



wwPDB EM Validation Summary Report ⓘ

Jun 17, 2026 – 07:04 pm BST

PDB ID : 9SLG / pdb_00009slg
EMDB ID : EMD-55001
Title : Doxycycline Bound E. coli Ribosome with Rearranged Peptidyl Transferase Centre
Authors : Stuart, W.S.; Isupov, M.N.; Harmer, N.J.
Deposited on : 2025-09-03
Resolution : 2.16 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:

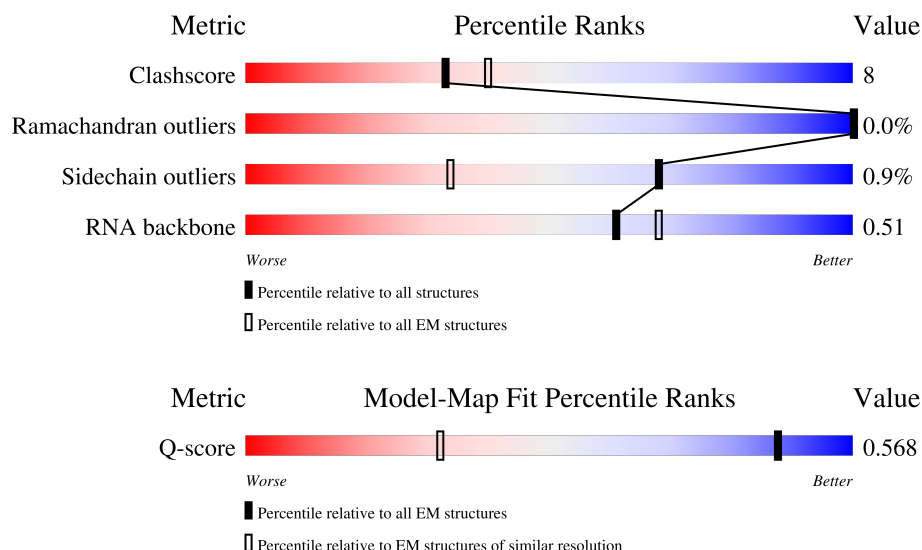
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.16 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	2609 (1.67 - 2.66)

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	0	55	13% 93% •
2	1	46	89% 9% •
3	2	65	94% 5% •

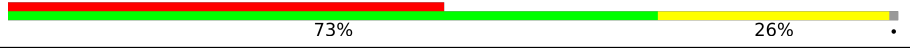
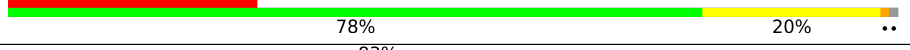
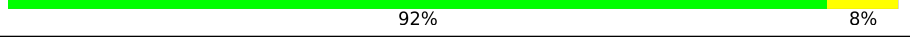
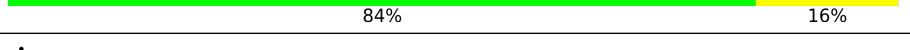
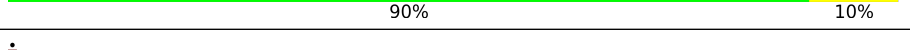
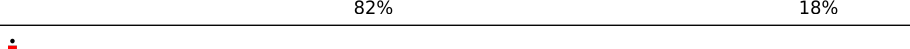
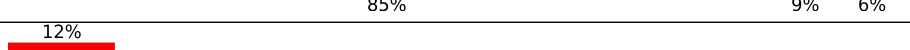
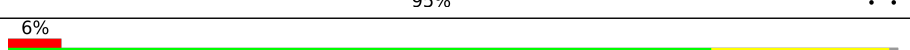
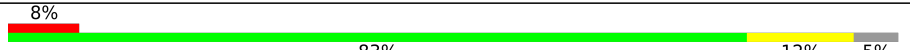
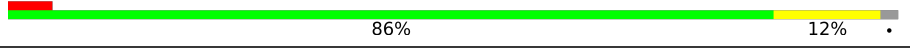
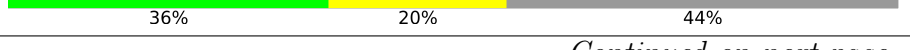
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Mol	Chain	Length	Quality of chain
4	3	38	
5	4	67	
6	A	1534	
7	B	241	
8	C	233	
9	D	206	
10	E	167	
11	F	131	
12	G	156	
13	H	130	
14	I	130	
15	J	103	
16	L	124	
17	M	118	
18	N	101	
19	O	89	
20	P	82	
21	Q	84	
22	R	75	
23	S	92	
24	T	87	
25	U	71	
26	Y	113	
27	a	2907	
28	b	120	

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Mol	Chain	Length	Quality of chain
29	c	273	
30	d	209	
31	f	179	
32	g	177	
33	h	149	
34	i	142	
35	j	123	
36	k	144	
37	l	136	
38	m	127	
39	n	117	
40	o	115	
41	p	118	
42	q	103	
43	r	110	
44	s	100	
45	t	104	
46	u	94	
47	v	85	
48	w	78	
49	x	63	
50	y	59	
51	z	57	
52	e	201	
53	6	234	

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Mol	Chain	Length	Quality of chain
54	K	129	 A horizontal bar chart showing the quality of chain K. The bar is divided into four segments: a red segment at the beginning labeled '15%', a large green segment labeled '80%', a yellow segment labeled '12%', and a small grey segment at the end labeled '8%'. The segments are separated by thin white lines.

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 150218 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Large ribosomal subunit protein bL33.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	0	53	Total	C	N	O	0	0
			436	281	80	75		

- Molecule 2 is a protein called Large ribosomal subunit protein bL34.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	1	46	Total	C	N	O	S	0	0
			377	228	90	57	2		

- Molecule 3 is a protein called Large ribosomal subunit protein bL35.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	64	Total	C	N	O	S	0	0
			504	323	105	74	2		

- Molecule 4 is a protein called Large ribosomal subunit protein bL36A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	3	38	Total	C	N	O	S	0	0
			302	185	65	48	4		

- Molecule 5 is a protein called Large ribosomal subunit protein bL31.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	4	67	Total	C	N	O	S	0	0
			529	328	100	95	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1534	Total	C	N	O	P	0	0
			32928	14691	6043	10660	1534		

- Molecule 7 is a protein called Small ribosomal subunit protein uS2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	226	Total	C	N	O	S	0	0
			1765	1116	317	324	8		

- Molecule 8 is a protein called Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	C	211	Total	C	N	O	S	0	0
			1653	1046	310	293	4		

- Molecule 9 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	D	205	Total	C	N	O	S	0	0
			1643	1026	315	298	4		

- Molecule 10 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	E	157	Total	C	N	O	S	0	0
			1152	717	218	211	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	151	ALA	GLU	variant	UNP P0A7W1

- Molecule 11 is a protein called Small ribosomal subunit protein bS6.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	F	105	Total	C	N	O	S	0	0
			853	539	154	153	7		

- Molecule 12 is a protein called Small ribosomal subunit protein uS7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	G	155	Total	C	N	O	S	0	0
			1229	767	237	221	4		

- Molecule 13 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	H	129	Total	C	N	O	S	0	0
			979	616	173	184	6		

- Molecule 14 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I	126	Total	C	N	O	S	0	0
			1010	628	202	177	3		

- Molecule 15 is a protein called Small ribosomal subunit protein uS10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	J	98	Total	C	N	O	S	0	0
			786	493	150	142	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	123	Total	C	N	O	S	0	0
			957	591	196	165	5		

- Molecule 17 is a protein called Small ribosomal subunit protein uS13.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	115	Total	C	N	O	S	0	0
			891	552	179	157	3		

- Molecule 18 is a protein called Small ribosomal subunit protein uS14.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	N	100	Total	C	N	O	S	0	0
			805	499	164	139	3		

- Molecule 19 is a protein called Small ribosomal subunit protein uS15.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	88	Total	C	N	O	S	0	0
			714	439	144	130	1		

- Molecule 20 is a protein called Small ribosomal subunit protein bS16.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	81	Total	C	N	O	S	0	0
			643	403	127	112	1		

- Molecule 21 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	Q	81	Total	C	N	O	S	0	0
			656	415	122	116	3		

- Molecule 22 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	67	Total	C	N	O	S	0	0
			554	350	104	99	1		

- Molecule 23 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	84	Total	C	N	O	S	0	0
			668	427	127	112	2		

- Molecule 24 is a protein called Small ribosomal subunit protein bS20.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	T	86	Total	C	N	O	S	0	0
			670	414	138	115	3		

- Molecule 25 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	70	Total	C	N	O	S	0	0
			590	366	125	98	1		

- Molecule 26 is a protein called Ribosome-associated inhibitor A.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	105	Total	C	N	O	S	0	0
			829	518	154	154	3		

- Molecule 27 is a RNA chain called 23S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	2907	Total	C	N	O	P	0	0
			62423	27854	11483	20179	2907		

- Molecule 28 is a RNA chain called 5S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	120	Total	C	N	O	P	0	0
			2568	1144	468	836	120		

- Molecule 29 is a protein called Large ribosomal subunit protein uL2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	c	271	Total	C	N	O	S	0	0
			2082	1288	423	364	7		

- Molecule 30 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	209	Total	C	N	O	S	0	0
			1566	980	288	294	4		

- Molecule 31 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	178	Total	C	N	O	S	0	0
			1420	905	251	258	6		

- Molecule 32 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	175	Total	C	N	O	S	0	0
			1313	826	241	244	2		

- Molecule 33 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	149	Total	C	N	O	S	0	0
			1111	699	197	214	1		

- Molecule 34 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	142	Total	C	N	O	S	0	0
			1129	714	212	199	4		

- Molecule 35 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	123	Total	C	N	O	S	0	0
			947	593	181	167	6		

- Molecule 36 is a protein called Large ribosomal subunit protein uL15.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	144	Total	C	N	O	S	0	0
			1053	654	207	190	2		

- Molecule 37 is a protein called Large ribosomal subunit protein uL16.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	136	Total	C	N	O	S	0	0
			1075	686	205	177	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
l	82	MS6	MET	conflict	UNP P0ADY7

- Molecule 38 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	m	119	Total	C	N	O	S	0	0
			951	588	195	163	5		

- Molecule 39 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	116	Total	C	N	O		0	0
			891	552	178	161			

- Molecule 40 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	114	Total	C	N	O	S	0	0
			917	574	179	163	1		

- Molecule 41 is a protein called Large ribosomal subunit protein bL20.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	117	Total	C	N	O		0	0
			947	604	192	151			

- Molecule 42 is a protein called Large ribosomal subunit protein bL21.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	103	Total	C	N	O	S	0	0
			816	516	153	145	2		

- Molecule 43 is a protein called Large ribosomal subunit protein uL22.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	110	Total	C	N	O	S	0	0
			857	532	166	156	3		

- Molecule 44 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	s	95	Total	C	N	O	S	0	0
			757	479	141	135	2		

- Molecule 45 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	t	103	Total	C	N	O		0	0
			789	498	148	143			

- Molecule 46 is a protein called Large ribosomal subunit protein bL25.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	u	94	Total	C	N	O	S	0	0
			753	479	137	134	3		

- Molecule 47 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	v	78	Total	C	N	O	S	0	0
			592	365	119	107	1		

- Molecule 48 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	w	77	Total	C	N	O	S	0	0
			624	388	129	105	2		

- Molecule 49 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	x	63	Total	C	N	O	S	0	0
			509	313	99	95	2		

- Molecule 50 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	y	58	Total	C	N	O	S	0	0
			449	281	87	79	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	z	56	Total	C	N	O	S	0	0
			444	269	94	80	1		

- Molecule 52 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	e	189	Total	C	N	O	S	0	0
			1453	912	260	276	5		

- Molecule 53 is a protein called Large ribosomal subunit protein uL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	6	130	Total	C	N	O	S	0	0
			993	623	180	188	2		

- Molecule 54 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	K	119	Total	C	N	O	S	0	0
			895	551	178	163	3		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	119	IAS	ASN	conflict	UNP P0A7R9

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
55	3	1	Total	Zn	0
			1	1	
55	4	1	Total	Zn	0
			1	1	

- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	132	Total	Mg	0
			132	132	
56	M	1	Total	Mg	0
			1	1	
56	a	305	Total	Mg	0
			305	305	
56	b	7	Total	Mg	0
			7	7	
56	c	1	Total	Mg	0
			1	1	
56	z	1	Total	Mg	0
			1	1	

- Molecule 57 is POTASSIUM ION (CCD ID: K) (formula: K).

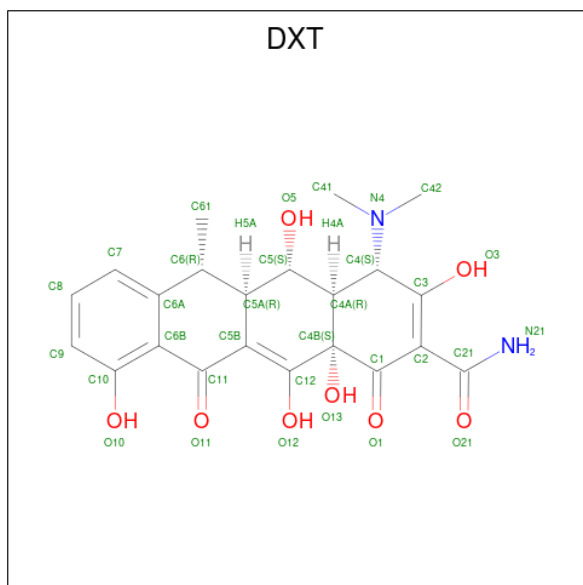
Mol	Chain	Residues	Atoms		AltConf
57	A	3	Total	K	0
			3	3	
57	a	69	Total	K	0
			69	69	
57	b	1	Total	K	0
			1	1	
57	c	3	Total	K	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
57	e	1	Total	K	0
			1	1	

- Molecule 58 is (4S,4AR,5S,5AR,6R,12AS)-4-(DIMETHYLAMINO)-3,5,10,12,12A-PENTAHYDROXY-6-METHYL-1,11-DIOXO-1,4,4A,5,5A,6,11,12A-OCTAHYDROTETRACENE-2-CARBOXAMIDE (CCD ID: DXT) (formula: C₂₂H₂₄N₂O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
58	a	1	Total	C	N	O	0
			32	22	2	8	

- Molecule 59 is water.

Mol	Chain	Residues	Atoms		AltConf
59	1	6	Total	O	0
			6	6	
59	2	15	Total	O	0
			15	15	
59	3	4	Total	O	0
			4	4	
59	A	1274	Total	O	0
			1274	1274	
59	B	1	Total	O	0
			1	1	
59	D	8	Total	O	0
			8	8	

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Mol	Chain	Residues	Atoms		AltConf
59	E	8	Total 8	O 8	0
59	F	3	Total 3	O 3	0
59	G	1	Total 1	O 1	0
59	H	17	Total 17	O 17	0
59	I	2	Total 2	O 2	0
59	J	3	Total 3	O 3	0
59	L	3	Total 3	O 3	0
59	N	2	Total 2	O 2	0
59	O	11	Total 11	O 11	0
59	P	7	Total 7	O 7	0
59	Q	4	Total 4	O 4	0
59	R	3	Total 3	O 3	0
59	S	1	Total 1	O 1	0
59	T	1	Total 1	O 1	0
59	U	6	Total 6	O 6	0
59	Y	1	Total 1	O 1	0
59	a	3472	Total 3472	O 3472	0
59	b	75	Total 75	O 75	0
59	c	51	Total 51	O 51	0
59	d	30	Total 30	O 30	0
59	f	1	Total 1	O 1	0

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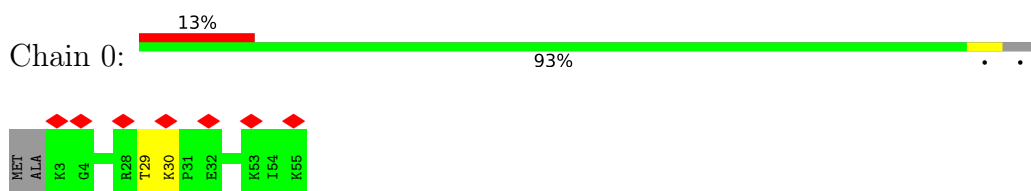
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Mol	Chain	Residues	Atoms		AltConf
59	i	8	Total 8	O 8	0
59	j	10	Total 10	O 10	0
59	k	26	Total 26	O 26	0
59	l	5	Total 5	O 5	0
59	m	13	Total 13	O 13	0
59	n	2	Total 2	O 2	0
59	o	8	Total 8	O 8	0
59	p	33	Total 33	O 33	0
59	q	10	Total 10	O 10	0
59	r	23	Total 23	O 23	0
59	s	8	Total 8	O 8	0
59	t	2	Total 2	O 2	0
59	u	1	Total 1	O 1	0
59	v	9	Total 9	O 9	0
59	w	5	Total 5	O 5	0
59	y	9	Total 9	O 9	0
59	z	14	Total 14	O 14	0
59	e	10	Total 10	O 10	0
59	K	7	Total 7	O 7	0

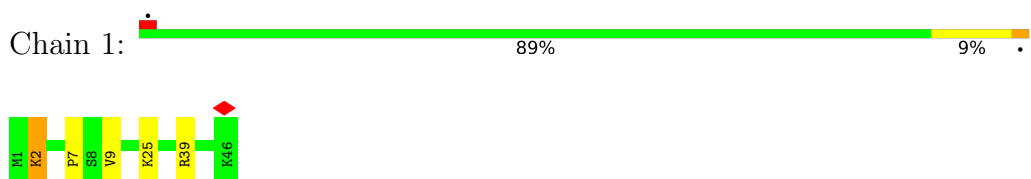
3 Residue-property plots [i](#)

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.

