



Full wwPDB EM Validation Report ⓘ

Jun 21, 2026 – 10:21 am BST

PDB ID : 9RJA / pdb_00009rja
EMDB ID : EMD-54009
Title : Manikomycin bound to the Escherichia coli 70S ribosome
Authors : Kaur, M.; Travin, D.; Berger, M.J.; Jangra, M.; Morici, M.; Safdari, H.A.; Guitor, A.K.; Koteva, K.; Xu, M.; Chen, X.; Vazquez-Laslop, N.; Mankin, A.S.; Wilson, D.N.; Wright, G.
Deposited on : 2025-06-12
Resolution : 2.45 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

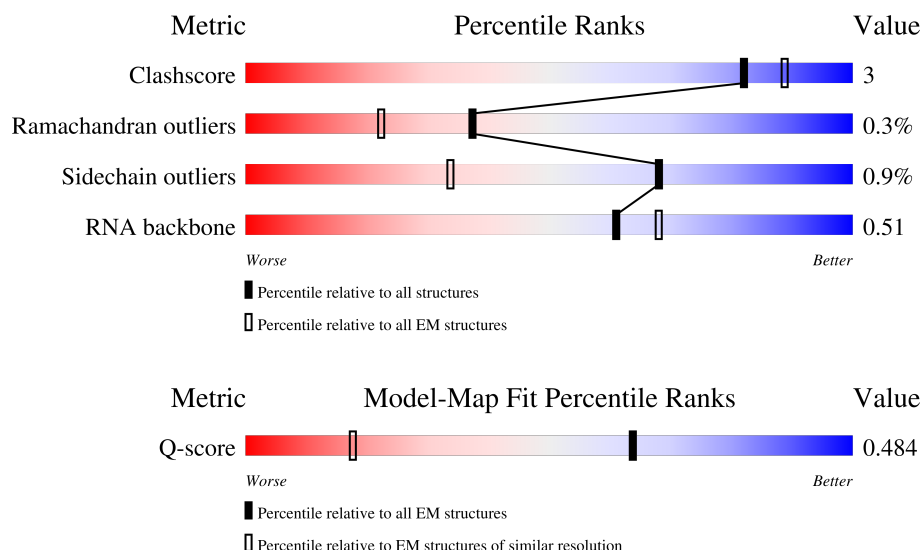
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 i

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

The reported resolution of this entry is 2.45 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	5931 (1.96 - 2.95)

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	25% 87% 5% 7%
2	1	46	93% 7%
3	2	65	88% 11%

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Mol	Chain	Length	Quality of chain
4	3	38	
5	C	233	
6	E	167	
7	F	135	
8	I	130	
9	J	103	
10	K	129	
11	L	124	
12	M	118	
13	N	101	
14	O	89	
15	P	82	
16	Q	84	
17	R	75	
18	X	12	
19	c	273	
20	d	209	
21	f	179	
22	h	149	
23	i	142	
24	j	123	
25	k	144	
26	l	136	
27	m	127	
28	n	117	

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Mol	Chain	Length	Quality of chain
29	p	118	
30	q	103	
31	r	110	
32	u	94	
33	v	85	
34	w	78	
35	x	63	
36	y	59	
37	z	57	
38	4	70	
39	a	2904	
40	b	120	
41	A	1542	
42	B	241	
43	D	206	
44	G	179	
45	H	130	
46	S	92	
47	T	87	
48	U	71	
49	e	201	
50	g	177	
51	o	115	
52	s	100	
53	t	104	

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Mol	Chain	Length	Quality of chain
54	Y	76	62% 66% 29%
55	Z	76	38% 72% 18% 7%
56	V	9	33% 67%
56	W	9	33% 56% 33% 11%

2 Entry composition

There are 62 unique types of molecules in this entry. The entry contains 140150 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	51	Total	C	N	O	0	0
			417	269	76	72		

- 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 Small ribosomal subunit protein uS3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	206	Total	C	N	O	S	0	0
			1624	1028	305	288	3		

- Molecule 6 is a protein called Small ribosomal subunit protein uS5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	156	Total	C	N	O	S	0	0
			1137	710	216	205	6		

- Molecule 7 is a protein called 30S ribosomal protein S6, fully modified isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	103	Total	C	N	O	S	0	0
			819	518	149	145	7		

- Molecule 8 is a protein called Small ribosomal subunit protein uS9.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	126	Total	C	N	O	S	0	0
			1014	630	204	177	3		

- Molecule 9 is a protein called Small ribosomal subunit protein uS10.

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

- Molecule 10 is a protein called Small ribosomal subunit protein uS11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	117	Total	C	N	O	S	0	0
			877	540	173	161	3		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 11 is a protein called Small ribosomal subunit protein uS12.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	121	Total	C	N	O	S	0	0
			942	582	193	162	5		

- Molecule 12 is a protein called Small ribosomal subunit protein uS13.

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

- Molecule 13 is a protein called Small ribosomal subunit protein uS14.

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

- Molecule 14 is a protein called Small ribosomal subunit protein uS15.

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

- Molecule 15 is a protein called 30S ribosomal protein S16.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	79	Total	C	N	O	S	0	0
			629	394	124	110	1		

- Molecule 16 is a protein called Small ribosomal subunit protein uS17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	79	Total	C	N	O	S	0	0
			641	406	120	112	3		

- Molecule 17 is a protein called Small ribosomal subunit protein bS18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	66	Total	C	N	O	S	0	0
			544	345	102	96	1		

- Molecule 18 is a RNA chain called mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	12	Total	C	N	O	P	0	0
			252	113	41	86	12		

- Molecule 19 is a protein called Large ribosomal subunit protein uL2.

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

- Molecule 20 is a protein called Large ribosomal subunit protein uL3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	208	Total	C	N	O	S	0	0
			1558	975	287	293	3		

- Molecule 21 is a protein called Large ribosomal subunit protein uL5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	f	177	Total	C	N	O	S	0	0
			1410	899	249	256	6		

- Molecule 22 is a protein called Large ribosomal subunit protein bL9.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	h	40	Total	C	N	O	S	0	0
			294	188	52	53	1		

- Molecule 23 is a protein called Large ribosomal subunit protein uL13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	i	141	Total	C	N	O	S	0	0
			1120	708	211	197	4		

- Molecule 24 is a protein called Large ribosomal subunit protein uL14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	j	123	Total	C	N	O	S	0	0
			946	593	181	166	6		

- Molecule 25 is a protein called 50S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	k	143	Total	C	N	O	S	0	0
			1043	649	206	186	2		

- Molecule 26 is a protein called Large ribosomal subunit protein uL16.

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

- Molecule 27 is a protein called Large ribosomal subunit protein bL17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	m	118	Total	C	N	O	S	0	0
			945	585	194	161	5		

- Molecule 28 is a protein called Large ribosomal subunit protein uL18.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	n	116	Total	C	N	O		0	0
			892	552	178	162			

- Molecule 29 is a protein called Large ribosomal subunit protein bL20.

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

- Molecule 30 is a protein called Large ribosomal subunit protein bL21.

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

- Molecule 31 is a protein called Large ribosomal subunit protein uL22.

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

- Molecule 32 is a protein called 50S ribosomal protein L25.

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

- Molecule 33 is a protein called Large ribosomal subunit protein bL27.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	v	84	Total	C	N	O	S	0	0
			628	388	126	113	1		

- Molecule 34 is a protein called Large ribosomal subunit protein bL28.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	w	77	Total	C	N	O	S	0	0
			625	388	129	106	2		

- Molecule 35 is a protein called Large ribosomal subunit protein uL29.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	x	59	Total	C	N	O	S	0	0
			486	300	95	90	1		

- Molecule 36 is a protein called Large ribosomal subunit protein uL30.

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

- Molecule 37 is a protein called Large ribosomal subunit protein bL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	z	54	Total	C	N	O	S	0	0
			429	260	91	77	1		

- Molecule 38 is a protein called Large ribosomal subunit protein bL31A.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	4	54	Total	C	N	O	S	0	0
			439	274	82	77	6		

- Molecule 39 is a RNA chain called 23S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	a	2747	Total	C	N	O	P	0	0
			59004	26328	10878	19051	2747		

- Molecule 40 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	b	114	Total	C	N	O	P	0	0
			2449	1090	454	791	114		

- Molecule 41 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	A	1488	Total	C	N	O	P	0	0
			31958	14260	5879	10331	1488		

- Molecule 42 is a protein called 30S ribosomal protein S2.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	B	197	Total	C	N	O	S	0	0
			1538	977	276	280	5		

- Molecule 43 is a protein called Small ribosomal subunit protein uS4.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	D	199	Total	C	N	O	S	0	0
			1602	1001	308	290	3		

- Molecule 44 is a protein called 30S ribosomal protein S7.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	G	147	Total	C	N	O	S	0	0
			1121	698	213	206	4		

- Molecule 45 is a protein called Small ribosomal subunit protein uS8.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	H	127	Total	C	N	O	S	0	0
			964	608	171	179	6		

- Molecule 46 is a protein called Small ribosomal subunit protein uS19.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	S	76	Total	C	N	O	S	0	0
			613	395	117	99	2		

- Molecule 47 is a protein called 30S ribosomal protein S20.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	T	80	Total	C	N	O	S	0	0
			630	390	131	106	3		

- Molecule 48 is a protein called Small ribosomal subunit protein bS21.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	U	64	Total	C	N	O	S	0	0
			534	336	109	88	1		

- Molecule 49 is a protein called Large ribosomal subunit protein uL4.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	e	199	Total	C	N	O	S	0	0
			1538	966	280	287	5		

- Molecule 50 is a protein called Large ribosomal subunit protein uL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	g	141	Total	C	N	O	S	0	0
			1058	666	194	196	2		

- Molecule 51 is a protein called Large ribosomal subunit protein bL19.

Mol	Chain	Residues	Atoms					AltConf	Trace
51	o	111	Total	C	N	O	S	0	0
			898	565	175	157	1		

- Molecule 52 is a protein called Large ribosomal subunit protein uL23.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	s	86	Total	C	N	O	S	0	0
			687	437	129	119	2		

- Molecule 53 is a protein called Large ribosomal subunit protein uL24.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	t	94	Total	C	N	O		0	0
			721	454	136	131			

- Molecule 54 is a RNA chain called A-site Phe-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	Y	74	Total	C	N	O	P	0	0
			1576	704	283	516	73		

- Molecule 55 is a RNA chain called P-Site Val-tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	Z	74	Total	C	N	O	P	0	0
			1582	705	287	516	74		

- Molecule 56 is a protein called Manikomycin.

Mol	Chain	Residues	Atoms				AltConf	Trace
56	V	9	Total	C	N	O	0	0
			84	50	22	12		
56	W	9	Total	C	N	O	0	0
			84	50	22	12		

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	3	1	Total	Zn	0
			1	1	
57	4	1	Total	Zn	0
			1	1	

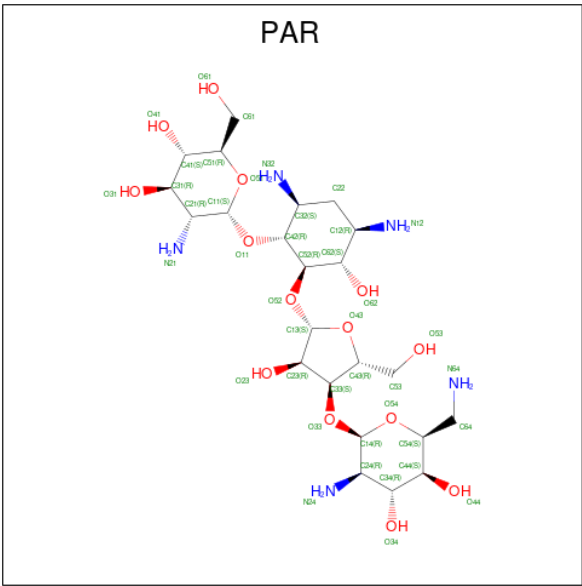
- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	c	1	Total	Mg	0
			1	1	
58	d	1	Total	Mg	0
			1	1	
58	f	1	Total	Mg	0
			1	1	
58	z	1	Total	Mg	0
			1	1	
58	a	207	Total	Mg	0
			207	207	
58	b	5	Total	Mg	0
			5	5	
58	A	93	Total	Mg	0
			93	93	

- Molecule 59 is POTASSIUM ION (CCD ID: K) (formula: K).

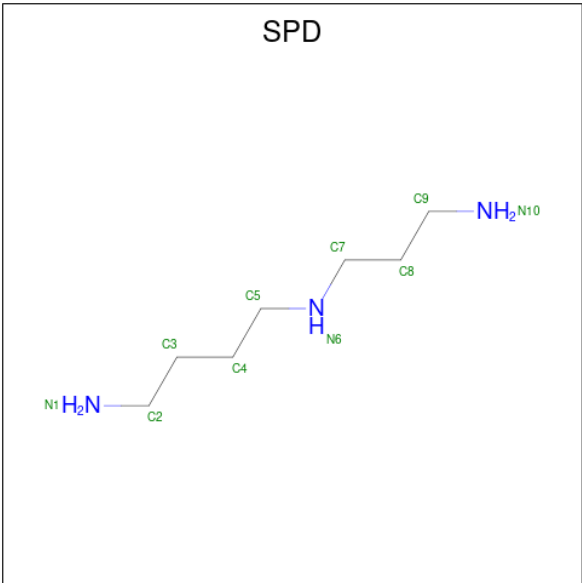
Mol	Chain	Residues	Atoms		AltConf
59	a	2	Total	K	0
			2	2	

- Molecule 60 is PAROMOMYCIN (CCD ID: PAR) (formula: C₂₃H₄₅N₅O₁₄).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
60	A	1	42	23	5	14	0

- Molecule 61 is SPERMIDINE (CCD ID: SPD) (formula: C₇H₁₉N₃).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	N	
61	A	1	10	7	3	0
61	A	1	10	7	3	0

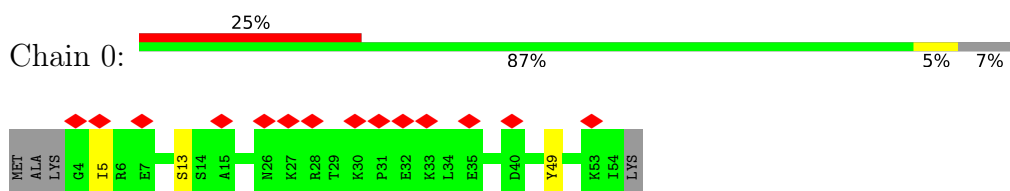
- Molecule 62 is water.

Mol	Chain	Residues	Atoms		AltConf
62	2	4	Total 4	O 4	0
62	w	1	Total 1	O 1	0
62	a	57	Total 57	O 57	0
62	V	3	Total 3	O 3	0

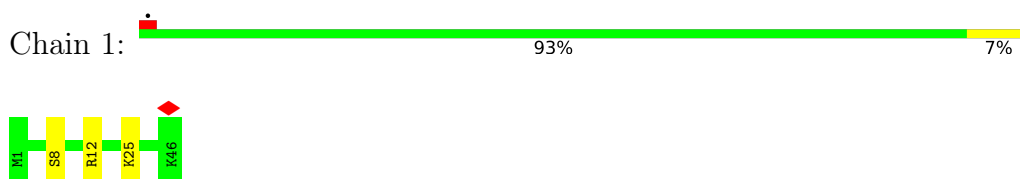
3 Residue-property plots [i](#)

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.

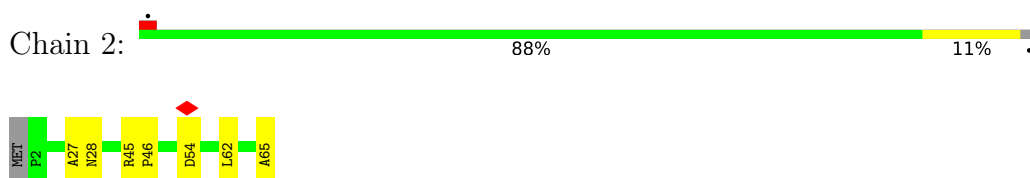
- Molecule 1: Large ribosomal subunit protein bL33



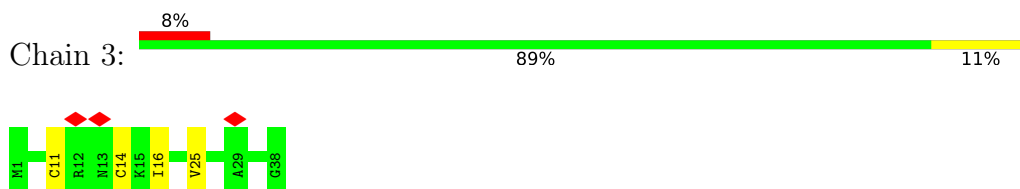
- Molecule 2: Large ribosomal subunit protein bL34



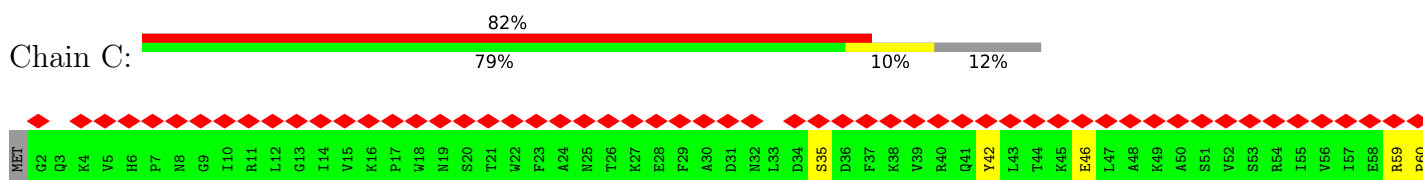
- Molecule 3: Large ribosomal subunit protein bL35

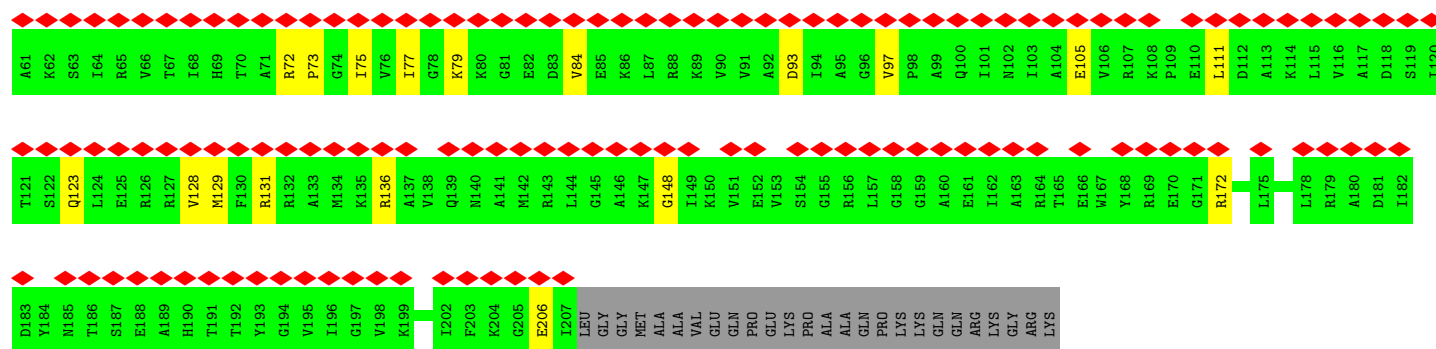


- Molecule 4: Large ribosomal subunit protein bL36A

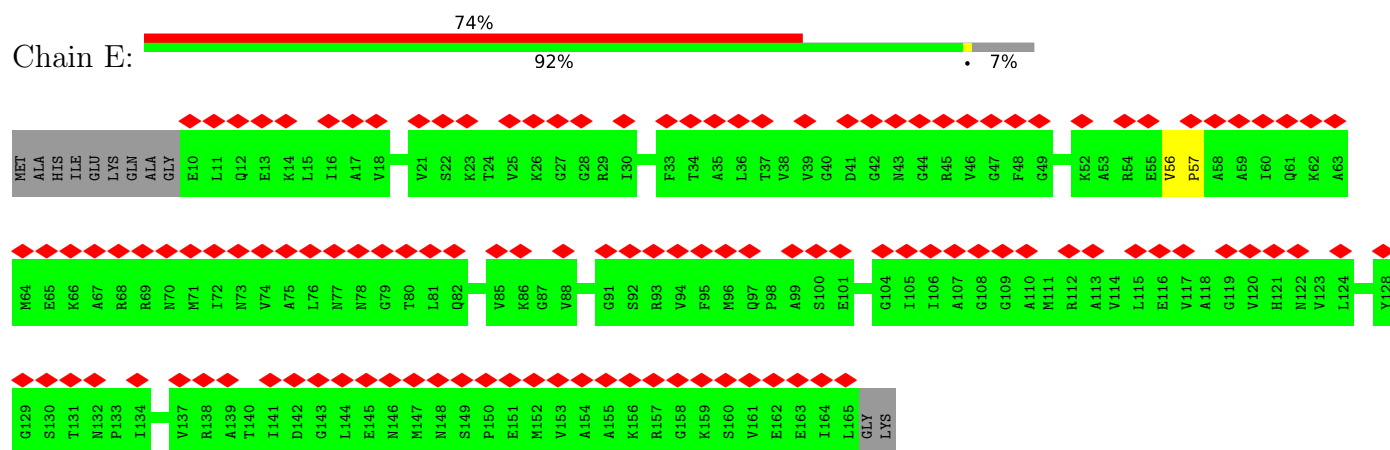


- Molecule 5: Small ribosomal subunit protein uS3

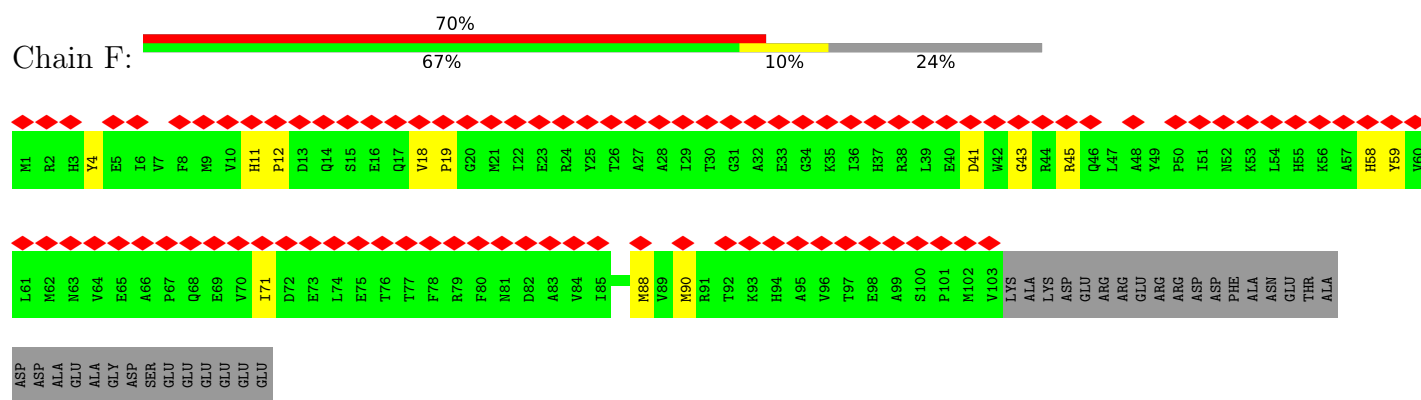




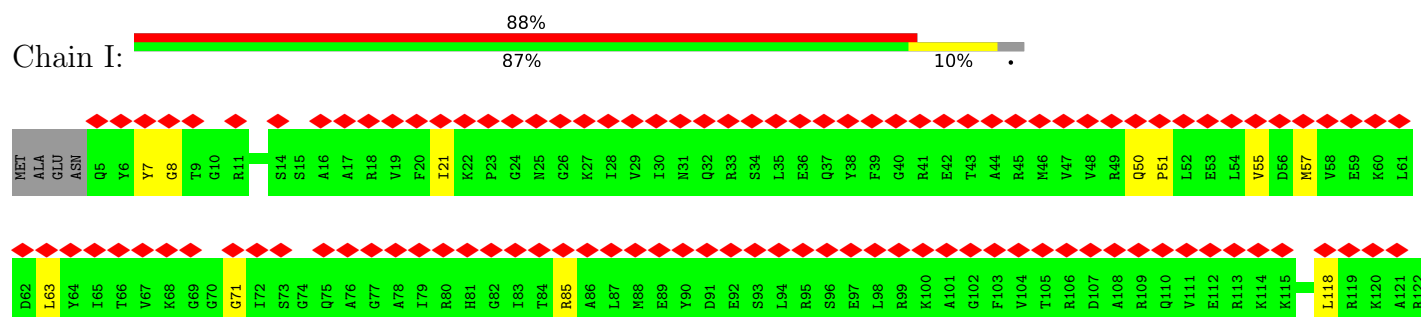
• Molecule 6: Small ribosomal subunit protein uS5

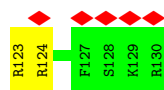


• Molecule 7: 30S ribosomal protein S6, fully modified isoform



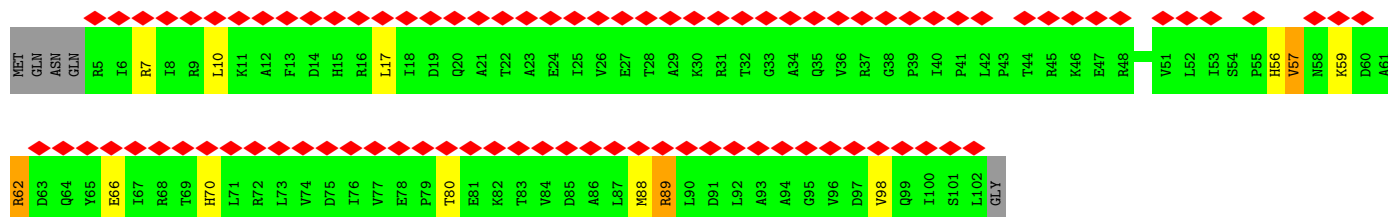
• Molecule 8: Small ribosomal subunit protein uS9





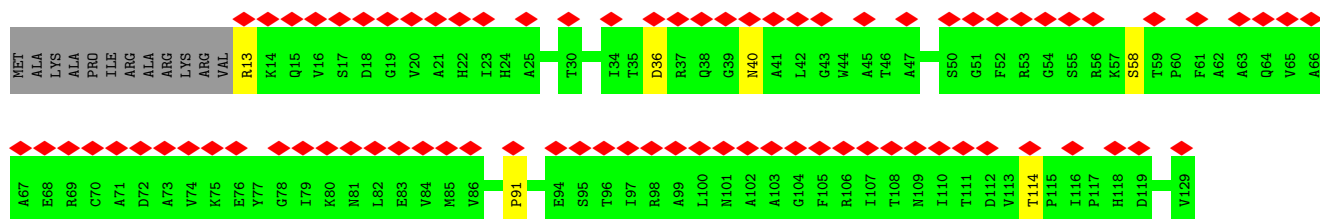
- Molecule 9: Small ribosomal subunit protein uS10

Chain J: 87%
83% 10% 5%



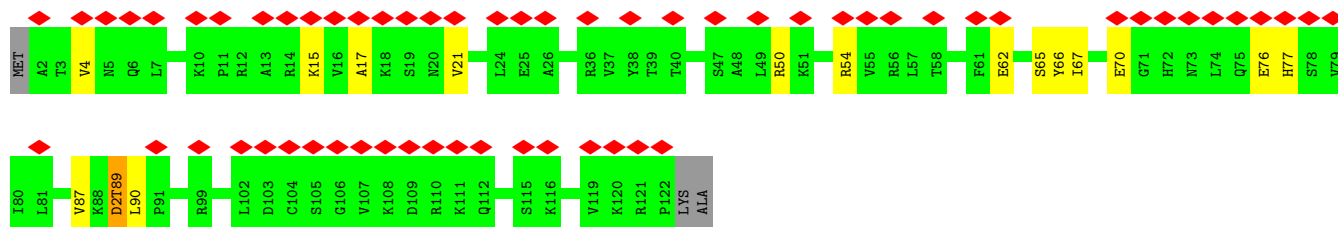
- Molecule 10: Small ribosomal subunit protein uS11

