



Full wwPDB EM Validation Report ⓘ

Jan 30, 2025 – 03:19 PM JST

PDB ID : 8HL3
EMDB ID : EMD-34868
Title : Cryo-EM Structures and Translocation Mechanism of Crenarchaeota Ribosome
Authors : Wang, Y.H.; Zhou, J.
Deposited on : 2022-11-28
Resolution : 4.80 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.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

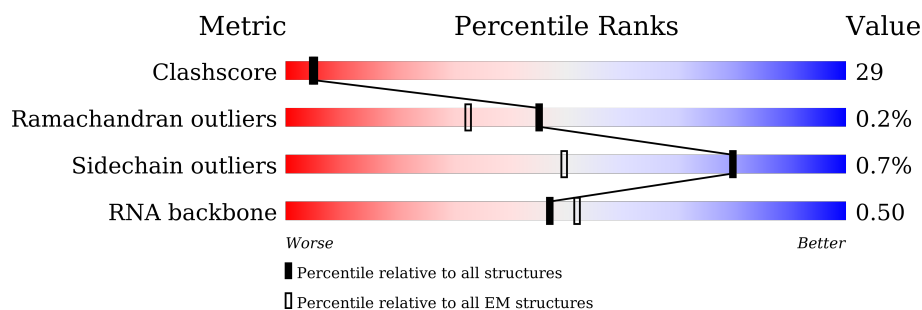
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

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

Mol	Chain	Length	Quality of chain
1	A23S	3022	
2	A16S	1503	
3	AEFG	729	
4	A5S	122	
5	AL2P	234	
6	AL3P	339	
7	AL4P	251	

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Mol	Chain	Length	Quality of chain	
8	AL5P	168	26%	100%
9	AL6P	181	23%	99%
10	ALX0	76	20%	99%
11	L10E	164	20%	99%
12	L13P	140	22%	100%
13	L141	86	20%	100%
13	L142	86	26%	100%
14	L14P	134	40%	99%
15	L15E	169	25%	100%
16	L18E	112	7%	98%
17	L18P	193	11%	98%
18	L19E	144	9%	99%
19	L22P	150	18%	97%
20	L23P	81	7%	100%
21	L24E	54	15%	100%
22	L24P	122	9%	100%
23	L29P	63	8%	100%
24	L30E	94	6%	100%
25	L30P	155	16%	100%
26	L31E	75	15%	100%
27	L32E	123	30%	98%
28	L34E	77	43%	94%
29	L37A	65	22%	98%
30	L37E	54	24%	100%
31	L39E	49	31%	98%

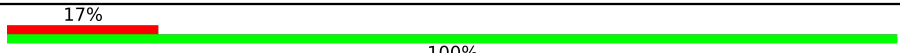
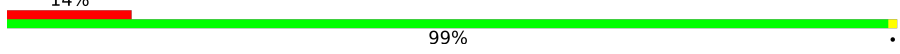
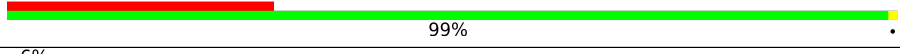
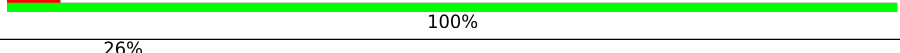
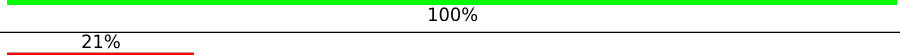
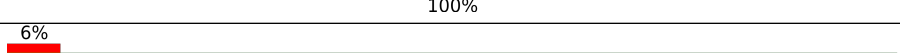
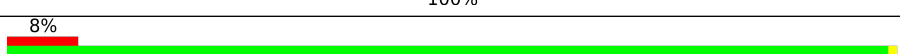
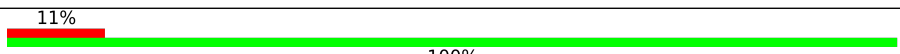
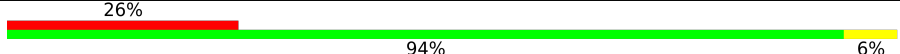
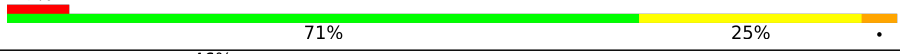
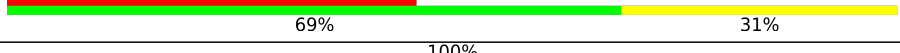


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Mol	Chain	Length	Quality of chain
32	L40E	55	47% 96% .
33	L44E	92	13% 100% .
34	L7A1	123	22% 100% .
34	L7A2	123	35% 99% .
34	SL7A	123	63% 100% .
35	L15P	144	5% 65% 35% .
36	L21E	97	18% 98% .
37	L45A	101	22% 96% .
38	L46A	70	43% 97% .
39	L47A	80	95% 96% .
40	AL1P	216	79% 99% .
41	AS2P	196	99% 99% .
42	AS4E	240	32% 99% .
43	AS4P	166	30% 99% .
44	AS5P	204	31% 100% .
45	AS6E	105	51% 100% .
46	AS8E	126	63% 100% .
47	AS8P	130	14% 99% .
48	S11P	128	50% 98% .
49	S12P	143	43% 97% .
50	S15P	149	19% 99% .
51	S17P	111	45% 99% .
52	S24E	96	32% 100% .
53	S27E	59	25% 100% .
54	S3AE	189	40% 99% .

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Mol	Chain	Length	Quality of chain
55	AS3P	201	
56	AS7P	193	
57	S10P	100	
58	S13P	147	
59	S14P	52	
60	S17E	62	
61	S19E	150	
62	S19P	115	
63	AS9P	136	
64	S28E	63	
65	S27A	54	
66	AETN	76	
66	APTN	76	
67	AMRN	13	
68	APTP	6	

2 Entry composition

There are 70 unique types of molecules in this entry. The entry contains 173506 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 23s rRNA (3000-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A23S	2996	Total	C	N	O	P	0	0
			64357	28673	11910	20778	2996		

- Molecule 2 is a RNA chain called 16s rRNA (1493-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A16S	1492	Total	C	N	O	P	0	0
			32040	14269	5925	10354	1492		

- Molecule 3 is a protein called Elongation factor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AEFG	725	Total	C	N	O	S	0	0
			5677	3609	984	1067	17		

- Molecule 4 is a RNA chain called 5s rRNA (122-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A5S	122	Total	C	N	O	P	0	0
			2609	1163	476	849	121		

- Molecule 5 is a protein called 50S ribosomal protein L2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	AL2P	234	Total	C	N	O	S	0	0
			1754	1101	344	307	2		

- Molecule 6 is a protein called 50S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AL3P	339	Total	C	N	O	S	0	0
			2695	1730	484	477	4		

- Molecule 7 is a protein called 50S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	AL4P	251	Total	C	N	O	S	0	0
			1926	1223	356	345	2		

- Molecule 8 is a protein called 50S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	AL5P	168	Total	C	N	O	S	0	0
			1343	854	253	232	4		

- Molecule 9 is a protein called 50S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AL6P	181	Total	C	N	O	S	0	0
			1431	920	246	264	1		

- Molecule 10 is a protein called 50S ribosomal protein L18Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	ALX0	76	Total	C	N	O	S	0	0
			629	403	110	115	1		

- Molecule 11 is a protein called 50S ribosomal protein L10e.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L10E	164	Total	C	N	O	S	0	0
			1310	837	239	227	7		

- Molecule 12 is a protein called 50S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L13P	140	Total	C	N	O	S	0	0
			1109	707	208	190	4		

- Molecule 13 is a protein called 50S ribosomal protein L14e.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L141	86	Total	C	N	O	S	0	0
			669	417	123	127	2		
13	L142	86	Total	C	N	O	S	0	0
			669	417	123	127	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L14P	134	Total	C	N	O	S	0	0
			1034	655	194	181	4		

- Molecule 15 is a protein called 50S ribosomal protein L15e.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L15E	169	Total	C	N	O	S	0	0
			1423	899	283	236	5		

- Molecule 16 is a protein called 50S ribosomal protein L18e.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L18E	112	Total	C	N	O	S	0	0
			895	576	163	153	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	L18P	193	Total	C	N	O	S	0	0
			1539	990	274	274	1		

- Molecule 18 is a protein called 50S ribosomal protein L19e.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	L19E	144	Total	C	N	O	0	0
			1206	753	247	206		

- Molecule 19 is a protein called 50S ribosomal protein L22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L22P	150	Total	C	N	O	S	0	0
			1223	782	225	213	3		

- Molecule 20 is a protein called 50S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L23P	81	Total	C	N	O	S	0	0
			650	419	109	121	1		

- Molecule 21 is a protein called 50S ribosomal protein L24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	L24E	54	Total	C	N	O	S	0	0
			441	282	80	73	6		

- Molecule 22 is a protein called 50S ribosomal protein L24.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	L24P	122	Total	C	N	O	S	0	0
			989	620	189	176	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	L29P	63	Total	C	N	O	S	0	0
			513	319	95	96	3		

- Molecule 24 is a protein called 50S ribosomal protein L30e.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	L30E	94	Total	C	N	O	S	0	0
			729	474	116	136	3		

- Molecule 25 is a protein called 50S ribosomal protein L30.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	L30P	155	Total	C	N	O	S	0	0
			1254	804	222	223	5		

- Molecule 26 is a protein called 50S ribosomal protein L31e.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	L31E	75	Total	C	N	O	S	0	0
			625	398	126	97	4		

- Molecule 27 is a protein called 50S ribosomal protein L32e.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	L32E	123	Total	C	N	O	S	0	0
			1010	650	193	166	1		

- Molecule 28 is a protein called 50S ribosomal protein L34e.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	L34E	77	Total	C	N	O	S	0	0
			629	395	119	110	5		

- Molecule 29 is a protein called 50S ribosomal protein L37Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	L37A	65	Total	C	N	O	S	0	0
			527	335	99	87	6		

- Molecule 30 is a protein called 50S ribosomal protein L37e.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L37E	54	Total	C	N	O	S	0	0
			436	267	94	69	6		

- Molecule 31 is a protein called 50S ribosomal protein L39e.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	L39E	49	Total	C	N	O	0	0
			414	265	88	61		

- Molecule 32 is a protein called 50S ribosomal protein L40E.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	L40E	55	Total	C	N	O	S	0	0
			439	273	89	72	5		

- Molecule 33 is a protein called 50S ribosomal protein L44e.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	L44E	92	Total	C	N	O	S	0	0
			753	474	144	129	6		

- Molecule 34 is a protein called 50S ribosomal protein L7Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	L7A1	123	Total	C	N	O	S	0	0
			935	593	155	184	3		
34	L7A2	123	Total	C	N	O	S	0	0
			935	593	155	184	3		
34	SL7A	123	Total	C	N	O	S	0	0
			935	593	155	184	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	L15P	94	Total	C	N	O	S	0	0
			752	487	131	133	1		

- Molecule 36 is a protein called 50S ribosomal protein L21e.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	L21E	97	Total	C	N	O	S	0	0
			785	502	152	129	2		

- Molecule 37 is a protein called DUF2280 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	L45A	101	Total	C	N	O	S	0	0
			816	515	141	156	4		

- Molecule 38 is a protein called Conserved protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	L46A	70	Total	C	N	O	S	0	0
			586	382	101	102	1		

- Molecule 39 is a protein called 50S ribosomal protein L47A.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	L47A	80	Total	C	N	O	S	0	0
			648	405	113	128	2		

- Molecule 40 is a protein called 50S ribosomal protein L1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	AL1P	216	Total	C	N	O	S	0	0
			1715	1096	303	312	4		

- Molecule 41 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	AS2P	196	Total	C	N	O	S	0	0
			1587	1022	277	286	2		

- Molecule 42 is a protein called 30S ribosomal protein S4e.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	AS4E	240	Total	C	N	O	S	0	0
			1925	1238	335	348	4		

- Molecule 43 is a protein called 30S ribosomal protein S4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	AS4P	166	Total	C	N	O	S	0	0
			1370	874	252	241	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
44	AS5P	204	Total	C	N	O	S	0	0
			1600	1028	277	287	8		

- Molecule 45 is a protein called 30S ribosomal protein S6e.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	AS6E	105	Total	C	N	O	S	0	0
			805	506	149	147	3		

- Molecule 46 is a protein called 30S ribosomal protein S8e.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	AS8E	126	Total	C	N	O	S	0	0
			993	619	187	187			

- Molecule 47 is a protein called 30S ribosomal protein S8.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	AS8P	130	Total	C	N	O	S	0	0
			1028	661	181	182	4		

- Molecule 48 is a protein called 30S ribosomal protein S11.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	S11P	128	Total	C	N	O	S	0	0
			960	595	190	173	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
49	S12P	143	Total	C	N	O	S	0	0
			1103	701	209	189	4		

- Molecule 50 is a protein called 30S ribosomal protein S15.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	S15P	149	Total	C	N	O	S	0	0
			1225	778	228	214	5		

- Molecule 51 is a protein called 30S ribosomal protein S17.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	S17P	111	Total	C	N	O	S	0	0
			885	557	165	160	3		

- Molecule 52 is a protein called 30S ribosomal protein S24e.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	S24E	96	Total	C	N	O	S	0	0
			759	479	133	147			

- Molecule 53 is a protein called 30S ribosomal protein S27e.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	S27E	59	Total	C	N	O	S	0	0
			458	294	83	76	5		

- Molecule 54 is a protein called 30S ribosomal protein S3Ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	S3AE	189	Total	C	N	O	S	0	0
			1545	1004	264	276	1		

- Molecule 55 is a protein called 30S ribosomal protein S3.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	AS3P	201	Total	C	N	O	S	0	0
			1576	1020	274	278	4		

- Molecule 56 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	AS7P	193	Total	C	N	O	S	0	0
			1537	969	285	279	4		

- Molecule 57 is a protein called 30S ribosomal protein S10.

Mol	Chain	Residues	Atoms					AltConf	Trace
57	S10P	100	Total	C	N	O	S	0	0
			824	522	154	142	6		

- Molecule 58 is a protein called 30S ribosomal protein S13.

Mol	Chain	Residues	Atoms					AltConf	Trace
58	S13P	147	Total	C	N	O	S	0	0
			1204	753	230	217	4		

- Molecule 59 is a protein called 30S ribosomal protein S14 type Z.

Mol	Chain	Residues	Atoms					AltConf	Trace
59	S14P	52	Total	C	N	O	S	0	0
			432	273	85	69	5		

- Molecule 60 is a protein called 30S ribosomal protein S17e.

Mol	Chain	Residues	Atoms				AltConf	Trace
60	S17E	62	Total	C	N	O	0	0
			517	326	92	99		

- Molecule 61 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
61	S19E	150	Total	C	N	O	S	0	0
			1239	801	223	213	2		

- Molecule 62 is a protein called 30S ribosomal protein S19.

Mol	Chain	Residues	Atoms					AltConf	Trace
62	S19P	115	Total	C	N	O	S	0	0
			968	620	181	162	5		

- Molecule 63 is a protein called 30S ribosomal protein S9.

Mol	Chain	Residues	Atoms					AltConf	Trace
63	AS9P	136	Total	C	N	O	S	0	0
			1096	692	200	197	7		

- Molecule 64 is a protein called 30S ribosomal protein S28e.

Mol	Chain	Residues	Atoms				AltConf	Trace
64	S28E	63	Total	C	N	O	0	0
			498	308	99	91		

- Molecule 65 is a protein called 30S ribosomal protein S27ae.

Mol	Chain	Residues	Atoms					AltConf	Trace
65	S27A	54	Total	C	N	O	S	0	0
			435	274	79	76	6		

- Molecule 66 is a RNA chain called tRNA (76-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
66	APTN	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		
66	AETN	76	Total	C	N	O	P	0	0
			1619	723	290	531	75		

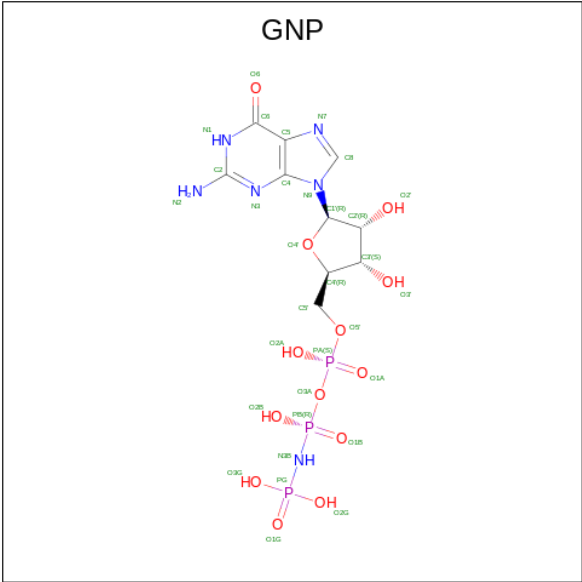
- Molecule 67 is a RNA chain called mRNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
67	AMRN	13	Total	C	N	O	P	0	0
			260	117	26	104	13		

- Molecule 68 is a protein called PHE-PHE-PHE-PHE-PHE-PHE.

Mol	Chain	Residues	Atoms				AltConf	Trace
68	APTP	6	Total	C	N	O	0	0
			67	54	6	7		

- Molecule 69 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
69	AEFG	1	Total	C	N	O	P	0
			32	10	6	13	3	

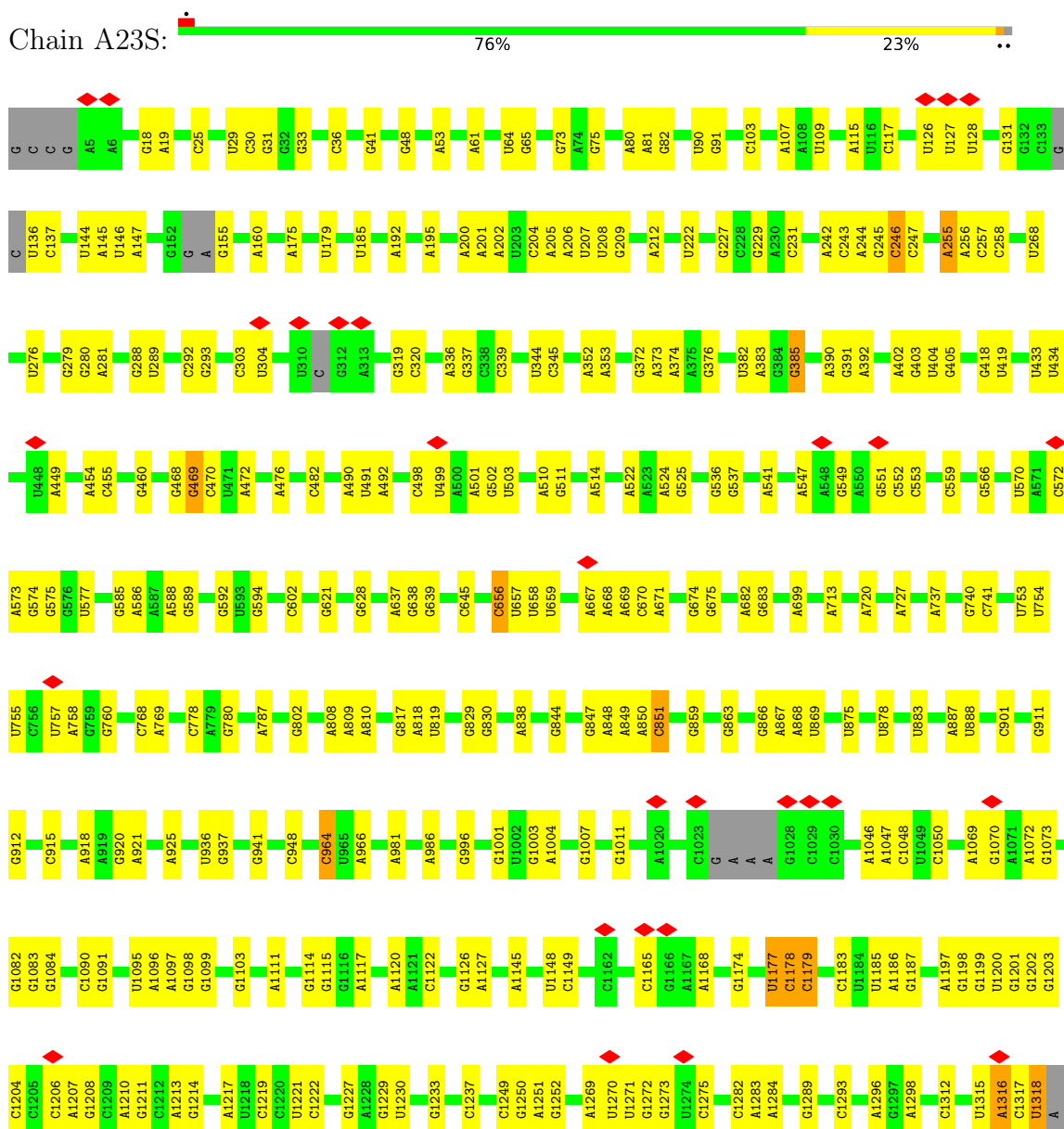
- Molecule 70 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

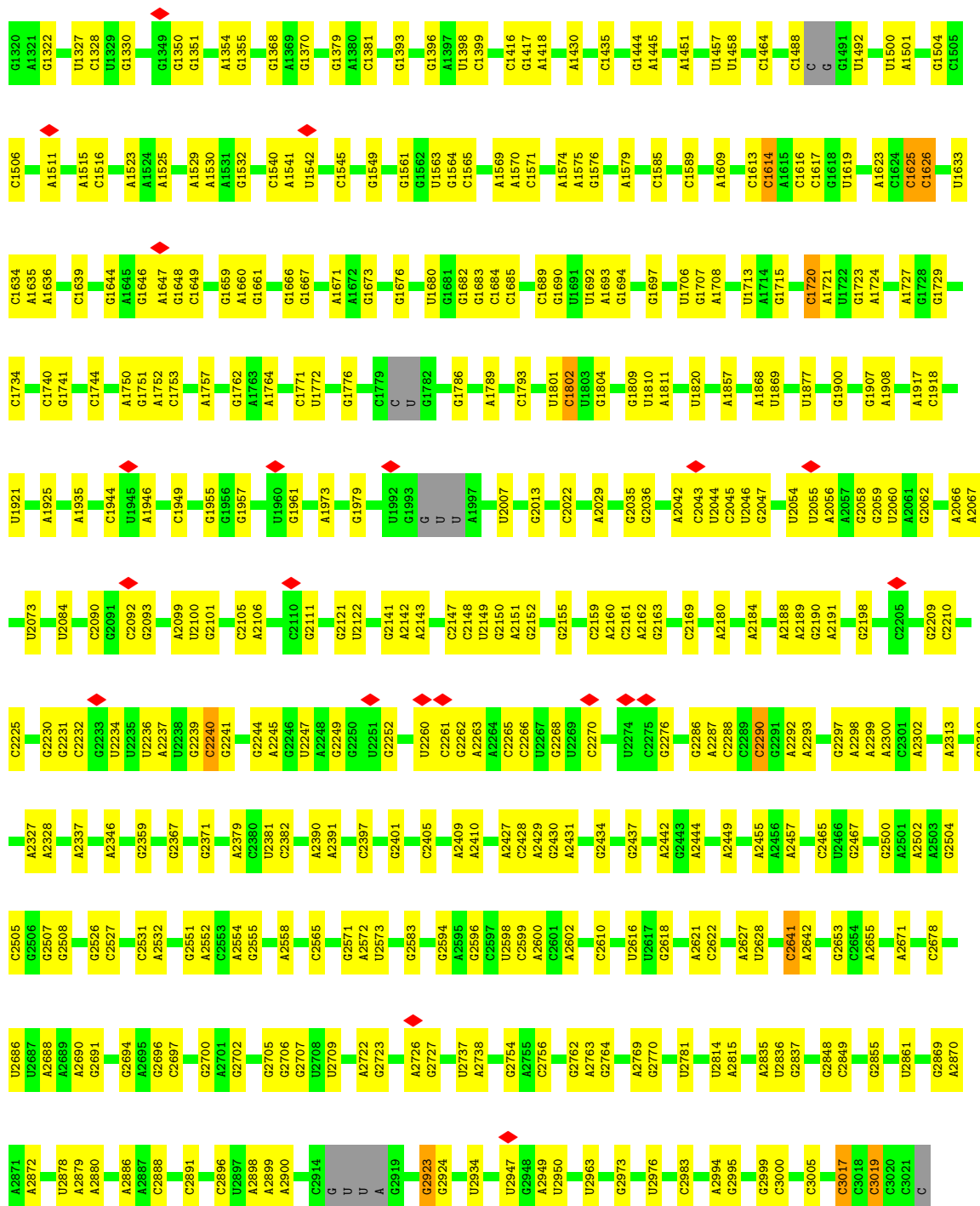
Mol	Chain	Residues	Atoms				AltConf
70	AS2P	29	Total	C	N	O	0
			146	87	29	30	
70	AS5P	21	Total	C	N	O	0
			105	63	21	21	
70	AS8P	7	Total	C	N	O	0
			35	21	7	7	

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

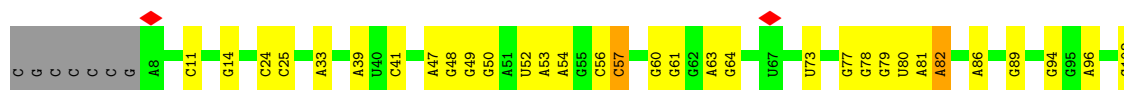
• Molecule 1: 23s rRNA (3000-MER)

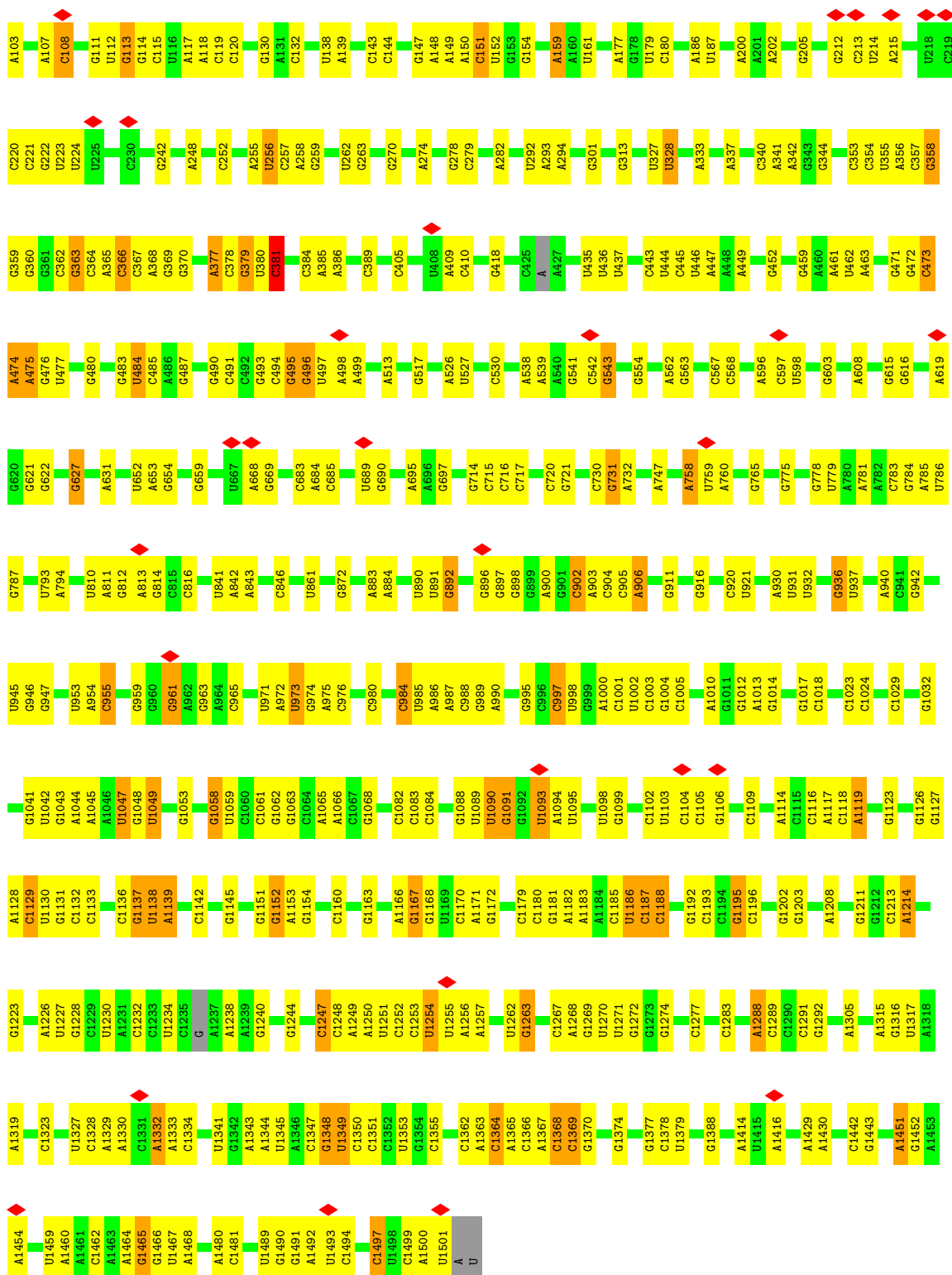




• Molecule 2: 16s rRNA (1493-MER)

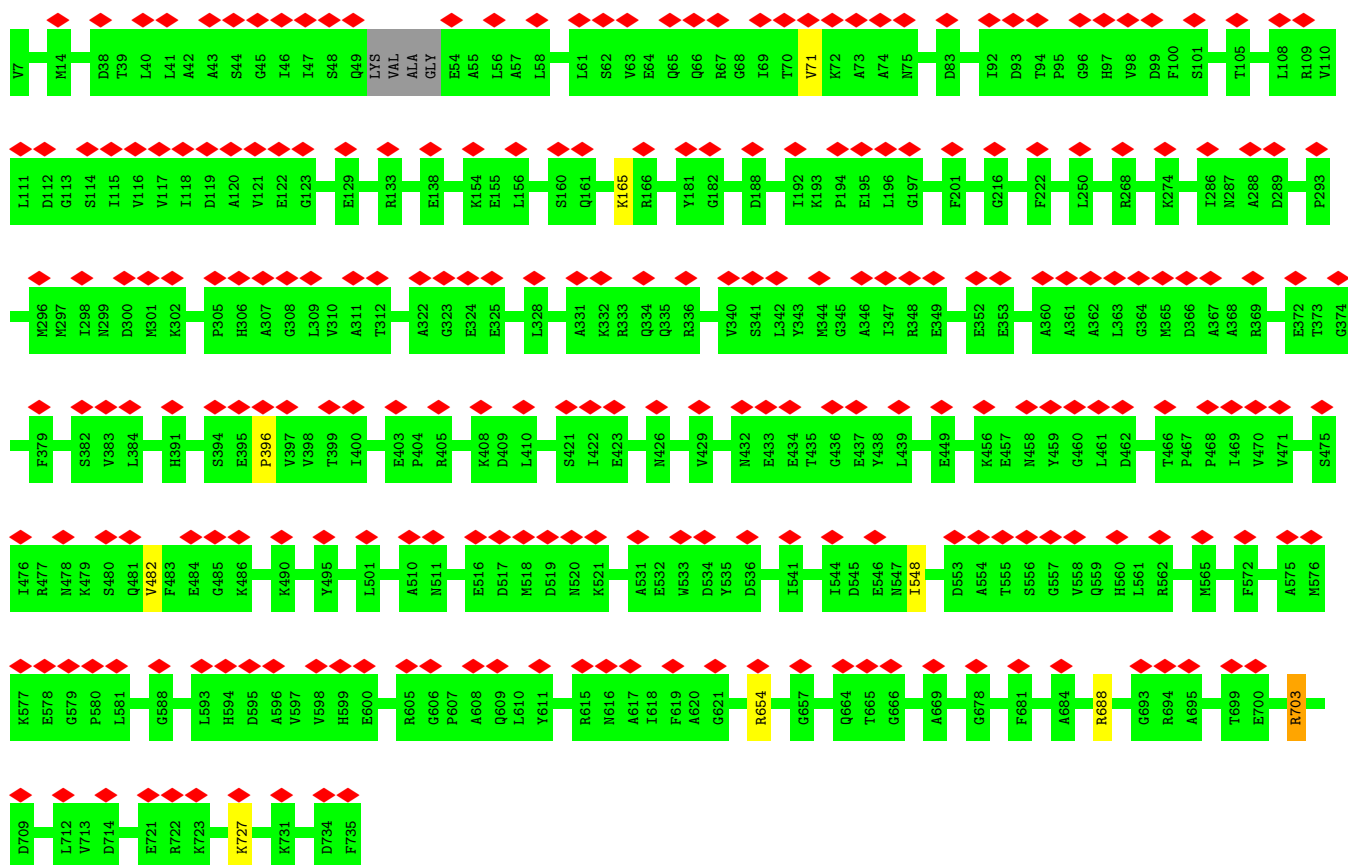
Chain A16S:



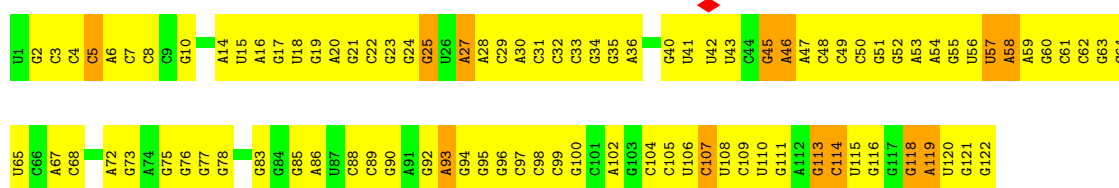


• Molecule 3: Elongation factor 2

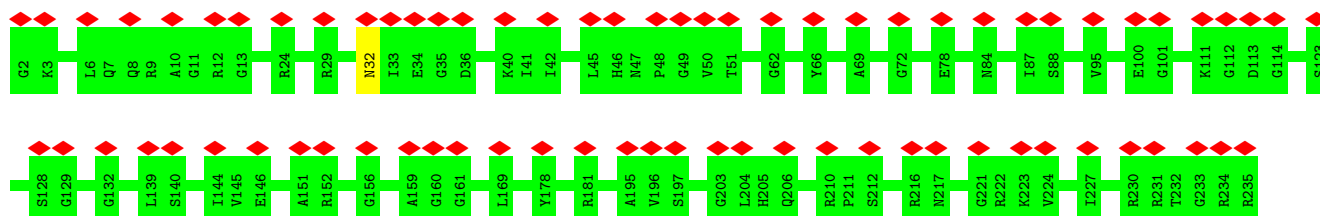




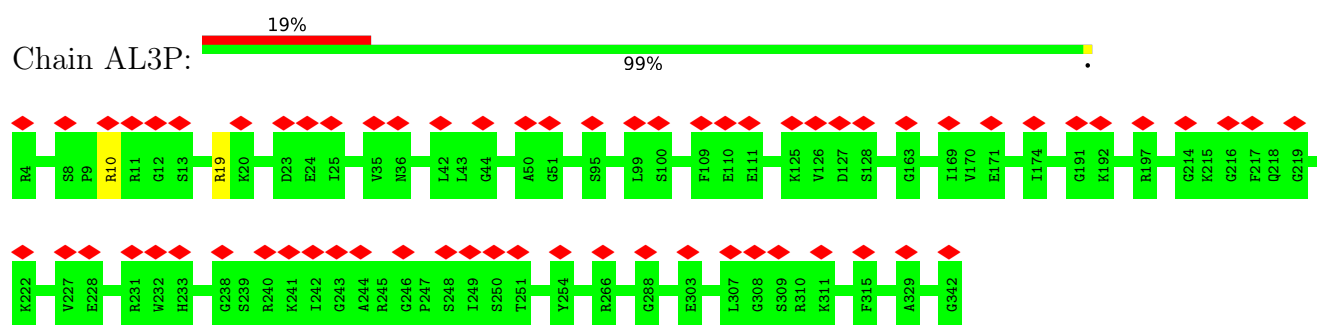
• Molecule 4: 5s rRNA (122-MER)



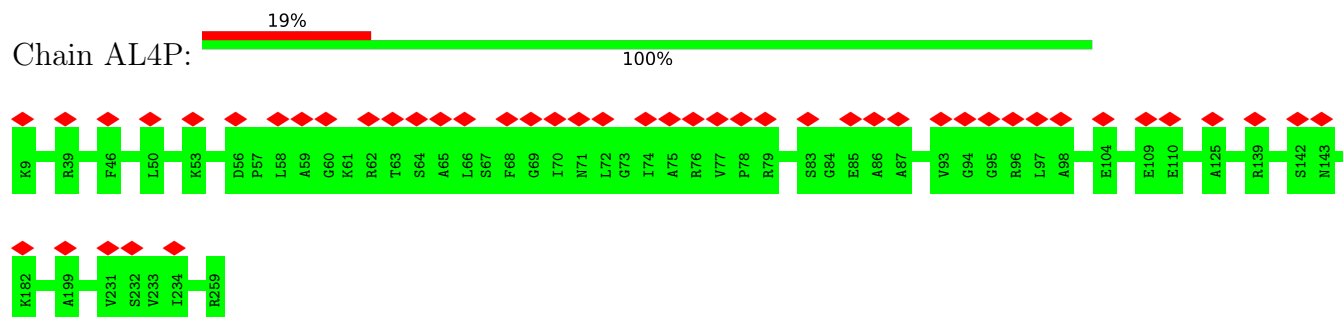
• Molecule 5: 50S ribosomal protein L2



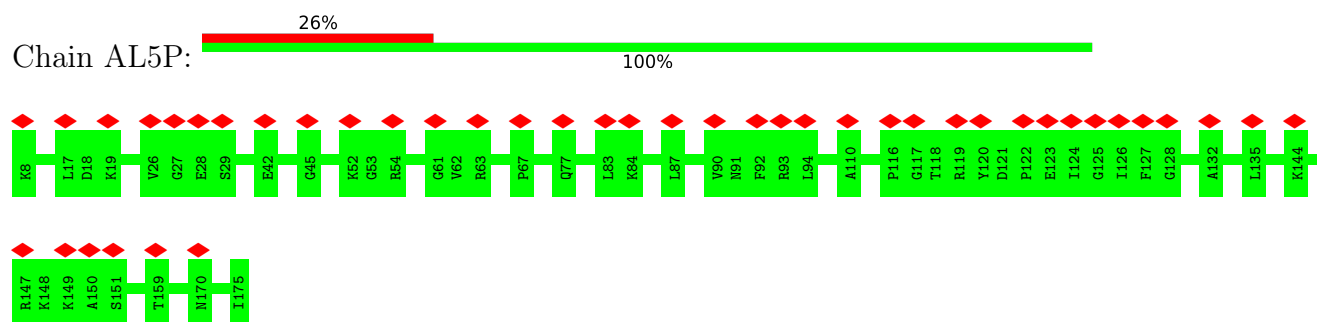
• Molecule 6: 50S ribosomal protein L3



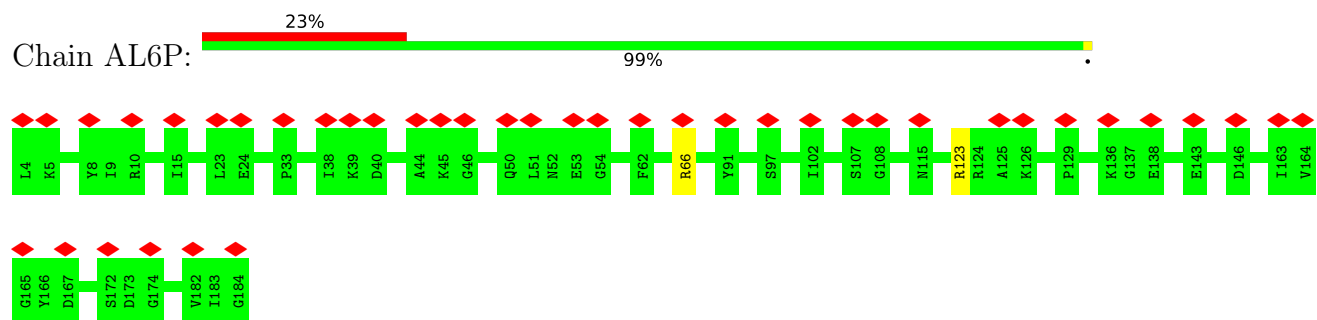
• Molecule 7: 50S ribosomal protein L4



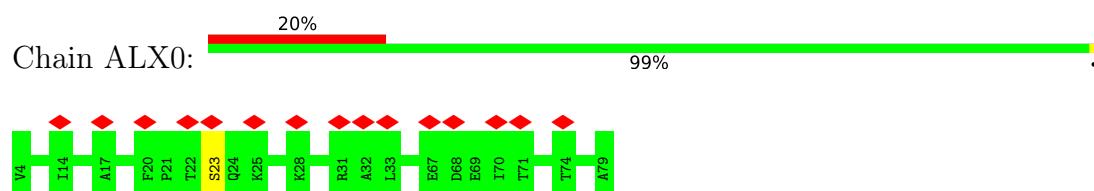
• Molecule 8: 50S ribosomal protein L5



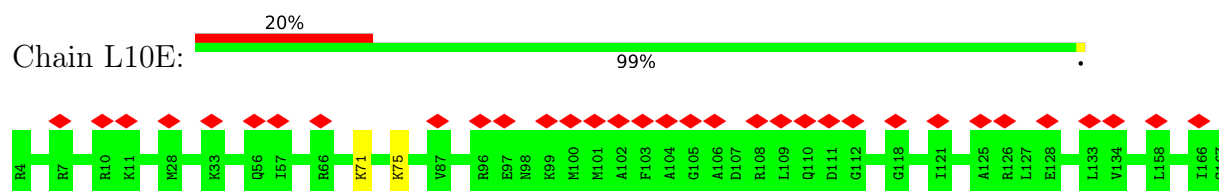
• Molecule 9: 50S ribosomal protein L6



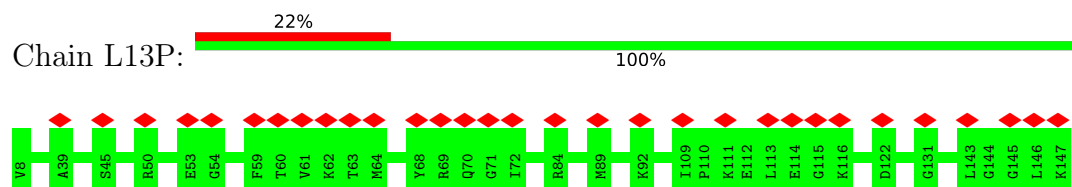
• Molecule 10: 50S ribosomal protein L18Ae



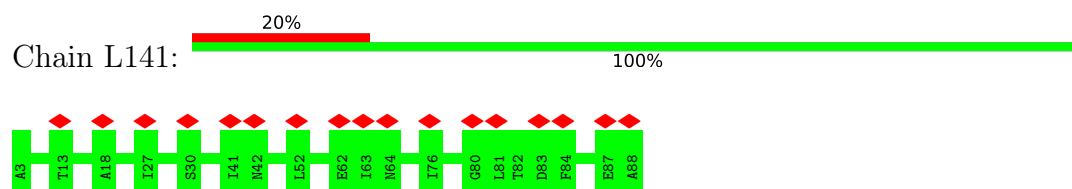
- Molecule 11: 50S ribosomal protein L10e



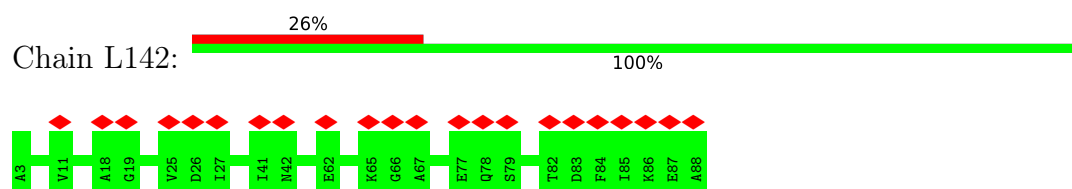
- Molecule 12: 50S ribosomal protein L13



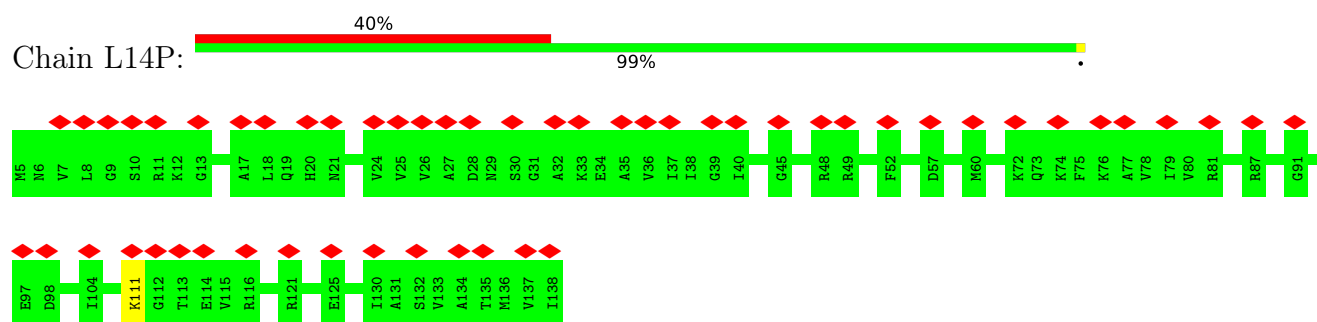
- Molecule 13: 50S ribosomal protein L14e



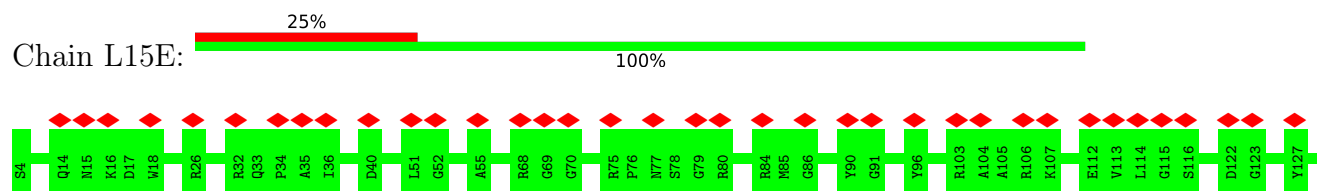
- Molecule 13: 50S ribosomal protein L14e

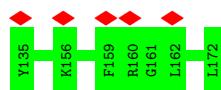


- Molecule 14: 50S ribosomal protein L14



- Molecule 15: 50S ribosomal protein L15e

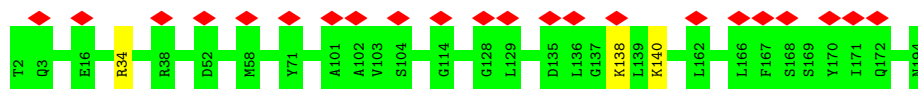




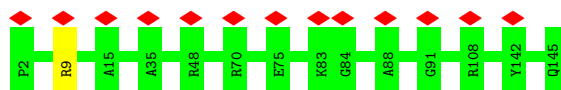
- Molecule 16: 50S ribosomal protein L18e



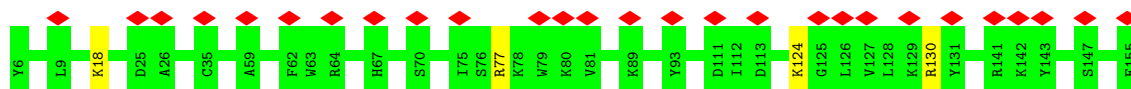
- Molecule 17: 50S ribosomal protein L18



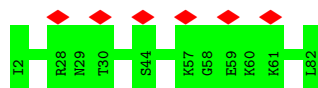
- Molecule 18: 50S ribosomal protein L19e



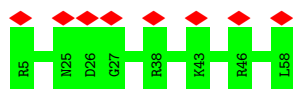
- Molecule 19: 50S ribosomal protein L22



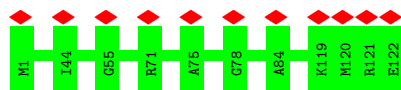
- Molecule 20: 50S ribosomal protein L23



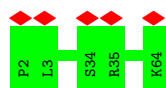
- Molecule 21: 50S ribosomal protein L24e



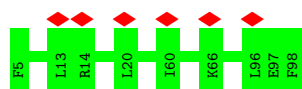
- Molecule 22: 50S ribosomal protein L24



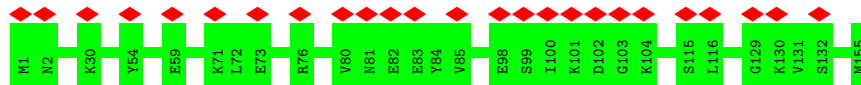
- Molecule 23: 50S ribosomal protein L29



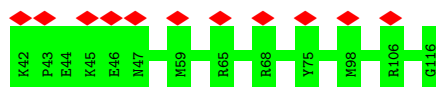
- Molecule 24: 50S ribosomal protein L30e



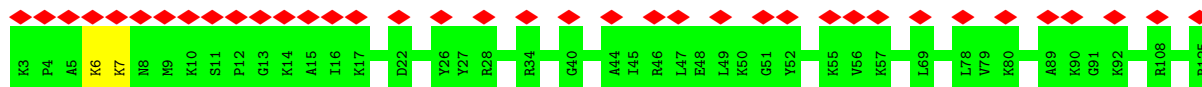
- Molecule 25: 50S ribosomal protein L30



- Molecule 26: 50S ribosomal protein L31e



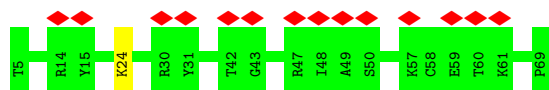
- Molecule 27: 50S ribosomal protein L32e



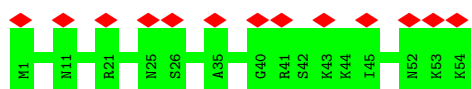
- Molecule 28: 50S ribosomal protein L34e



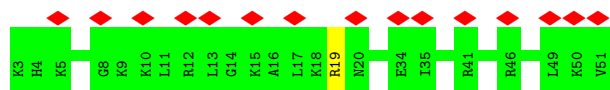
- Molecule 29: 50S ribosomal protein L37Ae



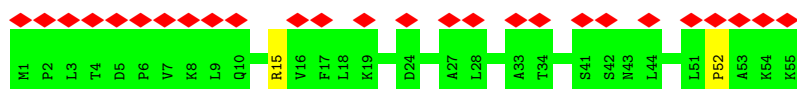
- Molecule 30: 50S ribosomal protein L37e



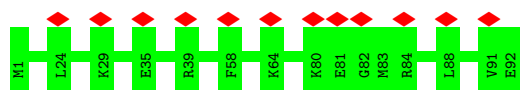
- Molecule 31: 50S ribosomal protein L39e



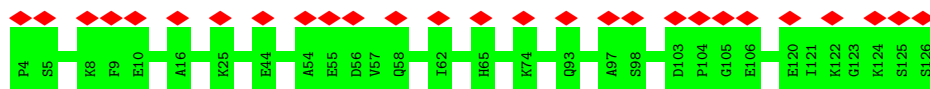
- Molecule 32: 50S ribosomal protein L40E



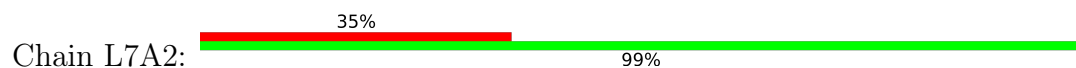
- Molecule 33: 50S ribosomal protein L44e

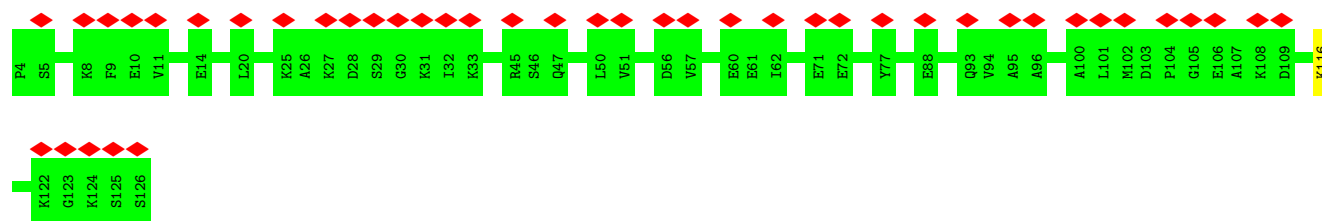


- Molecule 34: 50S ribosomal protein L7Ae

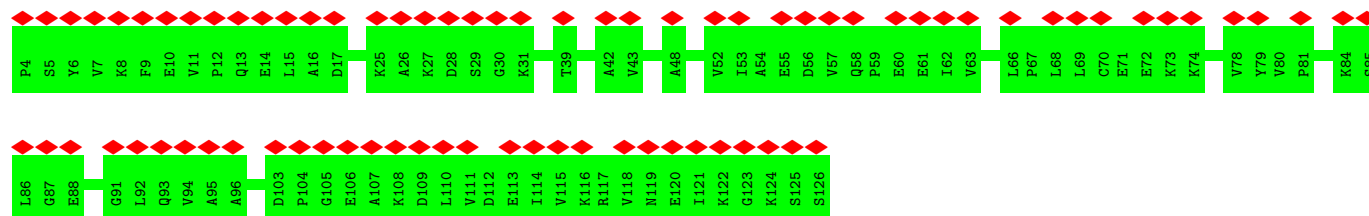


- Molecule 34: 50S ribosomal protein L7Ae

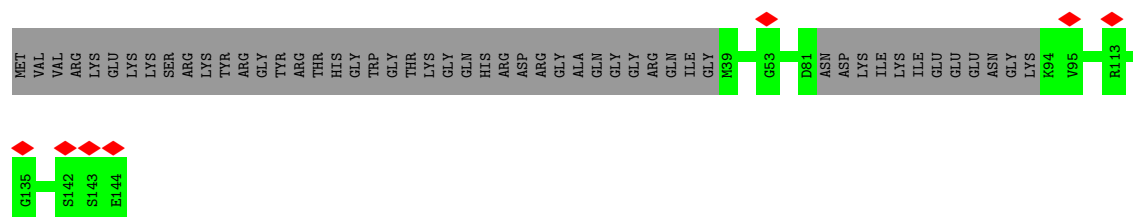




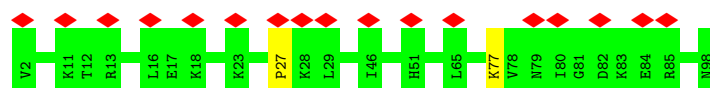
- Molecule 34: 50S ribosomal protein L7Ae



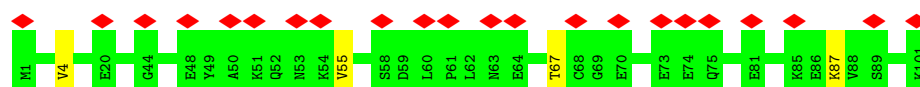
- Molecule 35: 50S ribosomal protein L15



- Molecule 36: 50S ribosomal protein L21e

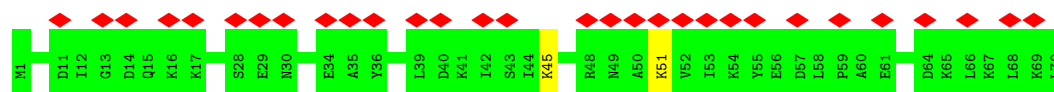


- Molecule 37: DUF2280 domain-containing protein

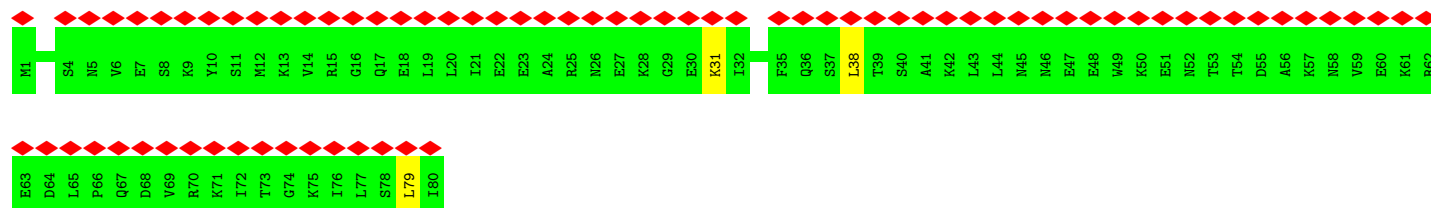


- Molecule 38: Conserved protein

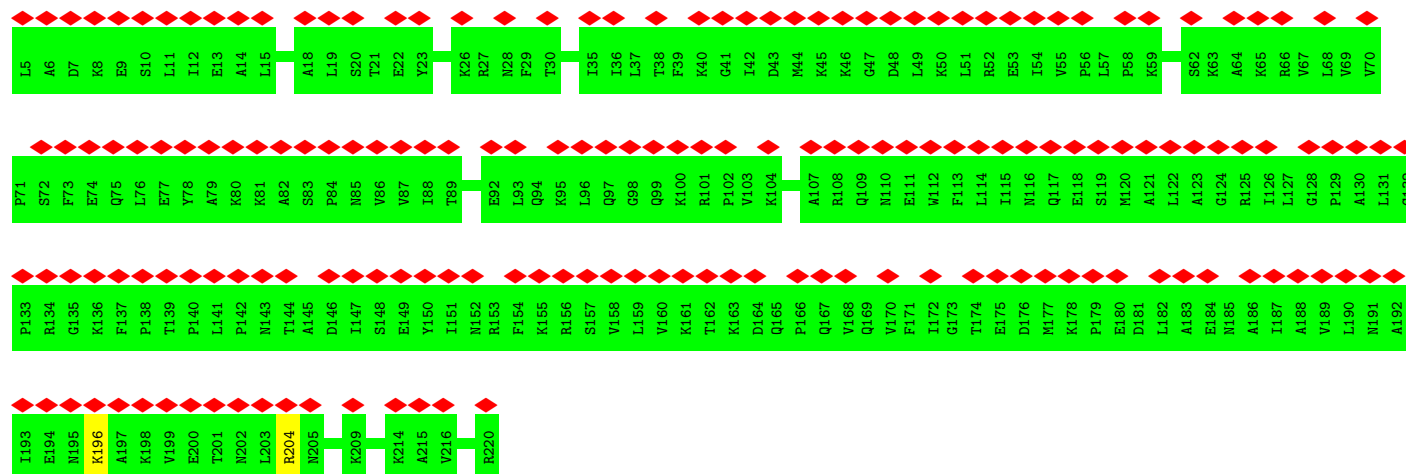
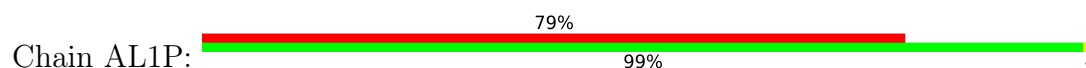




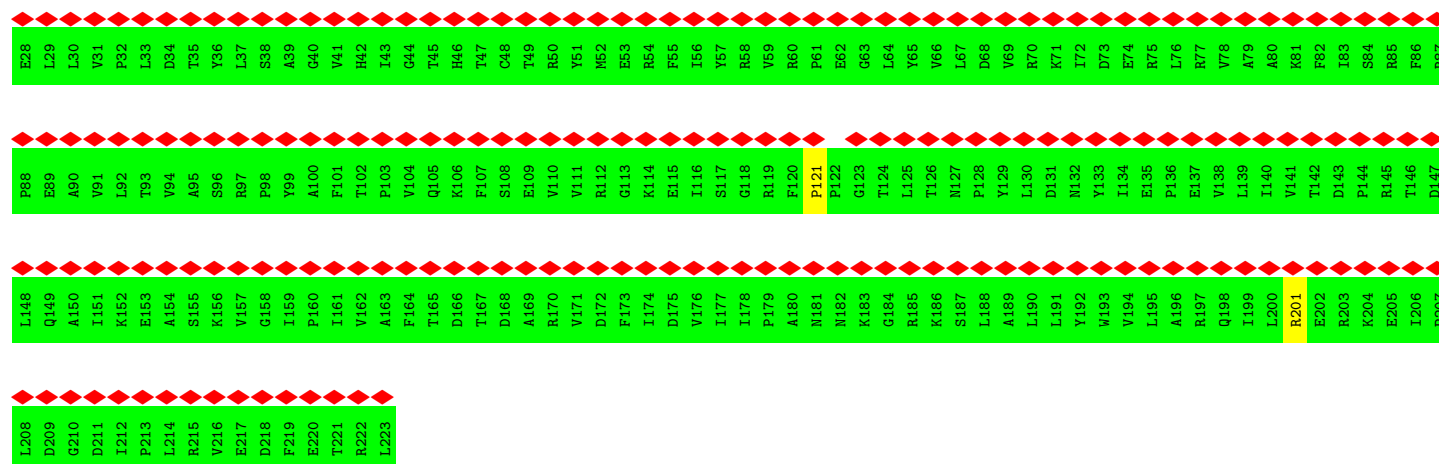
• Molecule 39: 50S ribosomal protein L47A