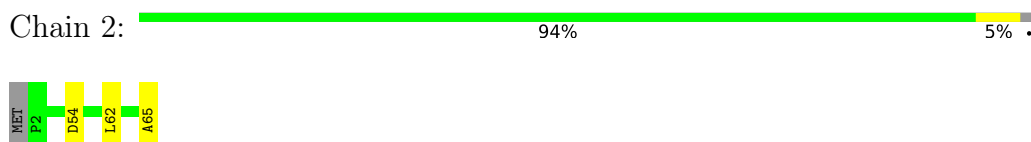
- Molecule 1: Large ribosomal subunit protein bL33



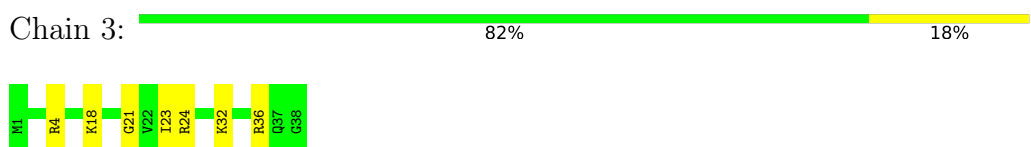
- Molecule 2: Large ribosomal subunit protein bL34



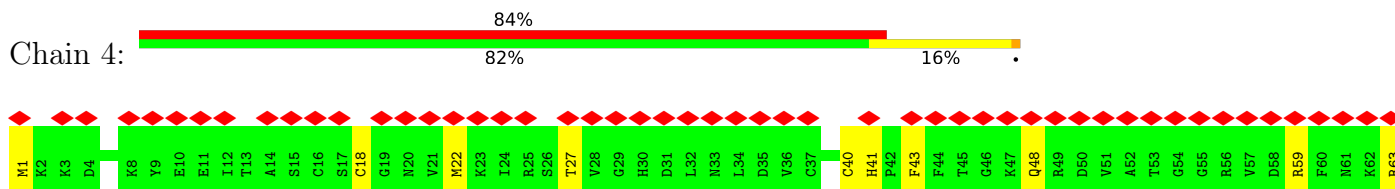
- Molecule 3: Large ribosomal subunit protein bL35

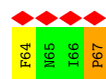


- Molecule 4: Large ribosomal subunit protein bL36A

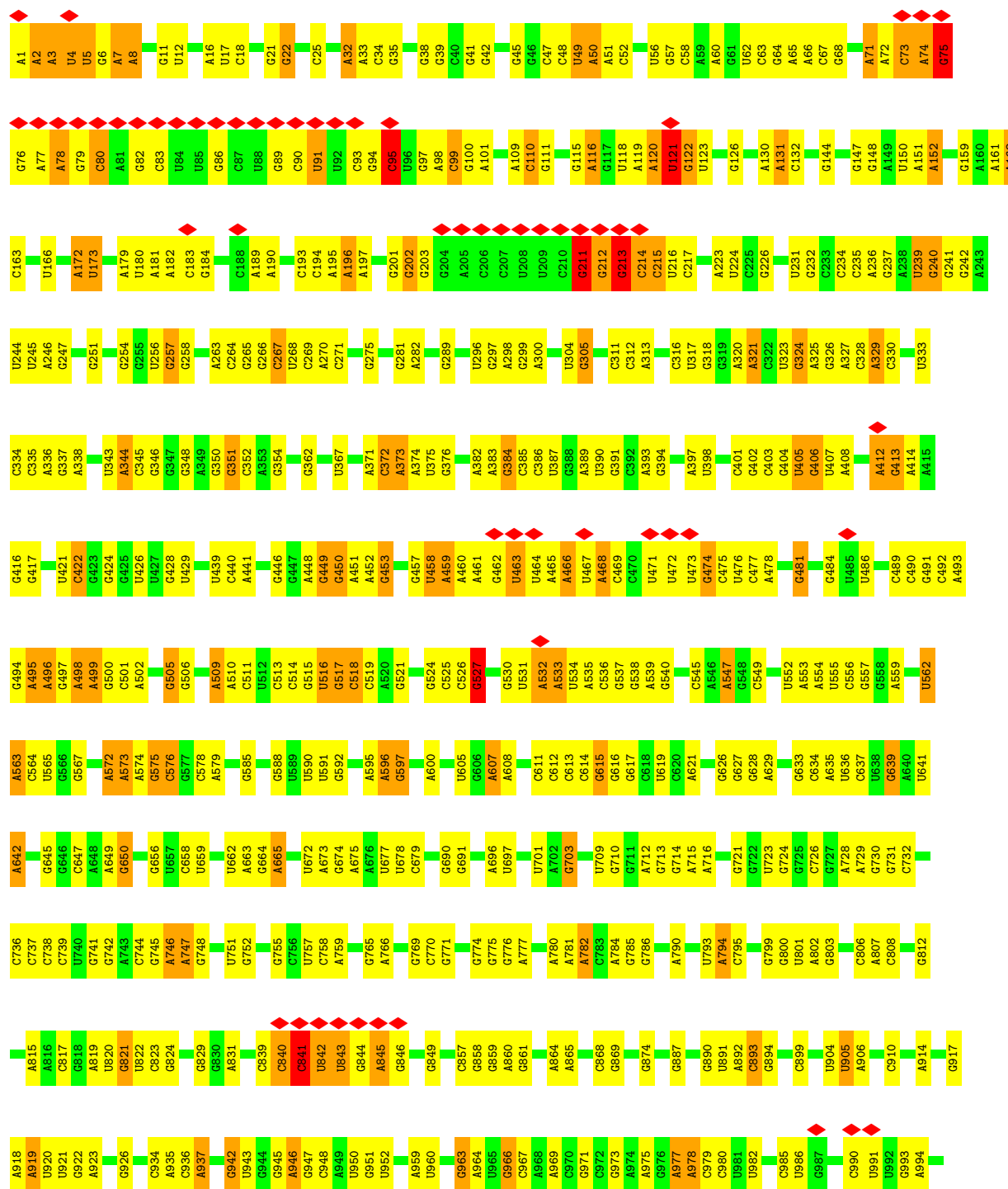


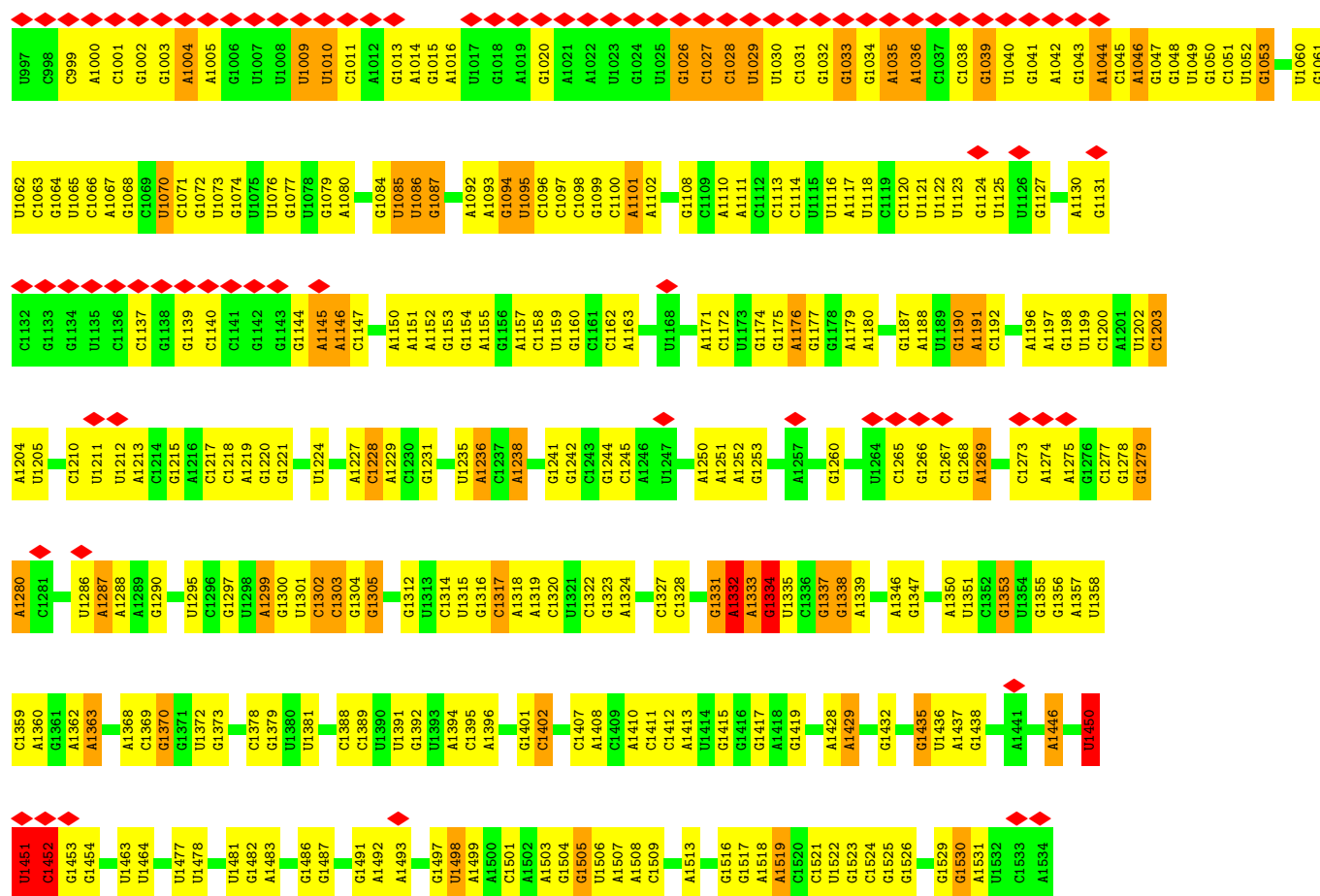
- Molecule 5: Large ribosomal subunit protein bL31



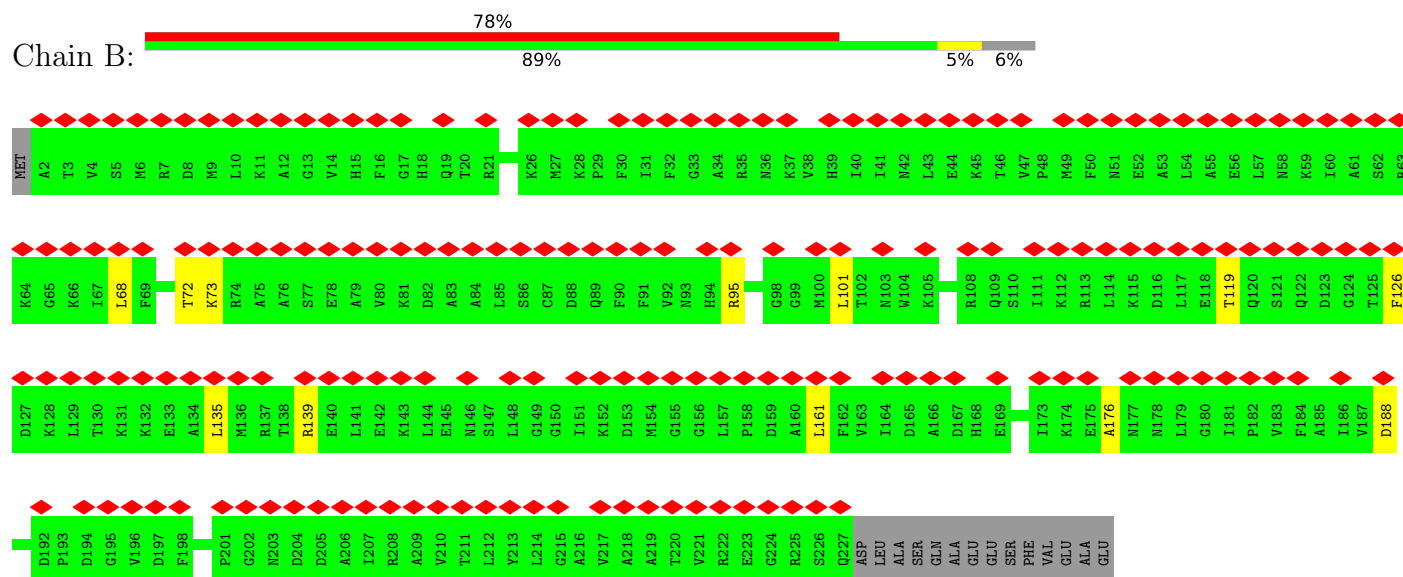


● Molecule 6: 16S ribosomal RNA

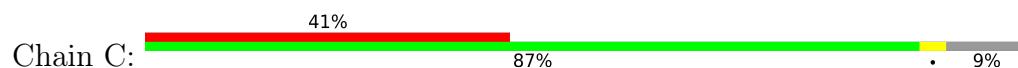


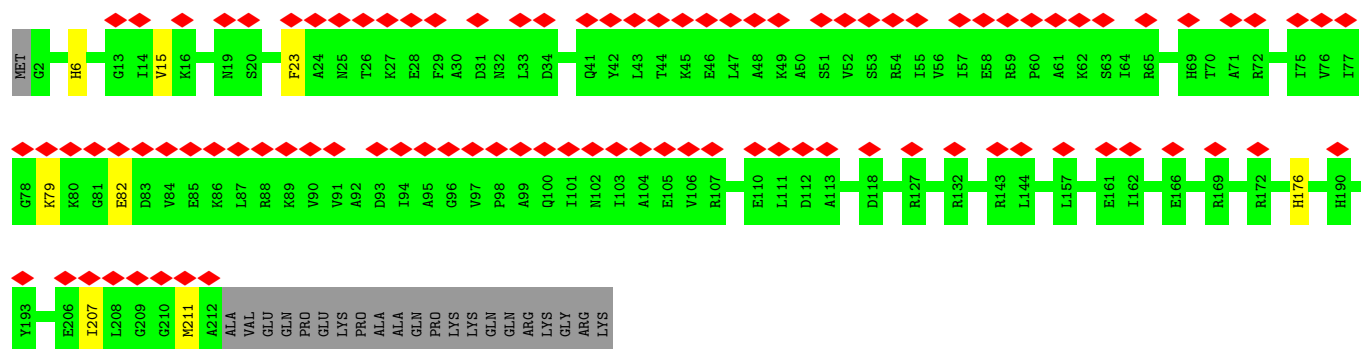


• Molecule 7: Small ribosomal subunit protein uS2

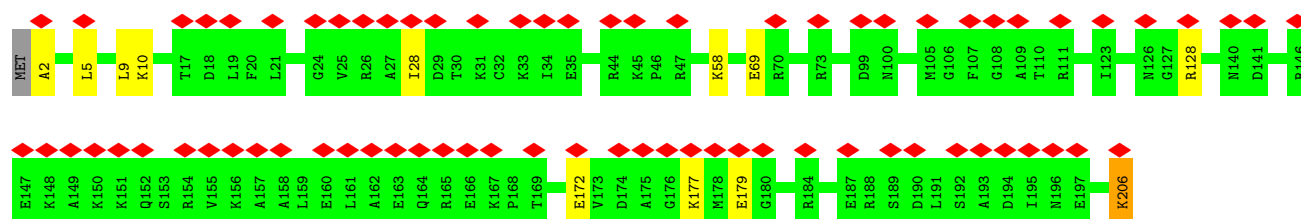


• Molecule 8: Small ribosomal subunit protein uS3

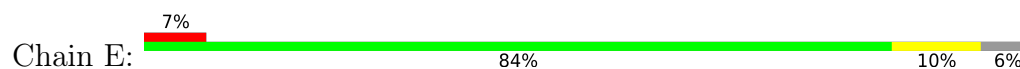




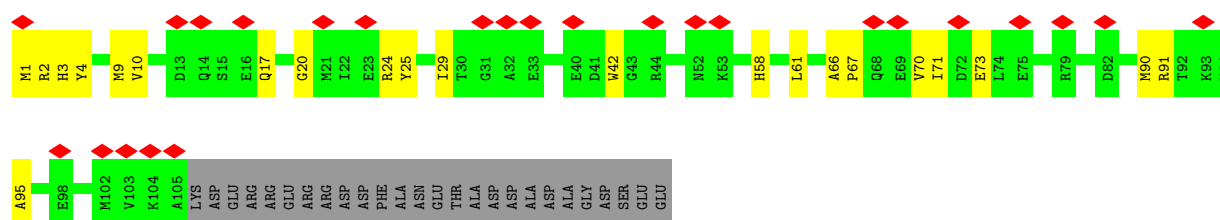
- Molecule 9: Small ribosomal subunit protein uS4



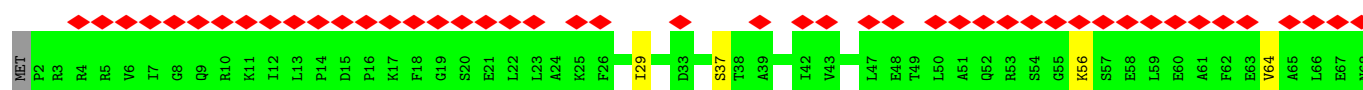
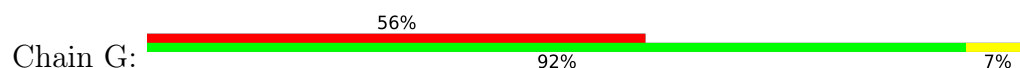
- Molecule 10: Small ribosomal subunit protein uS5

