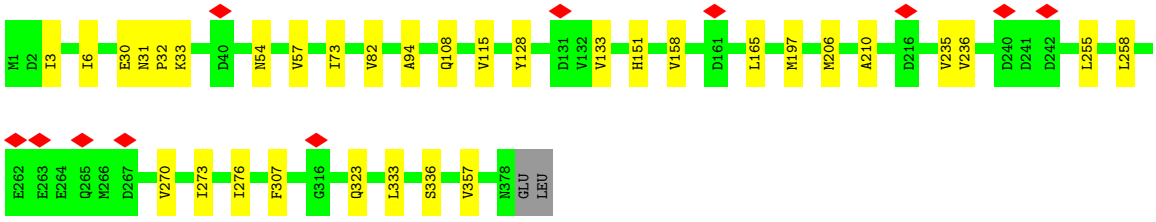




• Molecule 3: CBS domain protein

Chain 0:

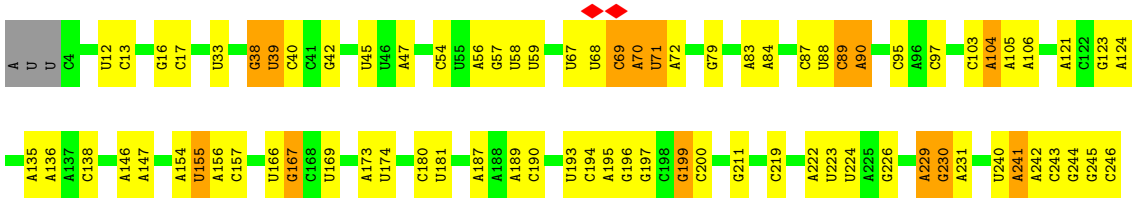


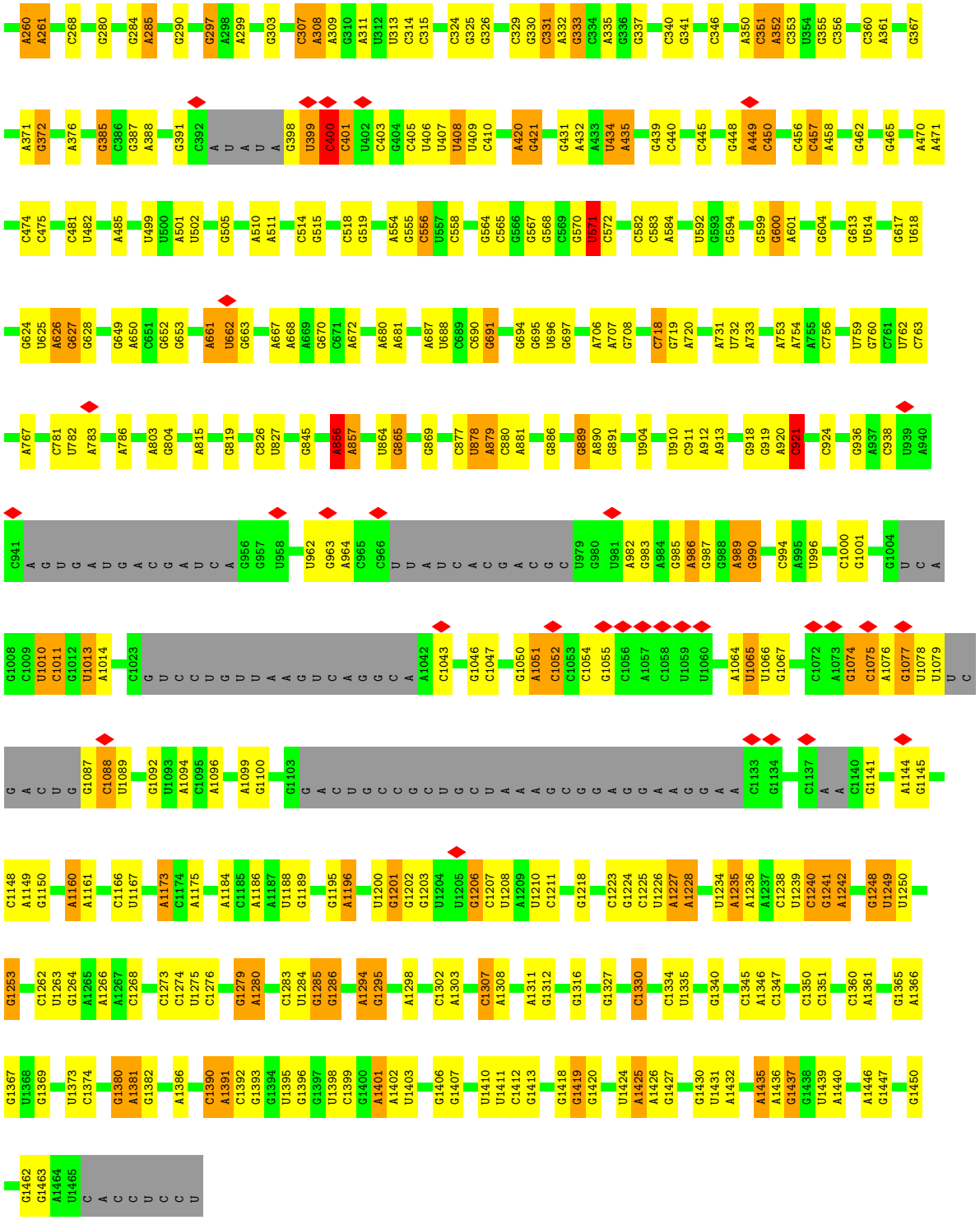


• Molecule 4: 16S rRNA

Chain 3:



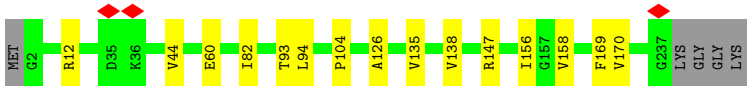




• Molecule 5: Large ribosomal subunit protein uL2

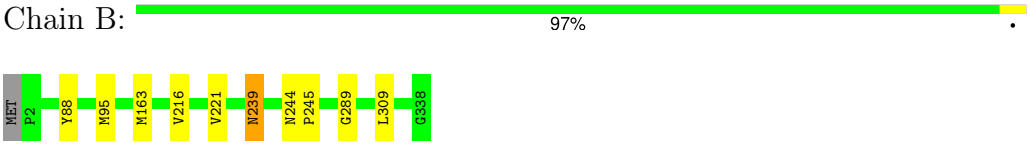
Chain A:





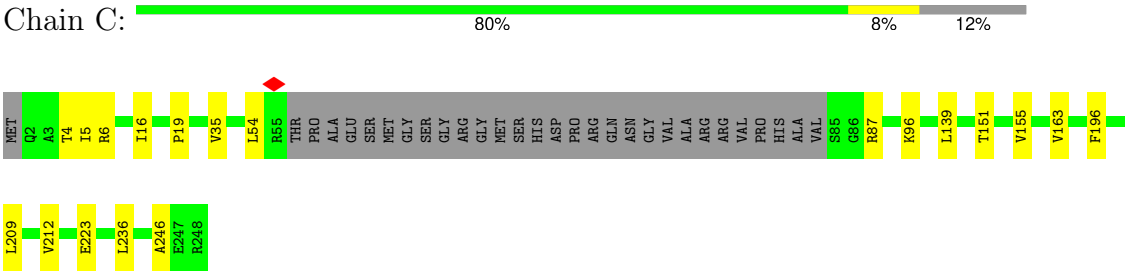
• Molecule 6: Large ribosomal subunit protein uL3

Chain B:



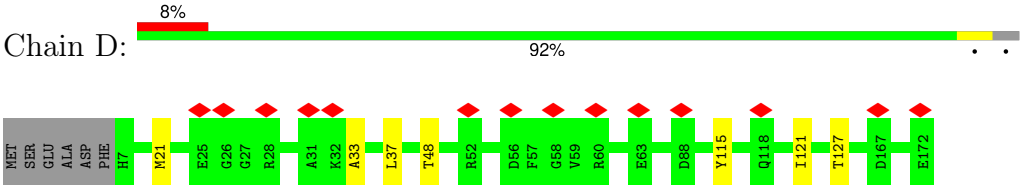
• Molecule 7: Large ribosomal subunit protein uL4

Chain C:



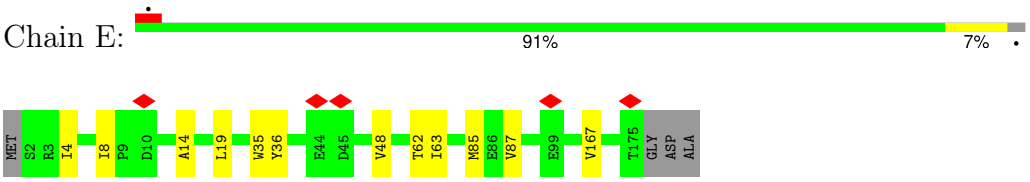
• Molecule 8: Large ribosomal subunit protein uL5

Chain D:



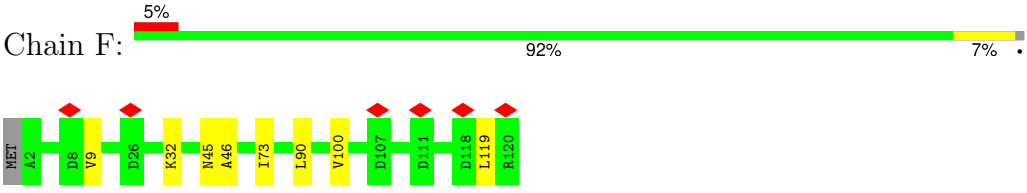
• Molecule 9: Large ribosomal subunit protein uL6

Chain E:



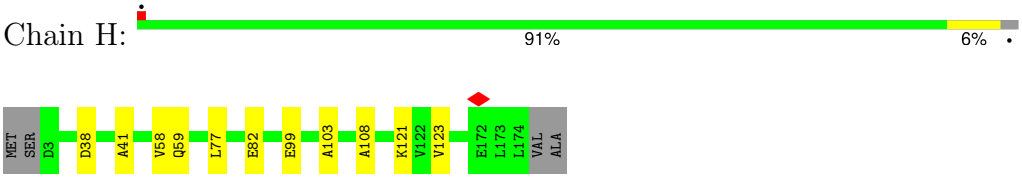
• Molecule 10: Large ribosomal subunit protein eL8

Chain F:



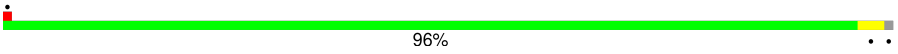
• Molecule 11: Large ribosomal subunit protein uL16

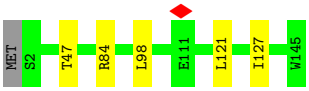
Chain H:



• Molecule 12: Large ribosomal subunit protein uL13

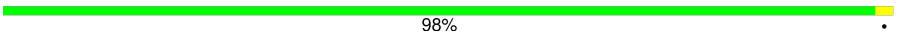
Chain J:





• Molecule 13: Large ribosomal subunit protein uL14

Chain K:

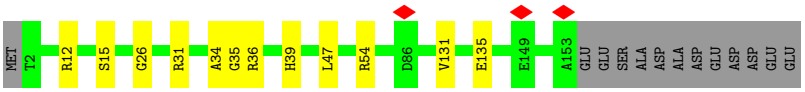




• Molecule 14: Large ribosomal subunit protein uL15

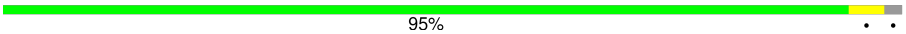
Chain L:

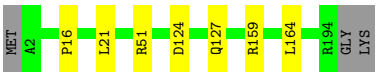




• Molecule 15: Large ribosomal subunit protein eL15

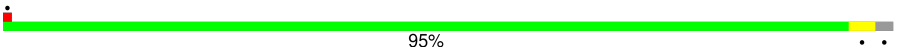
Chain M:

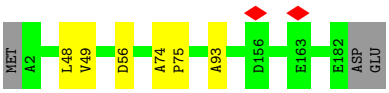




• Molecule 16: Large ribosomal subunit protein uL18

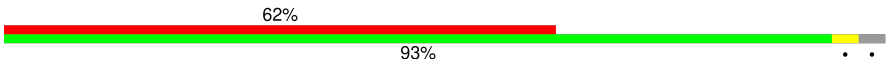
Chain N:

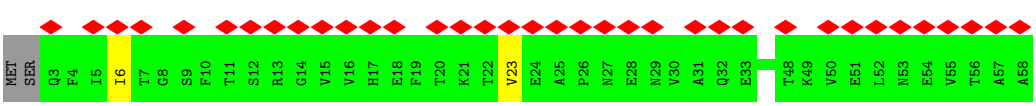




• Molecule 17: Large ribosomal subunit protein eL20

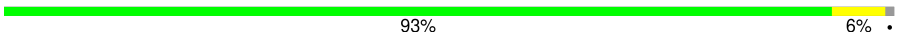
Chain O:





• Molecule 18: Large ribosomal subunit protein eL18

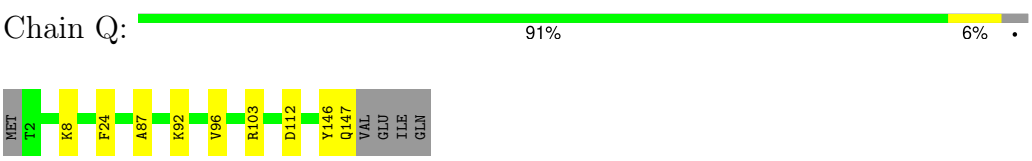
Chain P:





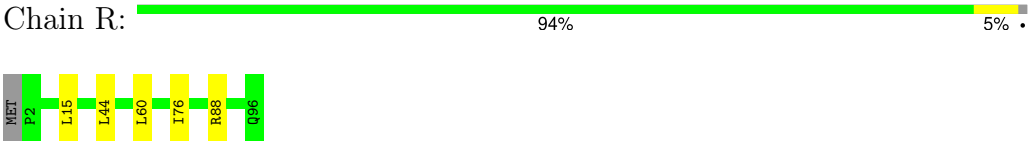
• Molecule 19: Large ribosomal subunit protein eL19

Chain Q:



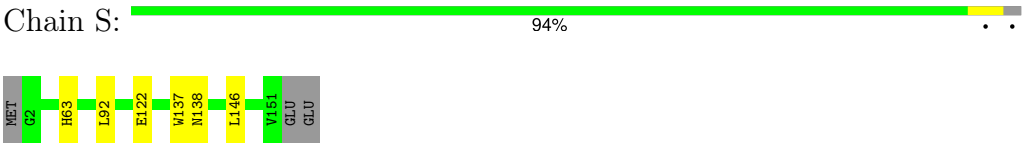
• Molecule 20: Large ribosomal subunit protein eL21

Chain R:



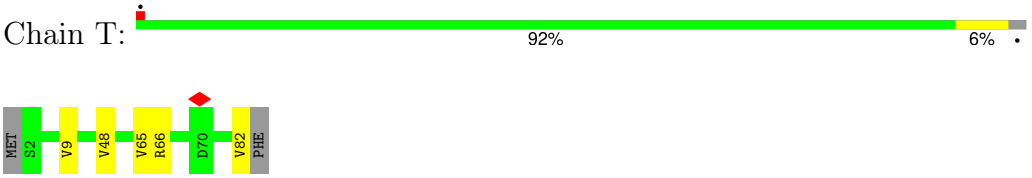
• Molecule 21: Large ribosomal subunit protein uL22

Chain S:



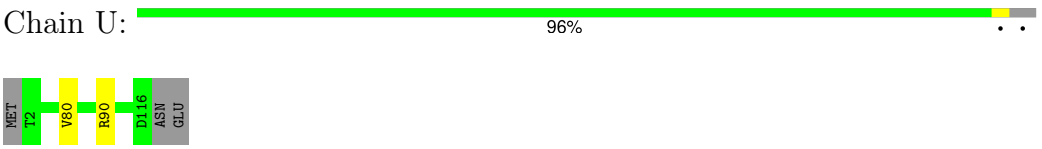
• Molecule 22: Large ribosomal subunit protein uL23

Chain T:



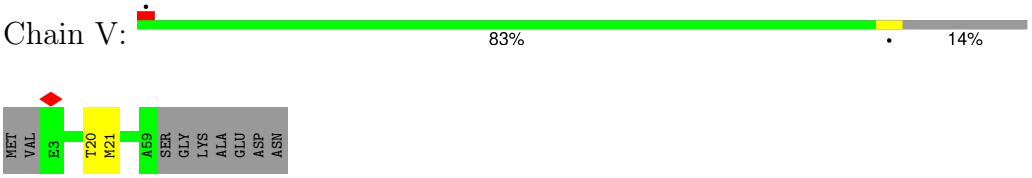
• Molecule 23: Large ribosomal subunit protein uL24

Chain U:



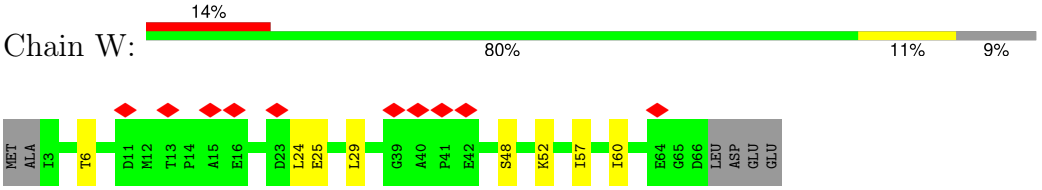
• Molecule 24: Large ribosomal subunit protein eL24

Chain V:



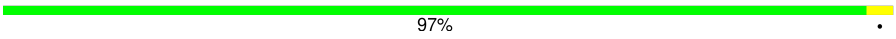
• Molecule 25: Large ribosomal subunit protein uL29

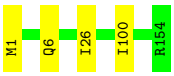
Chain W:



• Molecule 26: Large ribosomal subunit protein uL30

Chain X:

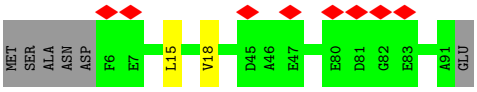




• Molecule 27: Large ribosomal subunit protein eL31

Chain Y:

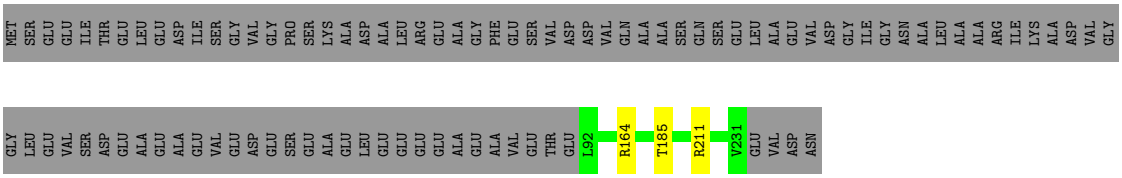




• Molecule 28: Large ribosomal subunit protein eL32

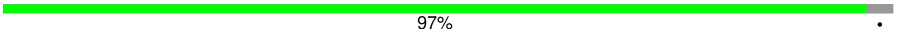
Chain Z:





• Molecule 29: Large ribosomal subunit protein eL37

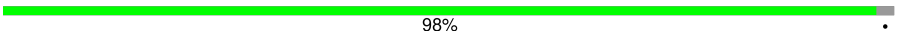
Chain a:





• Molecule 30: Large ribosomal subunit protein eL39

Chain b:

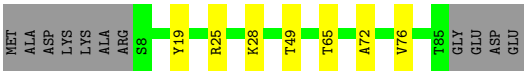




• Molecule 31: 50S ribosomal protein L37Ae

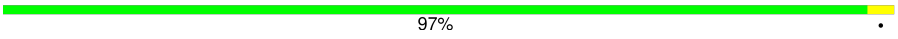
Chain c:

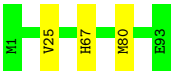




• Molecule 32: Large ribosomal subunit protein eL42

Chain d:

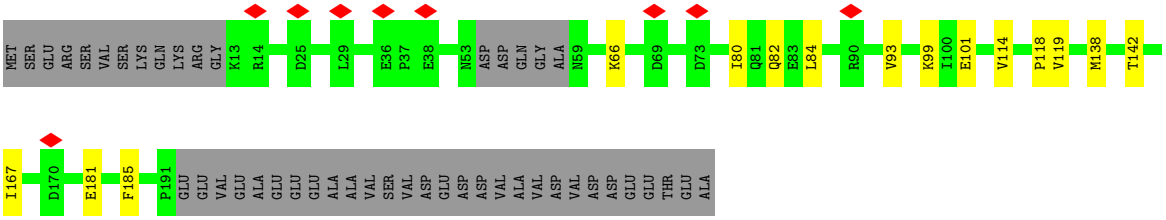




• Molecule 33: Small ribosomal subunit protein eS1

Chain e:





• Molecule 34: Small ribosomal subunit protein uS4

Chain f:

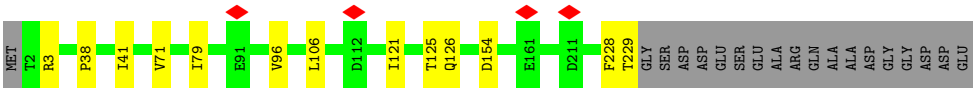




• Molecule 35: Small ribosomal subunit protein eS4

Chain g:

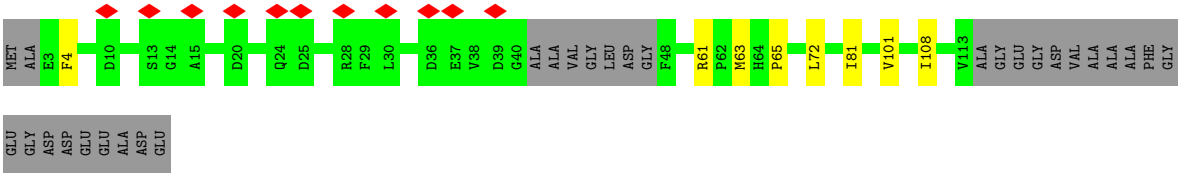




• Molecule 36: Small ribosomal subunit protein eS6

Chain h:

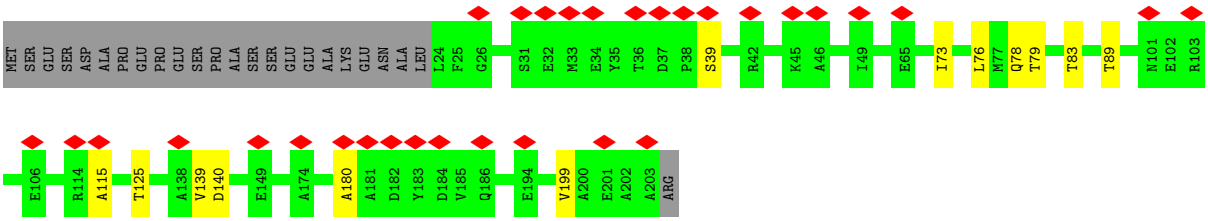




• Molecule 37: Small ribosomal subunit protein uS7

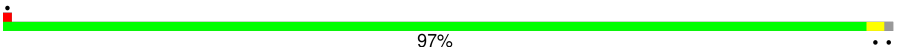
Chain i:

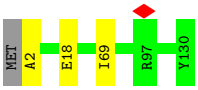




• Molecule 38: Small ribosomal subunit protein uS8

Chain j:





• Molecule 39: Small ribosomal subunit protein eS8

Chain k:

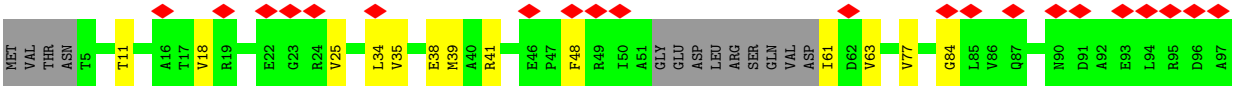


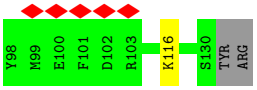


• Molecule 40: Small ribosomal subunit protein uS9

Chain l:



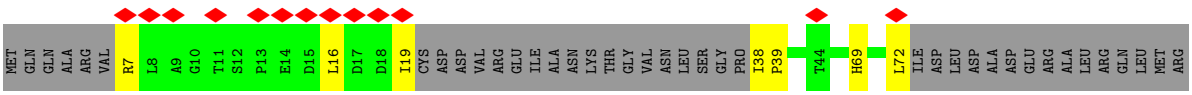




• Molecule 41: Small ribosomal subunit protein uS10

Chain m:



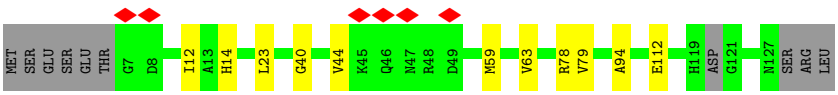




• Molecule 42: Small ribosomal subunit protein uS11

Chain n:

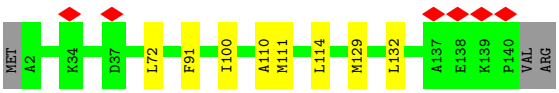




• Molecule 43: Small ribosomal subunit protein uS12

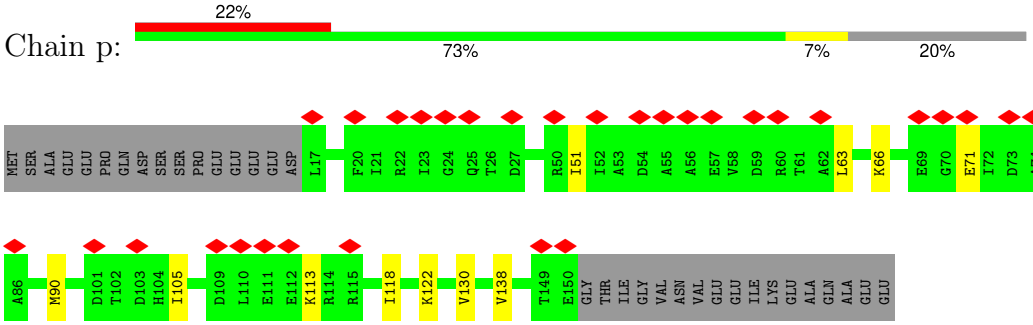
Chain o:





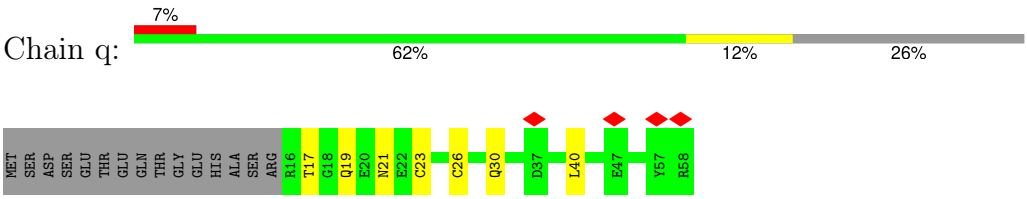
• Molecule 44: Small ribosomal subunit protein uS13

Chain p:



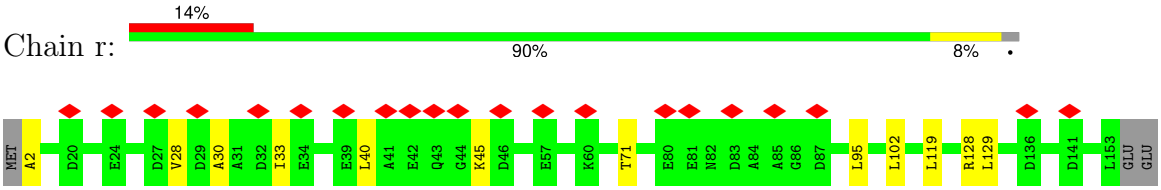
• Molecule 45: Small ribosomal subunit protein uS14

Chain q:



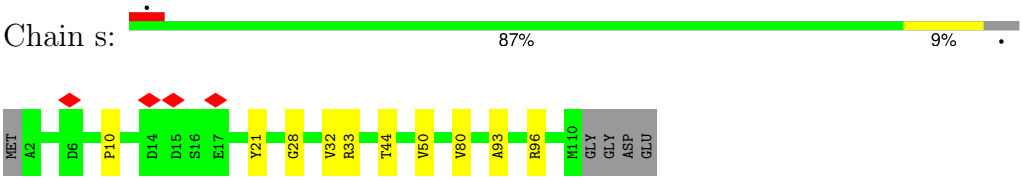
• Molecule 46: Small ribosomal subunit protein uS15

Chain r:



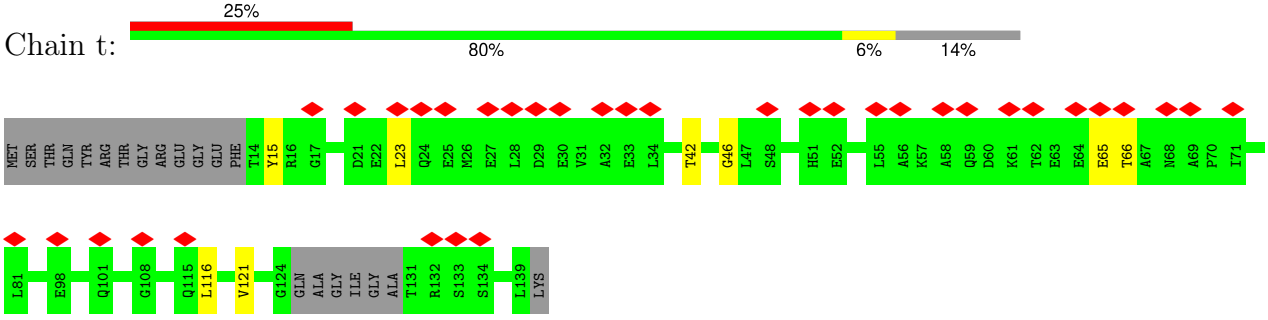
• Molecule 47: Small ribosomal subunit protein uS17

Chain s:



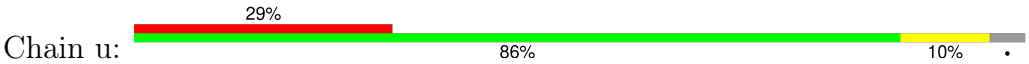
• Molecule 48: Small ribosomal subunit protein uS19

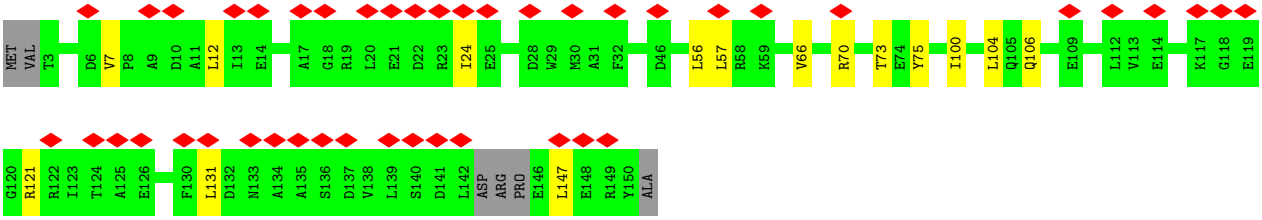
Chain t:



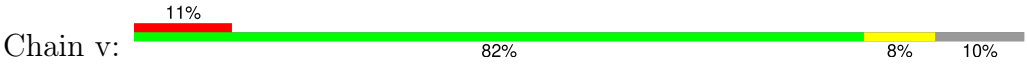
• Molecule 49: Small ribosomal subunit protein eS19

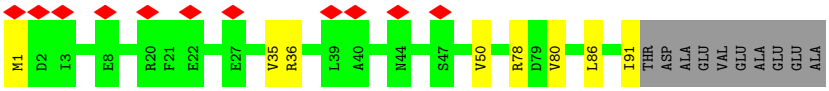
Chain u:



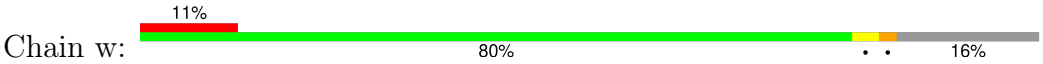


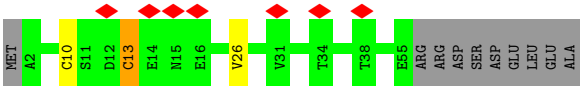
• Molecule 50: Small ribosomal subunit protein eS24





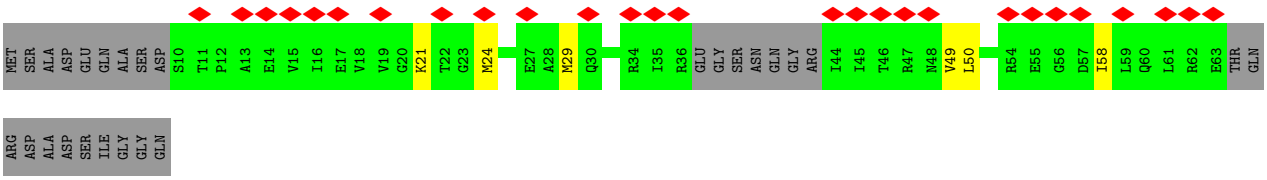
• Molecule 51: Small ribosomal subunit protein eS27





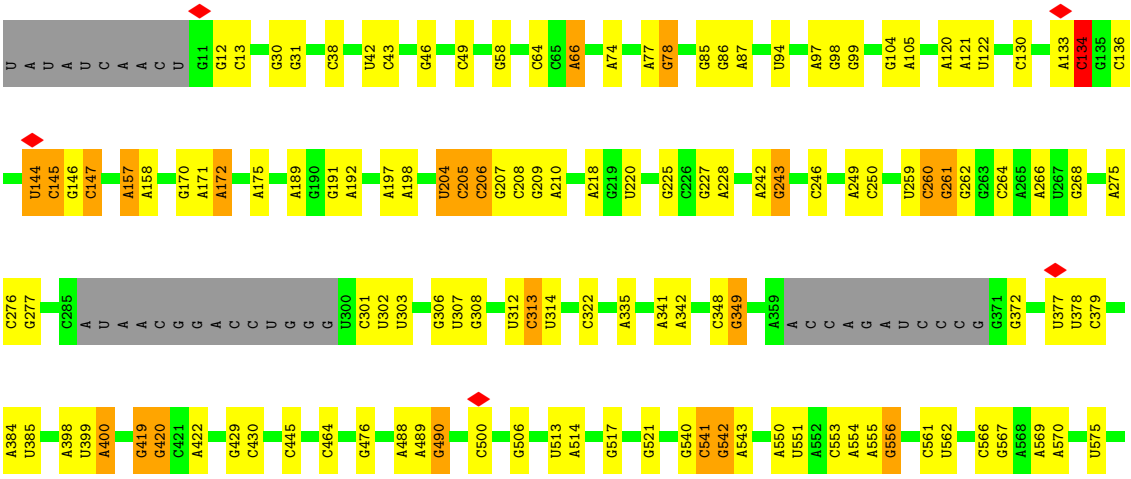
• Molecule 52: Small ribosomal subunit protein eS28

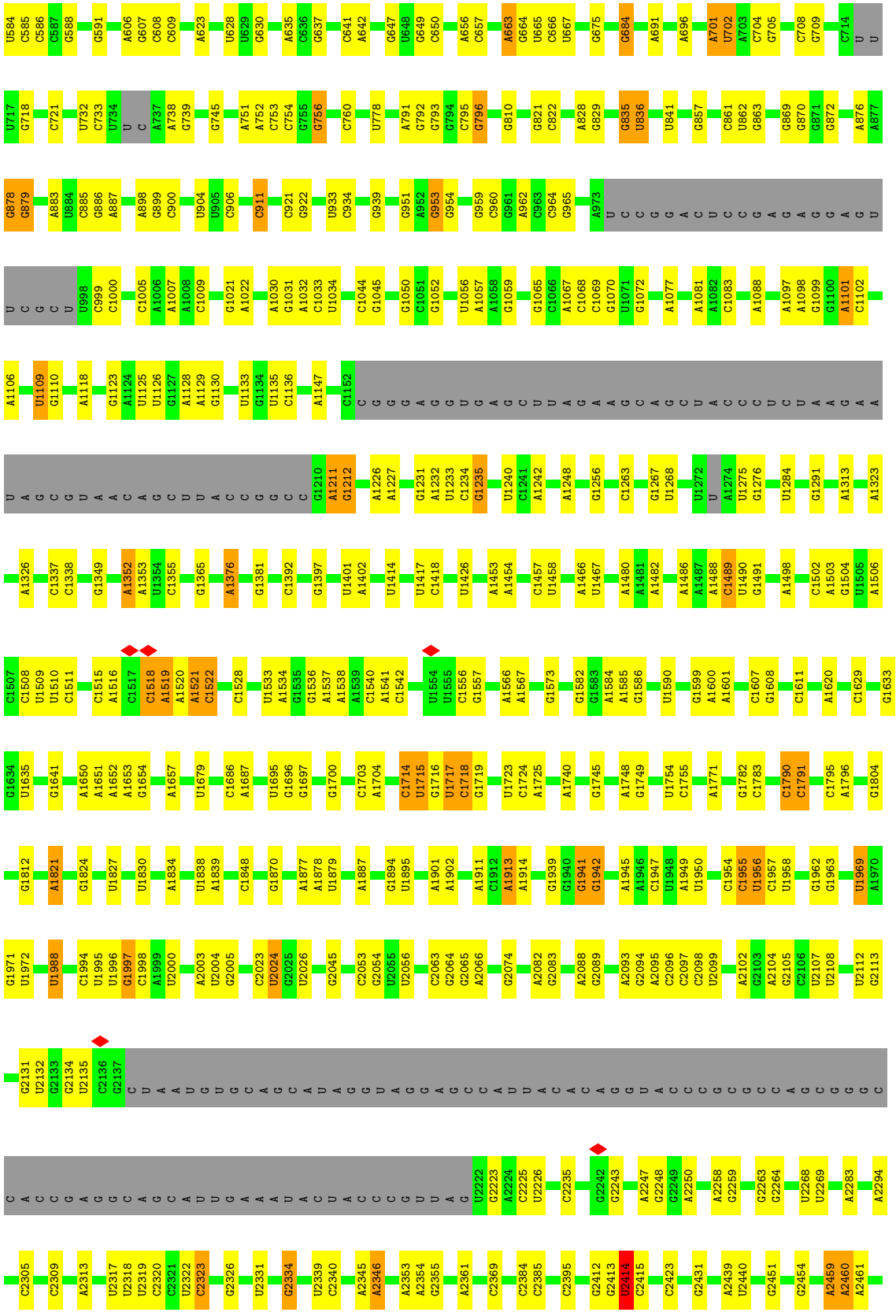


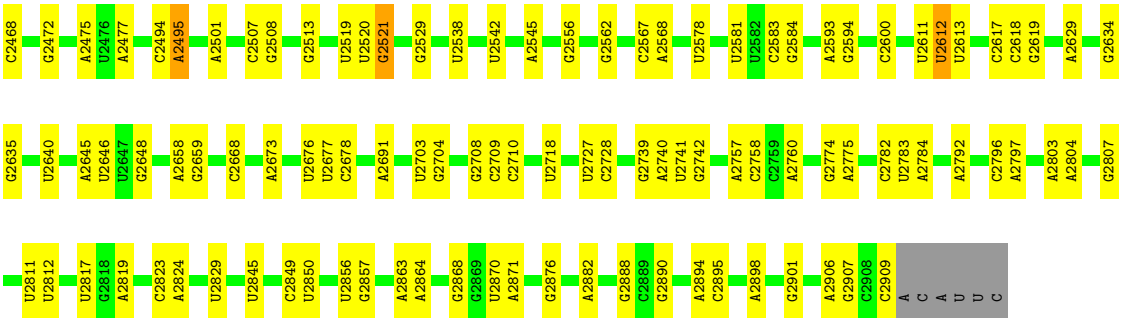


• Molecule 53: 23S rRNA








C2468
G2472
A2475
U2476
A2477
C2494
A2495
A2501
C2507
G2508
G2513
U2519
U2520
G2521
G2529
U2538
U2542
A2545
G2556
G2562
C2567
A2568
U2578
U2581
U2582
C2583
G2584
A2593
G2594
C2600
U2611
U2612
U2613
C2617
C2618
G2619
A2629
G2634
G2635
U2640
A2645
U2646
U2647
G2648
A2658
G2659
C2668
A2673
U2676
U2677
C2678
A2691
U2703
G2704
G2708
C2709
C2710
U2718
U2727
C2728
G2739
A2740
U2741
G2742
A2757
C2758
C2759
A2760
G2774
A2775
C2782
U2783
A2784
A2792
C2796
A2797
A2803
A2804
G2807
U2811
U2812
U2817
G2818
A2819
C2823
A2824
U2829
U2845
C2849
U2850
U2856
G2857
A2863
A2864
G2868
G2869
U2870
A2871
G2876
A2882
G2888
C2889
G2890
A2894
C2895
A2898
G2901
A2906
G2907
C2908
C2909
A
C
A
U
U
C

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	82088	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50.5081	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.756	Depositor
Minimum map value	-0.745	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.132	Depositor
Map size (Å)	466.39996, 466.39996, 466.39996	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AMP

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	2	0.45	0/2850	0.73	0/4439
2	4	0.34	0/1673	0.84	0/2598
3	0	0.18	0/3006	0.34	0/4066
4	3	0.44	0/32926	0.76	8/51344 (0.0%)
5	A	0.22	0/1803	0.35	0/2423
6	B	0.21	0/2666	0.32	0/3606
7	C	0.19	0/1701	0.33	0/2296
8	D	0.16	0/1319	0.32	0/1778
9	E	0.16	0/1373	0.32	0/1863
10	F	0.15	0/888	0.29	0/1208
11	H	0.19	0/1382	0.34	0/1859
12	J	0.21	0/1132	0.32	0/1527
13	K	0.20	0/1003	0.33	0/1346
14	L	0.21	0/1168	0.35	0/1567
15	M	0.22	0/1596	0.34	0/2133
16	N	0.18	0/1430	0.31	0/1945
17	O	0.13	0/440	0.31	0/592
18	P	0.18	0/896	0.31	0/1211
19	Q	0.20	0/1189	0.36	0/1583
20	R	0.20	0/752	0.31	0/1005
21	S	0.20	0/1189	0.36	0/1605
22	T	0.18	0/644	0.34	0/865
23	U	0.16	0/922	0.30	0/1247
24	V	0.19	0/467	0.28	0/625
25	W	0.15	0/491	0.27	0/662
26	X	0.20	0/1219	0.34	0/1653
27	Y	0.16	0/706	0.31	0/955
28	Z	0.19	0/1135	0.32	0/1520
29	a	0.23	0/437	0.35	0/575
30	b	0.19	0/421	0.33	0/556
31	c	0.21	0/615	0.36	0/823
32	d	0.22	0/766	0.33	0/1019