• Molecule 40: 50S ribosomal protein L1

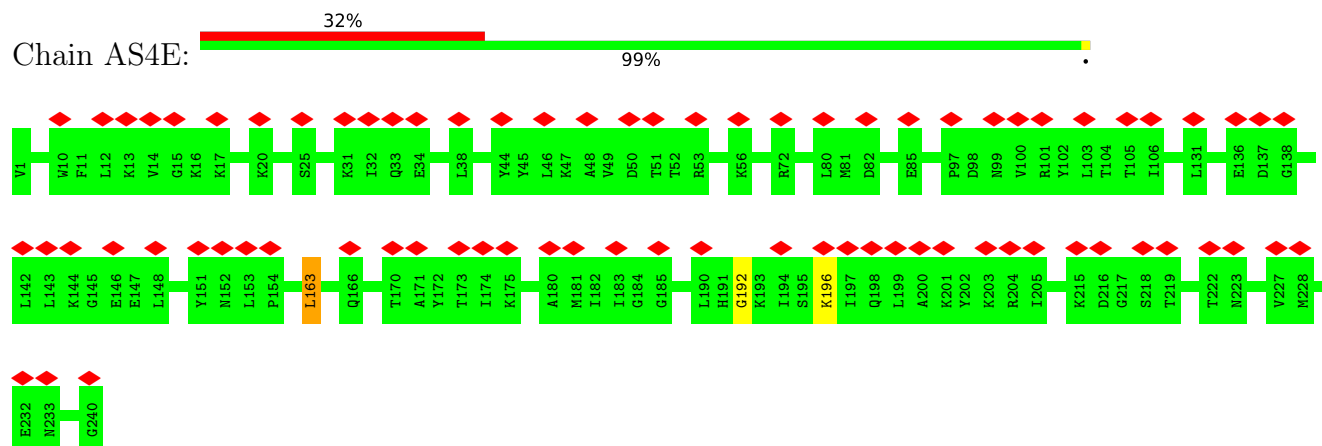


• Molecule 41: 30S ribosomal protein S2



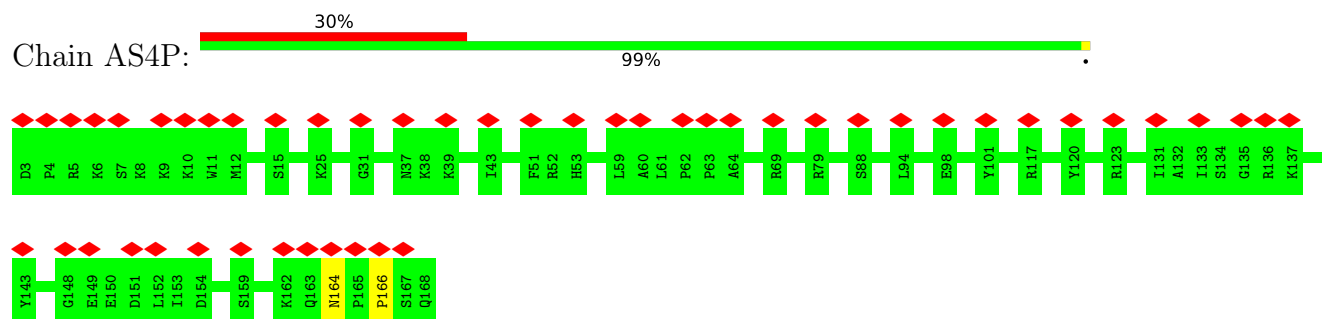
- Molecule 42: 30S ribosomal protein S4e

Chain AS4E:



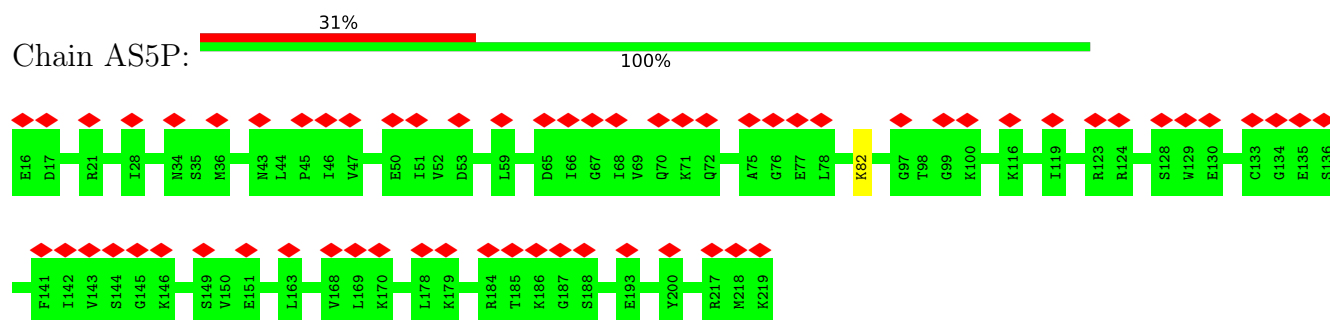
- Molecule 43: 30S ribosomal protein S4

Chain AS4P:



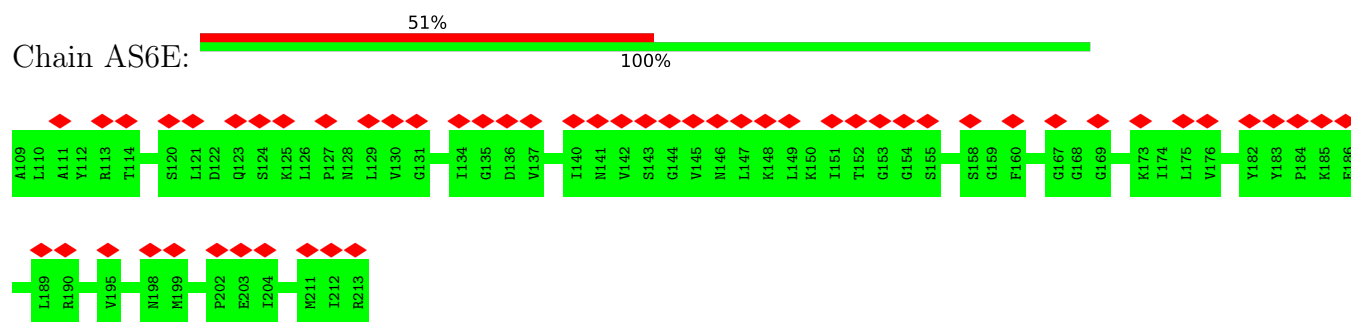
- Molecule 44: 30S ribosomal protein S5

Chain AS5P:

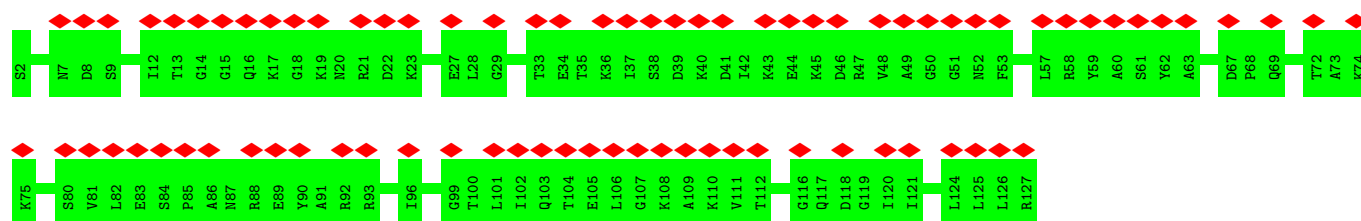


- Molecule 45: 30S ribosomal protein S6e

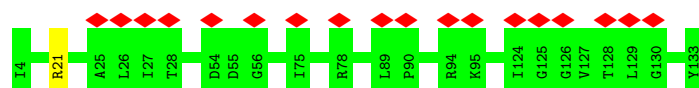
Chain AS6E:



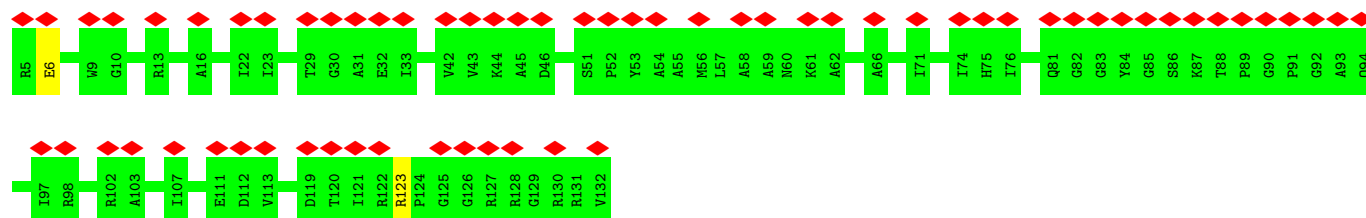
- Molecule 46: 30S ribosomal protein S8e



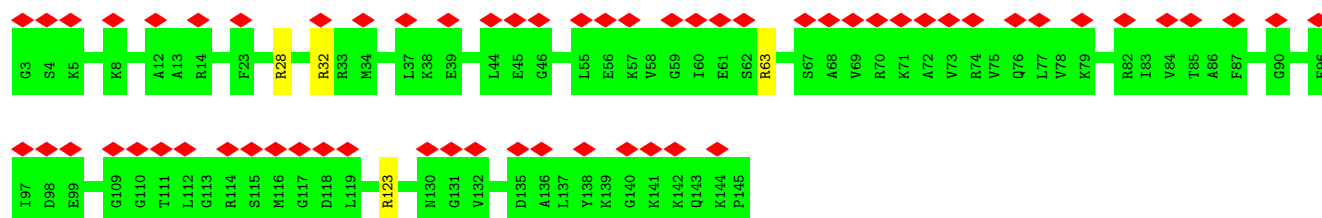
- Molecule 47: 30S ribosomal protein S8



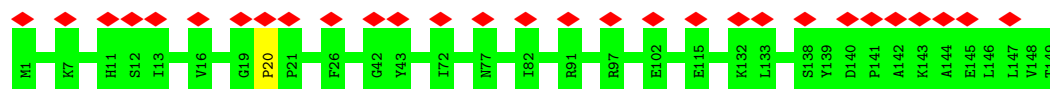
- Molecule 48: 30S ribosomal protein S11



- Molecule 49: 30S ribosomal protein S12

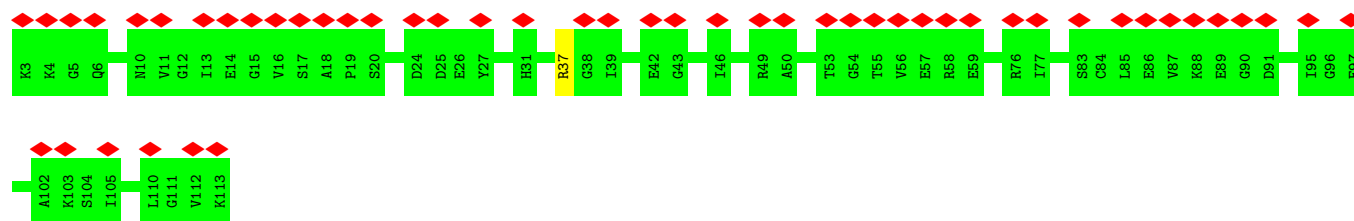


- Molecule 50: 30S ribosomal protein S15

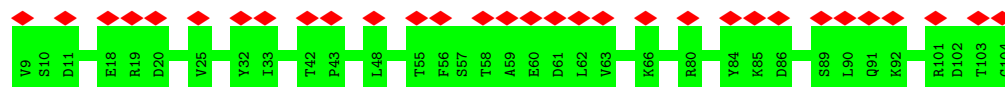


- Molecule 51: 30S ribosomal protein S17

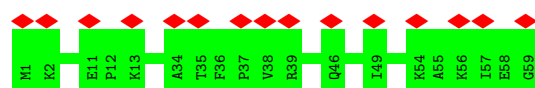




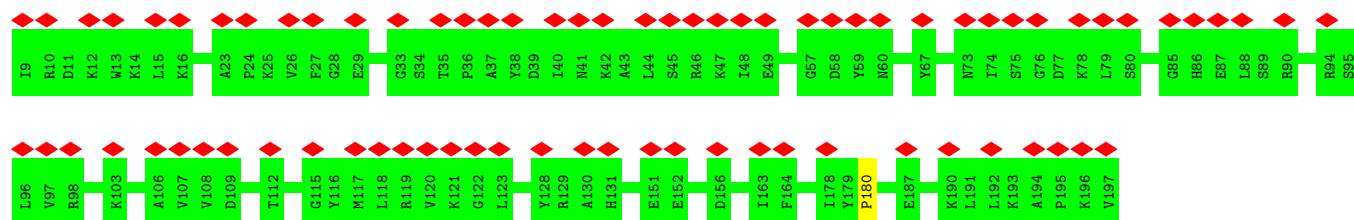
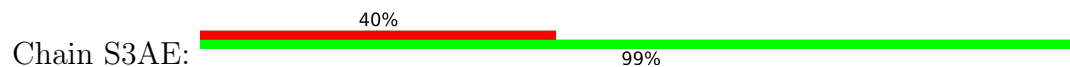
- Molecule 52: 30S ribosomal protein S24e



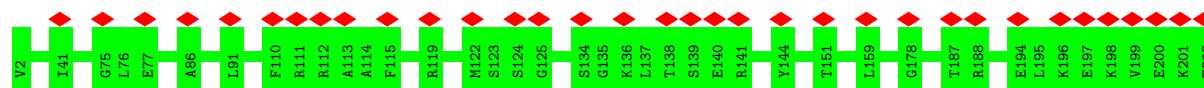
- Molecule 53: 30S ribosomal protein S27e



- Molecule 54: 30S ribosomal protein S3Ae

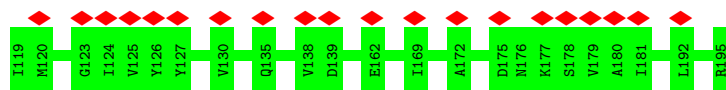


- Molecule 55: 30S ribosomal protein S3

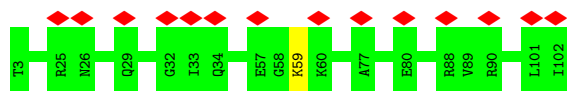


- Molecule 56: 30S ribosomal protein S7

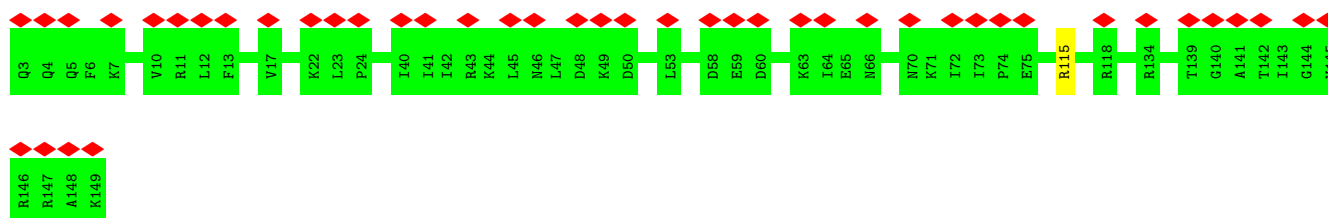




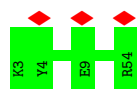
- Molecule 57: 30S ribosomal protein S10



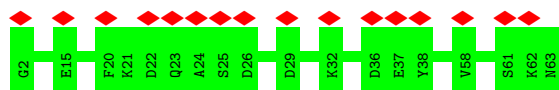
- Molecule 58: 30S ribosomal protein S13



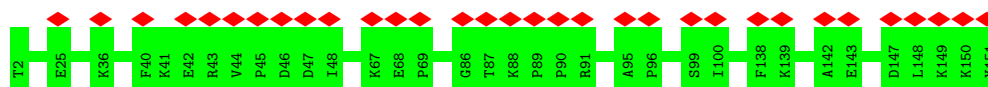
- Molecule 59: 30S ribosomal protein S14 type Z



- Molecule 60: 30S ribosomal protein S17e

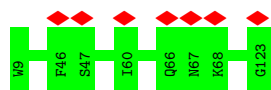


- Molecule 61: 30S ribosomal protein S19e



- Molecule 62: 30S ribosomal protein S19

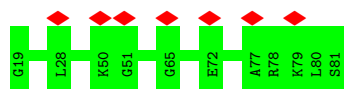




- Molecule 63: 30S ribosomal protein S9



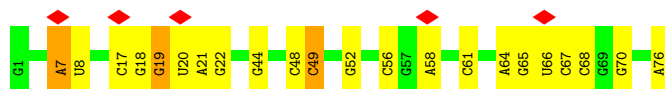
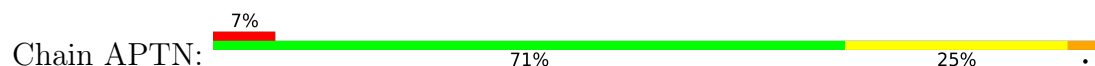
- Molecule 64: 30S ribosomal protein S28e



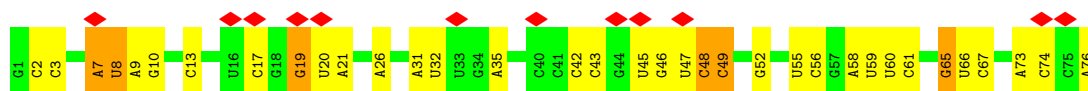
- Molecule 65: 30S ribosomal protein S27ae



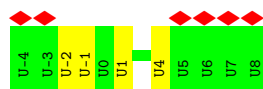
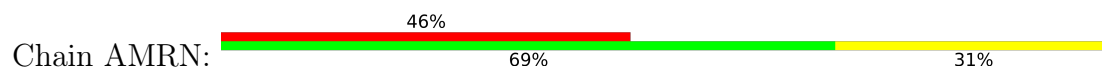
- Molecule 66: tRNA (76-MER)



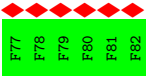
- Molecule 66: tRNA (76-MER)



- Molecule 67: mRNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')



- Molecule 68: PHE-PHE-PHE-PHE-PHE-PHE



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	2780	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	26.7	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.340	Depositor
Minimum map value	-0.241	Depositor
Average map value	0.027	Depositor
Map value standard deviation	0.087	Depositor
Recommended contour level	0.335	Depositor
Map size (Å)	413.06, 413.06, 413.06	wwPDB
Map dimensions	380, 380, 380	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.087, 1.087, 1.087	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A23S	0.47	5/72048 (0.0%)	0.88	108/112407 (0.1%)
2	A16S	0.67	63/35862 (0.2%)	1.26	516/55957 (0.9%)
3	AEFG	0.29	0/5771	0.53	0/7808
4	A5S	0.40	0/2917	0.74	0/4549
5	AL2P	0.30	0/1787	0.56	0/2409
6	AL3P	0.29	0/2758	0.55	0/3727
7	AL4P	0.28	0/1956	0.52	0/2635
8	AL5P	0.29	0/1364	0.57	0/1827
9	AL6P	0.29	0/1450	0.52	0/1949
10	ALX0	0.35	0/638	0.64	0/851
11	L10E	0.30	0/1334	0.58	0/1787
12	L13P	0.28	0/1123	0.56	0/1502
13	L141	0.27	0/673	0.51	0/900
13	L142	0.27	0/673	0.53	0/900
14	L14P	0.30	0/1054	0.56	0/1425
15	L15E	0.30	0/1458	0.59	0/1956
16	L18E	0.29	0/907	0.51	0/1214
17	L18P	0.29	0/1570	0.49	0/2115
18	L19E	0.28	0/1223	0.56	0/1622
19	L22P	0.30	0/1246	0.55	0/1671
20	L23P	0.29	0/655	0.50	0/874
21	L24E	0.31	0/451	0.53	0/599
22	L24P	0.28	0/1000	0.56	0/1329
23	L29P	0.24	0/513	0.52	0/678
24	L30E	0.30	0/738	0.50	0/985
25	L30P	0.31	0/1278	0.56	0/1713
26	L31E	0.29	0/632	0.61	0/837
27	L32E	0.29	0/1027	0.58	0/1366
28	L34E	0.30	0/642	0.70	0/854
29	L37A	0.32	0/542	0.62	0/726
30	L37E	0.33	0/445	0.58	0/585
31	L39E	0.27	0/422	0.59	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	L40E	0.28	0/443	0.63	0/587
33	L44E	0.28	0/763	0.53	0/1008
34	L7A1	0.28	0/946	0.43	0/1272
34	L7A2	0.26	0/946	0.44	0/1272
34	SL7A	0.26	0/946	0.52	0/1272
35	L15P	0.29	0/766	0.50	0/1023
36	L21E	0.30	0/800	0.54	0/1067
37	L45A	0.28	0/824	0.52	0/1094
38	L46A	0.29	0/595	0.51	0/793
39	L47A	0.25	0/652	0.53	1/870 (0.1%)
40	AL1P	0.25	0/1739	0.50	0/2338
41	AS2P	0.28	0/1621	0.56	1/2202 (0.0%)
42	AS4E	0.28	0/1956	0.58	1/2635 (0.0%)
43	AS4P	0.27	0/1399	0.57	0/1883
44	AS5P	0.28	0/1631	0.51	0/2200
45	AS6E	0.28	0/815	0.58	0/1093
46	AS8E	0.27	0/1005	0.57	0/1342
47	AS8P	0.28	0/1046	0.54	0/1410
48	S11P	0.27	0/976	0.61	0/1315
49	S12P	0.28	0/1120	0.59	0/1495
50	S15P	0.27	0/1250	0.55	0/1677
51	S17P	0.28	0/899	0.53	0/1203
52	S24E	0.28	0/769	0.52	0/1034
53	S27E	0.27	0/465	0.48	0/618
54	S3AE	0.28	0/1573	0.53	0/2115
55	AS3P	0.32	0/1599	0.53	0/2147
56	AS7P	0.34	0/1561	0.61	0/2105
57	S10P	0.33	0/840	0.58	0/1132
58	S13P	0.37	0/1221	0.63	0/1634
59	S14P	0.36	0/441	0.62	0/583
60	S17E	0.30	0/523	0.53	0/696
61	S19E	0.32	0/1267	0.56	0/1705
62	S19P	0.34	0/985	0.59	0/1310
63	AS9P	0.34	0/1115	0.58	0/1496
64	S28E	0.31	0/500	0.62	0/669
65	S27A	0.42	0/444	0.73	0/590
66	AETN	0.74	11/1809 (0.6%)	1.79	42/2819 (1.5%)
66	APTn	0.52	3/1809 (0.2%)	1.50	25/2819 (0.9%)
67	AMRN	0.29	0/285	0.95	0/438
68	APTP	0.28	0/72	0.32	0/93
All	All	0.46	82/186573 (0.0%)	0.90	694/275373 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	A16S	0	1
10	ALX0	0	1
28	L34E	0	2
42	AS4E	0	2
43	AS4P	0	1
48	S11P	0	1
50	S15P	0	1
56	AS7P	0	2
65	S27A	0	3
All	All	0	14

All (82) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A16S	381	C	C2-O2	-16.44	1.09	1.24
2	A16S	381	C	N1-C6	-15.46	1.27	1.37
66	AETN	65	G	C2-N2	-10.94	1.23	1.34
2	A16S	381	C	C4-C5	-9.17	1.35	1.43
2	A16S	1145	G	N9-C4	-8.99	1.30	1.38
2	A16S	1091	G	N9-C4	-8.93	1.30	1.38
66	AETN	65	G	N1-C2	-8.52	1.30	1.37
2	A16S	379	G	N1-C2	8.42	1.44	1.37
2	A16S	906	A	N9-C4	-8.41	1.32	1.37
2	A16S	1202	G	N9-C4	-8.31	1.31	1.38
2	A16S	381	C	N3-C4	-8.31	1.28	1.33
2	A16S	906	A	N3-C4	-8.16	1.29	1.34
2	A16S	1012	G	N9-C4	-8.12	1.31	1.38
2	A16S	14	G	N9-C4	-8.11	1.31	1.38
2	A16S	603	G	N9-C4	-8.01	1.31	1.38
2	A16S	622	G	N9-C4	-7.83	1.31	1.38
2	A16S	379	G	N9-C4	-7.82	1.31	1.38
2	A16S	154	G	N9-C4	-7.79	1.31	1.38
2	A16S	370	G	C2-N3	-7.44	1.26	1.32
66	AETN	7	A	N9-C4	-7.30	1.33	1.37
2	A16S	370	G	N3-C4	-7.25	1.30	1.35
2	A16S	242	G	N9-C4	-7.22	1.32	1.38
2	A16S	1168	G	N9-C4	-7.18	1.32	1.38
66	AETN	7	A	C6-N6	7.18	1.39	1.33
2	A16S	1348	G	N9-C4	-7.12	1.32	1.38
66	AETN	49	C	C5-C6	-6.97	1.28	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A16S	1168	G	N3-C4	-6.90	1.30	1.35
2	A16S	360	G	N9-C4	-6.87	1.32	1.38
2	A16S	61	G	N9-C4	-6.79	1.32	1.38
2	A16S	955	C	N1-C2	-6.75	1.33	1.40
2	A16S	370	G	N9-C4	-6.74	1.32	1.38
2	A16S	282	A	N9-C4	-6.62	1.33	1.37
66	AETN	49	C	C2-N3	6.59	1.41	1.35
66	AETN	49	C	N3-C4	-6.58	1.29	1.33
2	A16S	616	G	N7-C5	-6.57	1.35	1.39
66	APTN	7	A	N9-C4	-6.52	1.33	1.37
2	A16S	1263	G	N9-C4	-6.52	1.32	1.38
1	A23S	1179	C	N1-C6	-6.48	1.33	1.37
2	A16S	1012	G	N3-C4	-6.35	1.31	1.35
66	AETN	65	G	N3-C4	-6.25	1.31	1.35
2	A16S	1214	A	N3-C4	-6.21	1.31	1.34
2	A16S	33	A	N9-C4	-6.17	1.34	1.37
2	A16S	1131	G	N9-C8	-6.04	1.33	1.37
2	A16S	1452	G	C5-C6	-6.01	1.36	1.42
2	A16S	1332	A	C5-C6	-5.98	1.35	1.41
66	AETN	7	A	C2-N3	-5.96	1.28	1.33
66	AETN	65	G	C2-N3	-5.95	1.27	1.32
2	A16S	616	G	N3-C4	-5.90	1.31	1.35
2	A16S	1132	C	N1-C2	5.90	1.46	1.40
2	A16S	1192	G	N3-C4	-5.88	1.31	1.35
2	A16S	1192	G	N9-C4	-5.86	1.33	1.38
1	A23S	1318	U	C1'-N1	5.84	1.57	1.48
1	A23S	1179	C	C4-C5	-5.81	1.38	1.43
2	A16S	1319	A	C6-N1	-5.78	1.31	1.35
66	AETN	49	C	N1-C6	-5.76	1.33	1.37
66	APTN	19	G	C6-N1	-5.67	1.35	1.39
2	A16S	52	U	N3-C4	-5.63	1.33	1.38
2	A16S	1332	A	C8-N7	-5.59	1.27	1.31
2	A16S	82	A	N3-C4	-5.56	1.31	1.34
2	A16S	61	G	N7-C5	-5.55	1.35	1.39
2	A16S	567	C	N1-C2	5.50	1.45	1.40
2	A16S	1119	A	C6-N1	-5.50	1.31	1.35
2	A16S	1126	G	N9-C4	-5.50	1.33	1.38
66	APTN	19	G	N1-C2	-5.50	1.33	1.37
1	A23S	1315	U	C1'-N1	5.49	1.56	1.48
2	A16S	1263	G	C8-N7	-5.46	1.27	1.30
2	A16S	1145	G	N3-C4	-5.41	1.31	1.35
1	A23S	1316	A	C1'-N9	-5.41	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A16S	1452	G	N9-C4	-5.29	1.33	1.38
2	A16S	1024	C	N1-C2	-5.25	1.34	1.40
2	A16S	82	A	N9-C4	-5.23	1.34	1.37
2	A16S	1091	G	N3-C4	-5.23	1.31	1.35
2	A16S	716	C	N1-C2	5.20	1.45	1.40
2	A16S	14	G	N3-C4	-5.18	1.31	1.35
2	A16S	1083	C	N1-C6	-5.16	1.34	1.37
2	A16S	1091	G	C2-N3	-5.15	1.28	1.32
2	A16S	1202	G	N3-C4	-5.13	1.31	1.35
2	A16S	603	G	N3-C4	-5.11	1.31	1.35
2	A16S	627	G	N9-C4	-5.09	1.33	1.38
2	A16S	1083	C	C2-O2	-5.06	1.19	1.24
2	A16S	1263	G	N7-C5	-5.04	1.36	1.39
2	A16S	1180	C	N1-C2	-5.03	1.35	1.40