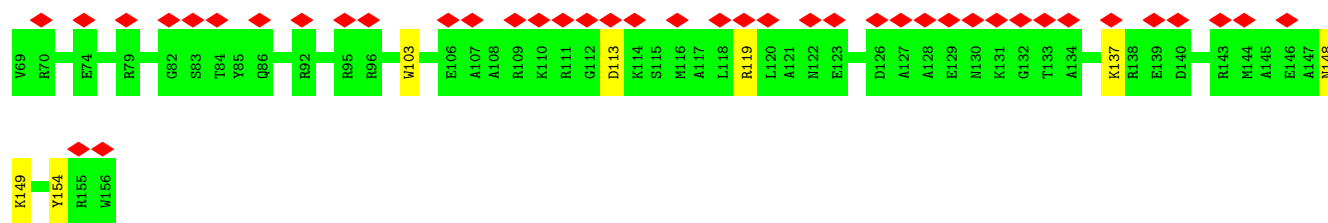


- Molecule 11: Small ribosomal subunit protein bS6

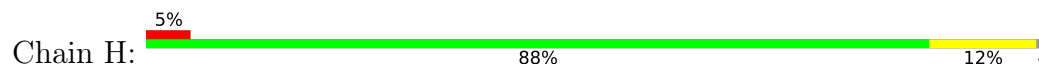


- Molecule 12: Small ribosomal subunit protein uS7

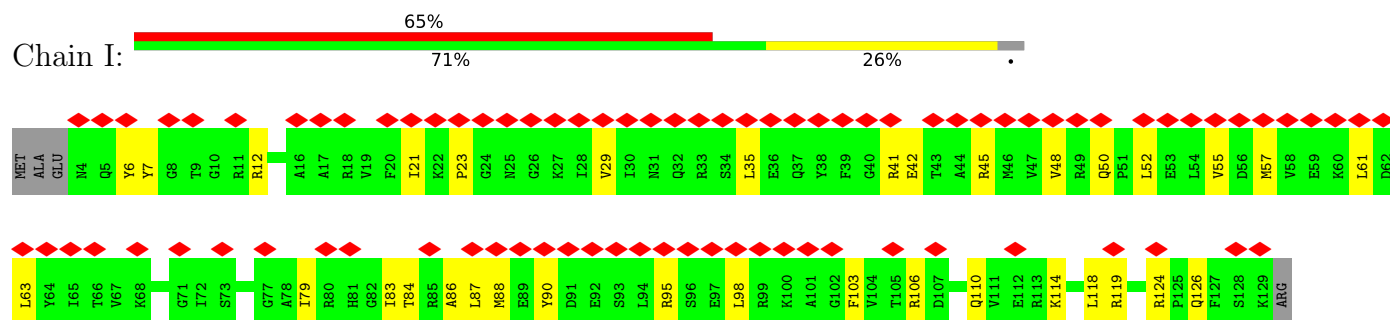




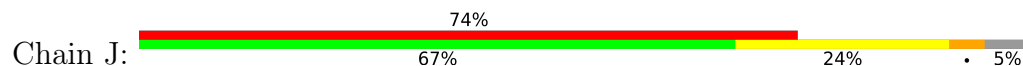
- Molecule 13: Small ribosomal subunit protein uS8



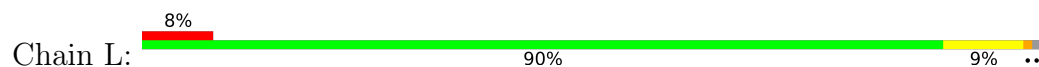
- Molecule 14: Small ribosomal subunit protein uS9



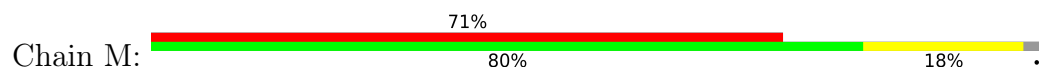
- Molecule 15: Small ribosomal subunit protein uS10

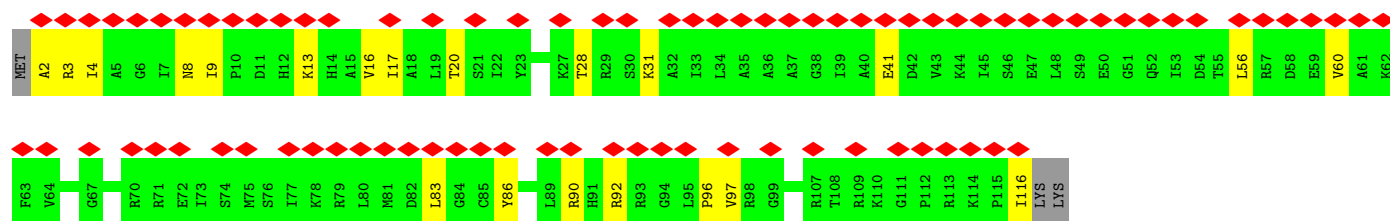


- Molecule 16: Small ribosomal subunit protein uS12

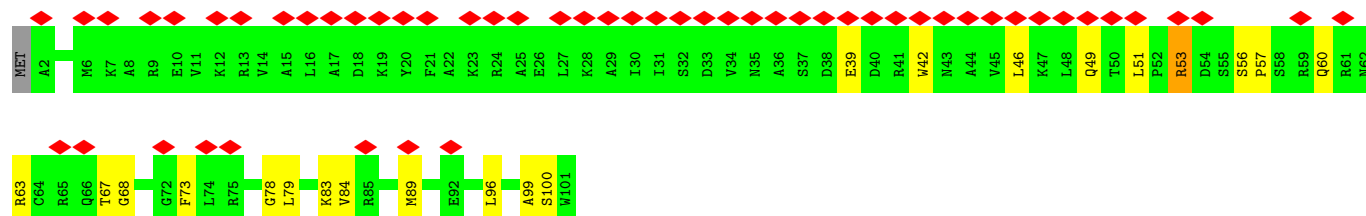
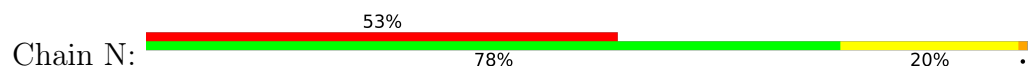


- Molecule 17: Small ribosomal subunit protein uS13

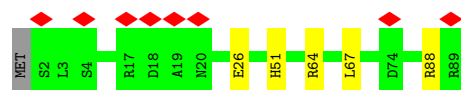




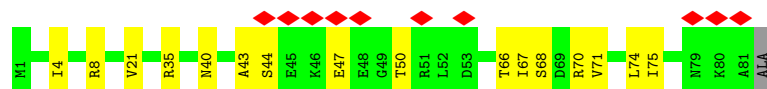
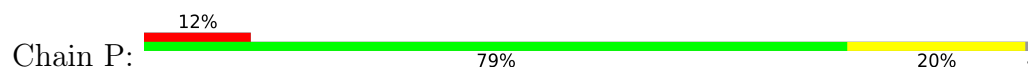
- Molecule 18: Small ribosomal subunit protein uS14



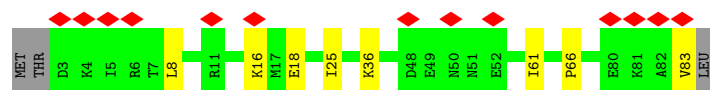
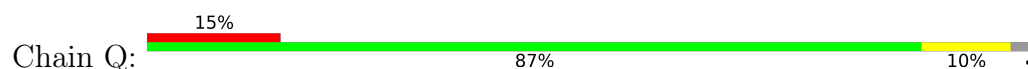
- Molecule 19: Small ribosomal subunit protein uS15



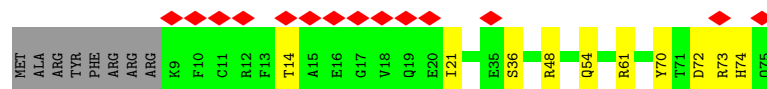
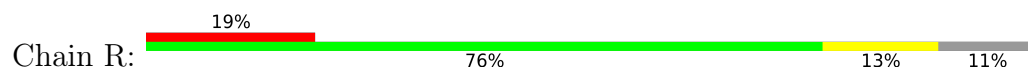
- Molecule 20: Small ribosomal subunit protein bS16



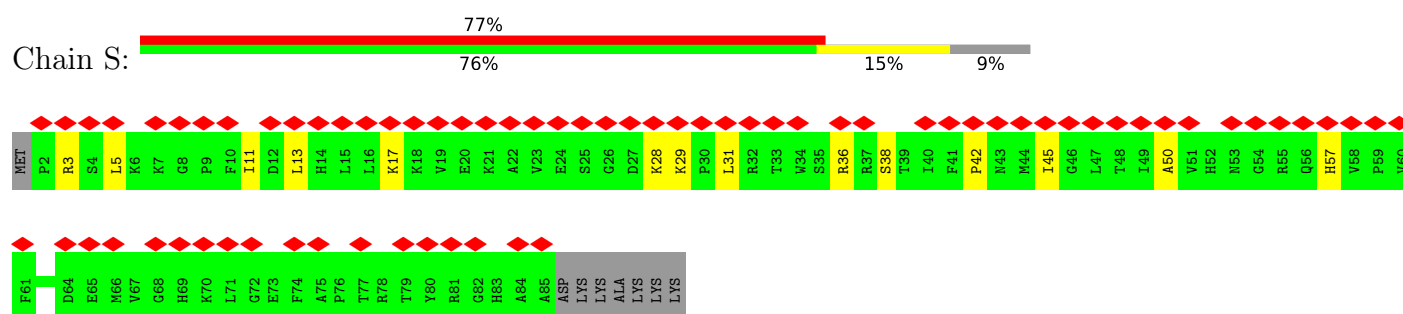
- Molecule 21: Small ribosomal subunit protein uS17



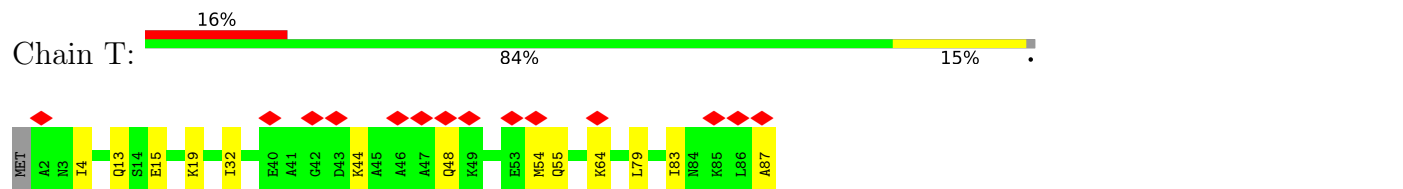
- Molecule 22: Small ribosomal subunit protein bS18



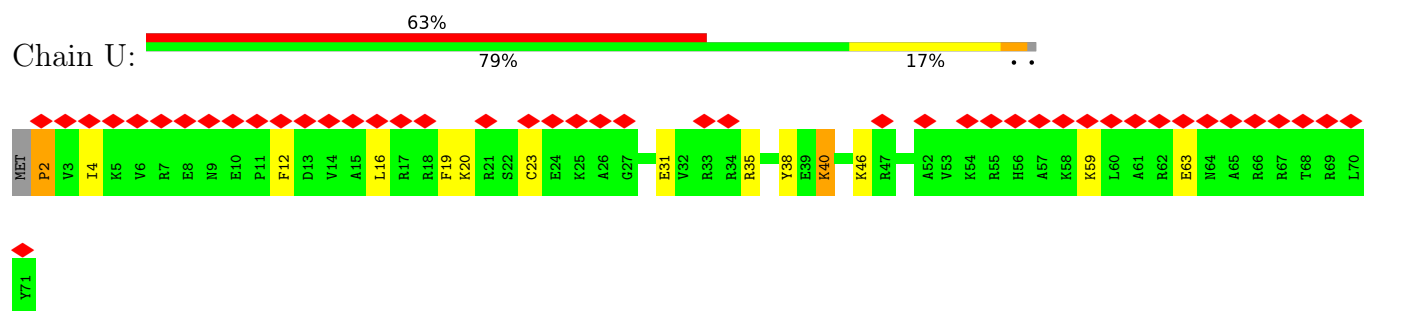
- Molecule 23: Small ribosomal subunit protein uS19



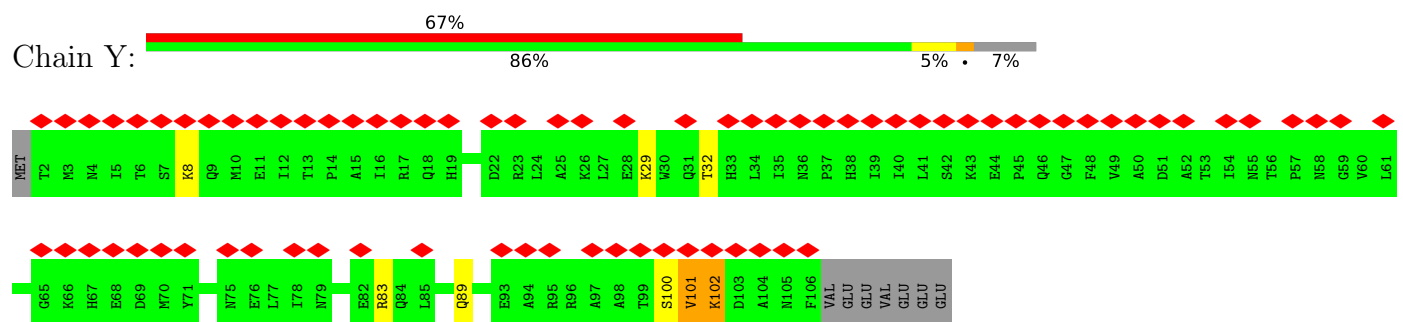
- Molecule 24: Small ribosomal subunit protein bS20