Chain K: 63%
86% 5% 9%



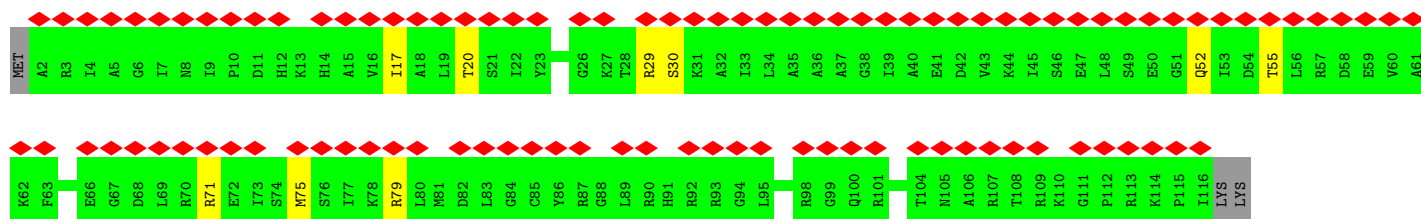
- Molecule 11: Small ribosomal subunit protein uS12

Chain L: 49%
85% 12% 2%

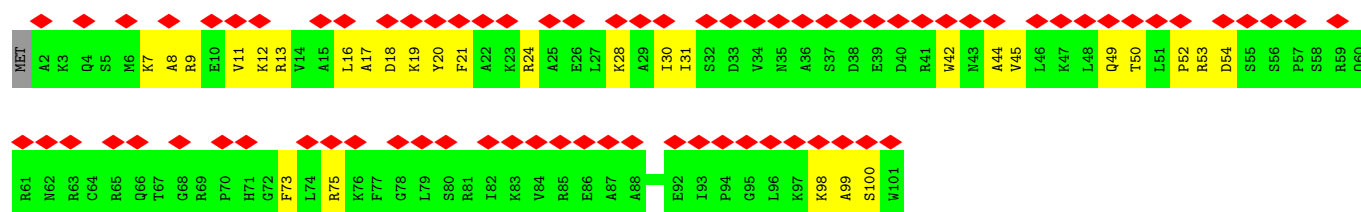
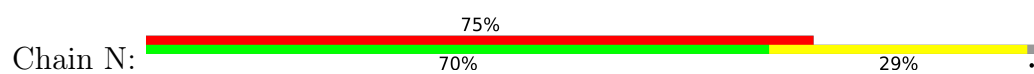


- Molecule 12: Small ribosomal subunit protein uS13

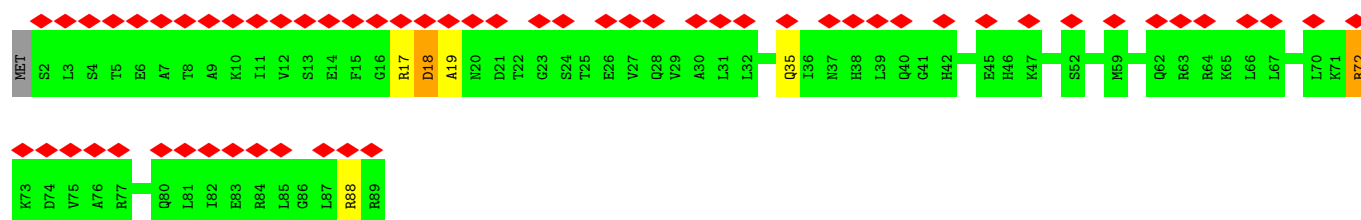
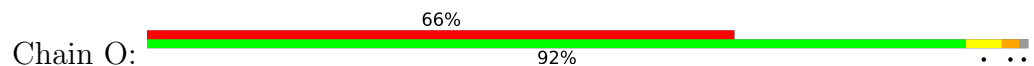
Chain M: 85%
90% 8% 1%



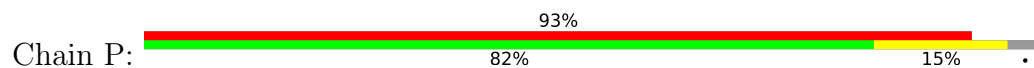
- Molecule 13: Small ribosomal subunit protein uS14



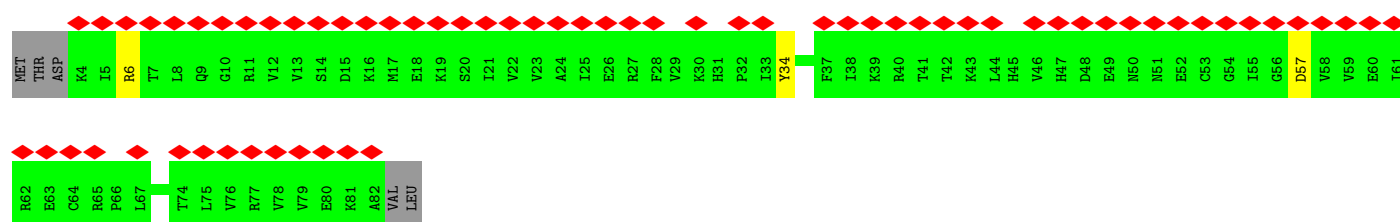
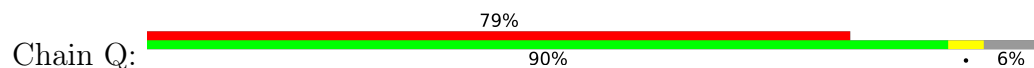
• Molecule 14: Small ribosomal subunit protein uS15



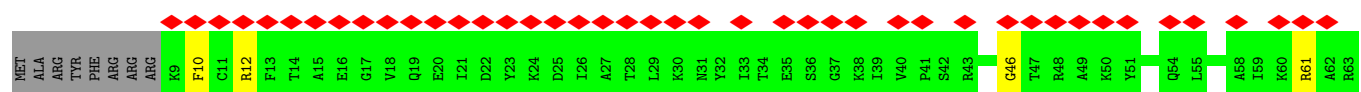
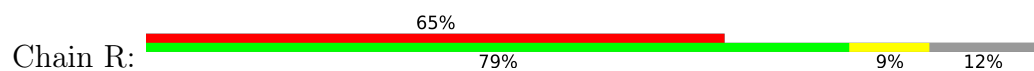
• Molecule 15: 30S ribosomal protein S16

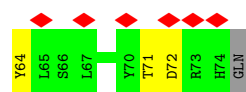


• Molecule 16: Small ribosomal subunit protein uS17

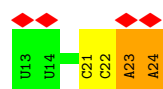


• Molecule 17: Small ribosomal subunit protein bS18

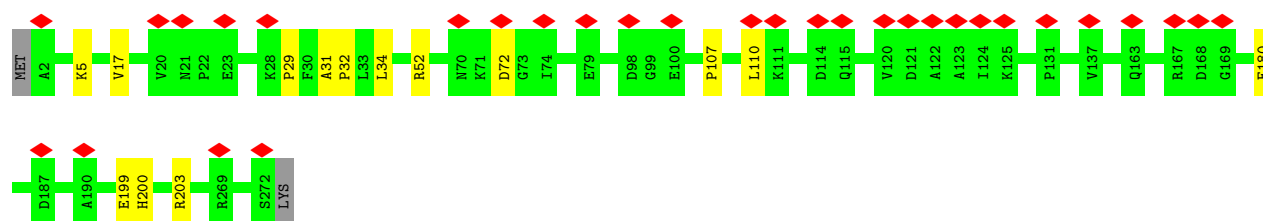




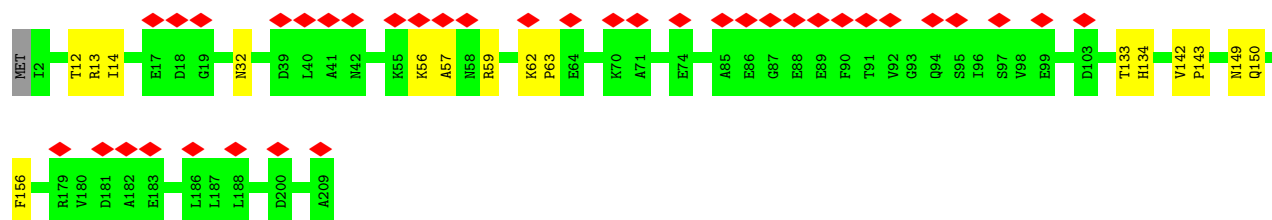
- Molecule 18: mRNA



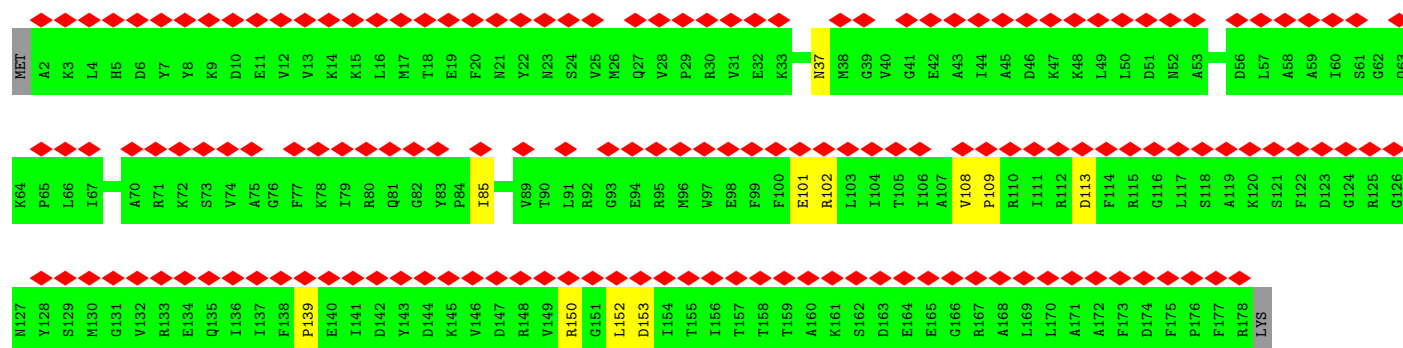
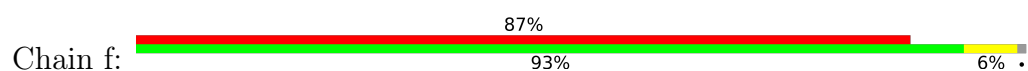
- Molecule 19: Large ribosomal subunit protein uL2



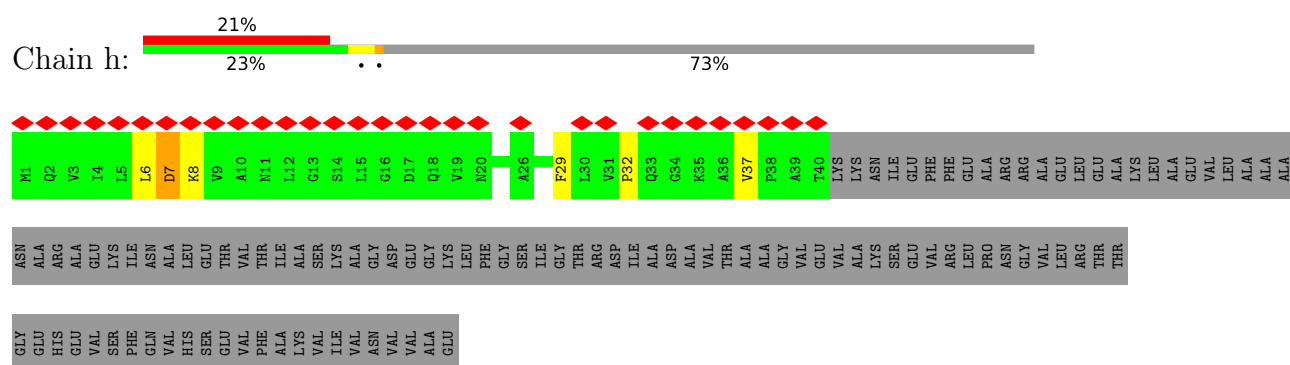
- Molecule 20: Large ribosomal subunit protein uL3



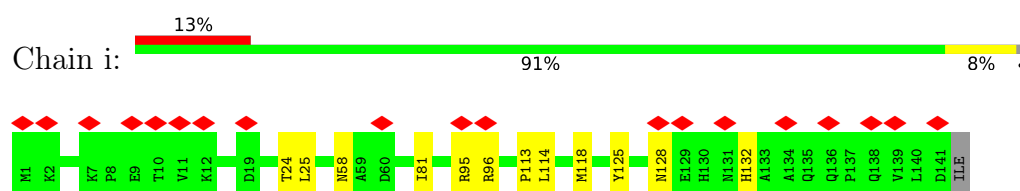
- Molecule 21: Large ribosomal subunit protein uL5



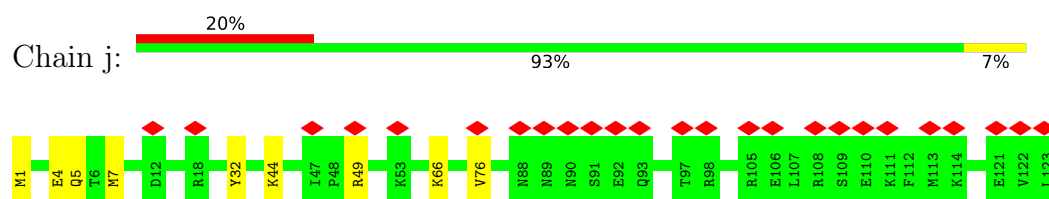
- Molecule 22: Large ribosomal subunit protein bL9



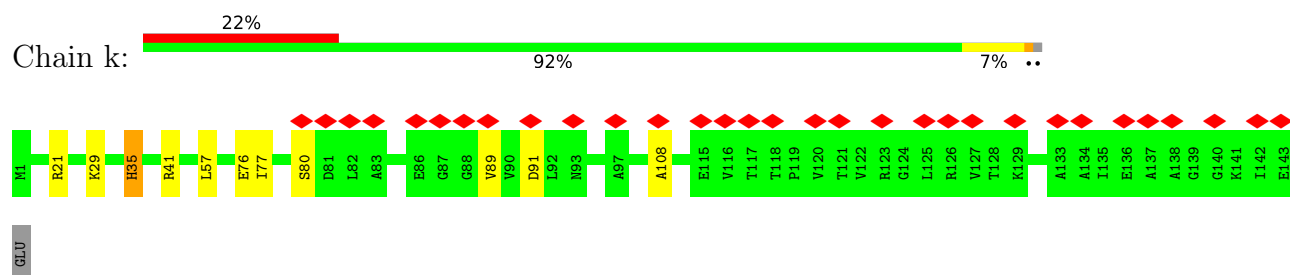
- Molecule 23: Large ribosomal subunit protein uL13



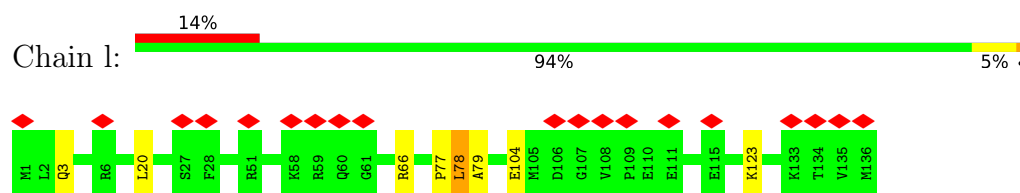
- Molecule 24: Large ribosomal subunit protein uL14



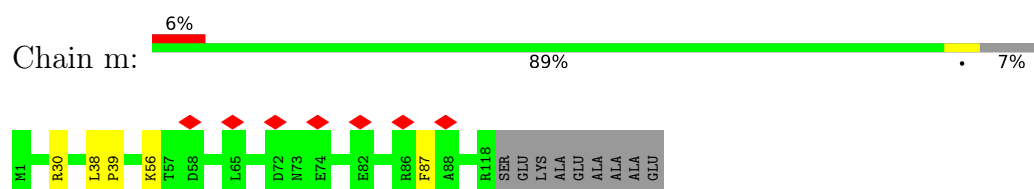
- Molecule 25: 50S ribosomal protein L15



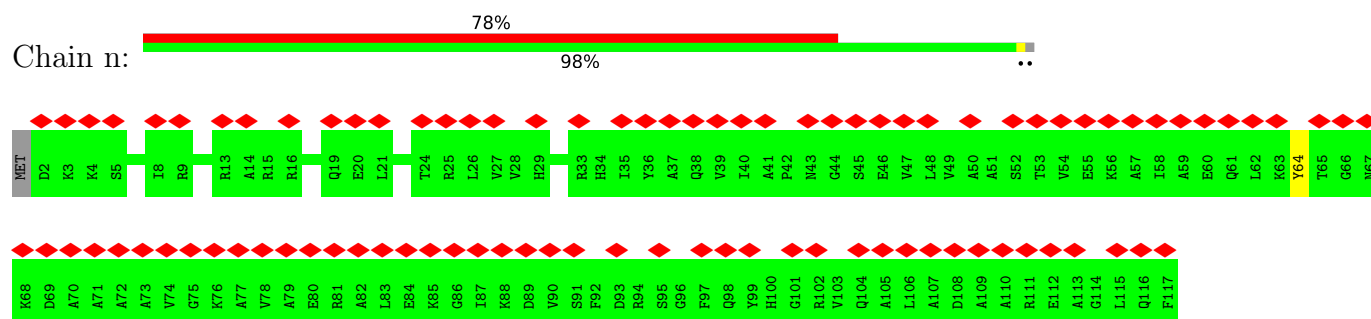
- Molecule 26: Large ribosomal subunit protein uL16



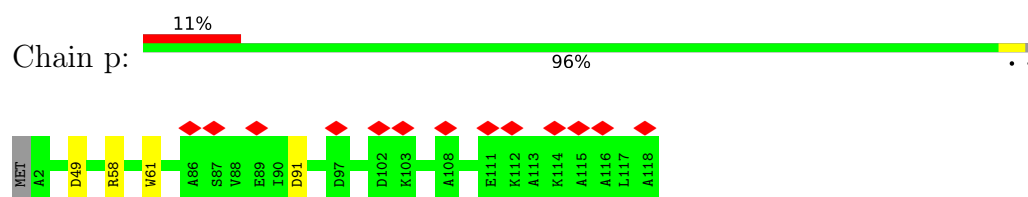
- Molecule 27: Large ribosomal subunit protein bL17



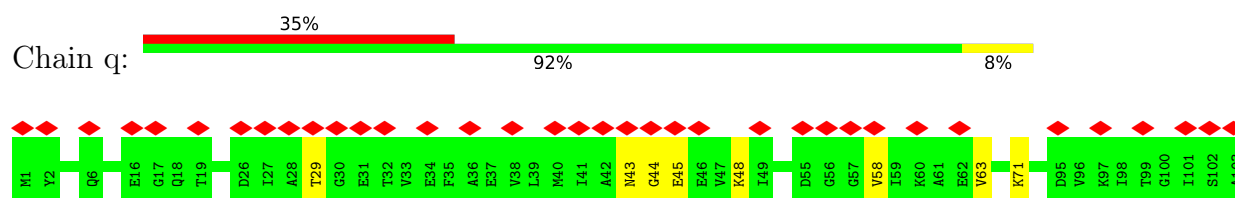
- Molecule 28: Large ribosomal subunit protein uL18



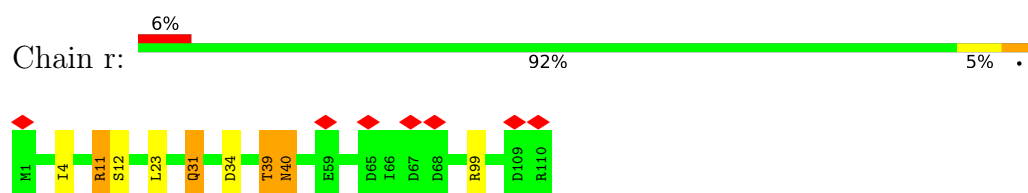
- Molecule 29: Large ribosomal subunit protein bL20



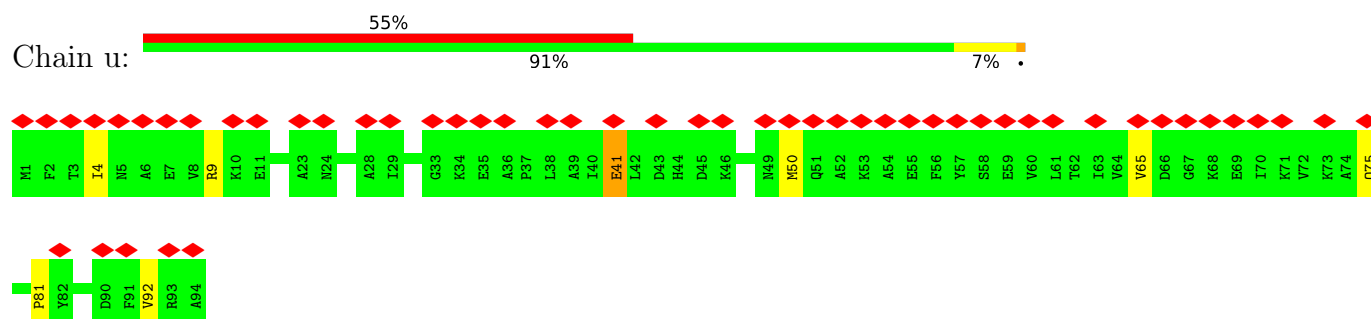
- Molecule 30: Large ribosomal subunit protein bL21



- Molecule 31: Large ribosomal subunit protein uL22

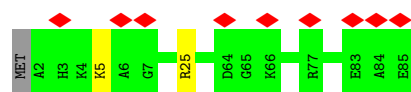


- Molecule 32: 50S ribosomal protein L25

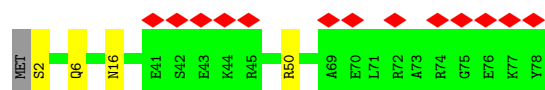


- Molecule 33: Large ribosomal subunit protein bL27

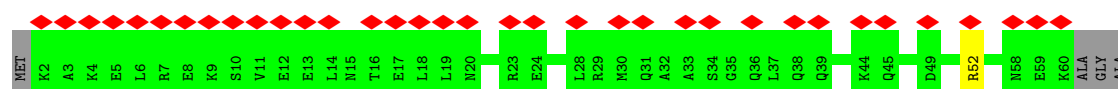
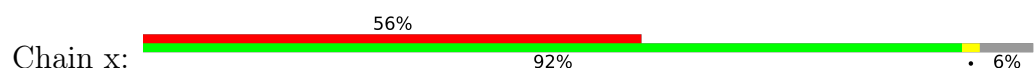




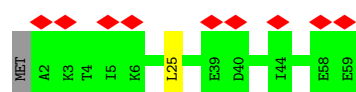
- Molecule 34: Large ribosomal subunit protein bL28



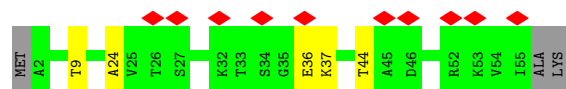
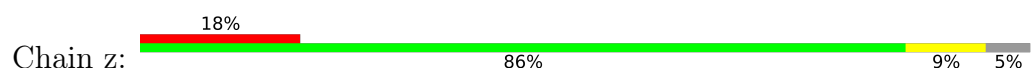
- Molecule 35: Large ribosomal subunit protein uL29



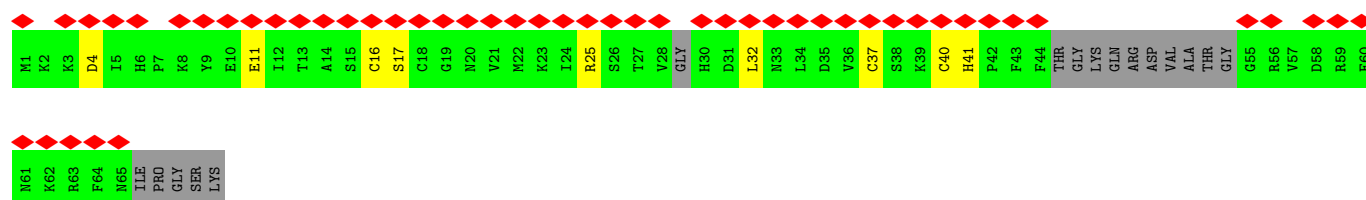
- Molecule 36: Large ribosomal subunit protein uL30



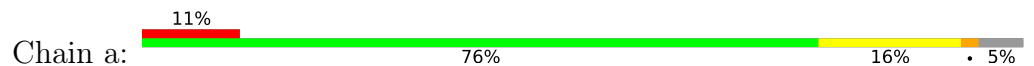
- Molecule 37: Large ribosomal subunit protein bL32



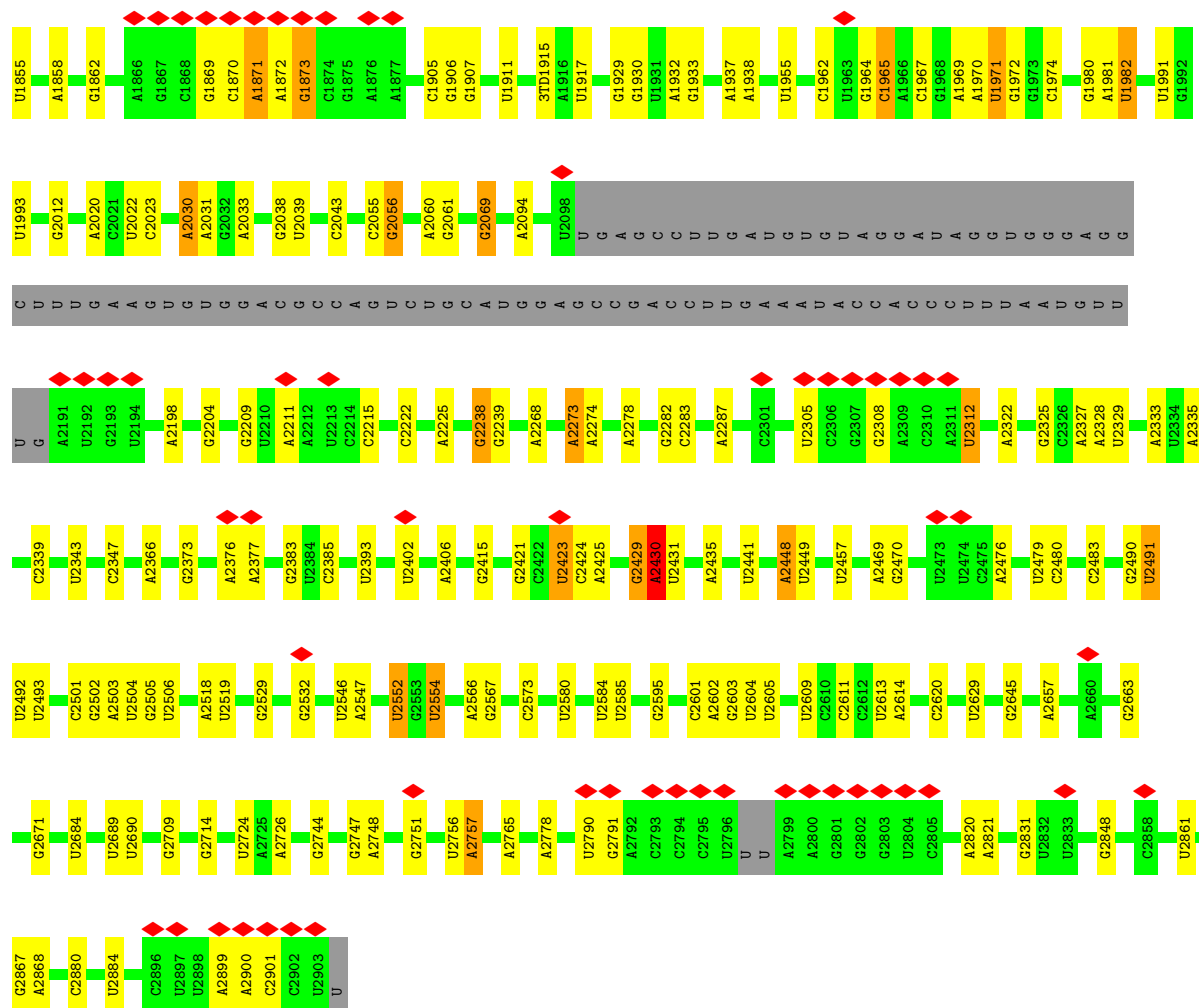
- Molecule 38: Large ribosomal subunit protein bL31A



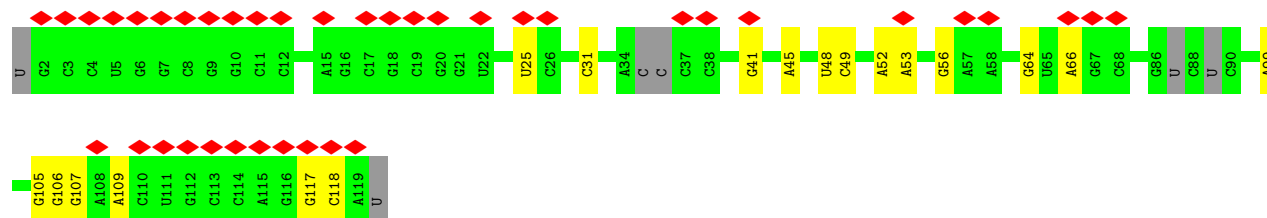
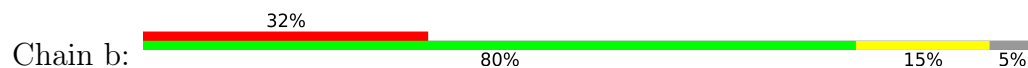
- Molecule 39: 23S rRNA