All (694) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	381	C	N1-C2-O2	-58.06	84.06	118.90
66	APTn	19	G	N3-C2-N2	33.20	143.14	119.90
2	A16S	381	C	N3-C2-O2	33.15	145.11	121.90
66	APTn	19	G	N1-C2-N2	-32.36	87.08	116.20
2	A16S	52	U	C5-C4-O4	26.36	141.71	125.90
2	A16S	381	C	C6-N1-C2	-23.75	110.80	120.30
2	A16S	52	U	N3-C4-O4	-22.06	103.96	119.40
2	A16S	381	C	C5-C6-N1	21.47	131.73	121.00
66	AETN	65	G	N1-C2-N3	21.39	136.73	123.90
66	AETN	65	G	N1-C6-O6	-19.75	108.05	119.90
66	AETN	7	A	C6-N1-C2	19.55	130.33	118.60
66	AETN	66	U	C5-C4-O4	-18.79	114.63	125.90
66	AETN	7	A	C5-C6-N6	17.80	137.94	123.70
2	A16S	1024	C	C6-N1-C2	-16.61	113.66	120.30
2	A16S	381	C	N3-C4-C5	-16.52	115.29	121.90
66	APTn	19	G	C5-C6-O6	16.33	138.40	128.60
66	APTn	56	C	N1-C2-O2	16.28	128.67	118.90
66	AETN	65	G	C5-C6-O6	15.62	137.97	128.60
66	AETN	65	G	N1-C2-N2	-15.55	102.21	116.20
66	AETN	65	G	C6-N1-C2	-15.54	115.78	125.10
2	A16S	1082	C	C6-N1-C2	-15.51	114.10	120.30
2	A16S	1023	C	C6-N1-C2	-15.48	114.11	120.30
66	AETN	66	U	N3-C4-O4	15.14	130.00	119.40
2	A16S	52	U	C2-N3-C4	14.47	135.68	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	1332	A	N9-C4-C5	-14.46	100.01	105.80
66	AETN	49	C	C4-C5-C6	14.21	124.50	117.40
66	AETN	65	G	N9-C4-C5	14.12	111.05	105.40
66	AETN	49	C	N1-C2-O2	-14.01	110.49	118.90
2	A16S	1083	C	C6-N1-C2	-14.01	114.70	120.30
66	AETN	7	A	N3-C4-N9	-13.97	116.22	127.40
2	A16S	1090	U	N3-C2-O2	-13.23	112.94	122.20
2	A16S	1452	G	C4-C5-N7	13.20	116.08	110.80
66	AETN	7	A	N1-C6-N6	-13.18	110.69	118.60
2	A16S	379	G	N3-C4-C5	13.17	135.18	128.60
66	APTN	19	G	C2-N3-C4	-13.02	105.39	111.90
2	A16S	1091	G	N3-C4-C5	13.01	135.10	128.60
1	A23S	246	C	N1-C2-O2	12.92	126.65	118.90
2	A16S	366	C	C2-N1-C1'	12.87	132.95	118.80
2	A16S	1180	C	C6-N1-C2	-12.84	115.16	120.30
2	A16S	1012	G	N3-C4-N9	-12.79	118.32	126.00
66	AETN	7	A	C5-C6-N1	-12.67	111.37	117.70
2	A16S	25	C	C6-N1-C2	-12.63	115.25	120.30
2	A16S	1364	C	N1-C2-O2	12.63	126.48	118.90
2	A16S	370	G	N3-C4-N9	-12.58	118.45	126.00
66	AETN	7	A	C6-C5-N7	12.40	140.98	132.30
2	A16S	57	C	C6-N1-C2	-12.33	115.37	120.30
66	APTN	19	G	N1-C6-O6	-12.31	112.51	119.90
2	A16S	717	C	C6-N1-C2	-12.14	115.44	120.30
2	A16S	144	C	C6-N1-C2	-12.12	115.45	120.30
66	APTN	56	C	N3-C2-O2	-12.05	113.47	121.90
2	A16S	379	G	N3-C4-N9	-11.90	118.86	126.00
2	A16S	568	C	C6-N1-C2	-11.89	115.54	120.30
2	A16S	1192	G	N3-C2-N2	-11.88	111.58	119.90
1	A23S	469	G	N9-C4-C5	-11.79	100.69	105.40
66	AETN	7	A	N1-C2-N3	-11.75	123.43	129.30
66	AETN	49	C	N3-C2-O2	11.74	130.12	121.90
2	A16S	1133	C	C6-N1-C2	-11.66	115.64	120.30
66	AETN	7	A	O4'-C1'-N9	11.63	117.50	108.20
2	A16S	1192	G	N3-C4-N9	-11.47	119.12	126.00
2	A16S	1091	G	N3-C4-N9	-11.42	119.15	126.00
2	A16S	354	C	C6-N1-C2	-11.41	115.73	120.30
66	AETN	7	A	C4-N9-C1'	-11.40	105.78	126.30
66	AETN	7	A	C8-N9-C1'	11.25	147.96	127.70
2	A16S	1132	C	C2-N1-C1'	11.19	131.10	118.80
2	A16S	603	G	N3-C4-N9	-11.16	119.30	126.00
2	A16S	52	U	N1-C2-N3	-11.12	108.23	114.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	14	G	N3-C4-N9	-11.09	119.34	126.00
2	A16S	906	A	N1-C2-N3	11.09	134.84	129.30
2	A16S	1145	G	N3-C4-N9	-11.06	119.36	126.00
2	A16S	1341	U	N3-C2-O2	-11.04	114.47	122.20
2	A16S	1145	G	N3-C4-C5	10.99	134.09	128.60
1	A23S	255	A	OP2-P-O3'	-10.98	81.05	105.20
1	A23S	1179	C	N1-C2-O2	10.97	125.48	118.90
2	A16S	381	C	C2-N3-C4	10.95	125.37	119.90
2	A16S	1082	C	C2-N1-C1'	10.93	130.82	118.80
2	A16S	1091	G	C2-N3-C4	-10.71	106.55	111.90
1	A23S	469	G	C4-C5-N7	10.69	115.08	110.80
2	A16S	242	G	N3-C4-C5	10.69	133.94	128.60
2	A16S	154	G	N3-C4-C5	10.62	133.91	128.60
2	A16S	1168	G	N3-C4-N9	-10.59	119.65	126.00
2	A16S	1319	A	N1-C6-N6	-10.56	112.26	118.60
2	A16S	1452	G	N9-C4-C5	-10.53	101.19	105.40
2	A16S	14	G	N3-C4-C5	10.50	133.85	128.60
66	AETN	7	A	N9-C4-C5	10.49	110.00	105.80
1	A23S	469	G	N3-C4-N9	10.48	132.29	126.00
2	A16S	603	G	N3-C4-C5	10.42	133.81	128.60
66	AETN	65	G	C4-C5-N7	-10.35	106.66	110.80
2	A16S	1168	G	C2-N3-C4	-10.35	106.73	111.90
2	A16S	1145	G	C2-N3-C4	-10.25	106.78	111.90
1	A23S	469	G	C6-C5-N7	-10.20	124.28	130.40
1	A23S	469	G	C8-N9-C1'	-10.19	113.75	127.00
2	A16S	906	A	N9-C4-C5	10.19	109.88	105.80
2	A16S	1132	C	N1-C2-O2	10.18	125.01	118.90
2	A16S	603	G	C2-N3-C4	-10.13	106.83	111.90
2	A16S	1012	G	N3-C4-C5	10.11	133.65	128.60
2	A16S	1263	G	C2-N3-C4	-10.08	106.86	111.90
2	A16S	892	G	C4-C5-N7	10.06	114.83	110.80
2	A16S	475	A	O5'-P-OP2	10.04	122.75	110.70
2	A16S	154	G	N3-C4-N9	-10.03	119.98	126.00
2	A16S	892	G	C6-C5-N7	-10.03	124.38	130.40
2	A16S	1012	G	C2-N3-C4	-10.03	106.89	111.90
2	A16S	1202	G	N3-C4-C5	10.01	133.60	128.60
2	A16S	14	G	C2-N3-C4	-9.98	106.91	111.90
66	AETN	7	A	N3-C4-C5	9.97	133.78	126.80
2	A16S	1082	C	N3-C2-O2	-9.94	114.94	121.90
66	AETN	49	C	N3-C4-N4	9.93	124.95	118.00
2	A16S	366	C	C6-N1-C1'	-9.90	108.92	120.80
2	A16S	61	G	C2-N3-C4	-9.89	106.96	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	AETN	65	G	C8-N9-C4	-9.87	102.45	106.40
2	A16S	1332	A	C4-C5-N7	9.85	115.62	110.70
1	A23S	246	C	C2-N1-C1'	9.82	129.60	118.80
66	APTN	19	G	N1-C2-N3	9.80	129.78	123.90
1	A23S	1179	C	C6-N1-C2	-9.75	116.40	120.30
1	A23S	255	A	OP1-P-O3'	-9.73	83.79	105.20
1	A23S	246	C	C6-N1-C1'	-9.67	109.19	120.80
2	A16S	1214	A	N9-C4-C5	9.62	109.65	105.80
2	A16S	1119	A	N1-C6-N6	-9.58	112.85	118.60
2	A16S	1093	U	C5-C4-O4	-9.56	120.16	125.90
2	A16S	716	C	C2-N1-C1'	9.55	129.31	118.80
2	A16S	381	C	C2-N1-C1'	9.46	129.21	118.80
2	A16S	616	G	C2-N3-C4	-9.46	107.17	111.90
66	AETN	7	A	C4-C5-C6	-9.45	112.28	117.00
2	A16S	567	C	C2-N1-C1'	9.45	129.19	118.80
1	A23S	2290	C	N1-C2-O2	9.43	124.56	118.90
2	A16S	363	G	C5-C6-O6	9.36	134.22	128.60
2	A16S	1369	C	N1-C2-O2	9.35	124.51	118.90
66	APTN	7	A	N3-C4-N9	-9.32	119.94	127.40
2	A16S	622	G	C2-N3-C4	-9.31	107.24	111.90
2	A16S	370	G	N9-C4-C5	9.26	109.10	105.40
1	A23S	1625	C	O4'-C1'-N1	9.25	115.60	108.20
1	A23S	469	G	C4-N9-C1'	9.21	138.47	126.50
2	A16S	1364	C	N3-C2-O2	-9.21	115.45	121.90
1	A23S	1179	C	C2-N1-C1'	9.20	128.92	118.80
2	A16S	370	G	C8-N9-C4	-9.17	102.73	106.40
2	A16S	1348	G	N3-C4-C5	9.15	133.18	128.60
2	A16S	112	U	N3-C4-O4	9.14	125.80	119.40
2	A16S	1202	G	C2-N3-C4	-9.12	107.34	111.90
2	A16S	622	G	N3-C4-C5	9.06	133.13	128.60
2	A16S	955	C	N1-C2-O2	-9.05	113.47	118.90
2	A16S	381	C	N3-C4-N4	9.02	124.32	118.00
2	A16S	622	G	N3-C4-N9	-8.97	120.62	126.00
2	A16S	1168	G	N1-C2-N3	8.96	129.27	123.90
2	A16S	1332	A	N3-C4-N9	8.95	134.56	127.40
2	A16S	242	G	C2-N3-C4	-8.93	107.44	111.90
2	A16S	1132	C	C6-N1-C1'	-8.91	110.11	120.80
2	A16S	154	G	C2-N3-C4	-8.88	107.46	111.90
2	A16S	215	A	N1-C6-N6	8.82	123.89	118.60
2	A16S	484	U	C4-C5-C6	8.82	124.99	119.70
2	A16S	1202	G	N3-C4-N9	-8.81	120.71	126.00
1	A23S	2641	C	N3-C2-O2	-8.80	115.74	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	1090	U	N1-C2-N3	8.77	120.16	114.90
2	A16S	1332	A	C6-C5-N7	-8.68	126.23	132.30
2	A16S	1024	C	C6-N1-C1'	8.66	131.19	120.80
2	A16S	360	G	C2-N3-C4	-8.63	107.58	111.90
2	A16S	892	G	N9-C4-C5	-8.63	101.95	105.40
2	A16S	1332	A	C8-N9-C4	8.62	109.25	105.80
2	A16S	716	C	N1-C2-O2	8.62	124.07	118.90
2	A16S	1192	G	N9-C4-C5	8.60	108.84	105.40
2	A16S	1180	C	C6-N1-C1'	8.58	131.09	120.80
2	A16S	366	C	C6-N1-C2	-8.53	116.89	120.30
2	A16S	370	G	C2-N3-C4	-8.52	107.64	111.90
2	A16S	360	G	N3-C4-C5	8.48	132.84	128.60
2	A16S	1319	A	C5-C6-N6	8.47	130.48	123.70
2	A16S	52	U	C4-C5-C6	-8.45	114.63	119.70
2	A16S	215	A	C5-C6-N6	-8.43	116.95	123.70
2	A16S	353	C	N1-C2-O2	8.38	123.93	118.90
2	A16S	906	A	C2-N3-C4	-8.38	106.41	110.60
2	A16S	57	C	N1-C2-N3	8.35	125.04	119.20
2	A16S	57	C	N3-C2-O2	-8.30	116.09	121.90
2	A16S	1497	C	C2-N1-C1'	8.29	127.92	118.80
2	A16S	61	G	N3-C4-C5	8.29	132.74	128.60
2	A16S	1451	A	N1-C2-N3	8.28	133.44	129.30
2	A16S	1179	C	C2-N1-C1'	8.27	127.90	118.80
2	A16S	1263	G	N3-C4-C5	8.27	132.74	128.60
2	A16S	1452	G	C5-C6-O6	-8.23	123.66	128.60
2	A16S	369	G	C4-C5-N7	8.22	114.09	110.80
2	A16S	1024	C	N1-C2-N3	8.22	124.95	119.20
2	A16S	1093	U	N3-C4-O4	8.21	125.14	119.40
2	A16S	1083	C	N1-C2-N3	8.20	124.94	119.20
2	A16S	616	G	C5-C6-N1	-8.19	107.41	111.50
2	A16S	567	C	N1-C2-O2	8.19	123.81	118.90
2	A16S	906	A	N3-C4-N9	-8.09	120.93	127.40
1	A23S	964	C	C2-N1-C1'	8.06	127.66	118.80
2	A16S	1370	G	C4-N9-C1'	-8.05	116.04	126.50
1	A23S	1179	C	C5-C6-N1	8.04	125.02	121.00
2	A16S	936	G	C4-N9-C1'	-8.02	116.08	126.50
2	A16S	495	G	O4'-C1'-N9	8.01	114.61	108.20
66	APTn	7	A	N9-C4-C5	8.01	109.00	105.80
2	A16S	363	G	N3-C4-N9	-8.01	121.19	126.00
2	A16S	354	C	C5-C6-N1	8.00	125.00	121.00
66	AETn	49	C	N3-C4-C5	-7.99	118.70	121.90
2	A16S	1185	C	C2-N1-C1'	7.97	127.56	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	921	U	N1-C2-N3	7.95	119.67	114.90
2	A16S	61	G	C5-N7-C8	-7.95	100.33	104.30
2	A16S	113	G	O4'-C1'-N9	7.93	114.54	108.20
2	A16S	892	G	N3-C2-N2	7.92	125.45	119.90
1	A23S	1179	C	N3-C2-O2	-7.91	116.36	121.90
66	AETN	7	A	C4-C5-N7	-7.91	106.75	110.70
2	A16S	1023	C	N3-C2-O2	-7.91	116.36	121.90
1	A23S	1683	G	N3-C4-N9	-7.89	121.26	126.00
66	AETN	65	G	O4'-C1'-N9	7.89	114.51	108.20
1	A23S	1802	C	C2-N1-C1'	7.88	127.47	118.80
2	A16S	1214	A	C8-N9-C4	-7.86	102.66	105.80
2	A16S	1024	C	C5-C6-N1	7.83	124.91	121.00
1	A23S	2265	C	N1-C2-O2	7.80	123.58	118.90
2	A16S	616	G	C8-N9-C4	-7.80	103.28	106.40
66	AETN	65	G	C6-C5-N7	7.77	135.06	130.40
2	A16S	1452	G	C5-N7-C8	-7.74	100.43	104.30
2	A16S	568	C	C6-N1-C1'	7.74	130.09	120.80
2	A16S	353	C	C2-N1-C1'	7.74	127.31	118.80
1	A23S	1683	G	N1-C6-O6	-7.74	115.26	119.90
2	A16S	1497	C	N1-C2-O2	7.73	123.54	118.90
2	A16S	248	A	N9-C4-C5	-7.73	102.71	105.80
2	A16S	1082	C	C5-C6-N1	7.72	124.86	121.00
1	A23S	3019	C	N1-C2-O2	7.68	123.51	118.90
1	A23S	1793	C	N3-C2-O2	-7.68	116.52	121.90
66	APTN	56	C	C2-N3-C4	7.68	123.74	119.90
1	A23S	1457	U	C2-N1-C1'	7.68	126.91	117.70
2	A16S	242	G	N3-C4-N9	-7.68	121.39	126.00
2	A16S	370	G	N3-C4-C5	7.68	132.44	128.60
2	A16S	717	C	C5-C6-N1	7.67	124.84	121.00
2	A16S	1132	C	N3-C2-O2	-7.67	116.53	121.90
2	A16S	1283	C	C6-N1-C2	-7.67	117.23	120.30
2	A16S	1126	G	C5-C6-O6	7.66	133.20	128.60
1	A23S	1683	G	C5-C6-O6	7.62	133.18	128.60
2	A16S	1126	G	N1-C6-O6	-7.60	115.34	119.90
66	AETN	66	U	C2-N1-C1'	7.58	126.80	117.70
2	A16S	1465	G	C4-N9-C1'	7.58	136.35	126.50
2	A16S	1369	C	N3-C2-O2	-7.58	116.59	121.90
2	A16S	370	G	N3-C2-N2	-7.58	114.60	119.90
1	A23S	469	G	N3-C2-N2	7.56	125.19	119.90
2	A16S	1119	A	C5-C6-N6	7.52	129.72	123.70
2	A16S	1180	C	N1-C2-N3	7.51	124.46	119.20
2	A16S	25	C	C5-C6-N1	7.51	124.75	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	1131	G	N3-C4-N9	7.51	130.50	126.00
2	A16S	1369	C	C2-N1-C1'	7.50	127.05	118.80
2	A16S	1047	U	N1-C2-O2	7.50	128.05	122.80
2	A16S	1168	G	N3-C4-C5	7.48	132.34	128.60
66	APTN	7	A	C2-N3-C4	-7.46	106.87	110.60
2	A16S	370	G	N1-C2-N3	7.45	128.37	123.90
2	A16S	366	C	N1-C2-O2	7.44	123.37	118.90
2	A16S	1129	C	C2-N1-C1'	7.43	126.98	118.80
2	A16S	1047	U	N3-C2-O2	-7.39	117.03	122.20
2	A16S	955	C	C6-N1-C1'	7.37	129.65	120.80
1	A23S	964	C	N1-C2-O2	7.34	123.30	118.90
2	A16S	1093	U	C2-N1-C1'	7.33	126.50	117.70
2	A16S	379	G	C4-N9-C1'	-7.33	116.97	126.50
2	A16S	1192	G	N1-C2-N2	7.32	122.79	116.20
2	A16S	1126	G	C2-N3-C4	-7.30	108.25	111.90
2	A16S	616	G	N7-C8-N9	7.30	116.75	113.10
2	A16S	720	C	C2-N1-C1'	7.30	126.83	118.80
2	A16S	1047	U	C2-N1-C1'	7.30	126.46	117.70
2	A16S	1370	G	C8-N9-C1'	7.30	136.49	127.00
2	A16S	56	C	C2-N1-C1'	7.29	126.82	118.80
2	A16S	144	C	C5-C6-N1	7.29	124.65	121.00
2	A16S	1179	C	N1-C2-O2	7.25	123.25	118.90
1	A23S	1683	G	C8-N9-C1'	7.25	136.42	127.00
2	A16S	716	C	C6-N1-C1'	-7.24	112.12	120.80
2	A16S	112	U	C2-N1-C1'	7.22	126.36	117.70
2	A16S	366	C	C5-C6-N1	7.21	124.61	121.00
2	A16S	1368	C	C6-N1-C2	-7.21	117.42	120.30
1	A23S	256	A	OP1-P-OP2	7.17	130.36	119.60
2	A16S	616	G	N1-C2-N3	7.17	128.20	123.90
66	APTN	49	C	C2-N1-C1'	7.17	126.69	118.80
2	A16S	1187	C	C4-C5-C6	7.15	120.97	117.40
2	A16S	1012	G	C8-N9-C1'	7.14	136.29	127.00
1	A23S	1683	G	C4-N9-C1'	-7.14	117.22	126.50
2	A16S	731	G	O4'-C1'-N9	7.14	113.91	108.20
2	A16S	370	G	C5-C6-O6	7.13	132.88	128.60
2	A16S	567	C	C6-N1-C1'	-7.13	112.24	120.80
2	A16S	1214	A	N1-C6-N6	-7.13	114.32	118.60
66	APTN	56	C	N3-C4-C5	-7.13	119.05	121.90
2	A16S	1202	G	C5-N7-C8	-7.13	100.74	104.30
2	A16S	1131	G	C8-N9-C1'	-7.12	117.75	127.00
2	A16S	543	G	C4-C5-N7	7.11	113.64	110.80
2	A16S	1126	G	N3-C4-N9	-7.09	121.74	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	1288	A	N1-C6-N6	-7.08	114.35	118.60
2	A16S	1348	G	N3-C4-N9	-7.08	121.75	126.00
2	A16S	1319	A	N1-C2-N3	-7.08	125.76	129.30
2	A16S	1288	A	C4-C5-C6	-7.08	113.46	117.00
2	A16S	1341	U	N1-C2-O2	7.08	127.75	122.80
2	A16S	151	C	C6-N1-C1'	7.07	129.28	120.80
2	A16S	89	G	N1-C2-N3	7.05	128.13	123.90
1	A23S	1802	C	N1-C2-O2	7.05	123.13	118.90
2	A16S	1214	A	N1-C2-N3	7.04	132.82	129.30
66	APTN	7	A	C6-C5-N7	7.03	137.22	132.30
2	A16S	1465	G	C8-N9-C1'	-7.02	117.88	127.00
2	A16S	627	G	N3-C4-C5	7.00	132.10	128.60
1	A23S	1626	C	N3-C2-O2	-6.97	117.02	121.90
2	A16S	159	A	N1-C6-N6	-6.96	114.42	118.60
2	A16S	363	G	N1-C6-O6	-6.96	115.72	119.90
66	APTN	7	A	C4-N9-C1'	-6.95	113.79	126.30
2	A16S	953	U	C5-C4-O4	-6.95	121.73	125.90
2	A16S	248	A	C4-C5-N7	6.94	114.17	110.70
2	A16S	1083	C	N3-C4-C5	-6.94	119.12	121.90
2	A16S	1288	A	C5-C6-N1	6.92	121.16	117.70
2	A16S	1126	G	N1-C2-N3	6.91	128.05	123.90
66	AETN	49	C	C2-N1-C1'	6.91	126.39	118.80
2	A16S	730	C	C2-N1-C1'	6.89	126.38	118.80
2	A16S	892	G	N3-C4-N9	6.89	130.13	126.00
2	A16S	1091	G	C5-N7-C8	-6.88	100.86	104.30
2	A16S	603	G	C8-N9-C1'	6.88	135.94	127.00
2	A16S	1192	G	N3-C4-C5	6.88	132.04	128.60
2	A16S	379	G	C8-N9-C1'	6.87	135.93	127.00
66	APTN	7	A	C8-N9-C1'	6.87	140.06	127.70
2	A16S	906	A	C5-C6-N6	6.86	129.19	123.70
1	A23S	1179	C	N3-C4-N4	6.86	122.80	118.00
2	A16S	143	C	N1-C2-O2	6.86	123.02	118.90
2	A16S	1133	C	C5-C6-N1	6.86	124.43	121.00
2	A16S	366	C	N1-C1'-C2'	6.85	122.91	114.00
2	A16S	1187	C	C2-N1-C1'	6.82	126.31	118.80
1	A23S	2290	C	N3-C2-O2	-6.82	117.12	121.90
2	A16S	1049	U	C2-N1-C1'	6.81	125.87	117.70
2	A16S	89	G	C2-N3-C4	-6.81	108.50	111.90
2	A16S	1024	C	N3-C4-C5	-6.81	119.18	121.90
1	A23S	1949	C	N3-C2-O2	-6.79	117.15	121.90
66	APTN	7	A	C5-C6-N6	6.78	129.13	123.70
2	A16S	1192	G	C6-C5-N7	6.76	134.46	130.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	61	G	N3-C4-N9	-6.76	121.94	126.00
1	A23S	1625	C	N3-C2-O2	-6.72	117.20	121.90
2	A16S	1023	C	C2-N1-C1'	6.72	126.19	118.80
2	A16S	57	C	C5-C4-N4	6.71	124.90	120.20
2	A16S	1452	G	N3-C4-C5	6.71	131.95	128.60
2	A16S	52	U	C5-C6-N1	6.70	126.05	122.70
2	A16S	1192	G	C5-C6-O6	6.69	132.61	128.60
1	A23S	3019	C	C2-N1-C1'	6.68	126.15	118.80
2	A16S	1083	C	C5-C4-N4	6.66	124.86	120.20
2	A16S	1093	U	O4'-C1'-N1	6.66	113.53	108.20
2	A16S	366	C	O4'-C1'-N1	6.66	113.53	108.20
2	A16S	1192	G	C8-N9-C1'	6.64	135.63	127.00
2	A16S	1332	A	C5-C6-N6	-6.63	118.39	123.70
2	A16S	379	G	C2-N3-C4	-6.62	108.59	111.90
1	A23S	964	C	N3-C2-O2	-6.61	117.27	121.90
66	AETN	66	U	C6-N1-C1'	-6.61	111.95	121.20
1	A23S	1683	G	N9-C4-C5	6.59	108.03	105.40
2	A16S	61	G	N7-C8-N9	6.58	116.39	113.10
2	A16S	567	C	N3-C2-O2	-6.58	117.29	121.90
2	A16S	14	G	C8-N9-C1'	6.58	135.55	127.00
2	A16S	82	A	C2-N3-C4	-6.57	107.31	110.60
2	A16S	1145	G	C8-N9-C1'	6.57	135.53	127.00
2	A16S	154	G	C8-N9-C1'	6.56	135.53	127.00
2	A16S	369	G	N9-C4-C5	-6.55	102.78	105.40
2	A16S	1012	G	N9-C4-C5	6.55	108.02	105.40
2	A16S	1452	G	C2-N3-C4	-6.54	108.63	111.90
1	A23S	1626	C	C6-N1-C2	-6.53	117.69	120.30
2	A16S	955	C	C6-N1-C2	-6.53	117.69	120.30
2	A16S	360	G	C5-N7-C8	-6.52	101.04	104.30
1	A23S	1918	C	N3-C2-O2	-6.52	117.33	121.90
2	A16S	1168	G	N9-C4-C5	6.52	108.01	105.40
2	A16S	1127	G	N3-C4-N9	-6.51	122.10	126.00
2	A16S	370	G	C8-N9-C1'	6.50	135.45	127.00
42	AS4E	163	LEU	CA-CB-CG	6.49	130.22	115.30
2	A16S	24	C	N1-C2-O2	6.48	122.79	118.90
2	A16S	120	C	N3-C2-O2	-6.48	117.36	121.90
2	A16S	1452	G	C6-C5-N7	-6.48	126.51	130.40
1	A23S	1625	C	C5-C4-N4	6.48	124.73	120.20
2	A16S	622	G	C5-N7-C8	-6.47	101.06	104.30
1	A23S	1435	C	N3-C2-O2	-6.47	117.37	121.90
2	A16S	1319	A	C6-N1-C2	6.47	122.48	118.60
2	A16S	151	C	N1-C2-O2	-6.46	115.02	118.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	716	C	N3-C2-O2	-6.45	117.38	121.90
2	A16S	112	U	C5-C4-O4	-6.45	122.03	125.90
2	A16S	56	C	N1-C2-O2	6.43	122.76	118.90
2	A16S	377	A	N1-C6-N6	6.43	122.46	118.60
2	A16S	1379	U	N1-C2-N3	6.43	118.76	114.90
2	A16S	1214	A	C6-N1-C2	-6.42	114.75	118.60
2	A16S	568	C	N1-C2-N3	6.42	123.69	119.20
2	A16S	354	C	C6-N1-C1'	6.42	128.50	120.80
1	A23S	1683	G	C6-C5-N7	6.41	134.25	130.40
2	A16S	256	U	N3-C2-O2	6.41	126.69	122.20
2	A16S	1131	G	C6-C5-N7	-6.41	126.55	130.40
2	A16S	484	U	N3-C4-O4	6.41	123.89	119.40
2	A16S	494	C	N3-C4-N4	6.41	122.49	118.00
2	A16S	1168	G	C5-C6-O6	6.41	132.44	128.60
2	A16S	1497	C	N3-C2-O2	-6.40	117.42	121.90
2	A16S	256	U	N1-C2-O2	-6.39	118.33	122.80
2	A16S	1364	C	C2-N1-C1'	6.39	125.83	118.80
1	A23S	1178	C	C2-N1-C1'	6.39	125.83	118.80
2	A16S	1012	G	N1-C2-N3	6.39	127.73	123.90
2	A16S	1378	C	N3-C2-O2	-6.39	117.43	121.90
1	A23S	3019	C	N3-C2-O2	-6.38	117.43	121.90
2	A16S	1127	G	C2-N3-C4	-6.38	108.71	111.90
2	A16S	1185	C	N1-C2-O2	6.37	122.72	118.90
2	A16S	1133	C	N1-C2-N3	6.36	123.65	119.20
2	A16S	1131	G	C4-N9-C1'	6.35	134.76	126.50
2	A16S	1023	C	N3-C4-C5	-6.35	119.36	121.90
1	A23S	3017	C	N3-C2-O2	-6.34	117.46	121.90
2	A16S	144	C	C6-N1-C1'	6.33	128.40	120.80
2	A16S	1465	G	N3-C4-C5	-6.33	125.44	128.60
2	A16S	328	U	C2-N1-C1'	6.33	125.29	117.70
2	A16S	1129	C	C6-N1-C1'	-6.32	113.21	120.80
2	A16S	367	C	C6-N1-C2	-6.31	117.78	120.30
2	A16S	25	C	C6-N1-C1'	6.31	128.37	120.80
2	A16S	1023	C	N1-C2-N3	6.30	123.61	119.20
2	A16S	1283	C	N3-C4-C5	-6.30	119.38	121.90
1	A23S	1683	G	O4'-C1'-N9	6.29	113.23	108.20
2	A16S	154	G	C4-N9-C1'	-6.29	118.33	126.50
2	A16S	543	G	N3-C4-C5	6.28	131.74	128.60
2	A16S	1179	C	C6-N1-C1'	-6.28	113.26	120.80
2	A16S	1465	G	N3-C4-N9	6.28	129.77	126.00
2	A16S	568	C	C5-C6-N1	6.28	124.14	121.00
2	A16S	61	G	N1-C6-O6	6.28	123.67	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	1133	C	C6-N1-C1'	6.27	128.32	120.80
2	A16S	159	A	N9-C4-C5	6.26	108.31	105.80
2	A16S	1180	C	C5-C6-N1	6.26	124.13	121.00
2	A16S	1192	G	N1-C6-O6	-6.26	116.14	119.90
1	A23S	246	C	N3-C2-O2	-6.25	117.52	121.90
2	A16S	920	C	N3-C2-O2	-6.25	117.52	121.90
2	A16S	360	G	C4-C5-N7	6.25	113.30	110.80
2	A16S	353	C	C6-N1-C1'	-6.24	113.31	120.80
1	A23S	339	C	N3-C2-O2	-6.24	117.53	121.90
66	APTN	49	C	C6-N1-C1'	-6.23	113.33	120.80
2	A16S	1263	G	N1-C6-O6	6.22	123.63	119.90
2	A16S	1369	C	O4'-C1'-N1	6.22	113.18	108.20
1	A23S	258	C	N3-C2-O2	-6.21	117.55	121.90
2	A16S	1192	G	C4-N9-C1'	-6.21	118.43	126.50
2	A16S	494	C	N3-C4-C5	-6.21	119.42	121.90
2	A16S	731	G	C8-N9-C4	6.20	108.88	106.40
2	A16S	921	U	C6-N1-C2	-6.20	117.28	121.00
2	A16S	1180	C	N1-C2-O2	-6.20	115.18	118.90
2	A16S	936	G	C8-N9-C1'	6.20	135.06	127.00
2	A16S	363	G	N3-C4-C5	6.17	131.68	128.60
2	A16S	353	C	N3-C2-O2	-6.16	117.59	121.90
1	A23S	1683	G	C4-C5-N7	-6.14	108.34	110.80
2	A16S	603	G	C5-N7-C8	-6.14	101.23	104.30
2	A16S	1049	U	N1-C2-O2	6.13	127.09	122.80
2	A16S	1129	C	N1-C2-O2	6.13	122.58	118.90
2	A16S	720	C	C6-N1-C1'	-6.12	113.45	120.80
2	A16S	892	G	N1-C6-O6	6.12	123.57	119.90
1	A23S	602	C	C2-N1-C1'	6.11	125.52	118.80
2	A16S	1179	C	N3-C2-O2	-6.11	117.62	121.90
2	A16S	1348	G	C5-N7-C8	-6.10	101.25	104.30
2	A16S	1499	C	C2-N1-C1'	6.10	125.51	118.80
66	APTN	7	A	N1-C6-N6	-6.09	114.94	118.60
2	A16S	1145	G	C5-N7-C8	-6.09	101.25	104.30
2	A16S	112	U	C4-C5-C6	6.09	123.35	119.70
2	A16S	1090	U	C2-N3-C4	-6.09	123.35	127.00
2	A16S	1452	G	N1-C6-O6	6.08	123.55	119.90
66	AETN	65	G	C2-N3-C4	-6.08	108.86	111.90
66	APTN	7	A	N3-C4-C5	6.08	131.05	126.80
2	A16S	731	G	C4-N9-C1'	-6.07	118.62	126.50
2	A16S	1023	C	C5-C6-N1	6.05	124.03	121.00
2	A16S	143	C	C2-N1-C1'	6.05	125.46	118.80
2	A16S	1370	G	O4'-C1'-N9	6.05	113.04	108.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	906	A	C4-C5-N7	-6.03	107.68	110.70
2	A16S	1192	G	C4-C5-N7	-6.03	108.39	110.80
2	A16S	151	C	C2-N1-C1'	-6.01	112.19	118.80
2	A16S	1452	G	C8-N9-C4	6.00	108.80	106.40
2	A16S	1462	C	C6-N1-C2	-6.00	117.90	120.30
2	A16S	370	G	N7-C8-N9	6.00	116.10	113.10
2	A16S	494	C	C2-N1-C1'	6.00	125.40	118.80
2	A16S	1049	U	N3-C2-O2	-6.00	118.00	122.20
1	A23S	1685	C	N3-C2-O2	-6.00	117.70	121.90
1	A23S	1918	C	N1-C2-O2	5.99	122.50	118.90
2	A16S	1185	C	C6-N1-C1'	-5.99	113.61	120.80
2	A16S	484	U	C2-N1-C1'	5.98	124.88	117.70
2	A16S	1195	G	C4-N9-C1'	5.98	134.27	126.50
2	A16S	1145	G	C4-N9-C1'	-5.97	118.74	126.50
1	A23S	1625	C	C6-N1-C2	-5.96	117.92	120.30
1	A23S	2290	C	C2-N1-C1'	5.96	125.35	118.80
2	A16S	1263	G	C6-C5-N7	-5.96	126.83	130.40
1	A23S	2641	C	N1-C2-O2	5.95	122.47	118.90
2	A16S	360	G	N3-C4-N9	-5.95	122.43	126.00
66	APTN	7	A	N1-C2-N3	5.95	132.27	129.30
2	A16S	215	A	C6-C5-N7	-5.94	128.14	132.30
2	A16S	282	A	C2-N3-C4	-5.94	107.63	110.60
2	A16S	936	G	N9-C1'-C2'	-5.94	105.47	112.00
2	A16S	242	G	C5-N7-C8	-5.93	101.34	104.30
1	A23S	2240	C	N1-C2-O2	5.92	122.45	118.90
1	A23S	1435	C	C6-N1-C2	-5.92	117.93	120.30
2	A16S	955	C	C2-N1-C1'	-5.92	112.29	118.80
2	A16S	82	A	C8-N9-C4	-5.90	103.44	105.80
1	A23S	3017	C	N1-C2-O2	5.90	122.44	118.90
2	A16S	973	U	OP2-P-O3'	5.89	118.17	105.20
2	A16S	1497	C	C6-N1-C2	-5.89	117.94	120.30
2	A16S	1213	C	N3-C2-O2	-5.87	117.79	121.90
2	A16S	24	C	C2-N1-C1'	5.86	125.25	118.80
2	A16S	1090	U	N1-C2-O2	5.85	126.90	122.80
1	A23S	1625	C	C6-N1-C1'	5.85	127.82	120.80
1	A23S	1720	C	N1-C2-O2	5.84	122.41	118.90
1	A23S	1625	C	N1-C2-N3	5.84	123.29	119.20
2	A16S	25	C	N1-C2-N3	5.84	123.29	119.20
2	A16S	1247	C	C2-N1-C1'	5.83	125.21	118.80
2	A16S	1263	G	C4-C5-N7	5.82	113.13	110.80
1	A23S	246	C	O4'-C1'-N1	5.81	112.85	108.20
2	A16S	215	A	N9-C4-C5	-5.81	103.48	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A23S	2265	C	N3-C2-O2	-5.81	117.83	121.90
2	A16S	1012	G	C4-N9-C1'	-5.80	118.95	126.50
2	A16S	143	C	N3-C2-O2	-5.78	117.85	121.90
2	A16S	494	C	C6-N1-C2	-5.78	117.99	120.30
2	A16S	603	G	C4-N9-C1'	-5.78	118.98	126.50
2	A16S	484	U	N3-C4-C5	-5.78	111.13	114.60
2	A16S	953	U	N3-C4-O4	5.78	123.45	119.40
1	A23S	482	C	N1-C2-O2	5.77	122.36	118.90
66	APTN	7	A	C4-C5-N7	-5.75	107.82	110.70
2	A16S	14	G	C4-N9-C1'	-5.75	119.03	126.50
2	A16S	358	G	N3-C4-C5	-5.75	125.73	128.60
1	A23S	2265	C	C2-N1-C1'	5.74	125.12	118.80
1	A23S	155	G	N3-C4-N9	-5.74	122.56	126.00
2	A16S	517	G	N3-C4-C5	5.74	131.47	128.60
1	A23S	2290	C	C6-N1-C1'	-5.73	113.92	120.80
2	A16S	717	C	N1-C2-N3	5.73	123.21	119.20
2	A16S	920	C	C2-N1-C1'	5.72	125.10	118.80
2	A16S	52	U	N3-C2-O2	5.72	126.20	122.20
66	AETN	65	G	N3-C4-N9	-5.71	122.57	126.00
2	A16S	215	A	C4-C5-N7	5.71	113.56	110.70
2	A16S	1093	U	C6-N1-C1'	-5.71	113.21	121.20
2	A16S	82	A	C5-C6-N6	5.70	128.26	123.70
2	A16S	369	G	C5-C6-N1	5.70	114.35	111.50
1	A23S	964	C	C6-N1-C1'	-5.69	113.97	120.80
2	A16S	242	G	C4-C5-N7	5.69	113.08	110.80
2	A16S	1024	C	N1-C2-O2	-5.69	115.49	118.90
1	A23S	2090	C	N3-C2-O2	-5.68	117.92	121.90
2	A16S	1083	C	C6-N1-C1'	5.68	127.62	120.80
1	A23S	1545	C	N1-C2-O2	5.67	122.31	118.90
2	A16S	1091	G	C8-N9-C1'	5.66	134.36	127.00
2	A16S	474	A	OP2-P-O3'	-5.65	92.76	105.20
2	A16S	906	A	C8-N9-C4	-5.65	103.54	105.80
1	A23S	1802	C	C6-N1-C1'	-5.65	114.02	120.80
2	A16S	1348	G	C2-N3-C4	-5.64	109.08	111.90
66	AETN	19	G	N3-C2-N2	5.64	123.85	119.90
2	A16S	358	G	N3-C4-N9	5.64	129.38	126.00
2	A16S	1465	G	C4-C5-C6	5.64	122.19	118.80
2	A16S	984	C	N1-C2-O2	5.64	122.28	118.90
2	A16S	1186	U	C5-C6-N1	5.63	125.52	122.70
2	A16S	1451	A	C6-N1-C2	-5.63	115.22	118.60
2	A16S	1497	C	C6-N1-C1'	-5.63	114.04	120.80
2	A16S	892	G	C5-N7-C8	-5.63	101.49	104.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	366	C	N3-C2-O2	-5.63	117.96	121.90
2	A16S	1131	G	N9-C4-C5	-5.61	103.15	105.40
2	A16S	1332	A	C8-N9-C1'	-5.61	117.59	127.70
2	A16S	1138	U	P-O3'-C3'	5.58	126.40	119.70
1	A23S	1614	C	N3-C2-O2	-5.58	118.00	121.90
2	A16S	621	G	N3-C4-N9	5.56	129.34	126.00
2	A16S	108	C	O4'-C1'-N1	-5.55	103.76	108.20
1	A23S	1178	C	C6-N1-C2	-5.55	118.08	120.30
66	AETN	49	C	C6-N1-C1'	-5.55	114.14	120.80
1	A23S	385	G	N1-C6-O6	-5.55	116.57	119.90
2	A16S	1370	G	C6-C5-N7	5.55	133.73	130.40
1	A23S	258	C	C6-N1-C2	-5.54	118.08	120.30
2	A16S	369	G	C6-N1-C2	-5.54	121.77	125.10
2	A16S	14	G	C5-N7-C8	-5.54	101.53	104.30
2	A16S	1349	U	N1-C2-O2	-5.53	118.93	122.80
2	A16S	1188	C	C5-C6-N1	5.53	123.77	121.00
2	A16S	1378	C	N1-C2-O2	5.53	122.22	118.90
1	A23S	1957	G	C5-C6-O6	5.53	131.92	128.60
2	A16S	248	A	C5-N7-C8	-5.53	101.14	103.90
2	A16S	56	C	C6-N1-C1'	-5.53	114.17	120.80
2	A16S	113	G	N1-C6-O6	-5.52	116.59	119.90
2	A16S	154	G	C5-N7-C8	-5.52	101.54	104.30
2	A16S	616	G	C4-C5-C6	5.52	122.11	118.80
66	AETN	49	C	C5-C4-N4	-5.51	116.34	120.20
2	A16S	61	G	C4-C5-N7	5.51	113.00	110.80
2	A16S	147	G	N1-C6-O6	-5.50	116.60	119.90
2	A16S	567	C	C6-N1-C2	-5.50	118.10	120.30
1	A23S	1179	C	C6-N1-C1'	-5.50	114.20	120.80
2	A16S	381	C	C4-C5-C6	-5.50	114.65	117.40
2	A16S	1091	G	C4-N9-C1'	-5.49	119.36	126.50
2	A16S	496	G	N3-C4-N9	5.49	129.29	126.00
2	A16S	1187	C	C6-N1-C1'	-5.49	114.21	120.80
2	A16S	717	C	C6-N1-C1'	5.49	127.39	120.80
66	APTIN	56	C	C6-N1-C2	-5.49	118.11	120.30
2	A16S	1369	C	C6-N1-C1'	-5.48	114.22	120.80
2	A16S	1083	C	C5-C6-N1	5.47	123.74	121.00
2	A16S	120	C	C2-N1-C1'	5.47	124.81	118.80
2	A16S	473	C	N1-C2-O2	5.47	122.18	118.90
2	A16S	730	C	N1-C2-O2	5.46	122.18	118.90
2	A16S	1213	C	C2-N1-C1'	5.46	124.81	118.80
2	A16S	1499	C	N1-C2-O2	5.45	122.17	118.90
2	A16S	543	G	N9-C4-C5	-5.45	103.22	105.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	730	C	C6-N1-C1'	-5.45	114.27	120.80
2	A16S	1126	G	N3-C4-C5	5.43	131.32	128.60
2	A16S	955	C	N1-C2-N3	5.43	123.00	119.20
2	A16S	1462	C	C2-N1-C1'	5.43	124.77	118.80
66	APTN	56	C	C5-C6-N1	5.43	123.71	121.00
2	A16S	1377	G	C5-C6-O6	-5.42	125.35	128.60
2	A16S	61	G	C5-C6-N1	-5.42	108.79	111.50
2	A16S	892	G	N1-C2-N2	-5.41	111.33	116.20
2	A16S	363	G	C6-C5-N7	5.41	133.65	130.40
1	A23S	385	G	C5-C6-O6	5.41	131.85	128.60
2	A16S	920	C	N1-C2-O2	5.40	122.14	118.90
2	A16S	147	G	N9-C4-C5	5.40	107.56	105.40
2	A16S	1187	C	N3-C2-O2	-5.39	118.12	121.90
2	A16S	543	G	C8-N9-C4	5.38	108.55	106.40
2	A16S	961	G	C2-N3-C4	5.38	114.59	111.90
2	A16S	543	G	C5-C6-O6	-5.38	125.37	128.60
2	A16S	1188	C	C2-N1-C1'	5.38	124.72	118.80
2	A16S	1332	A	N1-C2-N3	-5.38	126.61	129.30
66	AETN	8	U	C5-C4-O4	-5.37	122.68	125.90
1	A23S	829	G	N3-C4-N9	-5.36	122.78	126.00
1	A23S	1457	U	C6-N1-C1'	-5.36	113.69	121.20
2	A16S	56	C	N3-C2-O2	-5.36	118.15	121.90
2	A16S	906	A	N1-C6-N6	-5.35	115.39	118.60
1	A23S	1177	U	C2-N1-C1'	5.35	124.12	117.70
2	A16S	1127	G	N1-C2-N3	5.35	127.11	123.90
1	A23S	2022	C	N3-C2-O2	-5.34	118.17	121.90
2	A16S	82	A	C5-C6-N1	-5.34	115.03	117.70
2	A16S	496	G	N3-C4-C5	-5.34	125.93	128.60
1	A23S	1090	C	N3-C2-O2	-5.33	118.17	121.90
2	A16S	1126	G	C8-N9-C4	-5.33	104.27	106.40
2	A16S	622	G	C8-N9-C1'	5.33	133.93	127.00
2	A16S	363	G	C8-N9-C1'	5.32	133.92	127.00
2	A16S	1195	G	C8-N9-C1'	-5.32	120.09	127.00
2	A16S	1323	C	C2-N1-C1'	5.30	124.63	118.80
2	A16S	112	U	C6-N1-C1'	-5.30	113.78	121.20
2	A16S	120	C	N1-C2-O2	5.29	122.07	118.90
2	A16S	1058	G	O4'-C1'-N9	-5.29	103.97	108.20
39	L47A	79	LEU	CA-CB-CG	5.29	127.45	115.30
2	A16S	363	G	C4-N9-C1'	-5.28	119.63	126.50
2	A16S	1126	G	N7-C8-N9	5.28	115.74	113.10
1	A23S	1802	C	N3-C2-O2	-5.28	118.21	121.90
1	A23S	279	G	N3-C4-N9	-5.27	122.83	126.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	282	A	N3-C4-N9	-5.27	123.18	127.40
2	A16S	248	A	C5-C6-N6	-5.27	119.48	123.70
2	A16S	716	C	C6-N1-C2	-5.26	118.19	120.30
2	A16S	1223	G	N9-C4-C5	-5.26	103.30	105.40
2	A16S	89	G	N1-C2-N2	-5.26	111.47	116.20
2	A16S	494	C	N1-C2-O2	5.26	122.05	118.90
2	A16S	902	C	C2-N1-C1'	5.25	124.58	118.80
2	A16S	144	C	N1-C2-N3	5.25	122.88	119.20
2	A16S	758	A	P-O3'-C3'	5.24	125.99	119.70
2	A16S	1202	G	C4-C5-N7	5.24	112.90	110.80
1	A23S	851	C	N3-C2-O2	-5.24	118.24	121.90
2	A16S	1452	G	N3-C2-N2	5.23	123.56	119.90
66	AETN	7	A	N9-C1'-C2'	5.23	120.80	114.00
2	A16S	1167	G	N3-C4-N9	5.21	129.13	126.00
2	A16S	1348	G	C4-C5-N7	5.21	112.89	110.80
2	A16S	495	G	C4-C5-N7	-5.21	108.72	110.80
2	A16S	622	G	N1-C2-N3	5.21	127.02	123.90
2	A16S	256	U	C5-C4-O4	-5.20	122.78	125.90
2	A16S	377	A	C5-C6-N6	-5.20	119.54	123.70
2	A16S	1091	G	C4-C5-N7	5.20	112.88	110.80
1	A23S	2923	G	N1-C6-O6	-5.20	116.78	119.90
2	A16S	24	C	N3-C2-O2	-5.20	118.26	121.90
2	A16S	1292	G	N9-C4-C5	-5.19	103.32	105.40
1	A23S	2598	U	N1-C2-O2	5.19	126.43	122.80
2	A16S	33	A	C2-N3-C4	-5.18	108.01	110.60
1	A23S	656	C	N3-C2-O2	-5.18	118.28	121.90
2	A16S	151	C	N1-C2-N3	5.17	122.82	119.20
2	A16S	997	C	C2-N1-C1'	5.16	124.48	118.80
1	A23S	1178	C	N1-C2-O2	5.15	121.99	118.90
1	A23S	482	C	C2-N1-C1'	5.15	124.47	118.80
1	A23S	1545	C	N3-C2-O2	-5.15	118.29	121.90
2	A16S	82	A	N1-C2-N3	5.15	131.88	129.30
2	A16S	616	G	C6-C5-N7	-5.15	127.31	130.40
1	A23S	1103	G	N3-C4-N9	-5.14	122.91	126.00
2	A16S	1334	C	C2-N1-C1'	5.14	124.45	118.80
2	A16S	94	G	N3-C4-N9	-5.14	122.92	126.00
2	A16S	892	G	C5-C6-O6	-5.13	125.52	128.60
66	AETN	48	C	O4'-C1'-N1	5.12	112.30	108.20
41	AS2P	121	PRO	CA-N-CD	-5.12	104.33	111.50
2	A16S	1168	G	C8-N9-C1'	5.12	133.66	127.00
2	A16S	730	C	N3-C4-N4	5.11	121.58	118.00
2	A16S	57	C	N3-C4-N4	-5.11	114.42	118.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A16S	1127	G	C5-C6-O6	5.11	131.67	128.60
2	A16S	366	C	N3-C4-N4	5.11	121.58	118.00
2	A16S	14	G	N1-C2-N3	5.10	126.96	123.90
1	A23S	602	C	N1-C2-O2	5.10	121.96	118.90
2	A16S	1254	U	P-O3'-C3'	5.10	125.82	119.70
2	A16S	1152	G	N3-C2-N2	5.10	123.47	119.90
1	A23S	246	C	C4-C5-C6	-5.09	114.85	117.40
1	A23S	2598	U	C2-N1-C1'	5.09	123.81	117.70
1	A23S	1720	C	C2-N1-C1'	5.09	124.40	118.80
2	A16S	603	G	N1-C2-N3	5.09	126.95	123.90
2	A16S	1024	C	C5-C4-N4	5.09	123.76	120.20
1	A23S	469	G	N1-C2-N2	-5.09	111.62	116.20
2	A16S	1139	A	N1-C6-N6	5.09	121.65	118.60
1	A23S	1626	C	N1-C2-O2	5.08	121.95	118.90
2	A16S	1292	G	N3-C4-N9	5.08	129.05	126.00
2	A16S	1263	G	C5-C6-N1	-5.08	108.96	111.50
1	A23S	1614	C	C6-N1-C2	-5.08	118.27	120.30
2	A16S	354	C	N1-C2-N3	5.07	122.75	119.20
2	A16S	1137	G	N1-C2-N2	-5.07	111.64	116.20
2	A16S	370	G	C5-N7-C8	-5.07	101.77	104.30
2	A16S	627	G	C4-C5-N7	5.06	112.83	110.80
2	A16S	367	C	C5-C6-N1	5.06	123.53	121.00
2	A16S	1332	A	N1-C6-N6	5.06	121.63	118.60
1	A23S	1457	U	N1-C2-O2	5.05	126.33	122.80
2	A16S	1214	A	C4-C5-N7	-5.05	108.17	110.70
2	A16S	1139	A	C6-C5-N7	-5.05	128.77	132.30
2	A16S	61	G	C6-C5-N7	-5.04	127.38	130.40
2	A16S	1082	C	N3-C4-C5	-5.04	119.89	121.90
2	A16S	495	G	C5-N7-C8	5.04	106.82	104.30
2	A16S	1362	C	C6-N1-C2	-5.03	118.29	120.30
1	A23S	1179	C	C5'-C4'-O4'	5.02	115.12	109.10
2	A16S	82	A	N9-C4-C5	5.01	107.81	105.80
2	A16S	892	G	N7-C8-N9	5.01	115.61	113.10
2	A16S	1379	U	C6-N1-C2	-5.01	117.99	121.00
2	A16S	1131	G	C5-C6-O6	-5.00	125.60	128.60
2	A16S	1145	G	N1-C2-N3	5.00	126.90	123.90
2	A16S	358	G	C4-N9-C1'	5.00	133.00	126.50
2	A16S	1082	C	C6-N1-C1'	-5.00	114.80	120.80
2	A16S	1223	G	N3-C4-N9	5.00	129.00	126.00
2	A16S	1263	G	C5-N7-C8	-5.00	101.80	104.30