- Molecule 25: Small ribosomal subunit protein bS21

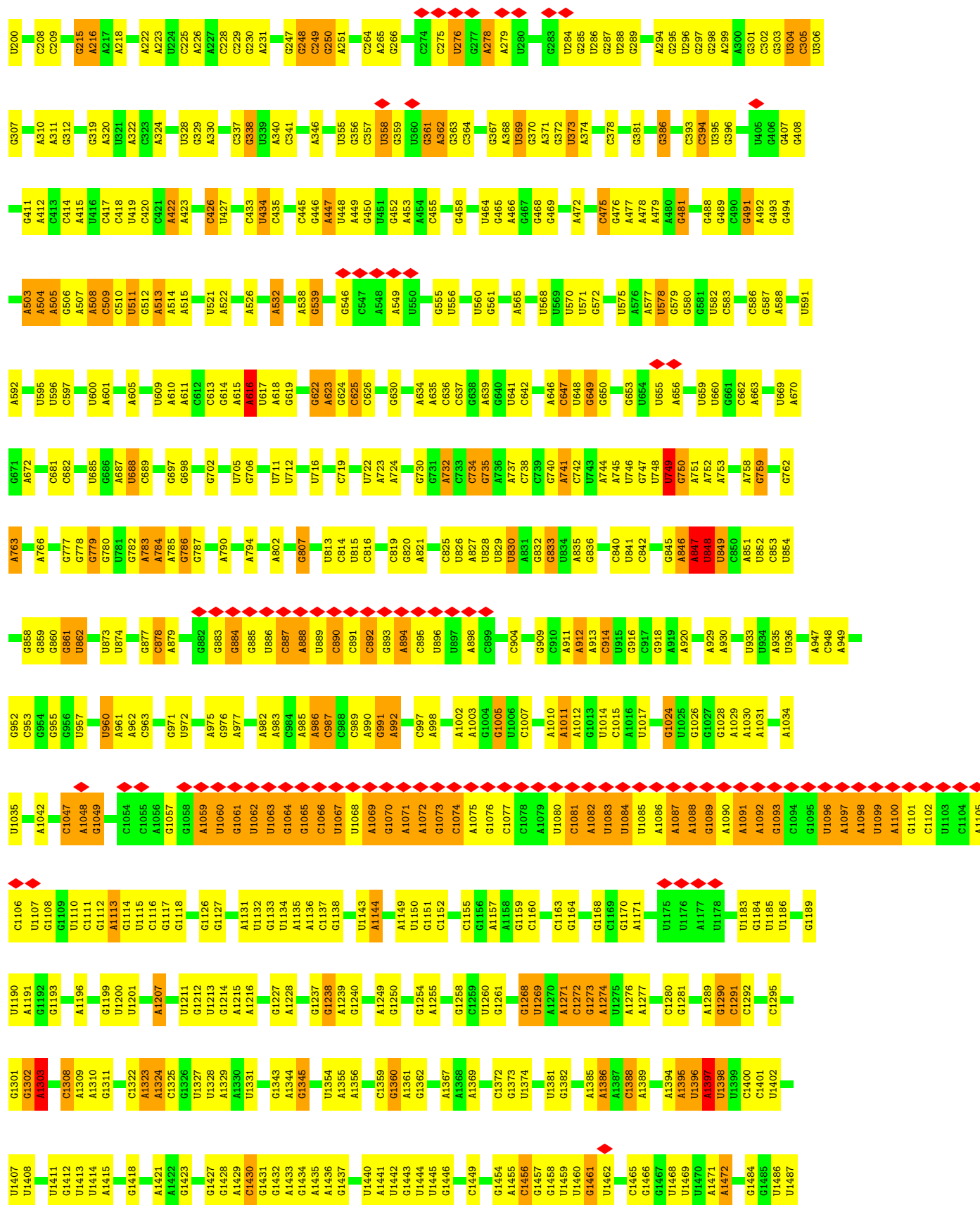


- Molecule 26: Ribosome-associated inhibitor A

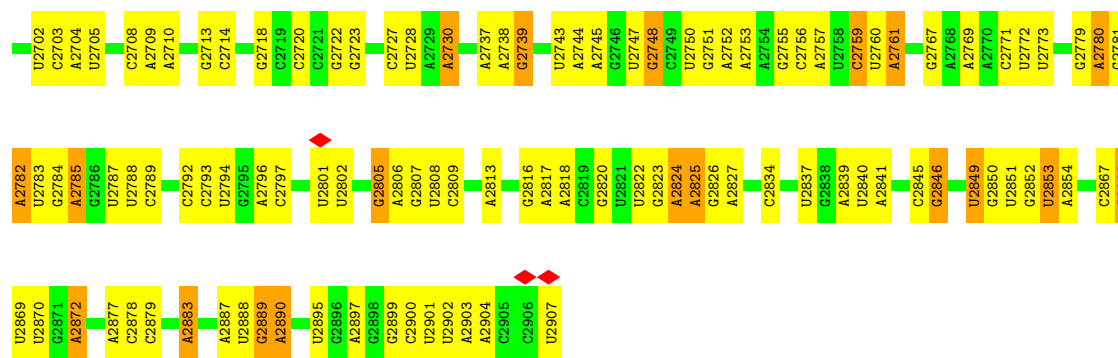


- Molecule 27: 23S ribosomal RNA

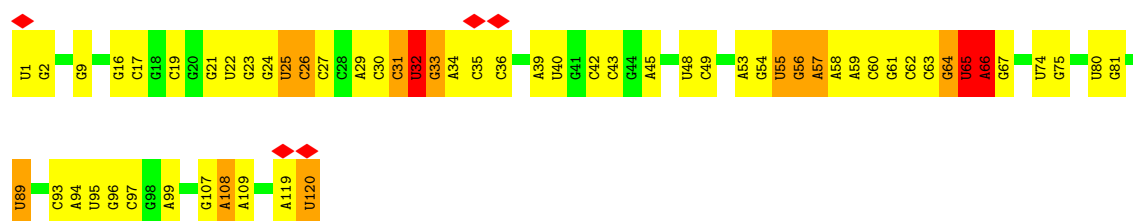




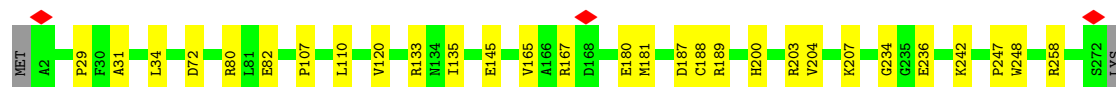
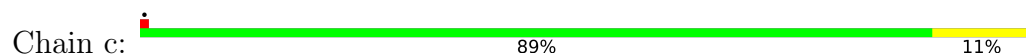




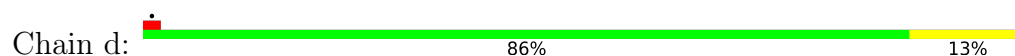
• Molecule 28: 5S ribosomal RNA



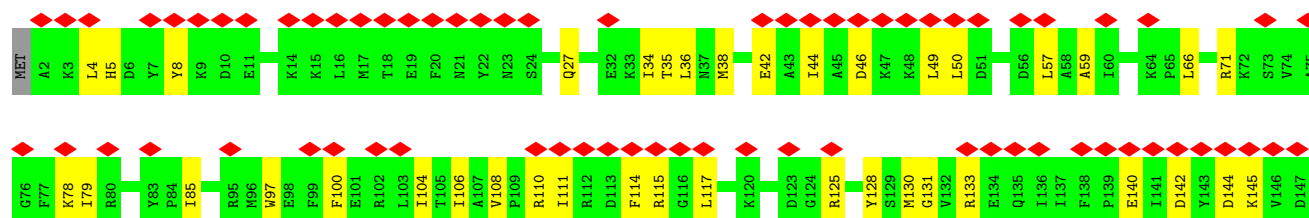
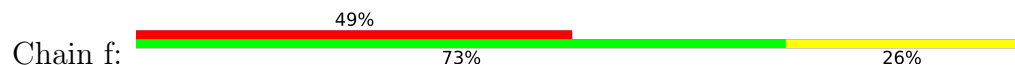
• Molecule 29: Large ribosomal subunit protein uL2

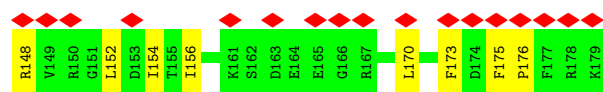


• Molecule 30: Large ribosomal subunit protein uL3

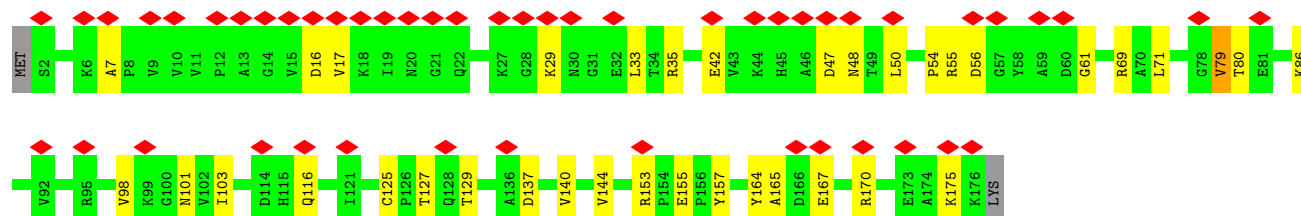
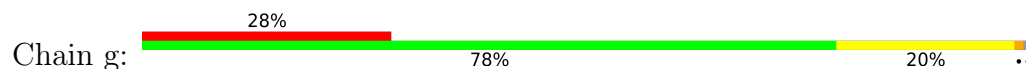


• Molecule 31: Large ribosomal subunit protein uL5

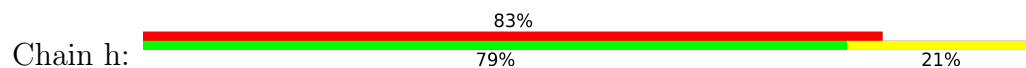




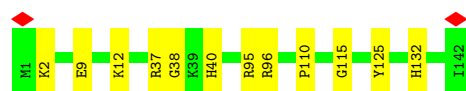
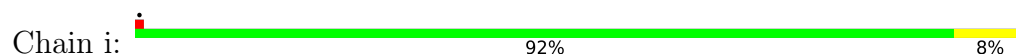
- Molecule 32: Large ribosomal subunit protein uL6



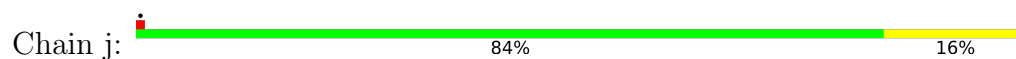
- Molecule 33: Large ribosomal subunit protein bL9



- Molecule 34: Large ribosomal subunit protein uL13

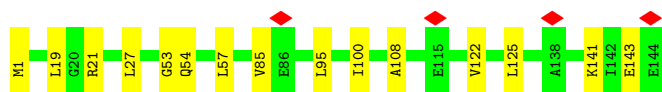


- Molecule 35: Large ribosomal subunit protein uL14

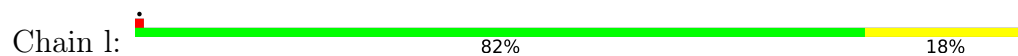


- Molecule 36: Large ribosomal subunit protein uL15

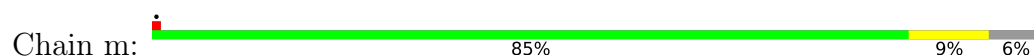




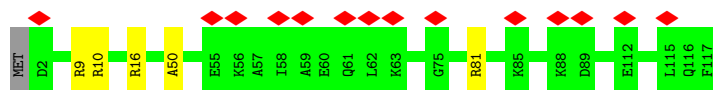
- Molecule 37: Large ribosomal subunit protein uL16



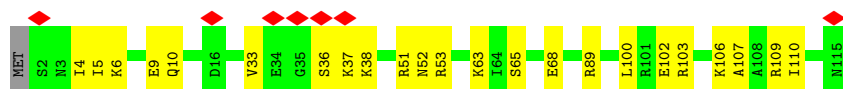
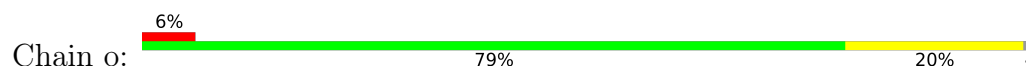
- Molecule 38: Large ribosomal subunit protein bL17



- Molecule 39: Large ribosomal subunit protein uL18



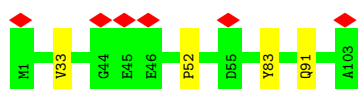
- Molecule 40: Large ribosomal subunit protein bL19



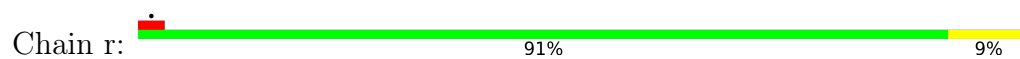
- Molecule 41: Large ribosomal subunit protein bL20



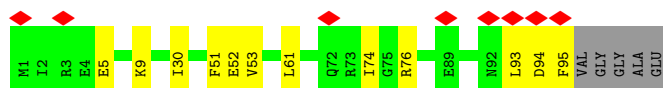
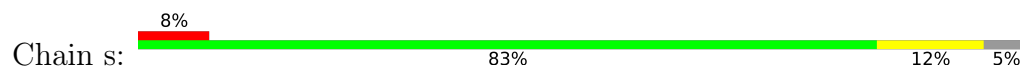
- Molecule 42: Large ribosomal subunit protein bL21



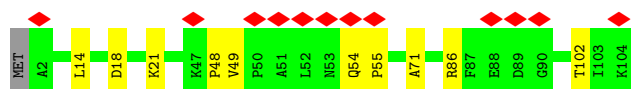
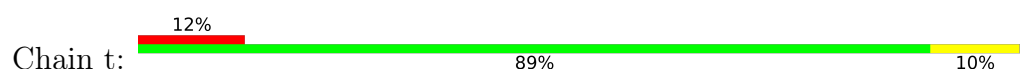
- Molecule 43: Large ribosomal subunit protein uL22



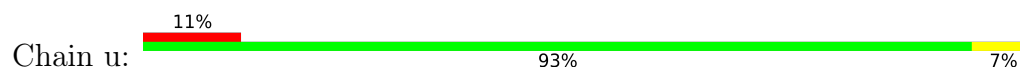
- Molecule 44: Large ribosomal subunit protein uL23



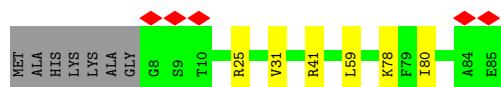
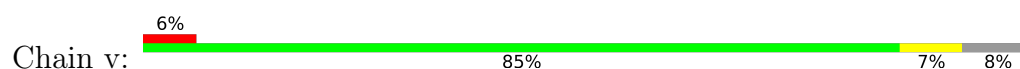
- Molecule 45: Large ribosomal subunit protein uL24



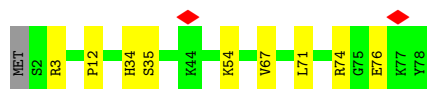
- Molecule 46: Large ribosomal subunit protein bL25



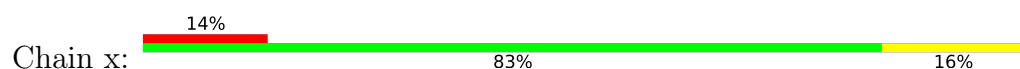
- Molecule 47: Large ribosomal subunit protein bL27



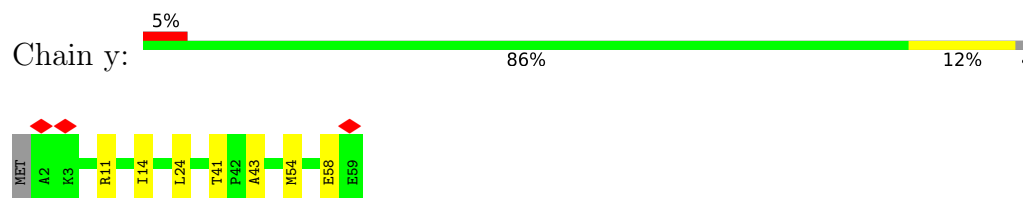
- Molecule 48: Large ribosomal subunit protein bL28



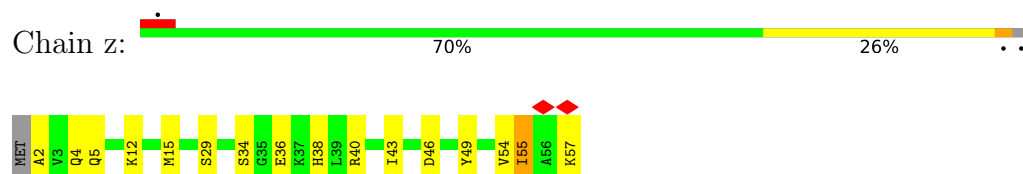
- Molecule 49: Large ribosomal subunit protein uL29



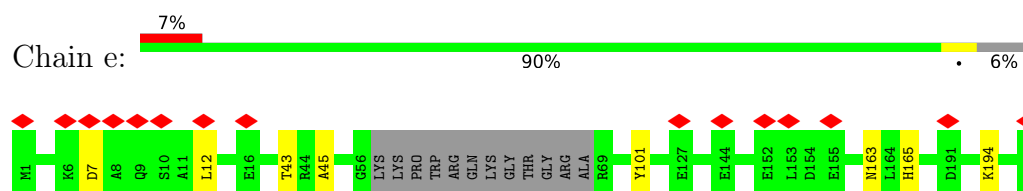
- Molecule 50: Large ribosomal subunit protein uL30



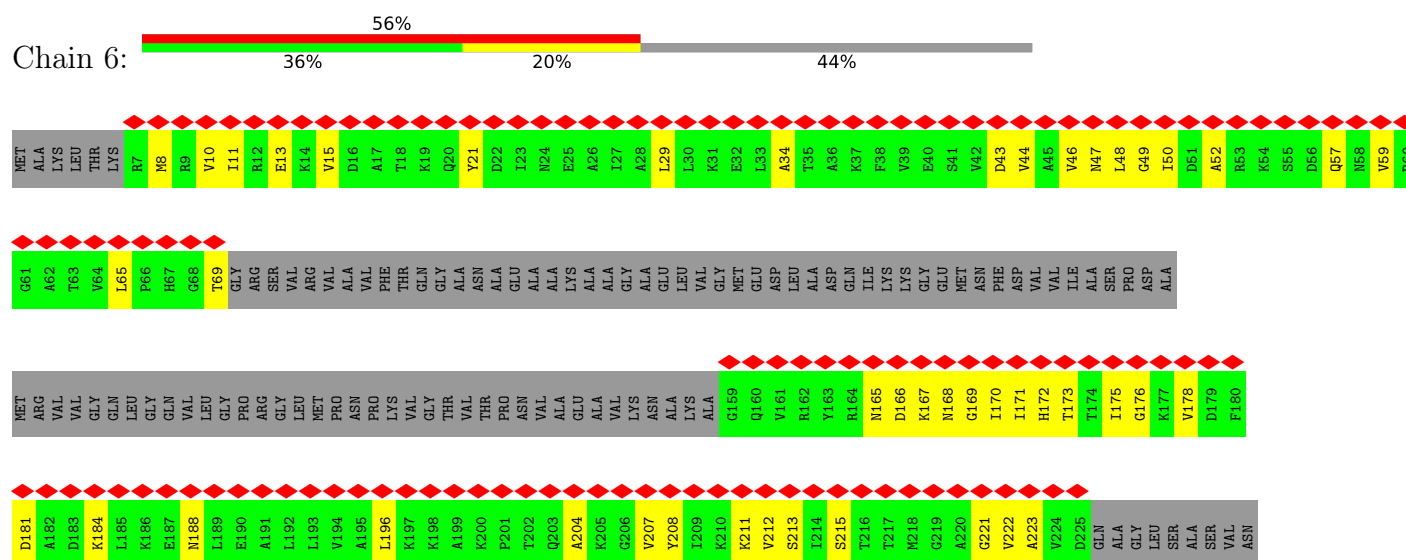
- Molecule 51: Large ribosomal subunit protein bL32



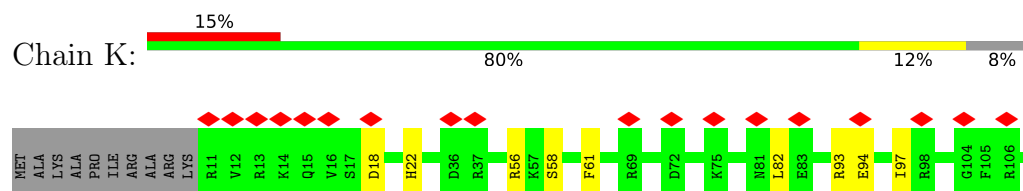
- Molecule 52: Large ribosomal subunit protein uL4



- Molecule 53: Large ribosomal subunit protein uL1



- Molecule 54: Small ribosomal subunit protein uS11





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215222	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45	Depositor
Minimum defocus (nm)	400	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.375	Depositor
Minimum map value	-0.101	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	387.0, 387.0, 387.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.645, 0.645, 0.645	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5MU, H2U, 2MG, 6MZ, IAS, G7M, MG, 4D4, MEQ, MA6, 4OC, 5MC, DXT, K, 1MG, ZN, OMC, D2T, MS6, 2MA, OMG, PSU, 3TD, OMU, UR3

