



wwPDB EM Validation Summary Report ⓘ

Jan 9, 2024 – 01:45 PM JST

PDB ID : 8HL1
EMDB ID : EMD-34866
Title : Cryo-EM Structures and Translocation Mechanism of Crenarchaeota Ribosome
Authors : Wang, Y.H.; Zhou, J.
Deposited on : 2022-11-28
Resolution : 3.93 Å(reported)

This is a wwPDB EM Validation Summary 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.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

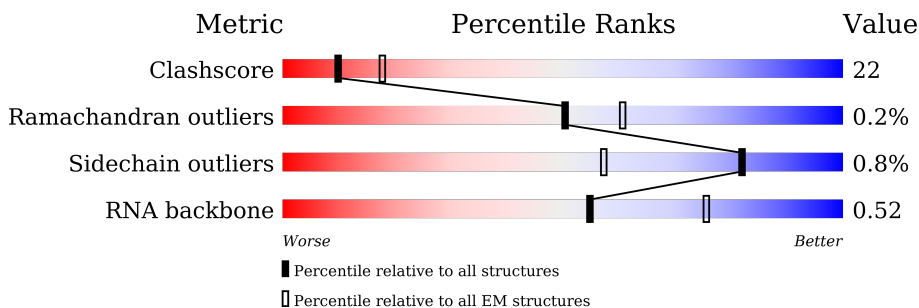
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.93 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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

Mol	Chain	Length	Quality of chain
1	A16S	1494	
2	A23S	3022	
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	12% 99%
9	AL6P	181	8% 100%
10	ALX0	76	13% 100%
11	L10E	164	11% 100%
12	L13P	140	11% 98%
13	L141	86	8% 100%
13	L142	86	9% 100%
14	L14P	134	16% 99%
15	L15E	169	6% 99%
16	L18E	112	• 98%
17	L18P	193	9% 99%
18	L19E	144	• 100%
19	L22P	150	7% 100%
20	L23P	81	9% 100%
21	L24E	54	• 100%
22	L24P	122	9% 98%
23	L29P	63	11% 100%
24	L30E	94	6% 99%
25	L30P	155	13% 100%
26	L31E	75	5% 100%
27	L32E	123	18% 98%
28	L34E	77	26% 96%
29	L37A	65	8% 98%
30	L37E	54	11% 100%
31	L39E	49	14% 98%

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Mol	Chain	Length	Quality of chain
32	L40E	55	35% 96%
33	L44E	92	100%
34	L7A1	123	7% 100%
34	L7A2	123	28% 100%
34	SL7A	123	89% 99%
35	L15P	144	65% 35%
36	L21E	97	6% 100%
37	L45A	101	20% 95% 5%
38	L46A	70	29% 99%
39	L47A	80	95% 99%
40	AL1P	216	63% 99%
41	AS3P	201	30% 100%
42	AS7P	193	58% 98%
43	S10P	100	47% 97%
44	S13P	147	56% 100%
45	S14P	52	29% 100%
46	S17E	62	42% 100%
47	S19E	150	55% 99%
48	S19P	115	36% 99%
49	AS9P	136	40% 100%
50	S28E	63	48% 100%
51	S27A	54	30% 98%
52	AS2P	196	49% 99%
53	AS4E	240	11% 98%
54	AS4P	166	8% 99%

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Mol	Chain	Length	Quality of chain
55	AS5P	204	8% 100%
56	AS6E	105	22% 98%
57	AS8E	126	17% 99%
58	AS8P	130	7% 99%
59	S11P	128	15% 100%
60	S12P	143	15% 99%
61	S15P	149	9% 99%
62	S17P	111	11% 98%
63	S24E	96	. 99%
64	S27E	59	. 100%
65	S3AE	189	12% 97%
66	AETN	76	7% 53% 42% 5%
66	APTN	76	. 71% 25%
67	AMRN	13	23% 46% 54%
68	APTP	6	83% 100%

2 Entry composition i

There are 70 unique types of molecules in this entry. The entry contains 173502 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 16s rRNA (1493-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A16S	1493	32063	14279	5930	10361	1493	0	0

- Molecule 2 is a RNA chain called 23s rRNA (3000-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	A23S	2995	64339	28665	11911	20768	2995	0	0

- Molecule 3 is a protein called Elongation factor 2.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- 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
			Total	C	N	O	S		
28	L34E	77	629	395	119	110	5	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 38 is a protein called Conserved protein.

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

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

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

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

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

- Molecule 41 is a protein called 30S ribosomal protein S3.

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

- Molecule 42 is a protein called 30S ribosomal protein S7.

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

- Molecule 43 is a protein called 30S ribosomal protein S10.

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

- Molecule 44 is a protein called 30S ribosomal protein S13.

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

- Molecule 45 is a protein called 30S ribosomal protein S14 type Z.

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

- Molecule 46 is a protein called 30S ribosomal protein S17e.

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

- Molecule 47 is a protein called 30S ribosomal protein S19e.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	S19E	149	Total	C	N	O	S	0	0
			1230	795	221	212	2		

- Molecule 48 is a protein called 30S ribosomal protein S19.

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

- Molecule 49 is a protein called 30S ribosomal protein S9.

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

- Molecule 50 is a protein called 30S ribosomal protein S28e.

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

- Molecule 51 is a protein called 30S ribosomal protein S27ae.

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

- Molecule 52 is a protein called 30S ribosomal protein S2.

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

- Molecule 53 is a protein called 30S ribosomal protein S4e.

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

- Molecule 54 is a protein called 30S ribosomal protein S4.

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

- Molecule 55 is a protein called 30S ribosomal protein S5.

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

- Molecule 56 is a protein called 30S ribosomal protein S6e.

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

- Molecule 57 is a protein called 30S ribosomal protein S8e.

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

- Molecule 58 is a protein called Small ribosomal subunit protein uS8.

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

- Molecule 59 is a protein called 30S ribosomal protein S11.

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

- Molecule 60 is a protein called 30S ribosomal protein S12.

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

- Molecule 61 is a protein called 30S ribosomal protein S15.

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

- Molecule 62 is a protein called 30S ribosomal protein S17.

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

- Molecule 63 is a protein called 30S ribosomal protein S24e.

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

- Molecule 64 is a protein called 30S ribosomal protein S27e.

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

- Molecule 65 is a protein called 30S ribosomal protein S3Ae.

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

- 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		

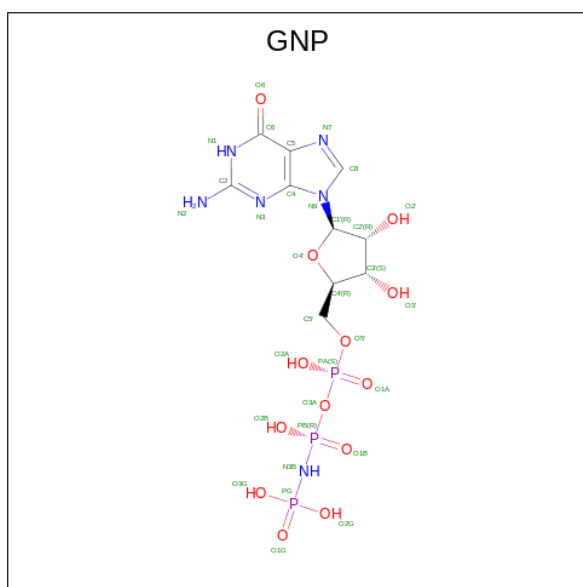
- Molecule 67 is a RNA chain called mRNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

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).



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

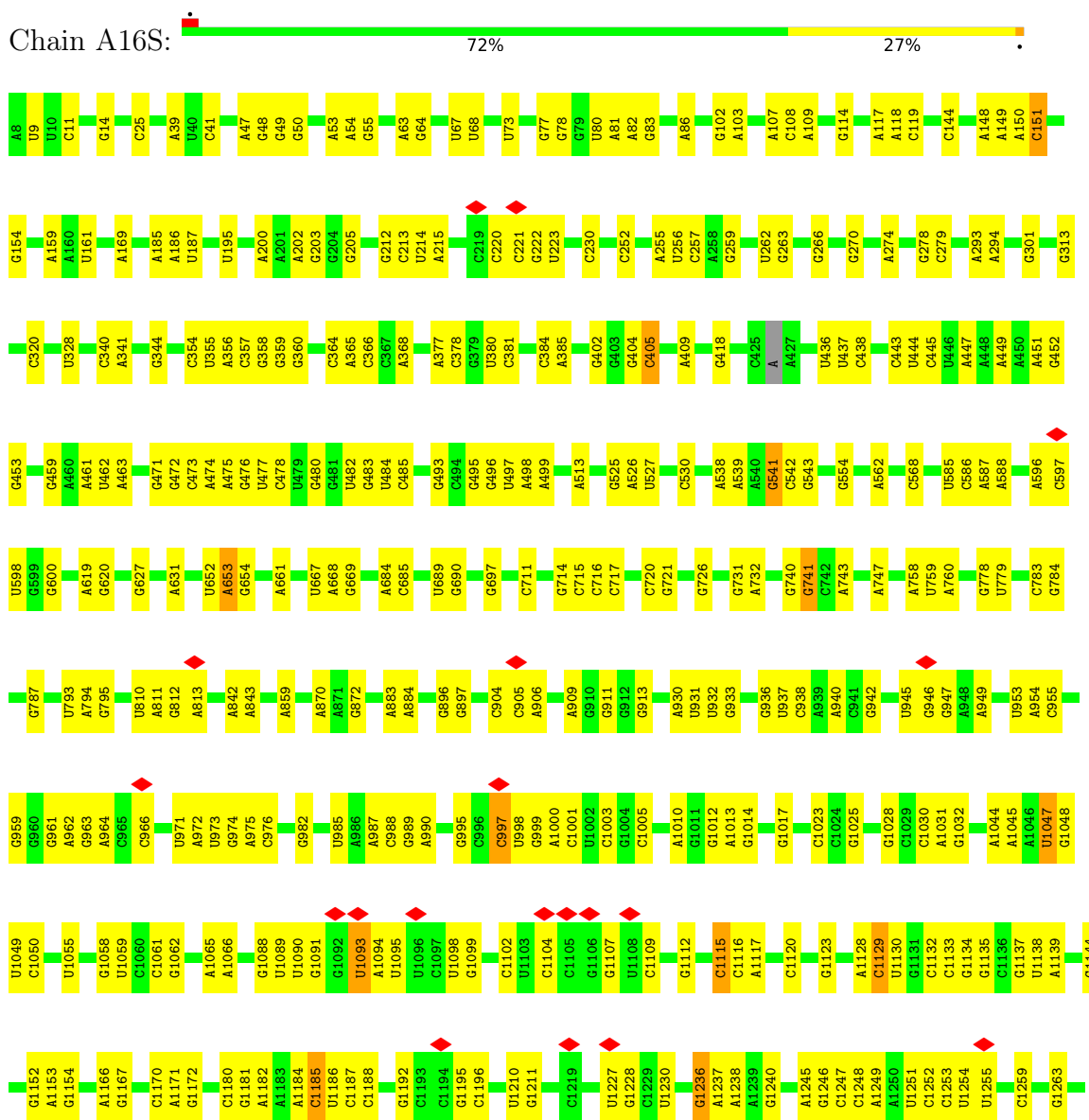
- Molecule 70 is UNKNOWN (three-letter code: UNK) (formula: C₄H₉NO₂) (labeled as "Ligand of Interest" by depositor).

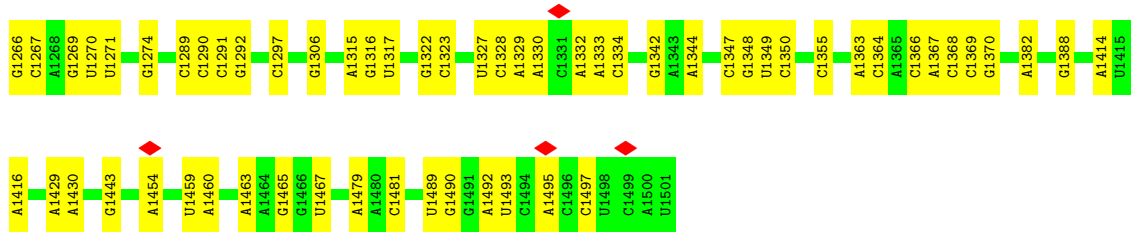
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
70	AS2P	34	171	102	34	35	0
70	AS5P	16	80	48	16	16	0
70	AS8P	7	35	21	7	7	0