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
33	e	0.14	0/1418	0.34	0/1913
34	f	0.14	0/1387	0.29	0/1869
35	g	0.17	0/1776	0.34	0/2414
36	h	0.16	0/793	0.31	0/1068
37	i	0.14	0/1430	0.31	0/1932
38	j	0.18	0/1013	0.37	0/1369
39	k	0.19	0/939	0.35	0/1261
40	l	0.14	0/917	0.32	0/1230
41	m	0.15	0/392	0.30	0/532
42	n	0.18	0/877	0.33	0/1187
43	o	0.17	0/1070	0.31	0/1428
44	p	0.14	0/1090	0.33	0/1457
45	q	0.22	0/366	0.49	0/479
46	r	0.16	0/1216	0.36	0/1639
47	s	0.19	0/871	0.31	0/1185
48	t	0.14	0/988	0.32	0/1333
49	u	0.13	0/1142	0.33	0/1541
50	v	0.17	0/752	0.39	0/1011
51	w	0.15	0/390	0.32	0/530
52	x	0.14	0/362	0.32	0/484
53	1	0.57	0/64903	0.77	15/101215 (0.0%)
All	All	0.44	0/154297	0.67	23/229571 (0.0%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	1	521	G	O4'-C1'-N9	6.97	113.78	108.20
53	1	66	A	O5'-C5'-C4'	6.96	114.97	109.40
53	1	134	C	C2-N1-C1'	6.84	126.33	118.80
53	1	1506	A	O5'-C5'-C4'	6.46	114.57	109.40
53	1	2414	U	O5'-C5'-C4'	5.61	113.88	109.40
53	1	2326	G	O5'-C5'-C4'	5.54	113.83	109.40
53	1	1077	A	O5'-C5'-C4'	5.50	113.80	109.40
4	3	297	G	O5'-C5'-C4'	5.48	113.79	109.40
53	1	1887	A	O5'-C5'-C4'	5.45	113.76	109.40
4	3	571	U	O5'-C5'-C4'	5.44	113.75	109.40
4	3	1369	G	O5'-C5'-C4'	5.38	113.70	109.40
4	3	921	C	C2-N1-C1'	5.36	124.69	118.80
53	1	953	G	O4'-C1'-N9	5.33	112.47	108.20
53	1	1969	U	O5'-C5'-C4'	5.30	113.64	109.40
53	1	796	G	O4'-C1'-N9	5.26	112.41	108.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	1	1352	A	O5'-C5'-C4'	5.20	113.56	109.40
4	3	662	U	O5'-C5'-C4'	5.19	113.55	109.40
4	3	400	C	N1-C2-O2	-5.15	115.81	118.90
4	3	211	G	O5'-C5'-C4'	5.14	113.51	109.40
53	1	1414	U	C2-N1-C1'	5.09	123.81	117.70
4	3	856	A	P-O3'-C3'	5.08	125.79	119.70
53	1	756	G	O5'-C5'-C4'	5.03	113.42	109.40
53	1	1827	U	O4'-C1'-N1	5.03	112.02	108.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2552	0	1298	9	0
2	4	1500	0	767	24	0
3	0	2969	0	2948	19	0
4	3	29421	0	14848	199	0
5	A	1769	0	1809	12	0
6	B	2607	0	2549	6	0
7	C	1680	0	1678	15	0
8	D	1298	0	1260	5	0
9	E	1352	0	1308	8	0
10	F	879	0	850	5	0
11	H	1358	0	1357	7	0
12	J	1116	0	1113	3	0
13	K	995	0	1044	1	0
14	L	1153	0	1102	10	0
15	M	1569	0	1595	5	0
16	N	1400	0	1364	5	0
17	O	434	0	429	1	0
18	P	888	0	904	4	0
19	Q	1177	0	1175	7	0
20	R	738	0	747	3	0
21	S	1165	0	1137	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	T	639	0	644	4	0
23	U	914	0	896	1	0
24	V	459	0	434	1	0
25	W	488	0	489	5	0
26	X	1201	0	1156	2	0
27	Y	692	0	673	1	0
28	Z	1117	0	1124	2	0
29	a	430	0	443	0	0
30	b	416	0	444	0	0
31	c	608	0	608	8	0
32	d	748	0	746	4	0
33	e	1398	0	1406	10	0
34	f	1367	0	1331	15	0
35	g	1745	0	1699	10	0
36	h	784	0	758	5	0
37	i	1410	0	1409	9	0
38	j	991	0	938	2	0
39	k	932	0	956	6	0
40	l	907	0	928	11	0
41	m	383	0	377	6	0
42	n	864	0	867	8	0
43	o	1058	0	1090	5	0
44	p	1076	0	1070	8	0
45	q	363	0	362	9	0
46	r	1202	0	1180	9	0
47	s	853	0	846	7	0
48	t	971	0	956	5	0
49	u	1126	0	1094	14	0
50	v	741	0	724	6	0
51	w	385	0	354	2	0
52	x	361	0	382	5	0
53	1	57971	0	29248	251	0
54	0	46	0	24	0	0
All	All	142666	0	96938	712	0