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	0	0.44	0/443	0.84	0/587
2	1	0.45	0/380	0.83	0/498
3	2	0.44	0/513	0.74	0/676
4	3	0.46	0/303	0.66	0/397
5	4	0.47	0/539	0.80	1/721 (0.1%)
6	A	0.45	1/36672 (0.0%)	0.76	86/57206 (0.2%)
7	B	0.55	0/1796	1.16	3/2420 (0.1%)
8	C	0.53	0/1680	1.03	0/2263
9	D	0.51	0/1665	1.12	0/2227
10	E	0.46	0/1165	0.76	0/1568
11	F	0.43	0/872	0.73	0/1178
12	G	0.53	0/1247	1.15	0/1672
13	H	0.41	0/989	0.71	0/1326
14	I	0.42	0/1022	0.77	0/1361
15	J	0.44	0/796	0.81	0/1077
16	L	0.61	0/960	0.95	1/1286 (0.1%)
17	M	0.44	0/900	0.83	0/1204
18	N	0.52	0/817	0.89	0/1088
19	O	0.41	0/722	0.83	0/964
20	P	0.41	0/653	0.75	0/877
21	Q	0.51	0/665	0.91	0/892
22	R	0.42	0/563	0.79	0/754
23	S	0.44	0/685	0.73	0/922
24	T	0.46	0/676	0.87	0/895
25	U	0.41	0/598	0.87	0/792
26	Y	0.58	0/842	1.00	0/1137
27	a	0.45	0/69339	0.72	102/108171 (0.1%)
28	b	0.47	0/2870	1.01	18/4473 (0.4%)
29	c	0.45	0/2121	0.72	0/2852
30	d	0.53	1/1576 (0.1%)	0.70	0/2119
31	f	0.41	0/1444	0.74	0/1937

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	g	0.45	0/1333	0.79	0/1805
33	h	0.42	0/1122	0.77	0/1515
34	i	0.41	0/1152	0.71	0/1551
35	j	0.40	0/956	0.71	0/1279
36	k	0.43	0/1062	0.77	0/1413
37	l	0.42	0/1073	0.73	0/1433
38	m	0.42	0/964	0.79	0/1289
39	n	0.44	0/901	0.79	0/1207
40	o	0.41	0/929	0.68	0/1242
41	p	0.42	0/960	0.82	0/1278
42	q	0.53	0/829	0.89	0/1107
43	r	0.43	0/864	0.73	0/1156
44	s	0.40	0/764	0.76	0/1021
45	t	0.40	0/797	0.73	0/1062
46	u	0.43	0/766	0.74	0/1025
47	v	0.42	0/599	0.66	0/792
48	w	0.42	0/634	0.75	0/846
49	x	0.38	0/510	0.83	0/677
50	y	0.46	0/453	0.75	0/605
51	z	0.44	0/450	0.79	0/599
52	e	0.51	0/1468	1.08	1/1975 (0.1%)
53	6	0.40	0/1000	0.72	0/1344
54	K	0.82	0/902	1.33	4/1215 (0.3%)
All	All	0.46	2/156001 (0.0%)	0.77	216/232976 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	d	165	MET	SD-CE	-13.28	1.46	1.79
6	A	89	G	C1'-N9	-7.11	1.37	1.48

The worst 5 of 216 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	1460	U	C4'-C3'-O3'	-20.00	79.40	109.40
27	a	1510	A	C1'-C2'-O2'	-19.05	79.83	108.40
28	b	64	G	C2'-C3'-O3'	-17.53	87.41	113.70
6	A	213	G	C2'-C3'-O3'	-15.87	89.89	113.70
6	A	4	U	C2'-C3'-O3'	-15.85	89.92	113.70

There are no chirality outliers.

There are no planarity outliers.

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	0	436	0	477	2	0
2	1	377	0	418	5	0
3	2	504	0	572	2	0
4	3	302	0	340	6	0
5	4	529	0	527	12	0
6	A	32928	0	16586	584	0
7	B	1765	0	1792	7	0
8	C	1653	0	1727	6	0
9	D	1643	0	1707	14	0
10	E	1152	0	1198	9	0
11	F	853	0	851	20	0
12	G	1229	0	1277	12	0
13	H	979	0	1031	11	0
14	I	1010	0	1057	37	0
15	J	786	0	828	24	0
16	L	957	0	1017	9	0
17	M	891	0	952	19	0
18	N	805	0	844	16	0
19	O	714	0	734	8	0
20	P	643	0	661	10	0
21	Q	656	0	695	6	0
22	R	554	0	573	16	0
23	S	668	0	693	12	0
24	T	670	0	719	10	0
25	U	590	0	629	18	0
26	Y	829	0	848	9	0
27	a	62423	0	31395	882	0
28	b	2568	0	1299	34	0
29	c	2082	0	2154	20	0
30	d	1566	0	1618	19	0
31	f	1420	0	1457	39	0
32	g	1313	0	1358	20	0
33	h	1111	0	1148	27	0
34	i	1129	0	1162	8	0
35	j	947	0	1023	14	0
36	k	1053	0	1129	11	0
37	l	1075	0	1145	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
38	m	951	0	994	6	0
39	n	891	0	923	4	0
40	o	917	0	962	19	0
41	p	947	0	1019	8	0
42	q	816	0	839	3	0
43	r	857	0	922	12	0
44	s	757	0	820	10	0
45	t	789	0	843	6	0
46	u	753	0	780	4	0
47	v	592	0	607	4	0
48	w	624	0	652	5	0
49	x	509	0	543	12	0
50	y	449	0	488	8	0
51	z	444	0	458	14	0
52	e	1453	0	1510	8	0
53	6	993	0	1048	32	0
54	K	895	0	905	22	0
55	3	1	0	0	0	0
55	4	1	0	0	0	0
56	A	132	0	0	0	0
56	M	1	0	0	0	0
56	a	305	0	0	0	0
56	b	7	0	0	0	0
56	c	1	0	0	0	0
56	z	1	0	0	0	0
57	A	3	0	0	0	0
57	a	69	0	0	0	0
57	b	1	0	0	0	0
57	c	3	0	0	0	0
57	e	1	0	0	0	0
58	a	32	0	21	0	0
59	1	6	0	0	0	0
59	2	15	0	0	0	0
59	3	4	0	0	0	0
59	A	1274	0	0	17	0
59	B	1	0	0	0	0
59	D	8	0	0	0	0
59	E	8	0	0	0	0
59	F	3	0	0	0	0
59	G	1	0	0	0	0
59	H	17	0	0	3	0
59	I	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
59	J	3	0	0	0	0
59	K	7	0	0	1	0
59	L	3	0	0	0	0
59	N	2	0	0	0	0
59	O	11	0	0	0	0
59	P	7	0	0	1	0
59	Q	4	0	0	0	0
59	R	3	0	0	0	0
59	S	1	0	0	0	0
59	T	1	0	0	0	0
59	U	6	0	0	0	0
59	Y	1	0	0	0	0
59	a	3472	0	0	38	0
59	b	75	0	0	0	0
59	c	51	0	0	1	0
59	d	30	0	0	1	0
59	e	10	0	0	0	0
59	f	1	0	0	0	0
59	i	8	0	0	0	0
59	j	10	0	0	1	0
59	k	26	0	0	1	0
59	l	5	0	0	0	0
59	m	13	0	0	0	0
59	n	2	0	0	0	0
59	o	8	0	0	0	0
59	p	33	0	0	0	0
59	q	10	0	0	0	0
59	r	23	0	0	0	0
59	s	8	0	0	0	0
59	t	2	0	0	0	0
59	u	1	0	0	0	0
59	v	9	0	0	0	0
59	w	5	0	0	0	0
59	y	9	0	0	3	0
59	z	14	0	0	0	0
All	All	150218	0	97975	1972	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 8.

The worst 5 of 1972 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)
25:U:12:PHE:HZ	54:K:97:ILE:HG22	1.06	1.15
22:R:14:THR:HG21	22:R:48:ARG:HD3	1.27	1.09
11:F:17:GLN:HE22	33:h:87:GLU:HG2	1.19	1.06
25:U:12:PHE:CZ	54:K:97:ILE:HG22	1.91	1.05
12:G:148:ASN:ND2	54:K:56:ARG:HH11	1.54	1.03

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	
1	0	51/55 (93%)	51 (100%)	0	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	58 (94%)	4 (6%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	4	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
7	B	224/241 (93%)	220 (98%)	4 (2%)	0	100	100
8	C	209/233 (90%)	205 (98%)	4 (2%)	0	100	100
9	D	203/206 (98%)	201 (99%)	2 (1%)	0	100	100
10	E	155/167 (93%)	149 (96%)	6 (4%)	0	100	100
11	F	103/131 (79%)	103 (100%)	0	0	100	100
12	G	153/156 (98%)	152 (99%)	1 (1%)	0	100	100
13	H	127/130 (98%)	122 (96%)	5 (4%)	0	100	100
14	I	124/130 (95%)	122 (98%)	2 (2%)	0	100	100
15	J	96/103 (93%)	93 (97%)	3 (3%)	0	100	100
16	L	120/124 (97%)	118 (98%)	2 (2%)	0	100	100
17	M	113/118 (96%)	108 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	N	98/101 (97%)	97 (99%)	1 (1%)	0	100	100
19	O	86/89 (97%)	84 (98%)	2 (2%)	0	100	100
20	P	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
21	Q	79/84 (94%)	76 (96%)	3 (4%)	0	100	100
22	R	65/75 (87%)	63 (97%)	2 (3%)	0	100	100
23	S	82/92 (89%)	78 (95%)	4 (5%)	0	100	100
24	T	84/87 (97%)	84 (100%)	0	0	100	100
25	U	68/71 (96%)	68 (100%)	0	0	100	100
26	Y	103/113 (91%)	100 (97%)	3 (3%)	0	100	100
29	c	269/273 (98%)	263 (98%)	6 (2%)	0	100	100
30	d	206/209 (99%)	200 (97%)	5 (2%)	1 (0%)	24	20
31	f	176/179 (98%)	168 (96%)	8 (4%)	0	100	100
32	g	173/177 (98%)	165 (95%)	8 (5%)	0	100	100
33	h	147/149 (99%)	142 (97%)	5 (3%)	0	100	100
34	i	140/142 (99%)	140 (100%)	0	0	100	100
35	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
36	k	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
37	l	132/136 (97%)	127 (96%)	5 (4%)	0	100	100
38	m	117/127 (92%)	112 (96%)	5 (4%)	0	100	100
39	n	114/117 (97%)	109 (96%)	5 (4%)	0	100	100
40	o	112/115 (97%)	110 (98%)	2 (2%)	0	100	100
41	p	115/118 (98%)	115 (100%)	0	0	100	100
42	q	101/103 (98%)	99 (98%)	2 (2%)	0	100	100
43	r	108/110 (98%)	106 (98%)	2 (2%)	0	100	100
44	s	93/100 (93%)	90 (97%)	3 (3%)	0	100	100
45	t	101/104 (97%)	94 (93%)	7 (7%)	0	100	100
46	u	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
47	v	76/85 (89%)	74 (97%)	2 (3%)	0	100	100
48	w	75/78 (96%)	75 (100%)	0	0	100	100
49	x	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
50	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
51	z	54/57 (95%)	54 (100%)	0	0	100	100
52	e	185/201 (92%)	183 (99%)	2 (1%)	0	100	100
53	6	126/234 (54%)	124 (98%)	2 (2%)	0	100	100
54	K	115/129 (89%)	112 (97%)	3 (3%)	0	100	100
All	All	5836/6230 (94%)	5694 (98%)	141 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
30	d	149	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	0	48/49 (98%)	48 (100%)	0	100	100
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	43
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	4	60/60 (100%)	59 (98%)	1 (2%)	53	60
7	B	187/199 (94%)	186 (100%)	1 (0%)	81	87
8	C	172/190 (90%)	172 (100%)	0	100	100
9	D	172/173 (99%)	170 (99%)	2 (1%)	63	70
10	E	118/125 (94%)	118 (100%)	0	100	100
11	F	91/112 (81%)	90 (99%)	1 (1%)	65	72
12	G	128/129 (99%)	127 (99%)	1 (1%)	73	79
13	H	104/105 (99%)	104 (100%)	0	100	100
14	I	104/107 (97%)	103 (99%)	1 (1%)	68	75
15	J	86/90 (96%)	80 (93%)	6 (7%)	14	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	L	102/103 (99%)	102 (100%)	0	100	100
17	M	93/96 (97%)	92 (99%)	1 (1%)	65	72
18	N	83/84 (99%)	81 (98%)	2 (2%)	43	47
19	O	76/77 (99%)	76 (100%)	0	100	100
20	P	65/65 (100%)	64 (98%)	1 (2%)	57	64
21	Q	75/78 (96%)	74 (99%)	1 (1%)	61	68
22	R	58/65 (89%)	58 (100%)	0	100	100
23	S	72/79 (91%)	72 (100%)	0	100	100
24	T	65/66 (98%)	64 (98%)	1 (2%)	57	64
25	U	60/61 (98%)	58 (97%)	2 (3%)	33	34
26	Y	90/98 (92%)	87 (97%)	3 (3%)	33	34
29	c	216/218 (99%)	216 (100%)	0	100	100
30	d	163/163 (100%)	162 (99%)	1 (1%)	78	84
31	f	149/150 (99%)	147 (99%)	2 (1%)	61	68
32	g	136/138 (99%)	131 (96%)	5 (4%)	30	30
33	h	114/114 (100%)	114 (100%)	0	100	100
34	i	116/116 (100%)	116 (100%)	0	100	100
35	j	104/104 (100%)	104 (100%)	0	100	100
36	k	103/103 (100%)	103 (100%)	0	100	100
37	l	107/107 (100%)	105 (98%)	2 (2%)	50	56
38	m	99/103 (96%)	99 (100%)	0	100	100
39	n	86/87 (99%)	86 (100%)	0	100	100
40	o	99/100 (99%)	99 (100%)	0	100	100
41	p	89/90 (99%)	89 (100%)	0	100	100
42	q	84/84 (100%)	83 (99%)	1 (1%)	63	70
43	r	93/93 (100%)	93 (100%)	0	100	100
44	s	82/84 (98%)	81 (99%)	1 (1%)	63	70
45	t	84/85 (99%)	84 (100%)	0	100	100
46	u	78/78 (100%)	77 (99%)	1 (1%)	61	68
47	v	59/63 (94%)	59 (100%)	0	100	100
48	w	67/68 (98%)	66 (98%)	1 (2%)	57	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	x	55/55 (100%)	53 (96%)	2 (4%)	31	31
50	y	48/49 (98%)	48 (100%)	0	100	100
51	z	47/48 (98%)	46 (98%)	1 (2%)	47	52
52	e	156/165 (94%)	156 (100%)	0	100	100
53	6	106/181 (59%)	105 (99%)	1 (1%)	70	77
54	K	91/98 (93%)	91 (100%)	0	100	100
All	All	4863/5079 (96%)	4820 (99%)	43 (1%)	68	77

5 of 43 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
32	g	56	ASP
42	q	33	VAL
32	g	79	VAL
32	g	153	ARG
46	u	12	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
24	T	78	ASN
29	c	251	GLN
54	K	101	ASN
26	Y	19	HIS
26	Y	89	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
27	a	2906/2907 (99%)	480 (16%)	0
28	b	119/120 (99%)	19 (15%)	0
6	A	1533/1534 (99%)	277 (18%)	31 (2%)
All	All	4558/4561 (99%)	776 (17%)	31 (0%)

5 of 776 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	A	3	A

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Mol	Chain	Res	Type
6	A	4	U
6	A	5	U
6	A	7	A
6	A	8	A