3 Residue-property plots [i](#)

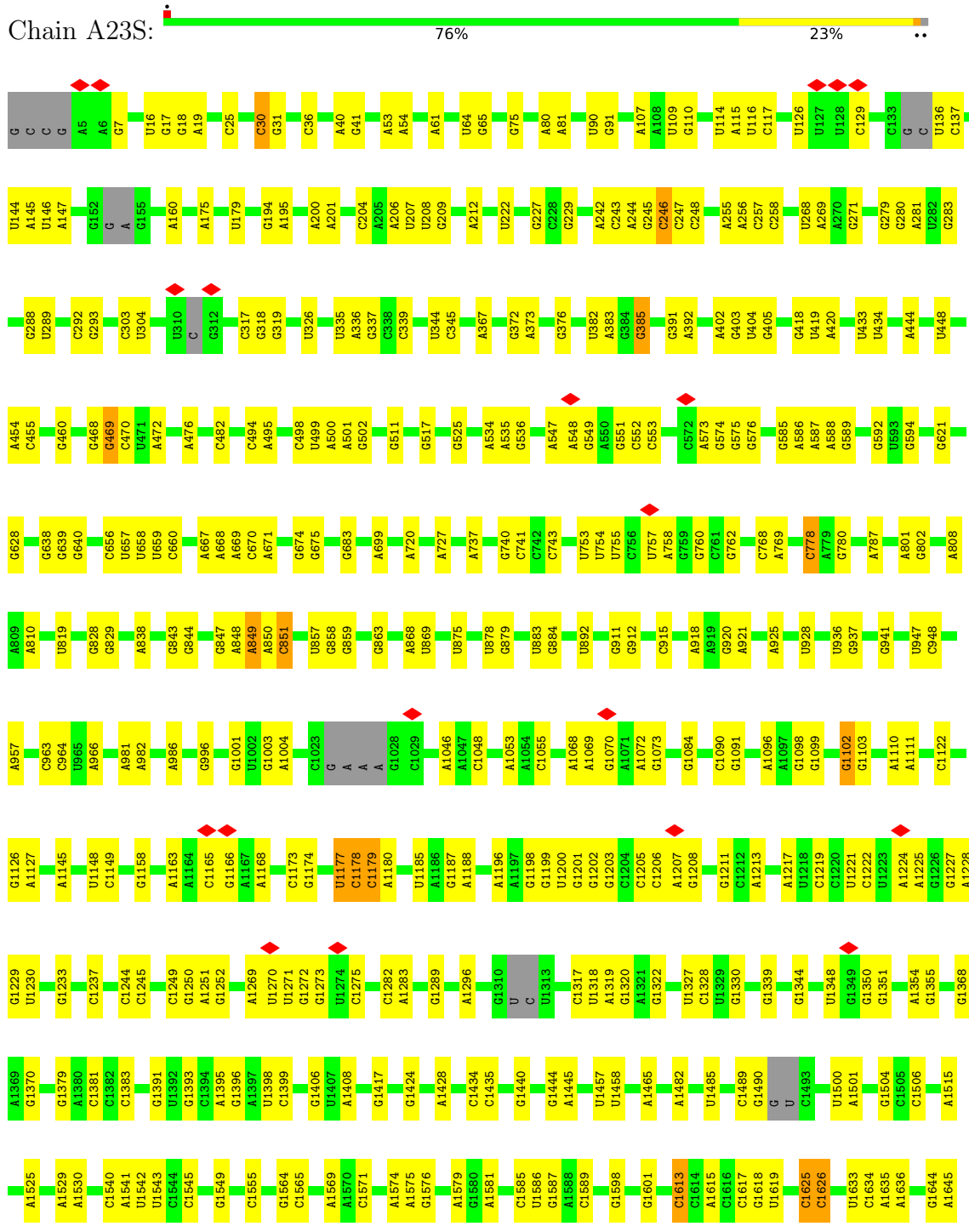
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

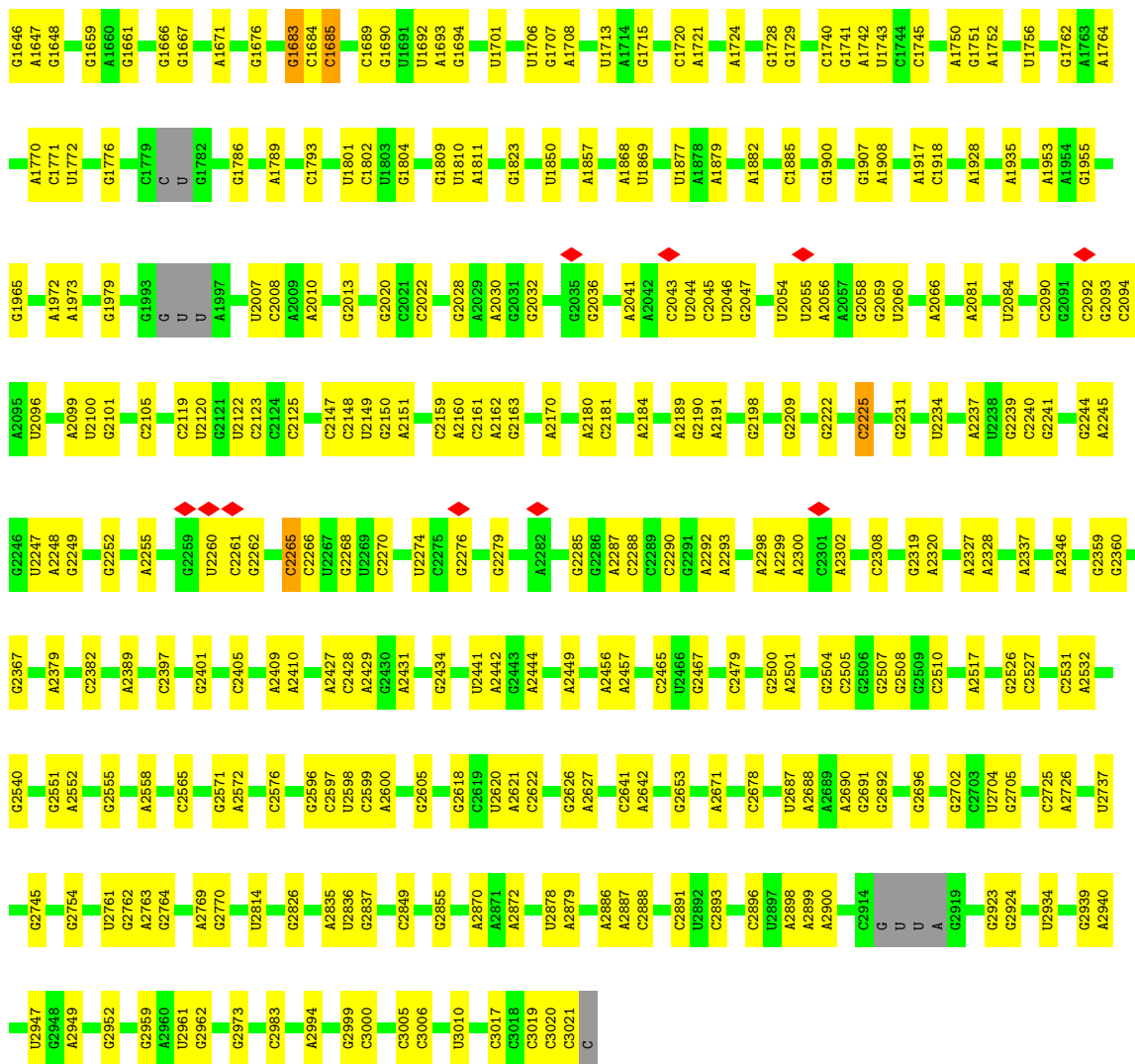
- Molecule 1: 16s rRNA (1493-MER)



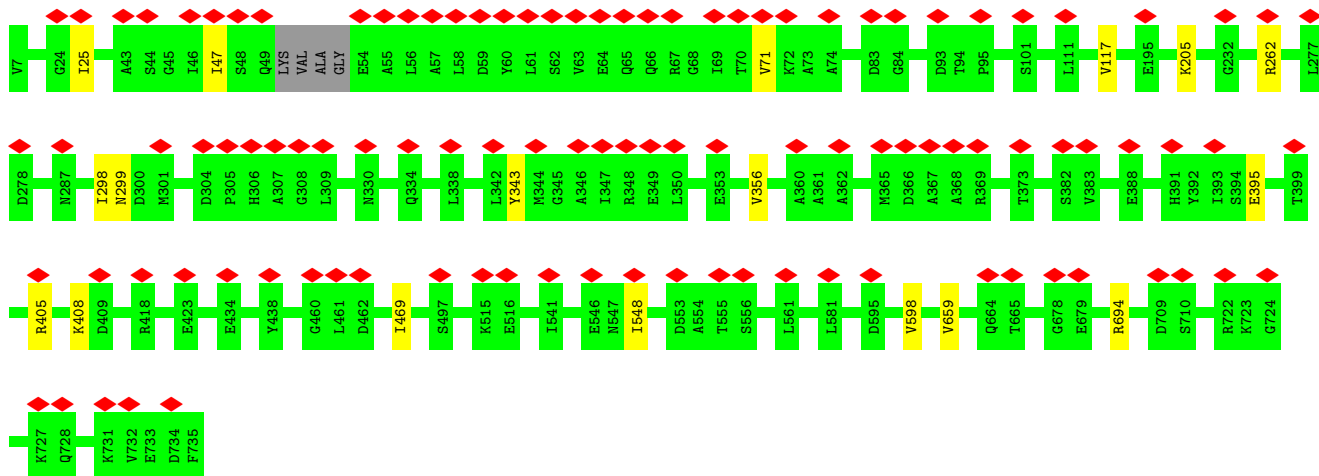


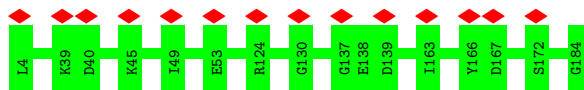
• Molecule 2: 23s rRNA (3000-MER)



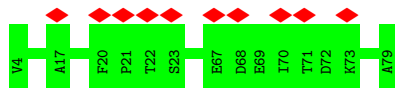


• Molecule 3: Elongation factor 2

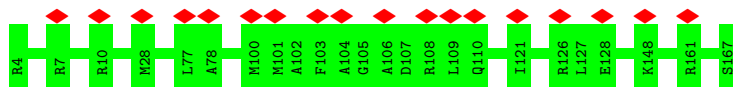




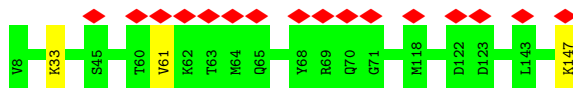
- Molecule 10: 50S ribosomal protein L18Ae



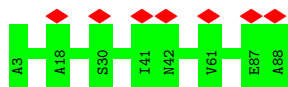
- Molecule 11: 50S ribosomal protein L10e



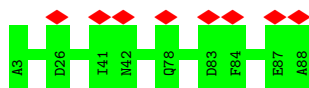
- Molecule 12: 50S ribosomal protein L13



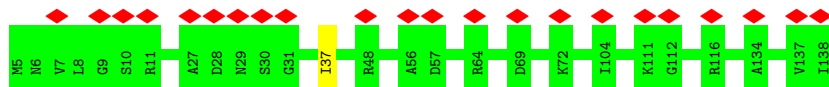
- Molecule 13: 50S ribosomal protein L14e



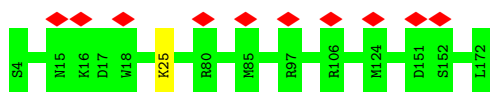
- Molecule 13: 50S ribosomal protein L14e



- Molecule 14: 50S ribosomal protein L14



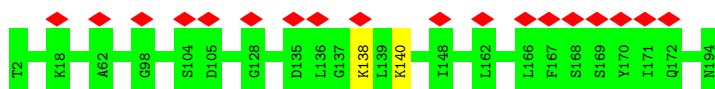
- Molecule 15: 50S ribosomal protein L15e



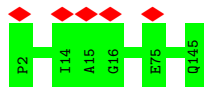
- Molecule 16: 50S ribosomal protein L18e



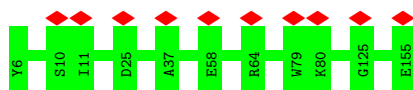
- Molecule 17: 50S ribosomal protein L18



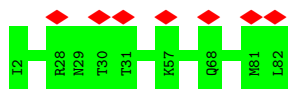
- Molecule 18: 50S ribosomal protein L19e



- Molecule 19: 50S ribosomal protein L22



- Molecule 20: 50S ribosomal protein L23



- Molecule 21: 50S ribosomal protein L24e

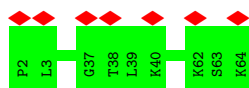


There are no outlier residues recorded for this chain.

- Molecule 22: 50S ribosomal protein L24



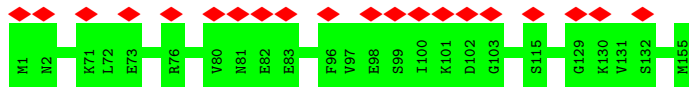
- Molecule 23: 50S ribosomal protein L29



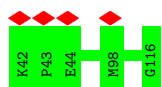
- Molecule 24: 50S ribosomal protein L30e



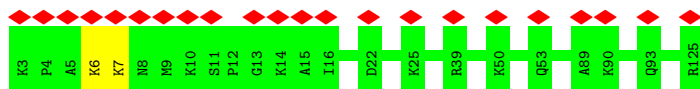
- Molecule 25: 50S ribosomal protein L30



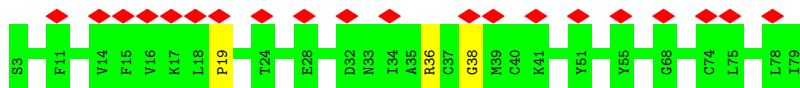
- Molecule 26: 50S ribosomal protein L31e



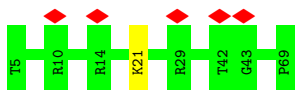
- Molecule 27: 50S ribosomal protein L32e



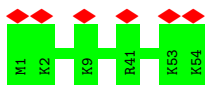
- Molecule 28: 50S ribosomal protein L34e



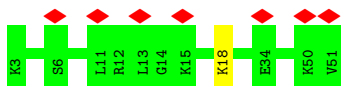
- Molecule 29: 50S ribosomal protein L37Ae



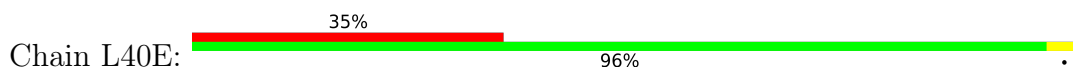
- Molecule 30: 50S ribosomal protein L37e



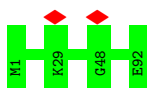
- Molecule 31: 50S ribosomal protein L39e



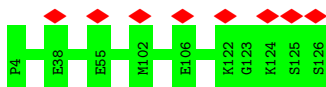
- Molecule 32: 50S ribosomal protein L40E



- Molecule 33: 50S ribosomal protein L44e

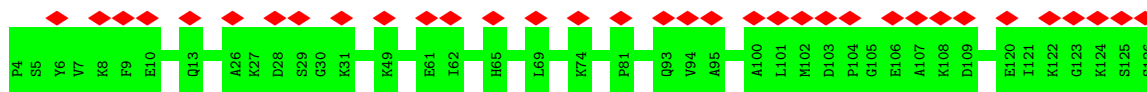


- Molecule 34: 50S ribosomal protein L7Ae

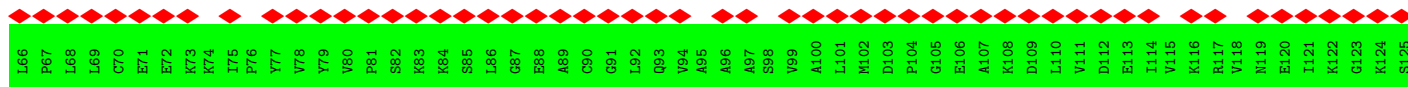
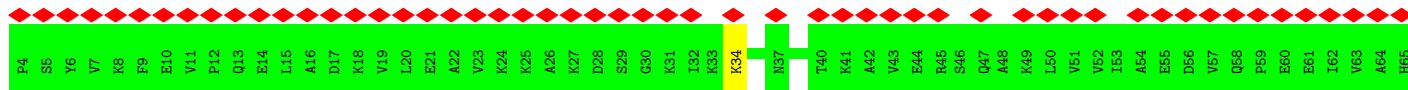