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

All (712) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:4:31:G:H22	2:4:39:C:H42	1.11	0.95
3:0:115:VAL:HG21	3:0:258:LEU:HD11	1.52	0.90
47:s:44:THR:HG22	47:s:50:VAL:HG12	1.60	0.81
50:v:1:MET:HE1	50:v:35:VAL:HG22	1.62	0.80
44:p:130:VAL:HG11	48:t:116:LEU:HD11	1.67	0.77
2:4:76:A:H8	53:1:2423:C:H42	1.32	0.76
42:n:79:VAL:HG21	42:n:94:ALA:HB1	1.70	0.72
2:4:31:G:H22	2:4:39:C:N4	1.87	0.70
2:4:38:A:HO2'	2:4:39:C:H6	1.38	0.70
53:1:691:A:H61	53:1:701:A:H5"	1.57	0.69
4:3:1264:G:H4'	45:q:17:THR:HG21	1.74	0.68
7:C:54:LEU:HD21	7:C:87:ARG:HE	1.58	0.67
22:T:9:VAL:HG21	22:T:82:VAL:HG22	1.77	0.67
10:F:9:VAL:HA	10:F:119:LEU:HD21	1.75	0.67
7:C:151:THR:O	7:C:155:VAL:HG23	1.95	0.66
22:T:9:VAL:HG12	22:T:9:VAL:O	1.95	0.66
4:3:762:U:HO2'	38:j:2:ALA:N	1.94	0.66
44:p:71:GLU:O	44:p:75:VAL:HG23	1.96	0.65
3:0:276:ILE:HD11	3:0:307:PHE:CE2	2.31	0.65
40:l:48:PHE:HZ	40:l:61:ILE:HD12	1.60	0.65
39:k:58:THR:HG21	39:k:117:VAL:HG21	1.78	0.64
13:K:128:ALA:HB3	13:K:131:ILE:HD11	1.80	0.64
25:W:6:THR:HG23	25:W:60:ILE:HD11	1.80	0.64
31:c:49:THR:HG23	31:c:65:THR:HG23	1.79	0.63
3:0:333:LEU:HD13	3:0:357:VAL:HG22	1.80	0.63
44:p:118:ILE:HG22	44:p:122:LYS:HD2	1.81	0.62
53:1:2082:A:H2'	53:1:2083:G:C8	2.33	0.62
2:4:37:A:H3'	2:4:38:A:H5"	1.80	0.62
6:B:88:TYR:HB3	6:B:95:MET:HE3	1.82	0.61
33:e:142:THR:HG23	33:e:167:ILE:HD11	1.81	0.61
23:U:80:VAL:HG23	23:U:90:ARG:HB2	1.82	0.61
44:p:63:LEU:HD12	44:p:66:LYS:HD2	1.83	0.61
53:1:1996:U:H3'	53:1:1997:G:C5'	2.30	0.61
20:R:15:LEU:HD21	20:R:44:LEU:HD13	1.83	0.60
33:e:118:PRO:HG3	33:e:142:THR:HG21	1.84	0.59
46:r:30:ALA:HA	46:r:71:THR:HG22	1.85	0.59
4:3:1234:U:OP1	49:u:73:THR:HG21	2.02	0.59
53:1:86:G:H22	53:1:104:G:H1'	1.68	0.59
2:4:38:A:O2'	2:4:39:C:H6	1.86	0.58
7:C:5:ILE:HD11	7:C:16:ILE:CG2	2.34	0.58
46:r:102:LEU:HD13	46:r:119:LEU:HA	1.85	0.58
4:3:1380:G:H4'	4:3:1381:A:OP1	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:575:U:H3	53:1:588:G:H22	1.50	0.58
4:3:229:A:O4’	4:3:231:A:C8	2.57	0.58
5:A:82:ILE:HG23	5:A:93:THR:HB	1.86	0.58
53:1:541:C:H5”	53:1:542:G:C8	2.38	0.58
49:u:7:VAL:HG21	49:u:12:LEU:HD12	1.86	0.58
3:0:273:ILE:HD12	3:0:276:ILE:HD12	1.84	0.57
3:0:73:ILE:HD12	3:0:94:ALA:HB3	1.85	0.57
4:3:989:A:H4’	4:3:990:G:O5’	2.03	0.57
34:f:50:LEU:HD12	34:f:102:ILE:HD11	1.87	0.57
4:3:229:A:H4’	4:3:230:G:O5’	2.05	0.57
8:D:127:THR:HG21	53:1:2340:C:H1’	1.86	0.57
35:g:79:ILE:HG22	35:g:96:VAL:HG21	1.87	0.56
40:l:34:LEU:HD21	49:u:147:LEU:HD11	1.86	0.56
53:1:2317:U:H2’	53:1:2318:U:C6	2.40	0.56
46:r:40:LEU:HD22	46:r:45:LYS:HD2	1.88	0.56
53:1:2856:U:H2’	53:1:2857:G:O4’	2.06	0.56
4:3:708:G:H4’	4:3:1446:A:H4’	1.87	0.56
37:i:125:THR:HG21	37:i:199:VAL:HG12	1.86	0.56
26:X:1:MET:HE2	26:X:100:ILE:HG22	1.86	0.56
53:1:835:G:H4’	53:1:836:U:OP2	2.05	0.56
5:A:135:VAL:HG21	5:A:147:ARG:HB3	1.88	0.55
51:w:26:VAL:HG23	51:w:26:VAL:O	2.05	0.55
53:1:878:G:H5’	53:1:879:G:OP1	2.07	0.55
4:3:763:C:OP1	46:r:2:ALA:HB2	2.05	0.55
5:A:158:VAL:HG21	31:c:72:ALA:HB1	1.88	0.55
40:l:48:PHE:CZ	40:l:61:ILE:HD12	2.41	0.55
4:3:599:G:H2’	4:3:600:G:C8	2.42	0.55
42:n:12:ILE:HG21	42:n:78:ARG:HE	1.70	0.55
11:H:99:GLU:HB3	11:H:123:VAL:HG11	1.89	0.55
20:R:60:LEU:HD12	20:R:76:ILE:HD12	1.89	0.55
53:1:1232:A:H2’	53:1:1233:U:O4’	2.07	0.54
53:1:1996:U:H3’	53:1:1997:G:H5”	1.88	0.54
36:h:65:PRO:HD2	36:h:81:ILE:HD11	1.88	0.54
4:3:1064:A:O4’	41:m:38:ILE:HD11	2.07	0.54
53:1:566:C:H2’	53:1:567:G:O4’	2.07	0.54
3:0:197:MET:HA	3:0:197:MET:HE2	1.89	0.54
53:1:42:U:H2’	53:1:43:C:C6	2.43	0.54
53:1:1509:U:H2’	53:1:1510:U:C6	2.43	0.54
42:n:79:VAL:HG12	42:n:112:GLU:O	2.08	0.54
3:0:73:ILE:HD13	3:0:82:VAL:HG13	1.90	0.54
37:i:78:GLN:O	37:i:79:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:E:35:TRP:CE2	12:J:127:ILE:HG22	2.43	0.53
8:D:21:MET:HE2	8:D:37:LEU:HB2	1.89	0.53
34:f:139:THR:HG22	34:f:141:VAL:H	1.74	0.53
4:3:12:U:H2'	4:3:13:C:C6	2.44	0.53
8:D:115:TYR:CD1	8:D:121:ILE:HD11	2.44	0.53
9:E:8:ILE:HD11	9:E:48:VAL:HG23	1.90	0.53
4:3:890:A:H2'	4:3:891:G:C8	2.44	0.53
11:H:38:ASP:OD1	11:H:41:ALA:HB2	2.09	0.53
37:i:73:ILE:O	37:i:89:THR:HG21	2.08	0.53
53:1:738:A:H2'	53:1:739:G:O4'	2.09	0.52
35:g:71:VAL:HG23	35:g:71:VAL:O	2.09	0.52
53:1:1748:A:H2'	53:1:1749:G:O4'	2.10	0.52
15:M:51:ARG:HH22	53:1:268:G:H3'	1.75	0.52
4:3:570:G:H3'	4:3:571:U:H5'	1.91	0.52
4:3:1054:C:H2'	4:3:1055:G:C8	2.45	0.52
15:M:51:ARG:NH2	53:1:268:G:OP1	2.43	0.52
48:t:15:TYR:HB3	48:t:23:LEU:HD11	1.92	0.52
53:1:1453:A:H2'	53:1:1454:A:C8	2.45	0.52
53:1:1901:A:H2'	53:1:1902:A:C8	2.44	0.52
33:e:82:GLN:HG3	33:e:185:PHE:HB3	1.92	0.52
2:4:27:U:N3	2:4:28:C:C5	2.77	0.51
25:W:25:GLU:O	25:W:29:LEU:HD23	2.09	0.51
44:p:105:ILE:HD13	44:p:113:LYS:HG3	1.92	0.51
53:1:1128:A:H2'	53:1:1129:A:C8	2.45	0.51
4:3:307:C:H1'	4:3:308:A:OP2	2.10	0.51
34:f:50:LEU:CD1	34:f:102:ILE:HD11	2.40	0.51
40:l:25:VAL:HG21	40:l:48:PHE:CE2	2.45	0.51
10:F:46:ALA:HB3	10:F:73:ILE:HD13	1.91	0.51
33:e:142:THR:CG2	33:e:167:ILE:HD11	2.41	0.51
34:f:151:GLU:O	34:f:154:VAL:HG12	2.10	0.51
2:4:12:C:H2'	2:4:13:C:O4'	2.10	0.51
4:3:878:U:H4'	4:3:879:A:OP2	2.09	0.51
32:d:25:VAL:HG21	32:d:80:MET:HE3	1.92	0.51
43:o:72:LEU:HD21	43:o:100:ILE:HD11	1.92	0.51
34:f:38:GLU:O	34:f:42:ARG:HG3	2.10	0.51
53:1:2494:C:H2'	53:1:2495:A:O4'	2.11	0.51
4:3:313:U:H2'	4:3:314:C:C6	2.46	0.51
4:3:329:C:O2'	4:3:330:G:H5'	2.11	0.51
35:g:96:VAL:HG22	35:g:106:LEU:CD2	2.40	0.51
4:3:434:U:H4'	4:3:435:A:OP1	2.11	0.51
21:S:122:GLU:HG2	21:S:138:ASN:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:25:ARG:O	31:c:28:LYS:HG2	2.11	0.51
35:g:79:ILE:CG2	35:g:96:VAL:HG21	2.41	0.51
53:1:1508:C:H2'	53:1:1509:U:C6	2.45	0.51
11:H:121:LYS:O	11:H:123:VAL:HG13	2.10	0.51
34:f:65:VAL:HG13	34:f:91:ILE:HG22	1.92	0.51
53:1:2225:C:H2'	53:1:2226:U:O4'	2.11	0.50
53:1:862:U:H2'	53:1:863:G:N7	2.26	0.50
4:3:880:C:C2	4:3:881:A:C8	3.00	0.50
33:e:84:LEU:HD11	33:e:181:GLU:HB3	1.93	0.50
49:u:57:LEU:HG	49:u:131:LEU:HD11	1.92	0.50
25:W:48:SER:O	25:W:52:LYS:HG2	2.11	0.50
53:1:1426:U:H5"	53:1:1717:U:O2'	2.12	0.50
53:1:1790:C:C2'	53:1:1791:C:O5'	2.59	0.50
5:A:94:LEU:HD13	5:A:156:ILE:HD11	1.94	0.50
3:0:270:VAL:HG11	3:0:273:ILE:HD13	1.94	0.50
2:4:38:A:O2'	2:4:39:C:C5'	2.60	0.50
39:k:58:THR:HG21	39:k:117:VAL:CG2	2.42	0.50
49:u:75:TYR:HD2	49:u:100:ILE:HD11	1.77	0.50
53:1:204:U:O2	53:1:204:U:O4'	2.29	0.50
53:1:732:U:H2'	53:1:733:C:C6	2.47	0.50
53:1:2134:G:H2'	53:1:2135:U:C6	2.47	0.50
53:1:1717:U:O2'	53:1:1718:C:P	2.69	0.50
3:0:54:ASN:HB3	3:0:57:VAL:HG23	1.93	0.49
4:3:558:C:C2	34:f:141:VAL:HG11	2.47	0.49
16:N:48:LEU:HD22	16:N:93:ALA:HB2	1.93	0.49
43:o:110:ALA:HB1	43:o:114:LEU:O	2.12	0.49
34:f:104:GLU:HA	34:f:109:THR:HG21	1.93	0.49
44:p:51:ILE:HD12	44:p:90:MET:HE1	1.93	0.49
4:3:856:A:H1'	4:3:857:A:OP2	2.11	0.49
53:1:2459:A:O2'	53:1:2460:A:H2'	2.11	0.49
4:3:667:A:H2'	4:3:668:A:C8	2.48	0.49
4:3:1294:A:H1'	4:3:1295:G:OP2	2.13	0.49
53:1:542:G:H2'	53:1:543:A:C8	2.47	0.49
1:2:3:A:N3	1:2:3:A:H2'	2.27	0.49
4:3:399:U:HO2'	4:3:400:C:H6	1.60	0.49
10:F:90:LEU:HD22	53:1:266:A:C6	2.48	0.49
53:1:398:A:C2	53:1:400:A:C6	3.01	0.49
53:1:1607:C:H2'	53:1:1608:G:O4'	2.13	0.49
53:1:2097:C:H2'	53:1:2098:C:C6	2.48	0.49
2:4:28:C:H2'	2:4:29:G:C8	2.48	0.49
7:C:5:ILE:HD11	7:C:16:ILE:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:L:36:ARG:HH12	14:L:47:LEU:HD23	1.77	0.49
53:1:649:G:H2'	53:1:650:C:C6	2.48	0.49
53:1:1489:C:H2'	53:1:1490:U:C6	2.48	0.49
4:3:652:G:H2'	4:3:653:G:C8	2.47	0.49
4:3:409:U:C4	4:3:410:C:C5	3.00	0.49
4:3:696:U:H2'	4:3:697:G:O4'	2.13	0.49
37:i:115:ALA:HB1	37:i:180:ALA:HB3	1.94	0.49
53:1:1521:A:H1'	53:1:1522:C:C6	2.47	0.48
4:3:16:G:H2'	4:3:17:C:C6	2.47	0.48
4:3:1238:C:C2	4:3:1239:U:C5	3.00	0.48
18:P:109:GLY:O	18:P:112:VAL:HG22	2.14	0.48
53:1:953:G:N3	53:1:2294:A:H2'	2.29	0.48
53:1:1533:U:H2'	53:1:1534:A:C8	2.48	0.48
4:3:1274:C:C2	4:3:1275:U:C5	3.00	0.48
5:A:158:VAL:HG23	31:c:76:VAL:CG2	2.44	0.48
7:C:139:LEU:HD11	7:C:163:VAL:HG11	1.95	0.48
14:L:12:ARG:O	53:1:904:U:C4	2.67	0.48
14:L:31:ARG:HD3	53:1:170:G:H4'	1.94	0.48
37:i:139:VAL:HG21	52:x:50:LEU:HB2	1.93	0.48
53:1:1838:U:H2'	53:1:1839:A:C8	2.48	0.48
4:3:400:C:H2'	4:3:401:C:C6	2.48	0.48
4:3:1077:G:H2'	4:3:1078:U:C6	2.49	0.48
7:C:35:VAL:HG13	7:C:223:GLU:HG3	1.95	0.48
8:D:21:MET:HE1	8:D:33:ALA:O	2.13	0.48
53:1:2353:A:H2'	53:1:2354:A:C8	2.48	0.48
2:4:32:C:H2'	2:4:33:C:O4'	2.14	0.48
4:3:594:G:OP1	46:r:2:ALA:HB3	2.14	0.48
4:3:936:G:H22	4:3:1160:A:P	2.37	0.48
40:l:18:VAL:HG21	40:l:84:GLY:HA3	1.96	0.48
53:1:30:G:H2'	53:1:31:G:O4'	2.13	0.48
53:1:821:G:O2'	53:1:857:G:H4'	2.13	0.48
53:1:933:U:H2'	53:1:934:C:C6	2.48	0.48
53:1:1518:C:H4'	53:1:1519:A:O5'	2.13	0.48
1:2:76:C:H3'	1:2:77:A:H5"	1.95	0.48
4:3:299:A:H5"	4:3:1399:C:O2'	2.14	0.48
53:1:1098:A:H2'	53:1:1099:G:O4'	2.13	0.48
4:3:706:A:H2'	4:3:707:A:O4'	2.14	0.48
4:3:989:A:H61	45:q:30:GLN:HE22	1.61	0.48
7:C:5:ILE:HD11	7:C:16:ILE:HG21	1.95	0.48
42:n:40:GLY:O	42:n:44:VAL:HG22	2.14	0.48
53:1:1533:U:H2'	53:1:1534:A:H8	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:2870:U:H2'	53:1:2871:A:O4'	2.14	0.48
4:3:680:A:H5'	46:r:102:LEU:HD21	1.95	0.48
4:3:1235:A:H2'	4:3:1236:A:C8	2.48	0.48
53:1:260:C:H1'	53:1:261:G:OP2	2.13	0.48
10:F:45:ASN:HB3	10:F:100:VAL:HG13	1.96	0.47
44:p:90:MET:O	44:p:90:MET:HG2	2.13	0.47
53:1:134:C:P	53:1:134:C:O4'	2.72	0.47
53:1:419:G:H4'	53:1:420:G:OP2	2.14	0.47
53:1:1954:C:C2'	53:1:1955:C:H5'	2.44	0.47
42:n:14:HIS:CE1	42:n:78:ARG:NH2	2.82	0.47
53:1:242:A:H4'	53:1:243:G:OP1	2.14	0.47
53:1:1033:C:H2'	53:1:1034:U:O4'	2.14	0.47
4:3:67:U:H2'	4:3:68:U:O4'	2.14	0.47
4:3:889:G:C2	4:3:890:A:C8	3.02	0.47
4:3:1054:C:H2'	4:3:1055:G:H8	1.80	0.47
4:3:1203:G:O2'	4:3:1206:G:H1'	2.15	0.47
4:3:1360:C:H2'	4:3:1361:A:C8	2.49	0.47
40:l:35:VAL:O	40:l:41:ARG:HB2	2.14	0.47
47:s:21:TYR:O	47:s:28:GLY:HA3	2.14	0.47
47:s:33:ARG:NH2	47:s:96:ARG:HA	2.29	0.47
53:1:2023:C:H2'	53:1:2024:U:O4'	2.14	0.47
4:3:169:U:H5	4:3:173:A:N7	2.12	0.47
11:H:58:VAL:HG22	11:H:59:GLN:H	1.79	0.47
53:1:1997:G:H3'	53:1:1998:C:H5"	1.96	0.47
4:3:1227:A:H2'	4:3:1227:A:N3	2.28	0.47
53:1:144:U:H4'	53:1:145:C:O5'	2.15	0.47
53:1:227:G:H2'	53:1:228:A:C8	2.49	0.47
4:3:690:C:H2'	4:3:691:G:O4'	2.14	0.47
43:o:129:MET:HE3	43:o:132:LEU:HB2	1.97	0.47
53:1:1488:A:H1'	53:1:1489:C:C6	2.50	0.47
53:1:2334:G:N3	53:1:2334:G:H2'	2.29	0.47
53:1:2823:C:C2	53:1:2824:A:C8	3.02	0.47
4:3:924:C:O2	45:q:19:GLN:HB2	2.14	0.47
11:H:77:LEU:HD12	11:H:82:GLU:HA	1.97	0.47
4:3:570:G:H5"	4:3:571:U:OP2	2.14	0.47
4:3:1373:U:H2'	4:3:1374:C:C6	2.50	0.47
7:C:209:LEU:HB2	7:C:212:VAL:HG21	1.97	0.47
24:V:20:THR:HG22	24:V:21:MET:N	2.30	0.47
36:h:65:PRO:CD	36:h:81:ILE:HD11	2.45	0.47
53:1:791:A:H2'	53:1:792:G:O4'	2.14	0.47
2:4:28:C:H2'	2:4:29:G:H8	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1425:A:H2'	4:3:1426:A:O4'	2.15	0.47
32:d:25:VAL:HG21	32:d:80:MET:CE	2.44	0.47
49:u:75:TYR:CD2	49:u:100:ILE:HD11	2.50	0.47
50:v:80:VAL:HG12	50:v:80:VAL:O	2.15	0.47
53:1:606:A:O4'	53:1:608:C:C6	2.68	0.47
53:1:2354:A:H2'	53:1:2355:G:C8	2.49	0.47
4:3:90:A:OP2	4:3:90:A:C8	2.68	0.46
4:3:583:C:C2	4:3:584:A:C8	3.03	0.46
4:3:1223:C:H2'	4:3:1224:G:O4'	2.14	0.46
19:Q:146:TYR:O	19:Q:147:GLN:C	2.58	0.46
4:3:135:A:H2'	4:3:136:A:O4'	2.15	0.46
4:3:1298:A:H1'	37:i:83:THR:HG21	1.96	0.46
4:3:1340:G:N2	4:3:1435:A:H8	2.14	0.46
28:Z:164:ARG:HD3	53:1:1323:A:C8	2.51	0.46
34:f:154:VAL:HG13	34:f:154:VAL:O	2.16	0.46
53:1:751:A:H2'	53:1:752:A:C8	2.50	0.46
53:1:1508:C:H2'	53:1:1509:U:H6	1.80	0.46
53:1:2849:C:H2'	53:1:2850:U:C6	2.50	0.46
2:4:26:G:C5	2:4:27:U:C5	3.04	0.46
4:3:1010:U:O2'	4:3:1011:C:P	2.74	0.46
4:3:1051:A:C5	4:3:1052:C:C6	3.03	0.46
4:3:1239:U:C2	4:3:1240:C:C5	3.04	0.46
15:M:16:PRO:HA	15:M:21:LEU:HD23	1.97	0.46
4:3:154:A:H2'	4:3:155:U:O2	2.15	0.46
4:3:350:A:H2'	4:3:351:C:O4'	2.15	0.46
4:3:1437:G:OP1	4:3:1440:A:H4'	2.16	0.46
53:1:1518:C:O2'	53:1:1519:A:OP2	2.32	0.46
53:1:1714:C:H4'	53:1:1715:U:O5'	2.16	0.46
4:3:242:A:H2'	4:3:243:C:C6	2.49	0.46
4:3:613:G:H2'	4:3:614:U:C6	2.51	0.46
31:c:19:TYR:HA	53:1:1821:A:H61	1.81	0.46
53:1:302:U:H2'	53:1:303:U:C6	2.51	0.46
53:1:708:C:H2'	53:1:709:G:O4'	2.15	0.46
41:m:16:LEU:HD11	41:m:69:HIS:HB2	1.98	0.46
14:L:35:GLY:HA3	14:L:39:HIS:CE1	2.51	0.46
4:3:38:G:HO2'	4:3:39:U:P	2.39	0.46
4:3:910:U:H2'	4:3:911:C:O4'	2.16	0.46
49:u:66:VAL:HG23	49:u:70:ARG:CG	2.46	0.46
53:1:2098:C:H2'	53:1:2099:U:C6	2.51	0.46
53:1:2414:U:H2'	53:1:2415:C:C6	2.51	0.46
53:1:2727:U:H2'	53:1:2728:C:C6	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1200:U:H2'	4:3:1201:G:O4'	2.16	0.46
50:v:50:VAL:O	50:v:91:ILE:HD11	2.16	0.46
53:1:307:U:H2'	53:1:308:G:O4'	2.16	0.46
53:1:2676:U:H2'	53:1:2677:U:C6	2.50	0.46
4:3:1241:G:HO2'	4:3:1242:A:P	2.38	0.45
7:C:236:LEU:O	7:C:236:LEU:HD23	2.16	0.45
53:1:2083:G:H22	53:1:2645:A:H2	1.62	0.45
53:1:2618:C:H2'	53:1:2619:G:C8	2.52	0.45
4:3:87:C:H2'	4:3:88:U:C6	2.51	0.45
11:H:58:VAL:HG22	11:H:59:GLN:N	2.31	0.45
40:l:38:GLU:O	40:l:39:MET:C	2.59	0.45
19:Q:87:ALA:HB2	53:1:793:G:H4'	1.98	0.45
49:u:104:LEU:HD13	49:u:121:ARG:HD2	1.98	0.45
53:1:134:C:H2'	53:1:134:C:O2	2.16	0.45
53:1:1101:A:H5"	53:1:1102:C:OP1	2.16	0.45
7:C:6:ARG:HH21	7:C:139:LEU:HD23	1.81	0.45
9:E:87:VAL:HG22	9:E:167:VAL:HG22	1.98	0.45
14:L:34:ALA:HB2	53:1:171:A:H5"	1.96	0.45
31:c:19:TYR:HA	53:1:1821:A:N6	2.31	0.45
53:1:608:C:C2	53:1:609:C:C5	3.05	0.45
53:1:702:U:H2'	53:1:745:G:O4'	2.16	0.45
53:1:861:C:H2'	53:1:862:U:O4'	2.16	0.45
4:3:879:A:H2'	4:3:880:C:H6	1.82	0.45
4:3:1340:G:H21	4:3:1435:A:H8	1.63	0.45
35:g:125:THR:HG22	35:g:126:GLN:N	2.32	0.45
50:v:78:ARG:HA	50:v:86:LEU:HD11	1.99	0.45
53:1:87:A:C2	53:1:105:A:C5	3.04	0.45
53:1:2104:A:H2'	53:1:2105:G:C8	2.51	0.45
4:3:1402:A:H2'	4:3:1403:U:C6	2.52	0.45
18:P:78:ALA:CB	18:P:102:LEU:HD22	2.46	0.45
53:1:2107:U:H2'	53:1:2108:U:C6	2.51	0.45
51:w:10:CYS:SG	51:w:13:CYS:N	2.90	0.45
53:1:1102:C:H1'	53:1:1109:U:N3	2.32	0.45
53:1:1490:U:H2'	53:1:1491:G:O4'	2.17	0.45
47:s:32:VAL:HG13	47:s:93:ALA:HB1	1.99	0.45
53:1:1956:U:H2'	53:1:1957:C:C6	2.52	0.45
2:4:38:A:O2'	2:4:39:C:P	2.75	0.45
4:3:989:A:H61	45:q:30:GLN:NE2	2.15	0.45
4:3:1207:C:H2'	4:3:1208:U:O4'	2.17	0.45
45:q:23:CYS:SG	45:q:40:LEU:HA	2.57	0.45
53:1:630:G:H2'	53:1:2063:C:C5	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:2709:C:O2'	53:1:2710:C:H5'	2.16	0.45
2:4:38:A:O2'	2:4:39:C:O5'	2.35	0.45
15:M:124:ASP:OD1	15:M:127:GLN:HG2	2.17	0.45
53:1:1540:C:H2'	53:1:1541:A:C8	2.52	0.45
4:3:240:U:P	39:k:54:ARG:HH22	2.39	0.44
4:3:518:C:H2'	4:3:519:G:O4'	2.17	0.44
4:3:1224:G:H2'	4:3:1225:C:O4'	2.16	0.44
4:3:1241:G:O2'	4:3:1242:A:P	2.75	0.44
22:T:48:VAL:HG13	22:T:65:VAL:HG13	1.99	0.44
53:1:2268:U:H2'	53:1:2269:U:C6	2.52	0.44
4:3:58:U:H2'	4:3:59:U:C6	2.52	0.44
4:3:420:A:H3'	4:3:421:G:H5"	1.99	0.44
4:3:1195:G:H2'	4:3:1196:A:O4'	2.17	0.44
53:1:1457:C:H2'	53:1:1458:U:C6	2.52	0.44
4:3:555:G:H2'	4:3:556:C:O4'	2.18	0.44
4:3:1065:U:O2	4:3:1065:U:O4'	2.35	0.44
53:1:1955:C:HO2'	53:1:1956:U:H6	1.63	0.44
3:0:108:GLN:HB2	3:0:255:LEU:HD11	1.99	0.44
33:e:118:PRO:HB2	33:e:138:MET:HE2	1.99	0.44
53:1:1231:G:OP2	53:1:2542:U:H4'	2.17	0.44
4:3:864:U:H2'	4:3:865:G:O4'	2.18	0.44
4:3:1446:A:H2'	4:3:1447:G:C8	2.52	0.44
53:1:665:U:H2'	53:1:666:C:C6	2.52	0.44
53:1:1097:A:H2'	53:1:1098:A:C8	2.53	0.44
53:1:1582:G:H1'	53:1:1601:A:H61	1.83	0.44
4:3:103:C:H5'	47:s:33:ARG:HD2	2.00	0.44
50:v:36:ARG:HG3	50:v:50:VAL:HG23	2.00	0.44
53:1:1128:A:N3	53:1:2513:G:O2'	2.51	0.44
53:1:2507:C:H2'	53:1:2508:G:O4'	2.18	0.44
53:1:488:A:N3	53:1:490:G:H5"	2.32	0.44
53:1:959:G:H2'	53:1:960:C:C6	2.53	0.44
53:1:2583:C:H2'	53:1:2584:G:O4'	2.18	0.44
53:1:2677:U:H2'	53:1:2678:C:C6	2.52	0.44
4:3:624:G:O2'	4:3:625:U:H5'	2.18	0.44
4:3:1275:U:H2'	4:3:1276:C:C6	2.52	0.44
4:3:1347:C:C2	4:3:1435:A:N6	2.85	0.44
4:3:1418:G:H3'	4:3:1419:G:H5"	2.00	0.44
17:O:6:ILE:CD1	17:O:23:VAL:HG22	2.48	0.44
39:k:110:ARG:HE	39:k:113:GLN:HG3	1.81	0.44
53:1:1240:U:H4'	53:1:1242:A:O4'	2.17	0.44
53:1:1955:C:O2'	53:1:1956:U:H6	2.01	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:0:133:VAL:HG21	3:0:151:HIS:CG	2.53	0.44
4:3:89:C:H4'	4:3:90:A:O5'	2.18	0.44
4:3:155:U:O2	4:3:155:U:O4'	2.35	0.44
4:3:1075:C:C2	4:3:1076:A:C8	3.05	0.44
4:3:1248:G:H4'	4:3:1249:U:O5'	2.18	0.44
26:X:6:GLN:HB2	26:X:26:ILE:HG21	1.99	0.44
53:1:1509:U:H2'	53:1:1510:U:H6	1.83	0.44
53:1:1521:A:N6	53:1:1657:A:H2'	2.33	0.44
4:3:405:C:H2'	4:3:406:U:C6	2.53	0.43
4:3:695:G:OP2	46:r:128:ARG:NH2	2.51	0.43
4:3:803:A:H2'	4:3:804:G:O4'	2.18	0.43
4:3:1412:C:H2'	4:3:1413:G:O4'	2.18	0.43
16:N:49:VAL:CG1	16:N:56:ASP:HB3	2.47	0.43
33:e:114:VAL:HG11	33:e:185:PHE:CE1	2.53	0.43
35:g:96:VAL:HG22	35:g:106:LEU:HD23	2.00	0.43
53:1:2053:C:H2'	53:1:2054:G:O4'	2.18	0.43
4:3:83:A:H4'	4:3:84:A:OP2	2.18	0.43
4:3:759:U:H4'	4:3:760:G:OP2	2.18	0.43
4:3:1253:G:H22	4:3:1279:G:H1'	1.82	0.43
7:C:236:LEU:HD23	7:C:236:LEU:C	2.44	0.43
32:d:67:HIS:CD2	32:d:80:MET:HE1	2.53	0.43
53:1:205:C:HO2'	53:1:206:C:P	2.37	0.43
53:1:1585:A:H2'	53:1:1585:A:N3	2.33	0.43
53:1:1877:A:C5	53:1:1878:A:C8	3.06	0.43
1:2:120:C:H2'	1:2:121:C:O4'	2.18	0.43
4:3:409:U:H2'	4:3:409:U:O2	2.17	0.43
4:3:1000:C:H2'	4:3:1001:G:H8	1.82	0.43
4:3:1099:A:O4'	41:m:39:PRO:HB2	2.18	0.43
4:3:1392:C:H2'	4:3:1393:G:O4'	2.19	0.43
7:C:4:THR:HB	7:C:6:ARG:HH11	1.84	0.43
9:E:8:ILE:HD13	9:E:14:ALA:HB3	2.00	0.43
10:F:32:LYS:HD2	10:F:90:LEU:HD21	2.00	0.43
49:u:56:LEU:HD11	49:u:100:ILE:HG12	1.99	0.43
53:1:1123:G:N2	53:1:1235:G:OP2	2.51	0.43
53:1:2611:U:H2'	53:1:2612:U:C6	2.53	0.43
4:3:68:U:H2'	4:3:69:C:H3'	2.01	0.43
4:3:1285:G:H5"	4:3:1286:G:OP1	2.18	0.43
4:3:1390:C:O2'	4:3:1391:A:P	2.76	0.43
7:C:19:PRO:CG	7:C:246:ALA:HB2	2.49	0.43
53:1:157:A:C2	53:1:445:C:C5	3.07	0.43
53:1:1067:A:H2'	53:1:1068:C:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:1566:A:H2'	53:1:1567:A:C8	2.53	0.43