5 of 31 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	A	532	A
6	A	1429	A
6	A	786	G
6	A	1452	C
6	A	1145	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	5MC	A	1407	6	18,22,23	0.97	1 (5%)	26,32,35	1.18	3 (11%)
6	G7M	A	527	6	23,26,27	1.78	2 (8%)	35,39,42	1.05	2 (5%)
27	2MG	a	2449	27	23,26,27	1.30	4 (17%)	32,38,41	2.29	7 (21%)
27	PSU	a	2608	27	18,21,22	1.42	2 (11%)	22,30,33	1.91	3 (13%)
27	5MC	a	1966	27	18,22,23	0.95	1 (5%)	26,32,35	1.18	4 (15%)
27	PSU	a	2508	27	18,21,22	0.81	0	22,30,33	1.56	4 (18%)
27	PSU	a	2461	27	18,21,22	1.44	2 (11%)	22,30,33	1.98	3 (13%)
27	OMG	a	2255	56,57,27	23,26,27	1.19	3 (13%)	33,38,41	2.09	8 (24%)
27	PSU	a	1915	27	18,21,22	1.41	2 (11%)	22,30,33	1.94	3 (13%)
27	5MU	a	749	27	19,22,23	1.48	5 (26%)	28,32,35	2.15	7 (25%)
27	1MG	a	747	27	22,26,27	1.18	2 (9%)	33,39,42	1.84	8 (24%)
27	OMU	a	2556	56,27	19,22,23	1.19	3 (15%)	26,31,34	1.99	6 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	MS6	l	82	37	5,7,8	0.76	0	2,7,9	1.90	1 (50%)
27	5MU	a	1943	57,27	19,22,23	1.58	5 (26%)	28,32,35	2.41	11 (39%)
27	6MZ	a	1620	27	22,25,26	1.55	4 (18%)	30,36,39	2.25	11 (36%)
30	MEQ	d	150	30	8,9,10	0.52	0	5,10,12	1.08	1 (20%)
27	G7M	a	2073	27	23,26,27	1.77	2 (8%)	35,39,42	1.03	2 (5%)
54	IAS	K	119	54	6,7,8	0.97	0	6,8,10	1.20	0
6	MA6	A	1518	6	23,26,27	1.55	5 (21%)	34,38,41	2.12	11 (32%)
6	4OC	A	1402	6	20,23,24	0.83	0	26,32,35	0.98	2 (7%)
27	3TD	a	1919	27	18,22,23	1.38	1 (5%)	22,32,35	1.72	2 (9%)
6	UR3	A	1498	6	19,22,23	1.14	1 (5%)	26,32,35	1.57	1 (3%)
27	PSU	a	2584	27	18,21,22	1.45	2 (11%)	22,30,33	2.20	7 (31%)
27	PSU	a	957	27	18,21,22	1.46	2 (11%)	22,30,33	2.12	5 (22%)
16	D2T	L	89	16	7,9,10	2.04	1 (14%)	6,11,13	2.87	4 (66%)
6	5MC	A	967	6	18,22,23	0.97	1 (5%)	26,32,35	1.10	4 (15%)
27	PSU	a	1921	27	18,21,22	1.43	3 (16%)	22,30,33	1.85	4 (18%)
27	PSU	a	2609	27	18,21,22	1.40	2 (11%)	22,30,33	2.03	3 (13%)
6	MA6	A	1519	6	23,26,27	1.56	5 (21%)	34,38,41	2.08	11 (32%)
27	PSU	a	748	56,27	18,21,22	1.49	2 (11%)	22,30,33	2.12	5 (22%)
27	H2U	a	2453	27	18,21,22	1.01	2 (11%)	21,30,33	1.87	2 (9%)
6	PSU	A	516	56,6	18,21,22	1.44	2 (11%)	22,30,33	2.26	5 (22%)
27	6MZ	a	2034	27	22,25,26	1.50	5 (22%)	30,36,39	2.38	11 (36%)
27	OMC	a	2502	56,27	19,22,23	0.79	0	26,31,34	1.16	1 (3%)
37	4D4	l	81	37	9,11,12	0.89	1 (11%)	8,13,15	0.86	1 (12%)
27	2MA	a	2507	56,27	22,25,26	1.54	5 (22%)	33,37,40	2.13	9 (27%)
27	2MG	a	1837	27	23,26,27	1.26	3 (13%)	32,38,41	2.33	7 (21%)

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
6	5MC	A	1407	6	-	0/7/25/26	0/2/2/2
6	G7M	A	527	6	-	3/7/25/26	0/3/3/3
27	2MG	a	2449	27	-	2/9/27/28	0/3/3/3
27	PSU	a	2608	27	-	0/7/25/26	0/2/2/2
27	5MC	a	1966	27	-	0/7/25/26	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PSU	a	2508	27	-	0/7/25/26	0/2/2/2
27	PSU	a	2461	27	-	0/7/25/26	0/2/2/2
27	OMG	a	2255	56,57,27	-	0/9/27/28	0/3/3/3
27	PSU	a	1915	27	-	0/7/25/26	0/2/2/2
27	5MU	a	749	27	-	2/7/25/26	0/2/2/2
27	1MG	a	747	27	-	0/7/25/26	0/3/3/3
27	OMU	a	2556	56,27	-	0/9/27/28	0/2/2/2
37	MS6	l	82	37	-	2/4/6/8	-
27	5MU	a	1943	57,27	-	2/7/25/26	0/2/2/2
27	6MZ	a	1620	27	-	3/9/27/28	0/3/3/3
30	MEQ	d	150	30	-	4/8/9/11	-
27	G7M	a	2073	27	-	1/7/25/26	0/3/3/3
54	IAS	K	119	54	-	2/7/7/8	-
6	MA6	A	1518	6	-	0/11/29/30	0/3/3/3
6	4OC	A	1402	6	-	0/9/29/30	0/2/2/2
27	3TD	a	1919	27	-	0/7/25/26	0/2/2/2
6	UR3	A	1498	6	-	2/7/25/26	0/2/2/2
27	PSU	a	2584	27	-	0/7/25/26	0/2/2/2
27	PSU	a	957	27	-	0/7/25/26	0/2/2/2
16	D2T	L	89	16	-	1/7/12/14	-
6	5MC	A	967	6	-	0/7/25/26	0/2/2/2
27	PSU	a	1921	27	-	0/7/25/26	0/2/2/2
27	PSU	a	2609	27	-	0/7/25/26	0/2/2/2
6	MA6	A	1519	6	-	2/11/29/30	0/3/3/3
27	PSU	a	748	56,27	-	2/7/25/26	0/2/2/2
27	H2U	a	2453	27	-	0/7/38/39	0/2/2/2
6	PSU	A	516	56,6	-	0/7/25/26	0/2/2/2
27	6MZ	a	2034	27	-	2/9/27/28	0/3/3/3
27	OMC	a	2502	56,27	-	0/9/27/28	0/2/2/2
37	4D4	l	81	37	-	0/11/12/14	-
27	2MA	a	2507	56,27	-	1/7/25/26	0/3/3/3
27	2MG	a	1837	27	-	0/9/27/28	0/3/3/3

The worst 5 of 81 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	527	G7M	C8-N7	7.24	1.46	1.33
27	a	2073	G7M	C8-N7	7.23	1.46	1.33
6	A	1518	MA6	C5-C4	4.72	1.47	1.39
16	L	89	D2T	CB-SB	-4.70	1.77	1.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1519	MA6	C5-C4	4.62	1.47	1.39

The worst 5 of 179 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	a	1837	2MG	C2-N3-C4	7.79	121.69	112.04
27	a	2449	2MG	C2-N3-C4	7.66	121.54	112.04
27	a	2453	H2U	C4-N3-C2	-7.39	119.66	125.79
6	A	516	PSU	N1-C2-N3	7.08	123.15	115.13
27	a	2507	2MA	C5-C4-N3	-7.00	119.32	127.19

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
30	d	150	MEQ	C-CA-CB-CG
6	A	527	G7M	C3'-C4'-C5'-O5'
27	a	748	PSU	C2'-C1'-C5-C4
27	a	749	5MU	C3'-C4'-C5'-O5'
27	a	2034	6MZ	C3'-C4'-C5'-O5'

There are no ring outliers.

15 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	527	G7M	1	0
27	a	2255	OMG	1	0
27	a	749	5MU	1	0
27	a	2556	OMU	1	0
27	a	1620	6MZ	1	0
54	K	119	IAS	1	0
6	A	1402	4OC	1	0
6	A	1498	UR3	1	0
27	a	2584	PSU	1	0
6	A	1519	MA6	2	0
6	A	516	PSU	1	0
27	a	2034	6MZ	2	0
27	a	2502	OMC	1	0
27	a	2507	2MA	1	0
27	a	1837	2MG	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 527 ligands modelled in this entry, 526 are monoatomic - 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	$\# Z > 2$
58	DXT	a	3001	56	33,35,35	1.91	7 (21%)	42,57,57	1.78	7 (16%)

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
58	DXT	a	3001	56	-	0/8/74/74	0/4/4/4

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	a	3001	DXT	C2-C21	-5.96	1.35	1.47
58	a	3001	DXT	C5B-C11	-4.09	1.37	1.47
58	a	3001	DXT	C2-C1	-3.76	1.36	1.45
58	a	3001	DXT	C4-N4	3.21	1.54	1.47
58	a	3001	DXT	C4B-C12	2.69	1.54	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	a	3001	DXT	O21-C21-N21	-7.09	106.30	122.88
58	a	3001	DXT	O21-C21-C2	4.17	127.83	120.67
58	a	3001	DXT	C2-C21-N21	3.51	125.87	118.75
58	a	3001	DXT	C4B-C1-C2	2.81	120.22	115.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	a	3001	DXT	C1-C4B-C12	2.46	112.77	109.88

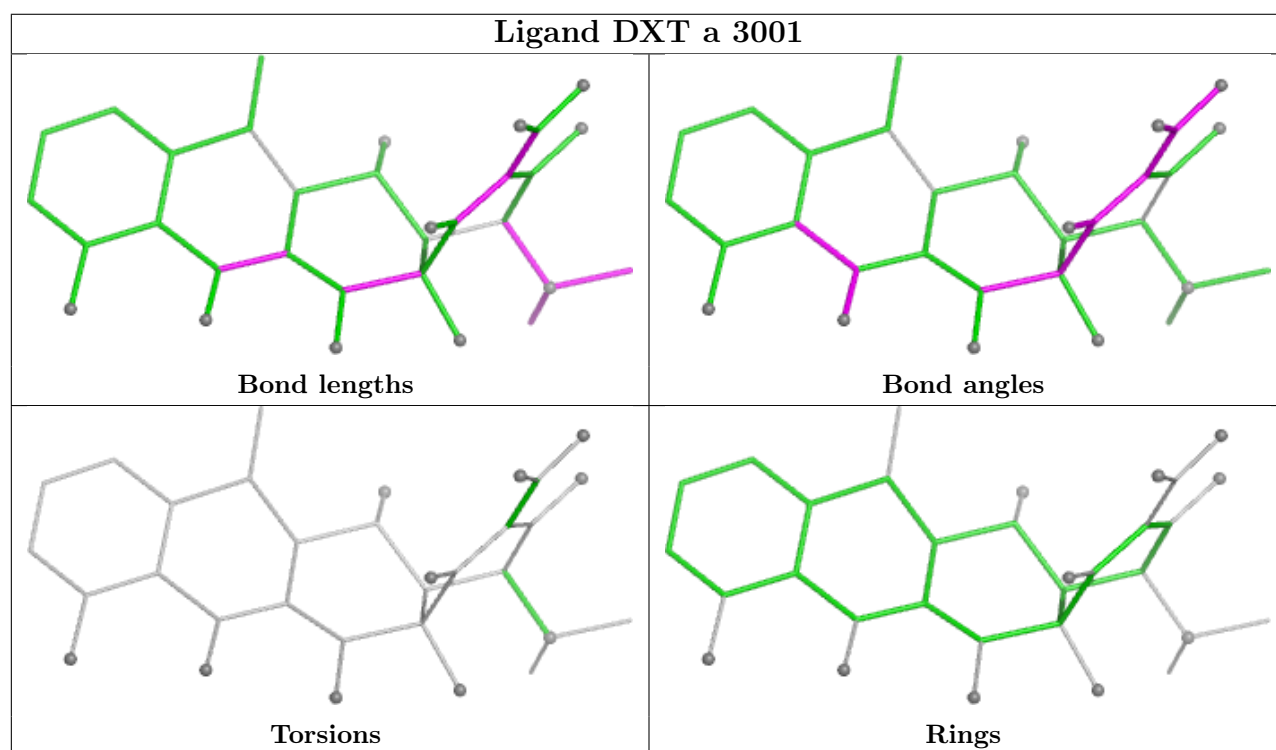
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

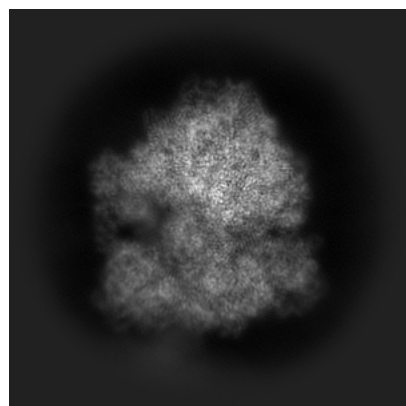
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55001. These allow visual inspection of the internal detail of the map and identification of artifacts.

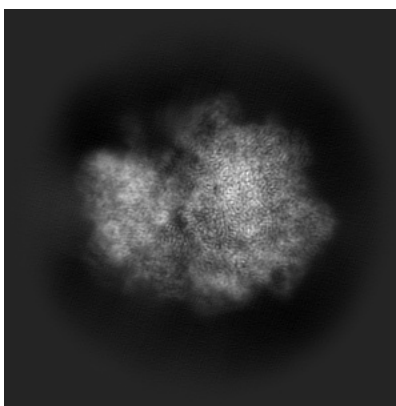
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

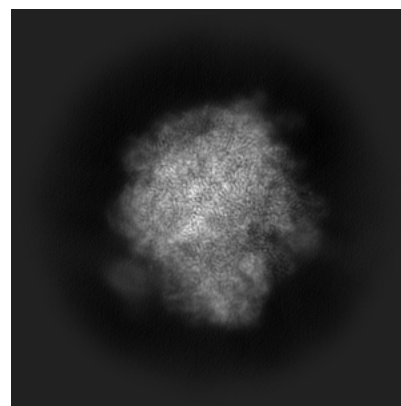
6.1.1 Primary map



X

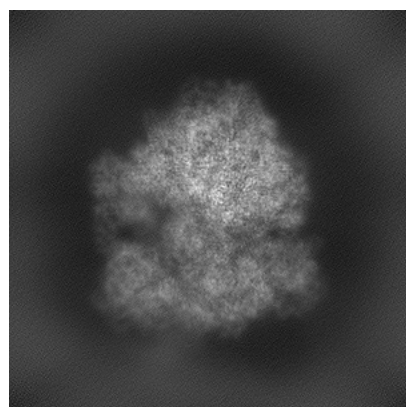


Y

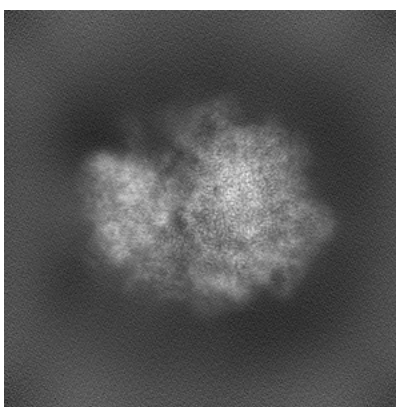


Z

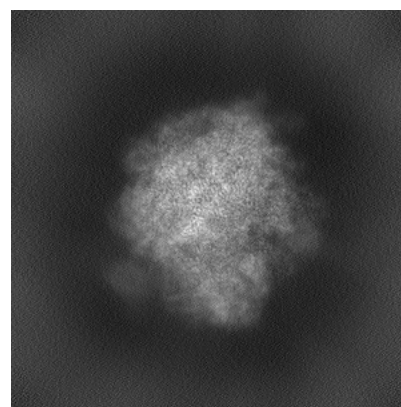
6.1.2 Raw map



X



Y

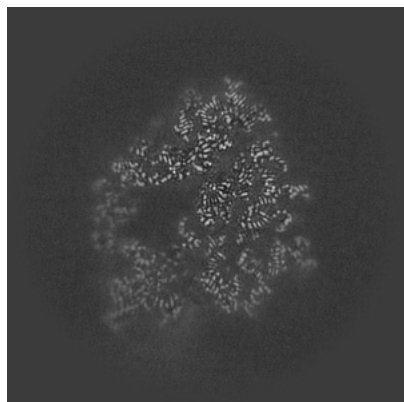


Z

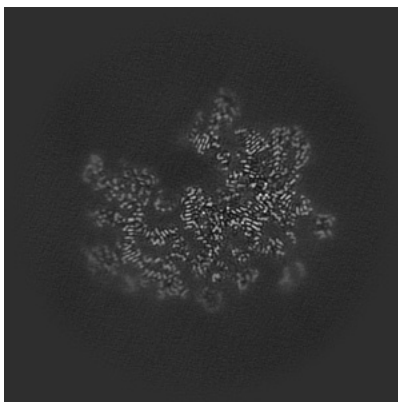
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

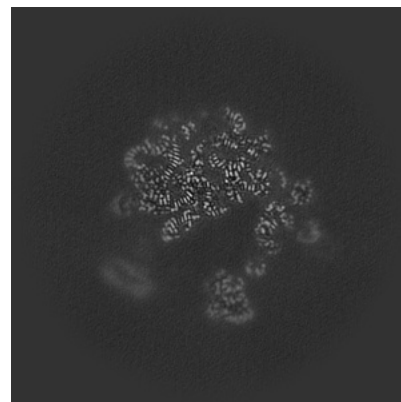
6.2.1 Primary map



X Index: 300

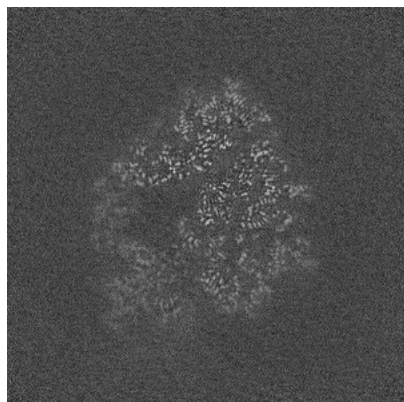


Y Index: 300

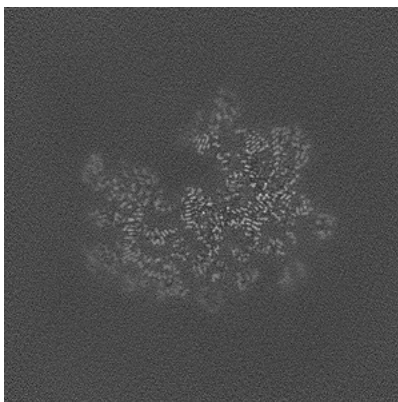


Z Index: 300

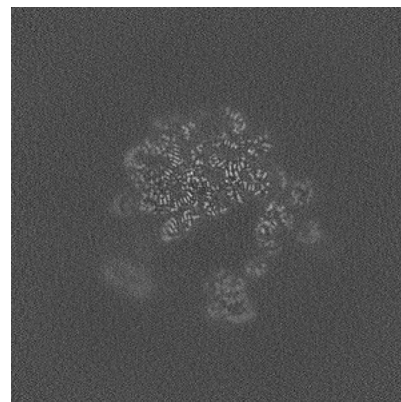
6.2.2 Raw map



X Index: 300



Y Index: 300

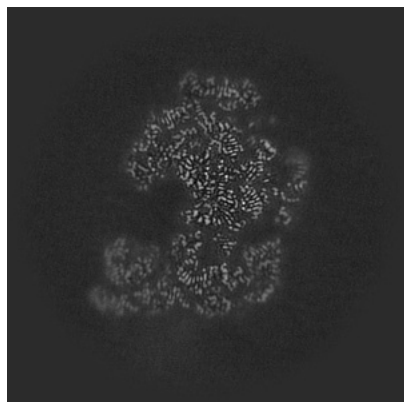


Z Index: 300

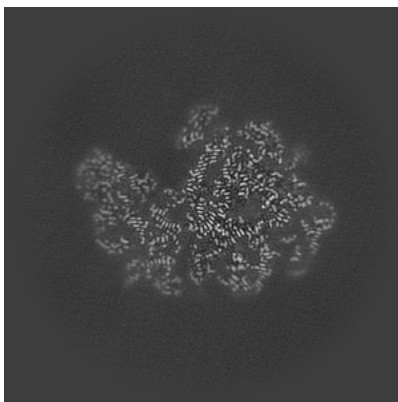
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