- Molecule 34: 50S ribosomal protein L7Ae

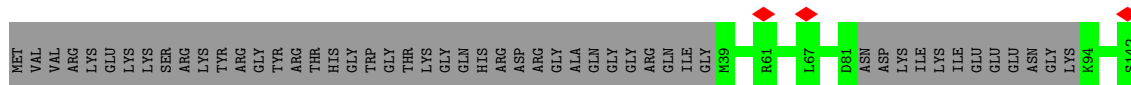




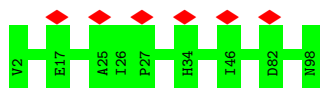
• Molecule 34: 50S ribosomal protein L7Ae



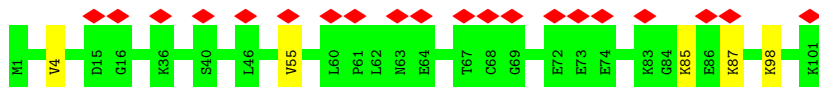
• Molecule 35: 50S ribosomal protein L15



• Molecule 36: 50S ribosomal protein L21e

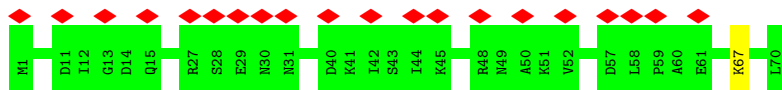


• Molecule 37: DUF2280 domain-containing protein

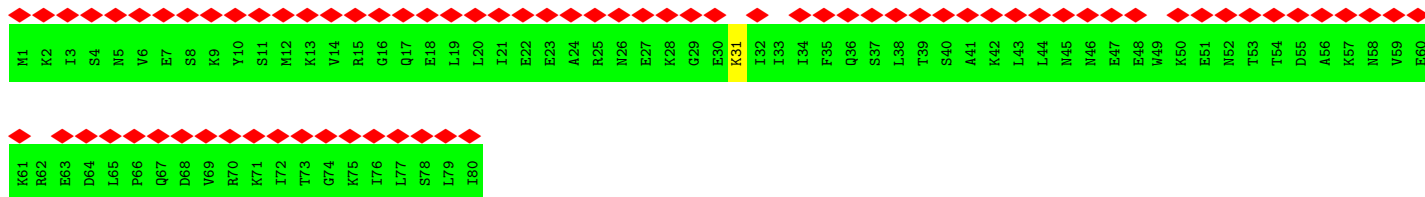


• Molecule 38: Conserved protein





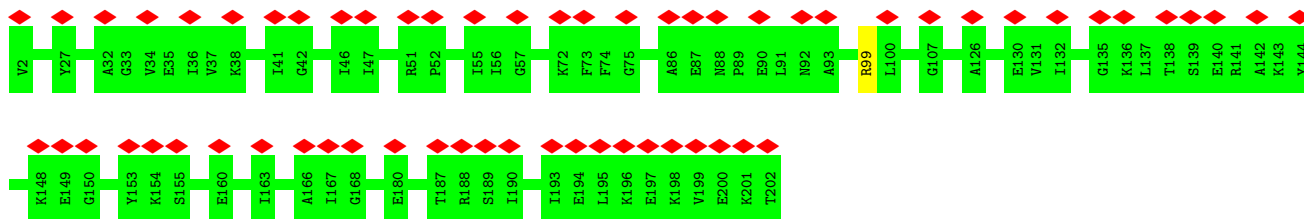
• Molecule 39: 50S ribosomal protein L47A



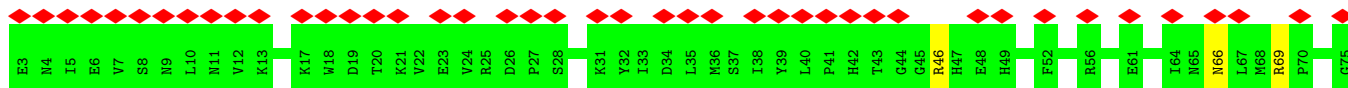
• Molecule 40: 50S ribosomal protein L1

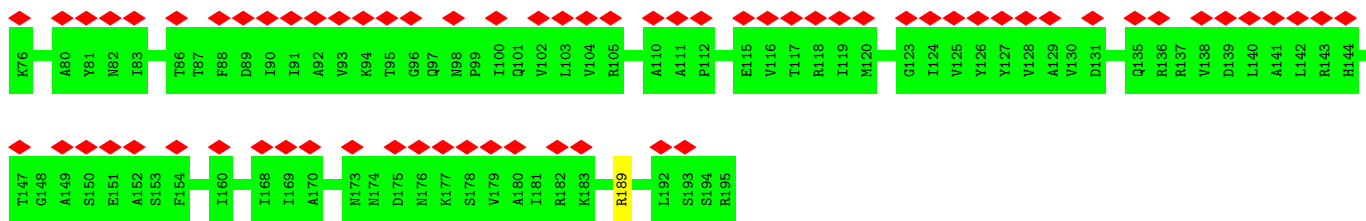


• Molecule 41: 30S ribosomal protein S3

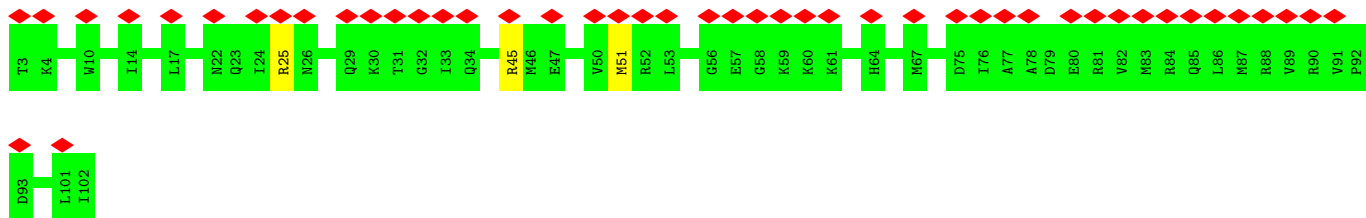


• Molecule 42: 30S ribosomal protein S7

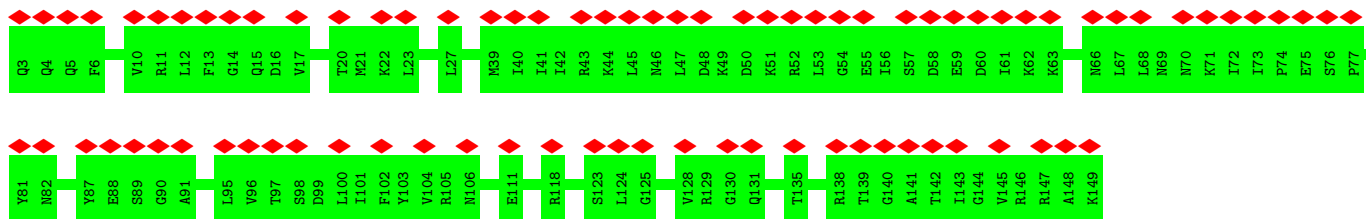




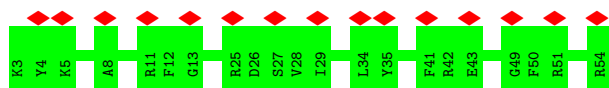
• Molecule 43: 30S ribosomal protein S10



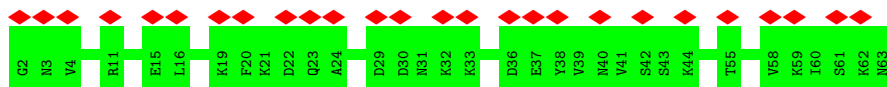
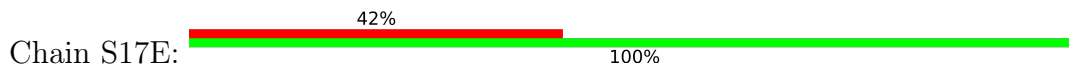
• Molecule 44: 30S ribosomal protein S13



• Molecule 45: 30S ribosomal protein S14 type Z

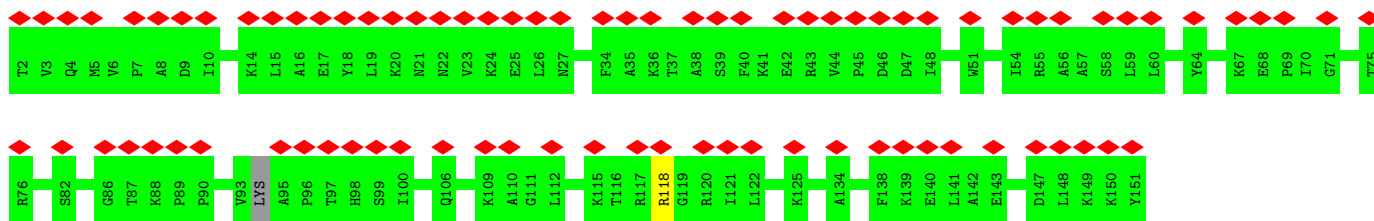


• Molecule 46: 30S ribosomal protein S17e

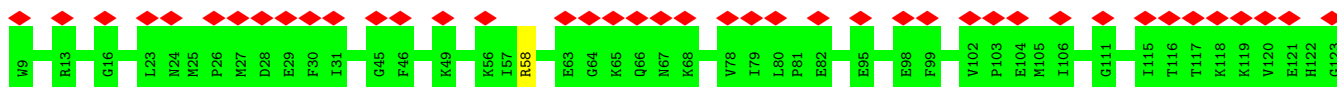


• Molecule 47: 30S ribosomal protein S19e

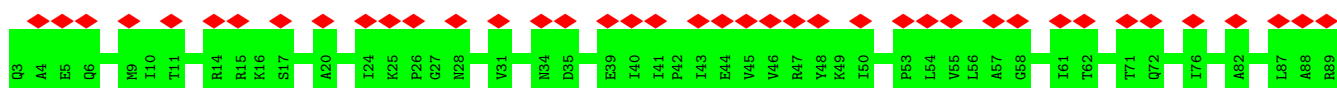
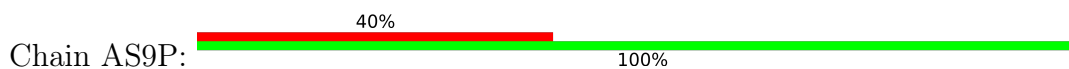




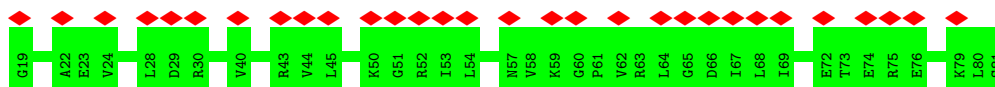
- Molecule 48: 30S ribosomal protein S19



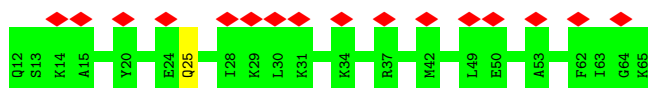
- Molecule 49: 30S ribosomal protein S9



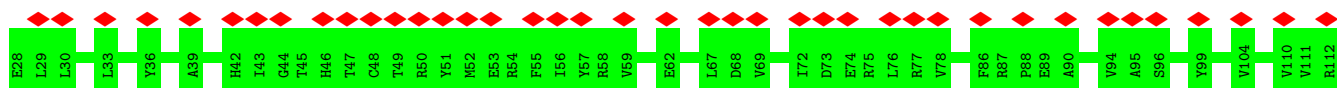
- Molecule 50: 30S ribosomal protein S28e

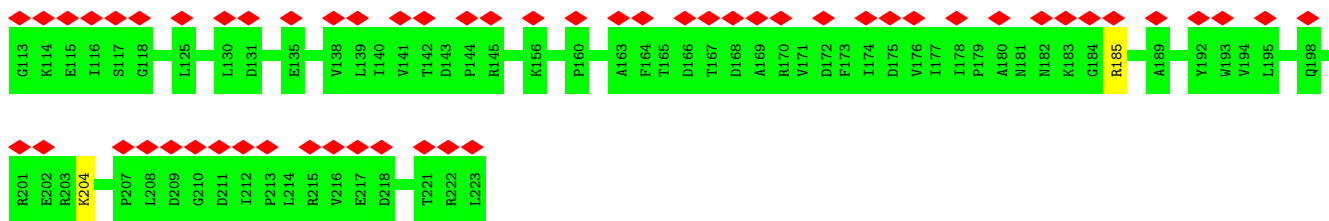


- Molecule 51: 30S ribosomal protein S27ae

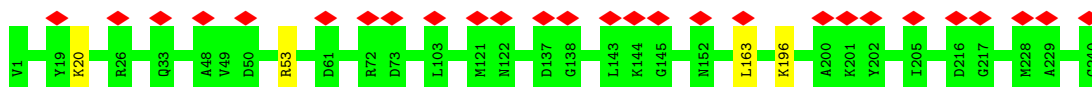


- Molecule 52: 30S ribosomal protein S2

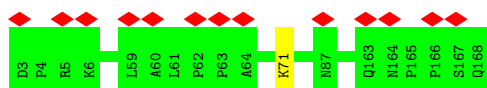




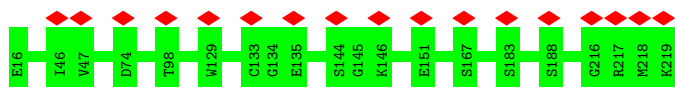
- Molecule 53: 30S ribosomal protein S4e