4:3:408:U:H1'	34:f:128:VAL:HG12	1.99	0.43
5:A:104:PRO:HG2	31:c:76:VAL:HG22	2.00	0.43
14:L:12:ARG:O	14:L:12:ARG:HG2	2.17	0.43
16:N:48:LEU:CD2	16:N:93:ALA:HB2	2.48	0.43
34:f:106:ARG:O	34:f:110:VAL:HG23	2.18	0.43
34:f:133:THR:HA	34:f:138:ARG:HA	2.00	0.43
53:1:999:C:H2'	53:1:1000:C:C6	2.53	0.43
53:1:1717:U:H2'	53:1:1718:C:OP1	2.18	0.43
4:3:1087:G:H2'	4:3:1088:C:O4'	2.18	0.43
4:3:1302:C:H2'	4:3:1303:A:H8	1.82	0.43
6:B:163:MET:HE1	6:B:309:LEU:HD21	1.99	0.43
7:C:196:PHE:HD2	7:C:236:LEU:HD22	1.83	0.43
8:D:48:THR:HG21	53:1:2339:U:H5'	1.99	0.43
12:J:84:ARG:HG3	12:J:98:LEU:HD22	2.00	0.43
4:3:385:G:C8	4:3:432:A:C2	3.07	0.43
5:A:169:PHE:O	5:A:170:VAL:HB	2.18	0.43
49:u:56:LEU:HD13	49:u:104:LEU:HG	2.01	0.43
53:1:429:G:H2'	53:1:430:C:O4'	2.18	0.43
53:1:637:G:O2'	53:1:1353:A:OP1	2.37	0.43
53:1:641:C:H2'	53:1:642:A:C8	2.54	0.43
53:1:1069:C:H2'	53:1:1070:G:O4'	2.18	0.43
53:1:1790:C:H2'	53:1:1791:C:O5'	2.18	0.43
53:1:2567:C:H2'	53:1:2568:A:O4'	2.19	0.43
4:3:243:C:H2'	4:3:244:G:O4'	2.18	0.43
33:e:101:GLU:HG2	33:e:119:VAL:HG13	1.99	0.43
48:t:65:GLU:O	48:t:66:THR:C	2.60	0.43
53:1:85:G:H2'	53:1:86:G:O4'	2.19	0.43
53:1:1510:U:H2'	53:1:1511:C:H6	1.84	0.43
53:1:2520:U:H2'	53:1:2521:G:O4'	2.18	0.43
4:3:340:C:H2'	4:3:341:G:O4'	2.18	0.43
32:d:67:HIS:NE2	32:d:80:MET:HE1	2.34	0.43
53:1:335:A:H61	53:1:349:G:C2'	2.32	0.43
53:1:1541:A:H2'	53:1:1542:C:C6	2.53	0.43
53:1:2258:A:H2'	53:1:2259:G:C8	2.54	0.43
53:1:2774:G:O6	53:1:2782:C:H5"	2.18	0.43
2:4:70:G:H2'	2:4:71:C:C6	2.53	0.43
4:3:87:C:H1'	4:3:333:G:H5'	2.00	0.43
4:3:260:A:H1'	4:3:261:A:OP2	2.18	0.43
4:3:570:G:O5'	4:3:571:U:H5'	2.19	0.43
4:3:718:C:H2'	4:3:719:G:O4'	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1013:U:H2'	4:3:1014:A:O4'	2.19	0.43
5:A:12:ARG:NH1	53:1:872:G:H5'	2.34	0.43
11:H:103:ALA:HB1	11:H:108:ALA:HB1	2.00	0.43
19:Q:103:ARG:HD3	53:1:1590:U:OP2	2.19	0.43
25:W:24:LEU:HD12	25:W:57:ILE:HD12	2.01	0.43
42:n:59:MET:O	42:n:63:VAL:HG23	2.19	0.43
49:u:24:ILE:HG22	49:u:106:GLN:HB3	2.01	0.43
53:1:218:A:O4'	53:1:220:U:C6	2.71	0.43
53:1:555:A:H3'	53:1:556:G:C5'	2.49	0.43
53:1:569:A:H2'	53:1:570:A:O4'	2.19	0.43
53:1:1714:C:H5"	53:1:1715:U:OP1	2.19	0.43
4:3:123:G:H2'	4:3:124:A:O4'	2.19	0.42
4:3:406:U:O2'	4:3:407:U:H5'	2.19	0.42
4:3:449:A:C4'	4:3:450:C:OP2	2.67	0.42
4:3:680:A:H2'	4:3:681:A:C8	2.54	0.42
4:3:1206:G:H2'	4:3:1207:C:C6	2.53	0.42
6:B:216:VAL:HA	6:B:221:VAL:HG22	2.01	0.42
19:Q:92:LYS:O	19:Q:96:VAL:HG23	2.18	0.42
35:g:228:PHE:O	35:g:229:THR:C	2.61	0.42
37:i:140:ASP:OD1	52:x:49:VAL:HG22	2.20	0.42
40:l:11:THR:HG22	40:l:11:THR:O	2.18	0.42
53:1:1056:U:H2'	53:1:1057:A:O4'	2.18	0.42
53:1:1997:G:H4'	53:1:1998:C:OP2	2.19	0.42
1:2:92:G:H2'	1:2:93:A:C8	2.55	0.42
2:4:37:A:H2'	2:4:38:A:H4'	2.00	0.42
4:3:1092:G:N2	4:3:1094:A:H62	2.17	0.42
19:Q:8:LYS:HG3	19:Q:24:PHE:CE2	2.54	0.42
33:e:66:LYS:HB2	33:e:80:ILE:HG21	2.01	0.42
53:1:828:A:H2'	53:1:829:G:O4'	2.18	0.42
1:2:114:G:H2'	1:2:115:C:C6	2.54	0.42
2:4:76:A:N1	53:1:2451:G:H2'	2.34	0.42
4:3:617:G:H2'	4:3:618:U:C6	2.54	0.42
4:3:1273:C:C2	4:3:1274:C:C5	3.07	0.42
9:E:85:MET:HE2	9:E:167:VAL:HG12	2.01	0.42
16:N:74:ALA:HB1	16:N:75:PRO:HD2	2.00	0.42
20:R:88:ARG:HE	53:1:2395:C:H5"	1.82	0.42
34:f:29:LEU:HD22	34:f:34:LEU:HB2	2.00	0.42
35:g:38:PRO:HD2	35:g:41:ILE:HD12	2.01	0.42
39:k:27:LEU:HD12	39:k:27:LEU:C	2.44	0.42
53:1:2322:U:H4'	53:1:2323:C:OP1	2.20	0.42
53:1:2345:A:H4'	53:1:2346:A:O5'	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:97:C:H5”	4:3:290:G:O2’	2.20	0.42
4:3:826:C:O2’	4:3:827:U:H5’	2.18	0.42
4:3:1074:G:H2’	4:3:1075:C:H6	1.83	0.42
4:3:1279:G:H1’	4:3:1280:A:OP2	2.19	0.42
18:P:90:ILE:HG21	18:P:96:THR:HG22	2.01	0.42
43:o:91:PHE:HB2	43:o:129:MET:HE1	2.02	0.42
52:x:21:LYS:HG2	52:x:29:MET:HE3	2.01	0.42
53:1:667:U:C5	53:1:684:G:C5	3.08	0.42
53:1:1417:U:H2’	53:1:1418:C:C6	2.54	0.42
53:1:2811:U:H2’	53:1:2812:U:C6	2.53	0.42
2:4:22:G:H2’	2:4:23:G:C8	2.54	0.42
4:3:1067:G:H5’	4:3:1228:A:O2’	2.20	0.42
4:3:1099:A:C2	4:3:1100:G:C5	3.07	0.42
9:E:36:TYR:CG	9:E:62:THR:HG21	2.55	0.42
14:L:54:ARG:HD2	53:1:696:A:O3’	2.20	0.42
36:h:63:MET:HE1	36:h:101:VAL:HG22	2.00	0.42
53:1:97:A:H2’	53:1:98:G:O4’	2.19	0.42
53:1:691:A:H61	53:1:701:A:C5’	2.30	0.42
53:1:795:C:C2’	53:1:796:G:H5’	2.50	0.42
53:1:2112:U:H2’	53:1:2113:G:O4’	2.19	0.42
3:0:165:LEU:HD22	3:0:235:VAL:HG11	2.01	0.42
4:3:156:A:C2	4:3:187:A:C5	3.07	0.42
4:3:626:A:H1’	4:3:627:G:OP2	2.19	0.42
5:A:158:VAL:HG23	31:c:76:VAL:HG21	2.01	0.42
16:N:48:LEU:HD22	16:N:93:ALA:CB	2.50	0.42
45:q:23:CYS:HB3	45:q:26:CYS:HB2	1.89	0.42
50:v:36:ARG:CG	50:v:50:VAL:HG23	2.49	0.42
53:1:1653:A:H2’	53:1:1654:G:O4’	2.20	0.42
53:1:1717:U:C2’	53:1:1718:C:OP1	2.67	0.42
53:1:2096:C:O2	53:1:2477:A:N1	2.53	0.42
4:3:457:C:H2’	4:3:458:A:O4’	2.20	0.42
4:3:1234:U:OP2	49:u:70:ARG:HD3	2.20	0.42
6:B:244:ASN:HA	6:B:245:PRO:C	2.45	0.42
53:1:553:C:H2’	53:1:554:A:O4’	2.20	0.42
53:1:2098:C:H2’	53:1:2099:U:H6	1.84	0.42
2:4:10:G:N2	2:4:26:G:H1’	2.35	0.42
4:3:199:G:C2	4:3:200:C:C6	3.08	0.42
4:3:387:G:O2’	4:3:388:A:H5’	2.20	0.42
37:i:76:LEU:HB2	37:i:89:THR:CG2	2.49	0.42
42:n:79:VAL:HG21	42:n:94:ALA:CB	2.43	0.42
46:r:95:LEU:HD12	46:r:129:LEU:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:1:2439:A:H2'	53:1:2440:U:C6	2.54	0.42
4:3:106:A:O2'	4:3:241:A:N3	2.51	0.42
4:3:439:G:H2'	4:3:440:C:O4'	2.20	0.42
4:3:1064:A:C4'	41:m:38:ILE:HD11	2.49	0.42
4:3:1381:A:H2'	4:3:1382:G:O4'	2.20	0.42
28:Z:185:THR:HG21	28:Z:211:ARG:HG2	2.01	0.42
37:i:39:SER:HB3	52:x:58:ILE:HD12	2.01	0.42
53:1:422:A:H1'	53:1:1913:A:C2	2.55	0.42
53:1:1376:A:N6	53:1:1397:G:H4'	2.35	0.42
53:1:1556:C:H2'	53:1:1557:G:O4'	2.19	0.42
53:1:1913:A:H2'	53:1:1914:A:O4'	2.20	0.42
53:1:2757:A:H2'	53:1:2758:C:C6	2.54	0.42
3:0:128:TYR:HB2	3:0:236:VAL:HG21	2.01	0.42
4:3:462:G:H5"	43:o:111:MET:HG2	2.02	0.42
4:3:481:C:H2'	4:3:482:U:C6	2.55	0.42
4:3:781:C:H2'	4:3:782:U:O4'	2.20	0.42
4:3:890:A:H2'	4:3:891:G:H8	1.83	0.42
4:3:1203:G:H2'	4:3:1227:A:N6	2.35	0.42
5:A:44:VAL:HG21	5:A:60:GLU:HB2	2.02	0.42
9:E:4:ILE:HD12	9:E:63:ILE:CG2	2.50	0.42
14:L:15:SER:HB2	53:1:1291:G:P	2.60	0.42
53:1:157:A:H2'	53:1:158:A:O4'	2.19	0.42
53:1:641:C:H2'	53:1:642:A:H8	1.85	0.42
53:1:964:C:H2'	53:1:965:G:C8	2.54	0.42
53:1:1515:C:C2	53:1:1516:A:C8	3.07	0.42
53:1:1754:U:H2'	53:1:1755:C:C6	2.54	0.42
53:1:2131:G:H2'	53:1:2132:U:O4'	2.20	0.42
2:4:24:A:H2'	2:4:25:C:C6	2.55	0.41
4:3:105:A:OP1	47:s:33:ARG:NE	2.53	0.41
4:3:180:C:N3	4:3:181:U:C5	2.88	0.41
4:3:241:A:H5'	39:k:46:SER:HB3	2.01	0.41
4:3:387:G:OP1	34:f:119:THR:HG21	2.20	0.41
4:3:1234:U:C5	49:u:70:ARG:HG3	2.55	0.41
4:3:1330:C:O4'	52:x:24:MET:HG3	2.20	0.41
27:Y:15:LEU:O	27:Y:18:VAL:HG22	2.20	0.41
45:q:23:CYS:SG	45:q:40:LEU:HD23	2.60	0.41
53:1:585:C:C2	53:1:586:C:C5	3.08	0.41
53:1:1135:U:H2'	53:1:1136:C:C6	2.55	0.41
1:2:59:C:H2'	1:2:60:U:C6	2.55	0.41
4:3:56:A:H4'	4:3:57:G:O5'	2.20	0.41
4:3:570:G:H3'	4:3:571:U:C5'	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:1240:C:H2'	4:3:1241:G:H8	1.85	0.41
5:A:126:ALA:HB1	5:A:138:VAL:CG1	2.51	0.41
36:h:4:PHE:HB3	36:h:108:ILE:HD13	2.02	0.41
53:1:1032:A:H2'	53:1:1033:C:O4'	2.20	0.41
53:1:2634:G:H2'	53:1:2635:G:O4'	2.19	0.41
53:1:2863:A:H2'	53:1:2864:A:C8	2.56	0.41
4:3:986:A:H2'	4:3:987:G:O4'	2.20	0.41
7:C:96:LYS:HB2	53:1:649:G:H4'	2.02	0.41
41:m:7:ARG:HA	41:m:72:LEU:HA	2.02	0.41
4:3:331:C:H4'	4:3:333:G:OP1	2.20	0.41
40:l:63:VAL:HG11	40:l:77:VAL:HG22	2.02	0.41
53:1:1129:A:H2'	53:1:1130:G:O4'	2.20	0.41
53:1:2384:C:H2'	53:1:2385:C:O4'	2.20	0.41
2:4:65:G:C2	2:4:66:C:C5	3.09	0.41
4:3:371:A:H2'	4:3:372:G:O4'	2.19	0.41
4:3:1350:C:H2'	4:3:1351:C:O4'	2.20	0.41
53:1:301:C:H2'	53:1:302:U:H6	1.86	0.41
53:1:488:A:H4'	53:1:489:A:OP1	2.20	0.41
53:1:1118:A:N3	53:1:1118:A:H3'	2.36	0.41
53:1:1226:A:H4'	53:1:1227:A:O5'	2.21	0.41
3:0:30:GLU:O	3:0:31:ASN:C	2.63	0.41
4:3:284:G:H5"	4:3:285:A:OP1	2.20	0.41
53:1:348:C:H2'	53:1:349:G:O4'	2.20	0.41
53:1:898:A:H2'	53:1:900:C:C5	2.55	0.41
53:1:1313:A:H4'	53:1:1338:C:H4'	2.02	0.41
53:1:1466:A:H2'	53:1:1467:U:C6	2.56	0.41
53:1:1994:C:H2'	53:1:1995:U:O4'	2.19	0.41
53:1:1996:U:H5"	53:1:1997:G:H5"	2.01	0.41
53:1:2318:U:H2'	53:1:2319:U:C6	2.55	0.41
53:1:2796:C:H2'	53:1:2797:A:O4'	2.21	0.41
3:0:323:GLN:HG2	3:0:336:SER:HB2	2.03	0.41
4:3:398:G:O2'	4:3:399:U:P	2.78	0.41
4:3:1050:G:C6	4:3:1051:A:H1'	2.56	0.41
5:A:12:ARG:HH11	53:1:872:G:H5'	1.86	0.41
46:r:28:VAL:HG21	46:r:33:ILE:HD11	2.01	0.41
53:1:663:A:H4'	53:1:664:G:O5'	2.20	0.41
53:1:911:C:O2'	53:1:933:U:H5"	2.21	0.41
53:1:1652:A:H2'	53:1:1653:A:C8	2.55	0.41
53:1:1878:A:C5	53:1:1879:U:C5	3.09	0.41
1:2:27:C:H2'	1:2:28:A:O4'	2.19	0.41
4:3:70:A:H1'	4:3:71:U:O5'	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:70:A:H1'	4:3:71:U:P	2.61	0.41
4:3:84:A:O2'	35:g:3:ARG:HB3	2.21	0.41
4:3:314:C:H2'	4:3:315:C:H6	1.84	0.41
4:3:360:C:H2'	4:3:361:A:O4'	2.20	0.41
4:3:1050:G:C5	4:3:1051:A:H1'	2.55	0.41
4:3:1076:A:C5	4:3:1077:G:C5	3.09	0.41
4:3:1316:G:OP2	40:l:116:LYS:HD3	2.21	0.41
14:L:131:VAL:O	14:L:135:GLU:HG2	2.20	0.41
19:Q:8:LYS:CD	53:1:1392:C:OP1	2.69	0.41
25:W:52:LYS:HE3	53:1:78:G:O3'	2.20	0.41
53:1:136:C:H2'	53:1:147:C:C5	2.55	0.41
53:1:301:C:C2	53:1:302:U:C5	3.09	0.41
53:1:1503:A:H2'	53:1:1504:G:C8	2.56	0.41
3:0:3:ILE:HG22	3:0:6:ILE:HD11	2.03	0.41
3:0:32:PRO:O	3:0:33:LYS:HB2	2.21	0.41
4:3:352:A:C2	4:3:353:C:C6	3.09	0.41
4:3:474:C:C2	4:3:475:C:C5	3.09	0.41
4:3:567:G:H2'	4:3:568:G:O4'	2.20	0.41
4:3:1173:A:O2'	48:t:121:VAL:HG21	2.20	0.41
4:3:1307:C:N3	45:q:21:ASN:HB2	2.36	0.41
19:Q:112:ASP:OD1	19:Q:112:ASP:C	2.63	0.41
22:T:66:ARG:HH22	53:1:1502:C:H5"	1.86	0.41
33:e:93:VAL:HG22	33:e:99:LYS:HD3	2.02	0.41
48:t:42:THR:O	48:t:46:GLY:O	2.39	0.41
53:1:550:A:O2'	53:1:551:U:H5'	2.21	0.41
53:1:753:C:H2'	53:1:754:C:C6	2.56	0.41
53:1:1782:G:H2'	53:1:1783:C:O4'	2.21	0.41
53:1:1941:G:O2'	53:1:1942:G:P	2.79	0.41
53:1:2098:C:C2	53:1:2099:U:C5	3.08	0.41
53:1:2645:A:H2'	53:1:2646:U:C6	2.55	0.41
4:3:297:G:O2'	4:3:1401:A:H4'	2.21	0.41
4:3:1166:C:C2	4:3:1167:U:C5	3.09	0.41
14:L:26:GLY:HA2	53:1:172:A:N7	2.35	0.41
15:M:159:ARG:HB2	15:M:164:LEU:HB2	2.03	0.41
18:P:26:VAL:HG21	18:P:112:VAL:HG21	2.03	0.41
21:S:63:HIS:HB3	53:1:1365:G:O5'	2.21	0.41
21:S:137:TRP:CE2	53:1:2045:G:H4'	2.56	0.41
53:1:313:C:C2	53:1:314:U:C5	3.09	0.41
53:1:1651:A:H2'	53:1:1652:A:C8	2.55	0.41
2:4:32:C:O5'	2:4:32:C:O2	2.39	0.40
4:3:146:A:H2'	4:3:147:A:C8	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:921:C:O2	4:3:921:C:C2'	2.69	0.40
38:j:18:GLU:HG3	38:j:69:ILE:HB	2.03	0.40
53:1:249:A:C8	53:1:250:C:C5	3.08	0.40
53:1:561:C:H2'	53:1:562:U:C6	2.56	0.40
53:1:1584:A:C2	53:1:1600:A:C8	3.09	0.40
53:1:1700:G:H1'	53:1:1704:A:N6	2.36	0.40
53:1:1795:C:H2'	53:1:1796:A:C8	2.56	0.40
53:1:1988:U:H6	53:1:2578:U:O2	2.04	0.40
1:2:44:A:C4	1:2:45:A:C8	3.09	0.40
1:2:77:A:OP1	1:2:77:A:H8	2.04	0.40
4:3:104:A:C2	4:3:173:A:C4	3.09	0.40
4:3:166:U:H2'	4:3:167:G:O4'	2.20	0.40
4:3:355:G:H2'	4:3:356:C:C6	2.57	0.40
4:3:449:A:H4'	4:3:450:C:H5'	2.03	0.40
4:3:1173:A:N3	4:3:1173:A:C2'	2.83	0.40
4:3:1262:C:C2	4:3:1263:U:C5	3.10	0.40
4:3:1307:C:C5	45:q:19:GLN:HG3	2.56	0.40
6:B:289:GLY:HA2	53:1:2890:G:H4'	2.03	0.40
35:g:121:ILE:HD12	35:g:154:ASP:HB2	2.03	0.40
40:l:34:LEU:CD2	49:u:147:LEU:HD21	2.52	0.40
53:1:208:C:H2'	53:1:209:G:O4'	2.20	0.40
53:1:1894:G:H2'	53:1:1895:U:O4'	2.20	0.40
2:4:37:A:HO2'	2:4:38:A:P	2.45	0.40
3:0:158:VAL:HG11	3:0:206:MET:SD	2.61	0.40
3:0:165:LEU:HD21	3:0:210:ALA:HB3	2.03	0.40
4:3:156:A:H2'	4:3:157:C:O4'	2.21	0.40
4:3:582:C:C2	4:3:583:C:C5	3.09	0.40
4:3:628:G:H5"	42:n:23:LEU:HD21	2.03	0.40
4:3:661:A:O2'	4:3:663:G:C8	2.73	0.40
4:3:1334:C:C2	4:3:1335:U:C5	3.09	0.40
21:S:92:LEU:HD21	21:S:146:LEU:HB2	2.04	0.40
34:f:124:ARG:O	34:f:128:VAL:HG23	2.21	0.40
47:s:10:PRO:HB2	47:s:80:VAL:HG22	2.03	0.40
53:1:206:C:H2'	53:1:207:G:O4'	2.21	0.40
53:1:335:A:N6	53:1:349:G:H2'	2.37	0.40
53:1:1050:G:C6	53:1:1065:G:C6	3.10	0.40
53:1:1957:C:H2'	53:1:1958:U:O4'	2.21	0.40
53:1:1996:U:O2	53:1:1996:U:O4'	2.39	0.40
4:3:564:G:H2'	4:3:565:C:C6	2.57	0.40
6:B:239:ASN:ND2	53:1:2538:U:O2	2.55	0.40
12:J:47:THR:HG22	12:J:121:LEU:CD1	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:h:61:ARG:NE	36:h:72:LEU:HD21	2.36	0.40
44:p:138:VAL:HG12	44:p:138:VAL:O	2.21	0.40
53:1:306:G:H2'	53:1:307:U:C6	2.57	0.40
53:1:1021:G:H2'	53:1:1022:A:C8	2.56	0.40
53:1:1211:A:H4'	53:1:1212:G:OP1	2.21	0.40
53:1:2703:U:H2'	53:1:2704:G:C8	2.57	0.40
4:3:241:A:H2'	4:3:242:A:C8	2.57	0.40
4:3:1210:U:H2'	4:3:1211:C:H6	1.85	0.40
9:E:19:LEU:HD13	9:E:35:TRP:CD1	2.56	0.40
41:m:16:LEU:O	41:m:19:ILE:HG22	2.22	0.40
53:1:656:A:H2'	53:1:657:C:C6	2.57	0.40
53:1:1267:G:H2'	53:1:1268:U:C6	2.56	0.40
53:1:1536:G:H2'	53:1:1537:A:O4'	2.21	0.40
53:1:2319:U:H2'	53:1:2320:C:C6	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	0	376/380 (99%)	368 (98%)	8 (2%)	0	100	100
5	A	234/241 (97%)	229 (98%)	5 (2%)	0	100	100
6	B	335/338 (99%)	335 (100%)	0	0	100	100
7	C	214/248 (86%)	208 (97%)	6 (3%)	0	100	100
8	D	164/172 (95%)	159 (97%)	5 (3%)	0	100	100
9	E	172/178 (97%)	168 (98%)	4 (2%)	0	100	100
10	F	117/120 (98%)	117 (100%)	0	0	100	100
11	H	170/176 (97%)	169 (99%)	1 (1%)	0	100	100
12	J	142/145 (98%)	139 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	K	130/132 (98%)	129 (99%)	1 (1%)	0	100	100
14	L	150/165 (91%)	146 (97%)	4 (3%)	0	100	100
15	M	191/196 (97%)	188 (98%)	3 (2%)	0	100	100
16	N	179/184 (97%)	177 (99%)	2 (1%)	0	100	100
17	O	54/58 (93%)	54 (100%)	0	0	100	100
18	P	113/116 (97%)	113 (100%)	0	0	100	100
19	Q	144/151 (95%)	144 (100%)	0	0	100	100
20	R	93/96 (97%)	93 (100%)	0	0	100	100
21	S	148/153 (97%)	145 (98%)	3 (2%)	0	100	100
22	T	79/83 (95%)	77 (98%)	2 (2%)	0	100	100
23	U	113/118 (96%)	112 (99%)	1 (1%)	0	100	100
24	V	55/66 (83%)	55 (100%)	0	0	100	100
25	W	62/70 (89%)	61 (98%)	1 (2%)	0	100	100
26	X	152/154 (99%)	150 (99%)	2 (1%)	0	100	100
27	Y	84/92 (91%)	82 (98%)	2 (2%)	0	100	100
28	Z	138/235 (59%)	138 (100%)	0	0	100	100
29	a	54/58 (93%)	53 (98%)	1 (2%)	0	100	100
30	b	47/50 (94%)	46 (98%)	1 (2%)	0	100	100
31	c	76/89 (85%)	73 (96%)	3 (4%)	0	100	100
32	d	91/93 (98%)	90 (99%)	1 (1%)	0	100	100
33	e	170/220 (77%)	164 (96%)	6 (4%)	0	100	100
34	f	167/175 (95%)	163 (98%)	4 (2%)	0	100	100
35	g	226/247 (92%)	218 (96%)	8 (4%)	0	100	100
36	h	100/133 (75%)	99 (99%)	1 (1%)	0	100	100
37	i	178/204 (87%)	173 (97%)	5 (3%)	0	100	100
38	j	127/130 (98%)	123 (97%)	4 (3%)	0	100	100
39	k	120/125 (96%)	116 (97%)	4 (3%)	0	100	100
40	l	113/132 (86%)	109 (96%)	4 (4%)	0	100	100
41	m	44/102 (43%)	43 (98%)	1 (2%)	0	100	100
42	n	116/130 (89%)	113 (97%)	3 (3%)	0	100	100
43	o	137/142 (96%)	136 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	p	132/167 (79%)	128 (97%)	4 (3%)	0	100	100
45	q	41/58 (71%)	39 (95%)	2 (5%)	0	100	100
46	r	150/155 (97%)	146 (97%)	4 (3%)	0	100	100
47	s	107/114 (94%)	107 (100%)	0	0	100	100
48	t	116/140 (83%)	110 (95%)	6 (5%)	0	100	100
49	u	141/151 (93%)	139 (99%)	2 (1%)	0	100	100
50	v	89/101 (88%)	88 (99%)	1 (1%)	0	100	100
51	w	52/64 (81%)	46 (88%)	6 (12%)	0	100	100
52	x	43/74 (58%)	39 (91%)	4 (9%)	0	100	100
All	All	6446/7121 (90%)	6317 (98%)	129 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	0	321/323 (99%)	321 (100%)	0	100	100
5	A	183/186 (98%)	183 (100%)	0	100	100
6	B	275/276 (100%)	274 (100%)	1 (0%)	84	92
7	C	177/200 (88%)	177 (100%)	0	100	100
8	D	141/146 (97%)	141 (100%)	0	100	100
9	E	151/153 (99%)	151 (100%)	0	100	100
10	F	93/94 (99%)	93 (100%)	0	100	100
11	H	144/147 (98%)	144 (100%)	0	100	100
12	J	118/119 (99%)	118 (100%)	0	100	100
13	K	106/106 (100%)	106 (100%)	0	100	100
14	L	111/122 (91%)	111 (100%)	0	100	100
15	M	159/161 (99%)	159 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	N	142/145 (98%)	142 (100%)	0	100	100
17	O	47/49 (96%)	47 (100%)	0	100	100
18	P	98/99 (99%)	98 (100%)	0	100	100
19	Q	117/122 (96%)	117 (100%)	0	100	100
20	R	78/79 (99%)	78 (100%)	0	100	100
21	S	121/124 (98%)	121 (100%)	0	100	100
22	T	75/77 (97%)	75 (100%)	0	100	100
23	U	100/103 (97%)	100 (100%)	0	100	100
24	V	47/54 (87%)	47 (100%)	0	100	100
25	W	51/56 (91%)	51 (100%)	0	100	100
26	X	132/132 (100%)	132 (100%)	0	100	100
27	Y	73/78 (94%)	73 (100%)	0	100	100
28	Z	115/188 (61%)	115 (100%)	0	100	100
29	a	47/49 (96%)	47 (100%)	0	100	100
30	b	46/47 (98%)	46 (100%)	0	100	100
31	c	62/70 (89%)	62 (100%)	0	100	100
32	d	77/77 (100%)	77 (100%)	0	100	100
33	e	152/190 (80%)	152 (100%)	0	100	100
34	f	145/149 (97%)	145 (100%)	0	100	100
35	g	190/203 (94%)	190 (100%)	0	100	100
36	h	83/98 (85%)	83 (100%)	0	100	100
37	i	151/171 (88%)	151 (100%)	0	100	100
38	j	102/103 (99%)	102 (100%)	0	100	100
39	k	99/102 (97%)	99 (100%)	0	100	100
40	l	92/106 (87%)	92 (100%)	0	100	100
41	m	42/90 (47%)	42 (100%)	0	100	100
42	n	87/97 (90%)	87 (100%)	0	100	100
43	o	108/111 (97%)	108 (100%)	0	100	100
44	p	114/142 (80%)	114 (100%)	0	100	100
45	q	38/51 (74%)	38 (100%)	0	100	100
46	r	131/134 (98%)	131 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
47	s	97/100 (97%)	97 (100%)	0	100 100
48	t	105/119 (88%)	105 (100%)	0	100 100
49	u	118/123 (96%)	118 (100%)	0	100 100
50	v	83/90 (92%)	83 (100%)	0	100 100
51	w	42/51 (82%)	41 (98%)	1 (2%)	43 65
52	x	40/60 (67%)	40 (100%)	0	100 100
All	All	5426/5872 (92%)	5424 (100%)	2 (0%)	100 100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	B	239	ASN
51	w	13	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
3	0	17	ASN
3	0	151	HIS
3	0	308	HIS
6	B	239	ASN
9	E	151	GLN
11	H	40	GLN
11	H	62	HIS
11	H	73	ASN
12	J	126	ASN
13	K	44	HIS
14	L	39	HIS
16	N	23	GLN
16	N	168	ASN
17	O	3	GLN
19	Q	119	GLN
20	R	77	ASN
22	T	15	ASN
22	T	74	GLN
23	U	44	ASN
23	U	93	GLN
25	W	61	GLN
26	X	27	HIS