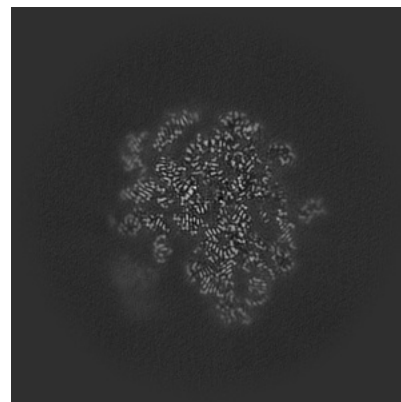
6.3.1 Primary map



X Index: 276

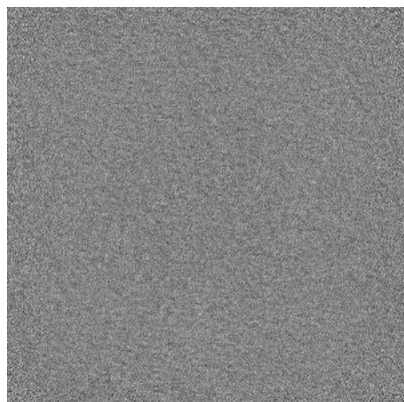


Y Index: 326

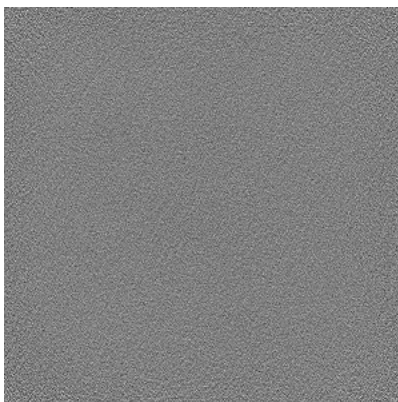


Z Index: 345

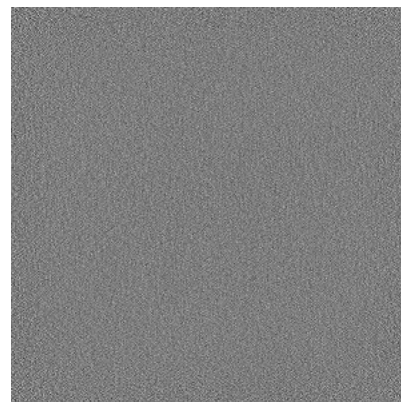
6.3.2 Raw map



X Index: 0



Y Index: 0

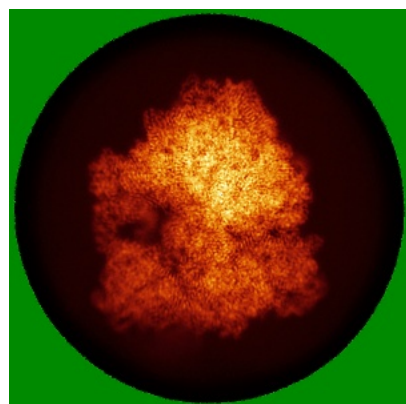


Z Index: 0

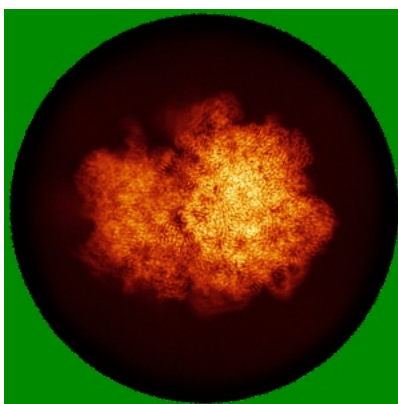
The images above show the largest variance slices of the map in three orthogonal directions.

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

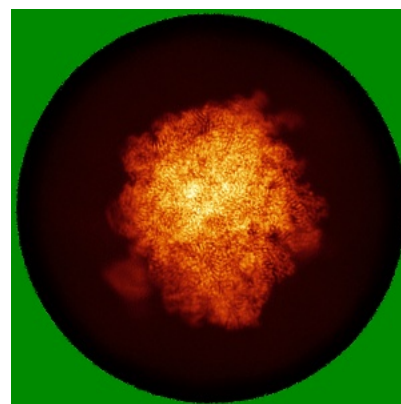
6.4.1 Primary map



X

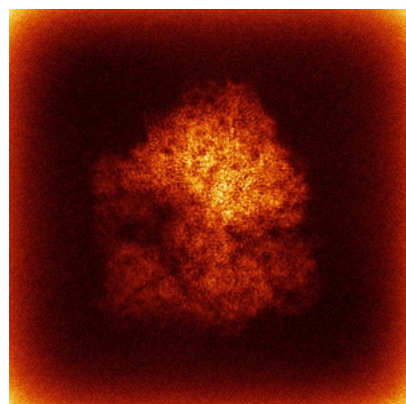


Y

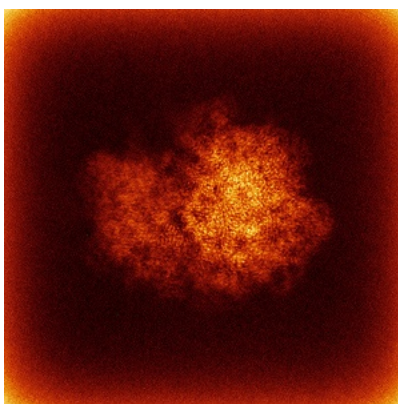


Z

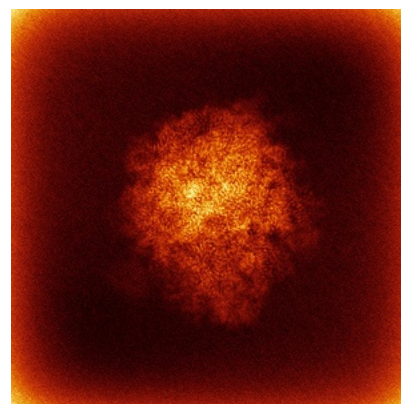
6.4.2 Raw map



X



Y



Z

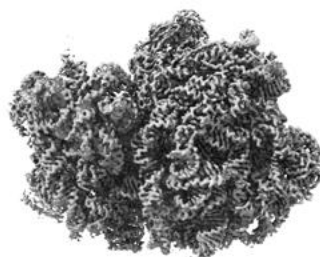
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



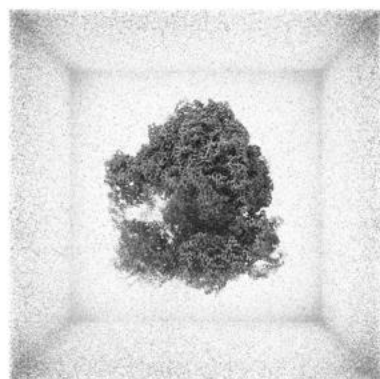
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

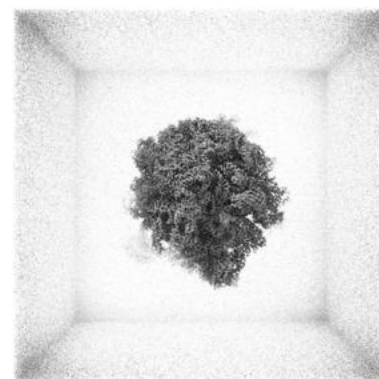
6.5.2 Raw map



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.

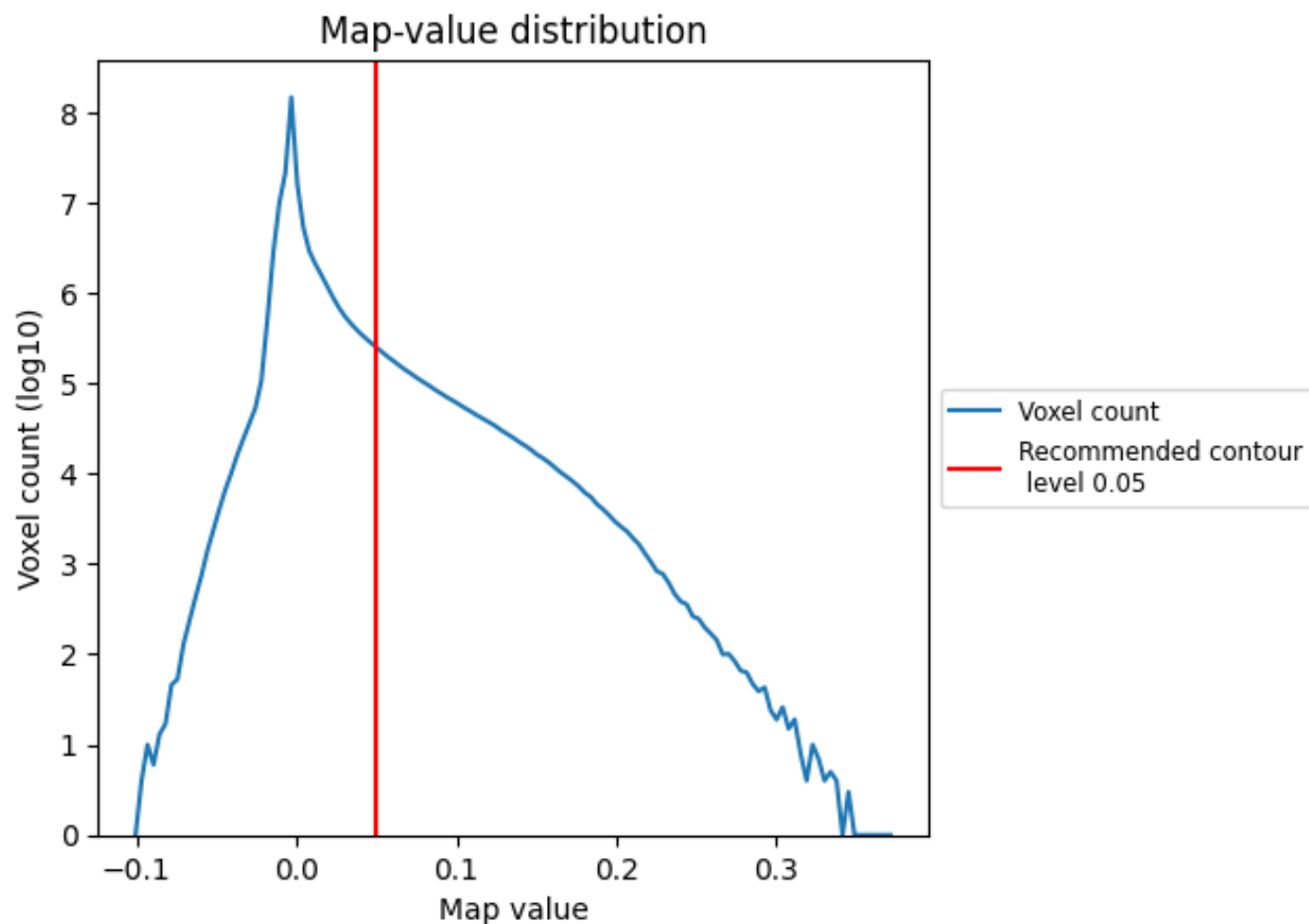
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

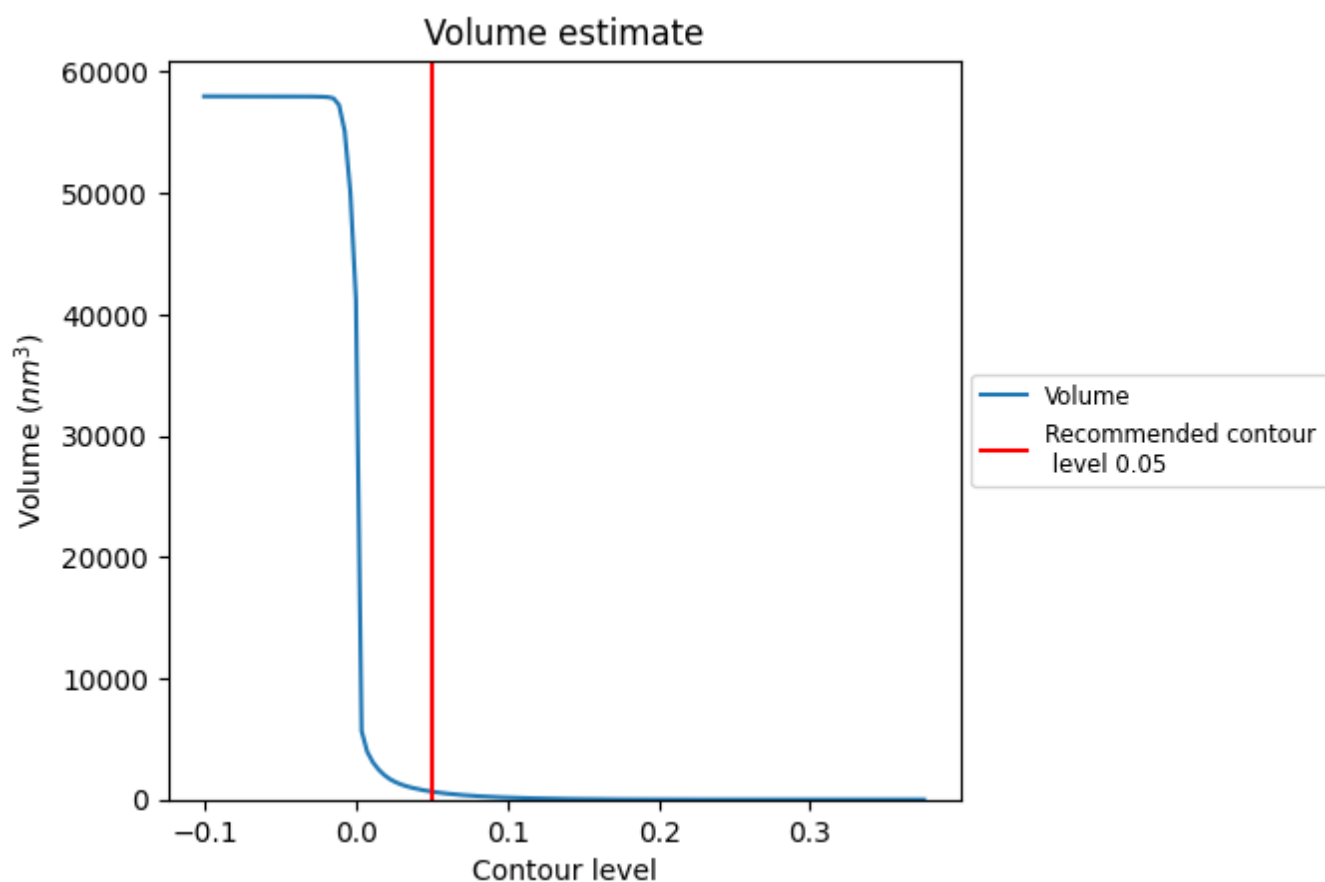
This section contains the results of statistical analysis of the map.

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.