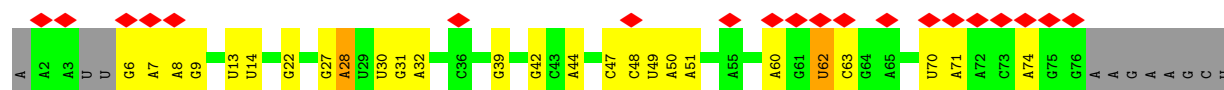




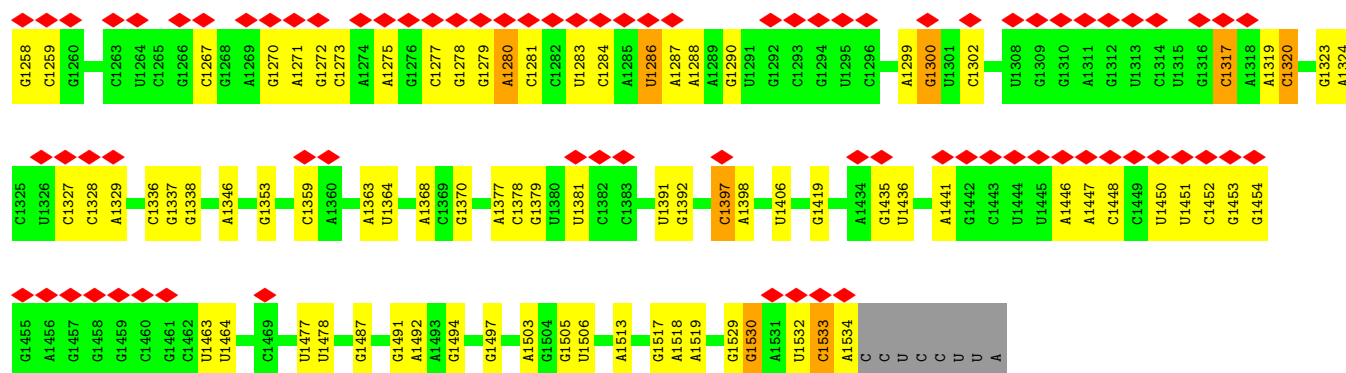
- Molecule 40: 5S rRNA



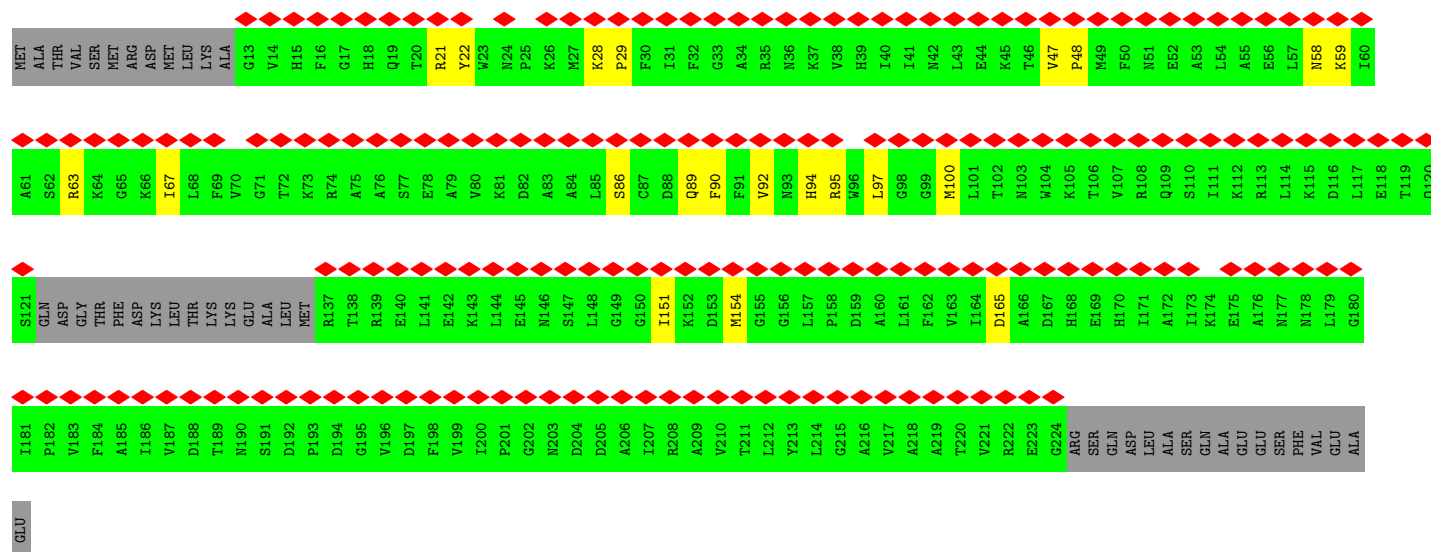
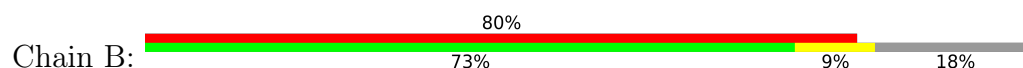
- Molecule 41: 16S rRNA



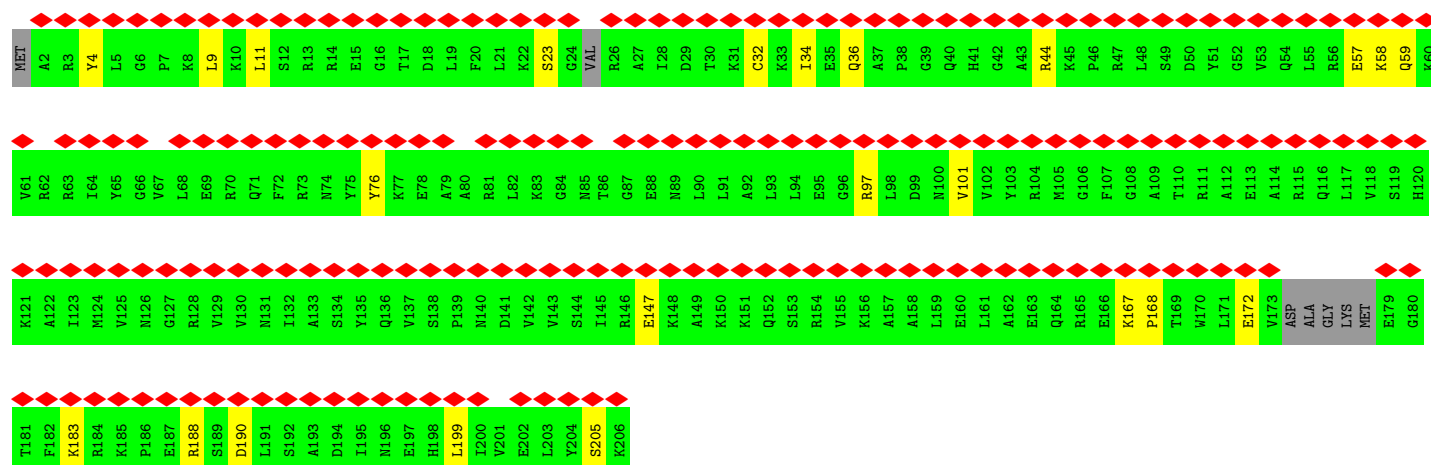
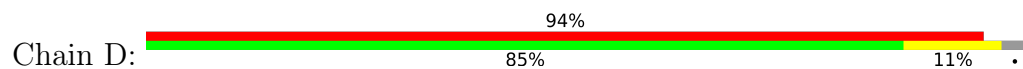




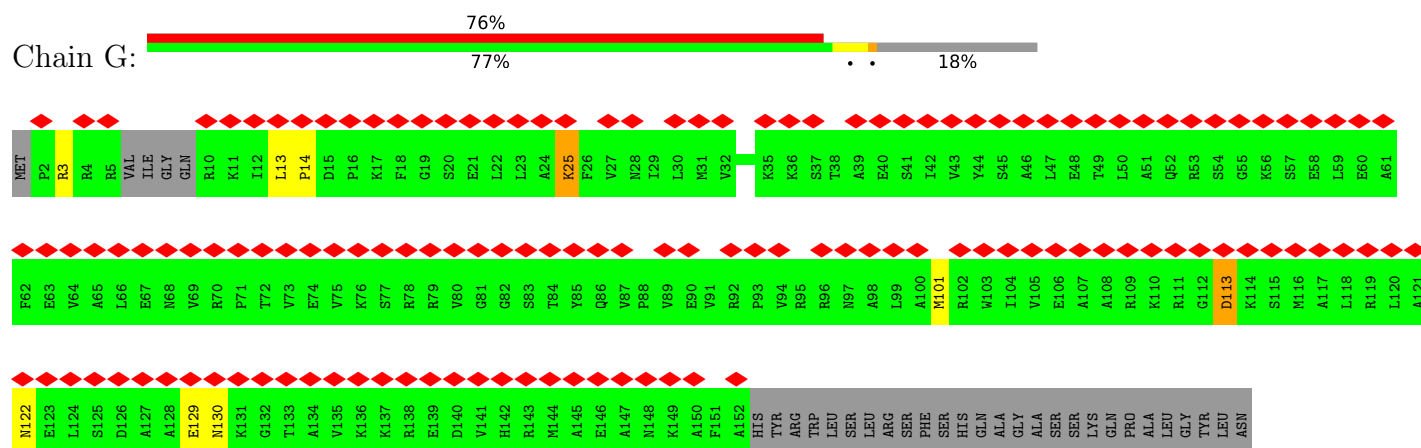
• Molecule 42: 30S ribosomal protein S2



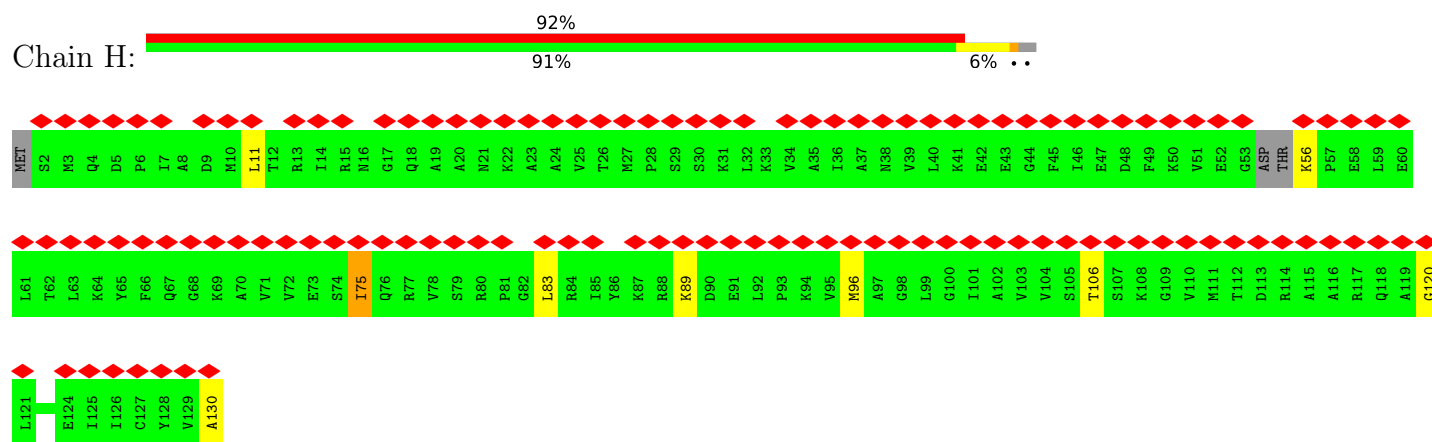
• Molecule 43: Small ribosomal subunit protein uS4



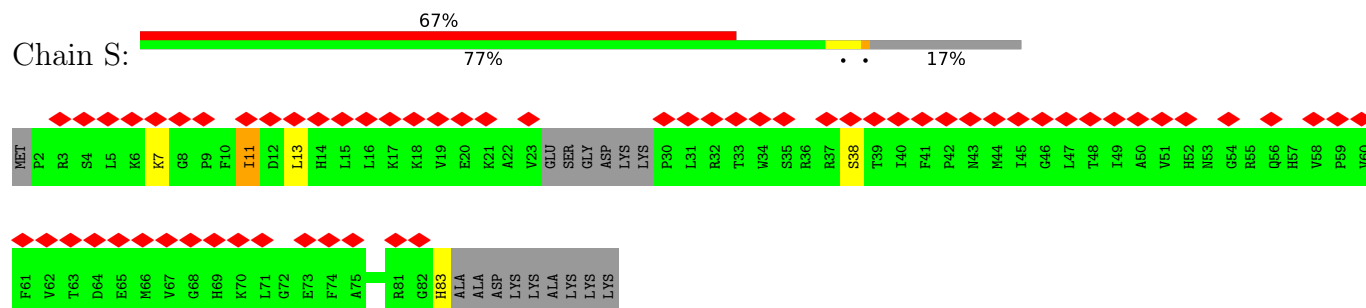
- Molecule 44: 30S ribosomal protein S7



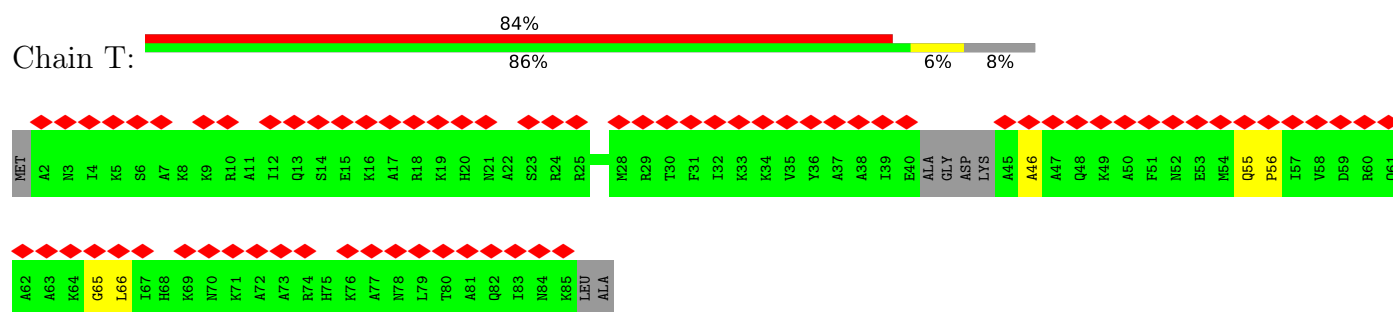
- Molecule 45: Small ribosomal subunit protein uS8



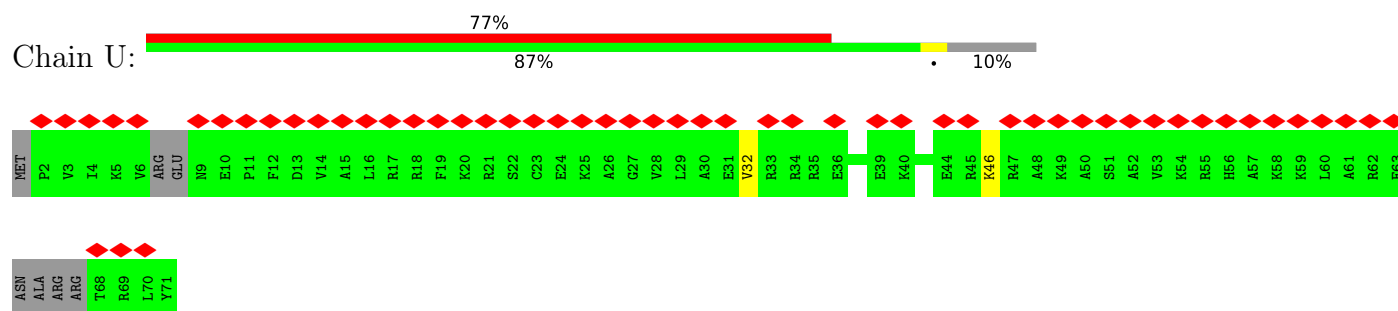
- Molecule 46: Small ribosomal subunit protein uS19



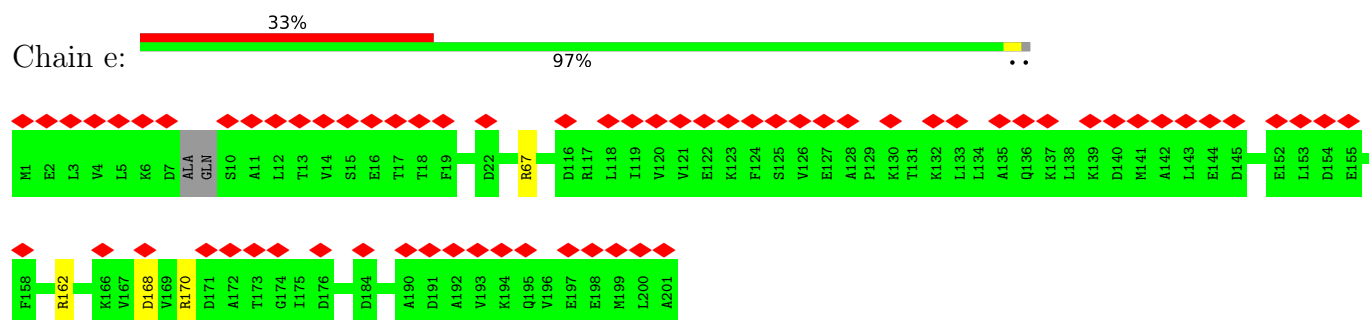
- Molecule 47: 30S ribosomal protein S20



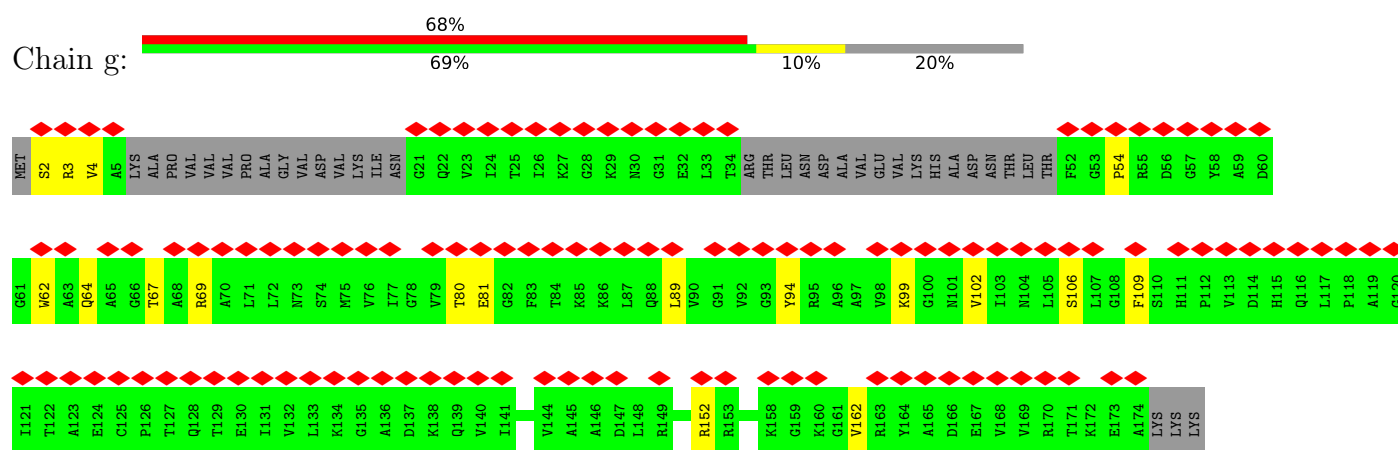
- Molecule 48: Small ribosomal subunit protein bS21



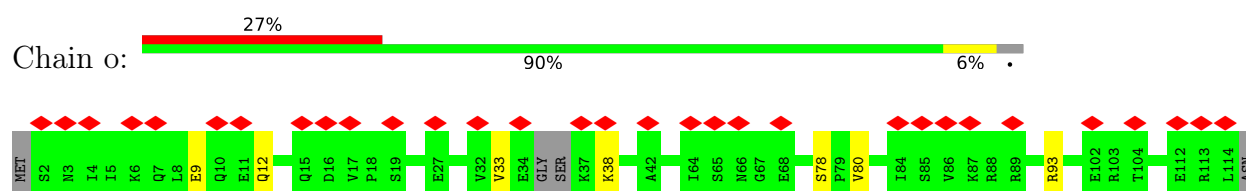
- Molecule 49: Large ribosomal subunit protein uL4



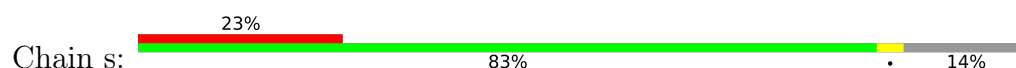
- Molecule 50: Large ribosomal subunit protein uL6

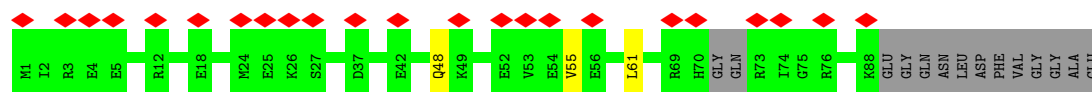


- Molecule 51: Large ribosomal subunit protein bL19

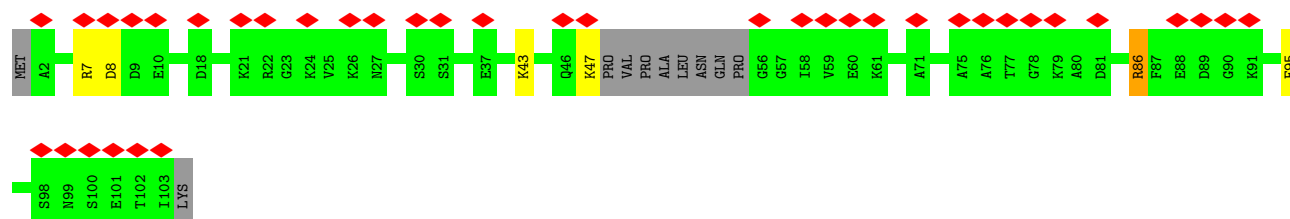
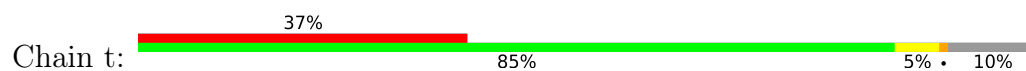


- Molecule 52: Large ribosomal subunit protein uL23

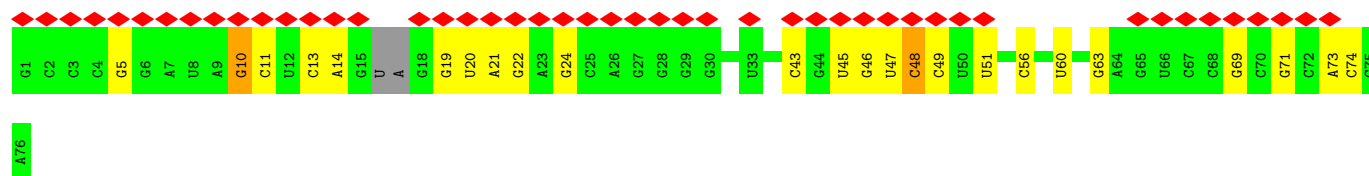




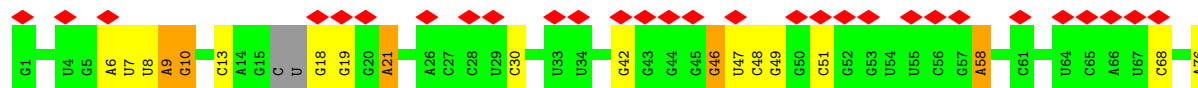
- Molecule 53: Large ribosomal subunit protein uL24



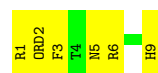
- Molecule 54: A-site Phe-tRNA



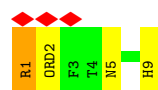
- Molecule 55: P-Site Val-tRNA



- Molecule 56: Manikomycin



- Molecule 56: Manikomycin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	340201	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 ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	0.274	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0256	Depositor
Map size (Å)	355.104, 355.104, 355.104	wwPDB
Map dimensions	432, 432, 432	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.58	0/424	0.83	0/565
2	1	0.77	0/380	0.91	0/498
3	2	0.80	0/513	0.91	0/676
4	3	0.65	0/303	0.86	0/397
5	C	0.52	0/1651	0.79	0/2225
6	E	0.58	0/1150	0.78	0/1549
7	F	0.51	0/838	0.81	0/1137
8	I	0.50	0/1026	0.80	0/1364
9	J	0.51	0/796	0.84	0/1077
10	K	0.60	0/884	0.84	0/1191
11	L	0.57	0/945	0.87	0/1268
12	M	0.51	0/900	0.86	0/1204
13	N	0.60	0/817	0.93	0/1088
14	O	0.53	0/722	0.86	0/964
15	P	0.53	0/639	0.87	0/859
16	Q	0.49	0/650	0.77	0/871
17	R	0.61	0/553	0.92	0/742
18	X	0.50	0/280	0.93	0/433
19	c	0.72	0/2121	0.86	0/2852
20	d	0.70	0/1568	0.85	0/2109
21	f	0.49	0/1434	0.84	0/1926
22	h	0.51	0/297	0.77	0/402
23	i	0.63	0/1143	0.80	0/1540
24	j	0.65	0/955	0.87	0/1279
25	k	0.81	0/1052	0.93	3/1401 (0.2%)
26	l	0.61	0/1072	0.83	0/1430
27	m	0.76	0/958	0.91	0/1281
28	n	0.56	0/902	0.82	0/1209
29	p	0.73	0/960	0.85	0/1278
30	q	0.60	0/829	0.81	0/1107
31	r	0.72	0/864	0.84	1/1156 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	u	0.55	0/766	0.83	0/1025
33	v	0.66	0/636	0.76	0/841
34	w	0.64	0/635	0.82	0/848
35	x	0.49	0/487	0.81	0/648
36	y	0.64	0/453	0.80	0/605
37	z	0.72	0/435	0.91	0/581
38	4	0.52	0/446	0.83	0/592
39	a	0.56	2/65510 (0.0%)	0.92	77/102191 (0.1%)
40	b	0.55	0/2737	0.86	1/4262 (0.0%)
41	A	0.57	0/35504	0.92	49/55373 (0.1%)
42	B	0.49	0/1567	0.86	0/2115
43	D	0.47	0/1622	0.89	0/2167
44	G	0.50	0/1134	0.84	0/1525
45	H	0.58	0/973	0.79	0/1302
46	S	0.53	0/629	0.81	0/846
47	T	0.50	0/635	0.96	0/840
48	U	0.55	0/540	0.88	0/714
49	e	0.69	0/1556	0.86	0/2091
50	g	0.52	0/1073	0.80	0/1447
51	o	0.67	0/909	0.84	1/1215 (0.1%)
52	s	0.57	0/692	0.80	0/923
53	t	0.58	0/725	0.78	0/961
54	Y	0.55	0/1760	0.78	0/2740
55	Z	0.55	0/1767	0.87	2/2751 (0.1%)
56	V	1.59	0/23	2.17	1/29 (3.4%)
56	W	2.12	1/23 (4.3%)	1.59	0/29
All	All	0.58	3/150863 (0.0%)	0.90	135/225739 (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
5	C	0	1
8	I	0	1
9	J	0	2
12	M	0	1
14	O	0	1
15	P	0	1
19	c	0	1
21	f	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
24	j	0	1
25	k	0	1
27	m	0	1
31	r	0	2
33	v	0	1
34	w	0	1
35	x	0	1
39	a	0	12
41	A	0	2
43	D	0	1
47	T	0	1
49	e	0	2
53	t	0	1
56	W	0	1
All	All	0	37

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	W	9	HIS	ND1-CE1	7.00	1.39	1.32
39	a	2069	G7M	O3'-P	5.45	1.61	1.56
39	a	2552	OMU	O3'-P	5.14	1.61	1.56