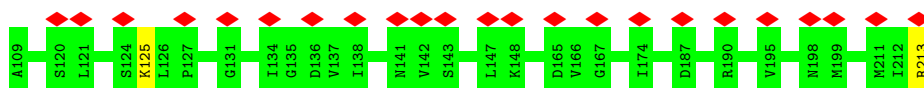
- Molecule 54: 30S ribosomal protein S4



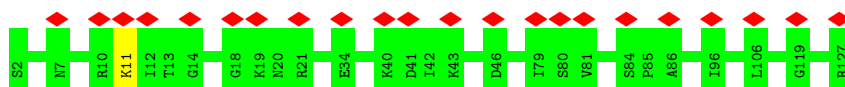
- Molecule 55: 30S ribosomal protein S5



- Molecule 56: 30S ribosomal protein S6e

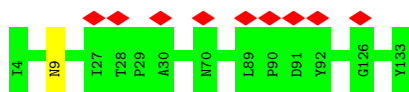


- Molecule 57: 30S ribosomal protein S8e

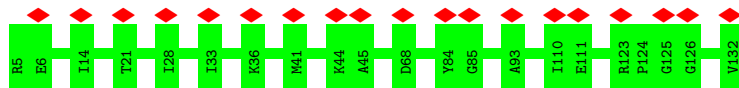


- Molecule 58: Small ribosomal subunit protein uS8





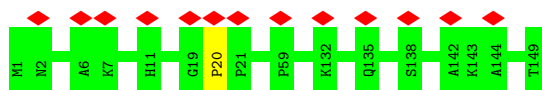
- Molecule 59: 30S ribosomal protein S11



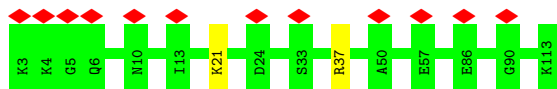
- Molecule 60: 30S ribosomal protein S12



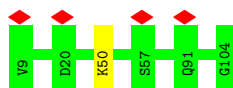
- Molecule 61: 30S ribosomal protein S15



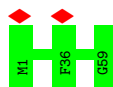
- Molecule 62: 30S ribosomal protein S17



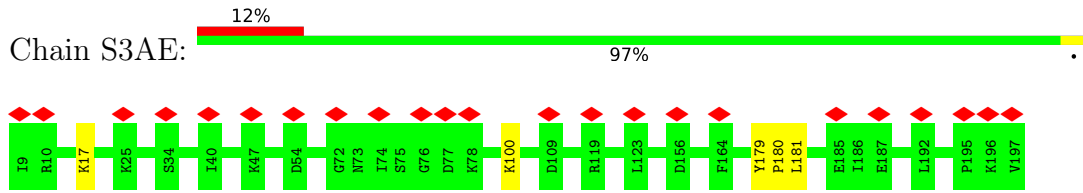
- Molecule 63: 30S ribosomal protein S24e



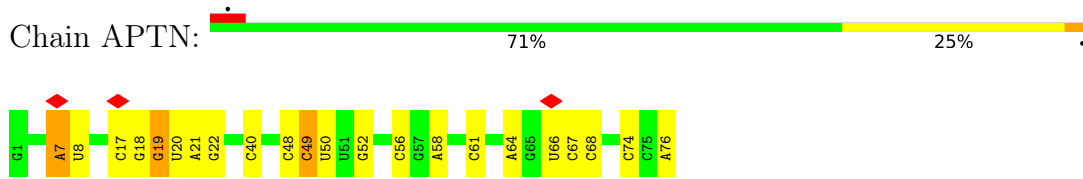
- Molecule 64: 30S ribosomal protein S27e



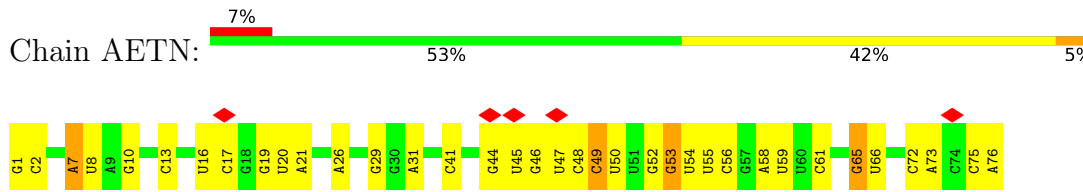
- Molecule 65: 30S ribosomal protein S3Ae



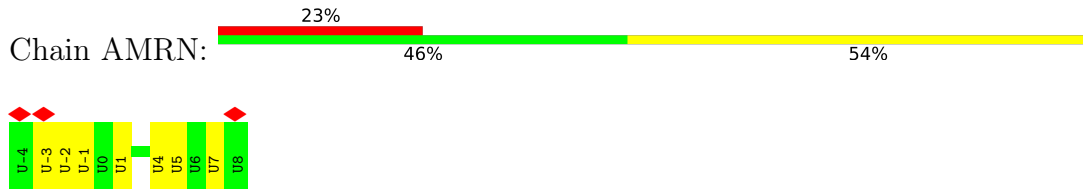
• Molecule 66: tRNA (76-MER)



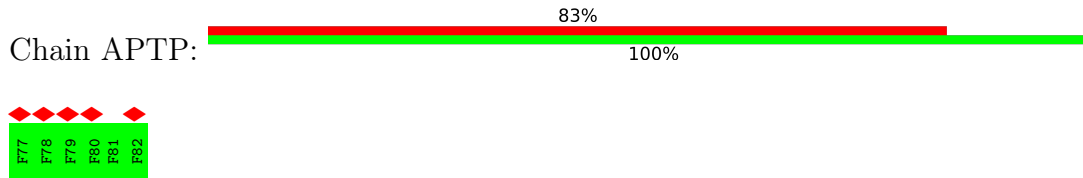
• Molecule 66: tRNA (76-MER)



• Molecule 67: mRNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*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	3841	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	1.282	Depositor
Minimum map value	-0.504	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.100	Depositor
Recommended contour level	0.33	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

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	A16S	0.56	6/35889 (0.0%)	0.90	61/56002 (0.1%)
2	A23S	0.43	1/72029 (0.0%)	0.88	109/112378 (0.1%)
3	AEFG	0.28	0/5771	0.54	1/7808 (0.0%)
4	A5S	0.34	0/2917	0.70	0/4549
5	AL2P	0.30	0/1787	0.55	0/2409
6	AL3P	0.29	0/2758	0.53	0/3727
7	AL4P	0.29	0/1956	0.55	0/2635
8	AL5P	0.28	0/1364	0.57	0/1827
9	AL6P	0.29	0/1450	0.49	0/1949
10	ALX0	0.32	0/638	0.62	0/851
11	L10E	0.30	0/1334	0.55	0/1787
12	L13P	0.28	0/1123	0.58	0/1502
13	L141	0.27	0/673	0.51	0/900
13	L142	0.27	0/673	0.51	0/900
14	L14P	0.30	0/1054	0.56	0/1425
15	L15E	0.32	0/1458	0.58	0/1956
16	L18E	0.28	0/907	0.51	0/1214
17	L18P	0.29	0/1570	0.49	0/2115
18	L19E	0.27	0/1223	0.54	0/1622
19	L22P	0.29	0/1246	0.50	0/1671
20	L23P	0.29	0/655	0.51	0/874
21	L24E	0.29	0/451	0.50	0/599
22	L24P	0.30	0/1000	0.57	0/1329
23	L29P	0.25	0/513	0.54	0/678
24	L30E	0.27	0/738	0.49	0/985
25	L30P	0.30	0/1278	0.55	0/1713
26	L31E	0.28	0/632	0.58	0/837
27	L32E	0.28	0/1027	0.53	0/1366
28	L34E	0.31	0/642	0.70	0/854
29	L37A	0.31	0/542	0.61	0/726
30	L37E	0.31	0/445	0.57	0/585
31	L39E	0.26	0/422	0.60	0/562

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	L40E	0.27	0/443	0.63	0/587
33	L44E	0.28	0/763	0.55	0/1008
34	L7A1	0.27	0/946	0.43	0/1272
34	L7A2	0.25	0/946	0.43	0/1272
34	SL7A	0.25	0/946	0.45	0/1272
35	L15P	0.28	0/766	0.49	0/1023
36	L21E	0.29	0/800	0.51	0/1067
37	L45A	0.27	0/824	0.56	0/1094
38	L46A	0.26	0/595	0.47	0/793
39	L47A	0.24	0/652	0.52	0/870
40	AL1P	0.26	0/1739	0.52	0/2338
41	AS3P	0.27	0/1599	0.51	0/2147
42	AS7P	0.26	0/1561	0.55	0/2105
43	S10P	0.25	0/840	0.55	0/1132
44	S13P	0.26	0/1221	0.55	0/1634
45	S14P	0.27	0/441	0.61	0/583
46	S17E	0.25	0/523	0.47	0/696
47	S19E	0.25	0/1257	0.51	0/1691
48	S19P	0.25	0/985	0.56	0/1310
49	AS9P	0.26	0/1115	0.54	0/1496
50	S28E	0.24	0/500	0.60	0/669
51	S27A	0.30	0/444	0.62	0/590
52	AS2P	0.27	0/1621	0.55	0/2202
53	AS4E	0.28	0/1956	0.55	0/2635
54	AS4P	0.28	0/1399	0.55	0/1883
55	AS5P	0.28	0/1631	0.52	0/2200
56	AS6E	0.28	0/815	0.57	0/1093
57	AS8E	0.27	0/1005	0.56	0/1342
58	AS8P	0.30	0/1046	0.57	0/1410
59	S11P	0.27	0/976	0.59	0/1315
60	S12P	0.29	0/1120	0.58	0/1495
61	S15P	0.28	0/1250	0.54	0/1677
62	S17P	0.28	0/899	0.56	0/1203
63	S24E	0.26	0/769	0.50	0/1034
64	S27E	0.27	0/465	0.49	0/618
65	S3AE	0.28	0/1573	0.54	0/2115
66	AETN	0.53	2/1809 (0.1%)	2.13	25/2819 (0.9%)
66	APTN	0.51	3/1809 (0.2%)	1.52	25/2819 (0.9%)
67	AMRN	0.25	0/285	0.86	0/438
68	APTP	0.33	0/72	0.34	0/93
All	All	0.41	12/186571 (0.0%)	0.81	221/275375 (0.1%)

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

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	AEFG	0	1
12	L13P	0	1
28	L34E	0	2
42	AS7P	0	1
51	S27A	0	1
53	AS4E	0	1
61	S15P	0	1
65	S3AE	0	2
All	All	0	10

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A16S	1236	G	C6-N1	37.36	1.65	1.39
1	A16S	1236	G	N3-C4	34.54	1.59	1.35
1	A16S	1236	G	N1-C2	33.69	1.64	1.37
1	A16S	1236	G	C2-N3	32.36	1.58	1.32
1	A16S	1236	G	C5-C4	28.52	1.58	1.38

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
66	AETN	61	C	N3-C2-O2	-49.60	87.18	121.90
66	AETN	61	C	N1-C2-O2	47.86	147.62	118.90
66	APTN	19	G	N3-C2-N2	33.59	143.42	119.90
66	APTN	19	G	N1-C2-N2	-32.19	87.23	116.20
66	AETN	29	G	N1-C2-N2	-28.30	90.73	116.20

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	AEFG	343	TYR	Peptide
42	AS7P	69	ARG	Peptide
12	L13P	61	VAL	Peptide
28	L34E	36	ARG	Peptide
28	L34E	38	GLY	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	A16S	32063	0	0	0	0
2	A23S	64339	0	0	0	0
3	AEFG	5677	0	0	0	0
4	A5S	2609	0	1324	47	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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	AS3P	1576	0	0	0	0
42	AS7P	1537	0	0	0	0
43	S10P	824	0	0	0	0
44	S13P	1204	0	0	0	0
45	S14P	432	0	0	0	0
46	S17E	517	0	0	0	0
47	S19E	1230	0	0	0	0
48	S19P	968	0	0	0	0
49	AS9P	1096	0	0	0	0
50	S28E	498	0	0	0	0
51	S27A	435	0	0	0	0
52	AS2P	1587	0	0	0	0
53	AS4E	1925	0	0	0	0
54	AS4P	1370	0	0	0	0
55	AS5P	1600	0	0	0	0
56	AS6E	805	0	0	0	0
57	AS8E	993	0	0	0	0
58	AS8P	1028	0	0	0	0
59	S11P	960	0	0	0	0
60	S12P	1103	0	0	0	0
61	S15P	1225	0	0	0	0
62	S17P	885	0	0	0	0
63	S24E	759	0	0	0	0
64	S27E	458	0	0	0	0
65	S3AE	1545	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	171	0	0	0	0
70	AS5P	80	0	0	0	0
70	AS8P	35	0	0	0	0
All	All	173502	0	1324	47	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 22.