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Mol	Chain	Res	Type
26	X	49	ASN
28	Z	122	GLN
30	b	42	ASN
32	d	18	HIS
32	d	20	HIS
35	g	62	HIS
35	g	123	ASN
37	i	87	GLN
37	i	110	GLN
37	i	176	GLN
38	j	32	ASN
38	j	113	HIS
41	m	63	HIS
42	n	16	HIS
42	n	95	GLN
49	u	83	ASN
50	v	15	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	119/122 (97%)	11 (9%)	1 (0%)
2	4	65/76 (85%)	13 (20%)	0
4	3	1363/1473 (92%)	239 (17%)	24 (1%)
53	1	2695/2915 (92%)	315 (11%)	15 (0%)
All	All	4242/4586 (92%)	578 (13%)	40 (0%)

All (578) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	23	G
1	2	24	U
1	2	25	U
1	2	28	A
1	2	55	U
1	2	56	A
1	2	66	G
1	2	75	U
1	2	77	A
1	2	94	U
1	2	114	G

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Mol	Chain	Res	Type
2	4	4	G
2	4	6	G
2	4	9	C
2	4	14	A
2	4	34	A
2	4	38	A
2	4	39	C
2	4	43	A
2	4	44	A
2	4	46	G
2	4	57	A
2	4	68	C
2	4	76	A
4	3	33	U
4	3	39	U
4	3	40	C
4	3	42	G
4	3	45	U
4	3	47	A
4	3	54	C
4	3	70	A
4	3	71	U
4	3	72	A
4	3	79	G
4	3	90	A
4	3	95	C
4	3	104	A
4	3	121	A
4	3	138	C
4	3	155	U
4	3	167	G
4	3	174	U
4	3	189	A
4	3	190	C
4	3	193	U
4	3	194	C
4	3	195	A
4	3	196	G
4	3	197	G
4	3	199	G
4	3	219	C
4	3	223	U

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Mol	Chain	Res	Type
4	3	224	U
4	3	226	G
4	3	230	G
4	3	241	A
4	3	245	G
4	3	246	C
4	3	260	A
4	3	261	A
4	3	268	C
4	3	280	G
4	3	285	A
4	3	303	G
4	3	307	C
4	3	308	A
4	3	309	A
4	3	311	A
4	3	324	C
4	3	325	G
4	3	326	G
4	3	331	C
4	3	332	A
4	3	333	G
4	3	335	A
4	3	337	G
4	3	346	C
4	3	351	C
4	3	352	A
4	3	367	G
4	3	372	G
4	3	376	A
4	3	385	G
4	3	391	G
4	3	399	U
4	3	400	C
4	3	401	C
4	3	403	C
4	3	408	U
4	3	420	A
4	3	421	G
4	3	431	G
4	3	434	U
4	3	435	A

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Mol	Chain	Res	Type
4	3	445	C
4	3	448	G
4	3	450	C
4	3	456	C
4	3	457	C
4	3	465	G
4	3	470	A
4	3	471	A
4	3	485	A
4	3	499	U
4	3	501	A
4	3	502	U
4	3	505	G
4	3	510	A
4	3	511	A
4	3	514	C
4	3	515	G
4	3	554	A
4	3	556	C
4	3	571	U
4	3	572	C
4	3	592	U
4	3	600	G
4	3	601	A
4	3	604	G
4	3	626	A
4	3	627	G
4	3	649	G
4	3	650	A
4	3	661	A
4	3	662	U
4	3	670	G
4	3	672	A
4	3	687	A
4	3	688	U
4	3	691	G
4	3	694	G
4	3	718	C
4	3	720	A
4	3	731	A
4	3	732	U
4	3	733	A

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Mol	Chain	Res	Type
4	3	753	A
4	3	754	A
4	3	756	C
4	3	767	A
4	3	783	A
4	3	786	A
4	3	815	A
4	3	819	G
4	3	845	G
4	3	857	A
4	3	865	G
4	3	869	G
4	3	877	C
4	3	878	U
4	3	879	A
4	3	886	G
4	3	889	G
4	3	904	U
4	3	912	A
4	3	913	A
4	3	918	G
4	3	919	G
4	3	920	A
4	3	921	C
4	3	938	C
4	3	962	U
4	3	963	G
4	3	964	A
4	3	982	A
4	3	983	G
4	3	985	G
4	3	986	A
4	3	990	G
4	3	994	C
4	3	996	U
4	3	1011	C
4	3	1013	U
4	3	1043	C
4	3	1046	G
4	3	1047	C
4	3	1051	A
4	3	1052	C

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Mol	Chain	Res	Type
4	3	1065	U
4	3	1066	U
4	3	1074	G
4	3	1075	C
4	3	1077	G
4	3	1079	U
4	3	1088	C
4	3	1089	U
4	3	1096	A
4	3	1141	G
4	3	1144	A
4	3	1145	G
4	3	1148	C
4	3	1149	A
4	3	1150	G
4	3	1160	A
4	3	1161	A
4	3	1173	A
4	3	1175	A
4	3	1184	A
4	3	1186	A
4	3	1188	U
4	3	1189	G
4	3	1196	A
4	3	1201	G
4	3	1202	G
4	3	1206	G
4	3	1218	G
4	3	1226	U
4	3	1227	A
4	3	1228	A
4	3	1235	A
4	3	1240	C
4	3	1242	A
4	3	1248	G
4	3	1249	U
4	3	1250	U
4	3	1253	G
4	3	1266	A
4	3	1268	C
4	3	1279	G
4	3	1280	A

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Mol	Chain	Res	Type
4	3	1283	C
4	3	1284	U
4	3	1285	G
4	3	1286	G
4	3	1294	A
4	3	1295	G
4	3	1307	C
4	3	1308	A
4	3	1311	A
4	3	1312	G
4	3	1327	G
4	3	1330	C
4	3	1345	C
4	3	1346	A
4	3	1365	G
4	3	1366	A
4	3	1367	G
4	3	1381	A
4	3	1386	A
4	3	1391	A
4	3	1395	U
4	3	1396	G
4	3	1398	U
4	3	1401	A
4	3	1406	G
4	3	1407	G
4	3	1410	U
4	3	1411	U
4	3	1419	G
4	3	1420	G
4	3	1424	U
4	3	1425	A
4	3	1427	G
4	3	1430	G
4	3	1432	A
4	3	1435	A
4	3	1436	A
4	3	1437	G
4	3	1439	U
4	3	1450	G
4	3	1462	G
4	3	1463	G

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Mol	Chain	Res	Type
53	1	12	G
53	1	13	C
53	1	38	C
53	1	46	G
53	1	49	C
53	1	58	G
53	1	64	C
53	1	66	A
53	1	74	A
53	1	77	A
53	1	78	G
53	1	94	U
53	1	99	G
53	1	120	A
53	1	121	A
53	1	122	U
53	1	130	C
53	1	134	C
53	1	144	U
53	1	145	C
53	1	146	G
53	1	147	C
53	1	157	A
53	1	172	A
53	1	175	A
53	1	189	A
53	1	191	G
53	1	192	A
53	1	197	A
53	1	198	A
53	1	204	U
53	1	205	C
53	1	206	C
53	1	210	A
53	1	225	G
53	1	243	G
53	1	246	C
53	1	259	U
53	1	260	C
53	1	261	G
53	1	262	G
53	1	264	C

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Mol	Chain	Res	Type
53	1	275	A
53	1	276	C
53	1	277	G
53	1	312	U
53	1	313	C
53	1	322	C
53	1	341	A
53	1	342	A
53	1	349	G
53	1	372	G
53	1	377	U
53	1	378	U
53	1	379	C
53	1	384	A
53	1	385	U
53	1	399	U
53	1	400	A
53	1	420	G
53	1	464	C
53	1	476	G
53	1	490	G
53	1	500	C
53	1	506	G
53	1	513	U
53	1	514	A
53	1	517	G
53	1	540	G
53	1	541	C
53	1	542	G
53	1	556	G
53	1	584	U
53	1	591	G
53	1	607	G
53	1	623	A
53	1	628	U
53	1	635	A
53	1	647	G
53	1	663	A
53	1	675	G
53	1	684	G
53	1	701	A
53	1	702	U

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Mol	Chain	Res	Type
53	1	704	C
53	1	705	G
53	1	718	G
53	1	721	C
53	1	756	G
53	1	760	C
53	1	778	U
53	1	810	G
53	1	822	C
53	1	836	U
53	1	841	U
53	1	869	G
53	1	870	G
53	1	876	A
53	1	878	G
53	1	879	G
53	1	883	A
53	1	885	C
53	1	886	G
53	1	887	A
53	1	899	G
53	1	906	C
53	1	911	C
53	1	921	C
53	1	922	G
53	1	939	G
53	1	951	G
53	1	954	G
53	1	962	A
53	1	1005	C
53	1	1007	A
53	1	1009	C
53	1	1030	A
53	1	1031	G
53	1	1044	C
53	1	1045	G
53	1	1052	G
53	1	1059	G
53	1	1072	G
53	1	1081	A
53	1	1083	C
53	1	1088	A

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Mol	Chain	Res	Type
53	1	1101	A
53	1	1106	A
53	1	1109	U
53	1	1110	G
53	1	1125	U
53	1	1126	U
53	1	1133	U
53	1	1147	A
53	1	1211	A
53	1	1212	G
53	1	1234	C
53	1	1235	G
53	1	1248	A
53	1	1256	G
53	1	1263	C
53	1	1275	U
53	1	1276	G
53	1	1284	U
53	1	1326	A
53	1	1337	C
53	1	1349	G
53	1	1352	A
53	1	1355	C
53	1	1376	A
53	1	1381	G
53	1	1401	U
53	1	1402	A
53	1	1480	A
53	1	1482	A
53	1	1486	A
53	1	1489	C
53	1	1498	A
53	1	1519	A
53	1	1520	A
53	1	1521	A
53	1	1522	C
53	1	1528	C
53	1	1538	A
53	1	1573	G
53	1	1586	G
53	1	1599	G
53	1	1611	C

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Mol	Chain	Res	Type
53	1	1620	A
53	1	1629	C
53	1	1633	G
53	1	1635	U
53	1	1641	G
53	1	1650	A
53	1	1679	U
53	1	1686	C
53	1	1687	A
53	1	1695	U
53	1	1696	G
53	1	1697	G
53	1	1703	C
53	1	1715	U
53	1	1716	G
53	1	1717	U
53	1	1718	C
53	1	1719	G
53	1	1723	U
53	1	1724	C
53	1	1725	A
53	1	1740	A
53	1	1745	G
53	1	1771	A
53	1	1791	C
53	1	1804	G
53	1	1812	G
53	1	1821	A
53	1	1824	G
53	1	1830	U
53	1	1834	A
53	1	1848	C
53	1	1870	G
53	1	1911	A
53	1	1913	A
53	1	1939	G
53	1	1942	G
53	1	1945	A
53	1	1947	C
53	1	1949	A
53	1	1950	U
53	1	1955	C

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Mol	Chain	Res	Type
53	1	1956	U
53	1	1962	G
53	1	1963	G
53	1	1969	U
53	1	1971	G
53	1	1972	U
53	1	1988	U
53	1	1997	G
53	1	2000	U
53	1	2003	A
53	1	2004	U
53	1	2005	G
53	1	2024	U
53	1	2026	U
53	1	2056	U
53	1	2064	G
53	1	2065	G
53	1	2066	A
53	1	2074	G
53	1	2088	A
53	1	2089	G
53	1	2093	A
53	1	2094	G
53	1	2095	A
53	1	2102	A
53	1	2223	G
53	1	2235	C
53	1	2243	G
53	1	2247	A
53	1	2248	G
53	1	2250	A
53	1	2263	G
53	1	2264	G
53	1	2283	A
53	1	2305	C
53	1	2309	C
53	1	2313	A
53	1	2323	C
53	1	2331	U
53	1	2334	G
53	1	2346	A
53	1	2361	A

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Mol	Chain	Res	Type
53	1	2369	C
53	1	2412	G
53	1	2413	G
53	1	2414	U
53	1	2431	G
53	1	2454	G
53	1	2459	A
53	1	2460	A
53	1	2461	A
53	1	2468	C
53	1	2472	G
53	1	2475	A
53	1	2495	A
53	1	2501	A
53	1	2519	U
53	1	2521	G
53	1	2529	G
53	1	2545	A
53	1	2556	G
53	1	2562	G
53	1	2581	U
53	1	2593	A
53	1	2594	G
53	1	2600	C
53	1	2612	U
53	1	2613	U
53	1	2617	C
53	1	2629	A
53	1	2640	U
53	1	2648	G
53	1	2658	A
53	1	2659	G
53	1	2668	C
53	1	2673	A
53	1	2691	A
53	1	2708	G
53	1	2718	U
53	1	2739	G
53	1	2740	A
53	1	2741	U
53	1	2742	G
53	1	2760	A

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Mol	Chain	Res	Type
53	1	2775	A
53	1	2784	A
53	1	2792	A
53	1	2803	A
53	1	2804	A
53	1	2807	G
53	1	2817	U
53	1	2819	A
53	1	2829	U
53	1	2845	U
53	1	2868	G
53	1	2876	G
53	1	2882	A
53	1	2888	G
53	1	2894	A
53	1	2895	C
53	1	2898	A
53	1	2901	G
53	1	2906	A
53	1	2907	G
53	1	2909	C

All (40) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	23	G
4	3	38	G
4	3	69	C
4	3	70	A
4	3	89	C
4	3	222	A
4	3	229	A
4	3	260	A
4	3	307	C
4	3	434	U
4	3	449	A
4	3	456	C
4	3	626	A
4	3	856	A
4	3	878	U
4	3	989	A
4	3	1010	U

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Mol	Chain	Res	Type
4	3	1149	A
4	3	1241	G
4	3	1248	G
4	3	1279	G
4	3	1294	A
4	3	1380	G
4	3	1390	C
4	3	1431	U
53	1	133	A
53	1	144	U
53	1	204	U
53	1	205	C
53	1	260	C
53	1	419	G
53	1	835	G
53	1	878	G
53	1	1518	C
53	1	1714	C
53	1	1717	U
53	1	1790	C
53	1	1941	G
53	1	2459	A
53	1	2783	U

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	AMP	0	401	-	25,25,25	1.39	4 (16%)	37,38,38	1.90	9 (24%)
54	AMP	0	402	-	25,25,25	1.38	5 (20%)	37,38,38	1.92	10 (27%)

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
54	AMP	0	401	-	-	3/10/26/26	0/3/3/3
54	AMP	0	402	-	-	0/10/26/26	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	0	401	AMP	C5-C4	4.40	1.46	1.39
54	0	402	AMP	C5-C4	4.34	1.46	1.39
54	0	401	AMP	C5-N7	-2.71	1.34	1.39
54	0	402	AMP	C5-C6	2.58	1.48	1.41
54	0	402	AMP	C5-N7	-2.45	1.34	1.39
54	0	401	AMP	C5-C6	2.29	1.47	1.41
54	0	402	AMP	C4-N9	-2.23	1.33	1.37
54	0	401	AMP	C4-N9	-2.20	1.33	1.37
54	0	402	AMP	C8-N7	2.14	1.35	1.31

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	0	402	AMP	C5-C4-N3	-5.37	119.33	126.72
54	0	401	AMP	C5-C4-N3	-5.32	119.40	126.72
54	0	401	AMP	N3-C4-N9	4.53	134.87	127.17
54	0	402	AMP	N3-C4-N9	4.26	134.41	127.17
54	0	401	AMP	N3-C2-N1	-3.96	122.59	128.58
54	0	402	AMP	N3-C2-N1	-3.84	122.76	128.58
54	0	402	AMP	C2-N3-C4	3.75	120.99	111.83
54	0	401	AMP	C2-N3-C4	3.55	120.51	111.83
54	0	402	AMP	C4-C5-N7	-3.52	106.56	110.58
54	0	401	AMP	C4-C5-N7	-3.23	106.89	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	0	401	AMP	C4-N9-C8	3.11	109.01	105.74
54	0	402	AMP	C4-N9-C8	3.04	108.93	105.74
54	0	401	AMP	C2-N1-C6	2.96	123.59	118.73
54	0	402	AMP	C5-N7-C8	2.70	107.69	103.45
54	0	401	AMP	C5-N7-C8	2.51	107.40	103.45
54	0	402	AMP	N9-C8-N7	-2.38	110.56	113.94
54	0	402	AMP	C6-C5-N7	2.38	136.68	132.09
54	0	402	AMP	C2-N1-C6	2.36	122.61	118.73
54	0	401	AMP	N9-C8-N7	-2.10	110.96	113.94

There are no chirality outliers.

All (3) torsion outliers are listed below:

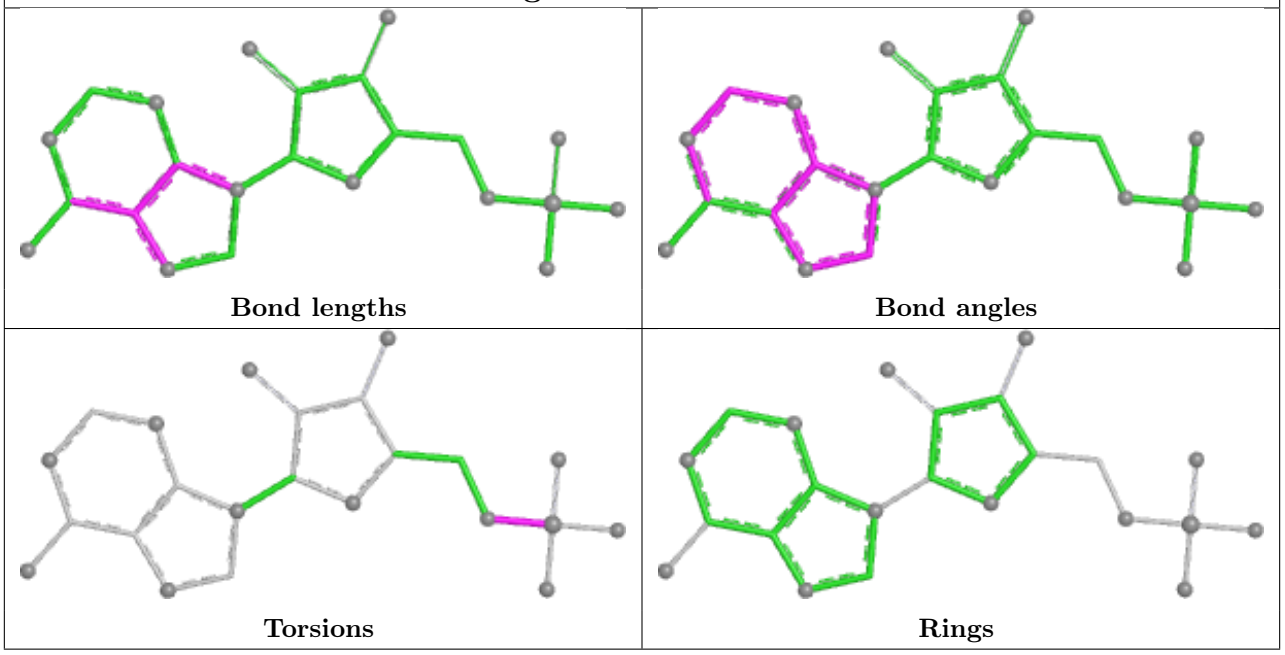
Mol	Chain	Res	Type	Atoms
54	0	401	AMP	C5'-O5'-P-O1P
54	0	401	AMP	C5'-O5'-P-O2P
54	0	401	AMP	C5'-O5'-P-O3P

There are no ring outliers.