All (135) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	A	599	C	O3'-P-O5'	-10.22	88.67	104.00
39	a	2490	G	O3'-P-O5'	-9.18	90.23	104.00
39	a	2546	U	O3'-P-O5'	-8.49	91.27	104.00
56	V	9	HIS	CA-CB-CG	-8.37	105.43	113.80
39	a	1025	G	O3'-P-O5'	8.12	116.18	104.00
39	a	204	A	O3'-P-O5'	-7.99	92.01	104.00
39	a	528	A	O3'-P-O5'	-7.99	92.01	104.00
41	A	1180	A	O3'-P-O5'	-7.98	92.03	104.00
39	a	247	G	O3'-P-O5'	-7.50	92.74	104.00
41	A	652	U	O3'-P-O5'	-7.46	92.82	104.00
25	k	35	HIS	CB-CA-C	7.45	125.24	110.42
39	a	1025	G	C2'-C3'-O3'	7.43	120.65	109.50
55	Z	8	U	O3'-P-O5'	-7.36	92.95	104.00
39	a	2601	C	O3'-P-O5'	-7.32	93.03	104.00
39	a	2493	U	O3'-P-O5'	-7.30	93.05	104.00
41	A	598	U	O3'-P-O5'	-7.29	93.07	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	781	A	O3'-P-O5'	-7.21	93.19	104.00
39	a	2492	U	O3'-P-O5'	-7.14	93.29	104.00
41	A	1290	G	O3'-P-O5'	-6.99	93.52	104.00
39	a	1905	C	O3'-P-O5'	-6.94	93.59	104.00
39	a	1373	A	O3'-P-O5'	-6.84	93.74	104.00
41	A	652	U	C2'-C3'-O3'	6.83	119.75	109.50
39	a	1246	A	O3'-P-O5'	-6.71	93.94	104.00
39	a	808	G	O3'-P-O5'	-6.66	94.01	104.00
39	a	1359	A	O3'-P-O5'	-6.64	94.04	104.00
41	A	1259	C	O3'-P-O5'	-6.63	94.05	104.00
39	a	2501	C	O3'-P-O5'	-6.59	94.11	104.00
41	A	339	C	O3'-P-O5'	-6.58	94.13	104.00
41	A	1220	G	O3'-P-O5'	-6.56	94.16	104.00
39	a	747	5MU	O3'-P-O5'	-6.55	94.18	104.00
39	a	329	G	O3'-P-O5'	-6.51	94.24	104.00
41	A	508	U	O3'-P-O5'	-6.48	94.28	104.00
39	a	2278	A	O3'-P-O5'	-6.38	94.43	104.00
39	a	1648	U	O3'-P-O5'	-6.38	94.44	104.00
39	a	1270	C	C2'-C3'-O3'	-6.36	104.17	113.70
39	a	2501	C	C4'-C3'-O3'	-6.34	103.49	113.00
41	A	500	G	O3'-P-O5'	-6.30	94.55	104.00
39	a	2423	U	O3'-P-O5'	-6.30	94.56	104.00
39	a	2611	C	O3'-P-O5'	-6.29	94.56	104.00
41	A	1377	A	O3'-P-O5'	-6.28	94.57	104.00
39	a	2222	C	O3'-P-O5'	-6.25	94.62	104.00
39	a	605	G	O3'-P-O5'	-6.24	94.64	104.00
25	k	35	HIS	CA-C-N	-6.23	112.99	121.84
25	k	35	HIS	C-N-CA	-6.23	112.99	121.84
41	A	288	A	O3'-P-O5'	-6.17	94.75	104.00
41	A	332	G	O3'-P-O5'	-6.16	94.76	104.00
39	a	972	A	O3'-P-O5'	-6.14	94.78	104.00
41	A	528	C	C4'-C3'-C2'	-6.13	96.47	102.60
41	A	757	U	O3'-P-O5'	-6.12	94.82	104.00
51	o	93	ARG	CA-CB-CG	-6.12	101.87	114.10
41	A	1336	C	O3'-P-O5'	-6.11	94.84	104.00
41	A	1088	G	O3'-P-O5'	-6.03	94.95	104.00
41	A	362	G	O3'-P-O5'	-6.03	94.96	104.00
41	A	978	A	O3'-P-O5'	-6.02	94.97	104.00
41	A	816	A	O3'-P-O5'	-6.00	95.00	104.00
41	A	725	G	O3'-P-O5'	-5.99	95.01	104.00
39	a	621	A	O3'-P-O5'	-5.97	95.05	104.00
41	A	921	U	O3'-P-O5'	-5.96	95.06	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	2620	C	O3'-P-O5'	-5.96	95.06	104.00
39	a	1328	A	O3'-P-O5'	-5.92	95.12	104.00
39	a	379	G	O3'-P-O5'	-5.90	95.15	104.00
39	a	2747	G	O3'-P-O5'	-5.86	95.20	104.00
41	A	557	G	O3'-P-O5'	-5.85	95.23	104.00
39	a	1974	C	O3'-P-O5'	-5.83	95.26	104.00
31	r	39	THR	CA-CB-OG1	-5.80	100.90	109.60
39	a	1981	A	C2'-C3'-O3'	-5.79	105.02	113.70
39	a	310	A	O3'-P-O5'	-5.78	95.33	104.00
39	a	731	C	O3'-P-O5'	-5.76	95.36	104.00
39	a	944	C	C4'-C3'-C2'	-5.74	96.86	102.60
39	a	982	C	C2'-C3'-O3'	-5.72	105.11	113.70
41	A	563	A	O3'-P-O5'	-5.71	95.44	104.00
41	A	1092	A	O3'-P-O5'	-5.67	95.50	104.00
39	a	579	G	O3'-P-O5'	-5.66	95.50	104.00
39	a	2479	U	O3'-P-O5'	-5.62	95.57	104.00
39	a	2012	G	O3'-P-O5'	-5.58	95.63	104.00
41	A	1124	G	C1'-O4'-C4'	-5.57	104.13	109.70
39	a	1293	C	O3'-P-O5'	-5.54	95.69	104.00
39	a	2519	U	O3'-P-O5'	-5.54	95.69	104.00
41	A	1320	C	O3'-P-O5'	-5.51	95.73	104.00
39	a	1565	C	O3'-P-O5'	-5.51	95.74	104.00
41	A	239	U	C2'-C3'-O3'	-5.49	105.47	113.70
39	a	1638	C	O3'-P-O5'	-5.49	95.77	104.00
39	a	1757	A	C4'-C3'-O3'	-5.48	104.78	113.00
41	A	1052	U	O3'-P-O5'	-5.45	95.83	104.00
39	a	816	C	O3'-P-O5'	-5.42	95.86	104.00
41	A	1128	C	O3'-P-O5'	-5.41	95.89	104.00
39	a	1810	A	O3'-P-O5'	-5.41	95.89	104.00
39	a	667	U	O3'-P-O5'	-5.39	95.91	104.00
39	a	2056	G	O3'-P-O5'	-5.38	95.93	104.00
39	a	60	G	O3'-P-O5'	-5.37	95.94	104.00
55	Z	13	C	O3'-P-O5'	-5.35	95.98	104.00
41	A	28	A	C4'-C3'-C2'	-5.35	97.25	102.60
39	a	827	U	C2'-C3'-O3'	-5.34	105.69	113.70
39	a	673	C	O3'-P-O5'	-5.34	95.99	104.00
39	a	2376	A	O3'-P-O5'	-5.33	96.00	104.00
41	A	8	A	O3'-P-O5'	-5.33	96.00	104.00
41	A	796	C	O3'-P-O5'	-5.32	96.03	104.00
39	a	2429	G	C2'-C3'-O3'	-5.30	105.76	113.70
39	a	495	G	O3'-P-O5'	-5.29	96.07	104.00
41	A	234	C	O3'-P-O5'	-5.28	96.08	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	a	1482	G	O3'-P-O5'	-5.27	96.09	104.00
39	a	409	G	O3'-P-O5'	-5.27	96.09	104.00
41	A	936	C	O3'-P-O5'	-5.27	96.10	104.00
39	a	404	A	C2'-C3'-O3'	5.26	117.39	109.50
41	A	597	G	O3'-P-O5'	-5.25	96.12	104.00
39	a	2430	A	C1'-O4'-C4'	-5.25	104.45	109.70
41	A	105	G	O3'-P-O5'	-5.25	96.13	104.00
41	A	711	G	O3'-P-O5'	-5.25	96.13	104.00
39	a	2094	A	O3'-P-O5'	-5.24	96.14	104.00
41	A	1221	G	O3'-P-O5'	-5.24	96.15	104.00
39	a	2022	U	C1'-C2'-O2'	-5.23	103.95	111.80
41	A	297	G	O3'-P-O5'	-5.22	96.17	104.00
39	a	2614	A	O3'-P-O5'	-5.22	96.17	104.00
41	A	890	G	O3'-P-O5'	-5.22	96.17	104.00
41	A	379	C	C3'-C2'-O2'	5.20	118.50	110.70
39	a	193	U	O3'-P-O5'	-5.20	96.20	104.00
39	a	748	G	C1'-O4'-C4'	-5.20	104.70	109.90
39	a	1971	U	C4'-C3'-O3'	-5.19	105.21	113.00
39	a	784	G	C2'-C3'-O3'	-5.18	105.93	113.70
39	a	1135	C	C4'-C3'-O3'	-5.18	105.23	113.00
39	a	1437	C	O3'-P-O5'	-5.17	96.25	104.00
39	a	1969	A	O3'-P-O5'	-5.15	96.27	104.00
40	b	66	A	O3'-P-O5'	-5.15	96.28	104.00
39	a	1416	G	O3'-P-O5'	-5.14	96.28	104.00
41	A	1187	G	O3'-P-O5'	-5.12	96.31	104.00
41	A	60	A	O3'-P-O5'	-5.11	96.34	104.00
39	a	1198	U	O3'-P-O5'	-5.10	96.35	104.00
39	a	1299	G	C2'-C3'-O3'	-5.10	106.05	113.70
41	A	352	C	O3'-P-O5'	-5.10	96.35	104.00
41	A	366	A	O3'-P-O5'	-5.09	96.36	104.00
41	A	379	C	O3'-P-O5'	-5.09	96.36	104.00
41	A	1125	U	C2'-C3'-O3'	5.05	117.08	109.50
39	a	2393	U	O3'-P-O5'	-5.04	96.44	104.00
39	a	22	C	O3'-P-O5'	-5.03	96.46	104.00
39	a	1500	G	O3'-P-O5'	-5.01	96.49	104.00

There are no chirality outliers.

All (37) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
41	A	362	G	Sidechain
41	A	587	G	Sidechain

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Mol	Chain	Res	Type	Group
5	C	206	GLU	Peptide
43	D	188	ARG	Sidechain
8	I	123	ARG	Sidechain
9	J	62	ARG	Sidechain
9	J	7	ARG	Sidechain
12	M	79	ARG	Sidechain
14	O	72	ARG	Sidechain
15	P	8	ARG	Sidechain
47	T	46	ALA	Peptide
56	W	1	DAR	Peptide
39	a	1025	G	Sidechain
39	a	249	C	Sidechain
39	a	2595	G	Sidechain
39	a	2645	G	Sidechain
39	a	2848	G	Sidechain
39	a	307	G	Sidechain
39	a	395	U	Sidechain
39	a	463	G	Sidechain
39	a	512	G	Sidechain
39	a	575	A	Sidechain
39	a	980	A	Sidechain
39	a	983	A	Sidechain
19	c	52	ARG	Sidechain
49	e	162	ARG	Sidechain
49	e	67	ARG	Sidechain
21	f	150	ARG	Sidechain
24	j	49	ARG	Sidechain
25	k	41	ARG	Sidechain
27	m	30	ARG	Sidechain
31	r	11	ARG	Sidechain
31	r	4	ILE	Peptide
53	t	86	ARG	Sidechain
33	v	25	ARG	Sidechain
34	w	16	ASN	Peptide
35	x	52	ARG	Sidechain

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	417	0	451	1	0
2	1	377	0	418	2	0
3	2	504	0	572	4	0
4	3	302	0	340	2	0
5	C	1624	0	1696	9	0
6	E	1137	0	1180	1	0
7	F	819	0	799	8	0
8	I	1014	0	1064	7	0
9	J	786	0	828	8	0
10	K	877	0	884	3	0
11	L	942	0	999	9	0
12	M	891	0	952	4	0
13	N	805	0	844	27	0
14	O	714	0	734	5	0
15	P	629	0	643	7	0
16	Q	641	0	682	2	0
17	R	544	0	565	4	0
18	X	252	0	128	3	0
19	c	2082	0	2154	7	0
20	d	1558	0	1606	10	0
21	f	1410	0	1444	5	0
22	h	294	0	314	3	0
23	i	1120	0	1151	8	0
24	j	946	0	1023	6	0
25	k	1043	0	1123	7	0
26	l	1075	0	1144	6	0
27	m	945	0	989	2	0
28	n	892	0	923	1	0
29	p	947	0	1019	3	0
30	q	816	0	839	4	0
31	r	857	0	922	6	0
32	u	753	0	780	4	0
33	v	628	0	642	1	0
34	w	625	0	652	1	0
35	x	486	0	518	0	0
36	y	449	0	488	1	0
37	z	429	0	440	5	0
38	4	439	0	432	5	0
39	a	59004	0	29704	130	0
40	b	2449	0	1242	9	0
41	A	31958	0	16106	229	0
42	B	1538	0	1552	12	0
43	D	1602	0	1662	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	G	1121	0	1143	6	0
45	H	964	0	1019	5	0
46	S	613	0	639	7	0
47	T	630	0	677	2	0
48	U	534	0	571	2	0
49	e	1538	0	1605	1	0
50	g	1058	0	1081	8	0
51	o	898	0	947	4	0
52	s	687	0	761	2	0
53	t	721	0	770	6	0
54	Y	1576	0	802	6	0
55	Z	1582	0	803	4	0
56	V	84	0	84	3	0
56	W	84	0	83	3	0
57	3	1	0	0	0	0
57	4	1	0	0	0	0
58	A	93	0	0	0	0
58	a	207	0	0	0	0
58	b	5	0	0	0	0
58	c	1	0	0	0	0
58	d	1	0	0	0	0
58	f	1	0	0	0	0
58	z	1	0	0	0	0
59	a	2	0	0	0	0
60	A	42	0	45	4	0
61	A	20	0	38	4	0
62	2	4	0	0	0	0
62	V	3	0	0	0	0
62	a	57	0	0	0	0
62	w	1	0	0	0	0
All	All	140150	0	93716	569	0