The worst 5 of 47 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:76:G:H1	4:A5S:106:U:H3	1.32	0.77
4:A5S:17:G:O6	4:A5S:68:C:N4	2.17	0.75
4:A5S:5:C:H2'	4:A5S:6:A:C8	2.34	0.62
4:A5S:41:U:O2'	4:A5S:46:A:N6	2.32	0.61
4:A5S:113:G:O2'	4:A5S:114:C:O5'	2.21	0.59

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	AEFG	721/729 (99%)	614 (85%)	96 (13%)	11 (2%)	10	45
5	AL2P	232/234 (99%)	215 (93%)	17 (7%)	0	100	100
6	AL3P	337/339 (99%)	301 (89%)	36 (11%)	0	100	100
7	AL4P	249/251 (99%)	234 (94%)	15 (6%)	0	100	100
8	AL5P	166/168 (99%)	146 (88%)	20 (12%)	0	100	100
9	AL6P	179/181 (99%)	170 (95%)	9 (5%)	0	100	100
10	ALX0	74/76 (97%)	64 (86%)	10 (14%)	0	100	100
11	L10E	162/164 (99%)	143 (88%)	19 (12%)	0	100	100
12	L13P	138/140 (99%)	122 (88%)	16 (12%)	0	100	100
13	L141	84/86 (98%)	74 (88%)	10 (12%)	0	100	100
13	L142	84/86 (98%)	78 (93%)	6 (7%)	0	100	100
14	L14P	132/134 (98%)	116 (88%)	16 (12%)	0	100	100
15	L15E	167/169 (99%)	159 (95%)	8 (5%)	0	100	100
16	L18E	110/112 (98%)	106 (96%)	4 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	L18P	191/193 (99%)	176 (92%)	15 (8%)	0	100	100
18	L19E	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
19	L22P	148/150 (99%)	138 (93%)	10 (7%)	0	100	100
20	L23P	79/81 (98%)	71 (90%)	8 (10%)	0	100	100
21	L24E	52/54 (96%)	48 (92%)	4 (8%)	0	100	100
22	L24P	120/122 (98%)	111 (92%)	9 (8%)	0	100	100
23	L29P	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
24	L30E	92/94 (98%)	89 (97%)	3 (3%)	0	100	100
25	L30P	153/155 (99%)	135 (88%)	18 (12%)	0	100	100
26	L31E	73/75 (97%)	68 (93%)	5 (7%)	0	100	100
27	L32E	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
28	L34E	75/77 (97%)	54 (72%)	20 (27%)	1 (1%)	12	47
29	L37A	63/65 (97%)	56 (89%)	7 (11%)	0	100	100
30	L37E	52/54 (96%)	45 (86%)	7 (14%)	0	100	100
31	L39E	47/49 (96%)	41 (87%)	6 (13%)	0	100	100
32	L40E	53/55 (96%)	35 (66%)	18 (34%)	0	100	100
33	L44E	90/92 (98%)	87 (97%)	3 (3%)	0	100	100
34	L7A1	121/123 (98%)	118 (98%)	3 (2%)	0	100	100
34	L7A2	121/123 (98%)	119 (98%)	2 (2%)	0	100	100
34	SL7A	121/123 (98%)	113 (93%)	8 (7%)	0	100	100
35	L15P	90/144 (62%)	84 (93%)	6 (7%)	0	100	100
36	L21E	95/97 (98%)	89 (94%)	6 (6%)	0	100	100
37	L45A	99/101 (98%)	82 (83%)	14 (14%)	3 (3%)	4	32
38	L46A	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
39	L47A	78/80 (98%)	72 (92%)	6 (8%)	0	100	100
40	AL1P	214/216 (99%)	194 (91%)	20 (9%)	0	100	100
41	AS3P	199/201 (99%)	182 (92%)	17 (8%)	0	100	100
42	AS7P	191/193 (99%)	157 (82%)	34 (18%)	0	100	100
43	S10P	98/100 (98%)	95 (97%)	3 (3%)	0	100	100
44	S13P	145/147 (99%)	130 (90%)	15 (10%)	0	100	100
45	S14P	50/52 (96%)	43 (86%)	7 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	S17E	60/62 (97%)	56 (93%)	4 (7%)	0	100	100
47	S19E	145/150 (97%)	134 (92%)	11 (8%)	0	100	100
48	S19P	113/115 (98%)	99 (88%)	14 (12%)	0	100	100
49	AS9P	134/136 (98%)	124 (92%)	10 (8%)	0	100	100
50	S28E	61/63 (97%)	55 (90%)	6 (10%)	0	100	100
51	S27A	52/54 (96%)	40 (77%)	12 (23%)	0	100	100
52	AS2P	194/196 (99%)	181 (93%)	13 (7%)	0	100	100
53	AS4E	238/240 (99%)	208 (87%)	30 (13%)	0	100	100
54	AS4P	164/166 (99%)	134 (82%)	30 (18%)	0	100	100
55	AS5P	202/204 (99%)	182 (90%)	20 (10%)	0	100	100
56	AS6E	103/105 (98%)	84 (82%)	19 (18%)	0	100	100
57	AS8E	124/126 (98%)	109 (88%)	15 (12%)	0	100	100
58	AS8P	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
59	S11P	126/128 (98%)	108 (86%)	18 (14%)	0	100	100
60	S12P	141/143 (99%)	119 (84%)	22 (16%)	0	100	100
61	S15P	147/149 (99%)	131 (89%)	16 (11%)	0	100	100
62	S17P	109/111 (98%)	99 (91%)	10 (9%)	0	100	100
63	S24E	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
64	S27E	57/59 (97%)	52 (91%)	5 (9%)	0	100	100
65	S3AE	187/189 (99%)	156 (83%)	30 (16%)	1 (0%)	29	66
68	APTP	4/6 (67%)	3 (75%)	1 (25%)	0	100	100
All	All	8720/8913 (98%)	7827 (90%)	877 (10%)	16 (0%)	50	79

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	AEFG	298	ILE
3	AEFG	356	VAL
3	AEFG	469	ILE
37	L45A	4	VAL
37	L45A	55	VAL

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AEFG	625/627 (100%)	620 (99%)	5 (1%)	81	88
5	AL2P	181/181 (100%)	180 (99%)	1 (1%)	86	91
6	AL3P	297/297 (100%)	296 (100%)	1 (0%)	92	95
7	AL4P	212/212 (100%)	210 (99%)	2 (1%)	78	87
8	AL5P	144/144 (100%)	143 (99%)	1 (1%)	84	90
9	AL6P	157/157 (100%)	157 (100%)	0	100	100
10	ALX0	68/68 (100%)	68 (100%)	0	100	100
11	L10E	137/137 (100%)	137 (100%)	0	100	100
12	L13P	121/121 (100%)	119 (98%)	2 (2%)	60	78
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%)	78	87
15	L15E	146/146 (100%)	145 (99%)	1 (1%)	84	90
16	L18E	98/98 (100%)	96 (98%)	2 (2%)	55	73
17	L18P	162/162 (100%)	160 (99%)	2 (1%)	71	83
18	L19E	126/126 (100%)	126 (100%)	0	100	100
19	L22P	131/131 (100%)	131 (100%)	0	100	100
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%)	106 (98%)	2 (2%)	57	75
23	L29P	59/59 (100%)	59 (100%)	0	100	100
24	L30E	83/83 (100%)	82 (99%)	1 (1%)	71	83
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%)	57	75
28	L34E	70/70 (100%)	70 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	L37A	53/53 (100%)	52 (98%)	1 (2%)	57	75
30	L37E	45/45 (100%)	45 (100%)	0	100	100
31	L39E	44/44 (100%)	43 (98%)	1 (2%)	50	70
32	L40E	50/50 (100%)	48 (96%)	2 (4%)	31	57
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%)	104 (100%)	0	100	100
34	SL7A	104/104 (100%)	103 (99%)	1 (1%)	76	85
35	L15P	78/118 (66%)	78 (100%)	0	100	100
36	L21E	85/85 (100%)	85 (100%)	0	100	100
37	L45A	91/91 (100%)	89 (98%)	2 (2%)	52	71
38	L46A	66/66 (100%)	65 (98%)	1 (2%)	65	79
39	L47A	74/74 (100%)	73 (99%)	1 (1%)	67	80
40	AL1P	189/190 (100%)	186 (98%)	3 (2%)	62	78
41	AS3P	165/165 (100%)	164 (99%)	1 (1%)	86	91
42	AS7P	166/166 (100%)	163 (98%)	3 (2%)	59	77
43	S10P	92/92 (100%)	89 (97%)	3 (3%)	38	62
44	S13P	129/129 (100%)	129 (100%)	0	100	100
45	S14P	45/45 (100%)	45 (100%)	0	100	100
46	S17E	57/57 (100%)	57 (100%)	0	100	100
47	S19E	133/134 (99%)	132 (99%)	1 (1%)	81	88
48	S19P	106/106 (100%)	105 (99%)	1 (1%)	78	87
49	AS9P	113/113 (100%)	113 (100%)	0	100	100
50	S28E	54/54 (100%)	54 (100%)	0	100	100
51	S27A	47/47 (100%)	47 (100%)	0	100	100
52	AS2P	174/174 (100%)	172 (99%)	2 (1%)	73	84
53	AS4E	210/210 (100%)	207 (99%)	3 (1%)	67	80
54	AS4P	149/149 (100%)	148 (99%)	1 (1%)	84	90
55	AS5P	174/174 (100%)	174 (100%)	0	100	100
56	AS6E	88/88 (100%)	86 (98%)	2 (2%)	50	70
57	AS8E	106/106 (100%)	105 (99%)	1 (1%)	78	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
58	AS8P	111/111 (100%)	110 (99%)	1 (1%)	78	87
59	S11P	94/94 (100%)	94 (100%)	0	100	100
60	S12P	116/116 (100%)	115 (99%)	1 (1%)	78	87
61	S15P	133/133 (100%)	133 (100%)	0	100	100
62	S17P	97/97 (100%)	95 (98%)	2 (2%)	53	72
63	S24E	84/84 (100%)	83 (99%)	1 (1%)	71	83
64	S27E	51/51 (100%)	51 (100%)	0	100	100
65	S3AE	170/170 (100%)	168 (99%)	2 (1%)	71	83
68	APTP	6/6 (100%)	6 (100%)	0	100	100
All	All	7656/7700 (99%)	7596 (99%)	60 (1%)	82	88

5 of 60 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
37	L45A	98	LYS
62	S17P	21	LYS
42	AS7P	46	ARG
60	S12P	22	LYS
65	S3AE	100	LYS

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A16S	1491/1494 (99%)	371 (24%)	52 (3%)
2	A23S	2986/3022 (98%)	649 (21%)	37 (1%)
4	A5S	121/122 (99%)	18 (14%)	1 (0%)
66	AETN	75/76 (98%)	31 (41%)	3 (4%)
66	APTN	75/76 (98%)	20 (26%)	1 (1%)
67	AMRN	12/13 (92%)	7 (58%)	0
All	All	4760/4803 (99%)	1096 (23%)	94 (1%)

5 of 1096 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A16S	9	U

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Mol	Chain	Res	Type
1	A16S	11	C
1	A16S	39	A
1	A16S	41	C
1	A16S	47	A

5 of 94 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	A23S	402	A
2	A23S	1250	G
2	A23S	547	A
2	A23S	1003	G
2	A23S	1646	G

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	3	29,34,34	1.53	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	3	-	2/14/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
69	AEFG	801	GNP	PB-O3A	3.87	1.63	1.59
69	AEFG	801	GNP	C6-N1	3.44	1.39	1.33
69	AEFG	801	GNP	PG-N3B	2.83	1.70	1.63
69	AEFG	801	GNP	PB-O1B	2.76	1.50	1.46
69	AEFG	801	GNP	PG-O1G	2.51	1.50	1.46

The worst 5 of 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	5.71	125.01	115.93
69	AEFG	801	GNP	C4-C5-C6	-3.13	117.81	120.80
69	AEFG	801	GNP	PB-O3A-PA	-2.92	122.35	132.62
69	AEFG	801	GNP	N3-C2-N1	-2.80	123.48	127.22

There are no chirality outliers.

All (2) torsion outliers are listed below:

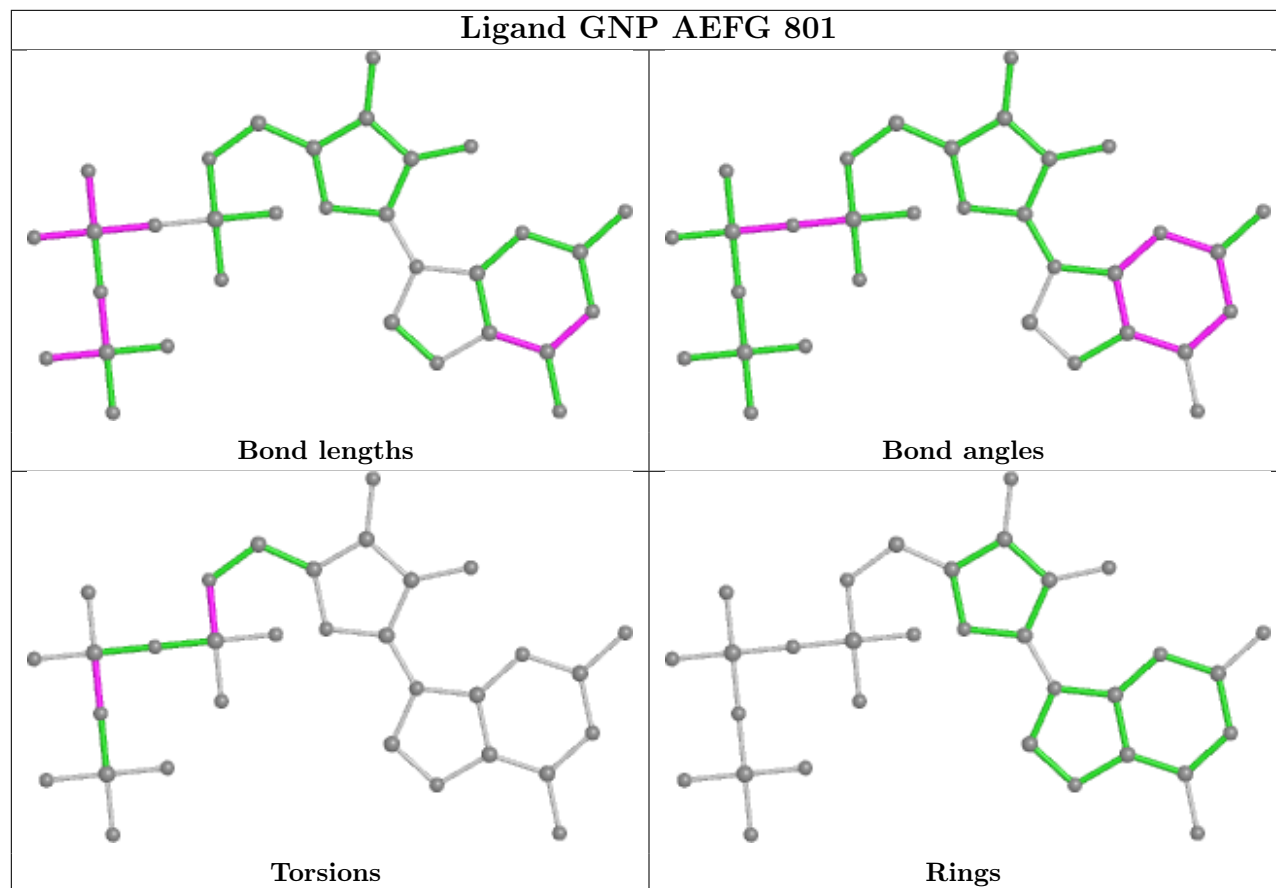
Mol	Chain	Res	Type	Atoms
69	AEFG	801	GNP	PG-N3B-PB-O1B
69	AEFG	801	GNP	C5'-O5'-PA-O1A

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.