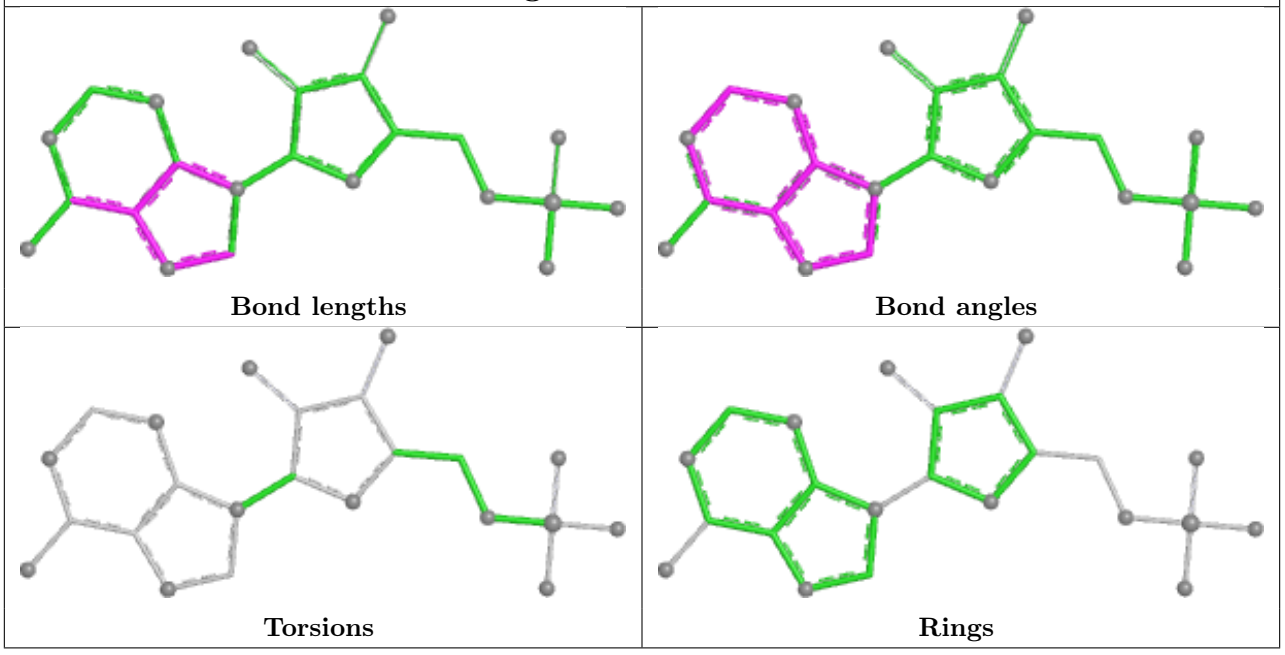
No monomer is involved in short contacts.

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 AMP 0 401



Ligand AMP 0 402



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

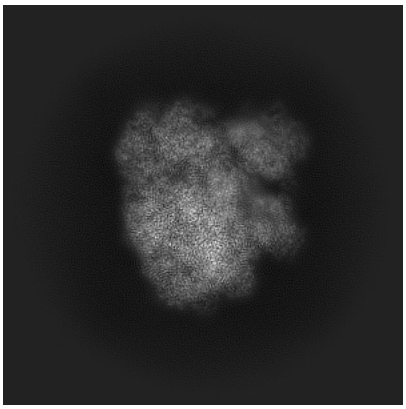
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-76336. These allow visual inspection of the internal detail of the map and identification of artifacts.

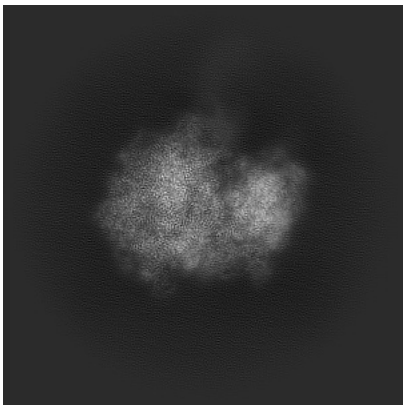
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

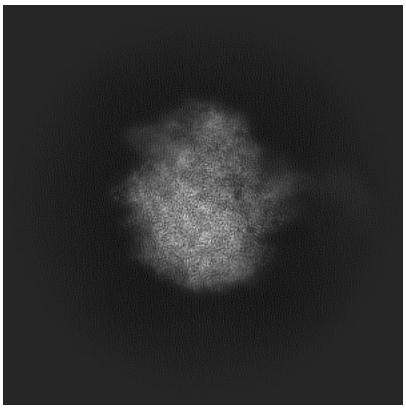
6.1.1 Primary map



X

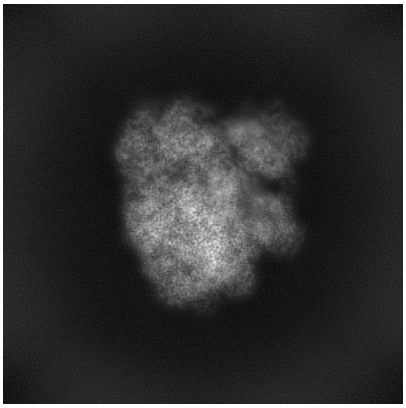


Y

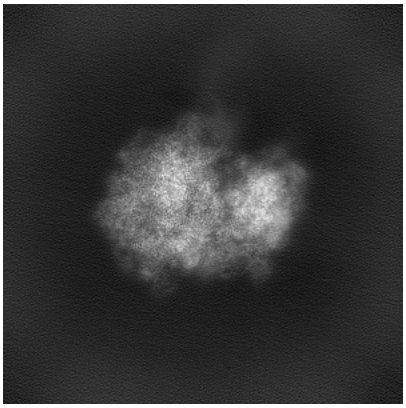


Z

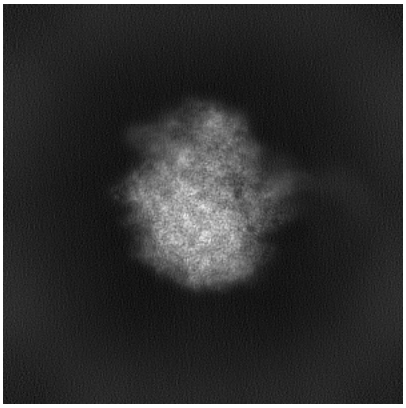
6.1.2 Raw map



X



Y

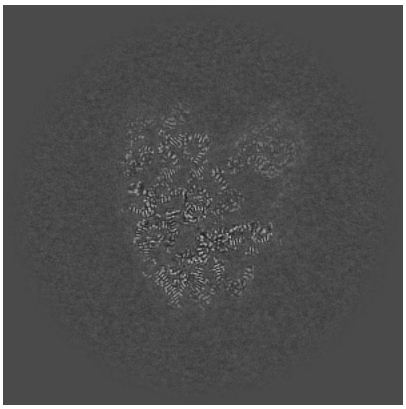


Z

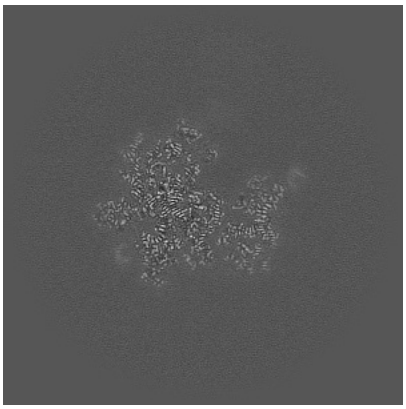
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

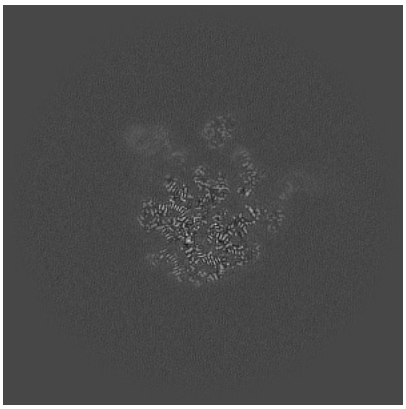
6.2.1 Primary map



X Index: 220

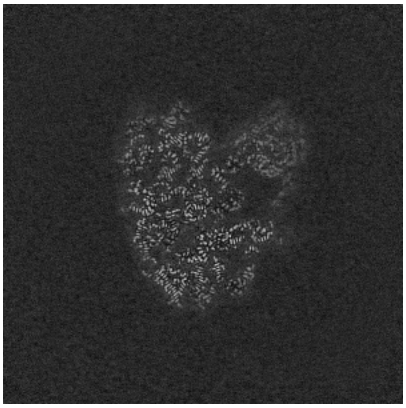


Y Index: 220

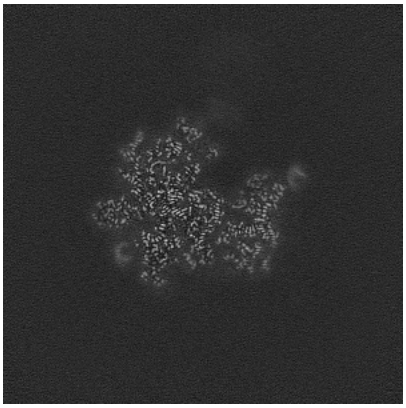


Z Index: 220

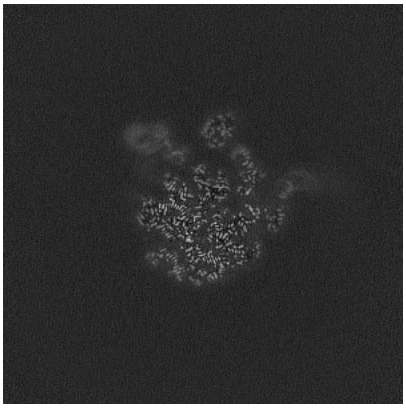
6.2.2 Raw map



X Index: 220



Y Index: 220

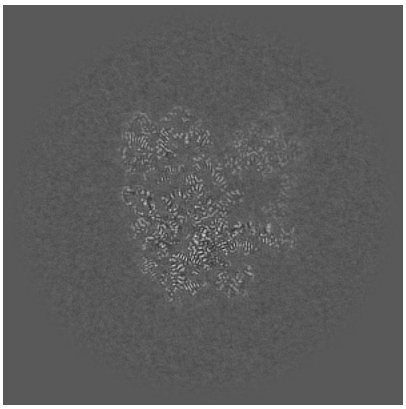


Z Index: 220

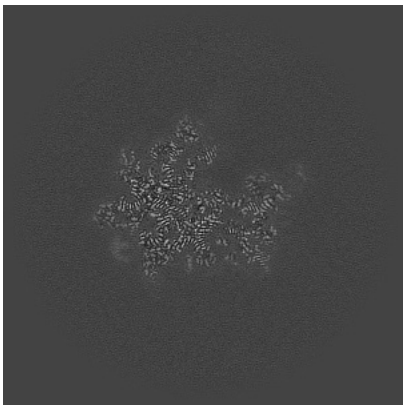
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

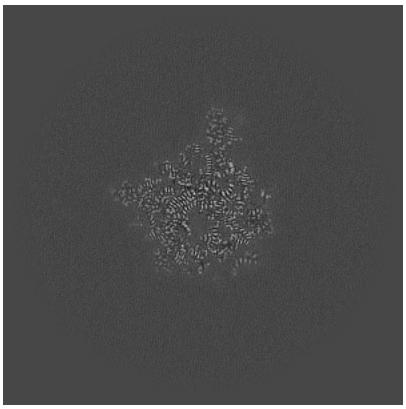
6.3.1 Primary map



X Index: 225

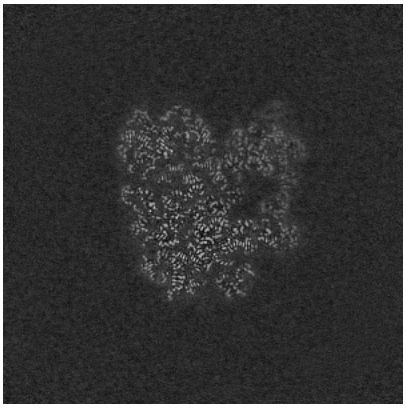


Y Index: 216

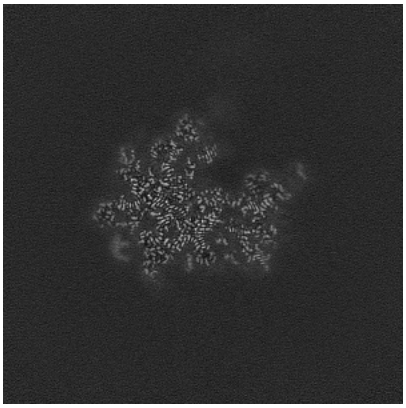


Z Index: 175

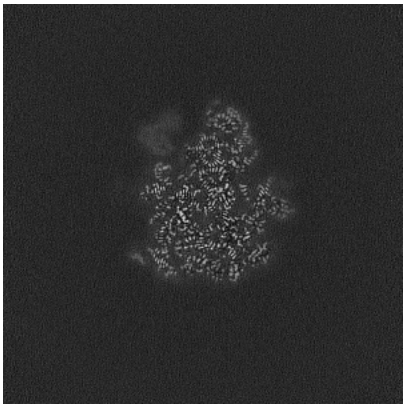
6.3.2 Raw map



X Index: 226



Y Index: 216

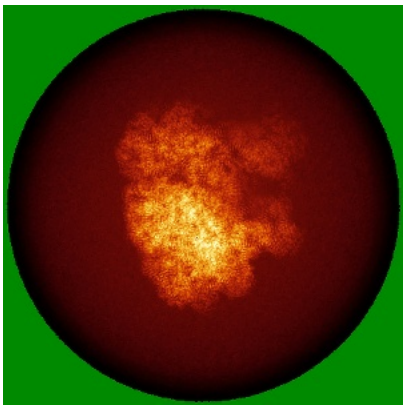


Z Index: 194

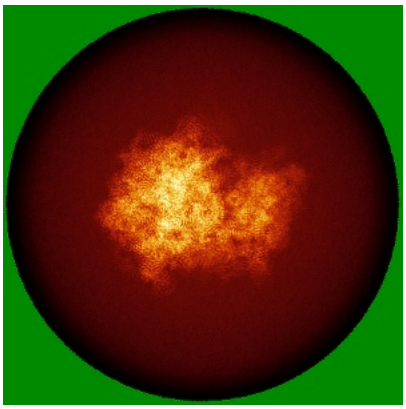
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

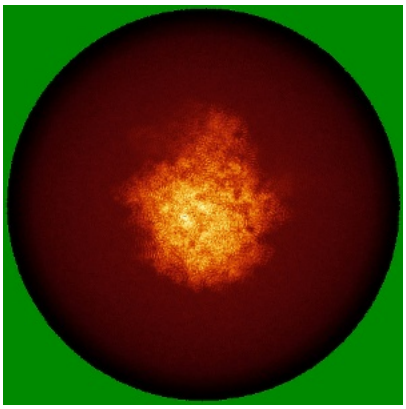
6.4.1 Primary map



X

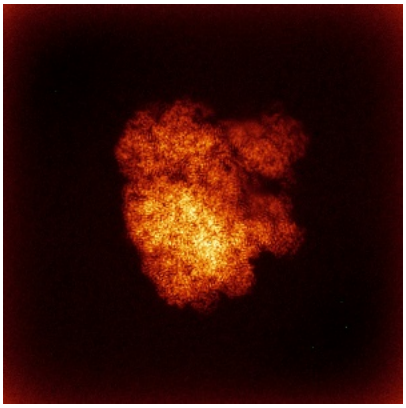


Y

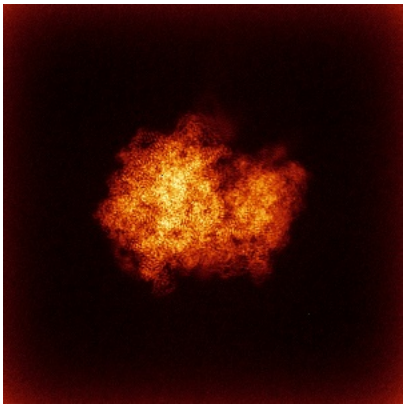


Z

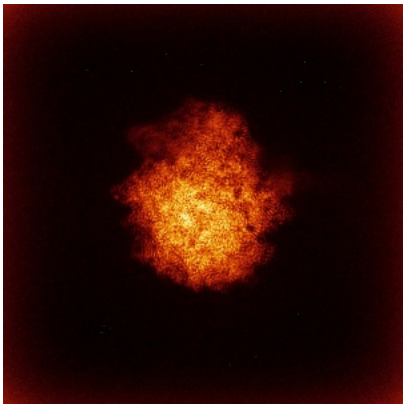
6.4.2 Raw map



X



Y

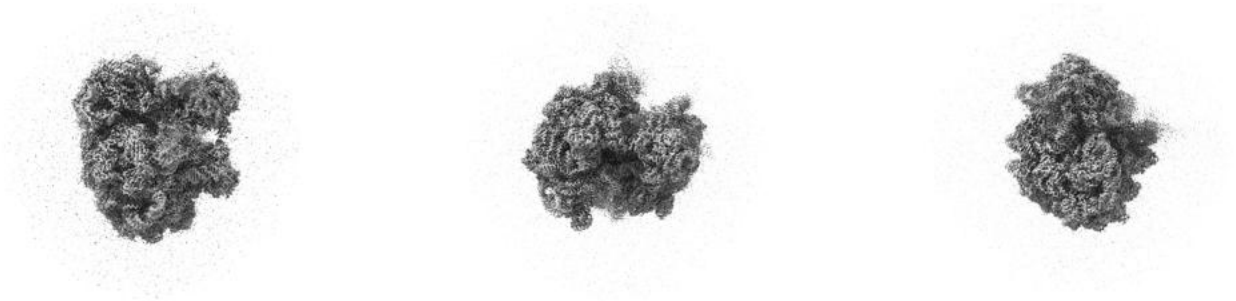


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.132. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

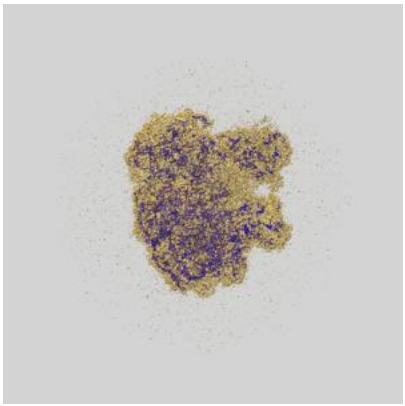
6.6 Mask visualisation (i)

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

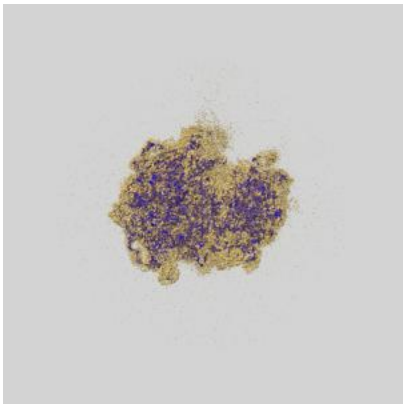
A mask typically either:

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

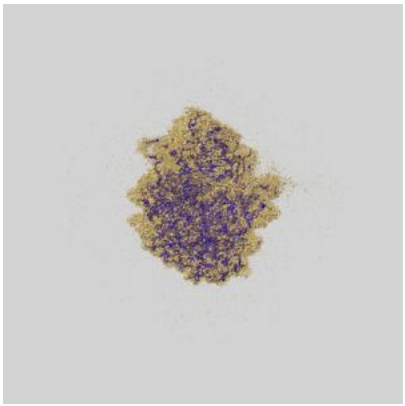
6.6.1 emd_76336_msk_1.map (i)