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

All (569) 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)
26:l:77:PRO:C	26:l:78:LEU:N	2.15	1.04
39:a:483:A:H5''	53:t:47:LYS:HD2	1.61	0.82
39:a:12:U:H2'	39:a:12:U:O2	1.79	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:1434:A:H2'	39:a:1435:G:C8	2.19	0.78
39:a:2209:G:H1	39:a:2215:C:H42	1.32	0.76
38:4:37:CYS:N	38:4:40:CYS:SG	2.59	0.75
39:a:2209:G:H1	39:a:2215:C:N4	1.83	0.75
41:A:606:G:N2	41:A:632:U:OP1	2.17	0.73
26:l:79:ALA:O	33:v:5:LYS:HB2	1.88	0.72
41:A:135:C:C5	41:A:136:C:C5	2.78	0.72
39:a:433:C:H5''	56:W:1:DAR:HE	1.55	0.71
41:A:384:G:H2'	41:A:385:C:C6	2.26	0.71
41:A:451:A:O2'	61:A:1695:SPD:N1	2.24	0.70
39:a:1434:A:H2'	39:a:1435:G:H8	1.56	0.70
34:w:6:GLN:HE21	34:w:50:ARG:H	1.41	0.69
41:A:1012:A:N6	41:A:1013:G:C6	2.61	0.68
39:a:2209:G:N2	39:a:2215:C:N3	2.39	0.68
39:a:549:G:H2'	39:a:550:C:H6	1.59	0.68
41:A:1012:A:C6	41:A:1013:G:C6	2.81	0.67
29:p:49:ASP:OD2	39:a:534:U:O2'	2.08	0.67
13:N:28:LYS:HD3	41:A:1317:C:OP2	1.94	0.67
41:A:1042:A:C6	41:A:1043:G:C6	2.82	0.67
41:A:343:U:H2'	41:A:345:C:C5	2.30	0.67
14:O:17:ARG:O	14:O:18:ASP:HB2	1.93	0.67
41:A:309:A:O2'	41:A:607:A:N1	2.21	0.66
41:A:138:G:C6	41:A:226:G:C6	2.84	0.66
26:l:77:PRO:O	26:l:78:LEU:N	2.28	0.65
41:A:63:C:OP1	41:A:383:A:N6	2.30	0.65
39:a:2431:U:OP2	56:V:1:DAR:NH1	2.26	0.65
39:a:896:A:H2'	54:Y:56:C:O2	1.96	0.64
31:r:39:THR:O	31:r:40:ASN:HB2	1.97	0.64
41:A:329:A:C2	41:A:332:G:C4	2.85	0.63
41:A:176:C:H2'	41:A:177:G:N3	2.14	0.63
51:o:78:SER:OG	51:o:80:VAL:HG12	1.99	0.63
39:a:894:U:H2'	39:a:895:U:O4'	1.99	0.63
39:a:2343:U:HO2'	39:a:2373:G:HO2'	1.47	0.63
32:u:9:ARG:HG2	32:u:41:GLU:HG2	1.80	0.62
41:A:404:G:H4'	41:A:439:U:O2	1.98	0.62
41:A:376:G:C2	41:A:389:A:C2	2.87	0.62
4:3:16:ILE:HD13	4:3:25:VAL:HG22	1.81	0.62
9:J:88:MET:O	9:J:89:ARG:CG	2.48	0.61
39:a:504:A:O2'	39:a:505:A:P	2.58	0.61
41:A:62:U:OP1	41:A:385:C:O2'	2.18	0.61
23:i:113:PRO:HD2	39:a:558:U:OP1	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:B:28:LYS:N	42:B:29:PRO:HD2	2.15	0.61
13:N:53:ARG:HH12	41:A:1220:G:P	2.23	0.61
17:R:71:THR:OG1	17:R:72:ASP:N	2.34	0.60
41:A:512:U:OP1	43:D:44:ARG:NH2	2.34	0.60
41:A:1130:A:H2'	41:A:1131:G:O4'	2.01	0.60
5:C:35:SER:OG	5:C:59:ARG:NH2	2.35	0.60
39:a:504:A:O2'	39:a:505:A:OP1	2.16	0.60
41:A:1012:A:C6	41:A:1013:G:C5	2.89	0.60
40:b:117:G:C6	40:b:118:C:C4	2.89	0.60
41:A:410:G:N1	41:A:431:A:OP2	2.28	0.59
41:A:1255:G:O2'	41:A:1258:G:N3	2.31	0.59
41:A:138:G:C5	41:A:226:G:C6	2.90	0.59
8:I:85:ARG:NH2	41:A:1119:C:OP1	2.35	0.59
4:3:11:CYS:SG	4:3:14:CYS:N	2.75	0.59
23:i:95:ARG:HD3	23:i:96:ARG:NH2	2.17	0.59
39:a:1872:A:H3'	39:a:1873:G:O4'	2.03	0.59
37:z:9:THR:CG2	39:a:2020:A:H5'	2.33	0.59
11:L:4:VAL:HG23	16:Q:34:TYR:HB3	1.85	0.59
20:d:12:THR:HG22	20:d:13:ARG:H	1.66	0.59
19:c:5:LYS:HD2	19:c:17:VAL:HG22	1.84	0.58
39:a:568:U:H1'	39:a:2030:6MZ:H9C1	1.85	0.58
42:B:100:MET:HE3	42:B:151:ILE:HD13	1.86	0.58
41:A:135:C:C4	41:A:136:C:C5	2.91	0.58
41:A:138:G:C4	41:A:226:G:C2	2.91	0.58
41:A:369:G:C2	41:A:370:C:C6	2.91	0.58
21:f:37:ASN:HB3	21:f:153:ASP:OD1	2.03	0.58
41:A:374:A:OP1	41:A:452:A:N6	2.26	0.58
41:A:1012:A:N6	41:A:1013:G:O6	2.37	0.58
41:A:544:G:OP1	43:D:59:GLN:NE2	2.27	0.58
9:J:66:GLU:HB2	13:N:99:ALA:HB2	1.85	0.57
41:A:533:A:O2'	41:A:535:A:OP2	2.19	0.57
54:Y:51:U:H3	54:Y:63:G:H1	1.51	0.57
41:A:429:U:H3'	43:D:9:LEU:HD12	1.86	0.57
30:q:29:THR:O	30:q:63:VAL:HB	2.04	0.57
13:N:53:ARG:NH1	41:A:1220:G:OP2	2.38	0.57
39:a:1722:A:H2'	39:a:1723:G:O4'	2.04	0.57
20:d:59:ARG:NH2	39:a:2831:G:OP2	2.35	0.56
20:d:156:PHE:CE1	23:i:81:ILE:HD13	2.40	0.56
41:A:49:U:O2	41:A:362:G:H1'	2.05	0.56
41:A:986:U:H2'	41:A:987:G:O4'	2.05	0.56
41:A:134:G:H1'	41:A:325:A:C5	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:784:G:H5'	39:a:785:G:OP1	2.05	0.56
41:A:306:A:C5	41:A:307:C:C5	2.93	0.56
41:A:401:C:O2'	41:A:621:A:N3	2.38	0.56
42:B:92:VAL:HG21	42:B:100:MET:HE1	1.88	0.56
39:a:2900:A:H2'	39:a:2901:C:O4'	2.06	0.55
41:A:337:G:H2'	41:A:338:A:C8	2.41	0.55
9:J:88:MET:O	9:J:89:ARG:HG2	2.06	0.55
41:A:160:A:C6	41:A:346:G:O6	2.60	0.55
32:u:4:ILE:HG12	32:u:50:MET:HE1	1.88	0.55
41:A:160:A:C6	41:A:346:G:C6	2.94	0.55
41:A:1130:A:H2'	41:A:1131:G:C8	2.42	0.55
41:A:1278:G:N3	41:A:1278:G:H2'	2.22	0.55
15:P:45:GLU:O	15:P:46:LYS:HB2	2.07	0.54
20:d:12:THR:HG23	51:o:9:GLU:OE2	2.07	0.54
39:a:549:G:H2'	39:a:550:C:C6	2.40	0.54
41:A:160:A:C5	41:A:346:G:O6	2.60	0.54
13:N:8:ALA:O	13:N:9:ARG:C	2.50	0.54
41:A:101:A:C6	41:A:102:G:N7	2.76	0.54
41:A:413:G:N2	41:A:428:G:O2'	2.39	0.54
41:A:98:A:C2	41:A:99:C:C2	2.96	0.54
30:q:29:THR:O	30:q:63:VAL:O	2.26	0.54
41:A:664:G:H22	41:A:741:G:H1	1.54	0.54
41:A:1532:U:C2'	41:A:1533:C:H5'	2.38	0.54
39:a:1778:U:H2'	39:a:1784:A:N6	2.23	0.53
39:a:2328:A:H2'	39:a:2329:U:C6	2.44	0.53
41:A:136:C:C4	41:A:137:U:C5	2.97	0.53
41:A:151:A:OP2	41:A:169:C:N4	2.41	0.53
41:A:98:A:C5	41:A:99:C:C4	2.96	0.53
42:B:47:VAL:HB	42:B:48:PRO:HD3	1.91	0.53
31:r:31:GLN:HE21	31:r:31:GLN:HA	1.74	0.53
7:F:11:HIS:ND1	7:F:12:PRO:HD2	2.24	0.53
11:L:87:VAL:HG11	11:L:90:LEU:HD12	1.91	0.53
41:A:410:G:H2'	41:A:429:U:C4	2.44	0.53
41:A:1323:G:H2'	41:A:1324:A:C8	2.44	0.52
38:4:11:GLU:HA	38:4:25:ARG:HA	1.91	0.52
39:a:2756:U:H1'	39:a:2757:A:H5''	1.92	0.52
41:A:1118:U:H2'	41:A:1119:C:O4'	2.10	0.52
49:e:168:ASP:OD2	49:e:170:ARG:NE	2.42	0.52
41:A:125:U:H2'	41:A:126:G:O4'	2.09	0.52
41:A:366:A:H2	41:A:394:G:O6	1.91	0.52
39:a:1182:G:H2'	39:a:1183:U:O4'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:A:101:A:C5	41:A:102:G:N7	2.78	0.52
41:A:103:U:O2'	41:A:172:A:N1	2.39	0.52
41:A:636:U:H2'	41:A:637:C:C6	2.44	0.52
39:a:141:G:H2'	39:a:142:A:O4'	2.09	0.52
39:a:1869:G:C6	39:a:1871:A:OP2	2.63	0.51
55:Z:9:A:O2'	55:Z:10:G:N7	2.44	0.51
32:u:75:GLN:HB2	32:u:92:VAL:HG23	1.91	0.51
13:N:19:LYS:HE3	13:N:20:TYR:CZ	2.46	0.51
41:A:138:G:C5	41:A:226:G:N1	2.79	0.51
13:N:75:ARG:NE	41:A:1359:C:OP2	2.33	0.51
15:P:51:ARG:NH1	41:A:627:G:OP1	2.43	0.51
15:P:51:ARG:HH12	41:A:627:G:P	2.33	0.51
47:T:55:GLN:HB3	47:T:56:PRO:HD3	1.92	0.51
39:a:2552:OMU:H6	39:a:2552:OMU:O5'	2.11	0.51
41:A:42:G:O2'	41:A:622:A:N1	2.35	0.51
25:k:77:ILE:HD13	25:k:108:ALA:HB1	1.93	0.50
39:a:1433:A:H2'	39:a:1434:A:O4'	2.11	0.50
41:A:410:G:H2'	41:A:429:U:C5	2.46	0.50
50:g:80:THR:OG1	50:g:81:GLU:N	2.43	0.50
41:A:347:G:N2	41:A:348:G:H1'	2.26	0.50
41:A:369:G:C2	41:A:370:C:C5	2.99	0.50
42:B:97:LEU:HB2	42:B:100:MET:HG3	1.93	0.50
44:G:13:LEU:HD12	44:G:14:PRO:HD2	1.93	0.50
13:N:16:LEU:O	13:N:19:LYS:N	2.34	0.50
19:c:31:ALA:N	19:c:32:PRO:CD	2.74	0.50
39:a:2:G:H2'	39:a:3:U:C6	2.47	0.50
39:a:543:G:H8	39:a:543:G:H5''	1.77	0.50
39:a:788:A:OP1	39:a:790:U:H5	1.95	0.50
39:a:1474:U:C4	39:a:1475:G:C6	2.99	0.50
17:R:61:ARG:NH1	41:A:736:C:OP1	2.44	0.50
20:d:14:ILE:HA	51:o:12:GLN:HE22	1.75	0.50
39:a:548:G:H2'	39:a:549:G:C1'	2.42	0.50
41:A:251:G:C6	41:A:266:G:C6	2.99	0.50
41:A:769:G:H4'	41:A:1513:A:H4'	1.93	0.50
26:l:66:ARG:NH1	26:l:104:GLU:OE2	2.44	0.50
41:A:110:C:H2'	41:A:111:G:O4'	2.11	0.49
25:k:76:GLU:C	25:k:77:ILE:HD12	2.37	0.49
41:A:945:G:C2	41:A:946:A:C8	3.00	0.49
41:A:1118:U:H1'	41:A:1179:A:C5	2.47	0.49
41:A:327:A:C4	41:A:329:A:C8	3.00	0.49
41:A:1130:A:H61	41:A:1144:G:H1'	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:A:142:G:C2	41:A:222:C:C2	3.00	0.49
14:O:88:ARG:NH2	39:a:714:U:OP2	2.46	0.49
39:a:183:C:H5''	56:W:1:DAR:HB2	1.93	0.49
7:F:18:VAL:HB	7:F:19:PRO:HD3	1.93	0.49
39:a:1872:A:C5	39:a:1873:G:H1'	2.47	0.49
41:A:677:U:H3	41:A:713:G:H22	1.61	0.49
42:B:94:HIS:O	42:B:95:ARG:C	2.56	0.49
25:k:77:ILE:CD1	25:k:108:ALA:HB1	2.42	0.49
41:A:374:A:N1	41:A:390:U:O2'	2.36	0.49
41:A:1272:G:H2'	41:A:1273:C:O4'	2.12	0.49
41:A:1450:U:H1'	41:A:1454:G:N2	2.28	0.49
54:Y:60:U:O2	54:Y:60:U:O5'	2.30	0.49
11:L:70:GLU:N	11:L:70:GLU:OE2	2.46	0.49
39:a:12:U:O2	39:a:12:U:C2'	2.54	0.49
41:A:326:G:O6	61:A:1696:SPD:N10	2.46	0.49
23:i:125:TYR:OH	23:i:132:HIS:NE2	2.42	0.49
37:z:36:GLU:OE2	37:z:44:THR:HB	2.13	0.49
41:A:1229:A:O2'	55:Z:30:C:OP1	2.30	0.49
43:D:9:LEU:HD13	43:D:32:CYS:HB3	1.95	0.48
14:O:72:ARG:NH2	41:A:754:C:OP1	2.46	0.48
11:L:50:ARG:HB3	11:L:66:TYR:HE1	1.79	0.48
39:a:1115:G:O2'	39:a:1116:G:O5'	2.30	0.48
41:A:160:A:H2'	41:A:161:A:O4'	2.13	0.48
41:A:1151:A:HO2'	41:A:1152:A:H8	1.62	0.48
11:L:21:VAL:HG21	41:A:553:A:H5''	1.94	0.48
27:m:56:LYS:HE2	27:m:87:PHE:O	2.14	0.48
41:A:598:U:H6	41:A:598:U:O5'	1.96	0.48
41:A:1530:G:N7	48:U:46:LYS:NZ	2.60	0.48
41:A:745:G:O2'	41:A:746:A:H5'	2.13	0.48
41:A:1016:A:N7	41:A:1017:U:H1'	2.28	0.48
13:N:24:ARG:NH2	41:A:1317:C:O4'	2.47	0.48
13:N:31:ILE:HG22	46:S:7:LYS:HG2	1.95	0.48
41:A:560:A:H4'	41:A:561:U:H5''	1.95	0.48
5:C:72:ARG:O	5:C:75:ILE:HG22	2.13	0.48
12:M:52:GLN:O	12:M:55:THR:OG1	2.27	0.48
41:A:1391:U:H2'	41:A:1392:G:C8	2.49	0.48
44:G:113:ASP:OD2	44:G:122:ASN:ND2	2.47	0.48
41:A:137:U:H1'	41:A:227:G:N2	2.28	0.48
41:A:227:G:H2'	41:A:228:A:C8	2.49	0.48
41:A:996:A:C6	41:A:997:U:C4	3.02	0.48
18:X:22:C:N4	18:X:23:A:H62	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:b:117:G:H2'	40:b:118:C:O4'	2.14	0.48
41:A:98:A:H2'	41:A:99:C:C6	2.49	0.48
41:A:635:A:H2'	41:A:636:U:C6	2.48	0.48
41:A:1169:A:H2'	41:A:1170:A:C8	2.49	0.48
9:J:10:LEU:HD22	9:J:98:VAL:HG22	1.96	0.48
39:a:644:A:H2'	39:a:645:C:O4'	2.14	0.48
39:a:2421:G:C2	56:V:3:DPN:HE2	2.48	0.48
41:A:121:U:O2'	41:A:122:G:OP1	2.22	0.48
44:G:25:LYS:HG2	44:G:101:MET:HE1	1.96	0.48
19:c:180:GLU:OE2	39:a:1799:G:O2'	2.22	0.47
26:l:20:LEU:HD13	32:u:81:PRO:HG2	1.95	0.47
39:a:548:G:H2'	39:a:549:G:H1'	1.95	0.47
41:A:98:A:C6	41:A:99:C:C4	3.02	0.47
50:g:4:VAL:O	50:g:69:ARG:HG2	2.13	0.47
6:E:56:VAL:N	6:E:57:PRO:HD2	2.29	0.47
41:A:657:U:H2'	41:A:658:C:H6	1.79	0.47
39:a:2532:G:O2'	39:a:2657:A:N1	2.47	0.47
10:K:58:SER:O	10:K:91:PRO:HG2	2.15	0.47
41:A:1126:U:O2	41:A:1280:A:O5'	2.32	0.47
41:A:1267:C:N3	41:A:1327:C:O2'	2.45	0.47
13:N:44:ALA:O	13:N:45:VAL:C	2.58	0.47
15:P:28:ARG:HD2	41:A:375:U:O2'	2.14	0.47
21:f:101:GLU:O	21:f:102:ARG:C	2.57	0.47
39:a:2273:A:H2'	39:a:2274:A:C8	2.50	0.47
50:g:64:GLN:O	50:g:67:THR:HG22	2.14	0.47
50:g:89:LEU:HD22	50:g:162:VAL:HG22	1.95	0.47
39:a:1296:G:OP1	39:a:2709:G:O2'	2.27	0.47
39:a:1409:U:H2'	39:a:1410:G:O4'	2.15	0.47
39:a:2506:U:C2	39:a:2585:U:O4	2.68	0.47
18:X:24:A:N6	41:A:1196:A:OP2	2.48	0.47
25:k:21:ARG:HA	39:a:811:U:H2'	1.97	0.47
40:b:117:G:C5	40:b:118:C:C5	3.03	0.47
41:A:453:G:C8	61:A:1695:SPD:H91	2.50	0.47
41:A:109:A:H2'	41:A:326:G:N2	2.30	0.47
23:i:125:TYR:HH	23:i:132:HIS:CD2	2.33	0.47
24:j:1:MET:HE3	24:j:32:TYR:CZ	2.50	0.47
39:a:140:C:H5''	39:a:141:G:C5	2.50	0.47
39:a:387:U:C4	39:a:388:G:O6	2.68	0.47
41:A:381:C:H2'	41:A:382:A:O4'	2.15	0.47
10:K:36:ASP:OD2	10:K:40:ASN:HB2	2.15	0.47
8:I:55:VAL:HG23	8:I:57:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:i:114:LEU:HG	23:i:118:MET:HE3	1.98	0.46
41:A:721:G:H4'	41:A:722:G:O4'	2.16	0.46
41:A:1494:G:O6	60:A:1601:PAR:H62	2.14	0.46
13:N:12:LYS:O	13:N:13:ARG:C	2.57	0.46
41:A:653:U:C2	45:H:56:LYS:HD2	2.51	0.46
41:A:1491:G:C5	60:A:1601:PAR:H21	2.50	0.46
13:N:7:LYS:O	13:N:11:VAL:HG23	2.15	0.46
37:z:9:THR:HG21	39:a:2020:A:H5'	1.97	0.46
41:A:1101:A:H4'	41:A:1102:A:O5'	2.14	0.46
11:L:89:D2T:OD2	41:A:523:A:N6	2.48	0.46
15:P:71:VAL:O	15:P:75:ILE:HG13	2.15	0.46
41:A:1157:A:C2	41:A:1181:G:C4	3.04	0.46
24:j:7:MET:HE1	24:j:44:LYS:HG3	1.97	0.46
39:a:1045:C:O2	39:a:1045:C:O4'	2.31	0.46
41:A:414:A:H2'	41:A:415:A:C8	2.51	0.46
43:D:57:GLU:HG2	43:D:199:LEU:HB2	1.98	0.46
50:g:2:SER:O	50:g:3:ARG:C	2.57	0.46
13:N:50:THR:HG21	46:S:13:LEU:HD23	1.98	0.46
19:c:29:PRO:HG2	19:c:34:LEU:HD11	1.96	0.46
39:a:1482:G:H1'	39:a:1509:A:H61	1.81	0.46
39:a:945:A:C4	39:a:2448:A:C2	3.04	0.46
39:a:1129:A:N6	39:a:2491:U:OP1	2.47	0.46
39:a:1528:A:H2'	39:a:1529:G:O4'	2.16	0.46
39:a:2327:A:H2'	39:a:2328:A:C8	2.50	0.46
41:A:126:G:OP1	41:A:605:U:O2'	2.32	0.46
25:k:89:VAL:HG12	25:k:91:ASP:OD1	2.15	0.46
41:A:354:G:C2	41:A:355:C:C6	3.03	0.46
13:N:16:LEU:O	13:N:17:ALA:C	2.59	0.46
13:N:49:GLN:NE2	46:S:11:ILE:O	2.43	0.46
39:a:2:G:C2	39:a:3:U:C2	3.05	0.46
39:a:1021:A:H3'	39:a:1021:A:N3	2.31	0.46
41:A:502:A:H2'	41:A:503:C:O4'	2.16	0.46
41:A:1149:C:H6	41:A:1149:C:O5'	1.99	0.46
41:A:1299:A:H2'	41:A:1300:G:H4'	1.97	0.46
31:r:11:ARG:NH1	31:r:99:ARG:O	2.49	0.45
41:A:994:A:C5	41:A:995:C:C5	3.04	0.45
52:s:48:GLN:HE21	52:s:55:VAL:H	1.64	0.45
21:f:108:VAL:N	21:f:109:PRO:CD	2.79	0.45
39:a:504:A:HO2'	39:a:505:A:P	2.30	0.45
39:a:1730:C:O2	39:a:1731:G:N1	2.49	0.45
41:A:379:C:H2'	41:A:380:G:O4'	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:84:A:N1	39:a:98:G:O2'	2.48	0.45
43:D:76:TYR:HH	43:D:205:SER:HG	1.59	0.45
5:C:77:ILE:HA	5:C:84:VAL:HB	1.98	0.45
41:A:412:A:C2	41:A:414:A:H1'	2.51	0.45
22:h:7:ASP:OD1	22:h:8:LYS:N	2.49	0.45
23:i:24:THR:O	23:i:25:LEU:C	2.60	0.45
41:A:620:C:H2'	41:A:621:A:C8	2.51	0.45
7:F:45:ARG:HD3	7:F:59:TYR:CD1	2.52	0.45
9:J:70:HIS:ND1	41:A:1152:A:OP1	2.35	0.45
13:N:16:LEU:O	13:N:18:ASP:N	2.49	0.45
38:4:40:CYS:O	38:4:41:HIS:C	2.59	0.45
39:a:3:U:H2'	39:a:4:U:C6	2.51	0.45
41:A:134:G:H2'	41:A:135:C:O4'	2.17	0.45
41:A:1283:U:H2'	41:A:1284:C:C6	2.52	0.45
27:m:38:LEU:HB3	27:m:39:PRO:HD3	1.99	0.45
39:a:542:C:H2'	39:a:543:G:H5''	1.98	0.45
41:A:1244:G:C6	41:A:1245:C:C4	3.04	0.45
16:Q:6:ARG:NH1	41:A:127:G:O2'	2.50	0.45
39:a:1720:U:H2'	39:a:1721:G:O4'	2.17	0.45
41:A:1286:U:C2	41:A:1288:A:OP1	2.70	0.45
52:s:61:LEU:HD12	52:s:61:LEU:C	2.42	0.45
54:Y:48:C:H5''	54:Y:48:C:H6	1.82	0.45
28:n:64:TYR:OH	40:b:52:A:N7	2.28	0.45
41:A:324:G:N2	41:A:327:A:C8	2.85	0.45
41:A:429:U:H4'	41:A:430:A:O5'	2.17	0.45
41:A:1092:A:H1'	41:A:1183:U:O4	2.17	0.45
2:1:12:ARG:NH1	39:a:465:G:OP1	2.48	0.44
41:A:369:G:N1	41:A:370:C:C4	2.85	0.44
41:A:1435:G:H2'	41:A:1436:U:C6	2.52	0.44
25:k:77:ILE:HD12	25:k:77:ILE:N	2.32	0.44
41:A:134:G:C2	41:A:135:C:H1'	2.52	0.44
41:A:135:C:H2'	41:A:136:C:H5'	1.99	0.44
41:A:1095:U:H2'	41:A:1096:C:O4'	2.18	0.44
41:A:1119:C:C2	41:A:1120:C:C6	3.05	0.44
40:b:117:G:C2	40:b:118:C:C2	3.05	0.44
41:A:402:G:H4'	41:A:620:C:O2	2.17	0.44
41:A:993:G:H2'	41:A:993:G:N3	2.33	0.44
44:G:129:GLU:O	44:G:130:ASN:C	2.60	0.44
39:a:1185:G:H5''	39:a:1186:G:OP1	2.17	0.44
41:A:136:C:C2	41:A:137:U:C6	3.06	0.44
53:t:7:ARG:O	53:t:8:ASP:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:A:138:G:C6	41:A:226:G:C5	3.06	0.44
41:A:1015:G:H2'	41:A:1016:A:O4'	2.18	0.44
36:y:25:LEU:HD11	39:a:930:G:H1'	2.00	0.44
39:a:493:G:H2'	39:a:494:G:O4'	2.18	0.44
39:a:1020:A:C2	39:a:1141:U:C2	3.06	0.44
39:a:2209:G:C2	39:a:2215:C:N3	2.86	0.44
41:A:147:G:H2'	41:A:148:G:C8	2.52	0.44
41:A:402:G:H5'	41:A:621:A:H1'	1.99	0.44
56:V:5:DSG:O	56:V:6:DAR:C	2.66	0.44
13:N:28:LYS:CD	41:A:1317:C:OP2	2.64	0.44
39:a:191:A:H2'	39:a:192:C:C6	2.53	0.44
39:a:1378:A:O2'	39:a:1380:G:N7	2.51	0.44
41:A:1237:C:C2'	41:A:1238:A:OP1	2.66	0.44
13:N:98:LYS:NZ	41:A:1189:U:OP1	2.51	0.44
20:d:62:LYS:N	20:d:63:PRO:CD	2.80	0.44
38:4:16:CYS:SG	38:4:17:SER:N	2.91	0.44
39:a:366:C:H2'	39:a:367:G:O4'	2.18	0.44
41:A:607:A:H2'	41:A:608:A:C8	2.53	0.44
41:A:946:A:H2'	41:A:947:G:C8	2.53	0.44
5:C:42:TYR:CZ	5:C:46:GLU:HG3	2.52	0.43
5:C:73:PRO:CG	5:C:105:GLU:HG2	2.48	0.43
39:a:221:A:N1	39:a:265:A:O2'	2.50	0.43
39:a:570:G:H2'	39:a:2030:6MZ:N7	2.33	0.43
39:a:1046:A:H3'	39:a:1047:G:C5'	2.48	0.43
41:A:6:G:H4'	41:A:298:A:H4'	1.99	0.43
41:A:1406:U:OP2	60:A:1601:PAR:H24	2.18	0.43
5:C:129:MET:HE1	5:C:131:ARG:HB2	1.98	0.43
40:b:48:U:H2'	40:b:49:C:C6	2.53	0.43
41:A:103:U:H1'	41:A:171:A:N1	2.33	0.43
41:A:130:A:N1	41:A:233:C:H1'	2.33	0.43
41:A:1397:C:H4'	41:A:1398:A:OP2	2.18	0.43
3:2:27:ALA:O	3:2:28:ASN:HB2	2.18	0.43
13:N:42:TRP:CH2	46:S:11:ILE:HG22	2.53	0.43
20:d:149:ASN:OD1	20:d:150:MEQ:N	2.50	0.43
29:p:91:ASP:C	29:p:91:ASP:OD1	2.60	0.43
46:S:11:ILE:HG13	46:S:38:SER:HB3	2.00	0.43
53:t:86:ARG:HG3	53:t:95:PHE:CE1	2.53	0.43
41:A:325:A:H2'	41:A:326:G:C8	2.54	0.43
41:A:604:G:H2'	41:A:605:U:O4'	2.18	0.43
41:A:1244:G:H2'	41:A:1245:C:O4'	2.18	0.43
17:R:10:PHE:N	17:R:46:GLY:HA3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:j:1:MET:HE3	24:j:32:TYR:CE2	2.52	0.43
30:q:43:ASN:O	30:q:44:GLY:C	2.61	0.43
39:a:499:U:H5''	53:t:43:LYS:HE2	2.01	0.43
39:a:2038:G:H2'	39:a:2039:U:O4'	2.17	0.43
41:A:1036:A:H2'	41:A:1037:C:O4'	2.19	0.43
42:B:90:PHE:CE1	42:B:154:MET:HA	2.54	0.43
42:B:92:VAL:CG2	42:B:100:MET:HE1	2.49	0.43
43:D:97:ARG:O	43:D:101:VAL:HG23	2.17	0.43
43:D:172:GLU:HG3	43:D:183:LYS:HD2	1.99	0.43
39:a:1050:A:H2'	39:a:1051:G:O4'	2.19	0.43
39:a:1050:A:C2	39:a:2751:G:C4	3.06	0.43
39:a:2430:A:N3	39:a:2430:A:H2'	2.34	0.43
41:A:1097:C:O2'	41:A:1169:A:O2'	2.34	0.43
41:A:1257:A:H3'	41:A:1258:G:H5'	2.01	0.43
41:A:1270:G:C4	41:A:1271:A:C8	3.07	0.43
19:c:199:GLU:O	19:c:200:HIS:C	2.61	0.43
41:A:429:U:C1'	41:A:430:A:H5''	2.49	0.43
41:A:1129:C:C1'	41:A:1146:A:H61	2.31	0.43
41:A:1157:A:H4'	41:A:1158:C:O5'	2.19	0.43
55:Z:21:A:N6	55:Z:46:G:H2'	2.34	0.43
8:I:50:GLN:N	8:I:51:PRO:HD2	2.33	0.43
39:a:2238:G:N3	39:a:2238:G:H2'	2.33	0.43
53:t:86:ARG:HG3	53:t:95:PHE:CD1	2.53	0.43
9:J:59:LYS:HE2	9:J:62:ARG:NH2	2.33	0.43
14:O:18:ASP:OD1	14:O:19:ALA:N	2.52	0.43
31:r:39:THR:O	31:r:40:ASN:CB	2.61	0.43
41:A:983:A:H5'	41:A:984:C:OP2	2.19	0.43
3:2:62:LEU:HB3	3:2:65:ALA:HB2	2.00	0.43
11:L:54:ARG:HB3	11:L:62:GLU:OE2	2.18	0.43
13:N:45:VAL:O	13:N:49:GLN:HG3	2.19	0.43
39:a:1746:A:H2'	39:a:1747:U:C6	2.54	0.43
43:D:4:TYR:CE2	43:D:11:LEU:HD11	2.54	0.43
43:D:147:GLU:OE1	43:D:147:GLU:N	2.52	0.43
3:2:54:ASP:HB3	25:k:57:LEU:HD22	2.00	0.42
8:I:71:GLY:HA2	41:A:1249:C:O2'	2.19	0.42
13:N:52:PRO:O	13:N:53:ARG:C	2.62	0.42
40:b:31:C:O2'	40:b:53:A:N1	2.31	0.42
42:B:67:ILE:H	42:B:89:GLN:NE2	2.17	0.42
50:g:109:PHE:CE1	50:g:152:ARG:NH2	2.87	0.42
12:M:71:ARG:O	12:M:75:MET:HG2	2.19	0.42
15:P:21:VAL:HG12	15:P:33:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:a:614:A:H3'	39:a:615:U:C5'	2.49	0.42
39:a:645:C:O2'	39:a:646:U:H5''	2.19	0.42
39:a:895:U:H3'	39:a:896:A:H5'	2.01	0.42
41:A:188:C:H2'	41:A:189:A:O4'	2.19	0.42
7:F:88:MET:HE3	17:R:64:TYR:CD2	2.54	0.42
8:I:7:TYR:CG	8:I:8:GLY:N	2.87	0.42
20:d:56:LYS:O	20:d:57:ALA:C	2.62	0.42
41:A:1279:G:O2'	41:A:1281:C:OP2	2.28	0.42
54:Y:10:G:H2'	54:Y:11:C:C6	2.55	0.42
39:a:1738:G:HO2'	39:a:1739:A:H8	1.65	0.42
39:a:2584:U:O5'	39:a:2584:U:H6	2.02	0.42
41:A:408:A:H2'	41:A:409:U:O4'	2.19	0.42
45:H:11:LEU:HD22	45:H:75:ILE:HD11	2.01	0.42
1:O:13:SER:HB2	1:O:49:TYR:CZ	2.54	0.42
42:B:28:LYS:N	42:B:29:PRO:CD	2.82	0.42
8:I:21:ILE:HG12	8:I:63:LEU:HD22	2.02	0.42
21:f:139:PRO:HB2	38:4:32:LEU:HD13	2.01	0.42
39:a:1141:U:H4'	39:a:1142:A:O4'	2.20	0.42
39:a:1313:U:O2	39:a:1313:U:C2'	2.68	0.42
39:a:1846:G:H2'	39:a:1847:A:O4'	2.19	0.42
41:A:50:A:O2'	41:A:360:G:N2	2.51	0.42
41:A:109:A:C6	41:A:326:G:C6	3.08	0.42
41:A:428:G:H8	41:A:428:G:OP1	2.01	0.42
41:A:1042:A:C6	41:A:1043:G:N1	2.88	0.42
3:2:45:ARG:N	3:2:46:PRO:HD2	2.35	0.42
39:a:144:A:H2'	39:a:145:C:C6	2.54	0.42
39:a:861:A:C2	39:a:917:A:C4	3.07	0.42
39:a:877:A:C2	39:a:899:A:C2	3.07	0.42
39:a:1584:U:H5''	39:a:1585:C:C5	2.55	0.42
41:A:268:U:H2'	41:A:269:C:C6	2.55	0.42
44:G:3:ARG:HG2	44:G:3:ARG:HH11	1.85	0.42
50:g:94:TYR:HA	50:g:106:SER:O	2.19	0.42
39:a:2339:C:O3'	40:b:41:G:N2	2.53	0.42
41:A:933:G:O6	44:G:3:ARG:NH2	2.51	0.42
41:A:1042:A:C5	41:A:1043:G:C6	3.08	0.42
41:A:1494:G:N7	60:A:1601:PAR:H222	2.35	0.42
51:o:33:VAL:HG22	51:o:38:LYS:HG3	2.02	0.42
7:F:43:GLY:HA2	7:F:58:HIS:CE1	2.54	0.42
12:M:29:ARG:O	12:M:30:SER:C	2.62	0.42
14:O:35:GLN:HE21	14:O:35:GLN:HA	1.84	0.42
19:c:203:ARG:HH21	19:c:203:ARG:HG3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:f:85:ILE:HD11	39:a:2312:U:H5'	2.02	0.42
39:a:1039:A:H2'	39:a:1040:A:O4'	2.19	0.42
39:a:2552:OMU:HM23	39:a:2554:U:C6	2.55	0.42
41:A:27:G:H2'	41:A:28:A:O4'	2.19	0.42
41:A:262:A:C6	41:A:263:A:C6	3.08	0.42
41:A:329:A:C6	41:A:332:G:C2	3.08	0.42
41:A:994:A:H2'	41:A:995:C:H5'	2.01	0.42
31:r:34:ASP:OD1	37:z:37:LYS:HE3	2.19	0.42
39:a:340:A:H2'	39:a:341:C:O4'	2.20	0.42
39:a:1869:G:O2'	39:a:1872:A:N6	2.53	0.42
41:A:151:A:C2	41:A:152:A:H1'	2.55	0.42
41:A:366:A:C2	41:A:394:G:O6	2.72	0.42
41:A:525:C:O5'	41:A:525:C:H6	2.03	0.42
45:H:89:LYS:HD3	45:H:120:GLY:HA2	2.01	0.42
50:g:54:PRO:HG3	50:g:62:TRP:CE2	2.54	0.42
9:J:88:MET:O	9:J:89:ARG:HG3	2.19	0.41
23:i:58:ASN:HD21	23:i:128:ASN:HD22	1.68	0.41
41:A:1271:A:C2	41:A:1272:G:C4	3.08	0.41
42:B:21:ARG:HD2	42:B:22:TYR:CZ	2.55	0.41
7:F:4:TYR:CD2	7:F:71:ILE:HG13	2.54	0.41
7:F:88:MET:HG2	7:F:90:MET:HE2	2.02	0.41
15:P:9:HIS:CD2	15:P:18:GLN:HG2	2.54	0.41
20:d:142:VAL:HB	20:d:143:PRO:HD2	2.00	0.41
39:a:273:G:C6	39:a:274:C:C4	3.08	0.41
39:a:857:G:H2'	39:a:858:G:O4'	2.21	0.41
39:a:1338:G:O2'	39:a:1393:A:N1	2.49	0.41
39:a:1421:G:C2	39:a:1422:G:C8	3.08	0.41
41:A:253:A:C6	41:A:274:A:N1	2.89	0.41
7:F:41:ASP:OD1	7:F:58:HIS:NE2	2.53	0.41
12:M:17:ILE:O	12:M:20:THR:OG1	2.36	0.41
13:N:30:ILE:O	13:N:31:ILE:C	2.62	0.41
19:c:107:PRO:HD2	19:c:110:LEU:HD22	2.01	0.41
41:A:1477:U:H2'	41:A:1478:U:C6	2.55	0.41
56:W:5:DSG:OD1	56:W:5:DSG:C	2.68	0.41
5:C:148:GLY:HA3	5:C:172:ARG:O	2.20	0.41
10:K:114:THR:HG21	48:U:32:VAL:HG21	2.03	0.41
11:L:50:ARG:NH2	41:A:522:C:H41	2.18	0.41
41:A:380:G:N2	41:A:382:A:H3'	2.34	0.41
5:C:128:VAL:HG11	5:C:136:ARG:HH22	1.85	0.41
13:N:20:TYR:O	13:N:21:PHE:C	2.64	0.41
39:a:871:U:H2'	39:a:872:U:C6	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:A:151:A:H2'	41:A:152:A:O4'	2.20	0.41
41:A:429:U:H1'	41:A:430:A:H5''	2.02	0.41
41:A:642:A:H1'	45:H:106:THR:O	2.20	0.41
41:A:1012:A:C5	41:A:1013:G:N7	2.88	0.41
41:A:1328:C:H2'	41:A:1329:A:O4'	2.20	0.41
43:D:167:LYS:HA	43:D:168:PRO:HD3	1.95	0.41
2:l:25:LYS:NZ	39:a:210:C:OP1	2.52	0.41
22:h:29:PHE:C	22:h:32:PRO:HD2	2.46	0.41
39:a:631:A:N3	39:a:2415:G:O2'	2.51	0.41
39:a:896:A:H2'	54:Y:56:C:C2	2.55	0.41
40:b:106:G:H2'	40:b:107:G:O4'	2.20	0.41
41:A:640:A:N7	41:A:641:U:C4	2.88	0.41
41:A:1119:C:N3	41:A:1120:C:C5	2.89	0.41
41:A:453:G:N7	61:A:1695:SPD:H72	2.36	0.41
41:A:994:A:C6	41:A:995:C:C5	3.09	0.41
9:J:56:HIS:O	9:J:57:VAL:HG22	2.21	0.41
5:C:123:GLN:OE1	5:C:136:ARG:NH2	2.54	0.41
11:L:76:GLU:O	11:L:77:HIS:HB2	2.20	0.41
13:N:42:TRP:HH2	46:S:11:ILE:HG22	1.86	0.41
24:j:66:LYS:HB3	24:j:66:LYS:HE2	1.83	0.41
31:r:23:LEU:HD22	37:z:24:ALA:HB2	2.03	0.41
39:a:1964:G:H4'	39:a:1965:C:OP2	2.21	0.41
41:A:431:A:H2'	41:A:432:A:O4'	2.21	0.41
41:A:640:A:C5	41:A:641:U:C4	3.09	0.41
41:A:838:G:H2'	41:A:839:C:O4'	2.21	0.41
41:A:955:U:O2'	46:S:83:HIS:HD2	2.03	0.41
41:A:1277:C:H2'	41:A:1278:G:H5''	2.03	0.41
41:A:1463:U:H2'	41:A:1464:U:C6	2.56	0.41
42:B:59:LYS:HG2	42:B:63:ARG:HH12	1.85	0.41
18:X:21:C:H2'	18:X:22:C:O4'	2.20	0.41
26:l:123:LYS:NZ	39:a:2483:C:N3	2.63	0.41
29:p:58:ARG:HA	29:p:61:TRP:CE3	2.56	0.41
39:a:483:A:H5''	53:t:47:LYS:CD	2.41	0.41
41:A:102:G:H2'	41:A:103:U:H6	1.86	0.41
41:A:374:A:H4'	41:A:451:A:OP1	2.21	0.41
41:A:429:U:O2	41:A:430:A:C8	2.74	0.41
41:A:1127:G:H1'	41:A:1280:A:C6	2.55	0.41
20:d:133:THR:O	20:d:134:HIS:C	2.64	0.40
30:q:44:GLY:O	30:q:45:GLU:HB2	2.21	0.40
39:a:1681:G:N3	39:a:1762:A:H2'	2.36	0.40
39:a:1820:U:H4'	39:a:1821:A:OP2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:A:42:G:N3	41:A:622:A:H2	2.18	0.40
41:A:1532:U:O2'	41:A:1533:C:H5'	2.21	0.40
22:h:6:LEU:O	22:h:7:ASP:HB2	2.22	0.40
24:j:4:GLU:O	24:j:5:GLN:HB2	2.20	0.40
39:a:2585:U:O2	39:a:2585:U:O4'	2.39	0.40
41:A:1042:A:N6	41:A:1043:G:O6	2.54	0.40
45:H:96:MET:SD	45:H:130:ALA:HB1	2.61	0.40
47:T:65:GLY:O	47:T:66:LEU:C	2.63	0.40
13:N:16:LEU:HB2	13:N:54:ASP:O	2.22	0.40
24:j:76:VAL:CG2	39:a:2684:U:H4'	2.52	0.40
39:a:284:U:H2'	39:a:285:G:O4'	2.22	0.40
39:a:984:A:N3	39:a:984:A:H2'	2.35	0.40
41:A:408:A:O3'	43:D:23:SER:OG	2.39	0.40
41:A:417:G:H5'	41:A:418:C:OP2	2.21	0.40
41:A:1118:U:H1'	41:A:1179:A:C4	2.57	0.40
41:A:1126:U:O2	41:A:1280:A:H2'	2.21	0.40
41:A:1126:U:O2	41:A:1280:A:H3'	2.21	0.40
8:I:118:LEU:HD22	8:I:124:ARG:HG2	2.03	0.40
13:N:73:PHE:CE2	13:N:75:ARG:HA	2.57	0.40
39:a:1169:A:H2'	39:a:1170:C:O4'	2.22	0.40
39:a:1980:G:O2'	39:a:1982:U:OP2	2.40	0.40
41:A:663:A:H5'	41:A:836:G:OP1	2.22	0.40
39:a:476:G:H4'	39:a:502:A:N1	2.36	0.40
39:a:1042:G:C6	39:a:1043:C:C4	3.09	0.40
39:a:1509:A:HO2'	39:a:1510:G:H8	1.66	0.40
39:a:1932:A:H2'	39:a:1933:G:O4'	2.21	0.40
41:A:137:U:C2	41:A:227:G:N1	2.90	0.40
41:A:182:A:N1	41:A:223:A:O2'	2.53	0.40
41:A:251:G:C6	41:A:266:G:O6	2.74	0.40
41:A:545:C:OP1	43:D:58:LYS:NZ	2.54	0.40
41:A:1012:A:C5	41:A:1013:G:C5	3.09	0.40
41:A:1257:A:H4'	41:A:1258:G:OP2	2.22	0.40
55:Z:18:G:H21	55:Z:58:A:H5'	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	0	49/55 (89%)	47 (96%)	2 (4%)	0	100	100
2	1	44/46 (96%)	44 (100%)	0	0	100	100
3	2	62/65 (95%)	60 (97%)	2 (3%)	0	100	100
4	3	36/38 (95%)	36 (100%)	0	0	100	100
5	C	204/233 (88%)	196 (96%)	7 (3%)	1 (0%)	24	32
6	E	154/167 (92%)	151 (98%)	3 (2%)	0	100	100
7	F	101/135 (75%)	99 (98%)	2 (2%)	0	100	100
8	I	124/130 (95%)	117 (94%)	7 (6%)	0	100	100
9	J	96/103 (93%)	90 (94%)	4 (4%)	2 (2%)	5	4
10	K	113/129 (88%)	108 (96%)	5 (4%)	0	100	100
11	L	118/124 (95%)	108 (92%)	9 (8%)	1 (1%)	16	20
12	M	113/118 (96%)	111 (98%)	2 (2%)	0	100	100
13	N	98/101 (97%)	88 (90%)	10 (10%)	0	100	100
14	O	86/89 (97%)	81 (94%)	4 (5%)	1 (1%)	10	11
15	P	77/82 (94%)	72 (94%)	4 (5%)	1 (1%)	9	9
16	Q	77/84 (92%)	72 (94%)	5 (6%)	0	100	100
17	R	64/75 (85%)	59 (92%)	5 (8%)	0	100	100
19	c	269/273 (98%)	256 (95%)	13 (5%)	0	100	100
20	d	205/209 (98%)	197 (96%)	8 (4%)	0	100	100
21	f	175/179 (98%)	168 (96%)	7 (4%)	0	100	100
22	h	38/149 (26%)	34 (90%)	3 (8%)	1 (3%)	4	2
23	i	139/142 (98%)	138 (99%)	1 (1%)	0	100	100
24	j	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
25	k	141/144 (98%)	134 (95%)	5 (4%)	2 (1%)	9	8
26	l	130/136 (96%)	126 (97%)	3 (2%)	1 (1%)	16	20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
27	m	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
28	n	114/117 (97%)	113 (99%)	1 (1%)	0	100	100
29	p	115/118 (98%)	114 (99%)	1 (1%)	0	100	100
30	q	101/103 (98%)	98 (97%)	3 (3%)	0	100	100
31	r	108/110 (98%)	105 (97%)	1 (1%)	2 (2%)	6	5
32	u	92/94 (98%)	90 (98%)	2 (2%)	0	100	100
33	v	82/85 (96%)	81 (99%)	1 (1%)	0	100	100
34	w	75/78 (96%)	75 (100%)	0	0	100	100
35	x	57/63 (90%)	57 (100%)	0	0	100	100
36	y	56/59 (95%)	55 (98%)	1 (2%)	0	100	100
37	z	52/57 (91%)	51 (98%)	1 (2%)	0	100	100
38	4	48/70 (69%)	45 (94%)	2 (4%)	1 (2%)	5	4
42	B	193/241 (80%)	186 (96%)	6 (3%)	1 (0%)	24	32
43	D	193/206 (94%)	183 (95%)	10 (5%)	0	100	100
44	G	143/179 (80%)	135 (94%)	8 (6%)	0	100	100
45	H	123/130 (95%)	119 (97%)	2 (2%)	2 (2%)	7	7
46	S	72/92 (78%)	72 (100%)	0	0	100	100
47	T	76/87 (87%)	73 (96%)	3 (4%)	0	100	100
48	U	58/71 (82%)	58 (100%)	0	0	100	100
49	e	195/201 (97%)	190 (97%)	5 (3%)	0	100	100
50	g	135/177 (76%)	128 (95%)	7 (5%)	0	100	100
51	o	107/115 (93%)	105 (98%)	2 (2%)	0	100	100
52	s	82/100 (82%)	80 (98%)	2 (2%)	0	100	100
53	t	90/104 (86%)	87 (97%)	3 (3%)	0	100	100
56	V	2/9 (22%)	2 (100%)	0	0	100	100
56	W	2/9 (22%)	2 (100%)	0	0	100	100
All	All	5321/5931 (90%)	5122 (96%)	183 (3%)	16 (0%)	37	45