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A16S	381	C	Sidechain
10	ALX0	23	SER	Peptide
42	AS4E	163	LEU	Peptide
42	AS4E	192	GLY	Peptide
43	AS4P	164	ASN	Peptide
56	AS7P	16	GLY	Peptide
56	AS7P	28	SER	Peptide
28	L34E	35	ALA	Peptide
28	L34E	36	ARG	Peptide
48	S11P	6	GLU	Peptide
50	S15P	20	PRO	Peptide
65	S27A	25	GLN	Peptide
65	S27A	26	ASP	Peptide
65	S27A	27	SER	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A23S	64357	0	0	0	0
2	A16S	32040	0	0	0	0
3	AEFG	5677	0	0	0	0
4	A5S	2609	0	1324	99	0
5	AL2P	1754	0	0	0	0
6	AL3P	2695	0	0	0	0
7	AL4P	1926	0	0	0	0
8	AL5P	1343	0	0	0	0
9	AL6P	1431	0	0	0	0
10	ALX0	629	0	0	0	0
11	L10E	1310	0	0	0	0
12	L13P	1109	0	0	0	0
13	L141	669	0	0	0	0
13	L142	669	0	0	0	0
14	L14P	1034	0	0	0	0
15	L15E	1423	0	0	0	0
16	L18E	895	0	0	0	0
17	L18P	1539	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	L19E	1206	0	0	0	0
19	L22P	1223	0	0	0	0
20	L23P	650	0	0	0	0
21	L24E	441	0	0	0	0
22	L24P	989	0	0	0	0
23	L29P	513	0	0	0	0
24	L30E	729	0	0	0	0
25	L30P	1254	0	0	0	0
26	L31E	625	0	0	0	0
27	L32E	1010	0	0	0	0
28	L34E	629	0	0	0	0
29	L37A	527	0	0	0	0
30	L37E	436	0	0	0	0
31	L39E	414	0	0	0	0
32	L40E	439	0	0	0	0
33	L44E	753	0	0	0	0
34	L7A1	935	0	0	0	0
34	L7A2	935	0	0	0	0
34	SL7A	935	0	0	0	0
35	L15P	752	0	0	0	0
36	L21E	785	0	0	0	0
37	L45A	816	0	0	0	0
38	L46A	586	0	0	0	0
39	L47A	648	0	0	0	0
40	AL1P	1715	0	0	0	0
41	AS2P	1587	0	0	0	0
42	AS4E	1925	0	0	0	0
43	AS4P	1370	0	0	0	0
44	AS5P	1600	0	0	0	0
45	AS6E	805	0	0	0	0
46	AS8E	993	0	0	0	0
47	AS8P	1028	0	0	0	0
48	S11P	960	0	0	0	0
49	S12P	1103	0	0	0	0
50	S15P	1225	0	0	0	0
51	S17P	885	0	0	0	0
52	S24E	759	0	0	0	0
53	S27E	458	0	0	0	0
54	S3AE	1545	0	0	0	0
55	AS3P	1576	0	0	0	0
56	AS7P	1537	0	0	0	0
57	S10P	824	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
58	S13P	1204	0	0	0	0
59	S14P	432	0	0	0	0
60	S17E	517	0	0	0	0
61	S19E	1239	0	0	0	0
62	S19P	968	0	0	0	0
63	AS9P	1096	0	0	0	0
64	S28E	498	0	0	0	0
65	S27A	435	0	0	0	0
66	AETN	1619	0	0	0	0
66	APTN	1619	0	0	0	0
67	AMRN	260	0	0	0	0
68	APTP	67	0	0	0	0
69	AEFG	32	0	0	0	0
70	AS2P	146	0	0	0	0
70	AS5P	105	0	0	0	0
70	AS8P	35	0	0	0	0
All	All	173506	0	1324	99	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 29.

All (99) 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)
4:A5S:41:U:O2'	4:A5S:46:A:N6	2.10	0.85
4:A5S:77:G:N2	4:A5S:105:C:O2	2.12	0.79
4:A5S:5:C:N4	4:A5S:120:U:O4	2.15	0.74
4:A5S:78:G:N2	4:A5S:104:C:O2	2.20	0.73
4:A5S:22:C:O2	4:A5S:63:G:N2	2.20	0.70
4:A5S:35:G:O2'	4:A5S:36:A:N7	2.29	0.66
4:A5S:75:G:H2'	4:A5S:76:G:H8	1.61	0.65
4:A5S:77:G:N1	4:A5S:105:C:N3	2.39	0.65
4:A5S:40:G:N2	4:A5S:45:G:OP2	2.29	0.64
4:A5S:85:G:H2'	4:A5S:86:A:C8	2.34	0.63
4:A5S:85:G:H2'	4:A5S:86:A:H8	1.62	0.63
4:A5S:95:G:H2'	4:A5S:96:G:H8	1.64	0.62
4:A5S:53:A:H2	4:A5S:54:A:H62	1.49	0.61
4:A5S:40:G:O2'	4:A5S:47:A:N1	2.35	0.58
4:A5S:45:G:N3	4:A5S:48:C:N4	2.40	0.58
4:A5S:98:C:H2'	4:A5S:99:C:C6	2.37	0.58
4:A5S:17:G:H2'	4:A5S:18:U:C6	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A5S:19:G:H2'	4:A5S:20:A:H8	1.67	0.58
4:A5S:75:G:H2'	4:A5S:76:G:C8	2.39	0.58
4:A5S:95:G:H2'	4:A5S:96:G:C8	2.39	0.58
4:A5S:106:U:H2'	4:A5S:107:C:C6	2.38	0.57
4:A5S:22:C:N3	4:A5S:63:G:N1	2.40	0.57
4:A5S:77:G:H2'	4:A5S:78:G:H8	1.71	0.55
4:A5S:57:U:H4'	4:A5S:58:A:O5'	2.07	0.55
4:A5S:62:C:H2'	4:A5S:63:G:H8	1.73	0.54
4:A5S:31:C:H2'	4:A5S:32:C:O4'	2.07	0.54
4:A5S:3:C:H2'	4:A5S:4:C:C6	2.43	0.54
4:A5S:25:G:N7	4:A5S:57:U:O2'	2.33	0.53
4:A5S:6:A:H5'	4:A5S:62:C:H4'	1.90	0.52
4:A5S:35:G:O6	4:A5S:45:G:H1'	2.10	0.52
4:A5S:109:C:H2'	4:A5S:110:U:C6	2.45	0.51
4:A5S:30:A:H61	4:A5S:56:U:H3	1.58	0.51
4:A5S:76:G:H1	4:A5S:106:U:H3	1.56	0.51
4:A5S:83:G:C6	4:A5S:100:G:C5	2.98	0.51
4:A5S:77:G:H2'	4:A5S:78:G:C8	2.44	0.51
4:A5S:104:C:H2'	4:A5S:105:C:H6	1.75	0.51
4:A5S:94:G:H2'	4:A5S:95:G:H8	1.75	0.50
4:A5S:97:C:H2'	4:A5S:98:C:C6	2.47	0.50
4:A5S:19:G:H2'	4:A5S:20:A:C8	2.47	0.50
4:A5S:105:C:H2'	4:A5S:106:U:H6	1.76	0.49
4:A5S:17:G:O6	4:A5S:67:A:N6	2.45	0.49
4:A5S:47:A:H2'	4:A5S:48:C:O4'	2.13	0.49
4:A5S:61:C:H2'	4:A5S:62:C:C6	2.47	0.49
4:A5S:94:G:H2'	4:A5S:95:G:C8	2.48	0.49
4:A5S:64:C:H2'	4:A5S:65:U:H6	1.78	0.48
4:A5S:105:C:H2'	4:A5S:106:U:C6	2.49	0.48
4:A5S:118:G:H2'	4:A5S:119:A:C8	2.48	0.48
4:A5S:5:C:H2'	4:A5S:6:A:C8	2.48	0.48
4:A5S:104:C:H2'	4:A5S:105:C:C6	2.49	0.47
4:A5S:114:C:H2'	4:A5S:115:U:C6	2.48	0.47
4:A5S:108:U:H2'	4:A5S:109:C:C6	2.50	0.46
4:A5S:51:G:C2	4:A5S:52:G:H1'	2.50	0.46
4:A5S:49:C:H2'	4:A5S:50:C:H6	1.80	0.46
4:A5S:20:A:H2'	4:A5S:21:G:H8	1.81	0.45
4:A5S:16:A:H5'	4:A5S:113:G:H5''	1.98	0.45
4:A5S:49:C:H2'	4:A5S:50:C:C6	2.52	0.45
4:A5S:64:C:H2'	4:A5S:65:U:C6	2.51	0.45
4:A5S:76:G:C2	4:A5S:107:C:C2	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A5S:46:A:C5	4:A5S:47:A:C8	3.04	0.45
4:A5S:35:G:C6	4:A5S:45:G:H1'	2.52	0.44
4:A5S:41:U:HO2'	4:A5S:46:A:N6	2.14	0.44
4:A5S:118:G:H2'	4:A5S:119:A:H8	1.83	0.44
4:A5S:60:G:C6	4:A5S:61:C:C2	3.05	0.44
4:A5S:72:A:H2'	4:A5S:73:G:H8	1.82	0.44
4:A5S:93:A:C2	4:A5S:94:G:H1'	2.52	0.44
4:A5S:25:G:O2'	4:A5S:28:A:N6	2.52	0.43
4:A5S:52:G:C2	4:A5S:53:A:C4	3.07	0.43
4:A5S:2:G:H3'	4:A5S:3:C:C6	2.53	0.43
4:A5S:20:A:H2'	4:A5S:21:G:C8	2.54	0.43
4:A5S:25:G:C6	4:A5S:57:U:C2	3.07	0.43
4:A5S:32:C:H2'	4:A5S:54:A:H61	1.82	0.43
4:A5S:121:G:H2'	4:A5S:122:G:C8	2.53	0.43
4:A5S:7:C:H2'	4:A5S:8:C:C6	2.54	0.42
4:A5S:115:U:H2'	4:A5S:116:G:H8	1.84	0.42
4:A5S:77:G:C2	4:A5S:106:U:C2	3.08	0.42
4:A5S:62:C:H2'	4:A5S:63:G:C8	2.54	0.42
4:A5S:27:A:C5	4:A5S:28:A:C8	3.08	0.42
4:A5S:54:A:H2'	4:A5S:55:G:O4'	2.20	0.42
4:A5S:92:G:H2'	4:A5S:93:A:C8	2.55	0.42
4:A5S:89:C:H2'	4:A5S:90:G:C8	2.55	0.42
4:A5S:109:C:H2'	4:A5S:110:U:H6	1.84	0.42
4:A5S:24:G:H2'	4:A5S:25:G:C8	2.55	0.42
4:A5S:14:A:O2'	4:A5S:15:U:H3'	2.20	0.42
4:A5S:34:G:H2'	4:A5S:35:G:O4'	2.20	0.42
4:A5S:4:C:HO2'	4:A5S:5:C:H6	1.61	0.41
4:A5S:22:C:H2'	4:A5S:23:G:H8	1.84	0.41
4:A5S:29:C:H2'	4:A5S:30:A:O4'	2.20	0.41
4:A5S:33:C:H2'	4:A5S:34:G:C8	2.54	0.41
4:A5S:85:G:C2	4:A5S:86:A:C5	3.08	0.41
4:A5S:31:C:C4	4:A5S:32:C:C2	3.08	0.41
4:A5S:23:G:C6	4:A5S:63:G:C6	3.08	0.41
4:A5S:73:G:C6	4:A5S:110:U:N3	2.89	0.41
4:A5S:27:A:C6	4:A5S:28:A:C4	3.09	0.41
4:A5S:54:A:H2'	4:A5S:55:G:C8	2.56	0.41
4:A5S:76:G:C6	4:A5S:77:G:C5	3.09	0.41
4:A5S:78:G:C2	4:A5S:105:C:C2	3.09	0.40
4:A5S:23:G:C4	4:A5S:63:G:C2	3.09	0.40
4:A5S:52:G:C6	4:A5S:53:A:C6	3.09	0.40
4:A5S:54:A:H2'	4:A5S:55:G:H8	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AEFG	721/729 (99%)	650 (90%)	66 (9%)	5 (1%)	19	56
5	AL2P	232/234 (99%)	219 (94%)	13 (6%)	0	100	100
6	AL3P	337/339 (99%)	305 (90%)	32 (10%)	0	100	100
7	AL4P	249/251 (99%)	237 (95%)	12 (5%)	0	100	100
8	AL5P	166/168 (99%)	153 (92%)	13 (8%)	0	100	100
9	AL6P	179/181 (99%)	166 (93%)	13 (7%)	0	100	100
10	ALX0	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
11	L10E	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
12	L13P	138/140 (99%)	125 (91%)	13 (9%)	0	100	100
13	L141	84/86 (98%)	75 (89%)	9 (11%)	0	100	100
13	L142	84/86 (98%)	72 (86%)	12 (14%)	0	100	100
14	L14P	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
15	L15E	167/169 (99%)	158 (95%)	9 (5%)	0	100	100
16	L18E	110/112 (98%)	107 (97%)	3 (3%)	0	100	100
17	L18P	191/193 (99%)	178 (93%)	13 (7%)	0	100	100
18	L19E	142/144 (99%)	136 (96%)	6 (4%)	0	100	100
19	L22P	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
20	L23P	79/81 (98%)	68 (86%)	11 (14%)	0	100	100
21	L24E	52/54 (96%)	50 (96%)	2 (4%)	0	100	100
22	L24P	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
23	L29P	61/63 (97%)	57 (93%)	4 (7%)	0	100	100
24	L30E	92/94 (98%)	90 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	L30P	153/155 (99%)	134 (88%)	19 (12%)	0	100	100
26	L31E	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
27	L32E	121/123 (98%)	108 (89%)	13 (11%)	0	100	100
28	L34E	75/77 (97%)	56 (75%)	18 (24%)	1 (1%)	10	42
29	L37A	63/65 (97%)	53 (84%)	10 (16%)	0	100	100
30	L37E	52/54 (96%)	49 (94%)	3 (6%)	0	100	100
31	L39E	47/49 (96%)	40 (85%)	7 (15%)	0	100	100
32	L40E	53/55 (96%)	38 (72%)	14 (26%)	1 (2%)	6	32
33	L44E	90/92 (98%)	83 (92%)	7 (8%)	0	100	100
34	L7A1	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
34	L7A2	121/123 (98%)	120 (99%)	1 (1%)	0	100	100
34	SL7A	121/123 (98%)	112 (93%)	9 (7%)	0	100	100
35	L15P	90/144 (62%)	83 (92%)	7 (8%)	0	100	100
36	L21E	95/97 (98%)	88 (93%)	6 (6%)	1 (1%)	12	46
37	L45A	99/101 (98%)	82 (83%)	14 (14%)	3 (3%)	3	22
38	L46A	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
39	L47A	78/80 (98%)	73 (94%)	4 (5%)	1 (1%)	10	42
40	AL1P	214/216 (99%)	199 (93%)	15 (7%)	0	100	100
41	AS2P	194/196 (99%)	183 (94%)	11 (6%)	0	100	100
42	AS4E	238/240 (99%)	217 (91%)	21 (9%)	0	100	100
43	AS4P	164/166 (99%)	137 (84%)	26 (16%)	1 (1%)	22	59
44	AS5P	202/204 (99%)	186 (92%)	16 (8%)	0	100	100
45	AS6E	103/105 (98%)	87 (84%)	16 (16%)	0	100	100
46	AS8E	124/126 (98%)	107 (86%)	17 (14%)	0	100	100
47	AS8P	128/130 (98%)	120 (94%)	8 (6%)	0	100	100
48	S11P	126/128 (98%)	111 (88%)	15 (12%)	0	100	100
49	S12P	141/143 (99%)	121 (86%)	20 (14%)	0	100	100
50	S15P	147/149 (99%)	132 (90%)	15 (10%)	0	100	100
51	S17P	109/111 (98%)	99 (91%)	10 (9%)	0	100	100
52	S24E	94/96 (98%)	90 (96%)	4 (4%)	0	100	100
53	S27E	57/59 (97%)	48 (84%)	9 (16%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
54	S3AE	187/189 (99%)	164 (88%)	22 (12%)	1 (0%)	25	64
55	AS3P	199/201 (99%)	185 (93%)	14 (7%)	0	100	100
56	AS7P	191/193 (99%)	159 (83%)	32 (17%)	0	100	100
57	S10P	98/100 (98%)	91 (93%)	7 (7%)	0	100	100
58	S13P	145/147 (99%)	124 (86%)	21 (14%)	0	100	100
59	S14P	50/52 (96%)	42 (84%)	8 (16%)	0	100	100
60	S17E	60/62 (97%)	53 (88%)	7 (12%)	0	100	100
61	S19E	148/150 (99%)	133 (90%)	15 (10%)	0	100	100
62	S19P	113/115 (98%)	101 (89%)	12 (11%)	0	100	100
63	AS9P	134/136 (98%)	122 (91%)	12 (9%)	0	100	100
64	S28E	61/63 (97%)	52 (85%)	9 (15%)	0	100	100
65	S27A	52/54 (96%)	39 (75%)	13 (25%)	0	100	100
68	APTP	4/6 (67%)	2 (50%)	2 (50%)	0	100	100
All	All	8723/8913 (98%)	7904 (91%)	805 (9%)	14 (0%)	45	78