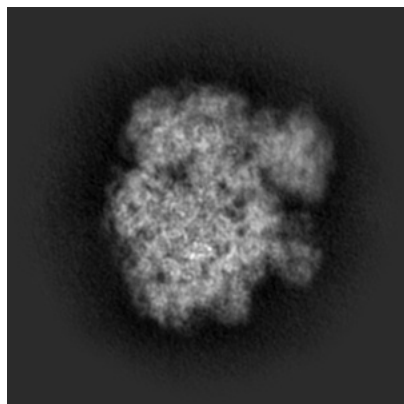
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34866. These allow visual inspection of the internal detail of the map and identification of artifacts.

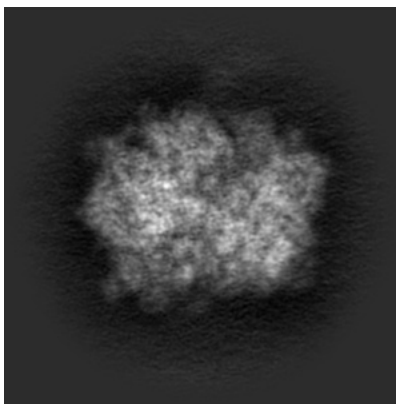
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

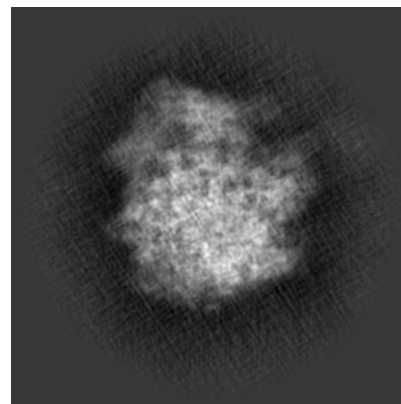
6.1.1 Primary map



X

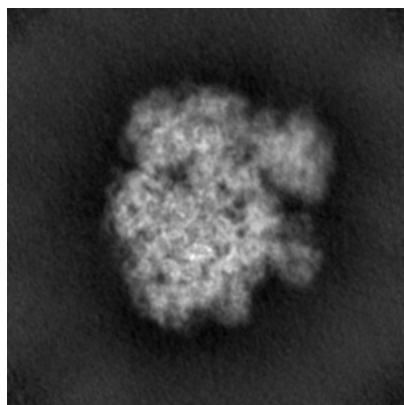


Y

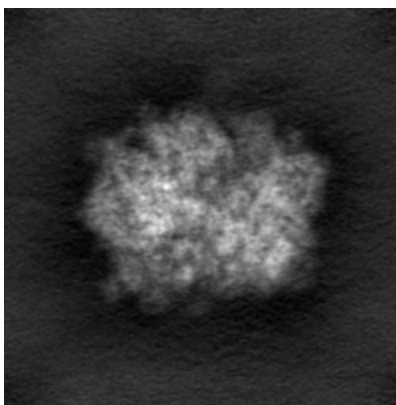


Z

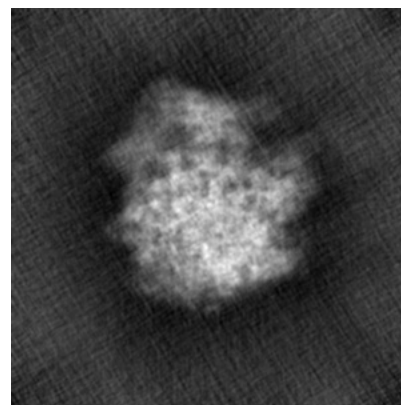
6.1.2 Raw map



X



Y

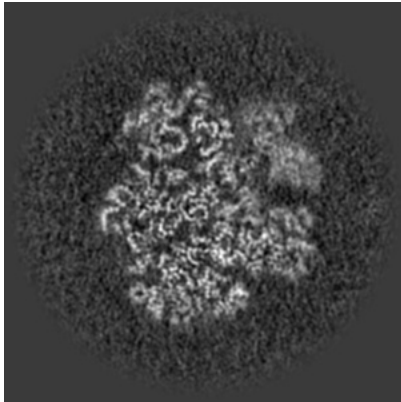


Z

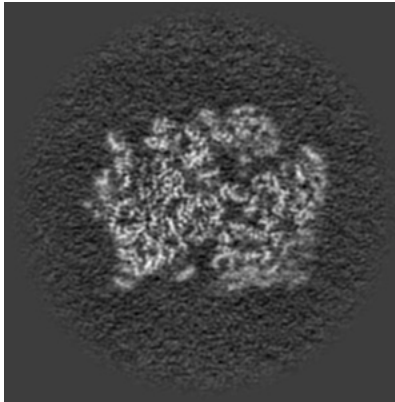
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

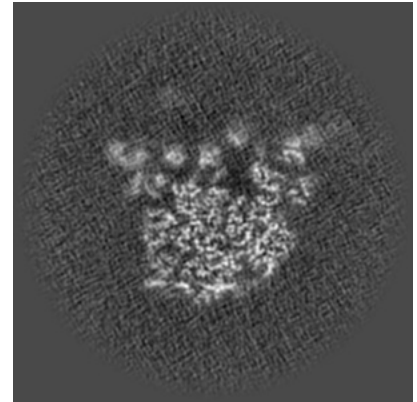
6.2.1 Primary map



X Index: 190

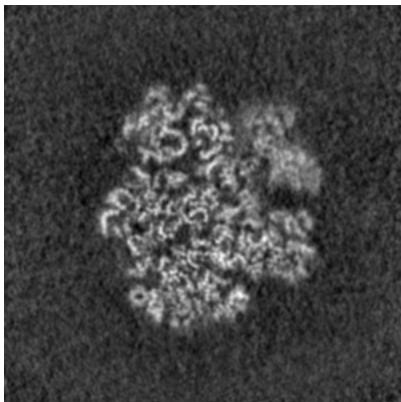


Y Index: 190

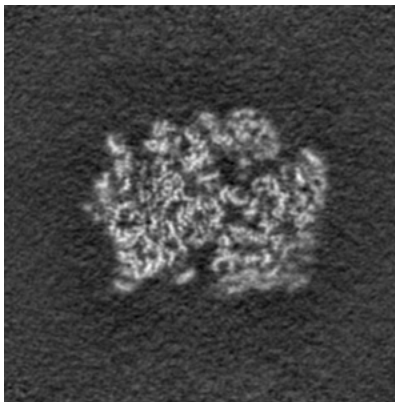


Z Index: 190

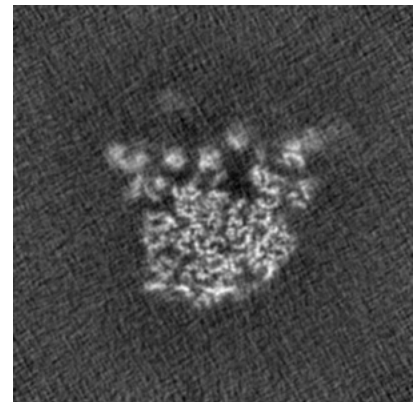
6.2.2 Raw map



X Index: 190



Y Index: 190

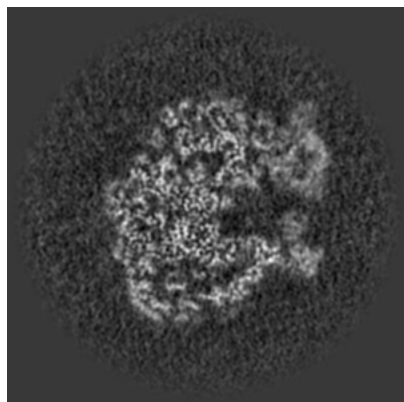


Z Index: 190

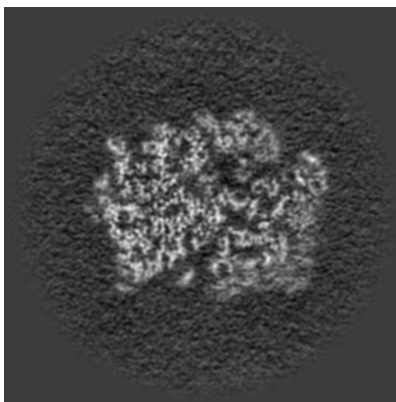
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

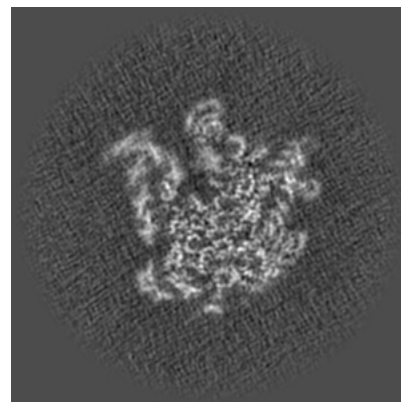
6.3.1 Primary map



X Index: 171

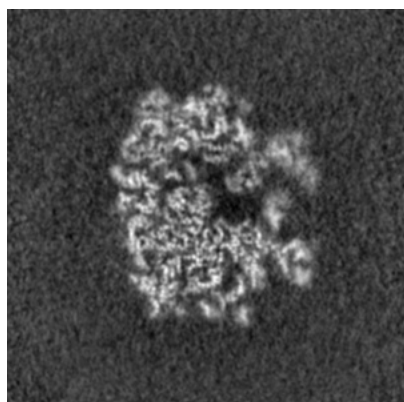


Y Index: 192

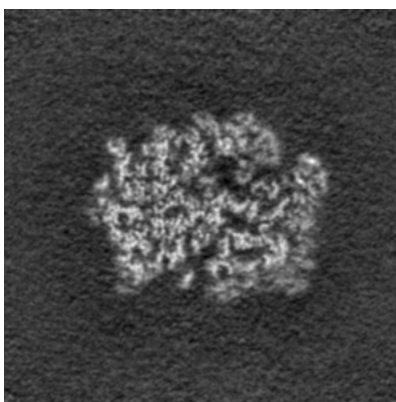


Z Index: 173

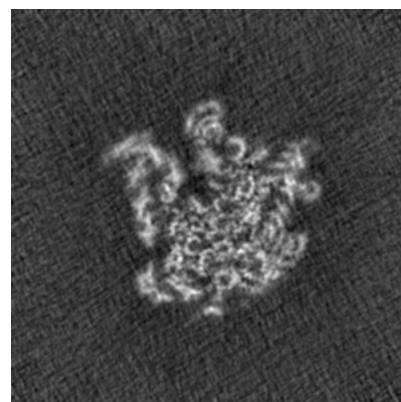
6.3.2 Raw map



X Index: 209



Y Index: 193

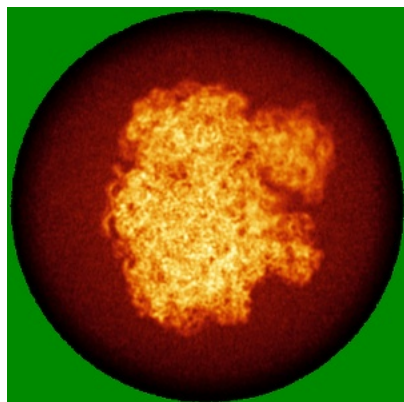


Z Index: 173

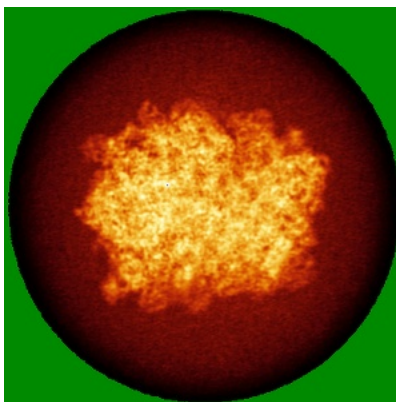
The images above show the largest variance slices of the map in three orthogonal directions.

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

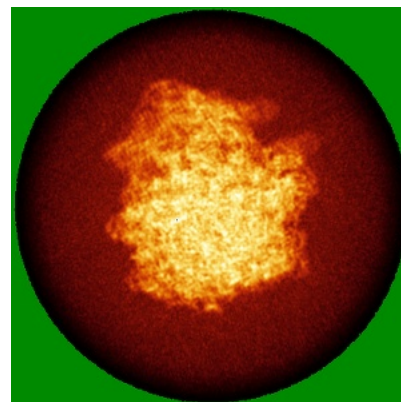
6.4.1 Primary map



X

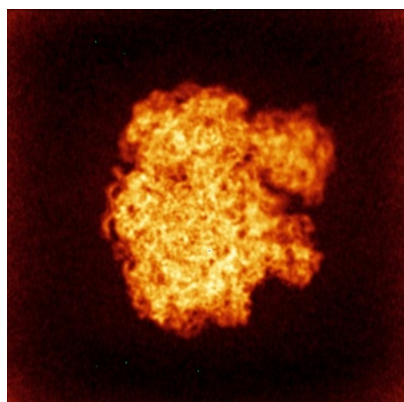


Y

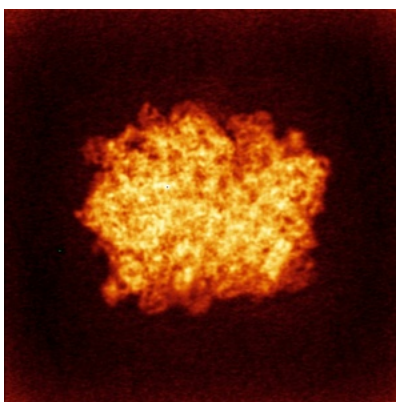


Z

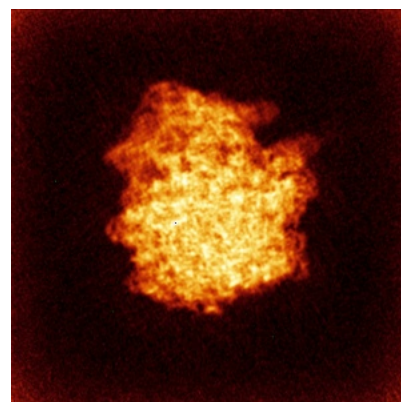
6.4.2 Raw map



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](#)

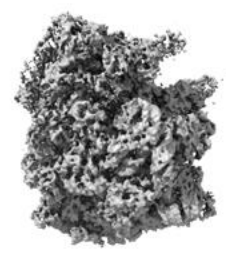
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.33. 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.