X



Y

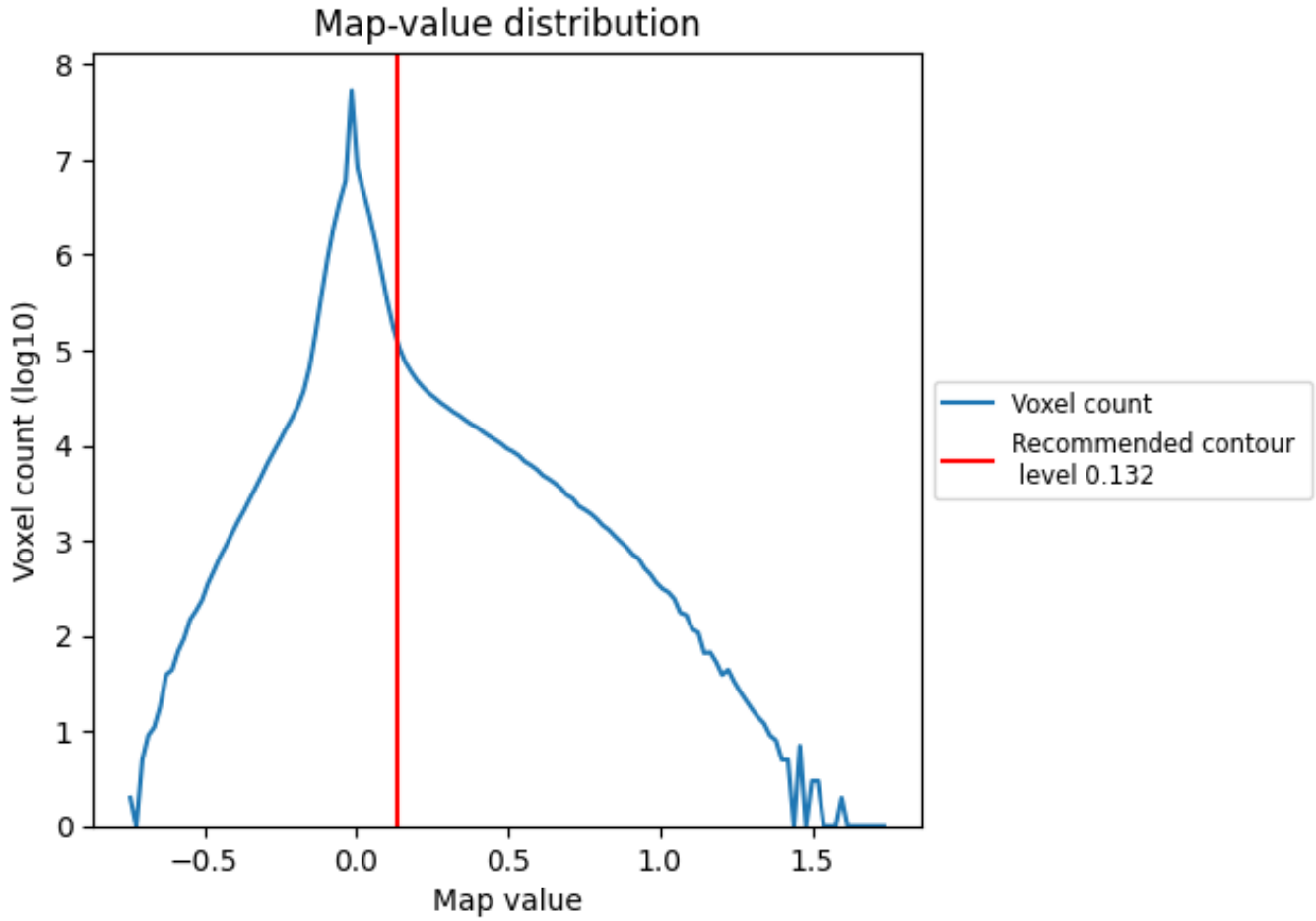


Z

7 Map analysis

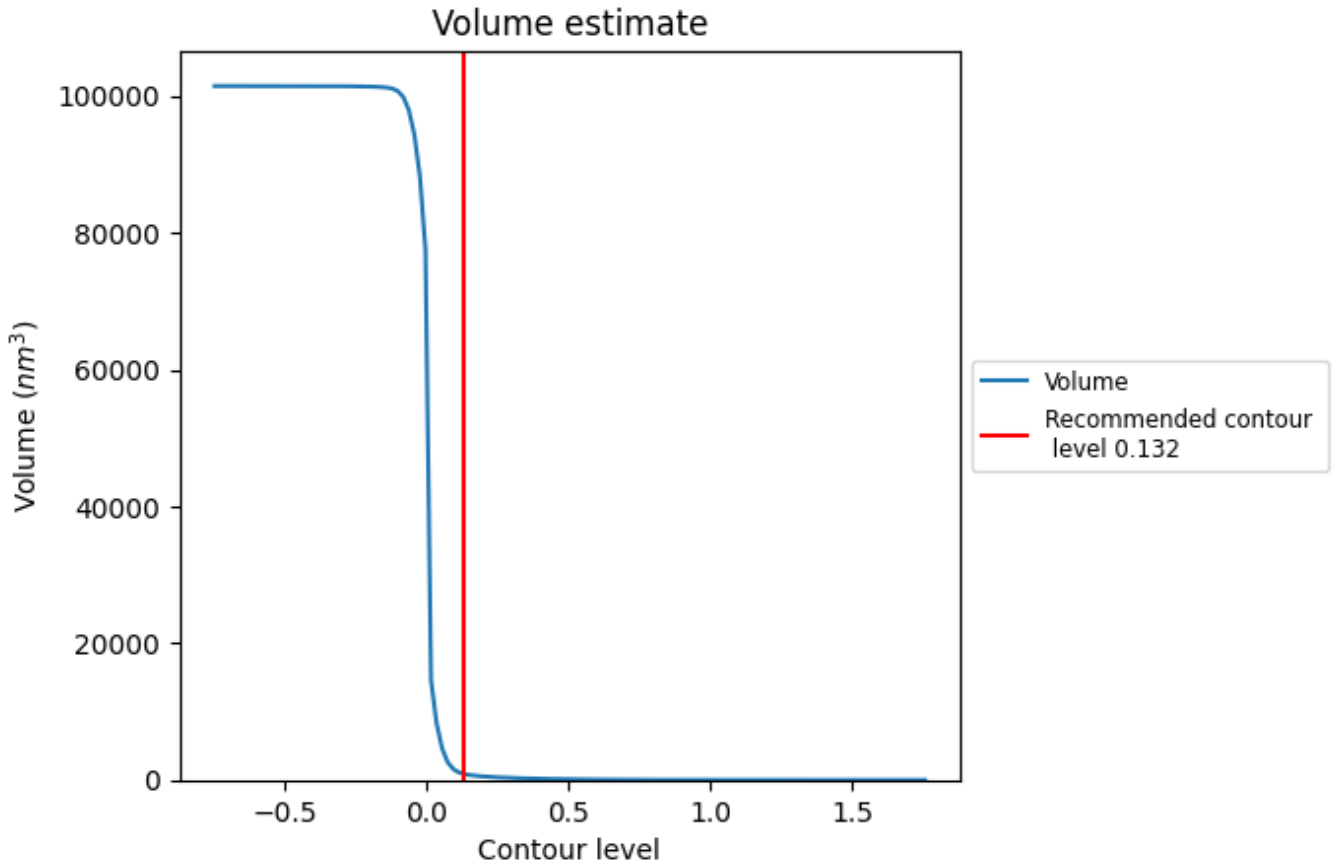
This section contains the results of statistical analysis of the map.

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.

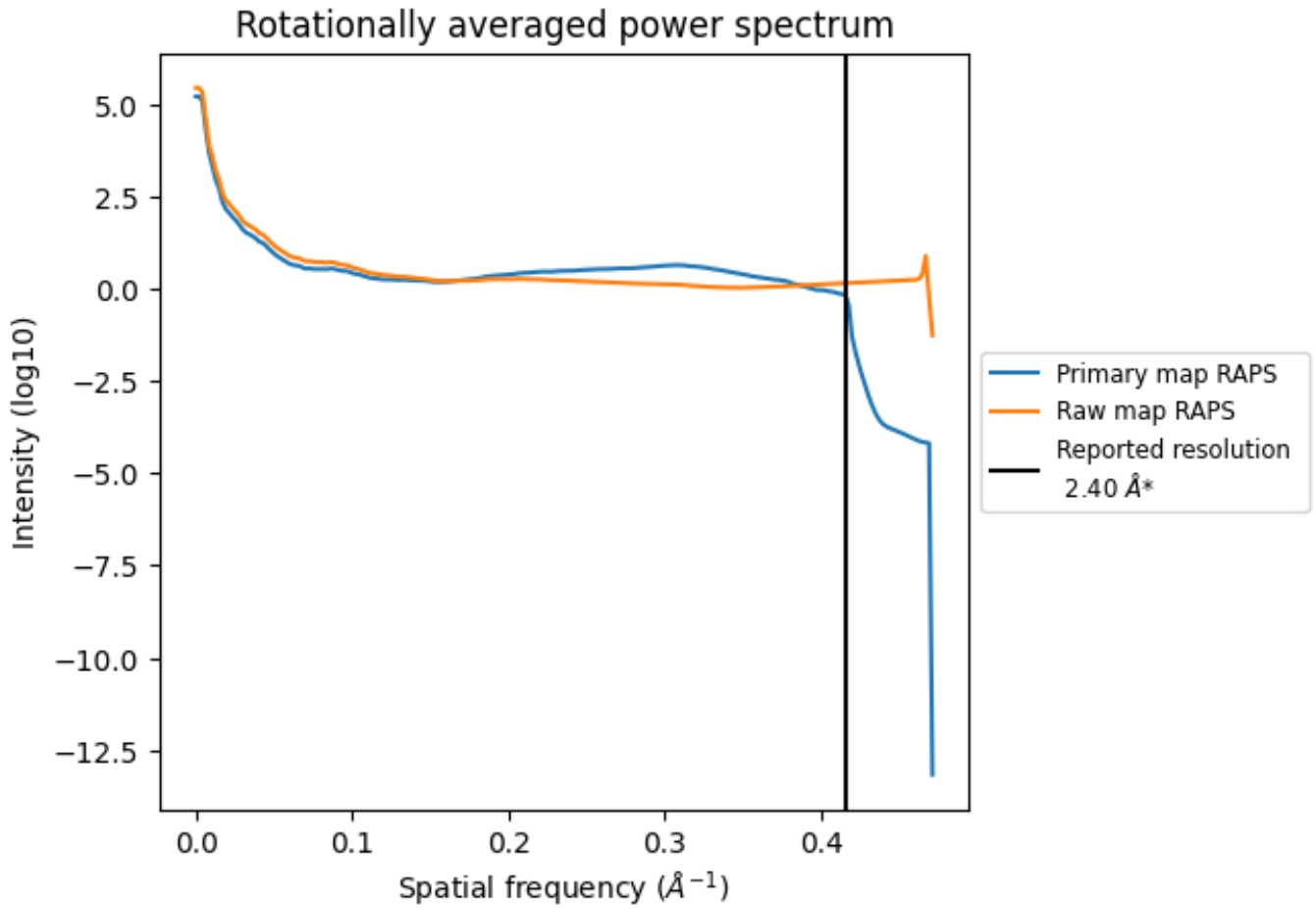
7.2 Volume estimate



The volume at the recommended contour level is 895 nm^3; this corresponds to an approximate mass of 809 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 (i)

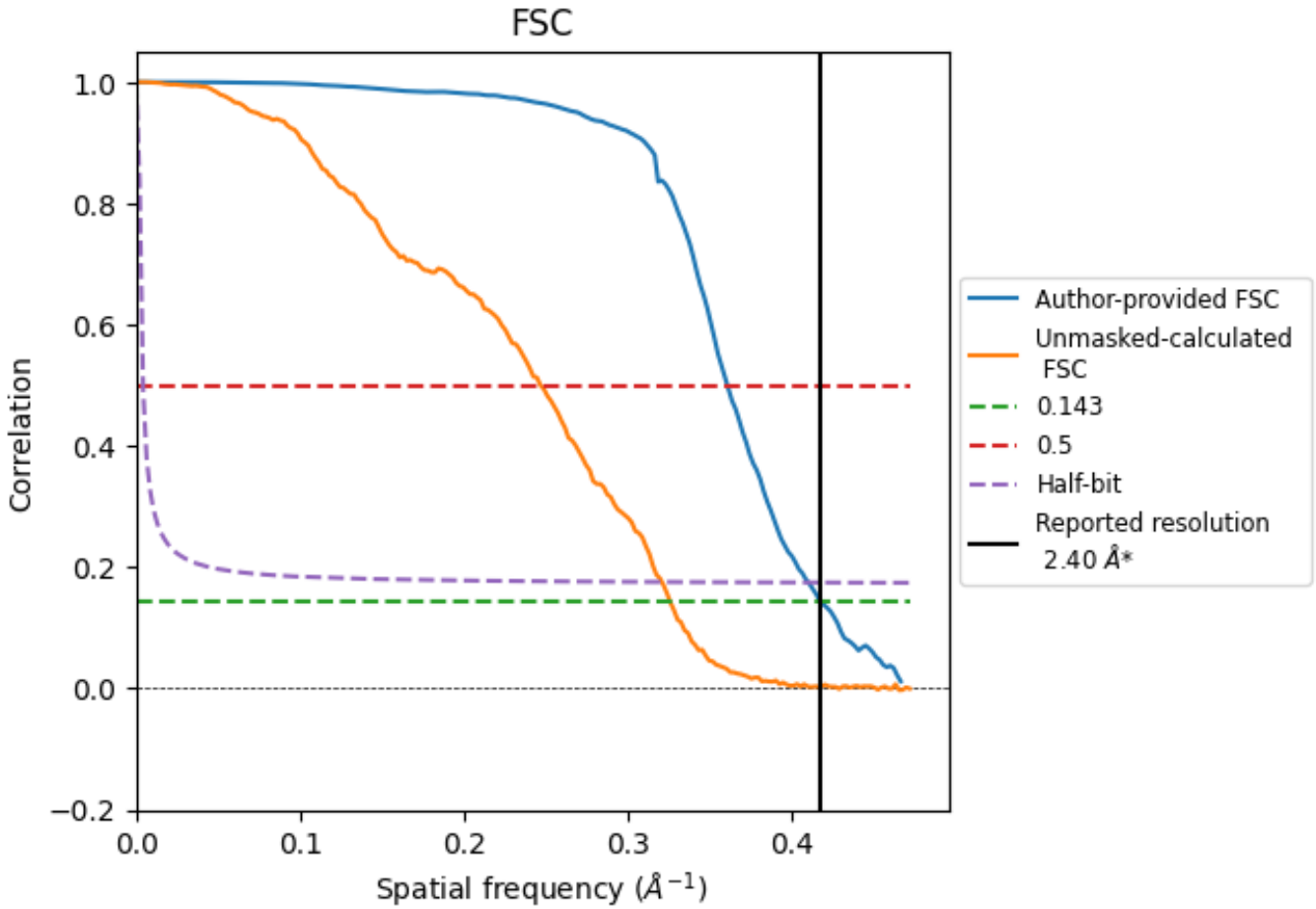


*Reported resolution corresponds to spatial frequency of 0.417 $Å^{-1}$

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 0.417 Å^{-1}

8.2 Resolution estimates (i)

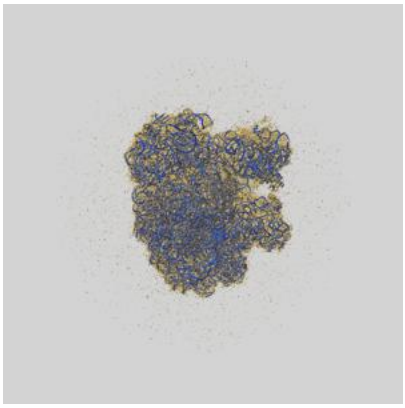
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.40	2.77	2.44
Unmasked-calculated*	3.07	4.06	3.12

*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 3.07 differs from the reported value 2.4 by more than 10 %

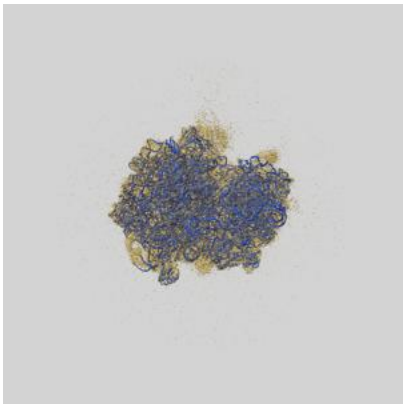
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-76336 and PDB model 12DM. Per-residue inclusion information can be found in section 3 on page 14.

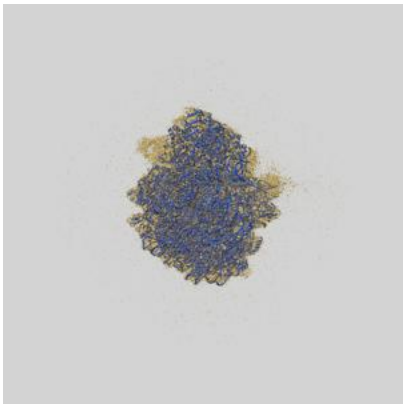
9.1 Map-model overlay



X



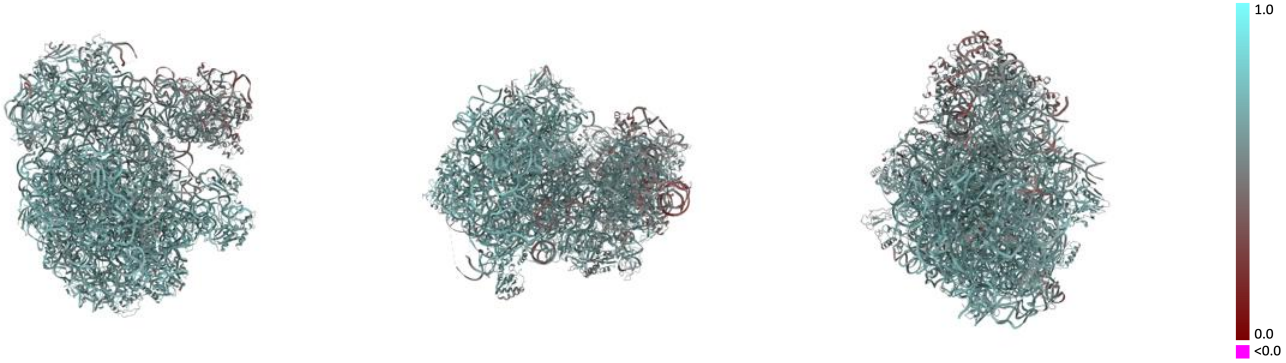
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.132 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.

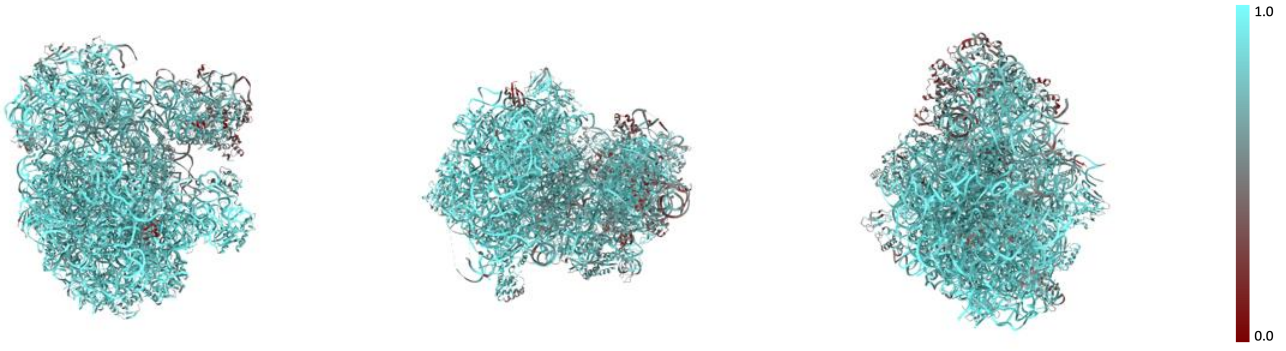
9.2 Q-score mapped to coordinate model (i)



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.

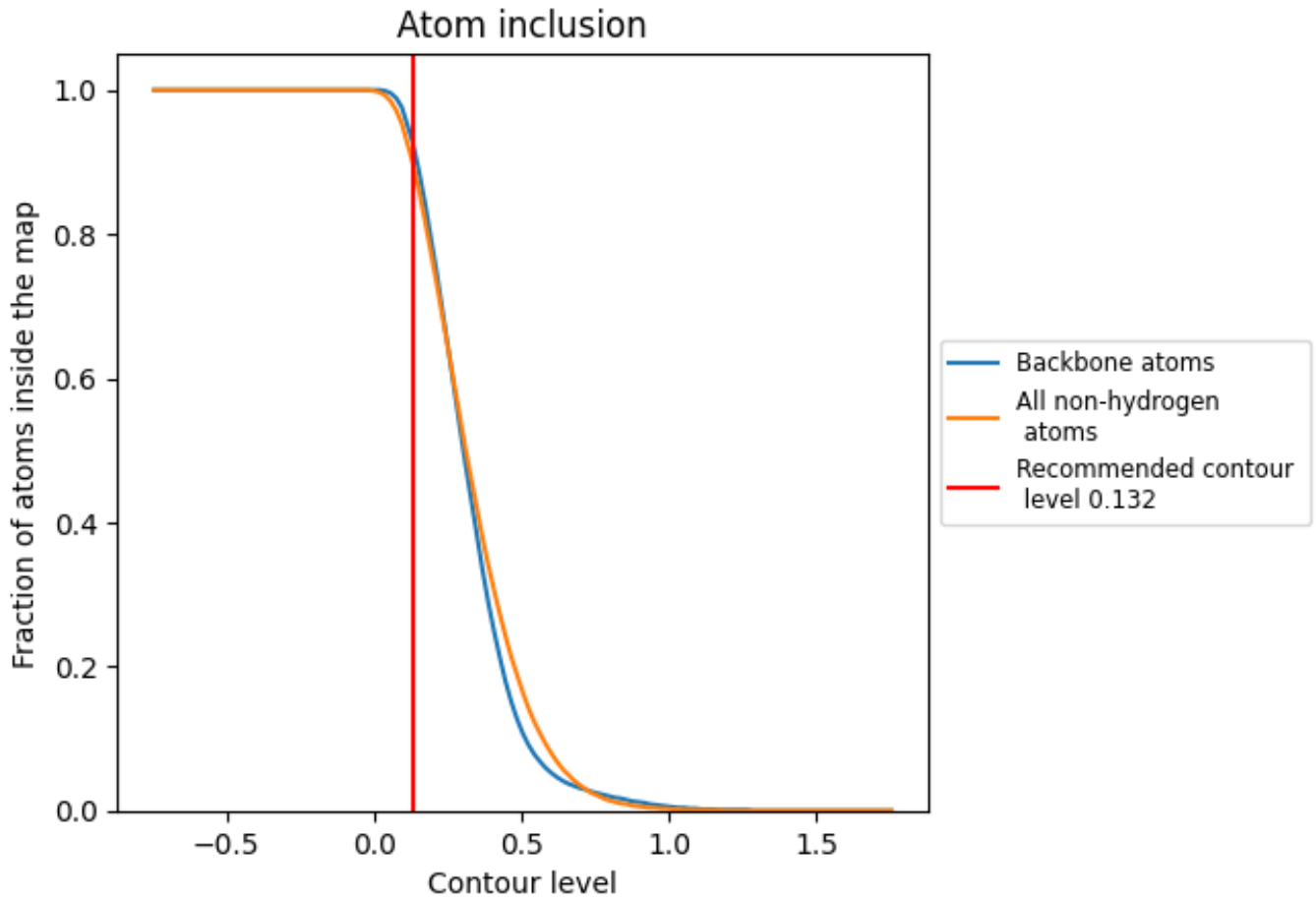
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.132).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 90% 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 (0.132) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9000	0.6300
0	0.8500	0.6290
1	0.9720	0.6600
2	0.9560	0.6360
3	0.9090	0.6080
4	0.6290	0.4760
A	0.9260	0.6640
B	0.9340	0.6700
C	0.8950	0.6480
D	0.7330	0.5770
E	0.8180	0.6120
F	0.7910	0.6020
H	0.9090	0.6550
J	0.9230	0.6640
K	0.9210	0.6640
L	0.8850	0.6410
M	0.9610	0.6790
N	0.8950	0.6410
O	0.3640	0.5280
P	0.8940	0.6430
Q	0.9250	0.6520
R	0.9470	0.6730
S	0.9270	0.6630
T	0.8210	0.6160
U	0.8900	0.6460
V	0.8880	0.6520
W	0.6330	0.5440
X	0.9230	0.6650
Y	0.8580	0.6410
Z	0.9210	0.6660
a	0.9670	0.6840
b	0.9070	0.6380
c	0.9120	0.6540
d	0.9360	0.6620
e	0.6930	0.5580



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Chain	Atom inclusion	Q-score
f	0.7360	0.5750
g	0.8330	0.6100
h	0.6800	0.5630
i	0.5880	0.5330
j	0.8560	0.6200
k	0.9220	0.6530
l	0.5910	0.5040
m	0.6060	0.5280
n	0.7870	0.5870
o	0.8320	0.6260
p	0.5690	0.5050
q	0.6610	0.5310
r	0.7330	0.5680
s	0.8790	0.6440
t	0.5300	0.4780
u	0.5600	0.4830
v	0.6430	0.5430
w	0.6220	0.5480
x	0.4070	0.4950