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	J	89	ARG
9	J	57	VAL

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Mol	Chain	Res	Type
14	O	18	ASP
31	r	40	ASN
11	L	17	ALA
15	P	64	GLY
25	k	35	HIS
38	4	4	ASP
25	k	29	LYS
45	H	83	LEU
5	C	60	PRO
22	h	7	ASP
31	r	12	SER
42	B	165	ASP
26	l	3	GLN
45	H	75	ILE

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	46/49 (94%)	45 (98%)	1 (2%)	45	60
2	1	38/38 (100%)	37 (97%)	1 (3%)	40	55
3	2	51/52 (98%)	51 (100%)	0	100	100
4	3	34/34 (100%)	34 (100%)	0	100	100
5	C	170/190 (90%)	166 (98%)	4 (2%)	43	58
6	E	115/126 (91%)	115 (100%)	0	100	100
7	F	85/116 (73%)	85 (100%)	0	100	100
8	I	104/107 (97%)	104 (100%)	0	100	100
9	J	86/90 (96%)	84 (98%)	2 (2%)	44	59
10	K	89/98 (91%)	88 (99%)	1 (1%)	65	76
11	L	101/103 (98%)	98 (97%)	3 (3%)	36	51
12	M	93/96 (97%)	93 (100%)	0	100	100
13	N	83/84 (99%)	82 (99%)	1 (1%)	63	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	O	76/77 (99%)	76 (100%)	0	100	100
15	P	64/65 (98%)	64 (100%)	0	100	100
16	Q	73/78 (94%)	72 (99%)	1 (1%)	59	72
17	R	57/65 (88%)	56 (98%)	1 (2%)	51	65
19	c	216/218 (99%)	215 (100%)	1 (0%)	81	87
20	d	162/163 (99%)	161 (99%)	1 (1%)	78	86
21	f	148/150 (99%)	146 (99%)	2 (1%)	59	72
22	h	31/114 (27%)	30 (97%)	1 (3%)	34	49
23	i	115/116 (99%)	115 (100%)	0	100	100
24	j	104/104 (100%)	104 (100%)	0	100	100
25	k	102/103 (99%)	101 (99%)	1 (1%)	68	77
26	l	107/107 (100%)	106 (99%)	1 (1%)	70	81
27	m	98/103 (95%)	98 (100%)	0	100	100
28	n	86/87 (99%)	86 (100%)	0	100	100
29	p	89/90 (99%)	89 (100%)	0	100	100
30	q	84/84 (100%)	81 (96%)	3 (4%)	31	45
31	r	93/93 (100%)	92 (99%)	1 (1%)	65	76
32	u	78/78 (100%)	76 (97%)	2 (3%)	40	55
33	v	61/63 (97%)	61 (100%)	0	100	100
34	w	67/68 (98%)	66 (98%)	1 (2%)	57	70
35	x	54/55 (98%)	54 (100%)	0	100	100
36	y	48/49 (98%)	48 (100%)	0	100	100
37	z	46/48 (96%)	46 (100%)	0	100	100
38	4	51/62 (82%)	51 (100%)	0	100	100
42	B	162/199 (81%)	160 (99%)	2 (1%)	63	74
43	D	168/173 (97%)	165 (98%)	3 (2%)	51	65
44	G	114/147 (78%)	112 (98%)	2 (2%)	51	65
45	H	102/105 (97%)	102 (100%)	0	100	100
46	S	67/79 (85%)	66 (98%)	1 (2%)	57	70
47	T	62/66 (94%)	62 (100%)	0	100	100
48	U	55/61 (90%)	55 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
49	e	164/165 (99%)	164 (100%)	0	100	100
50	g	107/138 (78%)	105 (98%)	2 (2%)	50	64
51	o	97/100 (97%)	97 (100%)	0	100	100
52	s	75/84 (89%)	75 (100%)	0	100	100
53	t	76/85 (89%)	76 (100%)	0	100	100
56	V	3/3 (100%)	3 (100%)	0	100	100
56	W	3/3 (100%)	3 (100%)	0	100	100
All	All	4460/4831 (92%)	4421 (99%)	39 (1%)	68	81

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	0	5	ILE
2	1	8	SER
5	C	79	LYS
5	C	93	ASP
5	C	97	VAL
5	C	111	LEU
9	J	17	LEU
9	J	80	THR
10	K	13	ARG
11	L	15	LYS
11	L	65	SER
11	L	67	ILE
13	N	100	SER
16	Q	57	ASP
17	R	12	ARG
19	c	72	ASP
20	d	32	ASN
21	f	113	ASP
21	f	152	LEU
22	h	37	VAL
25	k	80	SER
26	l	78	LEU
30	q	48	LYS
30	q	58	VAL
30	q	71	LYS
31	r	31	GLN
32	u	41	GLU
32	u	65	VAL

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Mol	Chain	Res	Type
34	w	2	SER
42	B	58	ASN
42	B	86	SER
43	D	34	ILE
43	D	36	GLN
43	D	190	ASP
44	G	25	LYS
44	G	113	ASP
46	S	11	ILE
50	g	99	LYS
50	g	102	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
4	3	13	ASN
5	C	100	GLN
5	C	140	ASN
6	E	70	ASN
6	E	73	ASN
6	E	82	GLN
7	F	46	GLN
8	I	32	GLN
10	K	38	GLN
10	K	118	HIS
11	L	112	GLN
13	N	4	GLN
13	N	35	ASN
13	N	66	GLN
14	O	35	GLN
14	O	40	GLN
15	P	9	HIS
15	P	63	GLN
15	P	79	ASN
19	c	53	HIS
19	c	197	ASN
23	i	47	HIS
23	i	86	GLN
23	i	128	ASN
23	i	136	GLN
26	l	97	GLN
28	n	29	HIS

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Mol	Chain	Res	Type
29	p	52	GLN
29	p	72	ASN
30	q	66	HIS
31	r	9	HIS
31	r	31	GLN
31	r	40	ASN
32	u	5	ASN
32	u	24	ASN
32	u	49	ASN
34	w	6	GLN
34	w	36	HIS
35	x	27	ASN
35	x	58	ASN
38	4	33	ASN
38	4	65	ASN
42	B	42	ASN
42	B	89	GLN
42	B	93	ASN
42	B	103	ASN
43	D	36	GLN
43	D	100	ASN
43	D	164	GLN
44	G	68	ASN
44	G	86	GLN
44	G	130	ASN
45	H	4	GLN
45	H	21	ASN
46	S	14	HIS
46	S	52	HIS
46	S	83	HIS
47	T	48	GLN
47	T	52	ASN
47	T	61	GLN
49	e	92	HIS
50	g	30	ASN
50	g	104	ASN
51	o	7	GLN
51	o	12	GLN
52	s	48	GLN
53	t	74	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	X	11/12 (91%)	2 (18%)	0
39	a	2742/2904 (94%)	323 (11%)	0
40	b	110/120 (91%)	7 (6%)	0
41	A	1483/1542 (96%)	218 (14%)	44 (2%)
54	Y	72/76 (94%)	18 (25%)	2 (2%)
55	Z	72/76 (94%)	15 (20%)	5 (6%)
All	All	4490/4730 (94%)	583 (12%)	51 (1%)

All (583) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
18	X	23	A
18	X	24	A
39	a	2	G
39	a	10	A
39	a	34	U
39	a	42	A
39	a	58	G
39	a	63	A
39	a	71	A
39	a	74	A
39	a	75	G
39	a	86	G
39	a	101	A
39	a	102	U
39	a	119	A
39	a	120	U
39	a	125	A
39	a	126	A
39	a	139	U
39	a	140	C
39	a	141	G
39	a	142	A
39	a	163	C
39	a	165	A
39	a	181	A
39	a	196	A
39	a	199	A
39	a	200	U
39	a	215	G
39	a	216	A
39	a	221	A
39	a	222	A

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Mol	Chain	Res	Type
39	a	248	G
39	a	265	A
39	a	272	A
39	a	278	A
39	a	282	A
39	a	285	G
39	a	289	G
39	a	310	A
39	a	311	A
39	a	329	G
39	a	330	A
39	a	361	G
39	a	362	A
39	a	386	G
39	a	404	A
39	a	405	U
39	a	411	G
39	a	412	A
39	a	420	C
39	a	425	G
39	a	451	U
39	a	456	C
39	a	481	G
39	a	491	G
39	a	503	A
39	a	504	A
39	a	505	A
39	a	509	C
39	a	530	G
39	a	531	C
39	a	532	A
39	a	533	G
39	a	543	G
39	a	544	C
39	a	545	U
39	a	546	U
39	a	547	A
39	a	549	G
39	a	563	A
39	a	573	U
39	a	575	A
39	a	586	A

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Mol	Chain	Res	Type
39	a	592	A
39	a	603	A
39	a	614	A
39	a	615	U
39	a	627	A
39	a	637	A
39	a	645	C
39	a	647	G
39	a	653	U
39	a	654	A
39	a	655	A
39	a	686	U
39	a	717	C
39	a	730	A
39	a	732	C
39	a	738	G
39	a	747	5MU
39	a	764	A
39	a	765	C
39	a	775	G
39	a	776	G
39	a	777	G
39	a	782	A
39	a	784	G
39	a	785	G
39	a	805	G
39	a	812	C
39	a	827	U
39	a	828	U
39	a	846	U
39	a	847	U
39	a	858	G
39	a	859	G
39	a	877	A
39	a	879	G
39	a	881	G
39	a	883	G
39	a	884	U
39	a	885	C
39	a	890	C
39	a	891	G
39	a	895	U

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Mol	Chain	Res	Type
39	a	896	A
39	a	897	C
39	a	898	C
39	a	905	A
39	a	910	A
39	a	914	G
39	a	927	A
39	a	931	U
39	a	934	U
39	a	946	C
39	a	961	C
39	a	974	G
39	a	983	A
39	a	984	A
39	a	985	C
39	a	996	A
39	a	1012	U
39	a	1013	C
39	a	1022	G
39	a	1025	G
39	a	1026	G
39	a	1033	U
39	a	1045	C
39	a	1047	G
39	a	1112	G
39	a	1115	G
39	a	1116	G
39	a	1122	G
39	a	1128	G
39	a	1129	A
39	a	1130	U
39	a	1132	U
39	a	1133	A
39	a	1134	A
39	a	1135	C
39	a	1136	G
39	a	1142	A
39	a	1171	G
39	a	1187	G
39	a	1253	A
39	a	1254	A
39	a	1256	G

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Mol	Chain	Res	Type
39	a	1271	G
39	a	1272	A
39	a	1273	U
39	a	1294	U
39	a	1300	G
39	a	1301	A
39	a	1338	G
39	a	1352	U
39	a	1365	A
39	a	1379	U
39	a	1383	A
39	a	1409	U
39	a	1411	U
39	a	1416	G
39	a	1419	A
39	a	1421	G
39	a	1428	C
39	a	1452	G
39	a	1453	A
39	a	1478	G
39	a	1482	G
39	a	1493	C
39	a	1509	A
39	a	1510	G
39	a	1515	A
39	a	1534	U
39	a	1535	A
39	a	1536	C
39	a	1537	G
39	a	1559	U
39	a	1569	A
39	a	1578	U
39	a	1585	C
39	a	1608	A
39	a	1609	A
39	a	1610	A
39	a	1647	U
39	a	1648	U
39	a	1674	G
39	a	1703	G
39	a	1713	A
39	a	1715	G

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Mol	Chain	Res	Type
39	a	1729	U
39	a	1730	C
39	a	1731	G
39	a	1732	C
39	a	1733	G
39	a	1738	G
39	a	1744	A
39	a	1750	G
39	a	1758	U
39	a	1764	C
39	a	1773	A
39	a	1782	U
39	a	1800	C
39	a	1801	A
39	a	1807	G
39	a	1808	A
39	a	1816	C
39	a	1829	A
39	a	1842	G
39	a	1847	A
39	a	1848	A
39	a	1855	U
39	a	1858	A
39	a	1862	G
39	a	1870	C
39	a	1871	A
39	a	1873	G
39	a	1906	G
39	a	1907	G
39	a	1929	G
39	a	1930	G
39	a	1937	A
39	a	1938	A
39	a	1955	U
39	a	1965	C
39	a	1967	C
39	a	1970	A
39	a	1971	U
39	a	1972	G
39	a	1982	U
39	a	1991	U
39	a	1993	U

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Mol	Chain	Res	Type
39	a	2023	C
39	a	2031	A
39	a	2033	A
39	a	2043	C
39	a	2055	C
39	a	2056	G
39	a	2060	A
39	a	2061	G
39	a	2069	G7M
39	a	2198	A
39	a	2204	G
39	a	2211	A
39	a	2225	A
39	a	2238	G
39	a	2239	G
39	a	2268	A
39	a	2273	A
39	a	2282	G
39	a	2283	C
39	a	2287	A
39	a	2305	U
39	a	2308	G
39	a	2312	U
39	a	2322	A
39	a	2325	G
39	a	2333	A
39	a	2335	A
39	a	2347	C
39	a	2366	A
39	a	2377	A
39	a	2383	G
39	a	2385	C
39	a	2402	U
39	a	2406	A
39	a	2423	U
39	a	2424	C
39	a	2425	A
39	a	2429	G
39	a	2430	A
39	a	2435	A
39	a	2441	U
39	a	2448	A

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Mol	Chain	Res	Type
39	a	2469	A
39	a	2470	G
39	a	2476	A
39	a	2480	C
39	a	2491	U
39	a	2502	G
39	a	2505	G
39	a	2518	A
39	a	2529	G
39	a	2547	A
39	a	2554	U
39	a	2566	A
39	a	2567	G
39	a	2573	C
39	a	2602	A
39	a	2603	G
39	a	2609	U
39	a	2613	U
39	a	2629	U
39	a	2663	G
39	a	2671	G
39	a	2689	U
39	a	2690	U
39	a	2714	G
39	a	2724	U
39	a	2726	A
39	a	2744	G
39	a	2748	A
39	a	2757	A
39	a	2765	A
39	a	2778	A
39	a	2790	U
39	a	2791	G
39	a	2820	A
39	a	2821	A
39	a	2861	U
39	a	2867	G
39	a	2868	A
39	a	2880	C
39	a	2884	U
39	a	2899	A
40	b	25	U

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Mol	Chain	Res	Type
40	b	45	A
40	b	56	G
40	b	64	G
40	b	99	A
40	b	105	G
40	b	109	A
41	A	9	G
41	A	13	U
41	A	14	U
41	A	22	G
41	A	31	G
41	A	32	A
41	A	39	G
41	A	44	A
41	A	47	C
41	A	48	C
41	A	51	A
41	A	71	A
41	A	74	A
41	A	94	G
41	A	95	C
41	A	119	A
41	A	120	A
41	A	121	U
41	A	122	G
41	A	131	A
41	A	141	G
41	A	143	A
41	A	144	G
41	A	163	C
41	A	164	G
41	A	166	U
41	A	181	A
41	A	182	A
41	A	183	C
41	A	197	A
41	A	202	G
41	A	204	G
41	A	226	G
41	A	240	G
41	A	245	U
41	A	247	G

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Mol	Chain	Res	Type
41	A	251	G
41	A	262	A
41	A	266	G
41	A	267	C
41	A	280	C
41	A	289	G
41	A	306	A
41	A	321	A
41	A	328	C
41	A	329	A
41	A	345	C
41	A	347	G
41	A	348	G
41	A	352	C
41	A	354	G
41	A	355	C
41	A	367	U
41	A	372	C
41	A	373	A
41	A	376	G
41	A	384	G
41	A	388	G
41	A	392	C
41	A	406	G
41	A	411	A
41	A	412	A
41	A	413	G
41	A	414	A
41	A	417	G
41	A	421	U
41	A	422	C
41	A	424	G
41	A	429	U
41	A	430	A
41	A	438	U
41	A	439	U
41	A	446	G
41	A	453	G
41	A	457	G
41	A	458	U
41	A	463	U
41	A	465	A

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Mol	Chain	Res	Type
41	A	467	U
41	A	468	A
41	A	469	C
41	A	478	A
41	A	479	U
41	A	481	G
41	A	484	G
41	A	486	U
41	A	500	G
41	A	511	C
41	A	518	C
41	A	524	G
41	A	528	C
41	A	530	G
41	A	531	U
41	A	533	A
41	A	536	C
41	A	547	A
41	A	559	A
41	A	572	A
41	A	573	A
41	A	576	C
41	A	577	G
41	A	579	A
41	A	628	G
41	A	633	G
41	A	650	G
41	A	651	C
41	A	653	U
41	A	661	G
41	A	665	A
41	A	723	U
41	A	724	G
41	A	746	A
41	A	748	G
41	A	755	G
41	A	777	A
41	A	793	U
41	A	794	A
41	A	815	A
41	A	817	C
41	A	821	G

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Mol	Chain	Res	Type
41	A	832	G
41	A	849	G
41	A	851	G
41	A	887	G
41	A	890	G
41	A	914	A
41	A	926	G
41	A	934	C
41	A	935	A
41	A	936	C
41	A	960	U
41	A	965	U
41	A	966	2MG
41	A	969	A
41	A	975	A
41	A	976	G
41	A	977	A
41	A	991	U
41	A	992	U
41	A	993	G
41	A	994	A
41	A	996	A
41	A	1004	A
41	A	1009	U
41	A	1036	A
41	A	1039	G
41	A	1042	A
41	A	1043	G
41	A	1044	A
41	A	1045	C
41	A	1046	A
41	A	1053	G
41	A	1065	U
41	A	1085	U
41	A	1094	G
41	A	1095	U
41	A	1099	G
41	A	1101	A
41	A	1125	U
41	A	1126	U
41	A	1132	C
41	A	1137	C

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Mol	Chain	Res	Type
41	A	1139	G
41	A	1140	C
41	A	1159	U
41	A	1171	A
41	A	1184	G
41	A	1196	A
41	A	1197	A
41	A	1213	A
41	A	1220	G
41	A	1225	A
41	A	1226	C
41	A	1227	A
41	A	1228	C
41	A	1238	A
41	A	1250	A
41	A	1257	A
41	A	1275	A
41	A	1280	A
41	A	1286	U
41	A	1287	A
41	A	1300	G
41	A	1302	C
41	A	1317	C
41	A	1319	A
41	A	1320	C
41	A	1337	G
41	A	1338	G
41	A	1346	A
41	A	1353	G
41	A	1363	A
41	A	1364	U
41	A	1368	A
41	A	1370	G
41	A	1378	C
41	A	1379	G
41	A	1381	U
41	A	1397	C
41	A	1419	G
41	A	1441	A
41	A	1446	A
41	A	1447	A
41	A	1448	C

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Mol	Chain	Res	Type
41	A	1451	U
41	A	1452	C
41	A	1453	G
41	A	1487	G
41	A	1492	A
41	A	1497	G
41	A	1503	A
41	A	1505	G
41	A	1506	U
41	A	1517	G
41	A	1529	G
41	A	1530	G
41	A	1533	C
41	A	1534	A
54	Y	5	G
54	Y	10	G
54	Y	14	A
54	Y	19	G
54	Y	20	U
54	Y	21	A
54	Y	22	G
54	Y	24	G
54	Y	43	C
54	Y	45	U
54	Y	46	G
54	Y	47	U
54	Y	48	C
54	Y	49	C
54	Y	69	G
54	Y	71	G
54	Y	73	A
54	Y	74	C
55	Z	6	A
55	Z	7	U
55	Z	9	A
55	Z	10	G
55	Z	19	G
55	Z	21	A
55	Z	42	G
55	Z	46	G
55	Z	47	U
55	Z	48	C

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Mol	Chain	Res	Type
55	Z	49	G
55	Z	51	C
55	Z	58	A
55	Z	68	C
55	Z	76	A

All (51) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
41	A	7	A
41	A	13	U
41	A	30	U
41	A	62	U
41	A	70	U
41	A	94	G
41	A	119	A
41	A	121	U
41	A	181	A
41	A	196	A
41	A	199	A
41	A	251	G
41	A	280	C
41	A	327	A
41	A	329	A
41	A	429	U
41	A	438	U
41	A	530	G
41	A	532	A
41	A	547	A
41	A	559	A
41	A	641	U
41	A	653	U
41	A	776	G
41	A	793	U
41	A	858	G
41	A	991	U
41	A	992	U
41	A	993	G
41	A	1035	A
41	A	1042	A
41	A	1045	C
41	A	1124	G

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Mol	Chain	Res	Type
41	A	1125	U
41	A	1139	G
41	A	1183	U
41	A	1225	A
41	A	1300	G
41	A	1319	A
41	A	1337	G
41	A	1446	A
41	A	1447	A
41	A	1451	U
41	A	1505	G
54	Y	13	C
54	Y	20	U
55	Z	6	A
55	Z	7	U
55	Z	9	A
55	Z	46	G
55	Z	48	C