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AEFG	396	PRO
3	AEFG	703	ARG
37	L45A	4	VAL
37	L45A	55	VAL
37	L45A	67	THR
28	L34E	19	PRO
39	L47A	38	LEU
3	AEFG	482	VAL
3	AEFG	71	VAL
3	AEFG	548	ILE
32	L40E	52	PRO
43	AS4P	166	PRO
36	L21E	27	PRO
54	S3AE	180	PRO

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AEFG	625/627 (100%)	620 (99%)	5 (1%)	79	85
5	AL2P	181/181 (100%)	180 (99%)	1 (1%)	84	88
6	AL3P	297/297 (100%)	295 (99%)	2 (1%)	81	87
7	AL4P	212/212 (100%)	212 (100%)	0	100	100
8	AL5P	144/144 (100%)	144 (100%)	0	100	100
9	AL6P	157/157 (100%)	155 (99%)	2 (1%)	65	77
10	ALX0	68/68 (100%)	68 (100%)	0	100	100
11	L10E	137/137 (100%)	135 (98%)	2 (2%)	60	75
12	L13P	121/121 (100%)	121 (100%)	0	100	100
13	L141	74/74 (100%)	74 (100%)	0	100	100
13	L142	74/74 (100%)	74 (100%)	0	100	100
14	L14P	110/110 (100%)	109 (99%)	1 (1%)	75	83
15	L15E	146/146 (100%)	146 (100%)	0	100	100
16	L18E	98/98 (100%)	96 (98%)	2 (2%)	50	69
17	L18P	162/162 (100%)	159 (98%)	3 (2%)	52	70
18	L19E	126/126 (100%)	125 (99%)	1 (1%)	79	85
19	L22P	131/131 (100%)	127 (97%)	4 (3%)	35	55
20	L23P	74/74 (100%)	74 (100%)	0	100	100
21	L24E	50/50 (100%)	50 (100%)	0	100	100
22	L24P	108/108 (100%)	108 (100%)	0	100	100
23	L29P	59/59 (100%)	59 (100%)	0	100	100
24	L30E	83/83 (100%)	83 (100%)	0	100	100
25	L30P	136/136 (100%)	136 (100%)	0	100	100
26	L31E	66/66 (100%)	66 (100%)	0	100	100
27	L32E	106/106 (100%)	104 (98%)	2 (2%)	52	70
28	L34E	70/70 (100%)	68 (97%)	2 (3%)	37	57
29	L37A	53/53 (100%)	52 (98%)	1 (2%)	52	70
30	L37E	45/45 (100%)	45 (100%)	0	100	100
31	L39E	44/44 (100%)	43 (98%)	1 (2%)	45	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	L40E	50/50 (100%)	49 (98%)	1 (2%)	50	69
33	L44E	84/84 (100%)	84 (100%)	0	100	100
34	L7A1	104/104 (100%)	104 (100%)	0	100	100
34	L7A2	104/104 (100%)	103 (99%)	1 (1%)	73	82
34	SL7A	104/104 (100%)	104 (100%)	0	100	100
35	L15P	78/118 (66%)	78 (100%)	0	100	100
36	L21E	85/85 (100%)	84 (99%)	1 (1%)	67	79
37	L45A	91/91 (100%)	90 (99%)	1 (1%)	70	80
38	L46A	66/66 (100%)	64 (97%)	2 (3%)	36	56
39	L47A	74/74 (100%)	73 (99%)	1 (1%)	62	76
40	AL1P	189/190 (100%)	187 (99%)	2 (1%)	70	80
41	AS2P	174/174 (100%)	173 (99%)	1 (1%)	84	88
42	AS4E	210/210 (100%)	209 (100%)	1 (0%)	86	90
43	AS4P	149/149 (100%)	149 (100%)	0	100	100
44	AS5P	174/174 (100%)	173 (99%)	1 (1%)	84	88
45	AS6E	88/88 (100%)	88 (100%)	0	100	100
46	AS8E	106/106 (100%)	106 (100%)	0	100	100
47	AS8P	111/111 (100%)	110 (99%)	1 (1%)	75	83
48	S11P	94/94 (100%)	93 (99%)	1 (1%)	70	80
49	S12P	116/116 (100%)	112 (97%)	4 (3%)	32	52
50	S15P	133/133 (100%)	133 (100%)	0	100	100
51	S17P	97/97 (100%)	96 (99%)	1 (1%)	73	82
52	S24E	84/84 (100%)	84 (100%)	0	100	100
53	S27E	51/51 (100%)	51 (100%)	0	100	100
54	S3AE	170/170 (100%)	170 (100%)	0	100	100
55	AS3P	165/165 (100%)	165 (100%)	0	100	100
56	AS7P	166/166 (100%)	165 (99%)	1 (1%)	84	88
57	S10P	92/92 (100%)	91 (99%)	1 (1%)	70	80
58	S13P	129/129 (100%)	128 (99%)	1 (1%)	79	85
59	S14P	45/45 (100%)	45 (100%)	0	100	100
60	S17E	57/57 (100%)	57 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
61	S19E	134/134 (100%)	134 (100%)	0	100	100
62	S19P	106/106 (100%)	106 (100%)	0	100	100
63	AS9P	113/113 (100%)	112 (99%)	1 (1%)	75	83
64	S28E	54/54 (100%)	54 (100%)	0	100	100
65	S27A	47/47 (100%)	47 (100%)	0	100	100
68	APTP	6/6 (100%)	6 (100%)	0	100	100
All	All	7657/7700 (99%)	7605 (99%)	52 (1%)	80	87

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

Mol	Chain	Res	Type
3	AEFG	165	LYS
3	AEFG	654	ARG
3	AEFG	688	ARG
3	AEFG	703	ARG
3	AEFG	727	LYS
5	AL2P	32	ASN
6	AL3P	10	ARG
6	AL3P	19	ARG
9	AL6P	66	ARG
9	AL6P	123	ARG
11	L10E	71	LYS
11	L10E	75	LYS
14	L14P	111	LYS
16	L18E	36	ARG
16	L18E	52	LYS
17	L18P	34	ARG
17	L18P	138	LYS
17	L18P	140	LYS
18	L19E	9	ARG
19	L22P	18	LYS
19	L22P	77	ARG
19	L22P	124	LYS
19	L22P	130	ARG
27	L32E	6	LYS
27	L32E	7	LYS
28	L34E	12	ARG
28	L34E	79	ILE
29	L37A	24	LYS
31	L39E	19	ARG

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Mol	Chain	Res	Type
32	L40E	15	ARG
34	L7A2	116	LYS
36	L21E	77	LYS
37	L45A	87	LYS
38	L46A	45	LYS
38	L46A	51	LYS
39	L47A	31	LYS
40	AL1P	196	LYS
40	AL1P	204	ARG
41	AS2P	201	ARG
42	AS4E	196	LYS
44	AS5P	82	LYS
47	AS8P	21	ARG
48	S11P	123	ARG
49	S12P	28	ARG
49	S12P	32	ARG
49	S12P	63	ARG
49	S12P	123	ARG
51	S17P	37	ARG
56	AS7P	46	ARG
57	S10P	59	LYS
58	S13P	115	ARG
63	AS9P	131	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A23S	2987/3022 (98%)	669 (22%)	32 (1%)
2	A16S	1489/1503 (99%)	404 (27%)	58 (3%)
4	A5S	121/122 (99%)	20 (16%)	1 (0%)
66	AETN	75/76 (98%)	34 (45%)	3 (4%)
66	APTN	75/76 (98%)	20 (26%)	1 (1%)
67	AMRN	12/13 (92%)	4 (33%)	0
All	All	4759/4812 (98%)	1151 (24%)	95 (1%)

All (1151) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A23S	18	G
1	A23S	19	A
1	A23S	25	C
1	A23S	29	U
1	A23S	30	C
1	A23S	31	G
1	A23S	33	G
1	A23S	36	C
1	A23S	41	G
1	A23S	48	G
1	A23S	53	A
1	A23S	61	A
1	A23S	64	U
1	A23S	65	G
1	A23S	73	G
1	A23S	75	G
1	A23S	80	A
1	A23S	81	A
1	A23S	82	G
1	A23S	90	U
1	A23S	91	G
1	A23S	103	C
1	A23S	107	A
1	A23S	109	U
1	A23S	115	A
1	A23S	117	C
1	A23S	126	U
1	A23S	127	U
1	A23S	128	U
1	A23S	131	G
1	A23S	137	C
1	A23S	144	U
1	A23S	145	A
1	A23S	146	U
1	A23S	147	A
1	A23S	160	A
1	A23S	175	A
1	A23S	179	U
1	A23S	185	U
1	A23S	192	A
1	A23S	195	A
1	A23S	200	A
1	A23S	201	A

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Mol	Chain	Res	Type
1	A23S	202	A
1	A23S	204	C
1	A23S	205	A
1	A23S	206	A
1	A23S	207	U
1	A23S	208	U
1	A23S	209	G
1	A23S	212	A
1	A23S	222	U
1	A23S	227	G
1	A23S	229	G
1	A23S	231	C
1	A23S	242	A
1	A23S	243	C
1	A23S	244	A
1	A23S	245	G
1	A23S	246	C
1	A23S	247	C
1	A23S	255	A
1	A23S	257	C
1	A23S	268	U
1	A23S	276	U
1	A23S	281	A
1	A23S	288	G
1	A23S	289	U
1	A23S	292	C
1	A23S	293	G
1	A23S	303	C
1	A23S	304	U
1	A23S	319	G
1	A23S	320	C
1	A23S	336	A
1	A23S	337	G
1	A23S	344	U
1	A23S	345	C
1	A23S	352	A
1	A23S	353	A
1	A23S	372	G
1	A23S	373	A
1	A23S	374	A
1	A23S	376	G
1	A23S	383	A

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Mol	Chain	Res	Type
1	A23S	385	G
1	A23S	390	A
1	A23S	391	G
1	A23S	392	A
1	A23S	403	G
1	A23S	405	G
1	A23S	418	G
1	A23S	419	U
1	A23S	433	U
1	A23S	434	U
1	A23S	449	A
1	A23S	454	A
1	A23S	455	C
1	A23S	460	G
1	A23S	468	G
1	A23S	469	G
1	A23S	470	C
1	A23S	472	A
1	A23S	476	A
1	A23S	490	A
1	A23S	491	U
1	A23S	492	A
1	A23S	498	C
1	A23S	499	U
1	A23S	501	A
1	A23S	502	G
1	A23S	503	U
1	A23S	510	A
1	A23S	511	G
1	A23S	514	A
1	A23S	522	A
1	A23S	524	A
1	A23S	525	G
1	A23S	536	G
1	A23S	537	G
1	A23S	541	A
1	A23S	547	A
1	A23S	549	G
1	A23S	551	G
1	A23S	552	C
1	A23S	553	C
1	A23S	559	C

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Mol	Chain	Res	Type
1	A23S	566	G
1	A23S	570	U
1	A23S	572	C
1	A23S	573	A
1	A23S	574	G
1	A23S	575	G
1	A23S	577	U
1	A23S	585	G
1	A23S	586	A
1	A23S	588	A
1	A23S	589	G
1	A23S	592	G
1	A23S	594	G
1	A23S	621	G
1	A23S	628	G
1	A23S	637	A
1	A23S	638	G
1	A23S	639	G
1	A23S	645	C
1	A23S	657	U
1	A23S	658	U
1	A23S	659	U
1	A23S	667	A
1	A23S	668	A
1	A23S	669	A
1	A23S	670	C
1	A23S	671	A
1	A23S	674	G
1	A23S	675	G
1	A23S	682	A
1	A23S	683	G
1	A23S	699	A
1	A23S	713	A
1	A23S	720	A
1	A23S	727	A
1	A23S	737	A
1	A23S	740	G
1	A23S	741	C
1	A23S	753	U
1	A23S	754	U
1	A23S	755	U
1	A23S	757	U

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Mol	Chain	Res	Type
1	A23S	758	A
1	A23S	760	G
1	A23S	768	C
1	A23S	769	A
1	A23S	778	C
1	A23S	780	G
1	A23S	787	A
1	A23S	802	G
1	A23S	808	A
1	A23S	809	A
1	A23S	810	A
1	A23S	817	G
1	A23S	818	A
1	A23S	819	U
1	A23S	830	G
1	A23S	838	A
1	A23S	844	G
1	A23S	847	G
1	A23S	848	A
1	A23S	849	A
1	A23S	850	A
1	A23S	851	C
1	A23S	859	G
1	A23S	863	G
1	A23S	866	G
1	A23S	867	A
1	A23S	868	A
1	A23S	869	U
1	A23S	875	U
1	A23S	878	U
1	A23S	883	U
1	A23S	887	A
1	A23S	888	U
1	A23S	901	C
1	A23S	911	G
1	A23S	912	G
1	A23S	915	C
1	A23S	918	A
1	A23S	920	G
1	A23S	921	A
1	A23S	925	A
1	A23S	936	U

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Mol	Chain	Res	Type
1	A23S	937	G
1	A23S	941	G
1	A23S	948	C
1	A23S	964	C
1	A23S	966	A
1	A23S	981	A
1	A23S	986	A
1	A23S	996	G
1	A23S	1001	G
1	A23S	1004	A
1	A23S	1007	G
1	A23S	1011	G
1	A23S	1046	A
1	A23S	1047	A
1	A23S	1048	C
1	A23S	1050	C
1	A23S	1069	A
1	A23S	1070	G
1	A23S	1072	A
1	A23S	1073	G
1	A23S	1082	G
1	A23S	1083	G
1	A23S	1084	G
1	A23S	1091	G
1	A23S	1095	U
1	A23S	1096	A
1	A23S	1097	A
1	A23S	1098	G
1	A23S	1099	G
1	A23S	1111	A
1	A23S	1114	G
1	A23S	1115	G
1	A23S	1117	A
1	A23S	1120	A
1	A23S	1122	C
1	A23S	1126	G
1	A23S	1127	A
1	A23S	1145	A
1	A23S	1148	U
1	A23S	1149	C
1	A23S	1165	C
1	A23S	1168	A

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Mol	Chain	Res	Type
1	A23S	1174	G
1	A23S	1177	U
1	A23S	1178	C
1	A23S	1179	C
1	A23S	1183	C
1	A23S	1185	U
1	A23S	1186	A
1	A23S	1187	G
1	A23S	1197	A
1	A23S	1198	G
1	A23S	1199	G
1	A23S	1200	U
1	A23S	1201	G
1	A23S	1202	G
1	A23S	1203	G
1	A23S	1204	C
1	A23S	1206	C
1	A23S	1207	A
1	A23S	1208	G
1	A23S	1210	A
1	A23S	1211	G
1	A23S	1213	A
1	A23S	1214	G
1	A23S	1217	A
1	A23S	1219	C
1	A23S	1221	U
1	A23S	1222	C
1	A23S	1227	G
1	A23S	1229	G
1	A23S	1230	U
1	A23S	1233	G
1	A23S	1237	C
1	A23S	1249	C
1	A23S	1250	G
1	A23S	1251	A
1	A23S	1252	G
1	A23S	1269	A
1	A23S	1270	U
1	A23S	1271	U
1	A23S	1272	G
1	A23S	1273	G
1	A23S	1275	C

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Mol	Chain	Res	Type
1	A23S	1282	C
1	A23S	1283	A
1	A23S	1284	A
1	A23S	1289	G
1	A23S	1293	C
1	A23S	1296	A
1	A23S	1298	A
1	A23S	1312	C
1	A23S	1316	A
1	A23S	1317	C
1	A23S	1318	U
1	A23S	1322	G
1	A23S	1328	C
1	A23S	1330	G
1	A23S	1350	G
1	A23S	1351	G
1	A23S	1354	A
1	A23S	1355	G
1	A23S	1368	G
1	A23S	1370	G
1	A23S	1379	G
1	A23S	1381	C
1	A23S	1393	G
1	A23S	1396	G
1	A23S	1398	U
1	A23S	1399	C
1	A23S	1416	C
1	A23S	1417	G
1	A23S	1418	A
1	A23S	1430	A
1	A23S	1444	G
1	A23S	1445	A
1	A23S	1451	A
1	A23S	1458	U
1	A23S	1464	C
1	A23S	1488	C
1	A23S	1492	U
1	A23S	1501	A
1	A23S	1504	G
1	A23S	1506	C
1	A23S	1511	A
1	A23S	1515	A

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Mol	Chain	Res	Type
1	A23S	1516	C
1	A23S	1523	A
1	A23S	1525	A
1	A23S	1529	A
1	A23S	1530	A
1	A23S	1532	G
1	A23S	1540	C
1	A23S	1541	A
1	A23S	1542	U
1	A23S	1549	G
1	A23S	1561	G
1	A23S	1563	U
1	A23S	1564	G
1	A23S	1565	C
1	A23S	1569	A
1	A23S	1570	A
1	A23S	1571	C
1	A23S	1574	A
1	A23S	1575	A
1	A23S	1576	G
1	A23S	1579	A
1	A23S	1585	C
1	A23S	1589	C
1	A23S	1609	A
1	A23S	1613	C
1	A23S	1614	C
1	A23S	1616	C
1	A23S	1617	C
1	A23S	1619	U
1	A23S	1623	A
1	A23S	1625	C
1	A23S	1626	C
1	A23S	1633	U
1	A23S	1634	C
1	A23S	1635	A
1	A23S	1636	A
1	A23S	1639	C
1	A23S	1644	G
1	A23S	1647	A
1	A23S	1648	G
1	A23S	1649	C
1	A23S	1659	G

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Mol	Chain	Res	Type
1	A23S	1660	A
1	A23S	1661	G
1	A23S	1666	G
1	A23S	1667	G
1	A23S	1671	A
1	A23S	1673	G
1	A23S	1676	G
1	A23S	1680	U
1	A23S	1682	G
1	A23S	1684	C
1	A23S	1690	G
1	A23S	1692	U
1	A23S	1693	A
1	A23S	1694	G
1	A23S	1697	G
1	A23S	1707	G
1	A23S	1708	A
1	A23S	1713	U
1	A23S	1715	G
1	A23S	1720	C
1	A23S	1721	A
1	A23S	1723	G
1	A23S	1724	A
1	A23S	1727	A
1	A23S	1729	G
1	A23S	1734	C
1	A23S	1740	C
1	A23S	1741	G
1	A23S	1744	C
1	A23S	1751	G
1	A23S	1752	A
1	A23S	1753	C
1	A23S	1757	A
1	A23S	1762	G
1	A23S	1764	A
1	A23S	1771	C
1	A23S	1772	U
1	A23S	1776	G
1	A23S	1786	G
1	A23S	1789	A
1	A23S	1801	U
1	A23S	1802	C

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Mol	Chain	Res	Type
1	A23S	1804	G
1	A23S	1809	G
1	A23S	1810	U
1	A23S	1811	A
1	A23S	1820	U
1	A23S	1857	A
1	A23S	1868	A
1	A23S	1869	U
1	A23S	1877	U
1	A23S	1900	G
1	A23S	1907	G
1	A23S	1908	A
1	A23S	1917	A
1	A23S	1921	U
1	A23S	1925	A
1	A23S	1935	A
1	A23S	1944	C
1	A23S	1946	A
1	A23S	1955	G
1	A23S	1961	G
1	A23S	1973	A
1	A23S	1979	G
1	A23S	2007	U
1	A23S	2013	G
1	A23S	2029	A
1	A23S	2035	G
1	A23S	2036	G
1	A23S	2042	A
1	A23S	2043	C
1	A23S	2044	U
1	A23S	2045	C
1	A23S	2046	U
1	A23S	2047	G
1	A23S	2054	U
1	A23S	2055	U
1	A23S	2056	A
1	A23S	2058	G
1	A23S	2059	G
1	A23S	2060	U
1	A23S	2062	G
1	A23S	2066	A
1	A23S	2067	A

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Mol	Chain	Res	Type
1	A23S	2073	U
1	A23S	2084	U
1	A23S	2092	C
1	A23S	2093	G
1	A23S	2099	A
1	A23S	2100	U
1	A23S	2101	G
1	A23S	2105	C
1	A23S	2106	A
1	A23S	2111	G
1	A23S	2121	G
1	A23S	2122	U
1	A23S	2141	G
1	A23S	2142	A
1	A23S	2143	A
1	A23S	2147	C
1	A23S	2148	C
1	A23S	2149	U
1	A23S	2150	G
1	A23S	2151	A
1	A23S	2152	G
1	A23S	2155	G
1	A23S	2159	C
1	A23S	2160	A
1	A23S	2161	C
1	A23S	2162	A
1	A23S	2163	G
1	A23S	2169	C
1	A23S	2180	A
1	A23S	2184	A
1	A23S	2188	A
1	A23S	2189	A
1	A23S	2190	G
1	A23S	2191	A
1	A23S	2198	G
1	A23S	2209	G
1	A23S	2210	C
1	A23S	2225	C
1	A23S	2230	G
1	A23S	2231	G
1	A23S	2232	C
1	A23S	2234	U

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Mol	Chain	Res	Type
1	A23S	2236	U
1	A23S	2237	A
1	A23S	2239	G
1	A23S	2240	C
1	A23S	2241	G
1	A23S	2244	G
1	A23S	2245	A
1	A23S	2247	U
1	A23S	2249	G
1	A23S	2252	G
1	A23S	2260	U
1	A23S	2261	C
1	A23S	2262	G
1	A23S	2263	A
1	A23S	2266	C
1	A23S	2268	G
1	A23S	2270	C
1	A23S	2276	G
1	A23S	2286	G
1	A23S	2287	A
1	A23S	2288	C
1	A23S	2290	C
1	A23S	2292	A
1	A23S	2293	A
1	A23S	2297	G
1	A23S	2298	A
1	A23S	2299	A
1	A23S	2300	A
1	A23S	2302	A
1	A23S	2313	A
1	A23S	2319	G
1	A23S	2327	A
1	A23S	2328	A
1	A23S	2337	A
1	A23S	2346	A
1	A23S	2359	G
1	A23S	2367	G
1	A23S	2371	G
1	A23S	2379	A
1	A23S	2381	U
1	A23S	2382	C
1	A23S	2390	A

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Mol	Chain	Res	Type
1	A23S	2391	A
1	A23S	2397	C
1	A23S	2401	G
1	A23S	2405	C
1	A23S	2409	A
1	A23S	2410	A
1	A23S	2427	A
1	A23S	2428	C
1	A23S	2429	A
1	A23S	2430	G
1	A23S	2431	A
1	A23S	2434	G
1	A23S	2437	G
1	A23S	2442	A
1	A23S	2444	A
1	A23S	2449	A
1	A23S	2455	A
1	A23S	2457	A
1	A23S	2465	C
1	A23S	2467	G
1	A23S	2500	G
1	A23S	2502	A
1	A23S	2504	G
1	A23S	2505	C
1	A23S	2507	G
1	A23S	2508	G
1	A23S	2526	G
1	A23S	2527	C
1	A23S	2531	C
1	A23S	2532	A
1	A23S	2551	G
1	A23S	2552	A
1	A23S	2554	A
1	A23S	2555	G
1	A23S	2558	A
1	A23S	2565	C
1	A23S	2571	G
1	A23S	2572	A
1	A23S	2573	U
1	A23S	2583	G
1	A23S	2594	G
1	A23S	2596	G

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Mol	Chain	Res	Type
1	A23S	2599	C
1	A23S	2600	A
1	A23S	2602	A
1	A23S	2610	C
1	A23S	2616	U
1	A23S	2618	G
1	A23S	2621	A
1	A23S	2622	C
1	A23S	2627	A
1	A23S	2628	U
1	A23S	2641	C
1	A23S	2642	A
1	A23S	2653	G
1	A23S	2655	A
1	A23S	2671	A
1	A23S	2678	C
1	A23S	2686	U
1	A23S	2688	A
1	A23S	2690	A
1	A23S	2691	G
1	A23S	2694	G
1	A23S	2696	G
1	A23S	2697	C
1	A23S	2700	G
1	A23S	2702	G
1	A23S	2705	G
1	A23S	2706	G
1	A23S	2707	G
1	A23S	2709	U
1	A23S	2722	A
1	A23S	2723	G
1	A23S	2726	A
1	A23S	2727	G
1	A23S	2737	U
1	A23S	2738	A
1	A23S	2754	G
1	A23S	2756	C
1	A23S	2762	G
1	A23S	2763	A
1	A23S	2764	G
1	A23S	2769	A
1	A23S	2770	G

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Mol	Chain	Res	Type
1	A23S	2781	U
1	A23S	2814	U
1	A23S	2815	A
1	A23S	2835	A
1	A23S	2836	U
1	A23S	2837	G
1	A23S	2848	G
1	A23S	2849	C
1	A23S	2855	G
1	A23S	2861	U
1	A23S	2869	G
1	A23S	2870	A
1	A23S	2872	A
1	A23S	2879	A
1	A23S	2880	A
1	A23S	2886	A
1	A23S	2888	C
1	A23S	2891	C
1	A23S	2896	C
1	A23S	2898	A
1	A23S	2899	A
1	A23S	2900	A
1	A23S	2924	G
1	A23S	2934	U
1	A23S	2947	U
1	A23S	2949	A
1	A23S	2950	U
1	A23S	2963	U
1	A23S	2973	G
1	A23S	2976	U
1	A23S	2983	C
1	A23S	2994	A
1	A23S	2995	G
1	A23S	2999	G
1	A23S	3000	C
1	A23S	3005	C
1	A23S	3017	C
1	A23S	3019	C
2	A16S	11	C
2	A16S	39	A
2	A16S	41	C
2	A16S	47	A

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Mol	Chain	Res	Type
2	A16S	48	G
2	A16S	49	G
2	A16S	50	G
2	A16S	53	A
2	A16S	54	A
2	A16S	57	C
2	A16S	60	G
2	A16S	64	G
2	A16S	73	U
2	A16S	77	G
2	A16S	78	G
2	A16S	79	G
2	A16S	80	U
2	A16S	81	A
2	A16S	82	A
2	A16S	86	A
2	A16S	96	A
2	A16S	103	A
2	A16S	107	A
2	A16S	108	C
2	A16S	111	G
2	A16S	113	G
2	A16S	114	G
2	A16S	115	C
2	A16S	117	A
2	A16S	118	A
2	A16S	119	C
2	A16S	130	G
2	A16S	132	C
2	A16S	139	A
2	A16S	148	A
2	A16S	149	A
2	A16S	150	A
2	A16S	151	C
2	A16S	152	U
2	A16S	159	A
2	A16S	161	U
2	A16S	177	A
2	A16S	180	C
2	A16S	186	A
2	A16S	187	U
2	A16S	200	A