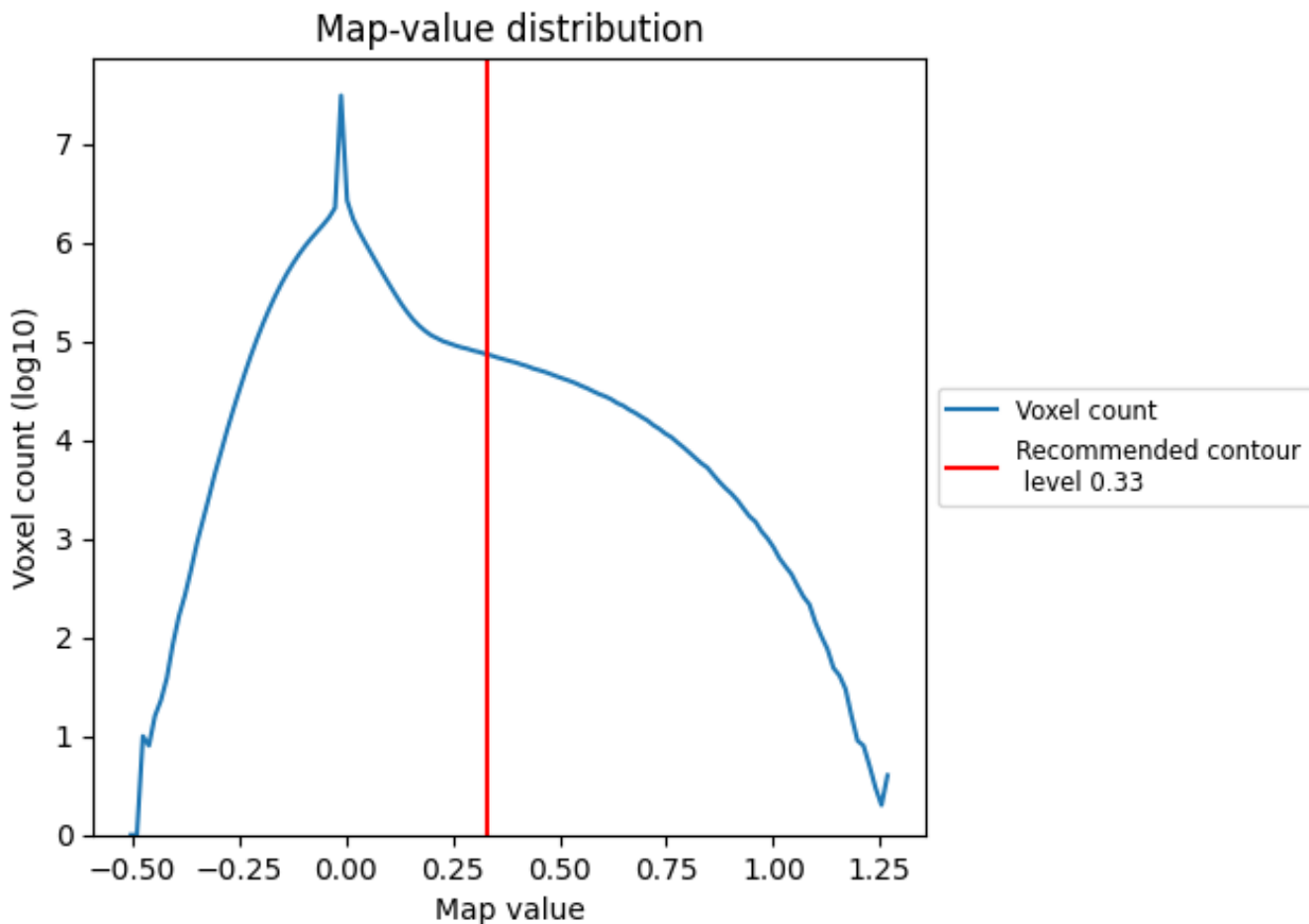
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

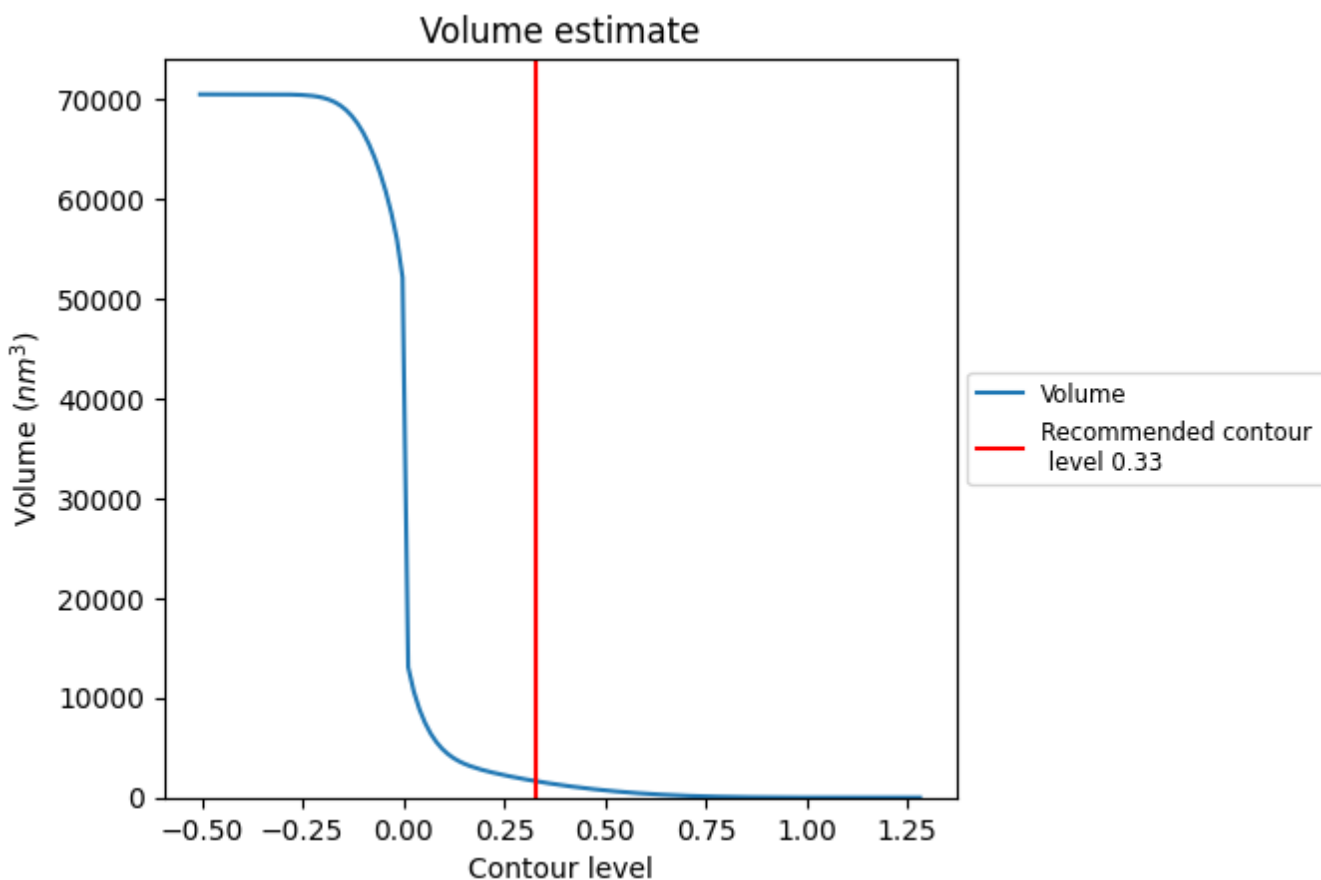
This section contains the results of statistical analysis of the map.

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.

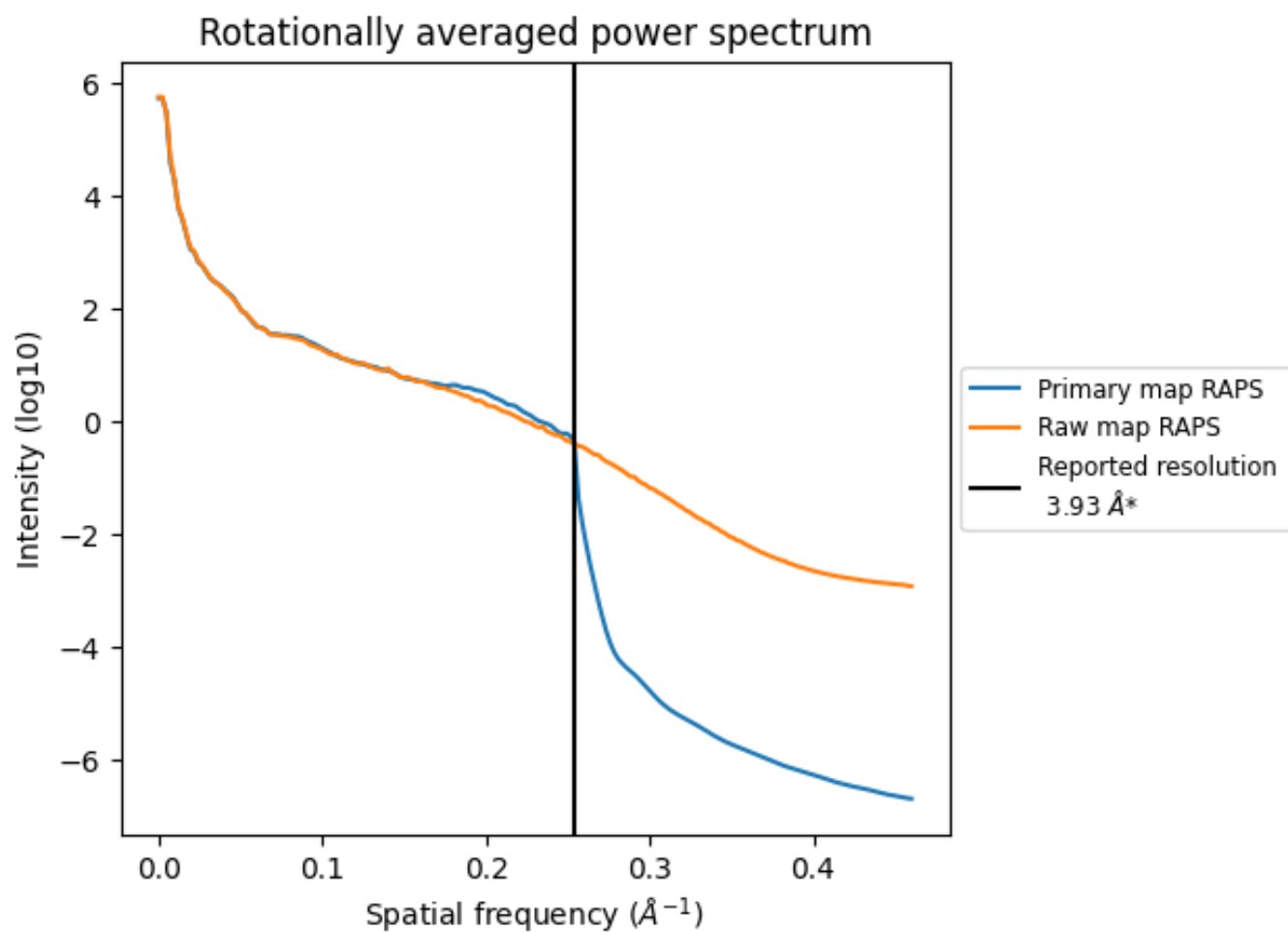
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 1637 nm³; this corresponds to an approximate mass of 1479 kDa.