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

52 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	$\# Z > 2$
41	2MG	A	1207	41	23,26,27	0.42	0	32,38,41	0.55	0
41	MA6	A	1519	41	23,26,27	0.40	0	34,38,41	0.80	2 (5%)
39	OMC	a	2498	58,39	19,22,23	0.50	0	26,31,34	0.50	0
39	6MZ	a	1618	39	22,25,26	0.50	0	30,36,39	0.68	0
39	2MG	a	1835	39	23,26,27	0.41	0	32,38,41	0.47	0
39	PSU	a	2580	58,39	18,21,22	0.64	0	22,30,33	1.02	1 (4%)
41	5MC	A	967	41	18,22,23	0.41	0	26,32,35	0.67	0
39	PSU	a	746	58,39	18,21,22	0.96	1 (5%)	22,30,33	0.71	0
39	2MA	a	2503	58,39	22,25,26	0.55	0	33,37,40	0.73	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	PSU	A	516	58,41	18,21,22	0.83	1 (5%)	22,30,33	0.71	0
39	PSU	a	2604	39	18,21,22	0.91	2 (11%)	22,30,33	0.85	1 (4%)
39	3TD	a	1915	39	18,22,23	0.84	1 (5%)	22,32,35	0.76	0
41	MA6	A	1518	41	23,26,27	0.33	0	34,38,41	0.74	1 (2%)
39	PSU	a	2504	39	18,21,22	1.09	1 (5%)	22,30,33	0.93	1 (4%)
26	MS6	l	82	26	5,7,8	0.44	0	2,7,9	0.40	0
41	5MC	A	1407	41	18,22,23	0.44	0	26,32,35	0.65	0
39	PSU	a	2457	39	18,21,22	0.96	1 (5%)	22,30,33	0.70	0
41	2MG	A	1516	41	23,26,27	0.44	0	32,38,41	0.47	0
39	2MG	a	2445	39	23,26,27	0.63	0	32,38,41	0.41	0
41	4OC	A	1402	41	20,23,24	0.32	0	26,32,35	0.57	0
10	IAS	K	119	10	6,7,8	0.94	0	6,8,10	0.90	0
20	MEQ	d	150	20	8,9,10	0.59	0	5,10,12	0.48	0
39	5MU	a	1939	39	19,22,23	0.55	0	28,32,35	0.41	0
39	5MU	a	747	39	19,22,23	0.55	0	28,32,35	0.63	1 (3%)
41	2MG	A	966	41	23,26,27	0.44	0	32,38,41	0.37	0
26	4D4	l	81	26	9,11,12	0.81	0	8,13,15	0.78	0
39	H2U	a	2449	39	18,21,22	0.88	1 (5%)	21,30,33	1.04	1 (4%)
39	G7M	a	2069	39	23,26,27	0.79	2 (8%)	35,39,42	0.69	0
39	OMG	a	2251	39,55	23,26,27	0.40	0	33,38,41	0.48	0
39	PSU	a	1917	39	18,21,22	0.85	1 (5%)	22,30,33	0.75	0
39	PSU	a	1911	39	18,21,22	0.84	1 (5%)	22,30,33	0.77	0
41	UR3	A	1498	41	19,22,23	0.53	0	26,32,35	0.71	0
39	6MZ	a	2030	39	22,25,26	0.85	1 (4%)	30,36,39	0.78	0
39	PSU	a	955	39	18,21,22	0.90	1 (5%)	22,30,33	0.73	0
39	1MG	a	745	39	22,26,27	0.73	0	33,39,42	0.54	0
41	G7M	A	527	41	23,26,27	0.79	1 (4%)	35,39,42	0.73	0
39	OMU	a	2552	39	19,22,23	0.50	0	26,31,34	0.50	0
56	ORD	V	2	56	6,7,8	1.77	2 (33%)	2,7,9	0.82	0
39	PSU	a	2605	39	18,21,22	0.86	1 (5%)	22,30,33	0.85	1 (4%)
56	ORD	W	2	56	6,7,8	1.34	1 (16%)	2,7,9	0.91	0
39	5MC	a	1962	39	18,22,23	0.55	0	26,32,35	0.69	1 (3%)
11	D2T	L	89	11	7,9,10	1.05	0	6,11,13	1.45	1 (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
41	2MG	A	1207	41	-	0/9/27/28	0/3/3/3
41	MA6	A	1519	41	-	3/11/29/30	0/3/3/3
39	OMC	a	2498	58,39	-	0/9/27/28	0/2/2/2
39	6MZ	a	1618	39	-	0/9/27/28	0/3/3/3
39	2MG	a	1835	39	-	0/9/27/28	0/3/3/3
39	PSU	a	2580	58,39	-	0/7/25/26	0/2/2/2
41	5MC	A	967	41	-	0/7/25/26	0/2/2/2
39	PSU	a	746	58,39	-	1/7/25/26	0/2/2/2
39	2MA	a	2503	58,39	-	3/7/25/26	0/3/3/3
41	PSU	A	516	58,41	-	0/7/25/26	0/2/2/2
39	PSU	a	2604	39	-	0/7/25/26	0/2/2/2
39	3TD	a	1915	39	-	0/7/25/26	0/2/2/2
41	MA6	A	1518	41	-	0/11/29/30	0/3/3/3
39	PSU	a	2504	39	-	0/7/25/26	0/2/2/2
26	MS6	l	82	26	-	0/4/6/8	-
41	5MC	A	1407	41	-	0/7/25/26	0/2/2/2
39	PSU	a	2457	39	-	0/7/25/26	0/2/2/2
41	2MG	A	1516	41	-	0/9/27/28	0/3/3/3
39	2MG	a	2445	39	-	1/9/27/28	0/3/3/3
41	4OC	A	1402	41	-	0/9/29/30	0/2/2/2
10	IAS	K	119	10	-	0/7/7/8	-
20	MEQ	d	150	20	-	3/8/9/11	-
39	5MU	a	1939	39	-	0/7/25/26	0/2/2/2
39	5MU	a	747	39	-	0/7/25/26	0/2/2/2
41	2MG	A	966	41	-	0/9/27/28	0/3/3/3
26	4D4	l	81	26	-	2/11/12/14	-
39	H2U	a	2449	39	-	0/7/38/39	0/2/2/2
39	G7M	a	2069	39	-	2/7/25/26	0/3/3/3
39	OMG	a	2251	39,55	-	0/9/27/28	0/3/3/3
39	PSU	a	1917	39	-	0/7/25/26	0/2/2/2
39	PSU	a	1911	39	-	0/7/25/26	0/2/2/2
41	UR3	A	1498	41	-	0/7/25/26	0/2/2/2
39	6MZ	a	2030	39	-	2/9/27/28	0/3/3/3
39	PSU	a	955	39	-	0/7/25/26	0/2/2/2
39	1MG	a	745	39	-	0/7/25/26	0/3/3/3
41	G7M	A	527	41	-	1/7/25/26	0/3/3/3
39	OMU	a	2552	39	-	0/9/27/28	0/2/2/2
56	ORD	V	2	56	-	0/5/6/8	-
39	PSU	a	2605	39	-	0/7/25/26	0/2/2/2
56	ORD	W	2	56	-	2/5/6/8	-
39	5MC	a	1962	39	-	0/7/25/26	0/2/2/2
11	D2T	L	89	11	-	1/7/12/14	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	V	2	ORD	CB-CA	-3.65	1.48	1.53
39	a	1915	3TD	C6-C5	3.23	1.39	1.35
39	a	2457	PSU	C6-C5	3.14	1.39	1.35
41	A	516	PSU	C6-C5	3.13	1.39	1.35
41	A	527	G7M	C8-N7	3.09	1.38	1.33
39	a	1917	PSU	C6-C5	3.00	1.38	1.35
39	a	1911	PSU	C6-C5	2.87	1.38	1.35
39	a	2604	PSU	C6-C5	2.79	1.38	1.35
39	a	2449	H2U	C2-N3	-2.75	1.33	1.38
39	a	2504	PSU	C6-C5	2.71	1.38	1.35
39	a	746	PSU	C6-C5	2.62	1.38	1.35
56	W	2	ORD	O-C	2.56	1.30	1.19
39	a	2030	6MZ	C8-N9	-2.55	1.32	1.37
39	a	2605	PSU	C6-C5	2.45	1.38	1.35
39	a	2069	G7M	C8-N7	2.28	1.37	1.33
39	a	955	PSU	C6-C5	2.17	1.37	1.35
39	a	2069	G7M	C5-C6	-2.09	1.36	1.43
39	a	2604	PSU	C4-C5	-2.06	1.38	1.44
56	V	2	ORD	O-C	2.05	1.28	1.19

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	A	1518	MA6	C2-N1-C6	3.12	119.12	111.75
41	A	1519	MA6	C2-N1-C6	2.98	118.78	111.75
39	a	2580	PSU	C3'-C2'-C1'	2.91	105.02	101.64
39	a	2449	H2U	N3-C2-N1	2.85	119.67	116.65
39	a	747	5MU	O3'-C3'-C4'	-2.47	103.91	111.05
41	A	1519	MA6	C2'-C3'-C4'	-2.28	98.22	102.64
11	L	89	D2T	OD1-CG-CB	-2.25	117.73	122.44
39	a	1962	5MC	C5-C6-N1	-2.24	121.03	123.34
39	a	2503	2MA	C5-C4-N3	-2.18	124.74	127.19
39	a	2604	PSU	C2'-C3'-C4'	-2.11	98.55	102.64
39	a	2504	PSU	C5-C6-N1	-2.10	118.96	122.11
39	a	2605	PSU	C2'-C3'-C4'	-2.01	98.74	102.64

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
20	d	150	MEQ	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
39	a	2030	6MZ	O4'-C4'-C5'-O5'
56	W	2	ORD	O-C-CA-CB
39	a	2030	6MZ	C3'-C4'-C5'-O5'
41	A	1519	MA6	O4'-C4'-C5'-O5'
20	d	150	MEQ	OE1-CD-CG-CB
20	d	150	MEQ	NE2-CD-CG-CB
41	A	1519	MA6	C3'-C4'-C5'-O5'
26	l	81	4D4	OB-CB-CG-CD
39	a	2503	2MA	O4'-C4'-C5'-O5'
41	A	1519	MA6	C4'-C5'-O5'-P
39	a	2069	G7M	O4'-C4'-C5'-O5'
11	L	89	D2T	CG-CB-SB-CB1
39	a	746	PSU	O4'-C1'-C5-C6
41	A	527	G7M	C4'-C5'-O5'-P
39	a	2069	G7M	C4'-C5'-O5'-P
39	a	2445	2MG	C3'-C4'-C5'-O5'
39	a	2503	2MA	O4'-C1'-N9-C8
26	l	81	4D4	O-C-CA-CB
39	a	2503	2MA	C4'-C5'-O5'-P
56	W	2	ORD	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	d	150	MEQ	1	0
39	a	2030	6MZ	2	0
39	a	2552	OMU	2	0
11	L	89	D2T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 316 ligands modelled in this entry, 313 are monoatomic - leaving 3 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
60	PAR	A	1601	-	45,45,45	0.40	0	64,67,67	0.56	0
61	SPD	A	1696	-	9,9,9	0.17	0	8,8,8	0.19	0
61	SPD	A	1695	-	9,9,9	0.15	0	8,8,8	0.18	0

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
60	PAR	A	1601	-	-	5/18/94/94	0/4/4/4
61	SPD	A	1696	-	-	2/7/7/7	-
61	SPD	A	1695	-	-	2/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
60	A	1601	PAR	C44-C54-C64-N64
60	A	1601	PAR	O54-C54-C64-N64
60	A	1601	PAR	C41-C51-C61-O61
60	A	1601	PAR	O51-C51-C61-O61
61	A	1695	SPD	C3-C4-C5-N6
61	A	1696	SPD	C2-C3-C4-C5
60	A	1601	PAR	C52-C42-O11-C11
61	A	1696	SPD	N6-C7-C8-C9
61	A	1695	SPD	C4-C5-N6-C7

There are no ring outliers.

3 monomers are involved in 8 short contacts:

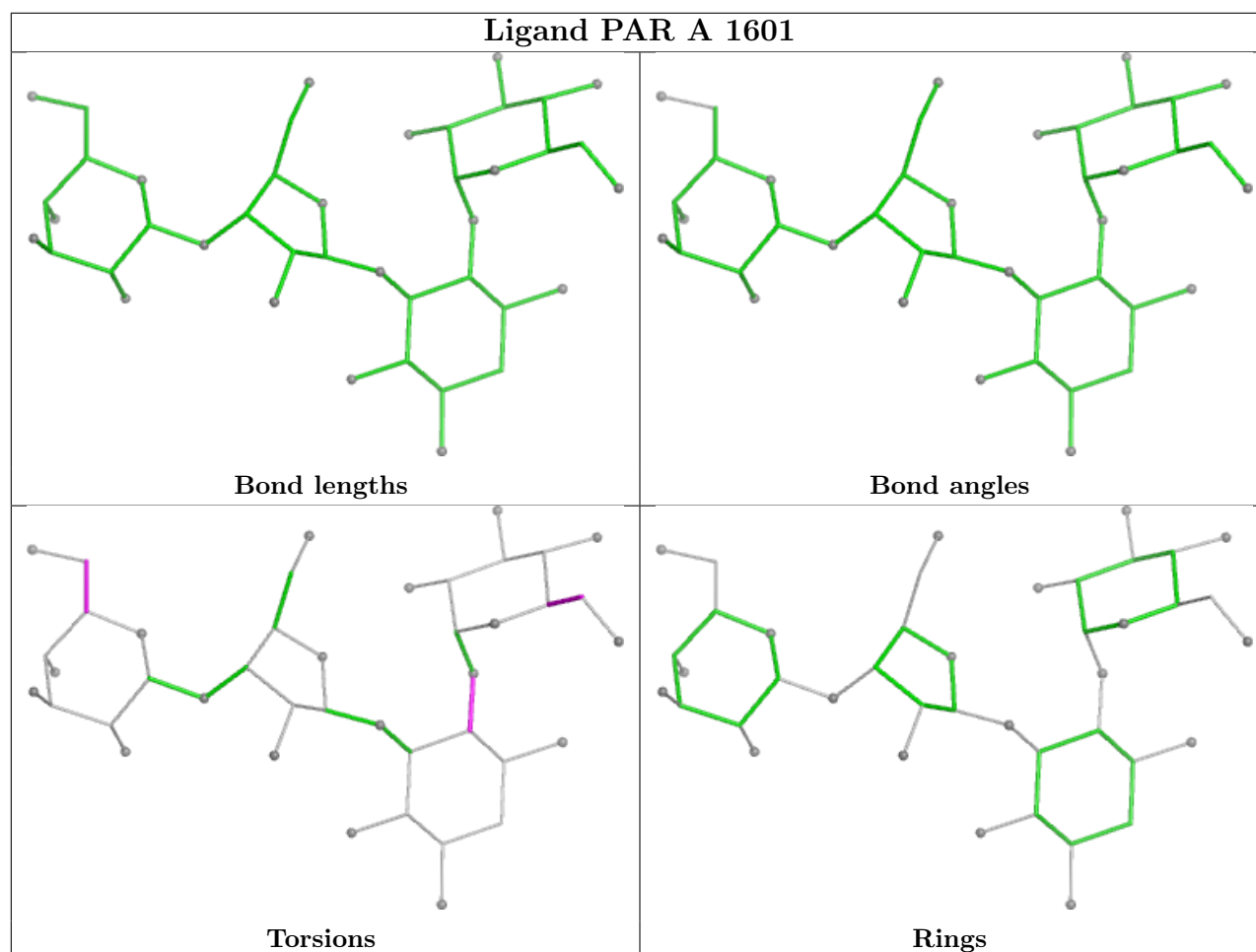
Mol	Chain	Res	Type	Clashes	Symm-Clashes
60	A	1601	PAR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
61	A	1696	SPD	1	0
61	A	1695	SPD	3	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
26	1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	77:PRO	C	78:LEU	N	2.15

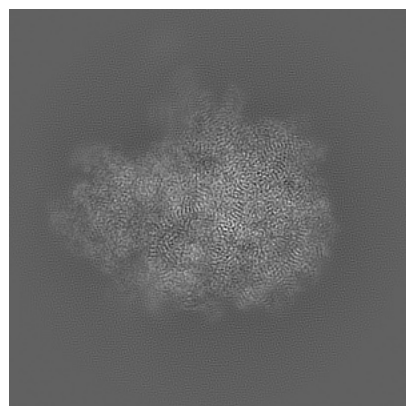
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54009. These allow visual inspection of the internal detail of the map and identification of artifacts.

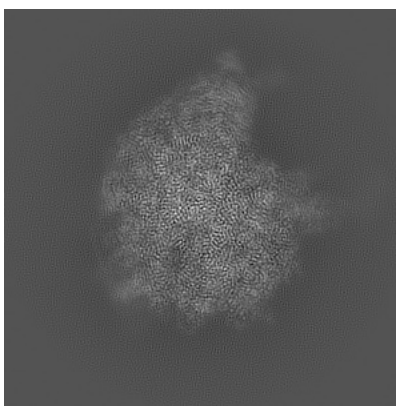
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

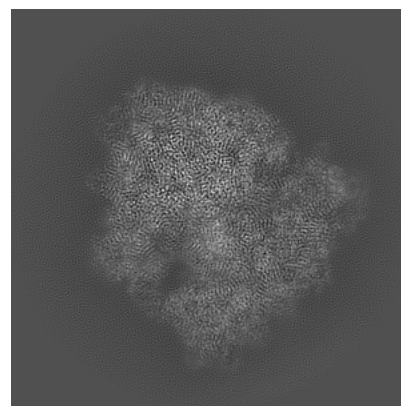
6.1.1 Primary map



X

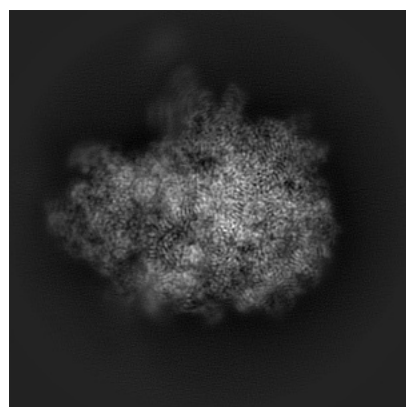


Y

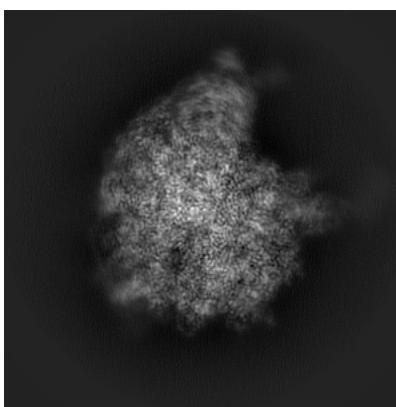


Z

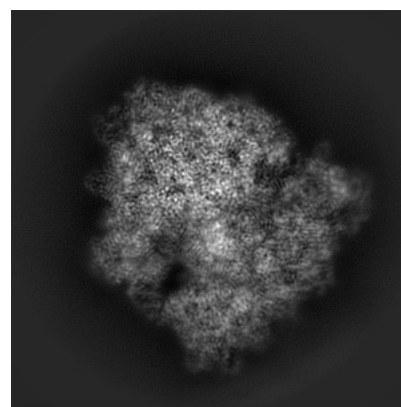
6.1.2 Raw map



X



Y

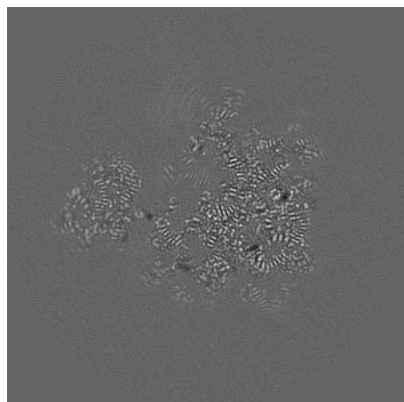


Z

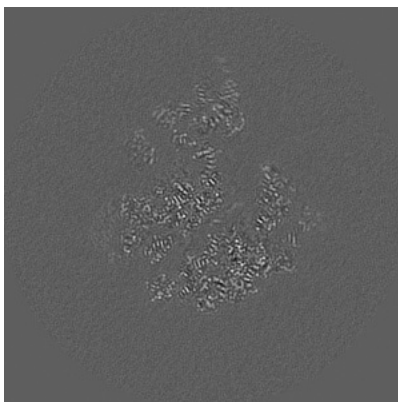
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

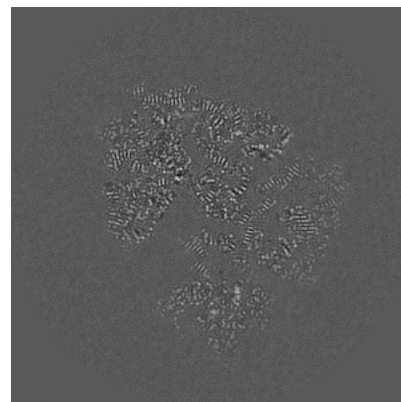
6.2.1 Primary map



X Index: 216

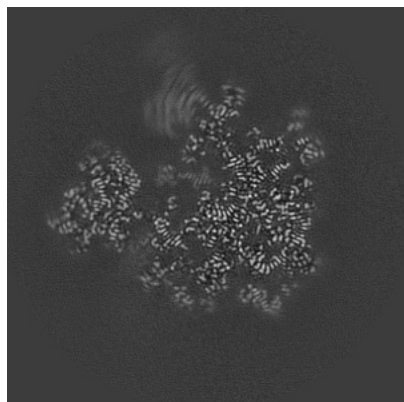


Y Index: 216

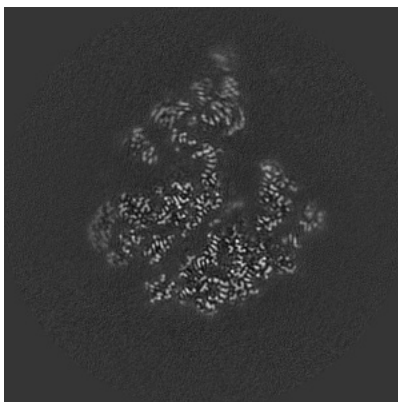


Z Index: 216

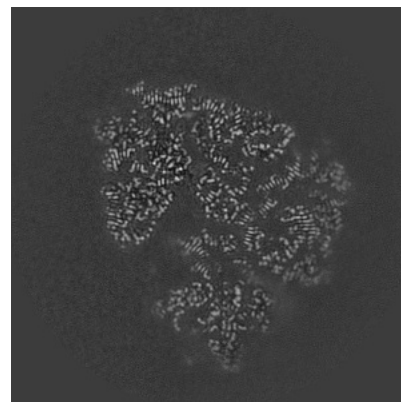
6.2.2 Raw map



X Index: 216



Y Index: 216

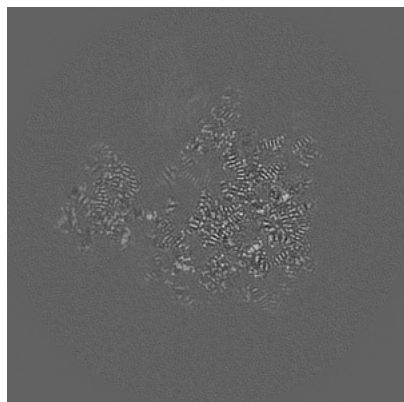


Z Index: 216

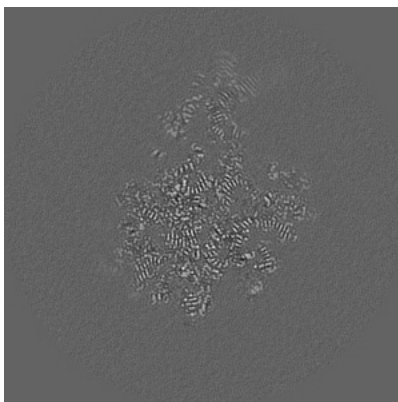
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

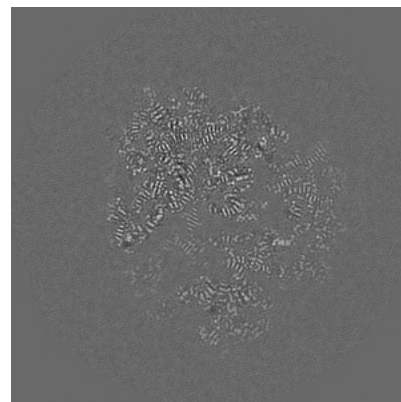
6.3.1 Primary map



X Index: 218

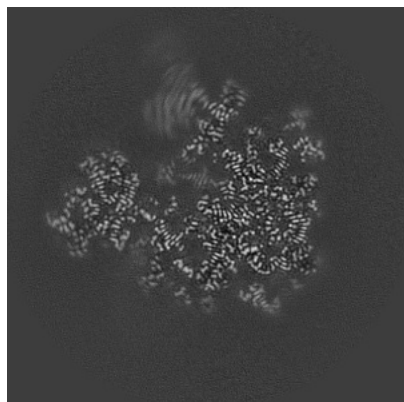


Y Index: 231

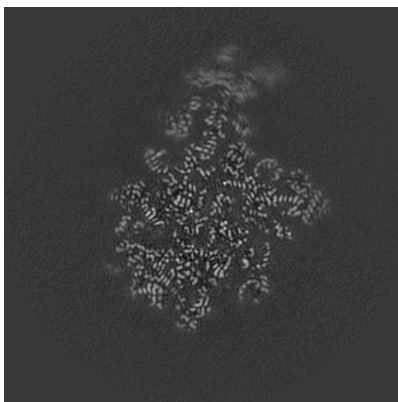


Z Index: 226

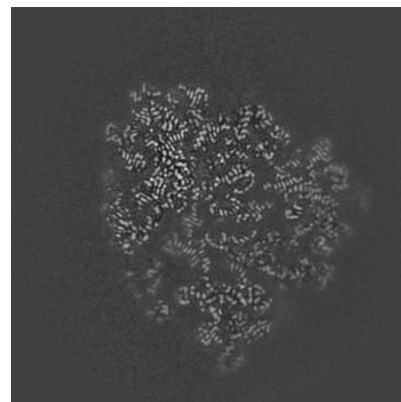
6.3.2 Raw map



X Index: 214



Y Index: 237

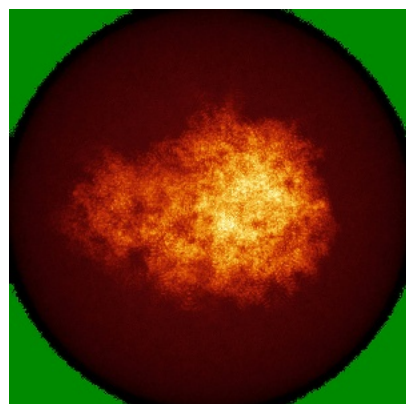


Z Index: 224

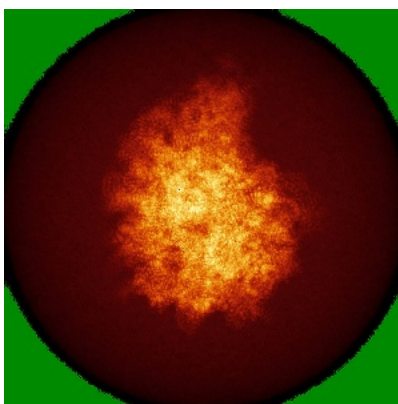
The images above show the largest variance slices of the map in three orthogonal directions.