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Mol	Chain	Res	Type
2	A16S	202	A
2	A16S	205	G
2	A16S	212	G
2	A16S	213	C
2	A16S	214	U
2	A16S	220	C
2	A16S	221	C
2	A16S	222	G
2	A16S	223	U
2	A16S	224	U
2	A16S	252	C
2	A16S	256	U
2	A16S	257	C
2	A16S	258	A
2	A16S	259	G
2	A16S	263	G
2	A16S	270	G
2	A16S	274	A
2	A16S	278	G
2	A16S	279	C
2	A16S	292	U
2	A16S	294	A
2	A16S	301	G
2	A16S	313	G
2	A16S	327	U
2	A16S	328	U
2	A16S	333	A
2	A16S	337	A
2	A16S	340	C
2	A16S	341	A
2	A16S	342	A
2	A16S	344	G
2	A16S	355	U
2	A16S	356	A
2	A16S	357	C
2	A16S	358	G
2	A16S	359	G
2	A16S	362	C
2	A16S	363	G
2	A16S	364	C
2	A16S	365	A
2	A16S	366	C

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Mol	Chain	Res	Type
2	A16S	368	A
2	A16S	377	A
2	A16S	378	C
2	A16S	379	G
2	A16S	380	U
2	A16S	381	C
2	A16S	385	A
2	A16S	386	A
2	A16S	389	C
2	A16S	405	C
2	A16S	409	A
2	A16S	410	C
2	A16S	418	G
2	A16S	435	U
2	A16S	436	U
2	A16S	437	U
2	A16S	443	C
2	A16S	444	U
2	A16S	445	C
2	A16S	446	U
2	A16S	447	A
2	A16S	449	A
2	A16S	452	G
2	A16S	459	G
2	A16S	461	A
2	A16S	462	U
2	A16S	463	A
2	A16S	472	G
2	A16S	473	C
2	A16S	474	A
2	A16S	475	A
2	A16S	476	G
2	A16S	477	U
2	A16S	480	G
2	A16S	483	G
2	A16S	484	U
2	A16S	485	C
2	A16S	487	G
2	A16S	490	G
2	A16S	491	C
2	A16S	493	G
2	A16S	495	G

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Mol	Chain	Res	Type
2	A16S	496	G
2	A16S	497	U
2	A16S	498	A
2	A16S	499	A
2	A16S	513	A
2	A16S	526	A
2	A16S	527	U
2	A16S	530	C
2	A16S	538	A
2	A16S	539	A
2	A16S	542	C
2	A16S	543	G
2	A16S	554	G
2	A16S	562	A
2	A16S	563	G
2	A16S	596	A
2	A16S	597	C
2	A16S	598	U
2	A16S	608	A
2	A16S	615	G
2	A16S	619	A
2	A16S	627	G
2	A16S	631	A
2	A16S	652	U
2	A16S	654	G
2	A16S	659	G
2	A16S	668	A
2	A16S	669	G
2	A16S	683	C
2	A16S	684	A
2	A16S	685	C
2	A16S	689	U
2	A16S	690	G
2	A16S	695	A
2	A16S	697	G
2	A16S	714	G
2	A16S	715	C
2	A16S	721	G
2	A16S	731	G
2	A16S	732	A
2	A16S	747	A
2	A16S	759	U

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Mol	Chain	Res	Type
2	A16S	760	A
2	A16S	765	G
2	A16S	775	G
2	A16S	779	U
2	A16S	781	A
2	A16S	783	C
2	A16S	784	G
2	A16S	785	A
2	A16S	787	G
2	A16S	793	U
2	A16S	794	A
2	A16S	810	U
2	A16S	811	A
2	A16S	812	G
2	A16S	813	A
2	A16S	814	G
2	A16S	816	C
2	A16S	841	U
2	A16S	842	A
2	A16S	843	A
2	A16S	846	C
2	A16S	861	U
2	A16S	872	G
2	A16S	884	A
2	A16S	890	U
2	A16S	891	U
2	A16S	892	G
2	A16S	896	G
2	A16S	897	G
2	A16S	898	G
2	A16S	900	A
2	A16S	902	C
2	A16S	903	A
2	A16S	904	C
2	A16S	905	C
2	A16S	906	A
2	A16S	911	G
2	A16S	916	G
2	A16S	930	A
2	A16S	931	U
2	A16S	932	U
2	A16S	936	G

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Mol	Chain	Res	Type
2	A16S	937	U
2	A16S	940	A
2	A16S	942	G
2	A16S	945	U
2	A16S	946	G
2	A16S	947	G
2	A16S	954	A
2	A16S	955	C
2	A16S	959	G
2	A16S	961	G
2	A16S	963	G
2	A16S	965	C
2	A16S	971	U
2	A16S	973	U
2	A16S	974	G
2	A16S	975	A
2	A16S	976	C
2	A16S	980	C
2	A16S	984	C
2	A16S	985	U
2	A16S	986	A
2	A16S	988	C
2	A16S	989	G
2	A16S	990	A
2	A16S	995	G
2	A16S	997	C
2	A16S	998	U
2	A16S	1000	A
2	A16S	1001	C
2	A16S	1002	U
2	A16S	1003	C
2	A16S	1004	G
2	A16S	1005	C
2	A16S	1010	A
2	A16S	1014	G
2	A16S	1017	G
2	A16S	1018	C
2	A16S	1029	C
2	A16S	1032	G
2	A16S	1041	G
2	A16S	1042	U
2	A16S	1043	G

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Mol	Chain	Res	Type
2	A16S	1044	A
2	A16S	1045	A
2	A16S	1047	U
2	A16S	1048	G
2	A16S	1049	U
2	A16S	1053	G
2	A16S	1058	G
2	A16S	1059	U
2	A16S	1061	C
2	A16S	1062	G
2	A16S	1063	G
2	A16S	1065	A
2	A16S	1066	A
2	A16S	1068	G
2	A16S	1084	C
2	A16S	1088	G
2	A16S	1089	U
2	A16S	1090	U
2	A16S	1091	G
2	A16S	1093	U
2	A16S	1094	A
2	A16S	1095	U
2	A16S	1098	U
2	A16S	1099	G
2	A16S	1102	C
2	A16S	1103	U
2	A16S	1104	C
2	A16S	1105	C
2	A16S	1106	G
2	A16S	1109	C
2	A16S	1114	A
2	A16S	1117	A
2	A16S	1118	C
2	A16S	1119	A
2	A16S	1123	G
2	A16S	1128	A
2	A16S	1129	C
2	A16S	1130	U
2	A16S	1136	C
2	A16S	1137	G
2	A16S	1138	U
2	A16S	1139	A

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Mol	Chain	Res	Type
2	A16S	1142	C
2	A16S	1152	G
2	A16S	1153	A
2	A16S	1154	G
2	A16S	1160	C
2	A16S	1163	G
2	A16S	1166	A
2	A16S	1167	G
2	A16S	1170	C
2	A16S	1171	A
2	A16S	1172	G
2	A16S	1181	G
2	A16S	1182	A
2	A16S	1183	A
2	A16S	1186	U
2	A16S	1187	C
2	A16S	1188	C
2	A16S	1193	C
2	A16S	1195	G
2	A16S	1196	C
2	A16S	1203	G
2	A16S	1208	A
2	A16S	1211	G
2	A16S	1214	A
2	A16S	1226	A
2	A16S	1228	G
2	A16S	1230	U
2	A16S	1232	C
2	A16S	1234	U
2	A16S	1238	A
2	A16S	1240	G
2	A16S	1244	G
2	A16S	1247	C
2	A16S	1248	C
2	A16S	1249	A
2	A16S	1250	A
2	A16S	1251	U
2	A16S	1252	C
2	A16S	1253	C
2	A16S	1254	U
2	A16S	1255	U
2	A16S	1256	A

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Mol	Chain	Res	Type
2	A16S	1257	A
2	A16S	1262	U
2	A16S	1263	G
2	A16S	1267	C
2	A16S	1268	A
2	A16S	1269	G
2	A16S	1270	U
2	A16S	1271	U
2	A16S	1272	G
2	A16S	1274	G
2	A16S	1277	C
2	A16S	1288	A
2	A16S	1289	C
2	A16S	1291	C
2	A16S	1305	A
2	A16S	1315	A
2	A16S	1316	G
2	A16S	1317	U
2	A16S	1327	U
2	A16S	1328	C
2	A16S	1329	A
2	A16S	1330	A
2	A16S	1332	A
2	A16S	1333	A
2	A16S	1343	A
2	A16S	1344	A
2	A16S	1345	U
2	A16S	1347	C
2	A16S	1348	G
2	A16S	1350	C
2	A16S	1351	C
2	A16S	1353	U
2	A16S	1355	C
2	A16S	1363	A
2	A16S	1364	C
2	A16S	1365	A
2	A16S	1366	C
2	A16S	1367	A
2	A16S	1368	C
2	A16S	1369	C
2	A16S	1374	G
2	A16S	1388	G

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Mol	Chain	Res	Type
2	A16S	1414	A
2	A16S	1416	A
2	A16S	1430	A
2	A16S	1443	G
2	A16S	1451	A
2	A16S	1454	A
2	A16S	1460	A
2	A16S	1464	A
2	A16S	1465	G
2	A16S	1466	G
2	A16S	1467	U
2	A16S	1468	A
2	A16S	1480	A
2	A16S	1481	C
2	A16S	1490	G
2	A16S	1491	G
2	A16S	1492	A
2	A16S	1493	U
2	A16S	1494	C
2	A16S	1497	C
2	A16S	1500	A
2	A16S	1501	U
4	A5S	5	C
4	A5S	10	G
4	A5S	25	G
4	A5S	27	A
4	A5S	42	U
4	A5S	43	U
4	A5S	45	G
4	A5S	46	A
4	A5S	58	A
4	A5S	59	A
4	A5S	68	C
4	A5S	88	C
4	A5S	93	A
4	A5S	102	A
4	A5S	107	C
4	A5S	111	G
4	A5S	113	G
4	A5S	114	C
4	A5S	118	G
4	A5S	119	A

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Mol	Chain	Res	Type
66	APTN	7	A
66	APTN	8	U
66	APTN	17	C
66	APTN	18	G
66	APTN	20	U
66	APTN	21	A
66	APTN	22	G
66	APTN	44	G
66	APTN	48	C
66	APTN	49	C
66	APTN	52	G
66	APTN	58	A
66	APTN	61	C
66	APTN	64	A
66	APTN	65	G
66	APTN	66	U
66	APTN	67	C
66	APTN	68	C
66	APTN	70	G
66	APTN	76	A
66	AETN	2	C
66	AETN	3	C
66	AETN	7	A
66	AETN	8	U
66	AETN	9	A
66	AETN	10	G
66	AETN	13	C
66	AETN	17	C
66	AETN	19	G
66	AETN	20	U
66	AETN	21	A
66	AETN	26	A
66	AETN	31	A
66	AETN	32	U
66	AETN	35	A
66	AETN	42	C
66	AETN	43	C
66	AETN	45	U
66	AETN	46	G
66	AETN	47	U
66	AETN	48	C
66	AETN	49	C

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Mol	Chain	Res	Type
66	AETN	52	G
66	AETN	55	U
66	AETN	56	C
66	AETN	58	A
66	AETN	59	U
66	AETN	60	U
66	AETN	61	C
66	AETN	65	G
66	AETN	67	C
66	AETN	73	A
66	AETN	74	C
66	AETN	76	A
67	AMRN	-2	U
67	AMRN	-1	U
67	AMRN	1	U
67	AMRN	4	U

All (95) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A23S	136	U
1	A23S	146	U
1	A23S	280	G
1	A23S	336	A
1	A23S	382	U
1	A23S	402	A
1	A23S	404	U
1	A23S	574	G
1	A23S	656	C
1	A23S	658	U
1	A23S	668	A
1	A23S	740	G
1	A23S	808	A
1	A23S	920	G
1	A23S	1003	G
1	A23S	1179	C
1	A23S	1198	G
1	A23S	1327	U
1	A23S	1500	U
1	A23S	1529	A
1	A23S	1646	G
1	A23S	1647	A

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Mol	Chain	Res	Type
1	A23S	1689	C
1	A23S	1706	U
1	A23S	1750	A
1	A23S	2046	U
1	A23S	2148	C
1	A23S	2240	C
1	A23S	2504	G
1	A23S	2835	A
1	A23S	2878	U
1	A23S	2923	G
2	A16S	47	A
2	A16S	49	G
2	A16S	63	A
2	A16S	102	G
2	A16S	117	A
2	A16S	138	U
2	A16S	179	U
2	A16S	220	C
2	A16S	255	A
2	A16S	262	U
2	A16S	293	A
2	A16S	340	C
2	A16S	364	C
2	A16S	384	C
2	A16S	444	U
2	A16S	445	C
2	A16S	471	G
2	A16S	475	A
2	A16S	484	U
2	A16S	526	A
2	A16S	541	G
2	A16S	653	A
2	A16S	758	A
2	A16S	778	G
2	A16S	786	U
2	A16S	883	A
2	A16S	936	G
2	A16S	972	A
2	A16S	973	U
2	A16S	987	A
2	A16S	989	G
2	A16S	997	C

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Mol	Chain	Res	Type
2	A16S	1000	A
2	A16S	1013	A
2	A16S	1065	A
2	A16S	1088	G
2	A16S	1093	U
2	A16S	1116	C
2	A16S	1138	U
2	A16S	1151	G
2	A16S	1152	G
2	A16S	1153	A
2	A16S	1166	A
2	A16S	1171	A
2	A16S	1227	U
2	A16S	1254	U
2	A16S	1269	G
2	A16S	1270	U
2	A16S	1316	G
2	A16S	1328	C
2	A16S	1329	A
2	A16S	1332	A
2	A16S	1349	U
2	A16S	1429	A
2	A16S	1442	C
2	A16S	1459	U
2	A16S	1489	U
2	A16S	1492	A
4	A5S	57	U
66	APTN	19	G
66	AETN	2	C
66	AETN	8	U
66	AETN	45	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 58 ligands modelled in this entry, 57 are unknown - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
69	GNP	AEFG	801	-	29,34,34	1.54	7 (24%)	33,54,54	2.13	6 (18%)

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
69	GNP	AEFG	801	-	-	4/14/38/38	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	AEFG	801	GNP	PB-O3A	3.73	1.63	1.59
69	AEFG	801	GNP	PG-N3B	3.12	1.71	1.63
69	AEFG	801	GNP	C6-N1	2.96	1.38	1.33
69	AEFG	801	GNP	PB-O1B	2.89	1.50	1.46
69	AEFG	801	GNP	PG-O1G	2.40	1.50	1.46
69	AEFG	801	GNP	PB-O2B	-2.31	1.50	1.56
69	AEFG	801	GNP	C5-C6	2.04	1.44	1.41

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
69	AEFG	801	GNP	C5-C6-N1	-8.31	112.07	123.43
69	AEFG	801	GNP	C2-N1-C6	5.79	125.13	115.93
69	AEFG	801	GNP	PB-O3A-PA	-3.15	121.51	132.62
69	AEFG	801	GNP	N3-C2-N1	-2.84	123.43	127.22
69	AEFG	801	GNP	C4-C5-C6	-2.65	118.26	120.80
69	AEFG	801	GNP	C2-N3-C4	-2.14	112.91	115.36

There are no chirality outliers.

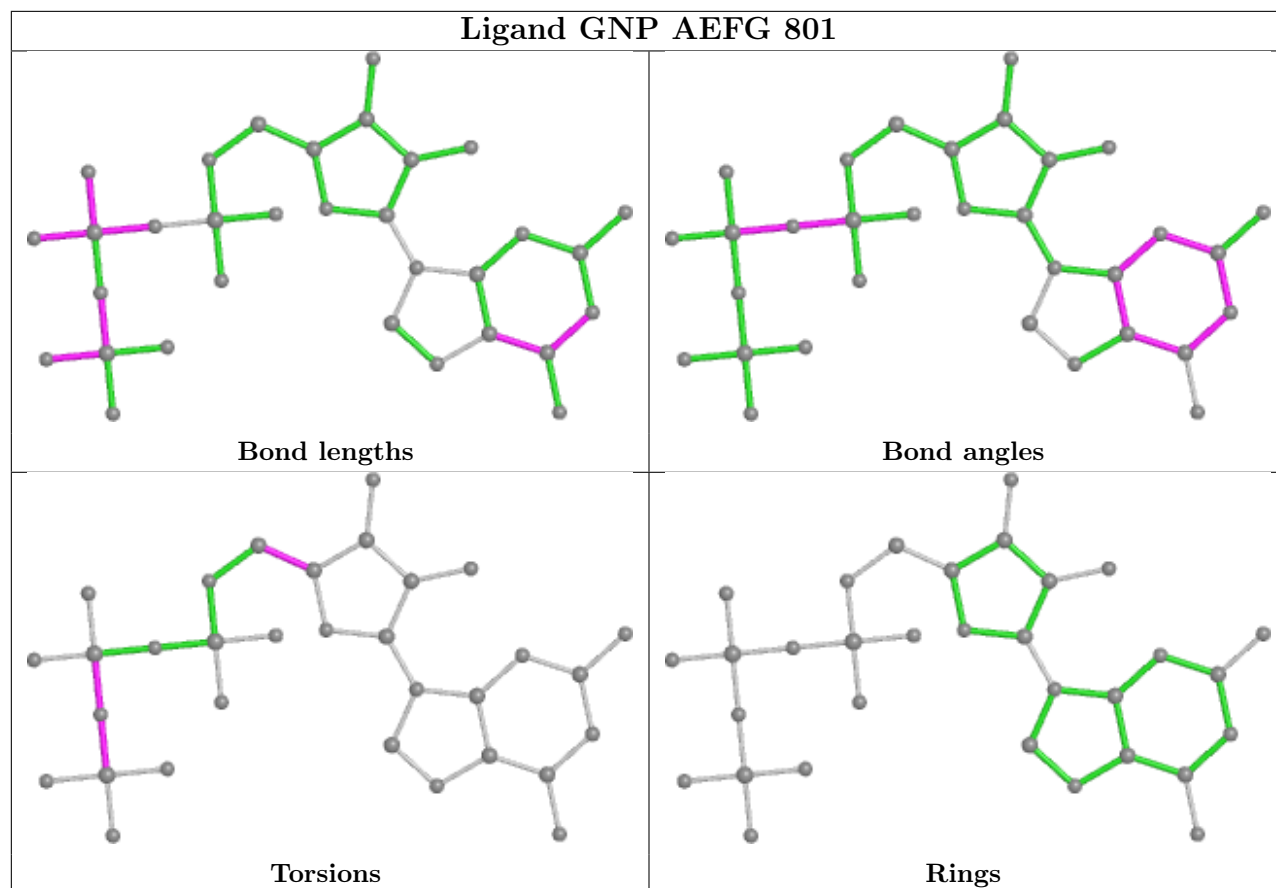
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
69	AEFG	801	GNP	PB-N3B-PG-O1G
69	AEFG	801	GNP	PG-N3B-PB-O1B
69	AEFG	801	GNP	O4'-C4'-C5'-O5'
69	AEFG	801	GNP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

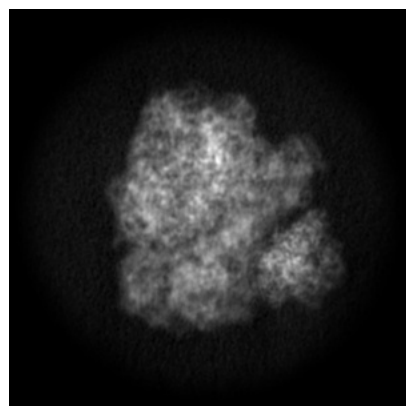
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34868. These allow visual inspection of the internal detail of the map and identification of artifacts.

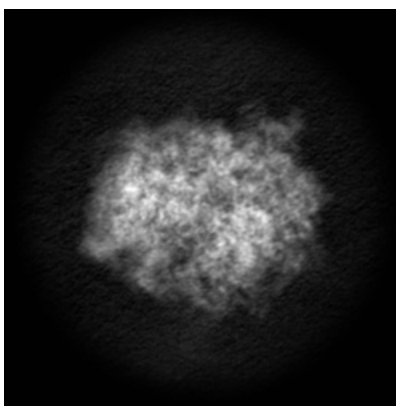
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

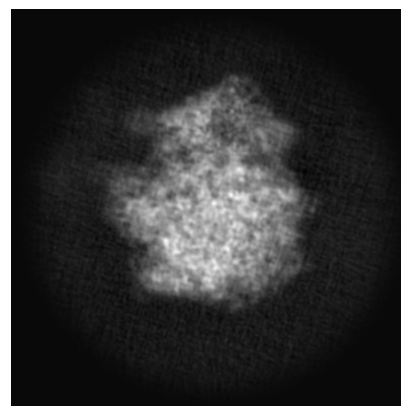
6.1.1 Primary map



X

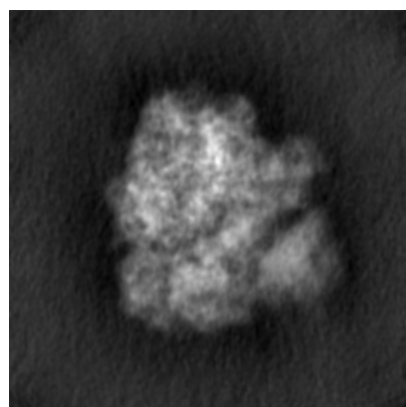


Y

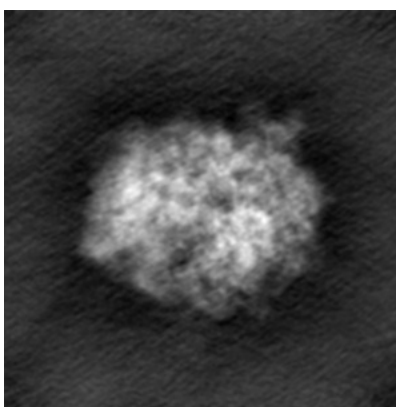


Z

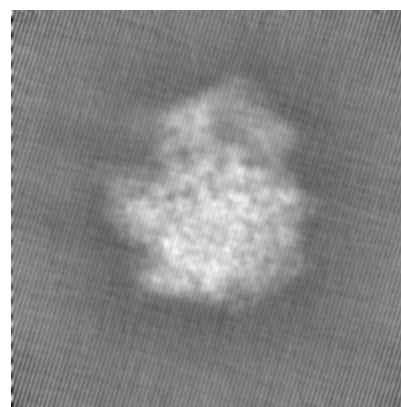
6.1.2 Raw map



X



Y

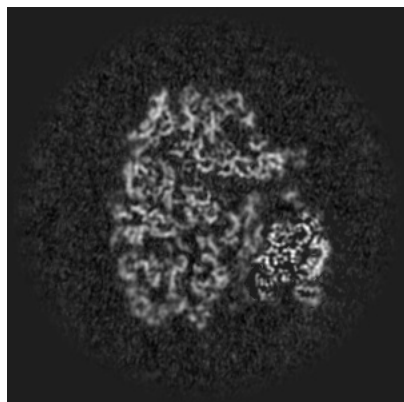


Z

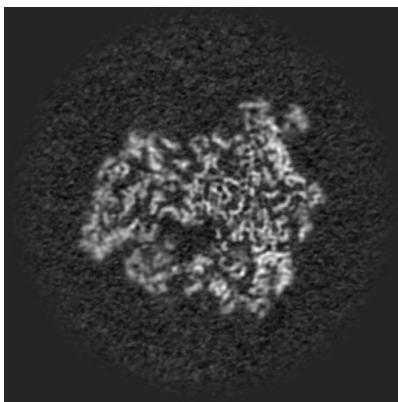
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

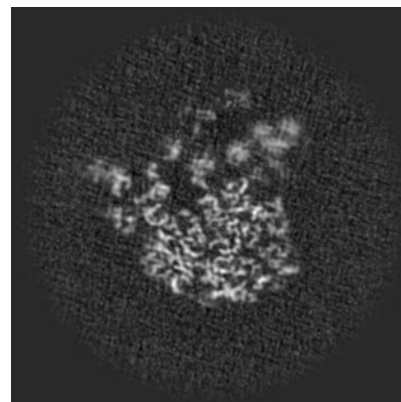
6.2.1 Primary map



X Index: 190

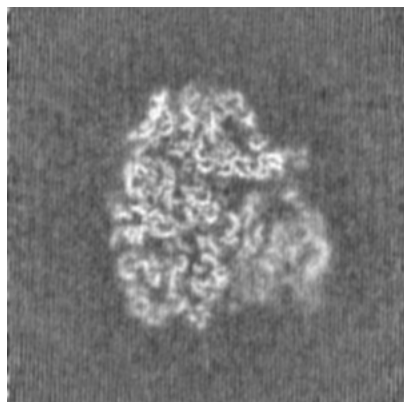


Y Index: 190

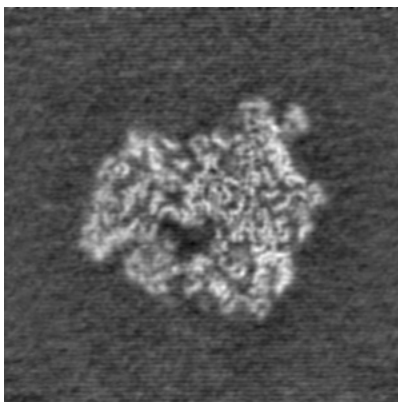


Z Index: 190

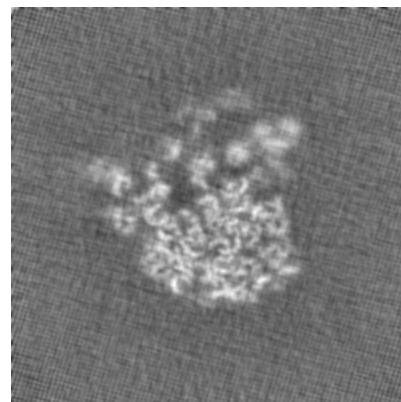
6.2.2 Raw map



X Index: 190



Y Index: 190

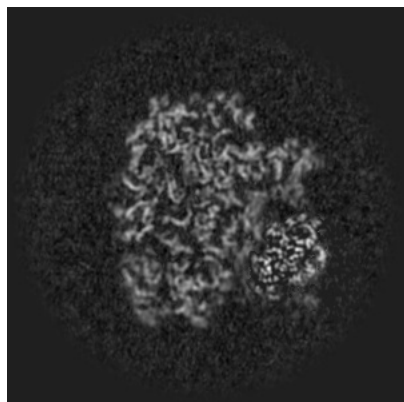


Z Index: 190

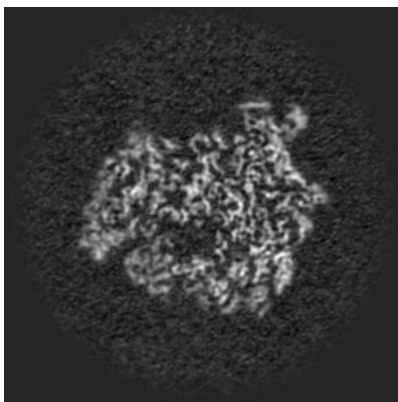
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

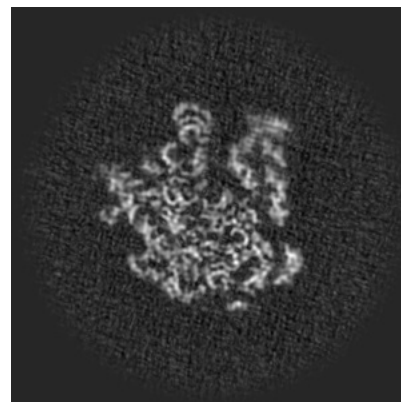
6.3.1 Primary map



X Index: 185

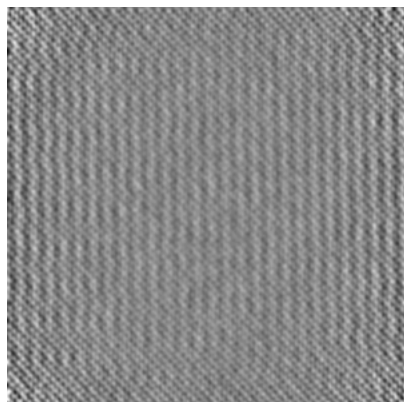


Y Index: 188

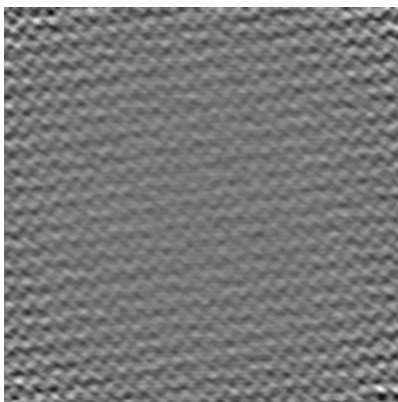


Z Index: 205

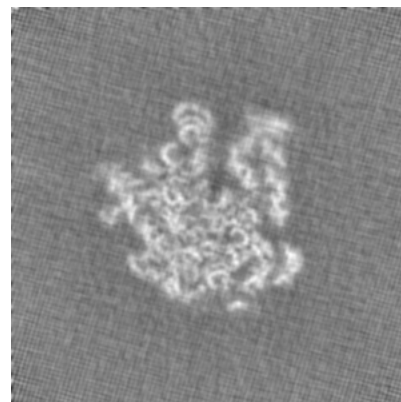
6.3.2 Raw map



X Index: 0



Y Index: 0

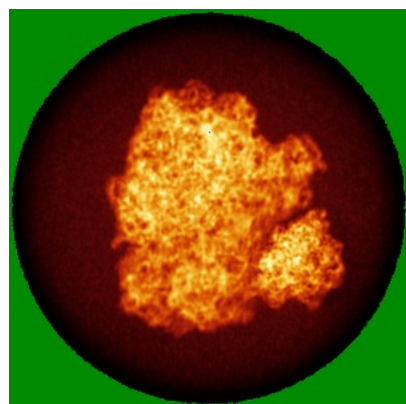


Z Index: 205

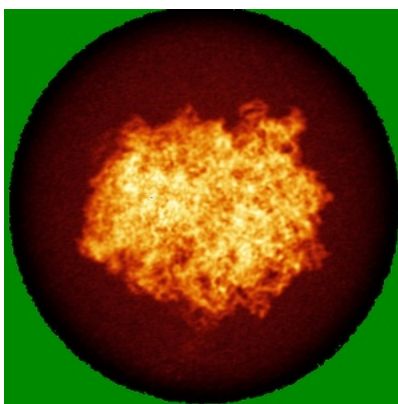
The images above show the largest variance slices of the map in three orthogonal directions.