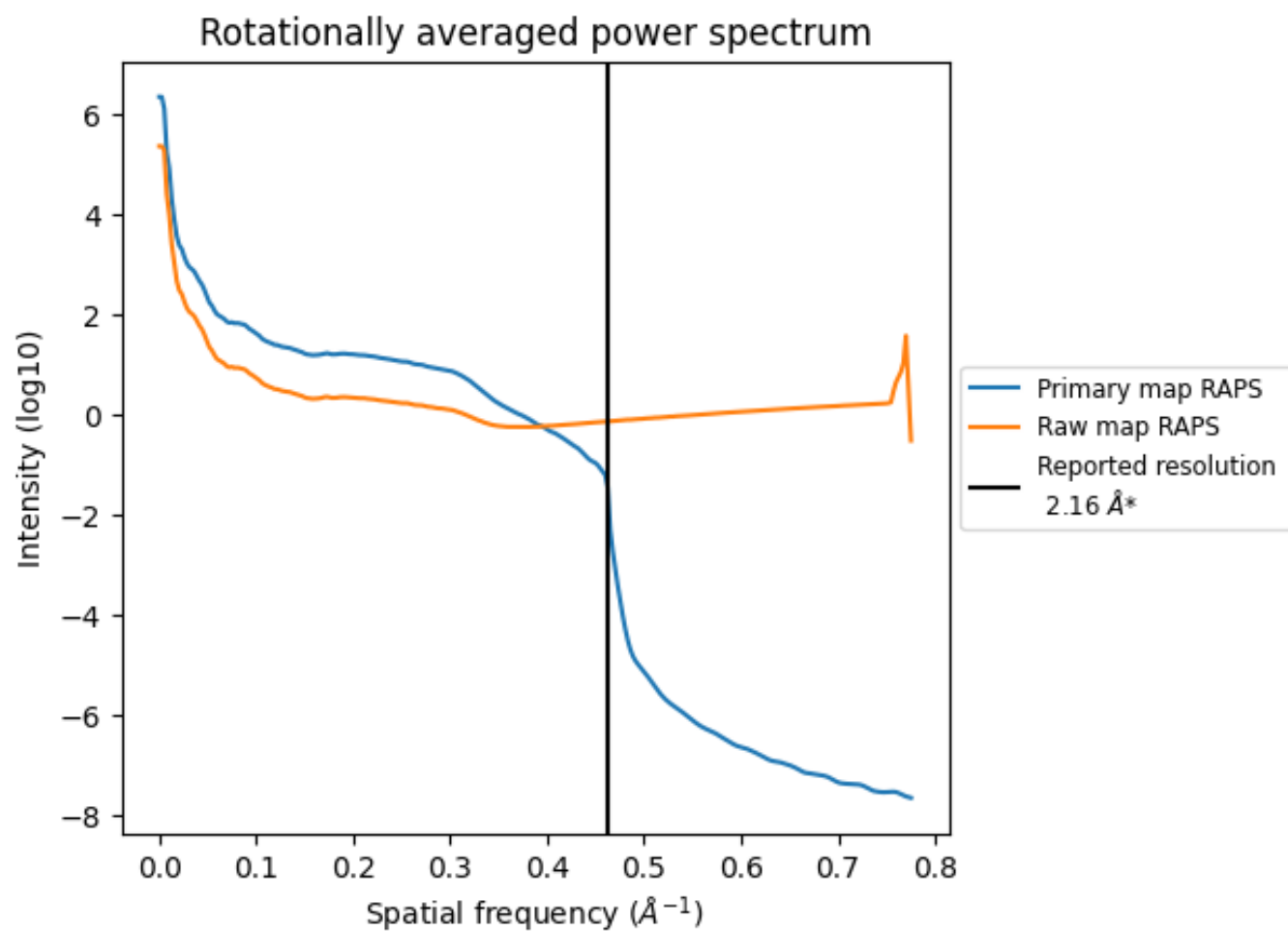
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 652 nm³; this corresponds to an approximate mass of 589 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 ⓘ

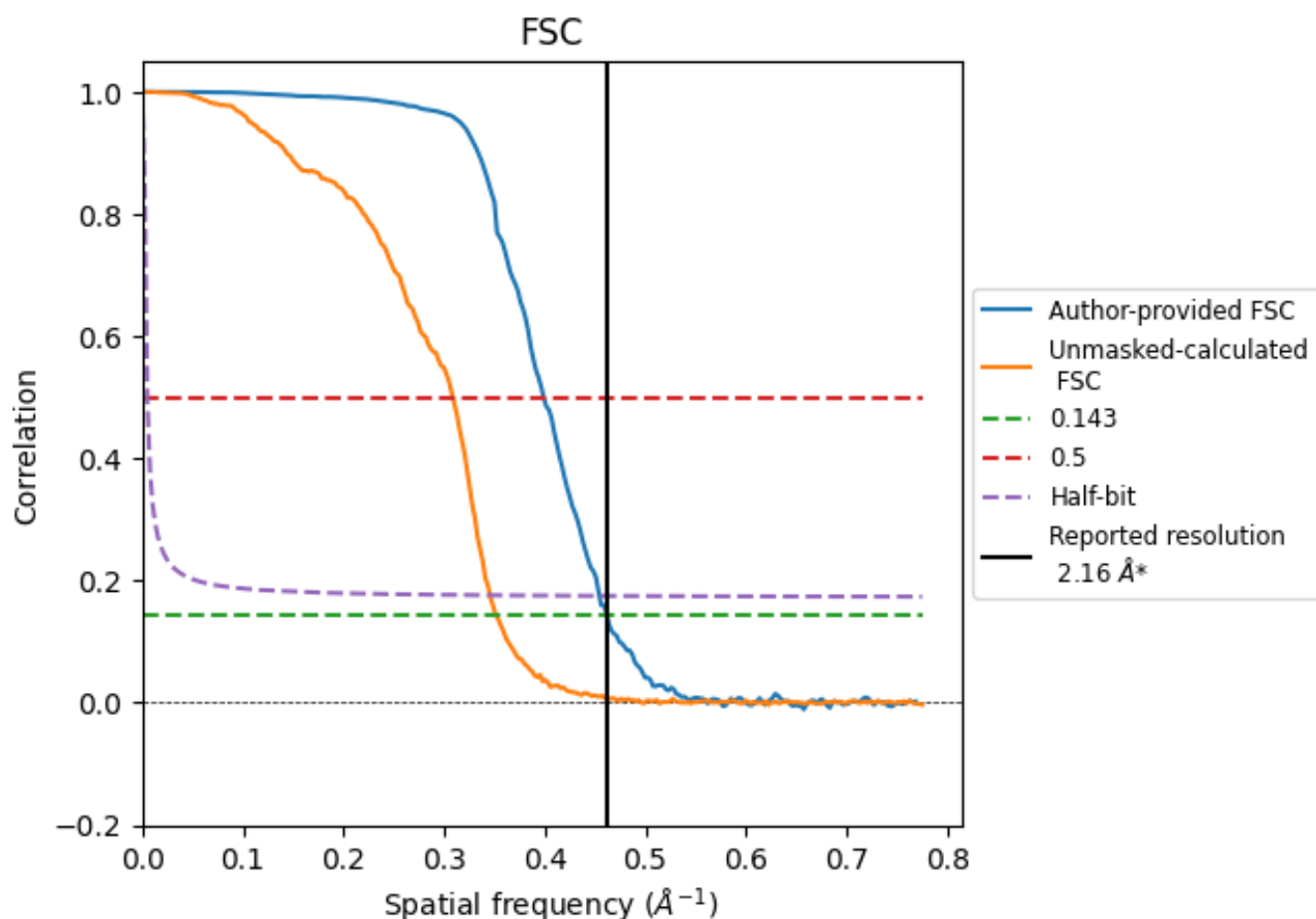


*Reported resolution corresponds to spatial frequency of 0.463 $\text{\AA}^{-1}$

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 0.463 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

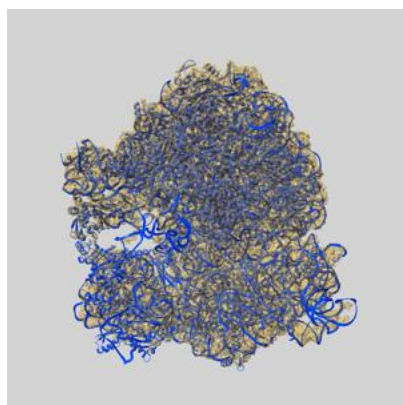
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.16	-	-
Author-provided FSC curve	2.16	2.51	2.20
Unmasked-calculated*	2.84	3.24	2.89

*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 2.84 differs from the reported value 2.16 by more than 10 %

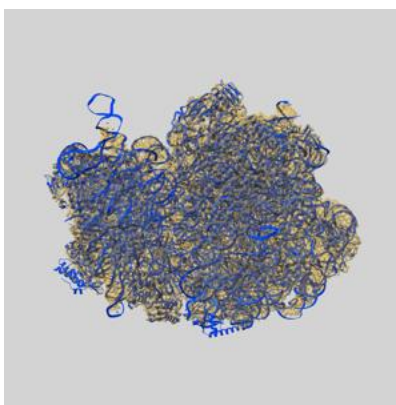
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55001 and PDB model 9SLG. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

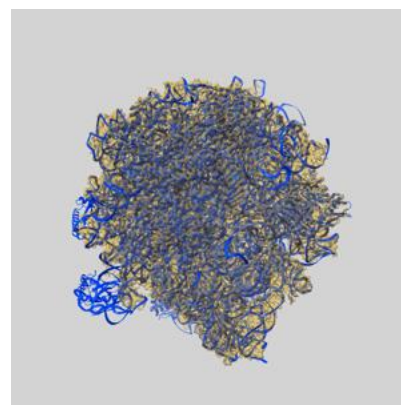
9.1 Map-model overlay [i](#)



X



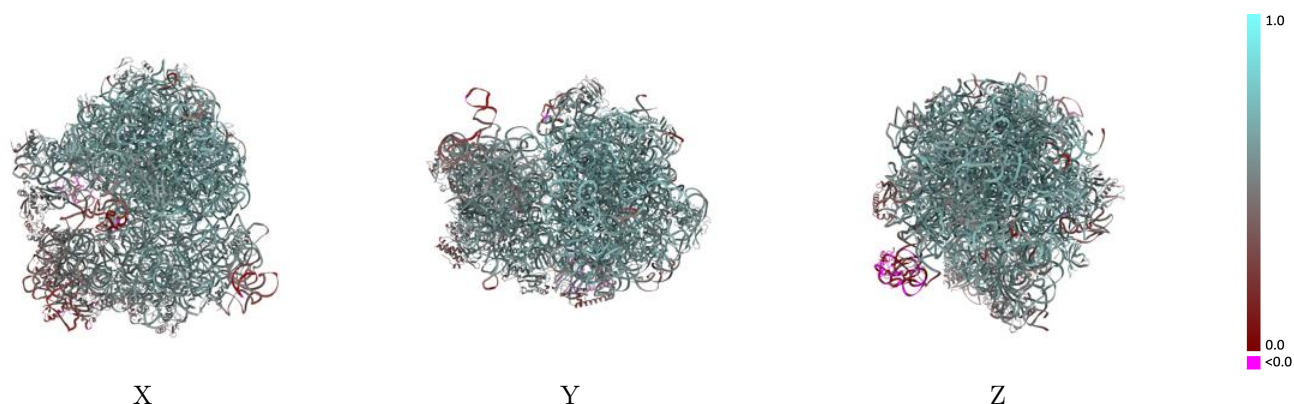
Y



Z

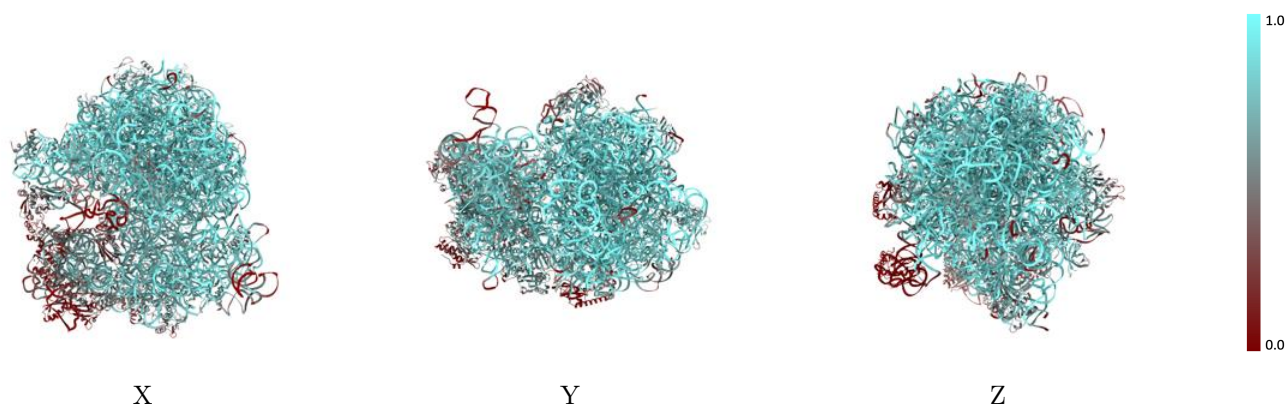
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



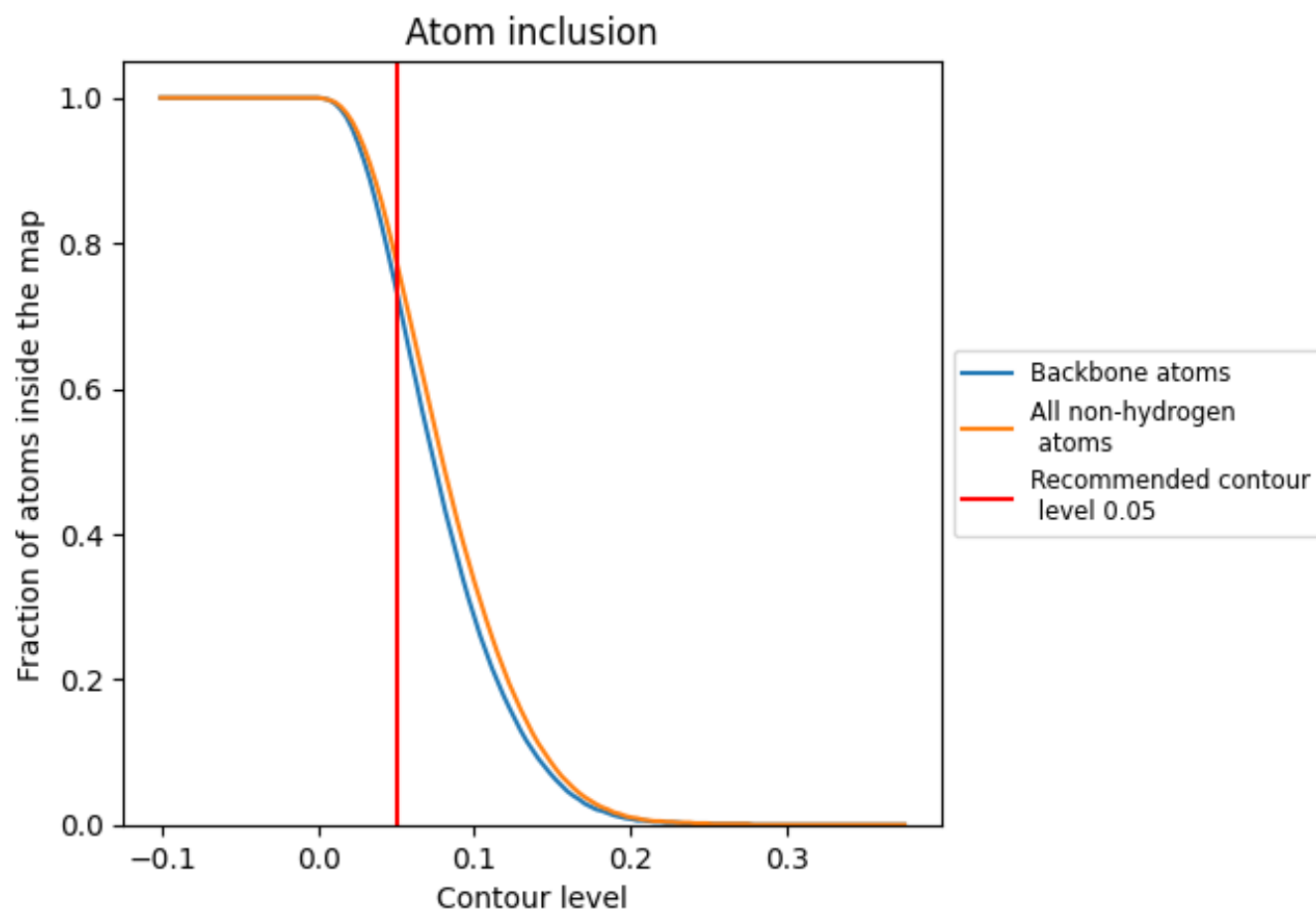
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 78% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7770	 0.5680
0	 0.7030	 0.5890
1	 0.9580	 0.6690
2	 0.9430	 0.6670
3	 0.8500	 0.6320
4	 0.2000	 0.3790
6	 0.0000	 0.1160
A	 0.7960	 0.5450
B	 0.2240	 0.4040
C	 0.4290	 0.4720
D	 0.5130	 0.5030
E	 0.6830	 0.5620
F	 0.5840	 0.5150
G	 0.3730	 0.4610
H	 0.6970	 0.5630
I	 0.2910	 0.4060
J	 0.2180	 0.3550
K	 0.6150	 0.5570
L	 0.7030	 0.6070
M	 0.2800	 0.4320
N	 0.3890	 0.4640
O	 0.7010	 0.5780
P	 0.6510	 0.5380
Q	 0.6480	 0.5670
R	 0.6150	 0.5260
S	 0.1900	 0.4190
T	 0.6150	 0.5390
U	 0.3040	 0.4310
Y	 0.2900	 0.4990
a	 0.8920	 0.6020
b	 0.8340	 0.5470
c	 0.9030	 0.6670
d	 0.8760	 0.6420
e	 0.7180	 0.5580
f	 0.4150	 0.4530



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Chain	Atom inclusion	Q-score
g	 0.5400	 0.5180
h	 0.1490	 0.4140
i	 0.8950	 0.6360
j	 0.8480	 0.6540
k	 0.8410	 0.6240
l	 0.8400	 0.6350
m	 0.9240	 0.6550
n	 0.6540	 0.5240
o	 0.8210	 0.6310
p	 0.9050	 0.6550
q	 0.7950	 0.6080
r	 0.8730	 0.6430
s	 0.7580	 0.5870
t	 0.6650	 0.5500
u	 0.7240	 0.5810
v	 0.8540	 0.6210
w	 0.8530	 0.6360
x	 0.6400	 0.5340
y	 0.8400	 0.6340
z	 0.8420	 0.6370