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

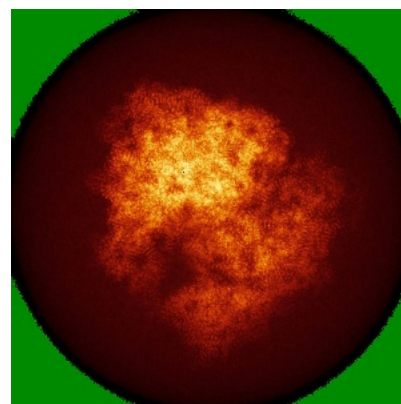
6.4.1 Primary map



X

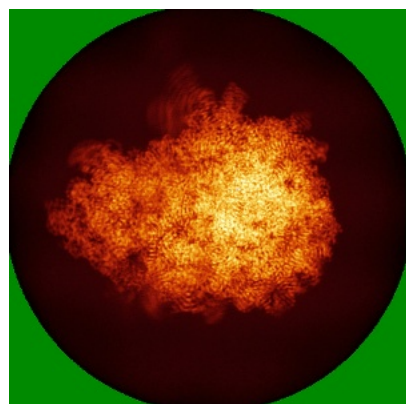


Y

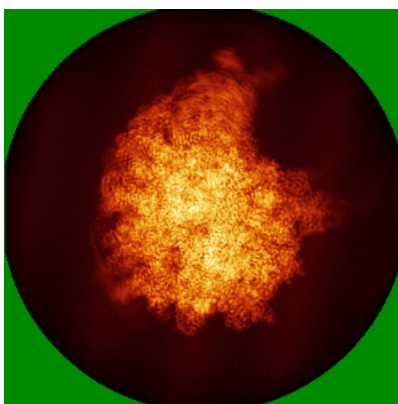


Z

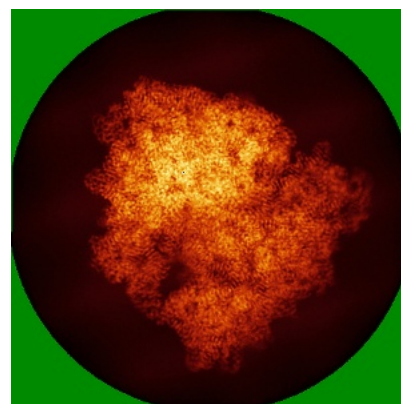
6.4.2 Raw map



X



Y

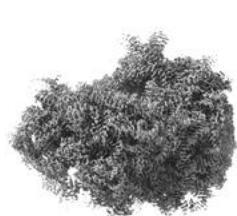


Z

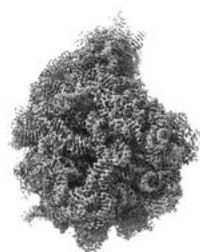
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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 0.0256. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

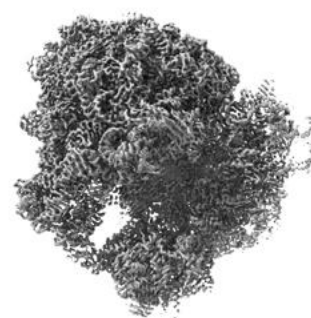
6.5.2 Raw map



X



Y



Z

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

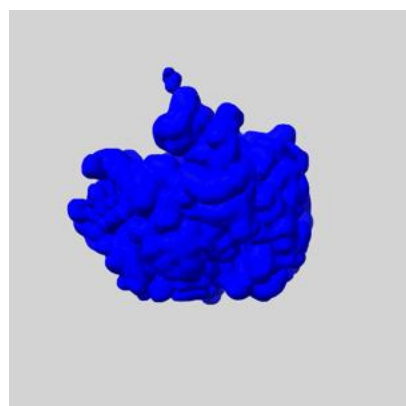
6.6 Mask visualisation [i](#)

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

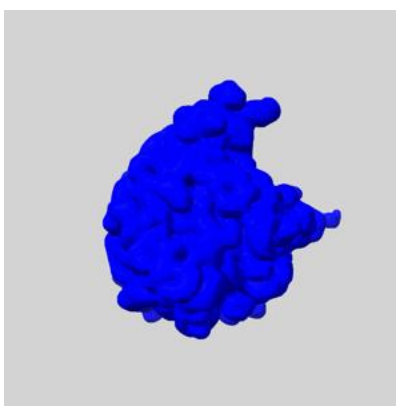
A mask typically either:

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

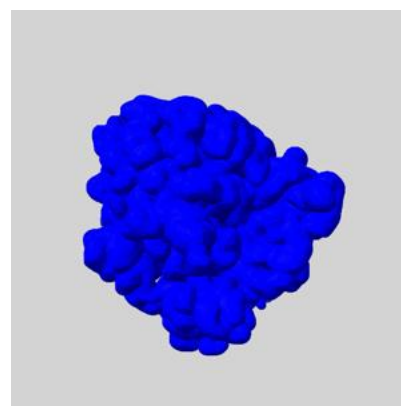
6.6.1 emd_54009_msk_1.map [i](#)



X



Y

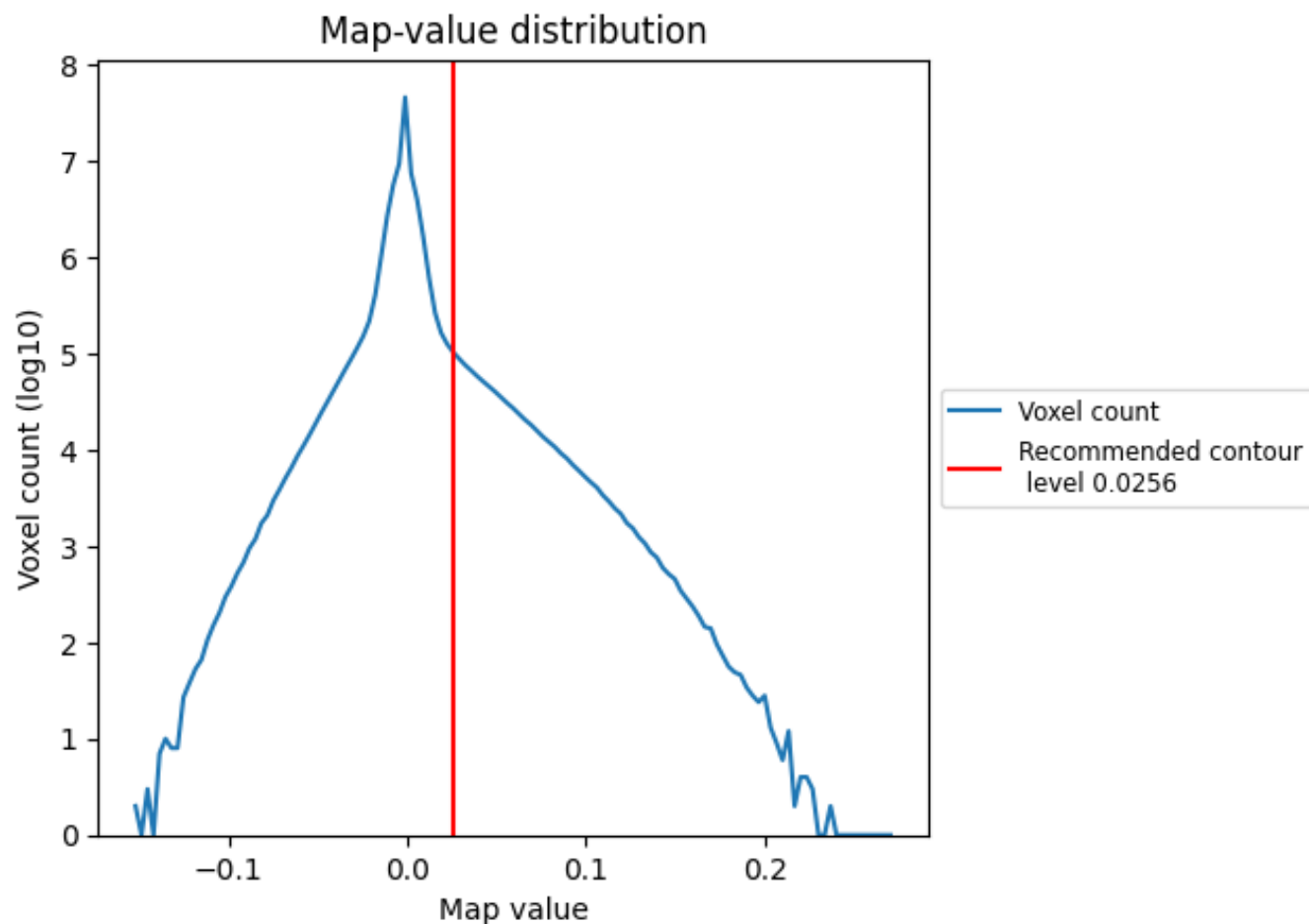


Z

7 Map analysis [i](#)

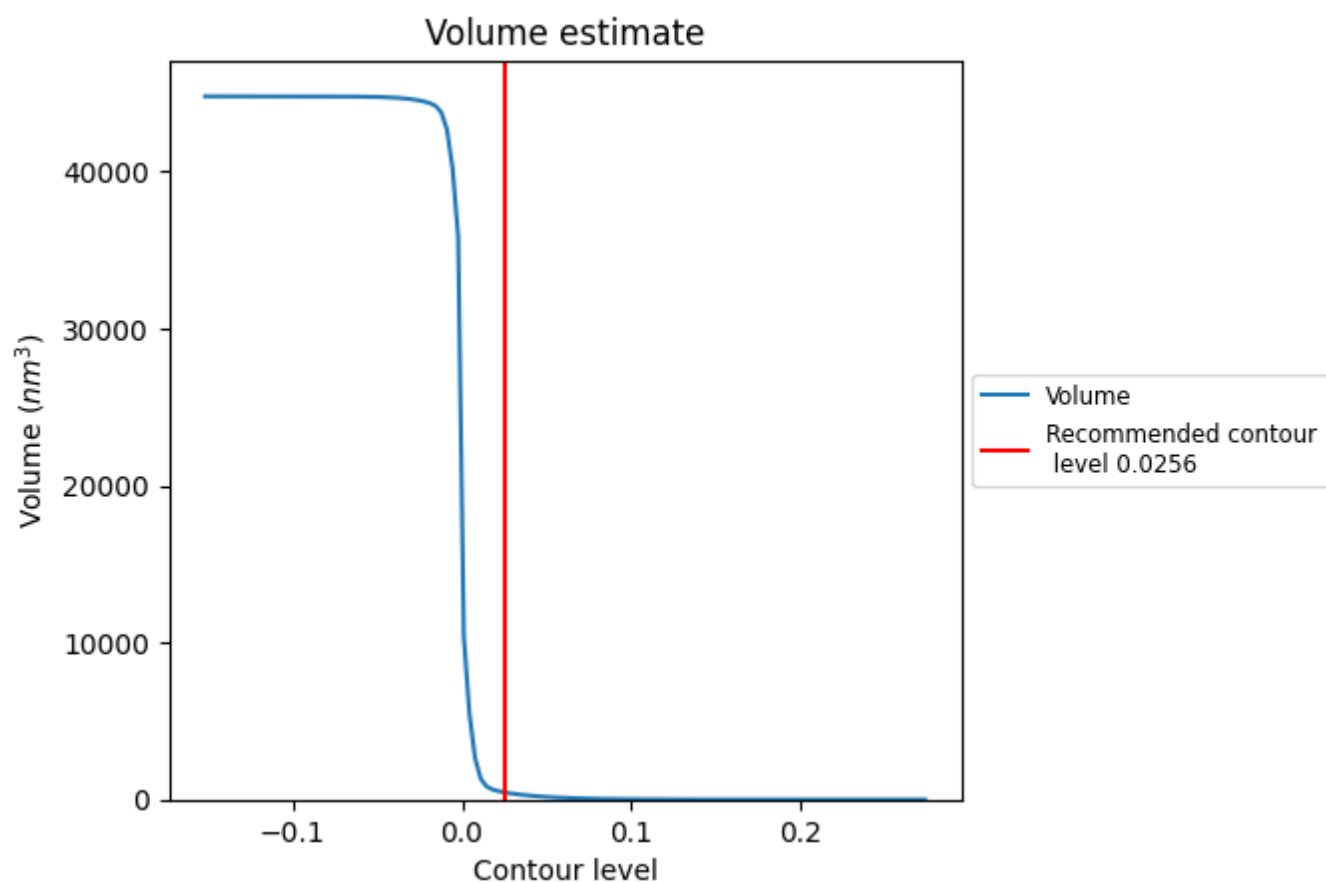
This section contains the results of statistical analysis of the map.

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.

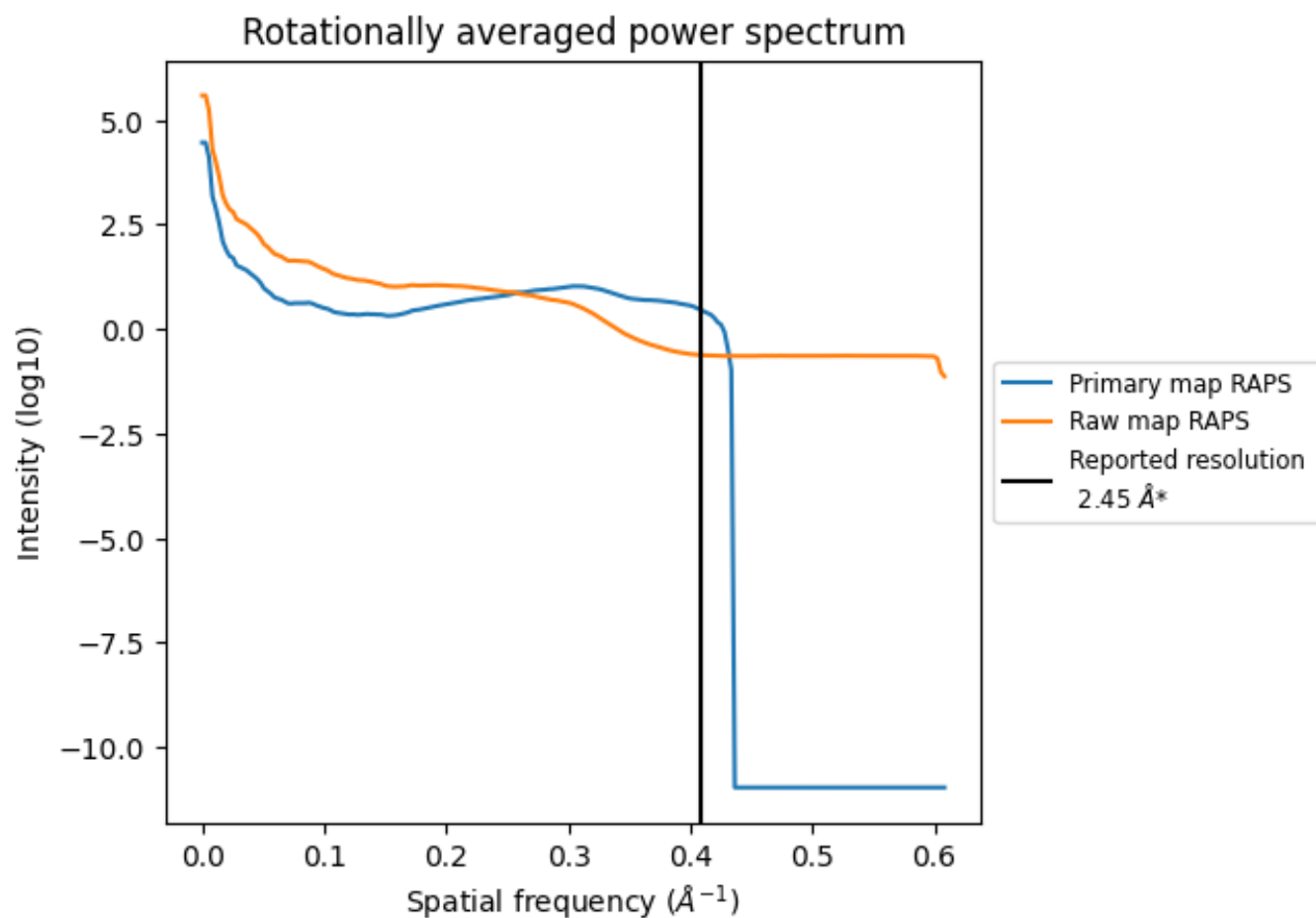
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 449 nm³; this corresponds to an approximate mass of 406 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 ⓘ

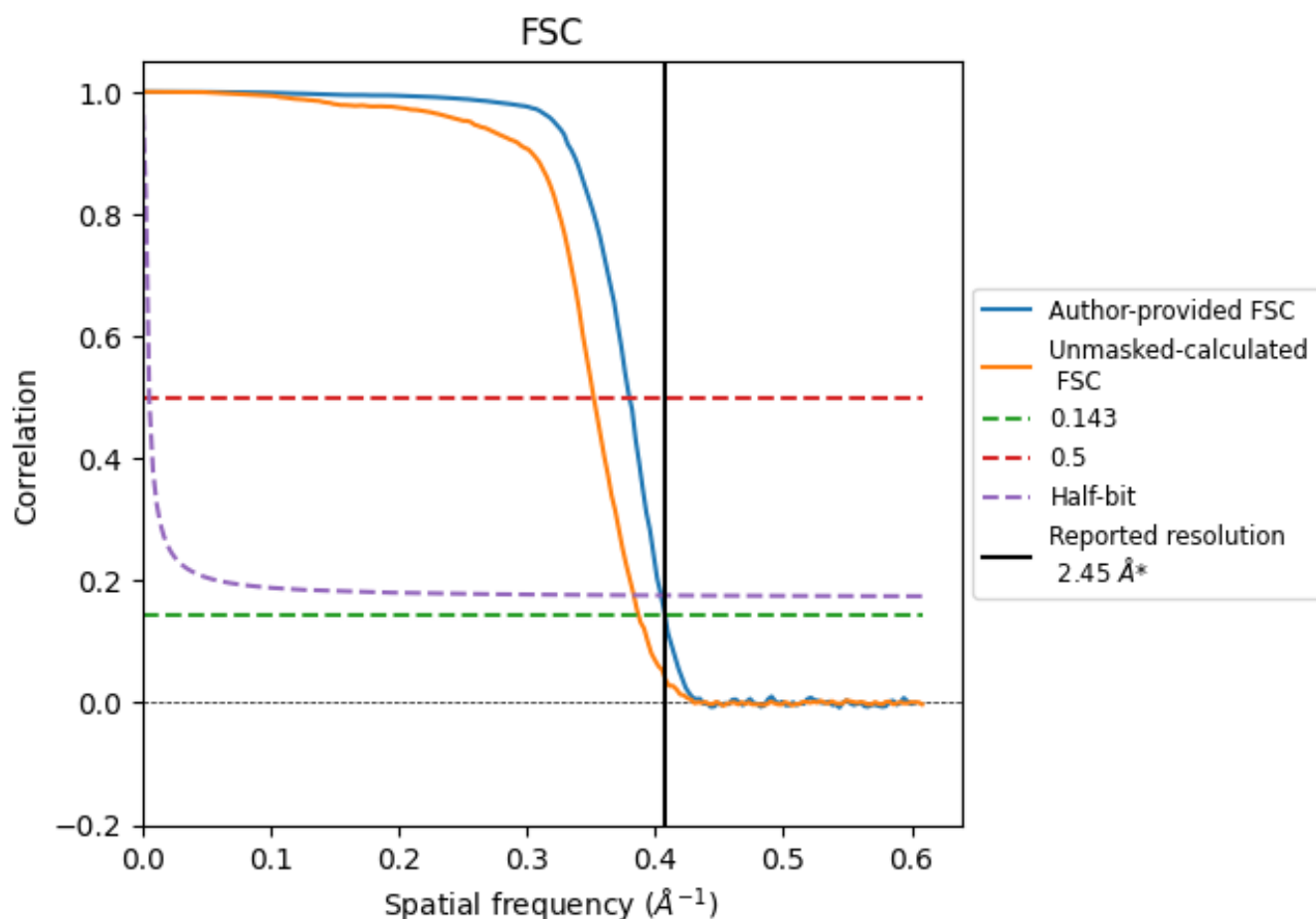


*Reported resolution corresponds to spatial frequency of 0.408 Å⁻¹

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 0.408 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

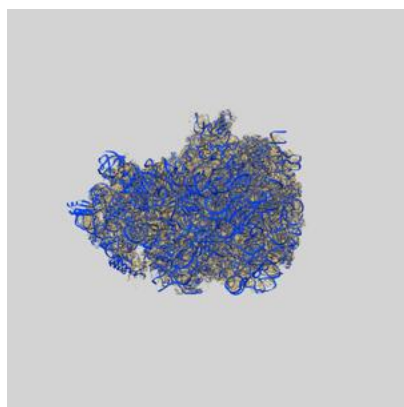
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.45	-	-
Author-provided FSC curve	2.45	2.63	2.47
Unmasked-calculated*	2.58	2.84	2.61

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

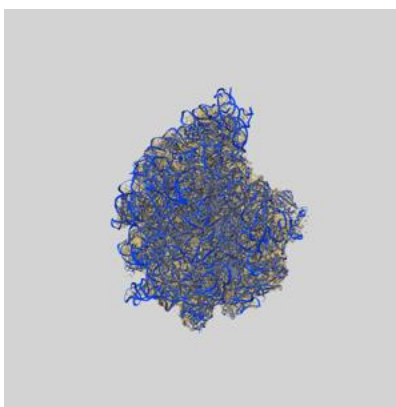
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54009 and PDB model 9RJA. Per-residue inclusion information can be found in section [3](#) on page [17](#).

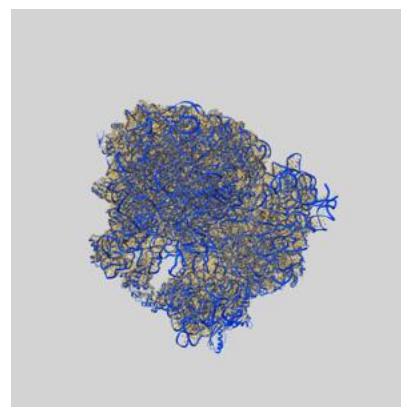
9.1 Map-model overlay [i](#)



X



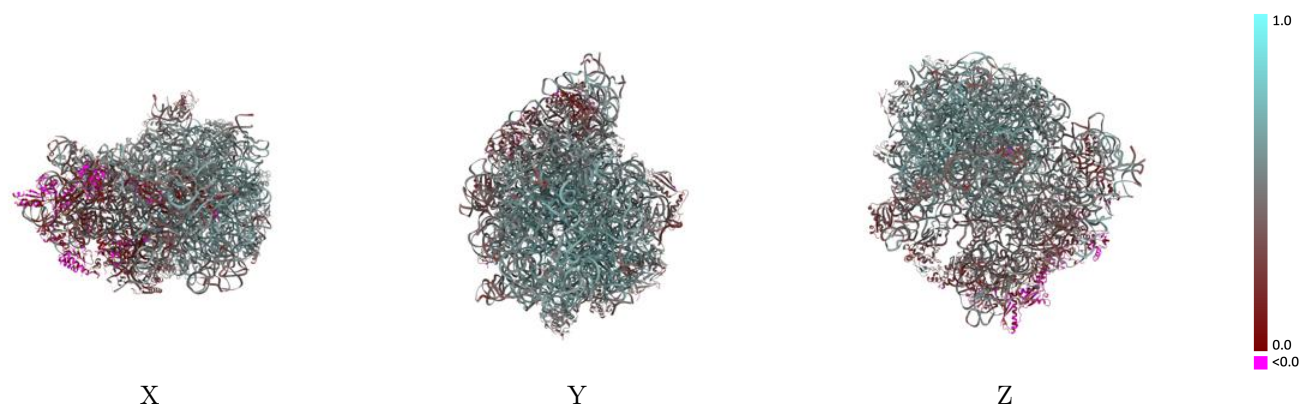
Y



Z

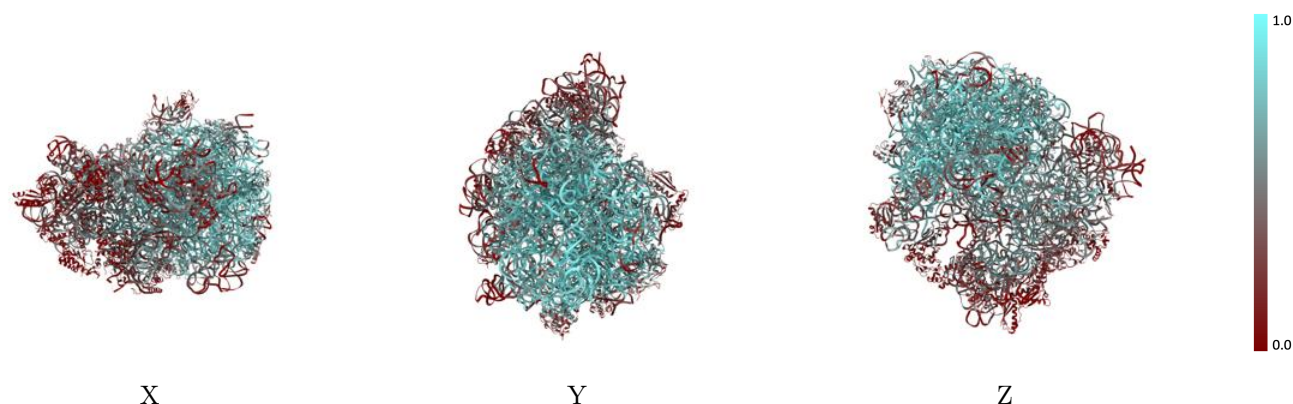
The images above show the 3D surface view of the map at the recommended contour level 0.0256 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



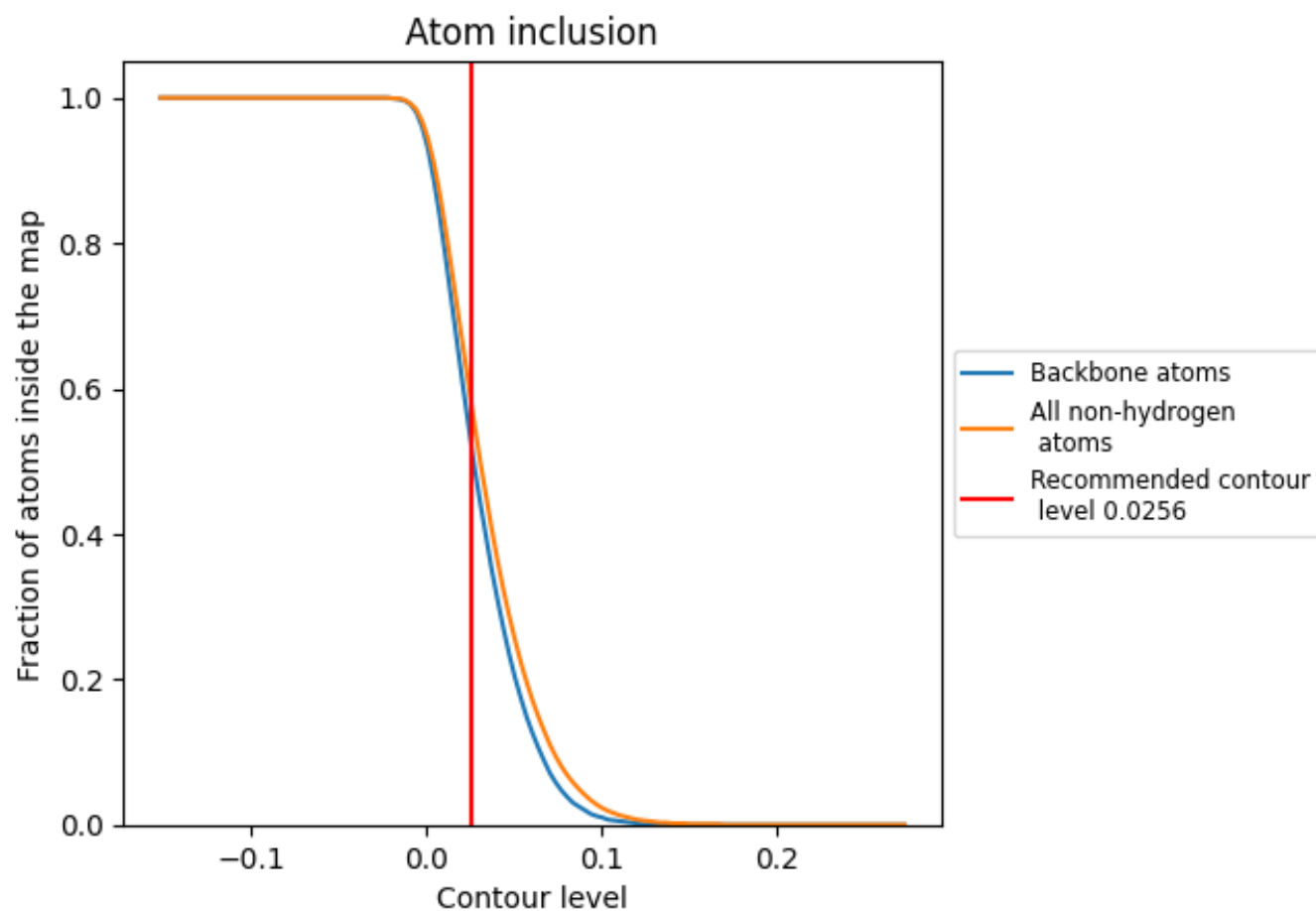
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0256).

9.4 Atom inclusion [i](#)



At the recommended contour level, 52% of all backbone atoms, 58% 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 (0.0256) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5830	 0.4840
0	 0.5600	 0.5460
1	 0.9240	 0.6660
2	 0.8960	 0.6450
3	 0.6380	 0.5090
4	 0.1740	 0.4800
A	 0.4990	 0.4330
B	 0.0890	 0.0930
C	 0.1370	 0.1010
D	 0.0960	 0.1210
E	 0.2420	 0.2170
F	 0.1780	 0.3080
G	 0.1630	 0.3090
H	 0.1760	 0.1660
I	 0.1410	 0.1780
J	 0.1020	 0.1020
K	 0.2980	 0.3940
L	 0.4140	 0.4180
M	 0.1920	 0.2990
N	 0.3000	 0.4020
O	 0.2910	 0.3130
P	 0.1170	 0.1360
Q	 0.2220	 0.3420
R	 0.2980	 0.3860
S	 0.2040	 0.3220
T	 0.1940	 0.2650
U	 0.1650	 0.2640
V	 0.8330	 0.6140
W	 0.5130	 0.5840
X	 0.4290	 0.4200
Y	 0.3370	 0.4830
Z	 0.4390	 0.4610
a	 0.7630	 0.5790
b	 0.5110	 0.4190
c	 0.7480	 0.5670



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Chain	Atom inclusion	Q-score
d	 0.6770	 0.5510
e	 0.5720	 0.5370
f	 0.1750	 0.3090
g	 0.2020	 0.3400
h	 0.2370	 0.3570
i	 0.7060	 0.5550
j	 0.6490	 0.5560
k	 0.6820	 0.5760
l	 0.6780	 0.5710
m	 0.7580	 0.5790
n	 0.2790	 0.3560
o	 0.5700	 0.4950
p	 0.7590	 0.5850
q	 0.5800	 0.5220
r	 0.7820	 0.6220
s	 0.5890	 0.5240
t	 0.4560	 0.4690
u	 0.3940	 0.4250
v	 0.7050	 0.5640
w	 0.6940	 0.5790
x	 0.3440	 0.4300
y	 0.6750	 0.5630
z	 0.7440	 0.6110