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

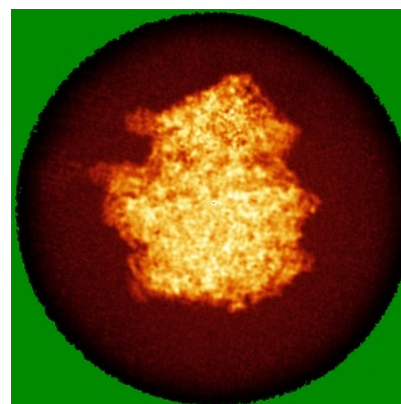
6.4.1 Primary map



X

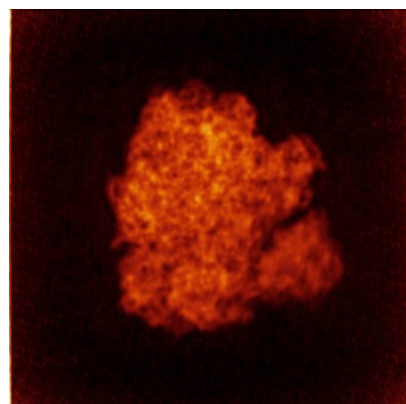


Y

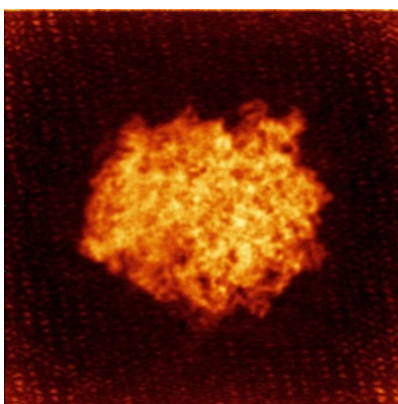


Z

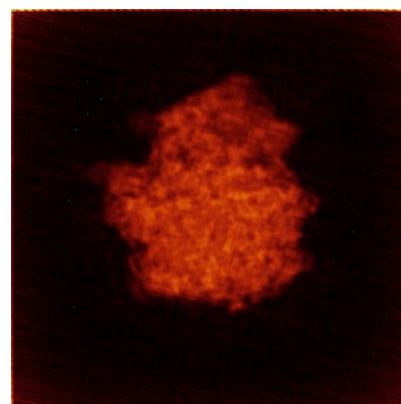
6.4.2 Raw map



X



Y

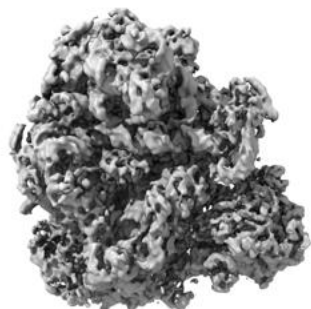


Z

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](#)

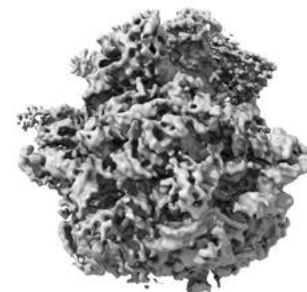
6.5.1 Primary map



X



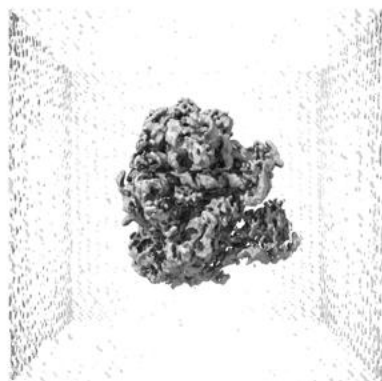
Y



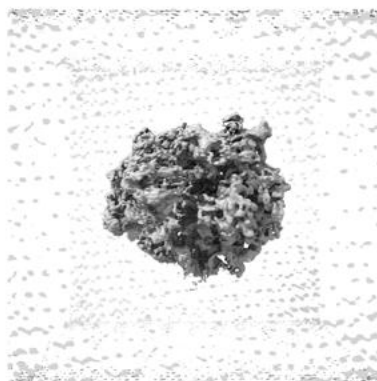
Z

The images above show the 3D surface view of the map at the recommended contour level 0.335. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

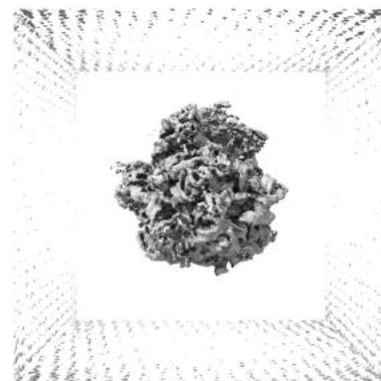
6.5.2 Raw map



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.

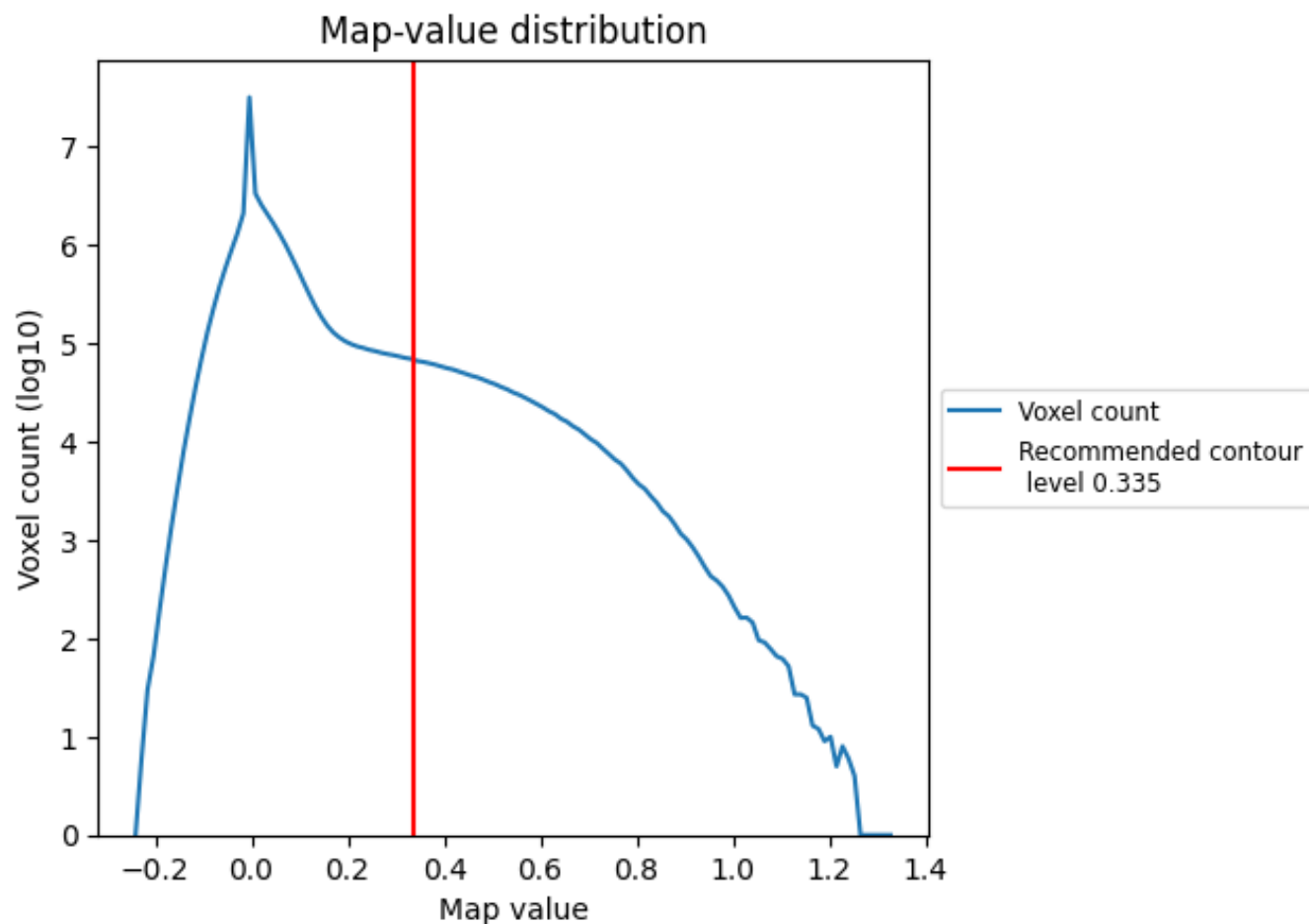
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

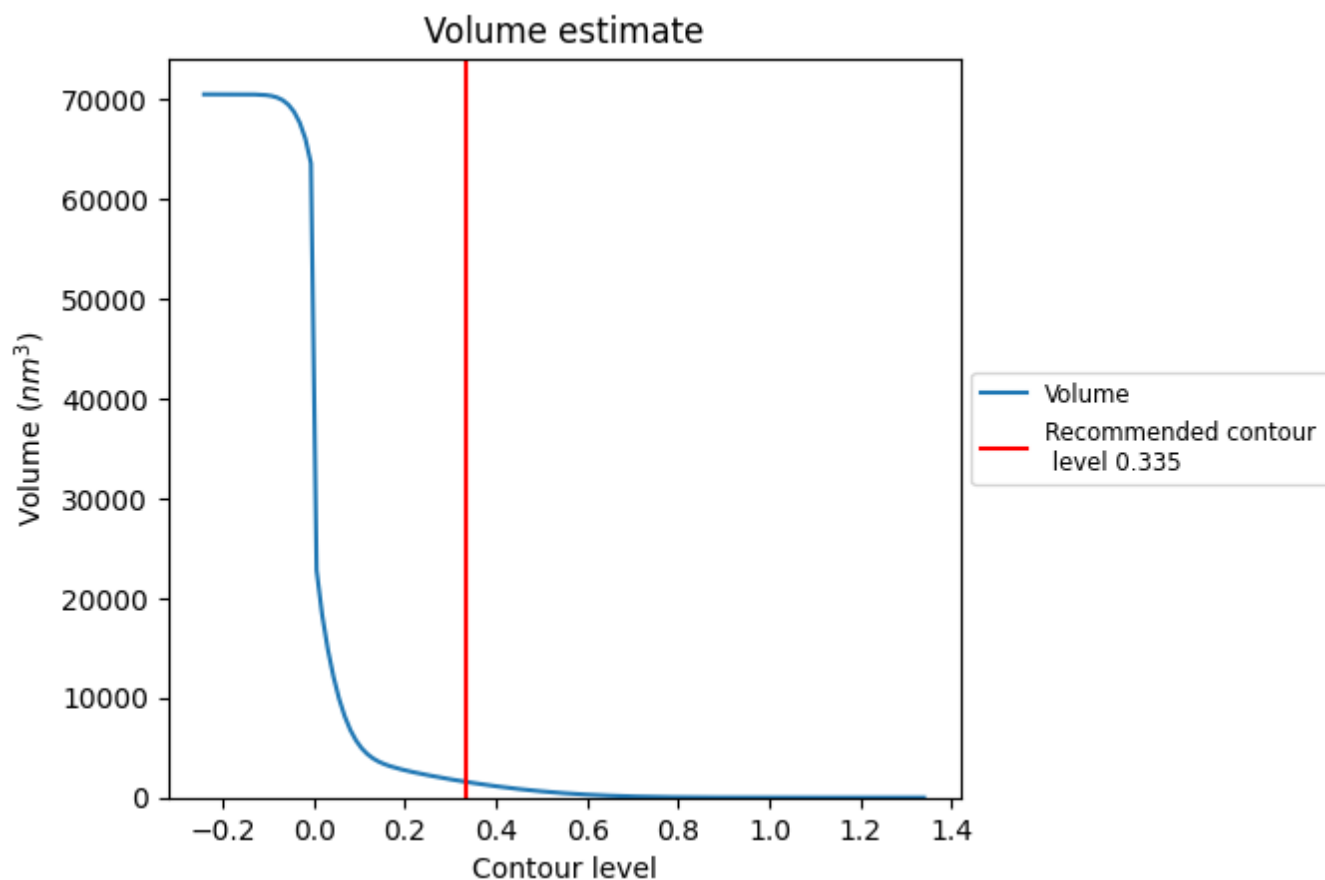
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

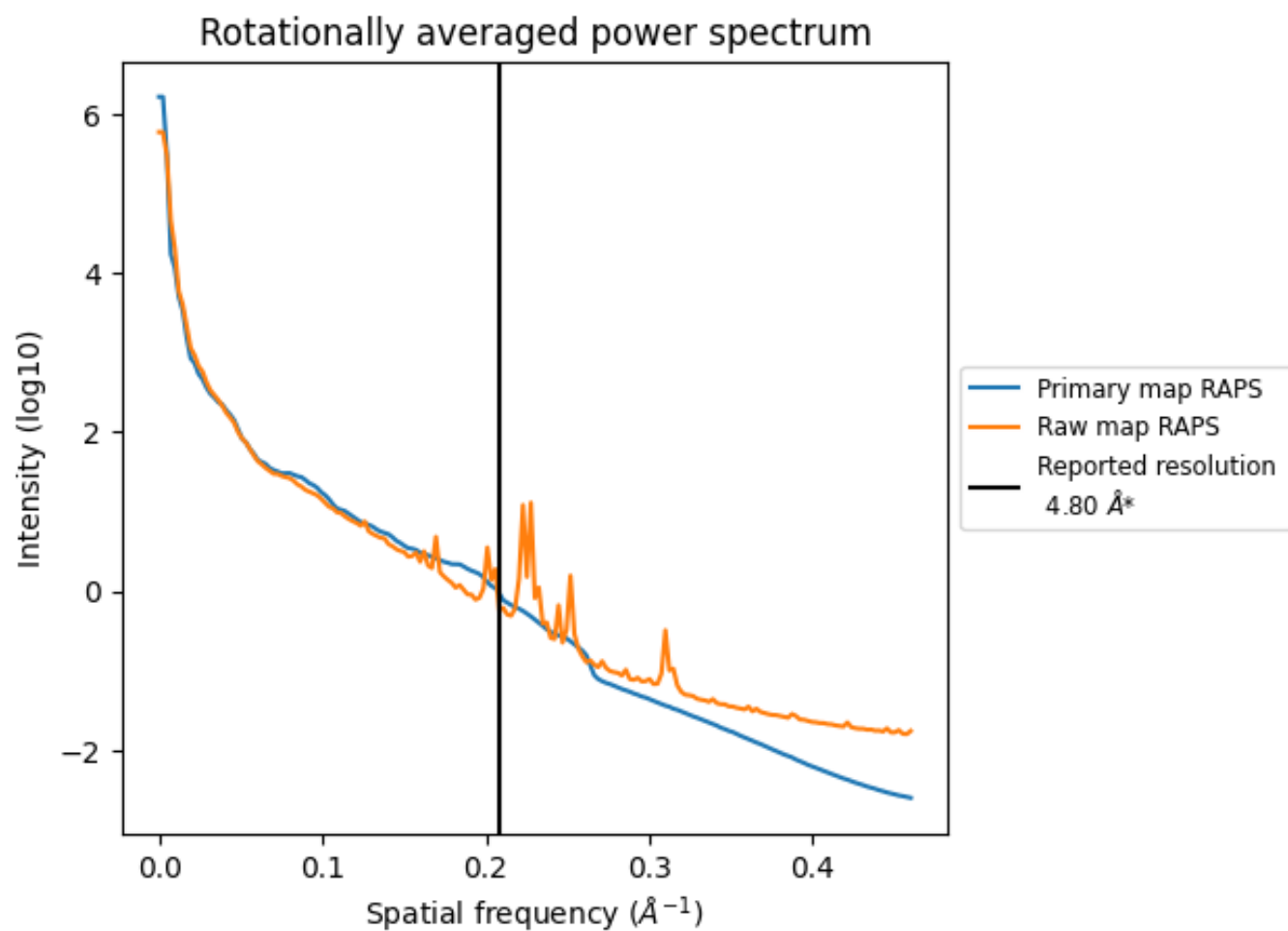
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1568 nm³; this corresponds to an approximate mass of 1417 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

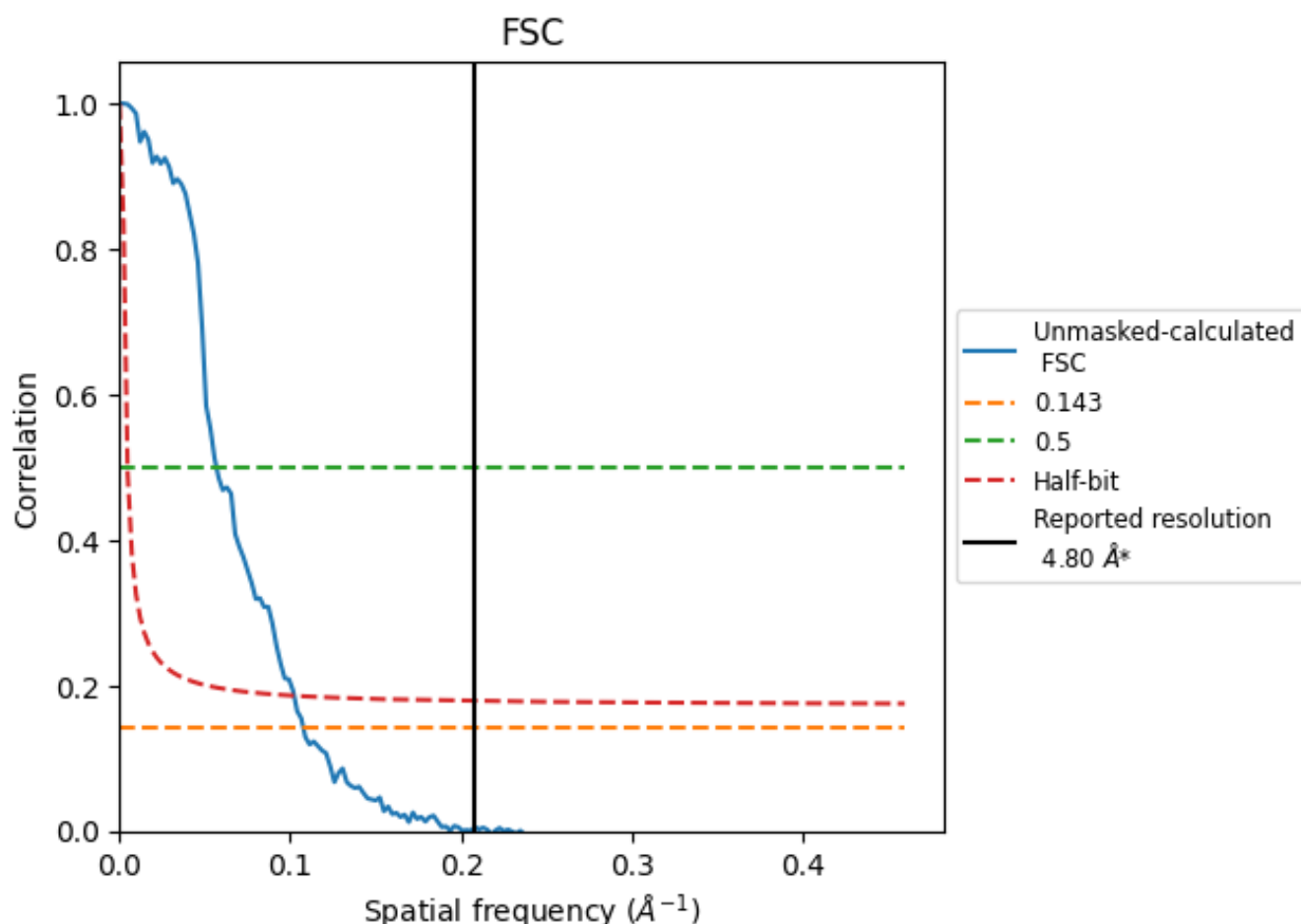


*Reported resolution corresponds to spatial frequency of 0.208 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.208 \AA^{-1}

8.2 Resolution estimates [i](#)

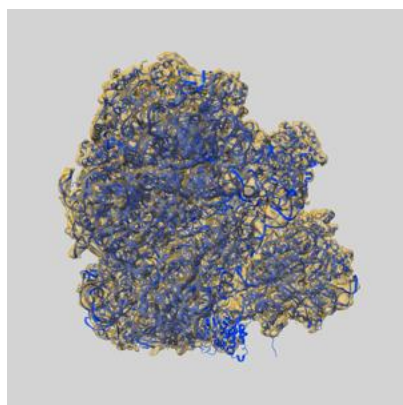
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.29	17.61	9.78

*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 9.29 differs from the reported value 4.8 by more than 10 %

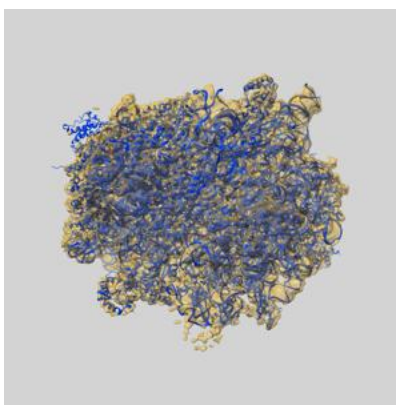
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-34868 and PDB model 8HL3. Per-residue inclusion information can be found in section 3 on page 17.

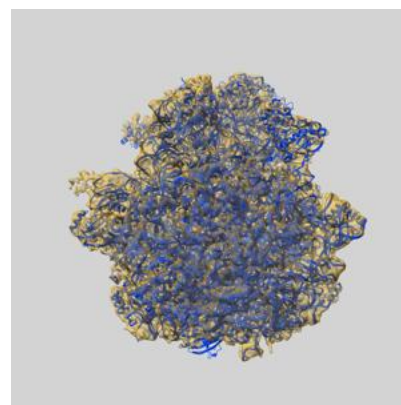
9.1 Map-model overlay [i](#)



X



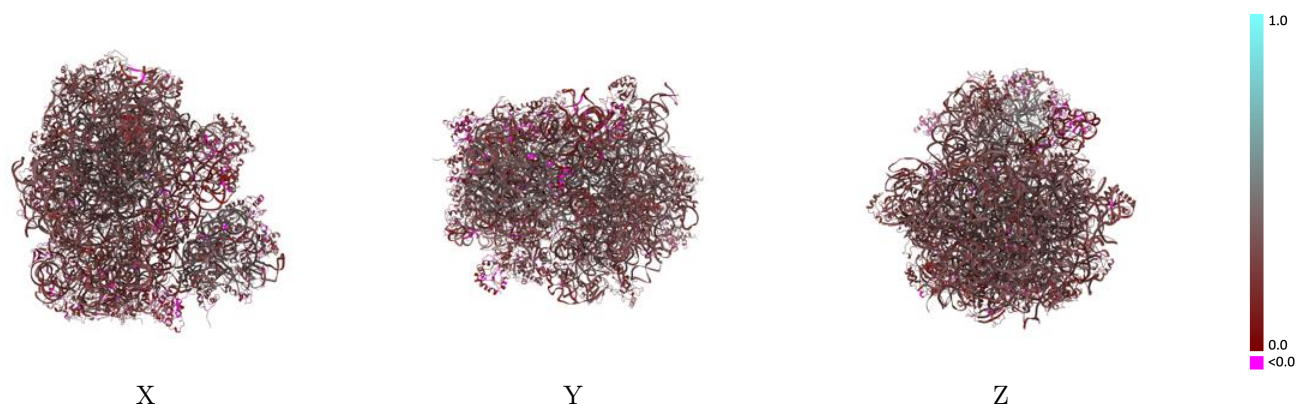
Y



Z

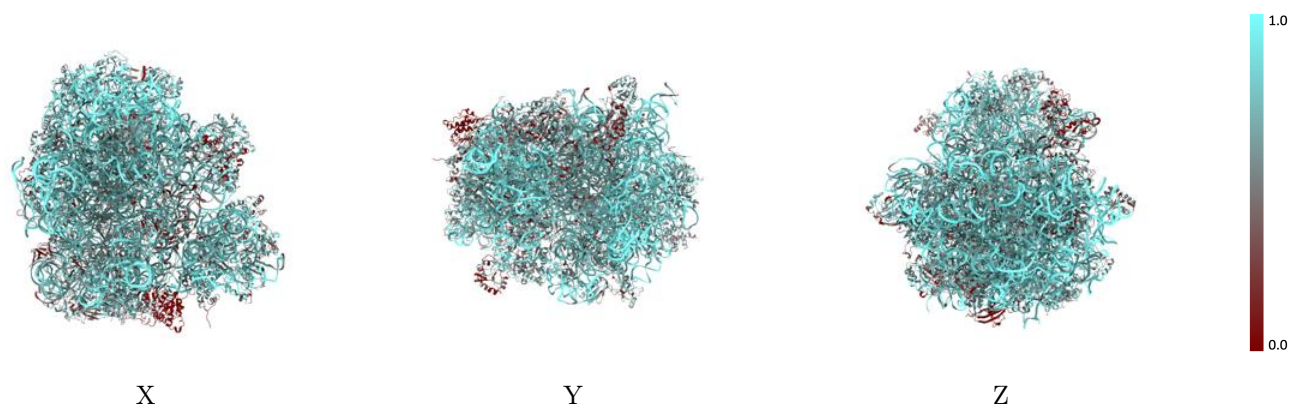
The images above show the 3D surface view of the map at the recommended contour level 0.335 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



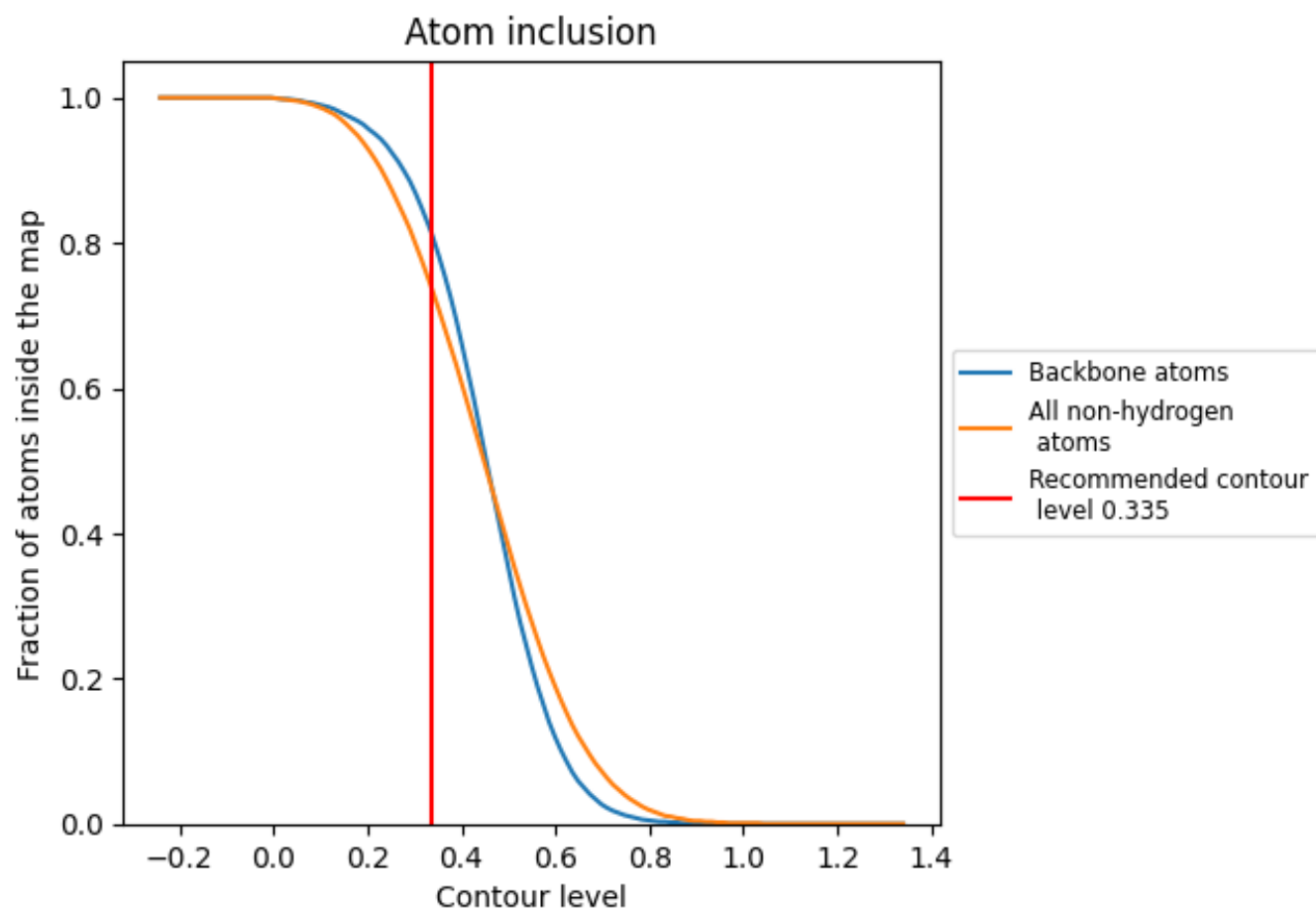
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.335).







































































9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 74% 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 (0.335) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7410	 0.2800
A16S	 0.8680	 0.2880
A23S	 0.8970	 0.3110
A5S	 0.9530	 0.3070
AEFG	 0.5210	 0.2300
AETN	 0.6420	 0.2070
AL1P	 0.2140	 0.1460
AL2P	 0.5250	 0.2920
AL3P	 0.5990	 0.2800
AL4P	 0.6000	 0.2790
AL5P	 0.5650	 0.2510
AL6P	 0.5700	 0.2640
ALX0	 0.5770	 0.2370
AMRN	 0.4270	 0.2160
APTN	 0.7640	 0.2460
APTP	 0.0600	 0.1340
AS2P	 0.0150	 0.1510
AS3P	 0.6280	 0.3560
AS4E	 0.5350	 0.2080
AS4P	 0.5480	 0.2140
AS5P	 0.4800	 0.2470
AS6E	 0.4030	 0.1890
AS7P	 0.5430	 0.2350
AS8E	 0.3090	 0.1870
AS8P	 0.6240	 0.2500
AS9P	 0.6830	 0.3530
L10E	 0.5720	 0.2760
L13P	 0.5920	 0.2440
L141	 0.6100	 0.2500
L142	 0.5750	 0.2440
L14P	 0.4510	 0.2740
L15E	 0.5660	 0.2750
L15P	 0.6510	 0.2760
L18E	 0.6680	 0.2810
L18P	 0.6350	 0.2570



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Chain	Atom inclusion	Q-score
L19E	 0.6420	 0.2730
L21E	 0.6080	 0.3040
L22P	 0.5760	 0.2740
L23P	 0.6050	 0.2750
L24E	 0.6530	 0.2920
L24P	 0.6540	 0.2670
L29P	 0.5990	 0.2370
L30E	 0.6470	 0.2730
L30P	 0.6150	 0.2440
L31E	 0.6310	 0.2870
L32E	 0.5010	 0.2790
L34E	 0.4700	 0.2070
L37A	 0.5860	 0.2710
L37E	 0.5660	 0.2760
L39E	 0.5700	 0.2450
L40E	 0.4290	 0.2110
L44E	 0.6560	 0.2810
L45A	 0.5520	 0.2570
L46A	 0.4220	 0.2670
L47A	 0.0380	 0.1890
L7A1	 0.5400	 0.2580
L7A2	 0.4780	 0.2390
S10P	 0.6800	 0.3340
S11P	 0.4000	 0.2340
S12P	 0.4140	 0.2550
S13P	 0.5920	 0.2480
S14P	 0.7570	 0.3900
S15P	 0.5850	 0.2180
S17E	 0.5890	 0.2460
S17P	 0.4360	 0.2330
S19E	 0.6200	 0.2540
S19P	 0.7330	 0.3570
S24E	 0.5230	 0.2150
S27A	 0.6560	 0.1610
S27E	 0.5640	 0.2180
S28E	 0.6360	 0.3410
S3AE	 0.4810	 0.2130
SL7A	 0.3420	 0.1270