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

7.3 Rotationally averaged power spectrum i

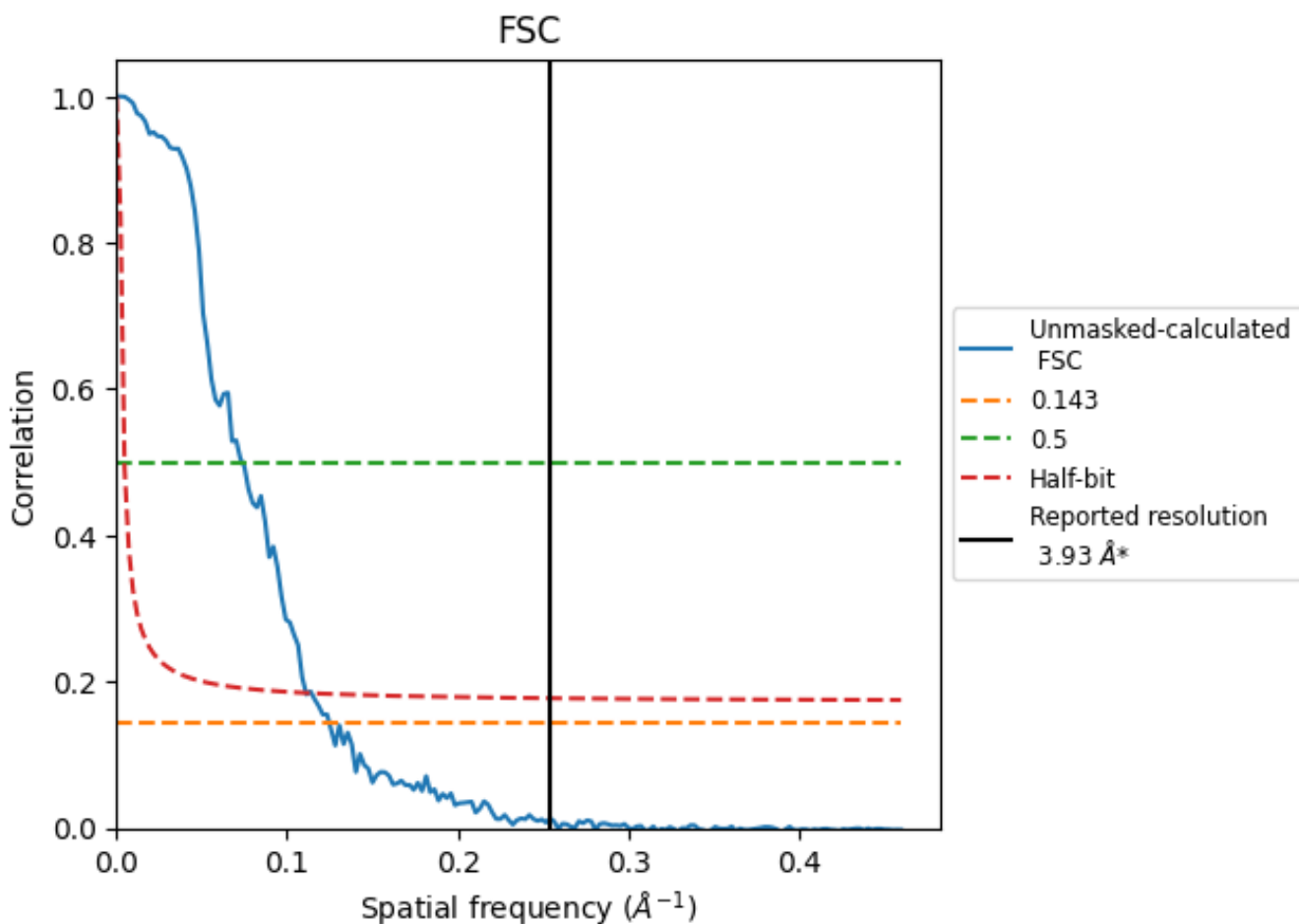


*Reported resolution corresponds to spatial frequency of 0.254 \AA^{-1}

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 0.254 Å⁻¹

8.2 Resolution estimates [i](#)

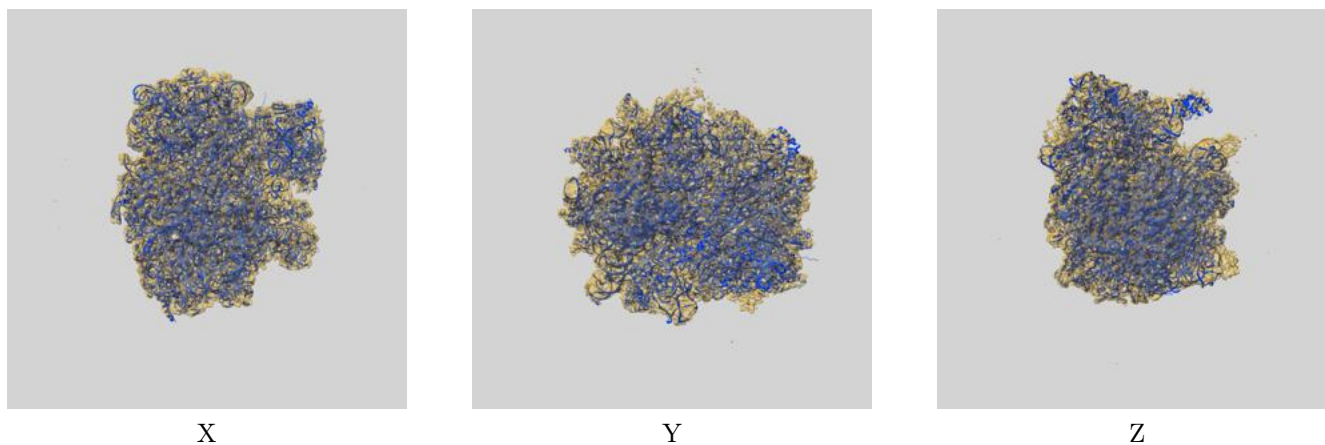
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.93	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.01	13.57	9.00

*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 8.01 differs from the reported value 3.93 by more than 10 %

9 Map-model fit [i](#)

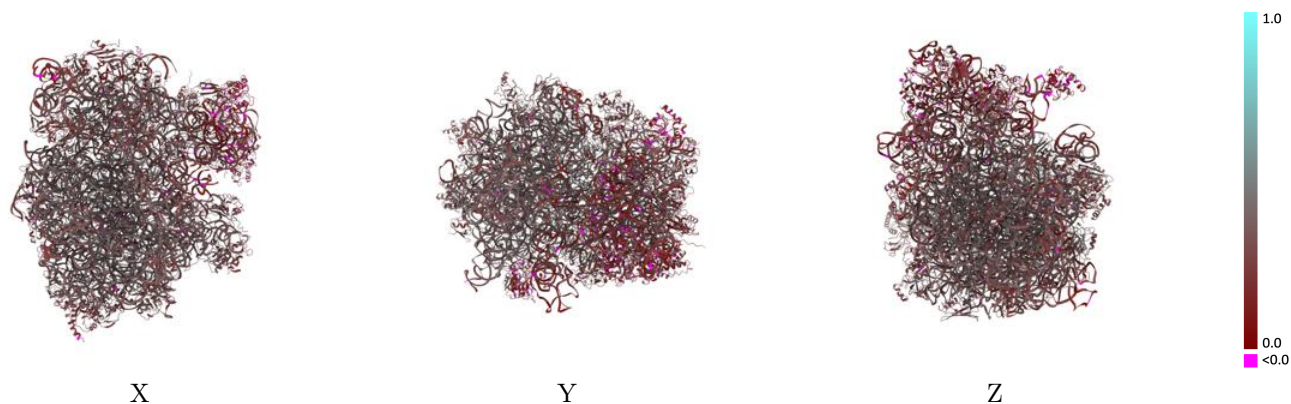
This section contains information regarding the fit between EMDB map EMD-34866 and PDB model 8HL1. Per-residue inclusion information can be found in section 3 on page 17.

9.1 Map-model overlay [i](#)



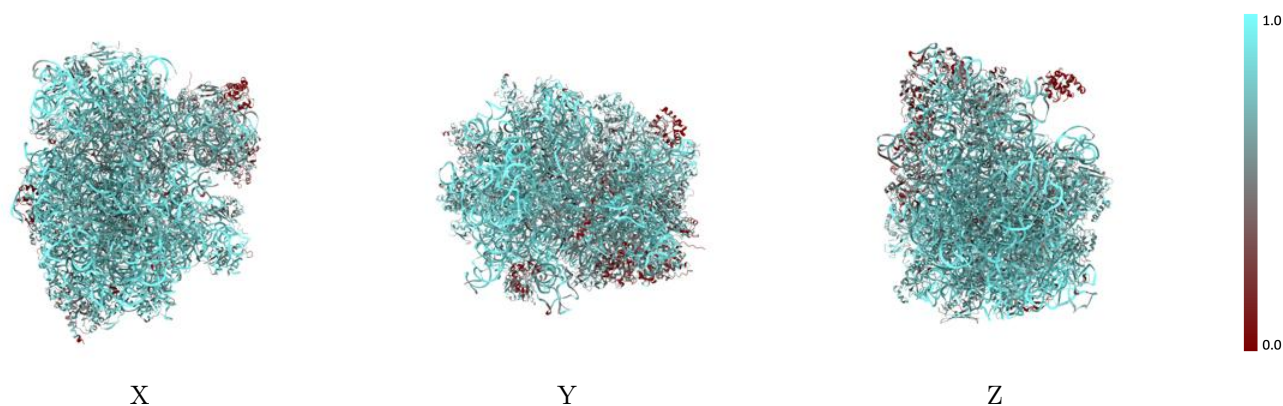
The images above show the 3D surface view of the map at the recommended contour level 0.33 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



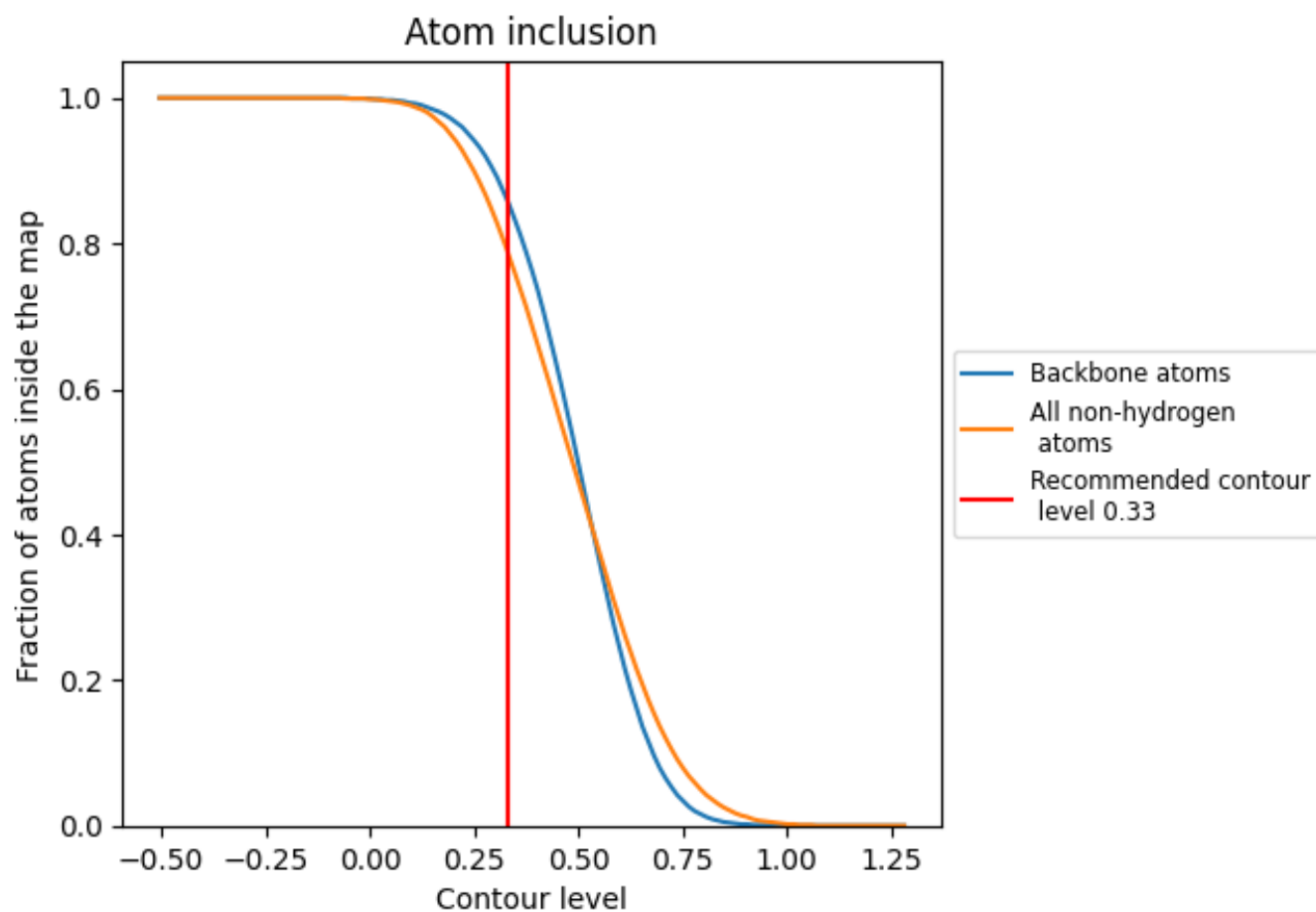
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.33).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 79% 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 (0.33) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7900	 0.3320
A16S	 0.8920	 0.3140
A23S	 0.9220	 0.3690
A5S	 0.9580	 0.3540
AEFG	 0.6340	 0.3100
AETN	 0.7700	 0.2280
AL1P	 0.3050	 0.1820
AL2P	 0.6650	 0.3980
AL3P	 0.7000	 0.3580
AL4P	 0.7020	 0.3600
AL5P	 0.6560	 0.2910
AL6P	 0.6880	 0.3430
ALX0	 0.6520	 0.3080
AMRN	 0.6500	 0.3000
APTN	 0.8690	 0.2930
APTP	 0.2690	 0.2070
AS2P	 0.4240	 0.2750
AS3P	 0.5340	 0.2690
AS4E	 0.6870	 0.3080
AS4P	 0.7090	 0.3020
AS5P	 0.6830	 0.3450
AS6E	 0.5920	 0.2800
AS7P	 0.3450	 0.1700
AS8E	 0.6290	 0.3220
AS8P	 0.7330	 0.3480
AS9P	 0.4420	 0.2080
L10E	 0.6620	 0.3610
L13P	 0.6690	 0.3260
L141	 0.6830	 0.3200
L142	 0.6670	 0.3130
L14P	 0.6160	 0.3870
L15E	 0.7020	 0.3830
L15P	 0.7420	 0.3790
L18E	 0.7540	 0.3600
L18P	 0.7260	 0.3190



Continued on next page...

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Chain	Atom inclusion	Q-score
L19E	 0.7170	 0.3670
L21E	 0.7050	 0.3960
L22P	 0.7150	 0.3680
L23P	 0.6410	 0.3620
L24E	 0.7720	 0.3800
L24P	 0.7120	 0.3470
L29P	 0.6330	 0.2920
L30E	 0.7190	 0.3320
L30P	 0.6880	 0.3130
L31E	 0.7180	 0.3670
L32E	 0.6250	 0.3610
L34E	 0.5760	 0.2580
L37A	 0.7090	 0.3850
L37E	 0.6520	 0.3720
L39E	 0.6660	 0.3430
L40E	 0.5180	 0.2910
L44E	 0.7530	 0.3840
L45A	 0.6190	 0.3150
L46A	 0.5350	 0.3500
L47A	 0.0670	 0.2470
L7A1	 0.6940	 0.3160
L7A2	 0.5280	 0.2820
S10P	 0.4600	 0.2320
S11P	 0.6110	 0.3220
S12P	 0.6080	 0.3690
S13P	 0.4020	 0.2010
S14P	 0.5680	 0.2560
S15P	 0.6960	 0.3120
S17E	 0.4950	 0.2390
S17P	 0.6830	 0.3650
S19E	 0.3690	 0.1860
S19P	 0.4940	 0.1980
S24E	 0.7350	 0.2920
S27A	 0.5650	 0.1530
S27E	 0.7720	 0.3140
S28E	 0.3930	 0.2580
S3AE	 0.6440	 0.2990
SL7A	 0.1540	 0.1530